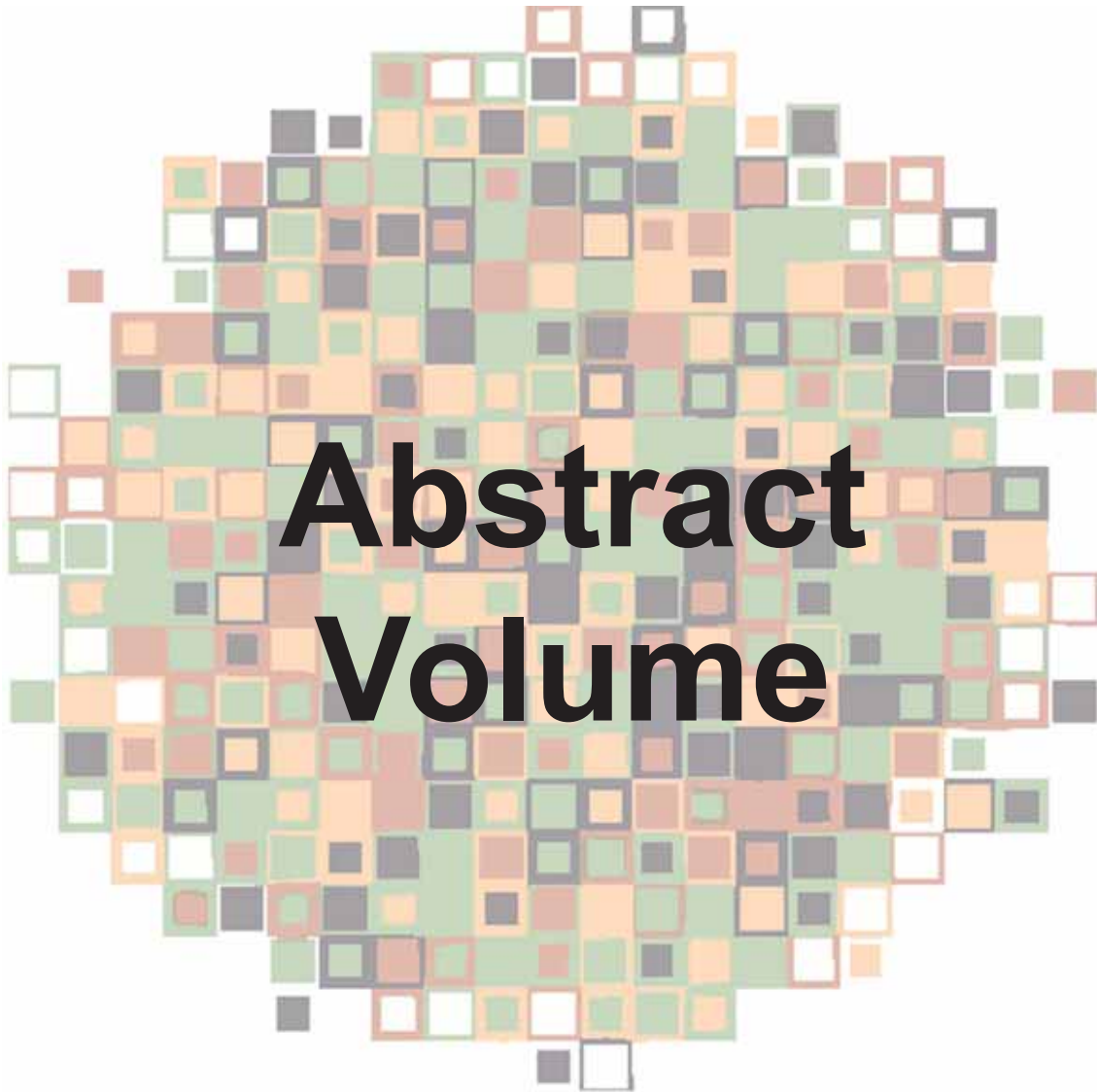




# MATHMOD VIENNA 2012



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I. Troch, F. Breitenecker, Eds.

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**Preprints**

**MATHMOD 2012 Vienna**

**Abstract Volume**

**Preface**



## Preface

At MATHMOD Vienna scientists and engineers using or developing models or interested in the development or application of various modelling tools are offered an opportunity to present ideas, methods and results and discuss their experiences or problems with experts of various areas of specialisation.

The scope of the *MATHMOD Conference Series* covers theoretic and applied aspects of various types of mathematical modelling. Comparison of modelling approaches, model simplification, modelling uncertainties, and port-based modelling are discussed. Besides applications of modelling in traditional areas such as engineering and natural sciences also new ones are of growing importance. The topics to be discussed during the conference reflect also the fact that mathematical modelling is now used more and more in industries. Numerical aspects are now often already part of the modelling process and, automation of modelling and the use of IT are of growing importance. All these facts can be recognized on one hand in the many MATHMOD minisymposia, which were organized by experts in various specific areas. And, on the other hand, also the many sessions, where classic submitted contributions will be presented and discussed, show the broad variety of the MATHMOD conference.

Moreover, it is to be observed that traditional classifications such as theory, applications, numerics, computer science, simulation etc. become more and more obsolete. Scientific work often presents new results in several areas. A look on the MATHMOD 2012 minisymposia illustrates this quite well and underlines the fact that working teams are now often already international:

*Bond Graph Modeling: Theory and Practice*

Dean Karnopp, Donald L. Margolis (Univ. California, USA)

*Classical and Quantum Circuits*

Wolfgang Mathis, Peter Russer (Univ. Hannover / Technical Univ. Munich, Germany)

*Cognitive Technical Systems: Modeling and Simulation*

Dirk Soeffker (University of Duisburg-Essen, Germany)

*Computational Micromagnetics*

Dirk Praetorius, Gino Hrkac, Thomas Schrefl, Dieter Suess (Vienna Univ. Of Technology, Austria / University of Sheffield, UK / Univ. Applied Sciences, St. Pölten, Austria)

*Control and Optimization in Mechatronics*

Georgy V. Kostin, Felix L. Chernousko (Russian Academy of Sciences, Moscow)

*Differential Equation Models in Cell-Biology*

Gabriela Schranz-Kirlinger, Peter Szmolyan (Vienna Univ. of Technology, Austria)

*Fractal Conservation Laws - Hyperbolic Conservation Laws Regularized by an Anomalous Diffusion*

Franz Achleitner, Anton Arnold (Vienna Univ. of Technology, Austria)

*Fractional Models*

J. A. Tenreiro Machado (Polytechnic Univ. Porto, Portugal)

*Mathematical Modeling for Decision Making in Epidemiology and Health Care*

Gottfried Endel, Nikolas Popper (Main Association of Austrian Social Security Institution / dwh Simulation Services, Vienna, Austria)

*Mathematical Modelling and Control of Bio-Chemical Processes*

Philippe Bogaerts, Jan Van Impe (Free Univ. Brussels / Catholic Univ. Leuven, Belgium)

*Model Reduction*

Bernard Haasdonk, Boris Lohmann (University Stuttgart / Technical Univ. Munich, Germany)

*Model-Based Analysis and Control for Distributed-Parameter Systems*

Thomas Meurer (Vienna Univ. of Technology, Austria)

*Modeling in Sport*

Arnold Baca Meurer (Univ. Vienna, Austria)

*Modeling of Dry Friction*

Alexander P. Ivanov, Felix L. Chernousko (Russian Academy of Sciences, Moscow, Russia)

*Modelling and Model Transformation in Automation Technologies*

Tina Krausser, Marius Lauder (RWTH Aachen, / Technical Univ. Darmstadt, Germany)

*Modelling and Simulation in and for Education*

Ildikó Perjési-Hámori, Andreas Körner (Univ. Pecs, Hungary/Vienna Univ. of Technology, Austria)

*Modelling and Simulation in Medicine and Pharmacy*

Maja Atanasijev-Kunc, Jože Drinovec, Aleš Mrhar (Univ. Ljubljana/Univ. Maribor, Slovenia)

*Modelling and Simulation of Water Treatment*

Esko Juuso (Univ. of Oulu, Finland)

*Modelling and Simulation to Support Sustainable Energy Production*

Esko Juuso (Univ. of Oulu, Finland)

*Models and Algorithms in Biotechnology*

Katharina Nöh, Eric von Lieres (Research Center Jülich, Germany)

*Multiscale Modeling and Simulation in Tissue Biomechanics*

Junuthula N. Reddy, Franco Maceri (Texas A&M Univ., USA / Univ. Rome 'Tor Vergata', Italy)

*Object-Oriented Modelling: New Challenges*

Francesco Casella, Gianni Ferretti (Polytechnical Univ. Milano, Italy)

*Optimal Control of ODE's and PDE's: Theory, Numerics and Applications*

Kurt Chudej, Hans Josef Pesch (University of Bayreuth, Germany)

*Vibrations in Engineering Systems*

Horst Ecker, Alois Steindl (Vienna Univ. of Technology, Austria)

Also the invited lectures reflect to some extent this wide spectrum of important topics of current interest, ranging from applications e.g. in engineering and biology to methodological and theoretic aspects of various types, and they clearly show, that scientific work now usually belongs to more than one area of classification:

- *Optimal Control of Dynamical Systems Governed by Partial Differential Equations*  
Hans Josef Pesch, Univ. of Bayreuth, Germany
- *Fourth Generation Wireless Channel Models*  
Christoph Mecklenbräuker, Vienna Univ. of Technology, Austria
- *Structure Preserving Model Order Reduction of Linear Time-Invariant Control Systems*  
Peter C. Müller, Univ. of Wuppertal, Germany
- *Modelling Prehistoric Mining*  
Kerstin Kowarik, Hans Reschreiter, Natural History Museum Vienna, Austria  
Gabriel Wurzer, Vienna Univ. of Technology, Austria
- *The Lattice-Boltzmann Method and Multiscale Hemodynamic: Recent Advances and Perspectives*  
Giuseppe Pontrelli, Consiglio Nazionale delle Ricerche, Roma, Italy



- *Model Order Reduction in Elastic Multibody Systems Using the Floating Frame of Reference Formulation*  
Christine Nowakowski, Univ. of Stuttgart, Germany
- *System Physics - A Modeling Approach to Fundamental Concepts*  
Werner Maurer, Univ. Applied Sciences, Zurich/Winterthur, Switzerland
- *Utilization of Buildings: Understand, Model, Simulate!*  
*The MoreSpace Project at TU Vienna*  
Dietmar Wiegand, Vienna Univ. of Technology, Austria
- *Structure and (Thermo)Dynamics of Biomolecular Complexes From Computer Simulation*  
Chris Oostenbrink, Univ. of Natural Resources and Life Sciences, Vienna, Austria
- *Physical Modeling Technology in Rand Model Designer*  
Yuri Senichenkov, St. Petersburg State Polytechnical University, Russian Federation
- *Evolution of Industrial Needs for Modelling & Simulation: New Challenges and New Opportunities*  
Agostino Bruzzone, Univ. of Genoa, Italy
- *Recognition and Classification of Human Motion Patterns*  
Arnold Baca, Univ. of Vienna, Austria

These *Preprint Volumes* compile the preprint abstracts and the preprint full contributions to MATHMOD 2012. Four contribution types have been provided. The classical contribution types are *MATHMOD Contribution* and *MATHMOD Minisymposium Contribution*, accepted by general peer review based on an extended review abstracts, or by review of the minisymposium organisers. MATHMOD 2012 also continues with a novelty introduced in MATHMOD 2009 – the type *MATHMOD Work-in-Progress Contribution*. Contributions of this type are intended for presentation of recent developments and work in progress in all areas of modelling and simulation. And last but not least, *MATHMOD Student Contributions* give e.g. PhD Students a chance to present themselves their own work.

While MATHMOD (minisymposium) contributions are orally presented in parallel sessions, work-in-progress contributions and student contributions – which both types have passed a review procedure analogous to the type MATHMOD contributions - are presented in plenary poster sessions.

For all contribution types the same publication possibilities are offered, as preprints based on the review abstracts and as proceedings based on review of the full preprint contribution.

MATHMOD 2012 comes with a new publication strategy. The need of *Proceedings* which are listed in scientific citation systems caused us to change from electronic CD-Proceedings with ISBN, but without DOI and without science citation index listing, towards electronic web publication on a renowned publication server with citation features. As MATHMOD conference series is an IFAC - sponsored conference series, our choice for web publication for the Proceedings was *IFAC-PapersOnLine.net*, the web publication server of IFAC, the International Federation of Automatic Control. All papers published on *IFAC-PapersOnLine.net* can be cited using the site ISSN, the event ISBN, and the individual paper DOI (Digital Object Identifier), and furthermore publications will be indexed in SCOPUS, etc. *IFAC-PapersOnLine.net*, developed as a partnership between IFAC and Elsevier, the IFAC Publisher, is *Open Access* in nature – no charge to individual for reading or downloading, up to a limit of 25 papers per calendar month.

MATHMOD participants have provided *Preprint Abstracts* of their contributions for the printed *MATHMOD 2012 Abstract Preprint Volume* and *Preprint Full Contributions* for the electronic *MATHMOD 2012 Full Contributions Preprint Volume* (USB Stick). These full preprint contributions will undergo a full-paper review for inclusion into *MATHMOD 2012 Proceedings* at *IFAC-PapersOnLine.net*.

The *Abstract Volume* (printed) and *Full Contribution Volume* (USB Stick) of these preprints, organised within the *ARGESIM Report Series* as ARGESIM Report no. AR-S38, start with the manuscripts (abstract, or full paper resp.) of the plenary lectures. Then follow the ‘classical’ MATHMOD contributions, arranged in sessions according to their main thematic point. Such a grouping is by no means easy because many contributions address several different aspects in a balanced manner, and the contributions show very strong inter-disciplinarity. So we decided for a first group with contributions on methods and theory, and for a second group dealing with identification in theory and application, and then followed by comprehensive application groups. Each group has been split in two to four sessions:

- Modelling Methods, Theory & Tools
- Identification, Estimation, & Calibration
- Mechatronics & Electrical Engineering
- Control Systems
- Biology, Physiology & Medicine
- Discrete Systems and Manufacturing
- Process Engineering

Next, abstracts, or full paper contributions resp., of the MATHMOD 2012 Minisymposia follow in the sequence given before. This sequence does not reflect a thematic order; the sequence is given by the submission sequence of minisymposia. Abstracts, or full contributions resp., of types *Work-in-Progress Contribution* and *Student Contribution* conclude the preprints, order sequence by submission.

The structure of these preprints will also be used for the *MATHMOD 2012 Proceedings* at *IFAC-PapersOnLine.net*, which will include all contributions, which will pass / which have already passed the full paper review.

As editors we wish to express our sincere thanks to all who have assisted us by making the idea of this symposium known within the scientific community or by acting as sponsor or cosponsor. We want to thank especially the members of the International Program Committee who assisted us in the reviewing process – some of them did indeed a tremendous work by reviewing some 20 extended abstracts in rather short time, and who have started reviewing the full preprint contributions for publication at *IFAC-PapersOnLine.net*. Further, we want to thank all colleagues who have done an excellent job by putting together MATHMOD minisymposia devoted to one main topic. Last but not least we like to thank IFAC for co-operation with a special publication arrangement, and the local ARGESIM team for their support in preparation of these Preprints.

Vienna, January 2012

Inge Troch and Felix Breiteneker

**Preprints**

**MATHMOD 2012 Vienna**

**Abstract Volume**

**Plenary Lectures**



# OPTIMAL CONTROL OF DYNAMICAL SYSTEMS GOVERNED BY PARTIAL DIFFERENTIAL EQUATIONS

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**Abstract.** When analyzing mathematical models for complex dynamical systems, their analysis and numerical simulation is often only a first step. Thereafter, one often wishes to complete the analysis by an optimization step to exploit inherent degrees of freedom for optimizing a desired performance index with the dynamical system as side condition. This generally leads to optimization problems of extremely high complexity if the underlying system is described by (time dependent) partial differential equations (PDEs) or, more generally, by a system of partial differential algebraic equations (PDAEs).

In the talk we will report on some of the latest achievements on the field of optimization with PDEs and exhibit the challenges we are facing and have to cope with to solve such tasks.

In the introduction three problems from engineering sciences are presented:

1. Hot cracking is a common risk in welding of aluminium alloys. According to a Russian patent this risk can be avoided by applying a so-called multi-beam laser welding technique. By two additional laser beams the thermal stress introduced by the main welding laser can be compensated, if the additional laser beams are optimally placed and sized while they must not melt on the material. Mathematically we obtain a semi-infinite optimization problem with PDE and inequality constraints.
2. Future concepts for intercontinental flights of passenger aircraft envisage aircraft which are able to fly at hypersonic speeds. Due to such high velocities the thermal heating of the aircraft is an issue which has to be taken into account. This multi-physics problem leads to an optimal control problem for a system of ordinary differential equations where the heating of the aircraft's body is modelled as a quasilinear heat equation with nonlinear boundary conditions. The temperature of the thermal protection system must be limited and plays the role of a state variable inequality in this ODE-PDE optimal control problem.
3. The main example, which will be discussed in detail in the second part of the talk, is concerned with the optimal control of certain fuel cell systems for an environmentally friendly production of electricity. Reaction-advection equations, a heat equation, additional ordinary as well as algebraic and integro equations sum up to a coupled system of up to 28 PDAEs of extremely high complexity. The inflow data into the anode inlet, the input data for the catalytic burner, and the amount of fed back from the cathode outlet are the control variables of this system.

After this motivation an outline of the mathematical theory of optimal control problems for one elliptic equation is given to depict the purpose of solving optimal control problems by first order necessary conditions. Thereafter two numerical concepts, namely *first optimize then discretize* and *First discretize then optimize* are discussed with respect to their pros and cons as well as an overlook on the mathematical toolbox from the literature is given.

The main part of the talk then deals with the results for optimal load changes when applying the two aforementioned methodologies including a method for the practical realisation of the computed optimal solutions based on model reduction techniques.

- [1] K. Chudej, H. J. Pesch, K. Sternberg. Optimal Control of Load Changes for Molten Carbonate Fuel Cell Systems: A Challenge in PDE Constrained Optimization. *SIAM J. on Applied Mathematics*, 70(2):621–639, 2009.
- [2] K. Chudej, H. J. Pesch, M. Wächter, G. Sachs, F. Le Bras. Instationary heat constrained trajectory optimization of a hypersonic space vehicle by ODE-PDE constrained optimal control. In A. Frediani, G. Butazzo, editors, *Variational Analysis and Aerospace Engineering*, pages 127–144. Springer, Berlin, 2009.
- [3] M. Hinze, R. Pinnau, M. Ulbrich, S. Ulbrich. *Optimization with PDE constraints*. Mathematical Modelling: Theory and Applications, volume 23, Springer, 2008.
- [4] V. Petzet. *Mathematische Optimierung und Sensitivitätsanalyse des Mehrstrahlschweißverfahrens zur Verhinderung der Heißrissbildung*. PhD thesis, University of Bayreuth, Germany, 2008.
- [5] A. Rund. *Beiträge zur Optimalen Steuerung partiell-differential algebraischer Gleichungen*. PhD thesis, University of Bayreuth, Germany, 2012.
- [6] K. Sundmacher, A. Kienle, H. J. Pesch, J. Berndt, G. Huppmann. *Molten Carbonate Fuel Cells — Modeling, Analysis, Simulation, and Control*. Wiley-VCH, 2007.
- [7] F. Tröltzsch. *Optimal Control of Partial Differential Equations: Theory, Methods and Applications*. Graduate Studies in Mathematics, AMS 2010.

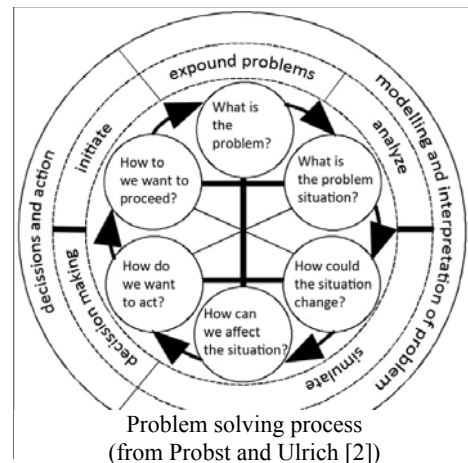
## UTILIZATION OF BUILDINGS: UNDERSTAND, MODEL, SIMULATE! THE MORESPACE PROJECT AT TU VIENNA

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Developers of real estate and infrastructure and builders in general are faced with the task of designing, steering and improving socio-technical systems. They deal with project organisation and with buildings and their use, all along its life-cycle – from the first idea up to the building’s demolition. Due to the dynamic and complexity inherent to such real world systems, almost all of the decisions faced by the aforementioned groups of people are based upon incomplete or insufficient information. To them models and simulations are worthless if they do not answer particular questions or provide valuable, additional information to support decision making processes.

In order for a model to provide vital information or support for decision making in urban and real estate development, especially concerning sustainability aspects, it is essential to assess the impacts of potential changes of built environment respecting its interrelationship with the systemic context. E.g. ecological builds constructed at the periphery of cities might increase the overall carbon emission in a certain region, due to fact that those who move into these buildings will now drive to their workplaces by car. To identify the potential scope for action a systemic perspective is necessary. According to Schalcher such a holistic view is only possible “if the interdependence of all human activity and natural events is consciously accepted and not neglected” [1]. Consequentially one of the main obstacles for a successful deployment of a simulation tool within (although not limited to) this area of application, is the identification not only of the system’s parameters but also of all external ones.



Drawing the border between these two sets of influencing factors is a very delicate task, as it is dependent of the objective target, the methodological approach and the subjective point of view or definition of the system. Following these steps one does obtain a dynamic model of the system at hand which becomes subject to in-depth analysis. Based on this dynamic model closed loops, main influencing factors and thus reasonable action can be identified. Only after such an analysis – and subsequent choice of rewarding search directions – does it become sensible to engage mathematical modelling and simulation to improve ecological and economical sustainability and replace experiences and assumptions by explicit knowledge. With the prior steps taken, simulation tools can now greatly aid the decision finding process, as they produce results that address the questions formulated.

At the Vienna University of Technology the shortage of lecture rooms was the incentive to develop a model to analyse and improve the utilisation of these rooms by means of a simulation and planning environment – called MoreSpace [3]. An extensive analysis of the given situation based on current booking data as well as a thorough inquiry about the room required showed the utilisation of rooms to be surprisingly low. The simulation model developed according to these insights, following the aforementioned principal guidelines for building utilization, allowed a further investigation of this situation; using the possibility of experimenting quickly showed that even small well directed changes to the booking procedure did show great impact by increasing the room capacity utilisation on one hand and merging free time slots to increase the disposability of lecture room space on the other hand. Thus it could be proven that not the quantity of lecture room is the main problem but the strategy used to utilise it. But only a very detailed and in depth analysis showed the source of the problem to be not based on the room structure itself but the behaviour of the surrounding system.

MoreSpace, a simulation and planning tool based on DEVS and planning heuristics ([3], [4]), has been developed within grants of Vienna University of Technology and by ZIT, the technology promotion agency of the City of Vienna; MoreSpace is intended for general use at universities, schools, and similar institutions which want to improve the utilization of their buildings.

[1] H. Schalcher: *Systems Engineering*. IBB, ETH Zürich, 2008.

[2] P. Gomez, and G. Probst: *Die Praxis des ganzheitlichen Problemlösens, vernetzt denken, unternehmerisch handeln, persönlich überzeugen*. Paul Haupt, Bern, 2001.

[3] S. Emrich, S. Tauböck, et al.: *MORE SPACE – A Hybrid Dynamic Approach for Modelling Lecture Room Management*. In Proc. MATHMOD 09 Vienna - CD Volume 2009, ISBN: 978-3-901608-35-3; 7 p.

[4] M. Bruckner, S. Tauböck, et al.: *A Combined Cellular Automata - DEVS Simulation For Room Management With Vacation Times*. In Proc. 7th EUROSIM Congress, ISBN: 978-80-01-04589-3; S. 555 - 560.

# STRUCTURE PRESERVING MODEL ORDER REDUCTION OF LINEAR TIME-INVARIANT CONTROL SYSTEMS

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## Abstract

The investigation of dynamical systems is based usually on a mathematical model. The increasing complexity of the systems leads generally to a large-scale model. In case of linear, time-invariant behaviour the state-space model is given by

$$\dot{\mathbf{x}}(t) = \mathbf{A} \mathbf{x}(t) + \mathbf{B} \mathbf{u}(t), \quad \mathbf{y}(t) = \mathbf{C} \mathbf{x}(t). \quad (1)$$

Simulation, analysis, control design of large-scale systems is difficult. Therefore, in many cases model order reduction methods will be applied to obtain more convenient models with smaller dimension  $r$  which represent hopefully a good approximation of the large-scale system. Assuming

$$\mathbf{x}_r = \mathbf{L} \mathbf{x}, \quad \mathbf{x} \approx \mathbf{R} \mathbf{x}_r, \quad (2)$$

where  $\mathbf{L}$  is the aggregation (or reduction) matrix and  $\mathbf{R}$  represents the expansion (or approximation) matrix, then the model of reduced order  $r$  is given by

$$\dot{\mathbf{x}}_r(t) = \mathbf{A}_r \mathbf{x}_r(t) + \mathbf{B}_r \mathbf{u}(t), \quad \mathbf{y}_r(t) = \mathbf{C}_r \mathbf{x}_r(t), \quad (3)$$

where

$$\mathbf{A}_r = \mathbf{L} \mathbf{A} \mathbf{R}, \quad \mathbf{B}_r = \mathbf{L} \mathbf{B}, \quad \mathbf{C}_r = \mathbf{C} \mathbf{R}. \quad (4)$$

The matrices  $\mathbf{L}$  and  $\mathbf{R}$  are required to be row- and column-regular of dimensions  $r \times n$  and  $n \times r$ . For consistency, additionally  $\mathbf{L} \mathbf{R} = \mathbf{I}_r$  is assumed (which is not really a restriction).

The analysis and design of system (1) will be carried out by the analysis and design of system (3). To get reasonable results the reduced-order model should approximate the behaviour of the large-scale system as good as possible. There are different methods to judge the quality of a “good” approximation, e.g. approximation of the transfer behaviour or preserving some structural properties. Here, in this contribution it will be dealt with preserving following features:

- Asymptotic stability
- Complete controllability
- Complete observability
- Steady-state accuracy
- Vanishing equation residuum
- Controller/observer design separation

The necessary and/or sufficient conditions on  $\mathbf{L}$ ,  $\mathbf{R}$  to preserve such important system properties are shown explicitly and discussed in detail.

## MODELLING PREHISTORIC MINING

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**Introduction.** Mining structures are among the most complex economical systems in prehistory. Until recently, research into prehistoric production processes has strongly focused on technological reconstruction. The complexity of production processes, their interconnectedness with the surrounding socioeconomic network and issues of quantification have, quite regrettably, been addressed to a much lesser extent. Simulation can contribute important insights into the latter problem areas, however, the lack of consistent methodological discussion on data collection, model building and comparability of results still represents a significant gap in research, which we address in our work.

**Archaeological Background.** Mining areas are not only characterized as centres of production, but also as centres of consumption - yielding high demands with respect to workforce, means of production (mining tools, raw materials) and means of consumption (food, clothes). The necessity of expert knowledge, intra- and superregional communication, traffic and trade networks further adds to the complexity. All these interdependent conditions demand an analytic approach combining different levels of observation, both spatially and in context of the model used.

**Method.** We argue that a consistent and methodical analysis of prehistoric mining structures can best be done by the *combination of several different simulation techniques* in connection with a *multidisciplinary database* drawing on experimental archaeology, ethnography and historical records. This combinational method, which we will demonstrate by using data gained through the modeling of the bronze age salt mining complex of Hallstatt/Austria (1458-1245 BC), lies at the core of our efforts.

In the course of our research, simulation tools allowing for extensive exploratory work with the existent archaeological model have been created and important insights in the working and production processes have been gained. The combination of these techniques allows for an analytic approach incorporating different levels of information. For example, we have used Agent-Based Simulation[1] (see Figure) to build a model of the working processes in one mining hall (breaking salt, collecting salt, transporting salt to the shaft), in order to gain insights into spatial organization, allocation of tasks and workload balance and to relate the time span of mining to the size of the workforce and the amount of mined salt. A System Dynamics Simulation[2] was applied to correlate the size of the workforce with food consumption and demand for mining tools. Through Process Simulation, we were able to display and analyze the workflow of an entire shaft system encompassing several mining halls.

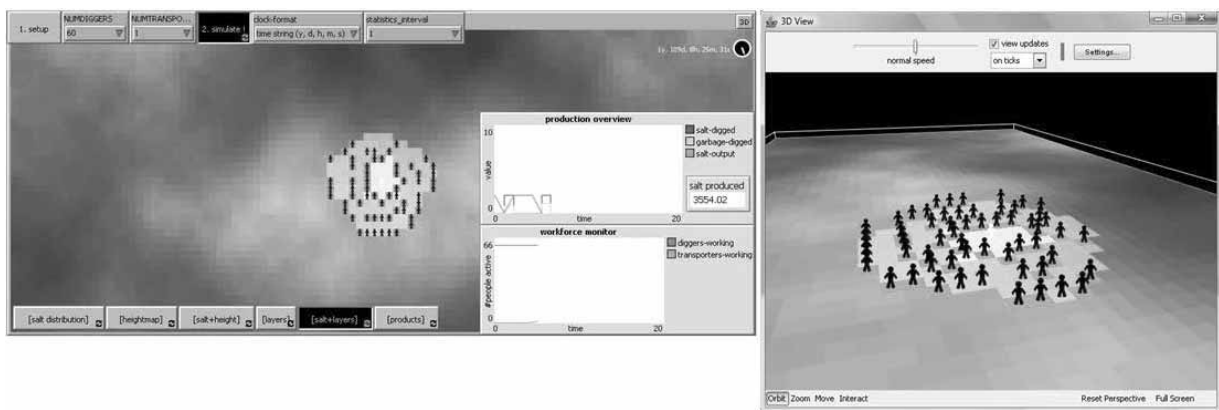


Figure: Example agent-based model used to simulate the mining process. An area with a typical salt distribution (purple) is mined by workers on different levels, using a stair-like strategy colour-coded yellow, green and cyan. The simulation computes the number of years to fully exploit the mine, dependent on number of workers, environment and stair strategy used.

- [1] Kowarik, K., Reschreiter, H., Wurzer, G., Totschnig, R., Rausch, A.: Mining with Agents - Agent-based Modeling of the Bronze Age Salt Mine of Hallstatt. In: Archäologie und Computer, ISBN 978-3-85161-016-1, Vienna, 2008, 1-19.
- [2] Kowarik, K., Reschreiter, H., Wurzer, G.: *Modeling a mine. Agentbased Modeling, Systemdynamics and Experimental Archaeology applied to the Bronze Age Saltmines of Hallstatt*. In: Mining in European History. SFB HiMAT, 2010, 44-52.



# THE LATTICE BOLTZMANN METHOD AND MULTISCALE HEMODYNAMICS: RECENT ADVANCES AND PERSPECTIVES

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The lattice Boltzmann method has emerged as a new and effective numerical technique of computational fluid dynamics, and offers an alternative to the discretization of the Navier-Stokes equations. It allows a physical modelling at an intermediate level between molecular scale and a continuum representation. As such, it is suitable for describing complex flows, as those in hemodynamics, where the microscopic kinetics plays a non-trivial role in determining macroscopic quantities.

Blood is a complex fluid containing a high volume fraction of red cells (RBC's) and other suspended elements in the plasma. A way to include the particulate nature of blood is presented here with the aim of studying flow dynamics both in large-scale vessels and in microcirculation. A key feature of the blood flowing in arteries is the shape of endothelium, that plays a number of important functions in the vascular system: its dysfunction may lead to several pathological states, including early development of atherosclerosis. The microscopic shape of the wall is addressed by the presence of endothelial cells, making the arterial boundary undulated [1]. In addition, the endothelium is coated by long-chained macromolecules and proteins which form a thin structure, called the endothelial surface layer (ESL) or glycocalyx. The glycocalyx has a *brushlike* structure and a mean thickness of 100nm for arterioles. It is believed that ESL acts as a transport barrier to prevent RBC's ballistic interaction with the endothelium and as sensor and a transducer of mechanical forces, such as the blood shear stress [2]. The main aim of this paper is to show that the inclusion in the model of crucial elements such as RBC's, the corrugated wall and the glycocalyx, can be modelled within a single unified computational framework.

The model is based on a modification of the standard lattice Boltzmann method (LBM) to account for a bi-component fluid, in the specific case plasma and RBC's. The latter are modelled as deformable, neutrally buoyant liquid drops constrained by a uniform interfacial tension and suspended in the plasma. LBM is based on a minimal kinetic Boltzmann equation in which representative particles evolve on a regular grid according to simple streaming and collision rules, designed in such a way as to preserve the basic symmetries of fluid mechanics [3]. The LBM exhibits a number of appealing features as a computational fluid dynamics solver, such as the simplicity of the stream-and-collide kinetics, its amenability to parallel computing and its ease in handling complex flows. However, if the standard LBM bears much of its conceptual simplicity and computational efficiency for being formulated over a uniform Cartesian mesh, on the other hand regular grids represent a severe limitation in modelling endothelium corrugations. Therefore, an effort has been directed to the goal of enhancing the geometrical flexibility of the LBM with a finite volume formulation that allows for irregular wall geometry and for a more complex rheological model for blood. Finally, the presence of the ESL is modelled by a thin porous layer of constant thickness over the corrugated wall surface. In such a layer, a repulsive body force density acts on the drop interface which approach the ESL region, impinging on the lumen. The idea is to solve a two-domain problem, whereby the bulk flow (in the lumen) is governed by the bi-component Navier-Stokes equations and the near-wall region by a porous-medium Brinkmann flow formulation.

Some numerical results illustrate the quality of the model in reproducing known rheological properties of blood as much as revealing the effect of RBC structuring on the wall shear stress. The average velocity of the drop is slower in the presence of the glycocalyx, which constitutes a hindrance for the lumen flow. Also, the mean deformation of a RBC is more pronounced in the ESL influence region, where it is subjected to the elastic force, which squeezes and lifts it, away from the wall, whilst making its shape more elongated. There are sensible wall shear stress differences in the cases without and with glycocalyx: in the latter case, a reduction of the shearing stress either at the wall and at the ESL top is evidenced.

[1] Pontrelli G., Köenig C.S. Halliday I., Spencer T.J., Collins M.W., Long Q. and Succi S., *Modelling wall shear stress in small arteries using the Lattice Boltzmann method: influence of the endothelial wall profile*, Med. Eng. Phys., 33 (7), 2011, 832-839.

[2] Weinbaum S., Tarbell J.M. and Damiano E.R., *The structure and the function of the endothelial glycocalyx layer*, Ann. Rev. Biom. Eng. 2007, 9 (6.1).

[3] Succi S. *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*, Oxford University Press, 2001.

# MODEL ORDER REDUCTION IN ELASTIC MULTIBODY SYSTEMS USING THE FLOATING FRAME OF REFERENCE FORMULATION

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**Introduction.** In the modern development process of technical products computer aided simulations are employed. In this way costly experiments and prototypes can be reduced. Thereby, shorter development periods and rising requirements like durability, efficiency or mass reduction which intensifies the usage of lightweight structures demand precise simulations. For systems which undergo large nonlinear working motions the multibody system approach is often most useful. Classical multibody systems (MBS) consist of rigid elements which are connected by ideal joints and coupling elements. For engineering applications, where the deformation of the bodies cannot be neglected, the method of elastic multibody systems (EMBS) has to be applied, see e.g. [1]. Typical applications are in the area of machine dynamics, vehicle dynamics, robotics, automation, biomechanics and energy systems.

**Elastic Multibody Dynamics.** Several methods have been suggested to capture both, the highly nonlinear motions and the deformations, see [1]. For systems where the elastic deformation is small compared to the rigid body motion, the floating frame of reference formulation can be used. It is one of the most common approaches in the field of modeling flexible multibody systems. The basic idea is to separate the motion of the body in a large nonlinear motion of the reference system and a linear elastic deformation with respect to the reference system. In this way the modeling of an EMBS can be split into two parts, on the one hand modeling the multibody dynamics and on the other hand modeling the flexibility.

**Model Reduction.** One basic instrument to describe the elastic deformation in combination with the floating frame of reference formulation is the linear Finite Element Method. The need of high precision and complex geometries leads to a fine spatial discretization. Mathematically the elasticity is described by a large set of linear ordinary differential equations

$$\mathbf{M}_e \cdot \ddot{\mathbf{q}}_e(t) + \mathbf{K}_e \cdot \mathbf{q}_e(t) = \mathbf{h}_e, \quad (1)$$

e.g. [2]. The matrices  $\mathbf{M}_e$  and  $\mathbf{K}_e$  are the mass and stiffness matrix and the vector  $\mathbf{q}_e$  the elastic coordinates of the flexible structure. The generalized surface and volume forces are summarized in the force vector  $\mathbf{h}_e$ . To consider the dissipative effects an additional damping term  $\mathbf{D}_e \cdot \dot{\mathbf{q}}_e$  is often introduced and can be approximated for example by viscous damping (Rayleigh damping).

Linear model reduction is a decisive component to simulate flexible multibody systems efficiently, see [2]. Thereby, the reduction of the equations of motion of each single elastic body is based on an approximation via projection. For this purpose the nodal displacement vector is projected into a first subspace of smaller dimension. The residual resulting from the first projection is eliminated by a projection to a second subspace, which is orthogonal to the residual. The projection of the equations of motion is called orthogonal if the subspaces are identical, otherwise it is called oblique, see [3]. The choice of the projection matrices is a crucial factor in the quality of the reduced model and task of the different reduction techniques. In the industrial setting the reduction methods based on modal reduction, sub-structuring and condensation, like component mode synthesis are still the state of the art. However, in the basic methods, information about the spatial distribution of the loads acting on the flexible body or information about the operation of the system are hardly taken into account and consequently the convergence of these approaches can be very slow. Modern reduction techniques based on Krylov subspaces, singular value decomposition (SVD) or Gramian matrices approximate the input to output mapping of a flexible body. In this way the distribution of the loads is taken into account and yields in a high accuracy of the reduced model. Furthermore, a-priori error bounds or efficient error estimators are available. An overview of the current state of developments can be found e.g. in [3].

- [1] Schwertassek, R., and Wallrapp, O.: Dynamik flexibler Mehrkörpersysteme (in German). Braunschweig: Vieweg, 1999.
- [2] Lehner, M.: Modellreduktion in elastischen Mehrkörpersystemen (in German). Dissertation, Schriften aus dem Institut für Technische und Numerische Mechanik der Universität Stuttgart, Band 10. Aachen: Shaker Verlag, 2007.
- [3] Antoulas, A.: Approximation of Large-Scale Dynamical Systems. Philadelphia: SIAM, 2005.

# SYSTEMS PHYSICS – A MODELING APPROACH TO FUNDAMENTAL CONCEPTS

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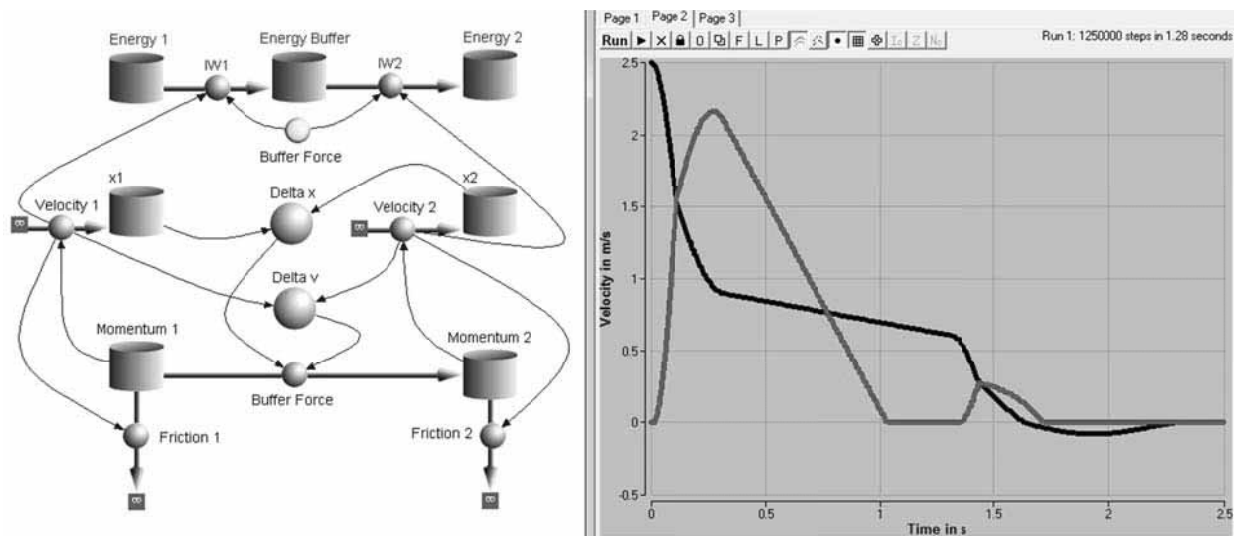
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“The book of nature is written in the language of mathematics” claimed Galilei in 1623. It is this language that creates a bottleneck on the way to understand basic laws of physics. Therefore teachers explain only the solution of some standard problems and students learn to parameterize some functions or put numbers in formulas. But they can’t explain what they are doing in their own words.

Systems Dynamics avoids the explicit use of differential equations with the help of bathtub- and feedback-thinking. Only four elements (reservoirs, pipes, feedback arrows and functions) are needed to model a dynamical system, such as a bouncing ball or the behavior of a predator-prey-system.

Systems Physics combines the modeling concept of System Dynamics with a unified description for all branches of classical physics known from bond graph theory [1]. In this model based approach students start by formulating the balance of a fundamental quantity (bathtub-thinking for volume, mass, electrical charge, momentum, angular momentum, entropy or amount of substance). Then they have to specify the currents and the rates of change (feedback-thinking). On a second layer they can add the balance of energy (bookkeeper-thinking).

The challenge of an introductory course is to convince the audience that physics is relevant, useful and coherent. Systems Physics can motivate people who are not expert in mathematics to think about the fundamental concepts of nature and technology. Some really new picture and the modeling approach help the students to understand the basic processes. Fig. 1 shows such a *system diagram* and the velocity-time-diagram for a freight wagon colliding with another.



**Figure 1:** System diagram (left) and velocity-time-diagram for a freight wagon colliding with another. Momentum balance, kinematics and energy balance form three levels of the model.

Systems Physics provides a consistent, coherent and relevant structure of physics. A huge number of dynamical systems can be modeled with the same heuristic approach. The equation of balance for substance like quantities like volume, mass, electric charge, momentum, angular momentum and entropy yields the backbone for such models. By adding the constitutive laws for accumulators and conductors we get the basic equations. In a third step we can add energy as a second substance like quantity. The energy balance analysis is often useful but not necessary for simple systems. But energy conservation becomes an inevitable requirement in more complex systems like thermodynamic accumulators.

Systems Physics has been developed on the basis of the Karlsruhe Physikkurs [2] and taught in different physics courses at Zurich University of Applied Sciences.

[1] Karnopp, D., Margolis, D., Rosenberg, R: *System dynamics: a unified approach*. Wiley, New York, 1990.

[2] Herrmann, F.: *Karlsruher Physikkurs*. Aulis, Hallbergmoos, 2003.

## FOURTH GENERATION WIRELESS CHANNEL MODELS

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**Abstract.** The dependability of next generation wireless systems will be a key demand for their evolution. The design and implementation of dependable wireless communication systems requires adequate models of the radio propagation channel in all relevant environments and scenarios. Wireless multiple-input multiple-output (MIMO) channels are prone to pathloss and several fading mechanisms. These induce a rich behavior in time, delay, frequency, Doppler shift, location, spatial separation and polarization [1] which determines channel capacity, packet reliability and network latency [2]. Three approaches have become state of the art: Tap delay models, ray-based models, and geometry- based stochastic models [3]. This contribution reviews their design, evolution, and validation methodology [4, 5] and highlights recent advances in this challenging field.

**Keywords:** radio propagation, multipath components, time-variance, model identification and validation.

- [1] A. F. Molisch, F. Tufvesson, J. Karedal, and C. F. Mecklenbräuer: A Survey on Vehicle-to-Vehicle Propagation Channels, IEEE Wireless Communications Magazine, Special Issue on "On-the-Road" communications, Vol. 16, No. 6, pp. 12–22, Dec. 2009.
- [2] C. F. Mecklenbräuer, A. F. Molisch, J. Karedal, F. Tufvesson, A. Paier, L. Bernadó, T. Zemen, O. Klemp, N. Czink: *Vehicular channel characterization and its implications for wireless system design and performance*, Proceedings of the IEEE, Special Issue on Vehicular Communications, Vol. 99, No. 7, July 2011. doi:10.1109/JPROC.2010.2101990.
- [3] J. Karedal, F. Tufvesson, N. Czink, A. Paier, C. Dumard, T. Zemen, C. F. Mecklenbräuer, A. F. Molisch: *A Geometry-Based Stochastic MIMO Model for Vehicle-to-Vehicle Communications*, IEEE Transactions for Wireless Communications, Vol. 8, No. 7, pp. 3646–3657, July 2009. doi:10.1109/TWC.2009.080753.
- [4] P.-J. Chung, D. Maiwald, N. Czink, C. F. Mecklenbräuer, B. H. Fleury: “Determining the number of propagation paths from broadband MIMO measurements via bootstrapped likelihoods and the false discovery rate criterion — Part I: Methodology,” in Proc. IEEE 2nd International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP 2007), St. Thomas, U.S. Virgin Islands, Dec. 12–14, 2007.
- [5] N. Czink, P.-J. Chung, D. Maiwald, B. H. Fleury, C. F. Mecklenbräuer: “Determining the number of propagation paths from broadband MIMO measurements via bootstrapped likelihoods and the false discovery rate criterion — Part II: Application,” in Proc. IEEE 2nd International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP 2007), St. Thomas, U.S. Virgin Islands, Dec. 12–14, 2007.

# STRUCTURE AND (THERMO)DYNAMICS OF BIOMOLECULAR COMPLEXES FROM COMPUTER SIMULATION

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**Abstract.** We will discuss methods to computationally describe the structure and dynamics of biomolecular complexes. Three main actors play a role in complexation: the biomolecular target (enzyme, receptor), the small molecule binding to it (inhibitor, agonist) and the solvent in which both are solvated. We will discuss the role of the individual actors and their influence on the prediction of binding poses. Moreover, their individual contributions in terms of enthalpy and entropy to the free energy of binding will be discussed. Subsequently, computational approaches to calculate the free energy of binding will be introduced, together with the use of thermodynamic cycles. These allows us to calculate relative free energies of binding for different ligands or to differently mutated proteins using non-physical transitions, which may be described in the context of molecular dynamics simulations. Examples of this approach will be given, showing the insight at a molecular level that may be obtained from the calculations.

## PHYSICAL MODELING OF HYBRID SYSTEMS IN RAND MODEL DESIGNER

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**Introduction.** Modern tools for modeling and simulation of complex dynamical systems are based on object-oriented modeling and maintain component modeling with oriented (“causal” modeling) and non-oriented (“physical” modeling) components.

Using state machine as a specification of event-driven component behaviour makes changes in algorithm of building current final system of algebraic-differential equations for “physical” modeling in comparison with “causal” modeling. For “physical” modeling this algorithm has greater time complexity. In spite of this we suggest performing a current final system during execution. It allows modeling hybrid systems without any limitation on type and structure of a local system of algebraic-differential equations.

For embedded systems it is very important providing breakneck computation speed. A possible way of decreasing model run-time is updating numerical methods. One of the basic auxiliary operations of numerical methods for solving algebraic-differential equations is solving linear system of algebraic equations. Modern solvers of algebraic-differential equations based on direct methods for solving linear algebraic systems of equations deal with general, band and sparse matrices. The list of practically important equation structures is bigger. It is possible to modify numerical methods for solving algebraic-differential equations taking in account different types of equation structure.

Modern industrial projects require special technology for debugging and testing. Jumbo size of whole model hybrid automation allows analysing separate trajectories only. Therefore information about separate trajectory should be manifold. It may be a list of visited states of total hybrid automation on trajectory and sequence of final systems, type and structure of final systems, Jacoby matrices values, sequence and results of discrete actions, etc.

Rand Model Designer ([www.rand-service.com](http://www.rand-service.com)) developed by MvStudium Group ([www.mvstudium.com](http://www.mvstudium.com)) is industrial visual environment for designing complex dynamical systems. In comparison with Model Vision Studium it maintains “causal” modeling event-driven systems, suitable for designing embedded systems, allows taking in count structure of solved systems, and has powerful instruments for testing and debugging large-scale models. Rand Model Designer is used in education, economics, ecology, ballistics, in industry for designing ship simulators.

- [1] Ascher U.M., Petzold L.R. *Computer methods for ordinary differential equations and differential-algebraic equations*, SIAM, 1998.
- [2] Breitenecker F., Proper N. Classification and evaluation of features in advanced simulators. Proceedings MATHMOD 09 Vienna, Full papers CD Volume.
- [3] Brown P.N., Hinmarsh A.G. Petzold L.R. *Using Krylov methods in solution of large-scale differential-algebraic systems*. Technical report. Numerical Mathematics Group, UCRL-JC-113507, 1993/  
<https://computation.llnl.gov/casc/nsde/pubs/221215.pdf>
- [4] Fritzson P. *Principles of Object-Oriented Modeling and Simulation with Modelica 2.1*. Wiley-IEEE Press, 2006
- [5] E. Hairer, G. Wanner. *Solving ordinary differential equations II*. Springer-Verlag, 1991, 1996.
- [6] Li S., Petzold L. *Design of new DASP for sensitivity analysis*. S. Technical Report, Department of Computer Science, University of California Santa Barbara, 1999.  
[www.cs.ucsb.edu/~cse/Files/LiPetz99.ps](http://www.cs.ucsb.edu/~cse/Files/LiPetz99.ps)
- [7] Pissanetzky S. *Sparse matrix technology*, Academic Press Inc., 1984.
- [8] Rumbaugh J., Jacobson I., Booch G. *The unified modeling language. Reference manual*. Second edition. Addison-Wesley, 2005.
- [9] Tiller M. *Introduction to physical modeling with Modelica*. The Springer international series in engineering and computer science. 2001.

## EVOLUTION OF INDUSTRIAL NEEDS FOR MODELLING & SIMULATION: NEW CHALLENGES AND NEW OPPORTUNITIES

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**Abstract.** The paper include an overview on Industrial requirements for applying Modelling & Simulation; the speech consider two different point of view: user needs and M&S evolution, the presentation couple the new expectations by the users with the potential of enabling technologies and innovative methodologies. Case Studies related to different projects are proposed as example for providing guidelines in term of identify critical issues as well as new R&D tracks that are expected to become strategic issues for future developments in this area. The evaluation of impact of M&S on Industry is presented considering several aspects (i.e. Profitability, quickness, robustness, competitiveness), in addition the presentation provide a guideline for identify conditions that support use of M&S in Industrial projects as well as cost drivers and risk/opportunity sources.

# METHODS FOR RECOGNITION AND CLASSIFICATION OF HUMAN MOTION PATTERNS A PREREQUISITE FOR INTELLIGENT DEVICES ASSISTING IN SPORTS ACTIVITIES

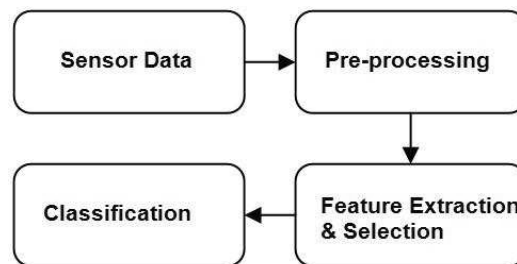
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**Introduction.** Technological systems are getting increasingly important for physical activity monitoring and assessment in general and for supervising load and performance in mass and elite sport in particular. Miniature sensors and computing devices are attached to the athletes or integrated into the sports equipment in order to acquire and process performance or load related data. Ubiquitous computing technologies are thus applied to implement systems, which provide athletes with feedback information on the quality of the motion just performed. Moreover, the acquired data may be used in order to adapt the sports equipment to the current needs of the athlete.

Due to the rapid progress in hardware capabilities and the potential of data processing methods, it is expected that “the emphasis in the future developments will shift to development of intelligent systems that could not only analyse the data but suggests strategies and interventions” [1]. Moreover, sports equipment will be able to sense new conditions in the environment and adapt accordingly thus showing the behaviour of adaptive systems.

**Recognition and Classification.** One main basis of almost any intelligent feedback system or adaptive system is the successful recognition or classification of patterns underlying the human motion just performed. This analysis does not only comprise kinematic parameters, but, moreover, also kinetic and physiological data. The figure illustrates the classification process.



*Statistical classification*

Different methods and models have proven to be useful for this kind of analysis. In the presentation, a survey of approaches most commonly applied is given. Pros and cons are discussed with regard to their applicability in intelligent devices supporting athletes. Practical applications are presented and experiences reported.

**Conclusions.** There are powerful weapons in our arsenal of computational methods for classification of human movement and physical activity. The choice of the method finally implemented depends on the type of the classification task. In particular, the complexity of the computations required and the available computing power have to be taken into consideration.

Many practical developments are able to differentiate between exercises. In order to provide adequate feedback in sport, however, often not the exercises are of interest, but a differentiation in execution of the individual exercise itself. Hence, small nuances have to be detected. This requires a careful training and adaptation of the classifiers selected.

- [1] Baca, A., Dabnichki, P., Heller, M., and Kornfeind, P. (2009). *Ubiquitous computing in sports: A review and analysis*. Journal of Sports Sciences, 27 (12) (2009), 1335-1346.



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## GENERATION OF RANDOM PARAMETERS OF BEHAVIORAL MODELS

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**Introduction.** Technology progress in IC design and semiconductor manufacturing has resulted in circuits with more functionality at lower prices for the last decades. This trend was mostly driven by decreasing the minimum feature sizes used in the fabrication process. With scaling also the impact of the variations increases. Front end variability is variability that impacts the devices. Back end variability results from steps creating the interconnects. Furthermore, it should be distinguished between variations from die-to-die and variations within a die [1]. It is now interesting in the design process to determine how the known randomness of process parameters influences the randomness of performance parameters of a system such as delay times and energy consumption. Violations of required limits of these parameters reduce the yield of the production. System studies in general can only be done with higher level models which we call behavioral models.

**Mathematical model.** A special problem in this context is to handle the influence of the intra-die variations on the parameters of behavioral models. Starting point for this paper is the subsequent problem: We consider two realizations  $i$  and  $j$  of the same subcircuit. The parameters  $(X_i, X_j)$  that characterize these components are jointly distributed and described by a cumulative distribution function (CDF)  $F(x_i, x_j)$ . Then the parameters  $(Y_i, Y_j)$  of the associated behavioral models are also jointly distributed and described by a CDF  $G(y_i, y_j)$ . All groups of two subcircuits with the same structure can be described in the same way.

To generate random parameters of behavioural models of two instances on a die, we modify an approach that bases on [2, 3]. Based on numerical experiments (or measurements), we can determine the matrix of Spearman's correlation coefficients (rank correlation coefficients) that characterizes  $G$ . Afterwards, jointly standard normal distributed values can be generated using the corresponding Pearson's correlation matrix. The results can be transformed into jointly uniform (0,1) distributed values followed by a transformation to the parameters of the behavioural models using a Generalized Lambda Distribution approach [4]. Marginal distributions and rank correlations are preserved [5].

In this way, the random parameters not only of two but of  $n$  behavioral models of the same subcircuit structure can be created. We briefly outline how the approach can be extended if different subcircuits shall be considered in one circuit.

**Examples.** Examples were prepared to compare Monte Carlo SPICE transistor level simulations with the results of Monte Carlo gate level simulations. In the first case, a path of digital gates was investigated. The second example is an adder structure. In both cases, we were interested in the energy consumption of the circuits. Furthermore, the path delay or delay was of interest in the first example. The results of SPICE level simulations and the behavioral gate level simulations are in good correspondence.

**Conclusion.** The presented approach is a step towards hierarchical statistical modeling of electronic circuits. This is a problem of high interest if semiconductor technologies move more and more to smaller geometries. The presented method focuses on the characterization of statistical properties of performance parameters and parameters of behavioral models. It considers inter-die and intra-die variations. After the characterization of the subcircuits, information about process parameter variations is no longer necessary. This option makes the approach attractive for the characterization of libraries of digital cells.

- [1] Srivastava, A.; Sylvester, D.; Blaauw, D. *Statistical Analysis and Optimization for VLSI: Timing and Power*. Springer, 2005.
- [2] Fackler, Paul, L: Generating Correlated Multidimensional Variates. 1999.  
Online: <http://www4.ncsu.edu/~pfackler/randcorr.ps>
- [3] Phoon, K.-K.; Quek, S.-T.; Huang, H.: Simulation of non-Gaussian process using fractal correlation. *Probabilistic Engineering Mechanics*, 19(2004), pp. 287-292.
- [4] Karian, Z.A.; Dudewicz, E.J.: *Fitting Statistical Distributions: The Generalized Lambda Distribution and Generalized Bootstrap Methods*. CRC Press, 2000.
- [5] Lange, A.; Sohrmann, C.; Jancke, R.; Haase, J.; Cheng, B.; Kovac, U.; Asenov, A.: A General Approach for Multivariate Statistical MOSFET Compact Modeling Preserving Correlations. In: *Proc. European Solid-State Device Research Conference, ESSCIRC 2011*, 12-16 September 2011, Helsinki, pp. 163-166, DOI: 10.1109/ESSDERC.2011.6044209

# EFFICIENT TRANSIENT SIMULATION OF NON-LINEAR DYNAMIC NETWORKS WITH DISCONTINUOUS FORCING

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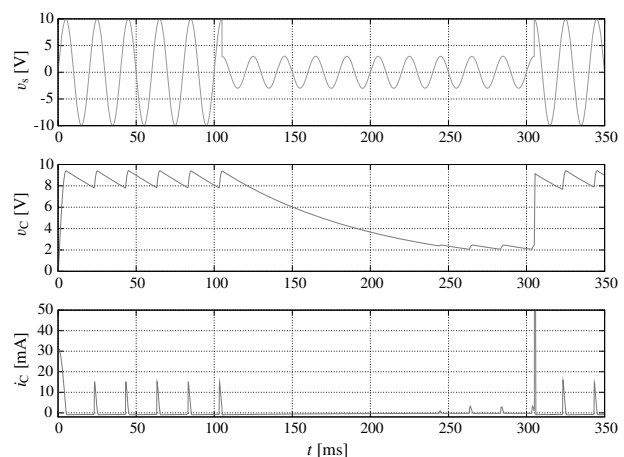
**Motivation.** New technologies produce more and more highly complex hybrid systems containing analogue components next to digital hardware and software. Approximately 80% of today's Systems on Chip (SoCs) are mixed-signal chips due to the International Technology Roadmap for Semiconductors (ITRS), 2007 Edition. Most of their input and output signals, e.g., signals from sensors and to actuators, are still analogue because our world and how we interact with it is analogue. However, major parts of the systems are mostly digital, circuits for signal processing and controls, for instance.

Co-simulation of digital and analogue components is normally done by coupling the various parts of a system via directed signals. Some of these signals may be considered as input signals with respect to the analogue parts, the others as output signals. Values of these input signals change at discrete points in time. The waveforms of prescribed quantities caused by these signals are therefore expected to be discontinuous. Usually, a common approach of most circuit simulators is to replace the steps in the stimulus functions by steep finite slopes. Then the resulting waveforms are continuous again but huge values in the derivatives of the network variables can be caused by these steep slopes. They may harm both, the simulation results and the simulation performance. Moreover, during the concept phase of a design process, appropriate rise and fall times of the logic gates' output voltages, for instance, are not known. Hence, discontinuities in input signals cannot be replaced by steep finite slopes.

**Approaches.** The determination of consistent initial values after a discontinuity in a forcing function of a prescribed quantity is discussed in a variety of publications. Recent approaches with numerical methods as in [1, 2, 3], for instance, yield consistent initial values but require that the regarded DAE systems are linear. Then the initial values can be determined by calculating the step response in the Laplace domain. The approach presented in this MATHMOD contribution is based on a transformation of the DAE system by substituting the time for a new independent variable. This substitution and a tailored function connecting the left- and right-hand limits of the values of the forcing functions at the discontinuities allow the numerical integration of the non-linear dynamic system between the events of discontinuities as well as the calculation of consistent initial values after each of these events. Note that only one DAE system is therefore needed to be set up.

Our method is described by applying it to the network equation system of a simple half wave rectifier. The results of the complete simulation of this example circuit are shown on the right. The calculation of the solution on the complete domain (0, 350 ms] is sequentially done. But the numerical method for calculating consistent initial values for the integration after the discontinuities can be the same as the one usually utilised to solve these DAE systems without discontinuous forcing (the resulting waveforms are red at discontinuities and blue otherwise). There is no difference to solving any other initial value problem.

**Conclusion.** An efficient and accurate method for the transient analysis of non-linear dynamic systems with discontinuities in the forcing functions of its prescribed quantities is presented. In contrast to recent approaches, the DAEs of the systems may be non-linear. For some special cases of DAE systems, generalised formulae for the calculation of the transformed equation system have been derived.



- [1] Barton, P.I. and Galán, S.: *Linear DAEs with Nonsmooth Forcing*. Technical Report, Massachusetts Institute of Technology, Cambridge, 2000.
- [2] Opal, A. and Vlach, J.: *Consistent Initial Conditions of Linear Switched Networks*. In: IEEE Trans. on Circuits and Systems, 37(3), 1990, 364–372.
- [3] Reißig, G., Boche, H., and Barton, P.I.: *On Consistent Initial Conditions for Linear Time-Invariant Differential-Algebraic Equations*. In: IEEE Trans. on Circuits and Systems I, 49(11), 2002, 1646–1648.

# COMPUTERIZED MODEL BASED FUNCTIONAL SAFETY ANALYSIS

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**Introduction** The functional correctness of a component is the guarantee that the component behaves the way it should and fulfills all the functional requirements of the system. In order to ensure functional correctness of a component it is necessary to perform a series of rigorous tests on the target device in the appropriate environment context. Skipping this phase and allowing for a component to be tested based on its design specification, without an actual hardware implementation, would make a significant contribution to reducing the skill, labor, time and money required to develop the component.

In this paper we present a novel approach to Functional Safety verification, where we integrate functional tests as full fledged components into a model based architecture developed using OpenModelica [2]. This model can then be used to generate a stochastic Bayesian model which in turn can be used to produce a Failure Mode Effect and Analysis (FMEA) table.

**A Combined Modeling Approach** We use Bayesian Networks for the specification of risk models that represent the key factors and their inter-relationships (a qualitative model) with probability distributions based on expert judgment or from observed data (a quantitative model).

To determine the possible failures of a design we rely on Failure modes and effects analysis (FMEA) [3].

These analysis techniques are integrated into a single tool suite, combined with the OpenModelica modeling tool, which allows for an intuitive and structured modeling process.

**Implementation** The proposed tool is implemented in C++ and Matlab is used for the generation of the causal nodes for the components of the model, which are written in Modelica using the OpenModelica tool. The implementation also relies on the Structural Modeling, Inference and Learning Engine (SMILE) library [1] for the creation of the Bayesian Network and the companion tool GeNie for visualizing the resulting BN.

Building the network consists of three tasks. The first of these is to identify the variables of importance along with their possible states. Once these are identified the next task is to identify the relationships between the variables and to express them through a graphical structure. The third and final task is to obtain the probabilities for the quantitative part of the network.

The troubleshooting problem in the context of a model can be expressed as follows “*Given a set of observations, which component is the most likely to be faulty?*”.

**Conclusion and Future Work** Using Bayesian Networks for diagnostics in the context of functional safety verification has both advantages and drawbacks.

A clear advantage is the direct correspondence of the network nodes to the real world components of the ECU. This simplifies the maintenance of the model.

The use of expert knowledge is also a plus. On the other hand it may become counter-effective when several experts are involved and a large amount of probabilities has to be elected.

In the near future the implementation will be rendered more portable and stable by replacing the Matlab tool by a node generation algorithm implemented in C++, which is now under development.

The next step, is to implement fault-tolerant control and diagnosis through a service oriented architecture in a more complex and realistic system, as opposed to the simplified example used for this paper.

- [1] Marek J. Druzdzel. Smile: Structural modeling, inference, and learning engine and genie: a development environment for graphical decision-theoretic models. In *Proceedings of the sixteenth national conference on Artificial intelligence and the eleventh Innovative applications of artificial intelligence conference innovative applications of artificial intelligence*, AAAI '99/IAAI '99, pages 902–903, Menlo Park, CA, USA, 1999. American Association for Artificial Intelligence.
- [2] Peter Fritzson. *Principles of Object-Oriented Modeling and Simulation with Modelica 2.1*. Wiley-IEEE Press, 1., auflage edition, January 2004.
- [3] R.E. McDermott, R.J. Mikulak, and M.R. Beaugard. *The basics of FMEA*. CRC Press, 2009.

# THE MATHEMATICAL MODELLING OF THERMAL TRACER PARTICLES IN NAVIER-STOKES FLUIDS

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## Summary

A key issue in fluid dynamics is the unique definition of the phase-space Lagrangian dynamics characterizing prescribed ideal fluids (i.e., continua), which is related to the dynamics of so-called *ideal tracer particles* (ITP) moving in the same fluids. These are by definition particles of infinitesimal size which do not produce significant perturbations of the fluid fields and do not interact among themselves. For Navier-Stokes (NS) fluids, the discovery by Tessarotto *et al.* (2005-2009) of the phase-space dynamical system advancing in time the state of the fluid has made possible, *in the case NS fluids*, the actual definition of these trajectories. In this paper we intend to pose the problem in the case of compressible/incompressible Navier-Stokes fluids based on the inverse kinetic theory which can be developed for their phase-space statistical description (see also accompanying extended paper [1]). In this paper we report the discovery of a subset of so-called *ideal tracer particles* (ITP [?]) belonging to Navier-Stokes (NS) fluids which are denoted as *thermal tracer particles* (TTP). Their states are found to be uniquely dependent on the local state of the fluid. This means that a suitable statistical ensemble of TTPs should reproduce exactly the dynamics of the fluid. In other words, it should be possible to determine the fluid fields characterizing the fluid state by means of suitable statistical averages on the ensemble of TTPs so that they satisfy *identically* the required set of fluid equations. The result applies to NS fluids described as mesoscopic, i.e., continuous fluids, which can be either viscous or inviscid, compressible or incompressible, thermal or isothermal, isentropic or non-isentropic. We shall assume that the state of these fluids is represented by an ensemble of observables  $\{Z(\mathbf{r}, t)\} \equiv \{Z_i(\mathbf{r}, t), i = 1, \dots, n\}$  (with  $n$  an integer  $\geq 1$ ), i.e., *fluid fields*, which can be *unambiguously prescribed* as continuous and suitably smooth functions, respectively, in  $\bar{\Omega} \times I$  and in the open set  $\Omega \times I$  (in the following to be identified with a bounded subset of  $\mathbb{R}^3$ ). We intend to show that, as a remarkable consequence, the phase-space dynamical system which advances in time (the states of) these particles can be *uniquely* prescribed in such a way to determine *self-consistently* the time evolution of the complete set of fluid equations characterizing the fluid. This implies that TTPs must reproduce *exactly* the dynamics of the fluid. In other words, by means of an appropriate statistical averages on the ensemble of the TTPs, it is possible to determine the time-evolution of the fluid state, in such a way that it *satisfies identically* the required set of fluid equations.

## References

- [1] Massimo Tessarotto, C. Asci, C. Cremaschini, A. Soranzo, Marco Tessarotto and G. Tironi, *Lagrangian dynamics of thermal tracer particles in Navier-Stokes fluids*, submitted (2011).

# GEOMETRIC MORPHOMETRICS AND FINITE ELEMENT ANALYSIS: FIRST RESULTS FROM A JOINT FORMALISM FOR MODELING STRAIN

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**Introduction; background in brief.** Finite element analysis (FEA) is a robust and widely exploited 20th-century approach to the computational approximation of partial differential equations, particularly for continuum mechanics. Geometric morphometrics (GMM), a more recent methodology, blends tools from computer vision and multivariate statistics in a toolkit for pattern analysis of shape variation that has been applied extensively in conjunction with deformable-template methods since 1990, especially within organismal biology and medical imaging. FEA works by (1) discretizing a body under analysis into a finite number of subdomains, (2) expressing the solution of the equation (e.g., shifts of the coordinates of the corners of the subdomains) in terms of a linear algebraic system accommodating continuities and boundary conditions among the subdomains, and (3) solving the resulting system of equations, which is often a very large one. The deformations are construed as if real, capable of validation by appropriate instrumentation. For GMM, in contrast, the implied deformations need not be realizable (e.g. a youngster's skull to the same skull twenty years later, or one elderly female's femur compared to another's). Rather, GMM is a praxis for statistical analysis of labelled point locations corresponding to any rearrangement of these labelled points in two or three dimensions. The typical GMM analysis proceeds by (1) erecting a list or mesh of homologically labelled points on two or more forms, (2) carrying out an appropriate statistical analysis of the locations of these points, and (3) visualizing the statistics by a simulated deformation, the *thin-plate spline*, back in the plane or volume of the original data. Step 2, the "appropriate statistical analysis," is usually realized as an analysis of the equivalence classes of the digitized data configurations under the operation of either the isometry group or the similarity group, the latter usually referred to as *Procrustes analysis*.

**Rationale.** GMM and FEA use the same raw data resources (marked points on internal or external bounding surfaces of objects of interest), and rely to some extent on the same partial differential equation (the biharmonic equation). In the absence of any canonical statistical method for finite-element studies, the possibility of a bridge between GMM and FEA is becoming a focus of active concern in several contemporary biosciences. To oversimplify only a little, GMM represents statistics without realism, whereas FEA represents realism without statistics. When it is organismal form we are studying, or an industrial form produced in indefinitely many copies, there is variation to be studied or controlled. Because they rely on the same information from nature, then, a fusion of GMM with FEA may prove capable of managing these information flows in the interest of the society that is manufacturing the objects or analyzing the organic forms.

**Strategy driving this MathMod presentation.** As a first step in this fusion, I explore the relation between the simplest scalar summaries of the two approaches, GMM and FEA, in what is probably the oldest context for elasticity studies: the *uniform cantilever* or *Euler-Bernoulli beam* subject to a load at the free end. In this setting there is no need for finite-element software, as the resulting deformation is known exactly (the effect on the neutral filament is a cubic polynomial). To prototype the exploration of GMM-FEA relationships in general, one produces a range of these deformations for various combinations of beam geometry and load and studies the patterns relating the separate GMM and FEA summaries. The central GMM summaries are *Procrustes distance* (a shape distance) and *Procrustes shape coordinates*; the central FEA summary is the strain energy of the resulting deformed beam.

**Results.** Neither the principal shape coordinates nor any of the other standard GMM statistical summaries correctly capture the energetics of the realistic Euler-Bernoulli elasticity model. However, when length and height of the beam are varied under conditions of constant end load, there is exact proportionality between strain energy and a nonstandard version of one common GMM scalar quantity, the Procrustes length of the deformation. The requirement that the report be common to the two methodologies (since they are working off the same geometric data) thus specifies the version of each that is appropriate for the reporting.

**Implications.** The information overlap between GMM and FEA approaches in this special case may serve as a prior conjecture in many other situations where geometric parameters are systematically varied in otherwise homogeneous simulations of empirical deformations. In the present setting, no finite element software was actually needed, as strain energy could be recovered from the simple kinematics of the load at the end of the beam. In more general contexts, strain energy will need to be produced as an integral of a functional on the strain tensor over all the elements of the analysis, and deformations that are less smooth will need to be described by another GMM scalar, the *bending energy*, as well as by this standard shape distance. The combination of the two may convey much of the information about strain concentrations and thereby lead to a good preliminary method for applied statistical analysis of finite-element computations under conditions of data variability around a realistically sculpted template (e.g., a femur), a problem for which there does not yet appear to be any suggestion of a standard method.

## ON MATHEMATICAL THEORY OF SELECTION: REPLICA DYNAMICS AND THE PRINCIPLE OF MINIMUM OF INFORMATION GAIN

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E.Szathmary and M.Smith [8] considered non-linear “parabolic” and “hyperbolic” models of prebiological evolution of replicating molecules. We show here that population heterogeneity can be a reasonable explanation for these unusual growth laws. We also consider the model of a community composed of populations that grow either parabolic or hyperbolic laws. We show that the frequencies of populations in the community follow the Pareto law and minimize the Tsallis relative entropy (non-additive information gain) at each time moment. Hence, the general principle of Minimum of Tsallis information gain is the underlying law for evolution of not only exponential, but also parabolic and hyperbolic selection systems.

- [1] Borland, L., Plastino, A.R., and Tsallis, S.: *Information gain within nonextensive thermostatistics*. Journal of Mathematical Physics, 39 (1998), 6490–6501.
- [2] von Forster, H., Mora, P.M., and Amiot, L.W.: *Doomsday: Friday, 13 November, A.D. 2026*. Science, 132 (1960), 1291-99.
- [3] Hofbauer, J., and Sigmund, K.: *Evolutionary game dynamics*. Bulletin of American Mathematical Society, 40 (2003), 479-519.
- [4] Karev, G.: *On mathematical theory of selection: continuous time population dynamics*. Journal of Mathematical Biology, 60 (2010), 107-129.
- [5] Karev, G.: *Principle of Minimum Discrimination Information and Replica Dynamics*. Entropy, 12 (2010), 1673-1695.
- [6] von Kiedrovski, G.: *Minimal replicator theory I: parabolic versus exponential growth*. Bioorganic Chemistry Frontiers, 3 (1993), 113-146.
- [7] Schuster, and P., Sigmund, K.: *Replicator Dynamics*. Journal of Theoretical Biology, 100 (1983), 533-538.
- [8] Szathmary, E., and Smith, M.: *From Replicators to Reproducers: the First Major Transitions Leading to Life*. Journal of Theoretical Biology, 187 (1997), 555-571.
- [9] Szathmary, E.: *The origin of replicators and reproducers*. Philosophical Transactions of the Royal Society B, 361 (2006), 1761-1776.



# MODELING OF INTERACTION OF MULTIPLE INTELLIGENT SYSTEMS IN A REAL-WORLD ENVIRONMENT

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**Introduction** In modern working environments, human operators work together with other humans as well as with technical systems. As technical systems and processes become more and more complex, supporting and assistance systems can help to increase the performance of the operators and the human-machines-system. This systems need a detailed understanding about the processes as well as of the operating units, which primarily involves understanding of interaction between multiple humans and 'intelligent' technical systems. Both humans and technical systems are equally referred to as intelligent systems (IS) here.

In this contribution, the interaction comprehension is achieved by the use of cognitive modeling approaches. Most current cognitive modeling approaches consider a single IS interacting with a dynamically changing environment. Accordingly, the main idea of this paper is based on the question how to model the complex system and the related dynamic interactions with more than two interacting IS with individual behavior. Two different solution approaches are proposed, the Integral Approach and the Empathy Approach.

**Cognitive modeling of multiple individuals** It is well known from psychology [2] that humans work with so-called mental models. The effect is to reduce the complexity of human interaction with the outside world by assuming constants in the structure of the outside world, which allows the prediction of the future based on those already known and experienced constants with a known structure. This leads to a knowledge-guided interaction behavior based on the use of the human cognition by cognitive functions, procedures, and routines. Within the contribution, cognition is based on the assumption of individual perception, awareness, and the individual ability to store, handle, and combine information. Here, a system showing this behavior is understood as an individual due to internal learning mechanisms in combination with an individual knowledge base which contains the mental model (refer to [1]).

In order to formalize the mental model for the use in cognitive technical systems, the Situation-Operator-Modeling (SOM) (refer to [3]) is applied. Within the SOM approach the processes in the real world are considered as sequences of scenes and actions, which are modeled as situations (time-fixed description of the considered system or problem) and operators (changes within the considered system), respectively.

**Modeling Approaches** Accordingly, in the 'Integral Approach', an integral and global perspective of all interacting IS and the environment is applied. This global perspective leads to an uniform description of all available aspects of the involved IS and the environment. The Integral Approach allows a global comprehension of the situation to be modeled. This requires all perceived information to be transferred between the involved IS immediately and without errors to constitute a global model, which is part of and synchronized between the involved IS. Accordingly, all involved IS contribute to the same shared mental model. However, if the synchronization is not possible due to communication problems, this approach will not work.

The second approach is based on the individual and distributed perspectives of each involved IS, so the approach is denoted as 'Empathy Approach'. In contrast to the Integral Approach, only the perceptions of the specific IS are considered when refining the individualized mental model. In this case, error-free communication (or communication at all) is not a requirement since each IS uses an individual model for the situation. This individual model is not shared with other IS, and the learning process is limited to the single IS. The knowledge base of the IS does not contain complete information about the others, only what is perceived from their (interaction) behavior and communicated by them.

**Application Example** The example to illustrate both proposed modeling approaches is taken as an advanced highway traffic scenario. Here, multiple vehicles and their human or technical intelligent drivers interact on a highway. If it is possible to model the traffic situation with the proposed cognitive approaches, the complexity of the traffic situation can be estimated by modeling the behavior of the drivers. This enables a supervision system to predict traffic behavior.

- [1] E. Ahle and D. Söffker. Interaction of intelligent and autonomous systems – part 1: Qualitative structuring of interaction. *Mathematical and Computer Modelling of Dynamical Systems*, 14(4):319–339, 2008.
- [2] J. Anderson. *Cognitive Psychology and Its Implications*. W.H. Freeman, New York, 5th edition, 2000.
- [3] D. Söffker. *Systemtheoretische Modellbildung der wissensgeleiteten Mensch-Maschine-Interaktion*. Berlin: Logos Wissenschaftsverlag, 2003. Also: Habilitation Thesis, Univ. Wuppertal, 2001.

# A MODEL OF INTERNAL INFORMATION STRUCTURE FOR PLANNING COORDINATED GROUP CONTROL

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The formation control and team behaviour simulation problems are significant items in modern agenda of optimal control and game theories [1,2]. The problems include a wide range of statements modelling real-time interaction of teams with finite membership.

The motion of participants of common movement may be treated in terms of system trajectories reflecting state, spatial, conceptual and organizational structures, results of observation and management. Participants may change their positions in accordance with consequent control decisions, step-wise formed on a symmetrical and discrete positional grid. Hence the common interaction may be split into multiple layers of respectively independent processes for couples of symmetrical systems.

The problem under consideration in the paper is connected with trajectory planning for the team of objects constrained in dynamics and overcoming nonconvex, disconnected obstacles under coordinated control. Research is partly motivated by applications in navigation and net tracing, where practical problems may be stated as geometrical, even planar ones. The crucial point for trajectory planning algorithms design is choice of adequate information structure. The requirement is to describe regularly complex circumstances with multiple obstacles and routes of team motion in case of objects limited in perception and conflicting interests.

A wide range of situations allows imbedding restrictions of object dynamics and observation in uncertainty of state position. Then the analysis of tubes of admissible trajectories is possible via guaranteed approach. It was shown in [3], that a priori choice of optimal tube and parameter approximation of obstacle are symmetrical problems. The structural symmetry and duality of problem statements and solutions for conjugate systems are essential properties in the optimal control theory under uncertainty. The duality property for control problems with set-membership description of disturbances and integral or extremal performance index [3] have been investigated on the base of operator presentation.

The possible application of results on duality of guaranteed estimation and control problems for the route design and choice is considered. Algorithms realizing coordinated control are based on separation property in problems of ensured control and estimation [4].

The triple  $C = (i)\{X, P, Q\}$  is called a hierarchical (i)-system if the following components are included.

- 1) *Topological region*  $X = \{X/Sc\}$ . Here  $X \subseteq V$  and  $Sc = \{cc, rc/ ec\}$  is a polar coordinate system.
- 2) *Graph of organizational structure*  $P = \{P, P\}$ . Here  $P = \{(i-1)C.m\}$  and  $P = \{(C, C^*)\} \subseteq P \times P$  is a binary relation.
- 3) *Border approximation*.  $Q = \{Q, Q\}$ ;  $Q = \{q=L_k\}$  lists  $Sc$ -ordered couples of links  $q$ ,  $Q$  is a structure matrix.

Presented model provide unified descriptions of organizational structure, trajectories and geography. Symmetry of hierarchical (i)-systems allows to describe complex shape of shoreline in advance as a solution of ensured estimation problem. Quality is evaluated by extremal induces. Then choice of trajectories may be interpreted in terms of control problem. Separation property of ensured control/estimation problems allows to split algorithmically procedures of coordinated control.

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- [1] Kurzanski A.B., Mitchel I.M., Varaiya P. *Optimization techniques for state-constrained control and obstacle problems*. Journ. of Optimization Theory and Appl. 2006. Vol. 128 (3), pp. 499-521.
- [2] Kurzanski, A.B. *On the problems of compound motion control*. Proc. Int. Conf. on Actual Problems of Stability and Control Theory. Yekaterinburg, Russia, Sept. 21-26 2009. p.103.
- [3] Kruglikov, S. V. *On the operator formalization of the separation property in problems of ensured control and estimation*. Proc. European Control Conf. Brussels, Belgium, July 1-4 1997. WE-E-13.
- [4] Kruglikov S.V. *Structural Properties of Guaranteed Control-Estimation Problems for Hierarchical Systems* the IPACS electronic library. 5th International Conference on Physics and Control (PhysCon 2011). September 5-8, 2011, León, Spain. <http://lib.physcon.ru/doc?id=0838a557d81f>

## CONTROL AND DESIGN OF COMPUTING SYSTEMS: WHAT TO MODEL AND HOW

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**Introduction.** The complexity of many computing system functionalities is nowadays abruptly increasing. To give just one example, consider the Linux scheduler. In the Kernel version 2.4.37.10 (September 2010) all of its code was contained in a single file of 1397 lines. In version 2.6.39.4 (August 2011) the scheduler code is spread among 13 files for a total of 17598 lines. Other examples could be given, but are omitted for space limitations.

Indeed, when such “explosions” are experienced, the overall design approach is to be somehow reconsidered. Observing the matter from a modelling-oriented standpoint, and not limiting the scope to the scheduler example, it can be noticed that hardly any computing systems functionality has been conceived and developed based on a dynamic model of some physical phenomenon to be controlled.

In the scheduler case, to stick to the example, the phenomenon is how the CPU is distributed among the running tasks, depending on control actions (the allotted timeslices) and exogenous disturbances (task blockings, resource contentions, and so on).

The situation just sketched has quite clear historical reasons. Suffice to say that, while in any other context controlled objects can be modelled based on physical (first) principles, this is not the case for computing systems, because there the “physics” is created by the system designer him/herself.

In the absence of a modelling framework, system design is carried out directly in an algorithmic setting, leaving the engineer without any means to assess its behaviour in the sense that term is given in the system and control theory domain.

While such a *scenario* could to date be tolerated, given the mentioned complexity rate increase, it cannot be assured that said tolerability will carry over to the future.

In fact, as “more physics” is created, the absence of a rigorous dynamic description of it may sooner or later pose intractable problems as for its governance. As a consequence, rigorous – and possibly simple – modelling frameworks to ground system design upon are needed.

**Paper outline.** The main message this paper wants to convey, is that if one accepts to re-design part of said system, such a framework can be found by (usefully) limiting the model scope to describing the real physical phenomenon on which the addressed aspects of the system behaviour depend. If this is done, surprisingly simple formalisms can be used—a noticeable example indeed of process/control co-design, and a relevant step forward with respect to previous research as presented e.g. in [1] and in the various papers quoted therein.

This paper concentrates on the modelling side of the problem, by showing the ideas above at work. Some words are spent on the consequent advantages in terms of system (and control) design, providing some examples based on parallel research on the matter such as [2], leaving however a deeper treatise to other works centred more on control than on modelling.

[1] Joseph L. Hellerstein, Yixin Diao, Sujay Parekh, and Dawn M. Tilbury. *Feedback Control of Computing Systems*. Wiley, September 2004.

[2] Alberto Leva and Martina Maggio. Feedback process scheduling with simple discrete-time control structures. *Control Theory Applications, IET*, 4(11):2331–2342, 2010.

*K-LINES* CLUSTERING WITH CONVEX AND PIECEWISE LINEAR (*CPL*) FUNCTIONS

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**Introduction.** Clustering algorithms are the basic tools for solving pattern recognition or data mining problems. The most popular iterative clustering algorithm is the *K-means*. The basic idea behind the *K-means* algorithm is to divide a given set of vectors into subsets around the *central points* (class prototypes). In the case of the *K-lines* clustering algorithms vectors are partitioned into *K* subsets by using the *central lines* in the *n*-dimensional feature space. The proposed *K-lines* clustering is based on minimizations of the *CPL* criterion functions.

**Content.** Data mining tools are used for transformation of data sets into needed information [6], [7]. Such tools are commonly used in a wide range of applications, such as marketing, forecasting, fraud detection or scientific discovery. Data mining can be viewed as a process of extracting hidden and possibly useful patterns or models from a given data set. The term *patterns* could mean regularities, such as trends, association rules or dependencies in an explored data set.

Clustering algorithms belongs to the most powerful tools of data mining. The most popular iterative clustering algorithm is the *K-means* [1], [6]. The basic idea in the *K-means* algorithm is linked to partitioning of a given set *C* of *m* vectors  $\mathbf{x}_j[n]$  ( $\mathbf{x}_j[n] \in R^n$ ) into subsets  $C_k$  around the *central points* (class prototypes)  $\mathbf{m}_k[n]$  ( $\mathbf{m}_k[n] \in R^n$ ) which had been computed (defined) earlier. In the next step, the central points  $\mathbf{m}_k[n]$  are modified in accordance with the subsets  $C_k$ . These steps are repeated until the central points  $\mathbf{m}_k[n]$  are stabilized in the successive steps.

Modifications of the *K-means* algorithm into the *K-planes* algorithm are based on computations of the *central planes*  $P_k$  for particular subsets  $C_k$  instead of the central points  $\mathbf{m}_k[n]$ . In accordance with the work [4], the central plane  $P_k$  that minimizes the sum of the squares of the  $L^2$  (*Euclidean*) distances to  $m_k$  points  $\mathbf{x}_j[n]$  in the subsets  $C_k$  is computed. The proposed solution can be achieved by using *singular value decomposition (SVD)* algorithms.

The *K-planes* algorithm based on the *central planes*  $P_k$  that minimize a special type of the convex and piecewise linear (*CPL*) criterion function  $\Phi_k(\mathbf{w}[n])$  ( $\mathbf{w}[n] \in R^n$ ) defined on feature vectors  $\mathbf{x}_j[n]$  from subsets  $C_k$  has been proposed in the work [5]. The basis exchange algorithms which are similar to linear programming allow to find the minimum of these *CPL* function  $\Phi_k(\mathbf{w}[n])$  efficiently, even in case of large, multidimensional data sets [3].

The *K-lines* clustering algorithm is described and analyzed in the presented work. The *K-lines* algorithm can be treated as a special case of the *K-planes* algorithm and is based on computations of the *central lines*  $l_k$  for particular subsets  $C_k$ . The minimization of the modified *CPL* criterion function  $\Psi_k(\mathbf{w}[n])$  allows to compute efficiently the *central line*  $l_k$  for the subset  $C_k$ .

- [1] Bobrowski L., and Bezdek J.C.: *C-means clustering with the  $L_1$  and  $L_\infty$  norms*. IEEE Transactions on Systems Man and Cybernetics, 21(3), 1991, 545-554.
- [2] Bobrowski L.: *CPL clustering based on linear dependencies*. In: Proc. MATHMOD 2009, Vienna, 2009.
- [3] Bobrowski L.: *Design of piecewise linear classifiers from formal neurons by some basis exchange technique*. Pattern Recognition, 24(9), 1991, 863-870.
- [4] Bobrowski L., and Łukaszuk T.: *Relaxed Linear Separability (RLS) Approach to Feature (Gene) Subset Selection*. Selected Works in Bioinformatics, Xuhua Xia (Ed.), INTECH, 2011, 103-118.
- [5] Bradley P. S., and Mangasarian O.L.: *K-plane clustering*. Journal of Global Optimization, 16, 2000, 23-32.
- [6] Duda O.R., Hart P.E., and Stork D.G.: *Pattern Classification*. J. Wiley, New York, 2001.
- [7] Hand D., Smyth P., and Mannila H.: *Principles of Data Mining*. MIT Press, Cambridge, 2001.
- [8] Wu T.T., Chen Y.F., Hastie T., Sobel E., and Lange K.: *Genome-wide association analysis by lasso penalized logistic regression*. Bioinformatics, 25(6), 2009, 714-721.

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# ONLINE REDUCED BASIS CONSTRUCTION PROCEDURE FOR MODEL REDUCTION OF PARAMETRIZED EVOLUTION SYSTEMS

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**Introduction** The reduced basis method is a model reduction technique for parametrized PDEs approximating the parameter-dependent solutions to the PDE in a low dimensional space. This reduced space is constructed by “snapshots” of high dimensional discrete solutions for selected parameters and is usually built up in advance in a costly offline phase. The space is suited to approximate well solutions for all parameters in a given parameter domain.

We propose a new approach where the reduced approximation space is constructed rapidly online using a set of precomputed reduced basis entities. As this reduced space is locally adapted it can be of small size. This results in a more efficient online simulation and an overall faster online phase. Furthermore we are flexible in the control of the approximation error and can assure the fulfillment of an approximation accuracy requirement. Our problem setting is a general discrete linear parameter-dependent evolution equation

$$\mathcal{L}_{h,\Delta t}^{\text{Im}} u_h^{k+1}(\mu) = \mathcal{L}_{h,\Delta t}^{\text{Ex}} u_h^k(\mu) + \Delta t b_h(t^k, \mu) \quad (1)$$

with discrete solutions  $u_h^k(\mu) := u_h(t^k, \mu)$  stemming from a discrete high dimensional function space  $X_h$  at time steps  $t^k = k\Delta t$  with  $1 \leq k \leq K$  and initial condition  $u_h^0(\mu) = u_0$ . Similar methods have been proposed in [1, 2] in the setting of dynamical systems using a POD model order reduction. An approach that also makes use of single precomputed bases for individual parameters in the framework of Krylov-subspace methods is [3].

**New method for online basis construction** During the preparing offline phase we construct a “dictionary” of reduced bases  $\mathcal{D} = \{b_e | 1 \leq e \leq E\}$  consisting of entities  $b_e := (\Phi_e, \mu_e)$  where the  $\mu_e \in \mathcal{M}_{\mathcal{D}}$  stem from a given set of parameters  $\mathcal{M}_{\mathcal{D}}$ . The entity bases  $\Phi_e$  contain precomputed POD-modes of the detailed solution trajectories to the high dimensional evolution scheme (1) for all parameters  $\mu_e \in \mathcal{M}_{\mathcal{D}}$ .

Based on this dictionary of bases we construct in the online phase for a given parameter  $\mu^*$  a local reduced basis  $\Phi(\mu^*)$  spanning up a locally adapted reduced space  $X_N = \text{span}\Phi(\mu^*)$ . This online construction is done iteratively by selecting and combining the next “nearest” entities to  $\mu^*$  from the dictionary  $\mathcal{D}$  using a rapidly evaluable distance function  $d(\mu^*, b_e)$ . We present and compare four different distance functions. An online-POD assures the linear independence and orthogonality of all basis functions in the newly constructed basis.

In order to conduct rapid online simulations we perform a Galerkin-projection of (1) onto the newly generated local reduced space  $X_N = \text{span}(\Phi(\mu^*))$  and solve the resulting low dimensional evolution scheme. The assembling of this low dimensional evolution scheme can also be done rapidly online by using precomputed projections of the operators.

Numerical experiments show that this new method of online constructed reduced bases outperforms the standard RB approach concerning online simulation time and approximation errors.

**Summary** We present a new online basis enrichment procedure for the reduced basis method in case of evolution equations, where instead of using a reduced space suited for the whole parameter domain we construct in the online phase for a given parameter a local reduced space using precomputed basis entities. As the so-constructed reduced space is locally adapted, it can be of smaller dimension than the reduced space in standard RB-methods. Hence, the online complexity is lower and online simulations are faster. Another advantage is the flexible control of the desired approximation error. If the dictionary contains sufficiently many precomputed bases, we can assure the fulfillment of any approximation error requirement, which is not the case in standard-RB where the fulfillment of the error tolerance can only be assured on a limited set of training parameters used during the basis construction.

- [1] D. Amsallem and C. Farhat. An online method for interpolating linear parametric reduced-order models. *SIAM J. Sci Comp*, 33, No.5:2169–2198, 2011.
- [2] U. Baur, C. Beattie, P. Benner, and S. Gucercin. Interpolatory projection methods for parameterized model reduction. *SIAM J. Sci Comp*, 33 No.5:2489–2518, 2011.
- [3] B. Lohmann and R. Eid. Efficient order reduction of parametric and nonlinear models by superposition of locally reduced models. In *Methoden und Anwendungen der Regelungstechnik. Erlangen-Münchener Workshops 2007 und 2008*, pages 27–36. Shaker Verlag, Aachen, 2009.

# REMODELING OF DYNAMICAL SYSTEMS TO BENEFIT NUMERICAL SIMULATIONS

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**Introduction.** Differential-algebraic equations (DAEs) are essential tools in the modeling of dynamical processes. For instance, the dynamical behavior of mechanical systems, electrical circuits and many other are often described by DAEs, in particular, of quasi-linear structure.

It is well known that the numerical treatment of DAEs is nontrivial in general and more complicated than the one of ordinary differential equations (ODEs). A classification of different types of DAEs lead to the development of several (independent) index concepts. As a rule of thumb, the higher the index of a DAE is, the more complicated is its numerical analysis and its numerical integration. A way out of this dilemma of a higher index is a *remodeling* of such dynamical systems, i.e., a *regularization* of such classes of DAEs.

In this article we present a regularization method for *quasi-linear DAEs* of the form

$$E(x, t)\dot{x} = k(x, t), \quad (1)$$

on the domain  $\mathbb{I} = [t_0, t_f]$  with initial values  $x(t_0) = x_0 \in \mathbb{R}^n$ , where  $E \in \mathcal{C}(\mathbb{R}^n \times \mathbb{I}, \mathbb{R}^{n,n})$  and  $k \in \mathcal{C}(\mathbb{R}^n \times \mathbb{I}, \mathbb{R}^n)$ . Furthermore,  $x : \mathbb{I} \rightarrow \mathbb{R}^n$  represent the *unknown variables*.

**Remodeling of Dynamical Systems.** In general, additionally to the constraints explicitly occurring in the DAE the solution of higher index DAEs is restricted by so called *hidden constraints*. Those constraints are hidden in the DAE, i.e., they are not explicitly stated as equations. These constraints impose additional consistency conditions on the initial values and provoke severe difficulties in the direct numerical integration of DAEs of higher index.

In this article we investigate a remodeling of a dynamical system modeled with a quasi-linear DAE (1) to benefit its numerical simulation. Such a remodeling should end in a *semi-implicit DAE* of the form

$$E_1(x, t)\dot{x} = k_1(x, t), \quad 0 = k_2(x, t) \quad (2)$$

with a full-rank leading matrix function  $E_1$  and where all constraints have to be stated in explicit form, i.e., no hidden constraints exist.

In this article we present an iterative procedure as a tool for the analysis of quasi-linear DAEs (1). This procedure determines in each iteration step a semi-implicit DAE of the form (2), where the index is lowered by one from each iteration step to the next. Furthermore, the number of differential equations decreases while the number of constraints increases. After the successfully termination of the procedure one obtains a so called strangeness-free form (2) with a full-rank leading matrix function  $E_1$  and where all constraints have to be stated in explicit form. This strangeness-free form (2) is equivalent to the original DAE (1) in the sense that both have the same solution set.

**Numerical Approach.** The strangeness-free formulation (2) is suited and preferable for the numerical integration using stiff ODE solvers like implicit Runge-Kutta methods or BDF methods.

The strangeness-free formulation (2) corresponds to the DAE system consisting of the set of all hidden constraints together with a selection of the original DAE (1) by use of a dynamical selector. On the other hand, the overdetermined DAE system consisting the (unselected) original DAE and all hidden constraints has the same solution set as the strangeness-free formulation (2). Therefore, it is possible to use adapted numerical integration schemes directly based on this overdetermined DAE system instead of the strangeness-free formulation (2). In Section 3 of this article we present the basic idea to integrate such overdetermined DAE systems.

**Conclusion.** We present a procedure as general tool for the regularization of quasi-linear DAEs of an arbitrary index. This procedure regularizes the quasi-linear DAEs by an iterative lowering of the index while maintaining all (hidden) constraints. The procedure ends with the strangeness-free form of the quasi-linear DAE which can be used as basis for numerical simulations or further numerical investigations of the dynamical system.

Furthermore, the basic idea to simulate such systems in an efficient and robust way is discussed and illustrated by an example using the software package GEOMS.

- [1] Steinbrecher, A. Analysis of quasi-linear differential-algebraic equations. Technical Report 11-2006, Institut für Mathematik, Technische Universität Berlin, Berlin, Germany. 2006.
- [2] Steinbrecher, A. Deflating type regularization method for quasi-linear differential-algebraic equations. Technical report, Institut für Mathematik, Technische Universität Berlin, Berlin, Germany. In preparation.

# ACCURACY OF PARAMETER SENSITIVITIES OF DAE SYSTEMS USING FINITE DIFFERENCE METHODS

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**Introduction.** This work is presenting a way for examining the accuracy of Finite Difference (FD) methods for computing parameter sensitivities of badly-scaled DAE systems. Due to their simple implementation, FD methods are commonly favoured especially when the underlying mathematical function is a hard-coded sophisticated simulator. Nevertheless, FD methods impose serious numerical problems if FD step sizes and solver tolerances w.r.t. the order of the FD scheme are not ideally selected. Judging the precision of the resulting parameter sensitivities is practically difficult.

**Methods.** An alternative for computing parameter sensitivities is to employ the direct method. This method is realized by direct numerical integration of the sensitivity equation system. Such systems are of high dimensions and direct integration can become inefficient from a runtime performance point of view. Nevertheless, the accuracy of the computed parameter sensitivities is controlled by the underlying solver. Common methods which utilize the structure of sensitivity equation systems exist. A modification of the method of Dickinson is employed [1]. Additionally, further significant runtime improvement is achieved by Automatic differentiation techniques for providing efficient representation of sensitivity equation systems. With the availability of powerful Automatic Differentiation (AD) tools for equation-based simulation languages like ADModelica [2, 3], there is a new possibility to examine step sizes of various FD schemes, solver tolerances and the resulting precision for realistic large scale examples. This can be done by comparing numerical parameter sensitivities with highly precise analytical solutions using direct integration of sensitivity equation systems generated by AD techniques.

**Results.** Based on a typical biochemical reaction network model, a benchmark for comparing the accuracy of the presented common methods is performed. It is shown with a realistically sized example that FD methods are actually more critical than usually assumed. This study encourages the employment of analytical techniques for computing parameter sensitivities of large-scale DAE-systems whenever possible, especially if accurate results of high-precision are effectively important.

- [1] Dickinson R. and Gelinas, R.: *Sensitivity analysis of ordinary differential equation systems - a direct method*. Journal of Computational Physics, (1976) 21, 123–143.
- [2] Elsheikh A. and Wiechert W.: *Automatic sensitivity analysis of DAE-systems generated from equation-based modeling languages*. In Advances in Automatic Differentiation, (2008) 235–246.
- [3] Elsheikh A., Noack, S. and Wiechert, W.: *Sensitivity analysis of Modelica applications via automatic differentiation*. In Modelica'2008: The 6th International Modelica Conference, (2008).

# STABILITY OF GLUED AND EMBEDDED GLASS PANES: DUNKERLEY STRAIGHT LINE AS A CONSERVATIVE ESTIMATE OF SUPERIMPOSED BUCKLING COEFFICIENTS

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**Introduction.** Lightweight structures can nowadays be stiffened efficiently by means of glued and embedded timber-glass composite panes. So far, glass has been mainly a filling building material. But a novel construction principle enables load transfer of horizontal forces via vitreous shear areas and compression diagonals within the glass. Hence, conventional stiffening methods such as wind bracing become dispensable [1].

In this talk we shall analyze the stability of the stiffening glass pane. This is one of the most important proofs within the sizing of stiffening timber-glass composite panes, and it presupposes the identification of the glass panes buckling coefficient. Due to the superposition of two bearing mechanisms (block setting and glueing) within one pane, the buckling coefficients – amongst others depending on the way of load application – have to be superimposed too. But while the stress tensor within the pane is a linear combination of the two applied forces, the buckling coefficient and therefore the buckling load is *not a linear function* of the critical compression force and the critical shear force. Hence, the related eigenvalue problem for the pane buckling has to be solved numerically for each pair of applied forces. To simplify the situation in real applications, the superimposed buckling coefficient can be approximated by the Dunkerley straight line, which is a linear interpolation between the coefficients of critical compression and shear forces.

First we present a numerical study of the accuracy of this approximation. Then we give a mathematical proof that the Dunkerley straight line represents a conservative estimate for the buckling coefficients in the present problem. So far, this fact was assumed to be known and “obvious”, but a rigorous justification was missing.

**Results.** In this talk we first present a PDE model (based on linear elasticity) for the stress tensor within the glass pane and the eigenvalue problem for buckling of the pane. These two equations (in weak formulation) are then solved subsequently with the software COMSOL, i.e. the computed stress field is an input coefficient for the eigenvalue problem of the plate equation. We are interested in the critical load that implies buckling, and it is determined by zero becoming an eigenvalue of the plate equation.

The maximum load is a non-linear function of the pressure and shear forces applied at the boundary of the pane. To provide a simplified analysis for the practitioner, we prove that the Dunkerley straight line represents a conservative estimate for superimposed buckling coefficients and therefore for the critical buckling load. This mathematically rigorous proof is based on an application of the generalized Dunkerley theorem for eigenvalue problems [3].

Here we extend our work from [2] by also including a uniform transversal load on the glass pane (e.g. due to wind forces or isochoric pressure within insulated glass). We shall assume small deflections of the pane (w.r.t. the glass thickness). Hence, the von Kármán plate equations become decoupled. In this linear regime, it turns out that the critical buckling loads are independent of the transversal force.

- [1] Hochhauser, W.: *Ein Beitrag zur Berechnung und Bemessung von geklebten und geklotzten Holz-Glas-Verbundscheiben*, PhD-thesis: TU Wien, 2011.
- [2] Neumann, L., Arnold, A., and Hochhauser, W.: *Zur Stabilität von geklebten und geklotzten Glasscheiben: Beurteilung der Dunkerley'schen Geraden zur Beulwertbestimmung*, submitted 2011.
- [3] Tarnai, T.: *Summation theorems concerning critical loads of bifurcation*, pp. 23–58 in *Structural Stability in Engineering Practice* (L. Kollár ed.), Taylor & Francis, London, 1999.



## DESIGN OF MODAL FILTERS EXACT ON MAXIMAL SPACES OF FUNCTIONS

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**Introduction.** For the control of linear distributed-parameter systems a lot of well-known concepts belong to the class of modal control, e.g. independent modal space control. For these concepts knowledge of the modal states of the system is mandatory, at least for the modes targeted for control. As an approach to extract the modal states from a set of measurements the implementation of modal filters was proposed as an alternative to state estimation via Luenberger observers, see [1], to address the problem of observation spillover caused by unmodeled dynamics.

Although the design of modal filters is not restricted to this class of problems, in the following, it will be referred to mechanical structures in order to illustrate the properties of the modal filters in concrete physical terms. In general, two approaches can be distinguished. The first approach uses spatially distributed sensors, e.g. piezoelectric films, realizing the filter properties through spatial shaping of the sensors. The second approach uses an array of discrete sensors, e.g. accelerometers or piezoelectric patches. In this context, the term discrete refers to sensors that are not tailored to be sensitive for a specific mode shape and cover only a small fraction of the structure.

In the second approach, which is investigated in this contribution, modal filtering is accomplished by a weighted sum of the single sensor outputs. The corresponding design problem involves the choice of proper weighting coefficients and locations for the elements of the sensor array. There are several methods to determine the weighting coefficients for a given set of sensors, including matching measured frequency response functions of the sensor array to desired shapes, see [3], and the method described in [1] where interpolation of the discrete measurements in conjunction with the orthogonality properties of the mode shapes is utilized. As for the sensor locations, besides using an equally spaced grid, various optimization methods, mainly based on finite dimensional models, are used to minimize observation spillover or the deviation from a desired frequency response function, see [2].

**Contribution.** In this contribution design guidelines for the use of the given degrees of freedom, e.g. sensor locations or geometry, are developed from examining the system of equations associated with the problem of transforming the measured outputs to a set of modal outputs. As the distributed-parameter systems under consideration exhibit an infinite number of mode shapes it will in general not be possible to obtain exact modal filtering with a finite number of discrete sensors. Thus, approximations containing a finite number of consecutive modes are considered. Consecutive, in this regard, refers to the frequencies associated with the mode shapes. This setup is reasonable since for a subsequent controller design one is in general interested in controlling modes in a specified frequency range. The design criterion utilized is to obtain filters that are exact for a maximum number of these consecutive modes. For the implementation of the proposed approach to the design of modal filters only information about a finite number of mode shapes and the corresponding frequencies along with accurate models of the behavior of the sensors are needed.

To illustrate the application of the given design guidelines two examples are considered. The first one being a cantilever beam with laminar piezoelectric sensors. In this case the sensor topology can be obtained without further optimization as long as the sensors are identical with respect to their dimensions and material properties and the number of sensors equals the number of modal coordinates to be observed. As a second example a simply-supported plate with point measurements of the displacement profile is considered. This configuration is used to demonstrate a case where the conditions on the sensor locations change according to the problem statement, namely the number of targeted modes, and where there are still degrees of freedom left for a subsequent optimization. In addition the use of equally spaced grids is discussed.

The proposed procedure yields design rules easy to apply, especially in cases where the number of sensors equals the number of modes to be observed. It is a clear advantage that, regarding the structure under consideration, only information about the mode shapes and, for an adequate ordering of the modes, the corresponding frequencies are needed. Another advantage is the possibility to handle various types of sensors within the same framework.

- [1] L. Meirovitch and H. Baruh. The Implementation of Modal Filters for Control of Structures. *Journal of Guidance, Control, and Dynamics*, 8(6):707–716, 1985.
- [2] C.C. Pagani Jr and M.A. Trindade. Optimization of modal filters based on arrays of piezoelectric sensors. *Smart Materials and Structures*, 18(9):095046, 2009.
- [3] A. Preumont, A. François, P. De Man, and V. Piefort. Spatial filters in structural control. *Journal of Sound and Vibration*, 265(1):61–79, 2003.

# A HIGH PERFORMANCE DYNAMIC MODEL FOR SOLVING A CLASS OF GEOMETRIC PROGRAMMING PROBLEMS

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The geometric programming (GP) problems arise in a wide variety of scientific and engineering applications, specially in engineering design, economics and statistic, manufacturing, and chemical equilibrium. In many engineering and scientific applications, a real-time solution is often desired. It is of great interest to develop some neural network models that could provide a real-time online solution for the GP problem.

We start with two classes of functions, monomials and posynomials. A monomial is a real valued function  $F$  of  $x$  with the form  $F(x) = cx_1^{a_1} x_2^{a_2} \dots x_n^{a_n}$ , where  $c > 0$ , and  $a_i \in \mathbb{R}$ . A posynomial is the sum of one or more monomials, namely  $F(x) = \sum_{k=1}^K c_k x_1^{a_{1k}} x_2^{a_{2k}} \dots x_n^{a_{nk}}$ , where each  $c_k$  is positive. A GP is an optimization problem of the form

$$\text{minimize } F_0(x) \quad (1)$$

subject to

$$F_k(x) \leq 1, \quad (k = 1, \dots, m), \quad (2)$$

$$G_p(x) = 1, \quad (p = 1, \dots, l), \quad (3)$$

where  $F_k$ s are posynomials for  $k = 0, \dots, m$  and all  $G_p$ s are monomials. Using logarithmic transformation of the variables  $x_i$ ,  $w_i = \log x_i$  (so  $x_i = e^{w_i}$ ), the above GP problem is transformed into a convex optimization problem as

$$\text{minimize } \log F_0(e^w) \quad (4)$$

subject to

$$\log F_k(e^w) \leq 1, \quad (k = 1, \dots, m), \quad (5)$$

$$\log G_p(e^w) = 1, \quad (p = 1, \dots, l). \quad (6)$$

In order to solve (4)-(6), we consider a general form of nonlinear convex optimization problem as following

$$\text{minimize } f(w) \quad (7)$$

subject to

$$g(w) \leq 0, \quad (8)$$

$$h(w) = 0, \quad (9)$$

where  $w \in \mathbb{R}^n$ ,  $f: \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $g(w): \mathbb{R}^n \rightarrow \mathbb{R}^m$ , the functions  $f, g_1, \dots, g_m$  are assumed to be convex and twice differentiable,  $h(w) = Aw - b$ ,  $A \in \mathbb{R}^{l \times n}$ ,  $\text{rank}(A) = l$ , ( $0 \leq l < n$ ) and  $b \in \mathbb{R}^l$ . It is well known (see Bazaraa et al. 1993) that  $w^* \in \mathbb{R}^n$  is an optimal solution (KKT point) of (7)-(9) if and only if there exist  $u^* \in \mathbb{R}^m$  and  $v^* \in \mathbb{R}^l$  such that  $(w^{*T}, u^{*T}, v^{*T})^T$  satisfies the following KKT system

$$\begin{cases} u^* \geq 0, \quad g(w^*) \leq 0, \quad u^{*T} g(w^*) = 0, \\ \nabla f(w^*) + \nabla g(w^*)^T u^* + \nabla h(w^*)^T v^* = 0, \\ h(w^*) = 0. \end{cases} \quad (10)$$

The aim is to construct a continuous-time dynamical system (recurrent neural network) that will settle down to the KKT point of the problem (7)-(9). A dynamic model for solving (7)-(9) and its dual is proposed as following

$$\frac{dw}{dt} = -(\nabla f(w) + \nabla g(w)^T (u + g(w))^+ + \nabla h(w)^T v), \quad (11)$$

$$\frac{du}{dt} = (u + g(w))^+ - u, \quad (12)$$

$$\frac{dv}{dt} = h(w). \quad (13)$$

It is shown that  $y^* = (w^{*T}, u^{*T}, v^{*T})^T$  is an equilibrium point of (11)-(13) if and only if  $y^*$  is a KKT point of (7)-(9). The proposed model is also proved to be Lyapunov stable by constructing a suitable Lyapunov function and the solution trajectory can converge globally to an optimal solution of the original GP problem. This neural network model has been successfully used for solving minimax problems (See Nazemi (2011)).

- [1] Bazaraa, M. S., Sherali, H. D., and Shetty, C. M. *Nonlinear Programming- Theory and Algorithms*. 2nd ed. New York: Wiley, 1993.
- [2] Nazemi, A. R. *A dynamical model for solving degenerate quadratic minimax problems with constraints*. Journal of Computational and Applied Mathematics, 236 (2011), 1282–1295.

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# A BEHAVIOURAL APPROACH IN EIV IDENTIFICATION: THE SISO CASE

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Errors-in-Variables (EIV) models refer to a stochastic environment where both the input and the output measurements of a process are affected by errors, modeled as additive noises [4]. The identification of a process in this context is usually oriented to the solution of diagnostic or filtering problems. In the second case the identification problem is not limited to the estimation of the model parameters but requires also the estimation of the covariance of the additive noises. The most simple EIV environment describes the measurement errors as mutually uncorrelated white processes, uncorrelated also with the (unknown) noiseless input and, consequently, with the noiseless output sequences. This context constitutes an extension to the dynamic case of the scheme introduced by Ragnar Frisch in 1934 and is thus known also as dynamic Frisch scheme [2].

The identification procedures that have been developed for this context have been strongly influenced by the work of Kalman on estimation schemes and are, in most cases, based on the properties of the sample covariance matrix of the observations,  $\Sigma$ . This approach has many advantages like computational efficiency and the possibility of defining a locus of admissible solutions,  $\mathcal{S}(\Sigma)$ , in the noise space where the solution of the identification problem can be selected by minimizing a suitable cost function [2]. Moreover, the properties of the data covariance matrix define a unitary framework where other identification procedures can be encompassed. On the other hand, the solutions defined by the locus  $\mathcal{S}(\Sigma)$  derive from algebraic properties of  $\Sigma$  that are not associated with corresponding properties of the system that has generated the noiseless data, with the only exception of the point defined by the true noise variances that can be discriminated, in all cases concerning real processes, only by introducing cost functions.

An alternative approach that fits very well the EIV context can be developed by considering a behavioural description for the process. In fact, in the EIV environment, the observed sequences  $u(\cdot)$ ,  $y(\cdot)$  can be seen as a non regular trajectory  $v$  to be decomposed, for solving the identification problem, into the sum of a regular trajectory  $\hat{v}$  defining the behaviour of the deterministic part of the process and into a stochastic one  $\tilde{v}$  [3]. Approaches of this kind, that are based on the total least squares concept, allow to identify the whole EIV model (parameters and noise variances) only when the noise covariance matrix is *a priori* known up to a scalar factor. This is true also for maximum likelihood (ML) identification procedures.

The approach proposed in this paper is based on the optimal solution of the EIV interpolation problem, i.e. the problem of partitioning  $v$  as  $\hat{v} + \tilde{v}$  when the EIV model is known [1]. In fact, the availability of a procedure for the optimal extraction of a regular trajectory from a noisy one, allows to devise a complete identification procedure, formulated as an optimization problem, once that a suitable criterion to discriminate different decompositions is introduced.

The extraction from the noisy observations of the optimal estimation of the noiseless data allows introducing selection criteria unavailable in covariance-based approaches. The criterion considered in the paper, for instance, is based on a condition that is assumed as satisfied in all traditional approaches, i.e. the orthogonality of  $\hat{v}$  and  $\tilde{v}$ . A drawback of behavioural EIV identification procedures concerns their heavier computational burden; the procedure proposed in the paper has limited this problem by taking advantage of the properties of the locus of solutions of the Frisch scheme,  $\mathcal{S}(\Sigma)$ . Computational efficiency, however, is not the primary goal of the considered approach whose possible advantages concern its large flexibility and possible extension to the case of mutually correlated and/or colored noise sequences as well as easy implementation for multivariable processes. A development of the considered approach that will also remarkably improve its efficiency will concern the application of optimal EIV filtering instead than interpolation algorithms [2].

Some Monte Carlo simulations have been performed on relatively short sequences of data (50, 100 and 200 samples); these simulations have shown a good degree of robustness and have led to accurate estimates of both model parameters and noise variances.

- [1] Guidorzi, R., Diversi, R., and Soverini, U. (2003). Optimal errors-in-variables filtering. *Automatica*, 39(2), 281–289.
- [2] Guidorzi, R., Diversi, R., and Soverini, U. (2008). The Frisch scheme in algebraic and dynamic identification problems. *Kybernetika*, 44(5), 585–616.
- [3] Roorda, B., and Heij, C. (1995). Global total least squares modeling of multivariable time series. *IEEE Transactions on Automatic Control*, 40, 50–63.
- [4] Söderström, T. (2007). Errors-in-Variables methods in system identification. *Automatica*, 43(6), 939–958.

## A STUDY ON THE INFLUENCE OF THE SAMPLING RATE ON THE IDENTIFICATION PROCESS ERRORS

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In this work we present a discussion on the problem of obtaining data for the purpose of identification of dynamic systems. To know the characteristics of such systems it is necessary to excite them with informative signals at a convenient sampling rate [1][2]. This stimulus is obtained by devices which frequently have the bandwidth smaller than that of the dynamics of the process under test. Because of that, we face two problems with the generation of the information necessary for the dynamic system identification: first, it is not possible to excite the system with frequencies close to the cut frequency (since the stimulator has the bandwidth smaller than the process) and, second, either the sampling frequency does not allow a good representation of the commanded frequencies or its influence on the discretization of the signal cannot be neglected (considering the relation between the values of the sampling rate and the highest frequency of process). Due to that, it is inevitable to make mistakes in the dynamics estimate.

In order to evaluate such mistakes we designed a test-bench based on two well-known transfer functions,  $G_1(s)$  and  $G_2(s)$ , implemented by one analog computer in tandem connection.  $G_1(s)$  is stimulated by a digital computer through an A/D converter (zero-order-hold type ZOH). The outputs of both  $G_1$  and  $G_2$  are both discretized and read by the same digital computer.

Regarding the dynamics  $G_1$ , and  $G_1 * G_2$  the dynamics of the ZOH was included because we made use of inputs generated digitally to produce a continuous action. It is important to point out that those equations take into account that the three measurements  $u(k)$ ,  $y_1(k)$  and  $y_2(k)$  are synchronized.

Through this scheme it is possible to evaluate several aspects of the identification process, such as the influence of the sampling rate, the input bandwidth, the choice of the input, the choice of the identification method and the influence of the ZOH presence in the process.

The selection of good excitation signals is an important step to guarantee the achievement of good models. The input signal must expose all of the relevant properties of the system. Other point in the experimental design is allocating the input power to those frequency bands where a good model is particularly important. Thus, it is necessary to determine which inputs will be used in the assessment. Two sorts of signals were chosen: multi-sine and swept sine [2]. Signals with different frequencies and bandwidths of each of them must be determined based on the dynamics under test, to permit a performance comparison among them.

The procedure begins with the use of a quite high sampling rate in such a way that the dynamics is perfectly identified since, by construction, it is already known. A typically good sampling frequency is about 10 times (or more) the bandwidth of the system. Both the time domain and the frequency domain methods must be chosen in order to identify the transfer functions proposed, and to allow it a later comparison. After choosing the input signals, they are implemented at different sampling rates, starting from the highest value of frequency (with which the effect of discretization is not noted), and then reducing it until it gets close to the Nyquist frequency (which is equal to twice the value of the dynamics bandwidth). It means that several experiments are performed with the same input and at different sampling rates.

The scheme set up tests allowed a qualitative assessment in the identification process, in view of the influence of sampling frequency, input types and methods of identification. Although only relative to some dynamics the results brought up important conclusions. It indicates the time domain method as the most appropriate when the input signal is generated digitally. Conversely, the method in the frequency domain is suitable for processes whose analog input is sampled (via A / D converter).

The tests also showed no significant trend for the selected type of input, as a function of the chosen method of identification as well as the dynamic identified. Contrary to expectation, the bandwidth of the process to be identified showed no significant influence on the frequency of sampling used, when used the appropriate method.

[1] L. Ljung, *System Identification*, 2<sup>nd</sup> Ed. Prentice-Hall, New Jersey, 1999

[2] R. Pintelon & J. Schoukens, *System Identification: A Frequency Domain Approach*, IEEE Press, New York, 2001.

[3] Leite Filho, W.C. & Carrijo, D.S., "Hardware in the Loop Scheme to Verify the Influence of the Inertial Platform Dynamics", *Proc. of 6<sup>th</sup> Inter. Conference on Mathematical Problems in Engineering and Aerospace Sciences*, Budapest, Hungary, 2006.

# PARAMETER IDENTIFICATION OF TIME-DELAY SYSTEMS: A FLATNESS BASED APPROACH

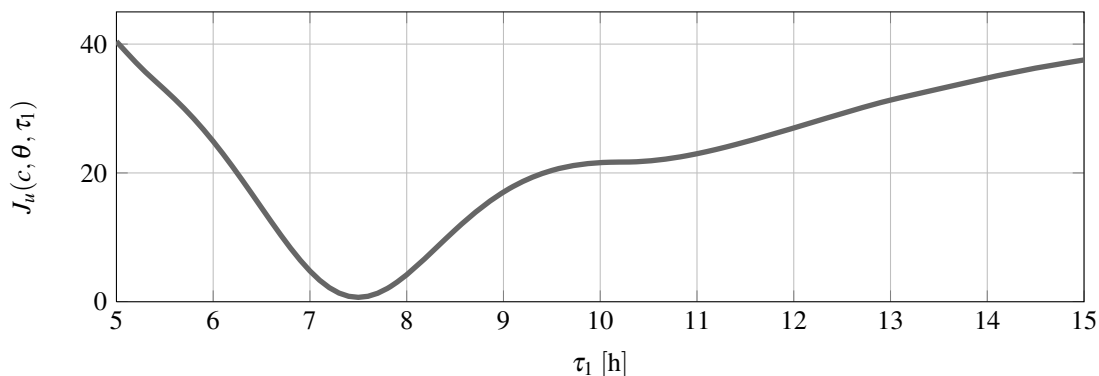
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**Introduction.** The use of mathematical models is widely established in various fields of application. To name but a few of their major applications, mathematical models can improve the controller design of complex technical systems or are able to facilitate the understanding of highly complex biochemical systems. No matter what mathematical models are used for, however, they fail to perform the intended task if they are badly parameterized. In general, during the process of parameterization one tries to make differences between simulation results and measurement data as small as possible. Under the assumption of a suitable model candidate this is done by choosing optimal model parameters. Unfortunately, the majority of used models cannot be solved analytically. For example, many dynamical processes are described by systems of ordinary differential equations (ode's). Usually, analytical solutions do not exist. Although quite efficient numerical routines are available they usually slow down the parameterization process dramatically. The situation is even more demanding if one has to deal with processes that are described by delay differential equations (dde's). Commonly, standard dde solvers show a lack of efficiency as well as of robustness, i.e., they are likely to fail to solve the underlying dde system. Consequently, it would be of great benefit to eliminate any need of numerical ode/dde solvers.

**Methods.** As an alternative, the concept of flat inputs [2, 3] is applied to facilitate the parameter identification process of delay differential equations. The key aspect is to transform the dde system into an algebraic input/output representation, i.e., the inputs of the system are expressed analytically by the outputs and derivatives thereof. Now, the objective of parameterization is to minimize differences between these flat inputs and the physical inputs of the related process. As no numerical dde solver is involved there is a significant speedup of the parameter identification step. In addition, the presented approach is closely linked to optimal experimental design for parameter identification. In particular, the reformulation of the cost function also affects parameter sensitivities. Using the same measurement data it is possible that previously insensitive model parameters become sensitive. In addition to its merits, the presented approach has two possible shortcomings: a) the determination of flat inputs  $u^{flat}(t)$  for a given output configuration and b) to cope well with measurement noise. To overcome the first problem, a heuristic approach is introduced. Here, a structural analysis is used to figure out at which states possible flat inputs have to act on. The issue of measurement imperfection is addressed by the concept of functional data analysis [1]. Instead of real measurement data, surrogate output functions are applied to determine flat inputs. All results are demonstrated for the example of a mathematical model of the influenza A virus production. For instance, the related time-delay parameter  $\tau_1 = 7.5$  h is identified reliably with a minimum of computational effort (Fig. 1).



The cost function based on flat inputs  $J_u(c, \theta, \tau_1)$  is evaluated at different time-delay parameter values  $\tau_1$ . In detail, an optimizer is initialized iteratively at 100 different  $\tau_1$  values,  $\tau_1 \in [5, 15]$  h. The overall cpu-time is less than 10 seconds in this case.

- [1] Ramsay J. O., and Silverman B. W.: *Functional Data Analysis*. Springer, New York, 2005.
- [2] Waldherr S., and Zeitz M.: *Conditions for the existence of a flat input*. International Journal of Control, 81 (2008), 439–443.
- [3] Waldherr S., and Zeitz M. *Flat inputs in the MIMO case*. In: IFAC Symposium on Nonlinear Control Systems, University of Bologna - Italy, 2010.

# A DATA-DRIVEN ONLINE IDENTIFICATION AND CONTROL OPTIMIZATION APPROACH APPLIED TO A HYBRID ELECTRIC POWERTRAIN SYSTEM

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This contribution describes the control optimization of the electric current flow within a hybrid electric powertrain system and hence its power and energy management strategy. Power and energy management are methods applied to hybrid electric powertrain systems as they occur e.g. in modern vehicles. Hereby the electric current flow within the powertrain, i.e. between its system components, is controlled regarding predefined control objectives such as the power or energy availability with respect to a load profile applied to this system. For the realization of these control algorithms at least one additional degree of freedom for the current flow has to be provided, which typically occurs in electric topologies with multiple power sources or electric storage elements. Typical energy storage elements in this context are batteries (accumulators), supercapacitors, etc. The electric power supply is realized by the electric grid, generators, fuel cell systems, solar modules etc. Typical electrical elements necessary to realize the control of the electric current flow between the power sources and the storage elements and thus the power and energy management are controllable DC/DC converters, inverters, and rectifiers as e.g. utilized within motor controller systems. As shown in [1] the application of power and energy management has, dependent on its parameter choice, a significant influence on central system properties as energy efficiency, vehicle drivability and component life time. This makes the application of optimization approaches of the electric power flow control evident and thus necessary for efficient applications. For the optimization of the power and energy management it is essential to take the characteristics of a load profile (given or assumed) applied to the powertrain into consideration. In [2] it is shown that the application of an optimization loop is a suitable method for offline-optimization of the electric current flow control. In addition and for the first time an online-applicable optimization method of the power and energy management strategy is introduced in this contribution. Its realization contains a system identification algorithm capable of being implemented within online applications and, based on this, a suitable control optimization including a predictive approach. The control objectives to be optimized in this context are the energy consumption, the power availability, and deterioration aspects of the system and its components. The algorithm is demonstrated using the example of a fuel cell/supercap-based hybrid electric powertrain system. After a brief description of the system and operation details, the results of the identification process in relation to the real behavior as well as the optimization algorithm are presented. Applying typical driving cycles to this system it can be shown that a significant improvement of this approach compared with classical power and energy methods can be achieved. The main scientific and practical question remains: what can be assumed about the future behavior of the workload (applied to the system) and how can the control be optimized for the unknown future behavior. Mathematically expressed: How exact the system behavior has to be identified (from the last measurements) in relation to the principally unknown character of the upcoming future load in relations to the different optimization goals.

- [1] M. Marx, M. Oezbek, D. Söffker, *Powermanagement Investigations on a Fuel Cell-based Hybrid HiL Powertrain*. - SAE 2010 World Congress, April, Detroit, 2010.
- [2] M. Marx, D. Söffker, *Integrated Optimization of the Powermanagement System of a Hybrid Electric Powertrain System*. 7th IEEE Vehicle Power and Propulsion Conference, Chicago, IL, USA, Sept. 6-9, 2011.



# COMBUSTION ENGINE AIR INTAKE THEORETICAL MODELLING, MODEL-VERIFICATION & APPLICATION TO OPTIMAL VALVE ACTUATION

S. Studener

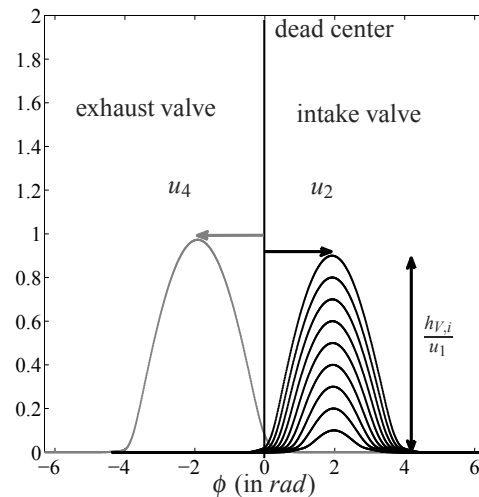
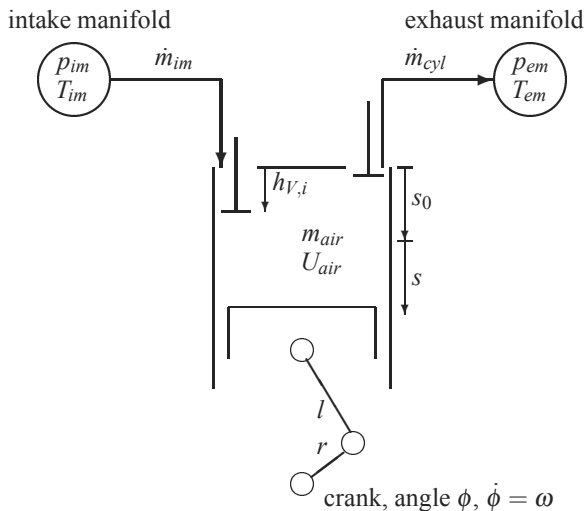
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**Introduction.** Positive displacement machines with internal combustion are one of the most important technological developments of the past century. They have become the most frequently encountered source of propulsion energy in passenger cars. One reason for this is, that this source of propulsion energy does rely on the large energy density of liquid hydrocarbons, which is very hard to be beaten for by alternative propulsion concepts. In spite of all the research efforts that have been made, internal combustion engines still have potential for improvements, which are hard to be realized without model based control and optimization. From a control engineer's point of view, the positive displacement machine with internal combustion is a non-linear, time periodic plant. It is the time periodicity, whose frequency varies with the number of revolutions, that makes the application of contemporary control techniques a challenge [1]. The amount of air, that is aspirated by the engine's cylinders, limits the amount of fuel, that can be burned inside and hence limits the power, the engine is able to deliver [2]. Estimating and optimizing the air intake rate of a positive displacement machine with internal combustion is one of the major sources of engine control development time and cost today.



**Content.** In this contribution a theoretical model for the air intake of a four stroke internal combustion engine is derived from first principles, the conservation of mass and the conservation of energy. The opening angle of both the intake as well as the exhaust valve, as well as the variable valve lift are considered as plant inputs, which may be manipulated to maximize the air intake rate and hence the power, the engine delivers. After a formal connection between state-of-the-art mean value models and the crank angle resolved physical model has been established, the theoretical model is verified by comparing the model output to steady state data collected at an engine test bench. The pressure loss in the intake valve is considered a disturbance of the ideal cylinder filling dynamics, which is estimated using non-linear optimization techniques. The intended purpose of physical model building for the cylinder air intake is prediction of the air intake rate and computation of optimal valve control action before a lot of effort is put into a real experiment at the engine test bench. A significant reduction of operating time and cost consumed by the real engine test bench can be achieved, if a small subset of steady state measurements are used to compute a meta-model for the pressure loss. Since the model errors are of sole deterministic nature, in this contribution the Kriging Predictor is chosen as a suitable meta-model [3]. The combination of the black-box pressure loss model and the air intake model allows for prediction of the air intake rate at unknown operating points of the engine with sufficient accuracy.

- [1] L. Guzzella: *Introduction to Modeling and Control of Internal Combustion Engine Systems*. Springer, Berlin, 2010.
- [2] R. Pischinger: *Thermodynamik der Verbrennungskraftmaschine*. Springer, Berlin, 2009.
- [3] T.W. Simpson and J.D. Peplinski and P.N. Koch and J.K. Allen: *Metamodels for Computer-based Engineering Design: Survey and Recommendations*. In: *Engineering with Computers*, Vol.17, 2001.

# ROBUST GAUSSIAN PROCESS MODELLING FOR ENGINE CALIBRATION

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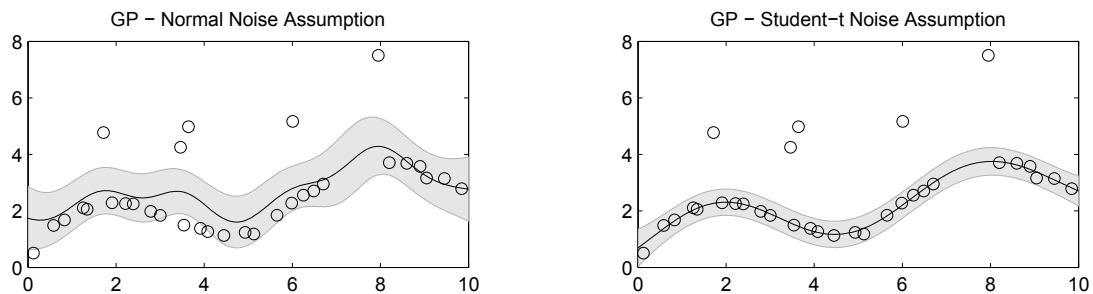
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**Introduction.** The performance of model-based engine calibration is highly dependent on the type of modelling which is used. A problem for state of the art algorithms for engine calibration arises, if outliers occur in the measurement data. Since outliers are not considered in recent types of modelling for engine calibration, they always have to be removed before training, either manually, or by simple leave-one-out cross validation algorithms, which cannot be adopted very efficiently, if there are many outliers in the measurements, which is shown in the paper. Therefore, there is a need for a new type of modelling for engine calibration, which is robust to outliers.

**State of the art modelling in engine calibration.** Common types of modelling for engine calibration are discussed in [1]. Training for polynomials, Tree-based Models, the MLP Networks and Least-Squares Support Vector Machines is performed by minimizing the sum of squares error function on the training data. This minimization of the sum of squares error function is equivalent to a maximization of the likelihood function under a conditional Gaussian noise distribution of these models. Instead of using the least squares approach, the Relevance Vector Machines and Gaussian Processes directly use a normal noise assumption for modelling in engine calibration. In the paper, the drawbacks of a normal noise assumption regarding outliers are illustrated and a possible solution with a Student's-t noise assumption is presented.

**Robust Gaussian process modelling.** In the paper the formulas for the training of the hyperparameters of the Gaussian process and the formulas for the prediction are discussed. Since we use a Student's-t noise assumption for modelling, inference becomes analytically intractable and several methods for approximation are discussed. As computational speed is an important factor in the task of engine calibration, we follow the approach of [2], which is based on the Laplace approximation. Further, some remarks on the implementation are given and a simple theoretical example of a comparison between Gaussian process regression with a normal noise assumption and Student's-t noise assumption is shown in the paper and in the figure below. In the figure it clearly can be seen, that the five outliers distort the model with the normal noise assumption. This is a serious problem with state of the art models for engine calibration, if quantities of an engine should be modeled, where the risk of outliers is high. With the new approach on the right, the modelling is robust to outliers in the measurement data.



Comparison of Gaussian process regression with normal noise assumption (left), which is state of the art in engine calibration, and Student's-t noise assumption (right). The training data (circles), the predicted mean (solid line) and the predicted variance (confidence interval) are plotted.

**Application to a diesel engine.** In the last section a Gaussian process model with a normal noise assumption is applied on NOx and soot measurements of a diesel engine and compared to a Student's-t noise assumption. Since the NOx emissions can be measured relatively well, no outliers occur in the measurement data and the model with the Student's-t noise assumption gives pretty much the same result as the model with the normal noise assumption. The performance of both models for NOx is quite good, but it is shown that this is not the case for the soot emissions. Since the soot emissions are much harder to measure, outliers occur in the measurement data. These outliers will distort the model with the normal noise assumption. It is shown, that this is not a problem if one uses a Gaussian process modelling with a Student's-t noise assumption. With this modelling a better fit on the training data is achieved and the prediction of the validation data is very accurate.

- [1] Berger B., Rauscher F., and Lohmann B.: *Analysing Gaussian Processes for Stationary Black-Box Combustion Engine Modelling*. In: Proceedings of the 18th IFAC World Congress, 2011, Milano, Italy
- [2] Vanhatalo J., Jylänki P., and Vehtari A.: *Gaussian process regression with Student-t likelihood*. In: Proceedings of Advances in Neural Information Processing Systems, 2009.

## OPTIMAL EXPERIMENT DESIGN FOR CALIBRATING AN AIRPATH MODEL OF A DIESEL ENGINE

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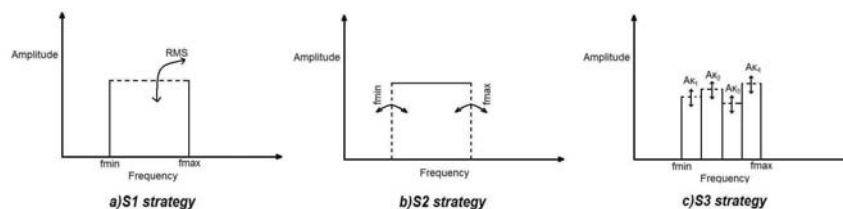
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**Introduction.** Mathematical models become more and more indispensable tools for engine manufacturers. As nonlinear dynamic models based on first-principles are preferred by practitioners, model calibration or parameter estimation is often a time consuming task. The use of optimally designed dynamic inputs can reduce the experimental burden and increase the accuracy of the estimated parameters. The current paper presents the calibration and validation of a Diesel engine airpath model using optimally designed inputs.

**Content.** The airpath model used is similar to the one described in [1] and the dynamic parameters have to be estimated based on measurement from an engine test bench. Optimal experiments are designed using a random phase multisine discretization [2] instead of traditionally used polynomial discretizations [3] in order to cope with the requirements of fast variations and operating around fixed setpoints. The current paper proposes three strategies based on the allowed degrees of freedom for the multisines (see Figure). In the first strategy the root mean square (RMS) value is optimized. The second strategy includes the optimization of the frequency bands, whereas the amplitudes vary for the different frequencies in the third strategy.



Schematic diagram of the input structure for every strategy

The airpath model is characterized by the combination of physical equations with static maps. The model contains five parameters describing the dynamic behavior which have to be estimated, i.e., the volume of the intake and exhaust manifold  $V_i$  and  $V_x$ , the turbocharger efficiency  $\eta_n$ , the time constants of the turbocharger and exhaust gas recirculation  $\tau_{vgt}$  and  $\tau_{egr}$ . Hence, four model inputs, i.e., the valve positions of the exhaust gas recirculation and variable geometry turbocharger  $X_{egr}$  and  $X_{vgt}$ , the injected fuel mass  $W_f$  and the engine speed  $n$  have to be designed in order to yield as informative outputs for the intake pressure (MAP) and fresh air flow (MAF) as possible. These two outputs mentioned above are used for model calibration.

**Results.** The procedure of the *modeling cycle* has been followed. The preliminary step involved a verification of the model's structural and practical identifiability. A sensitivity analysis of the outputs with respect to the inputs revealed that all parameters can be estimated. Then a sequential approach followed for choosing the appropriate parameters. This sequential part included the loop: *Experiment, Parameter Estimation, Confidence Interval Computation* and *Design of Experiments* according to the results of the Confidence Interval. This sequential procedure has been applied in the current study.

The inputs have been optimized using each of the three strategies based on random phase multisines. Also a comparison to white noise has been made. The designed inputs have been applied to the test-bench and the dynamic parameters have been successfully estimated. The 95 % error bounds were significantly smaller than the parameter values. Finally, a validation of the calibrated model has been successfully performed.

**Acknowledgements.** This research is supported by Projects OT/10/035, PFV/10/002 (Center-of-Excellence Optimization in Engineering) of the Research Council of the K.U. Leuven, Project KP/09/005 (SCORES4CHEM) of the Industrial Research Council of the K.U. Leuven, the Belgian Program on Interuniversity Poles of Attraction, initiated by the Belgian Federal Science Policy Office and the industry project ACCM. Dries Telen has a Ph.D grant of the Institute for the Promotion of Innovation through Science and Technology in Flanders (IWT-Vlaanderen). J. Van Impe holds the chair Safety Engineering sponsored by the Belgian chemistry and life sciences federation essenscia. The scientific responsibility is assumed by its authors.

- [1] S. Puchner, B. Winkler-Ebner, D. Alberer, and L. del Re.: *Optimization based mean value model of turbocharged diesel engines*. In: MATHMOD 2009.
- [2] R. Pintelon and J. Schoukens.: *System Identification, A Frequency Domain Approach*. IEEE Press, 2001.
- [3] G. Franceschini and S. Macchietto. Model-based design of experiments for parameter precision: State of the art. *Chemical Engineering Science*, 63(19):4846-4872, 2008.

# EVOLUTIONARY ALGORITHMS FOR THE AUTOMATIC CALIBRATION OF SIMULATION MODELS FOR THE VIRTUAL ENGINE APPLICATION

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**Motivation** The automotive industry is, based on the sales, the most important industry section in Germany and other countries. Because of many various boundary conditions, like  $CO_2$  and fuel reduction, the calibration of the engine control unit is growing up for the development of the whole system automotive. Traditional calibration methods fail because of the increasing complexity of the optimization tasks and the huge measurement effort. A one dimensional engine process simulation in combination with a physical combustion model can significantly contribute to essential parts of engine calibration. For an accurate reproduction of the reality the simulation model must be calibrated. Factors are used as calibration parameters, which take influence on various combustion values. With the help of an automatic optimization routine the time effort can be reduced significantly for the adjustment with constant or increasing accuracy.

Therefore, the main target of this contribution is the improvement of the simulation and optimization techniques. For this aspect an evolutionary algorithm, which is a combination of a genetic algorithm and an evolutionary strategy, is used for the optimization task. Evolutionary optimization methods are stochastic searching methods, which are leaned on the naturally biological evolution. They work simultaneously with a number of potential solutions and they are variable, robust and powerful. They give the opportunity to solve complex and multi-criteria problems in a reasonable time. Further advantages of this approach are the better results and the time saving. The presented evolutionary algorithm for the automatic calibration of simulation models for the virtual engine application has been evaluated by simulations.

**Approach** To reduce the measuring effort at engine test benches one dimensional engine process simulations can provide a valuable contribution. To use these virtual methods effectively, a method for the automatic adjustment of the simulation models is developed. Therefore, a combination of a calculation on the local computer and a simulation on a computing cluster is used.

In the field of the virtual application of engine control unit functions an exact reproduction of the fresh air mass situated in the cylinder is necessary. To calibrate the load change uniquely with the help of measurements, the influences on the results are studied and a suitable calibration method is developed.

As soon as the load measuring at the engine is exactly enough synchronized, the calibration of the combustion can be started. Therefore, to simulate the engine combustion with changing operating points defined among other things, like engine speed, throttle angle, wastegate angle at the turbocharger, valve timing on intake and exhaust, intake valve lift and air-fuel ratio, a physical combustion model with an integrated turbulence model is used, which must be adapted to the engine by only a few calibration parameters, that cannot be measured directly [2]. These parameters are adapted automatically to each combustion engine with the help of a powerful evolutionary algorithm optimizer.

Already in the sixties of the 20th century several persons have tried to apply the principles of the biological evolution like the "survival of the fittest" on optimization problems. Independently of each other the genetic algorithms [1], the genetic programming and the evolutionary strategies [3] have been developed, which build together the classic evolutionary algorithms. Every evolutionary procedure works during the optimization on a number of potential solutions (the population), which are improved through little changes to reach an acceptable solution quality at the end of the optimization. Similar to the natural evolution, which is based on the three steps reproduction, variation and selection, the evolutionary algorithms are also divided in such phases and are complemented with additional phases to suit the algorithms to the given problem.

With the use of such an algorithm a clearly time saving can be reached by the calibration and the global error minimum can be found. With such a calibrated simulation model miscellaneous tasks can be realised by the parameterization of the engine control unit functions, from the load measuring up to the engine torque model.

- [1] D. E. Goldberg and J. H. Holland. Genetic algorithms and machine learning. In *Machine Learning 3: 95-99*, 1988.
- [2] Ulrich Knoll, Susanne Zaglauer, Sebastian Grasreiner, and Prof. Dr.-Ing. Christian Hasse. Automatisierte Kalibrierung von Simulationsmodellen zur virtuellen Motorapplikation. In *Fachtagung AUTOREG 2011*, 2011.
- [3] Hans-Paul Schwefel. *Numerische Optimierung von Computer-Modellen mittels der Evolutionsstrategie*. Birkhäuser Verlag, Basel und Stuttgart, 1977.

## ON IMPROVING PROBABILITY MODELS IN SYSTEM IDENTIFICATION

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A solution of the following problem is presented. Given a known model represented by a discrete probability distribution  $\bar{q} = (q_1, q_2, \dots, q_n)$ , and information  $\tilde{D}$ , a new improved model represented by a probability distribution  $\bar{p}$  is found which is associated with  $\bar{q}$  such that  $\tilde{D} = D(\bar{p}|\bar{q})$ , where  $D(\bar{p}|\bar{q})$  represents the relative information between the two probability distributions. The improved probability distributions  $\bar{p}$  have been chosen to be those which become local minima of the discrete entropy. The fundamental properties of such models and natural effects how to use information are studied.

The resulting solutions depend on the existence and value of two roots of a nonlinear equation. The corresponding solutions take on a *positive* and *negative* sense in that the form of the probability distribution can be enhanced or reduced. We therefore refer to the *positive* and *negative* effect of information. The behavior of the related entropy function is studied and reasons for this behavior stated. It is the justification of our approach. To study the negative and positive effects of information in order to improve some models used in identification.

This study indicates a potential to improve models during identification process when knowing an extra information. It was shown that the uncertainty of the probability distribution related to a set of probabilities can be increased or decreased by the use of relative information. This effect on the probability distributions can be characterized by the choice of the *positive* or *negative* roots of the derived solution equation. By appropriate choice, the original shape of the distribution can be enhanced, or reduced, or even inverted. It can form an alternative approach to known methods using e.g. conditional probabilities or information criteria.

Note that the calculation of the mutual information,  $I$  is a special case of the calculation of the relative information  $D$ . Therefore, we can approach the use of this type of information in a similar manner. Given a known joint probability distribution,  $\bar{r}^*$ , we look for a joint probability distribution  $\bar{r}$  which is associated with  $\bar{r}^*$  through the known mutual information  $\tilde{I}$ . It represents the relation  $\bar{r}^* \xrightarrow{\tilde{I}} \bar{r}$  with  $\tilde{I} = D(\bar{r}|\bar{r}^*)$ .

# MEASUREMENT, IDENTIFICATION AND VERIFICATION OF HIERARCHICAL SIMULATION MODEL OF THE CAR DRIVER

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Driving a car requires such a dynamic characteristics of the driver, allowing respond properly to unexpected situations in traffic. Unpredictable situations in the driving of the car are likely because the traffic on the road is crowded. Therefore, the research activity concerned with the possibility application of so-called "intelligent systems to support driver's decision." For such applications in transport uses the term "intelligent transport systems". Their implementation is made possible by new advances in automation and information technology. This article explains a new conceptual model of driver behavior, which is able to characterize the response of the driver in the car from "intelligent control system driver/car/traffic situation" point of view. The article outlined the verification of this model by measuring the human reactions in real time. This model is presented at Fig.1. Author of this subscription started with measurement and verification of driver's linear model with constant parameters [1], continued with linear model with variable parameters [2] and design of hierarchical model of driver decision making [3], which is partly verified in this subscription.

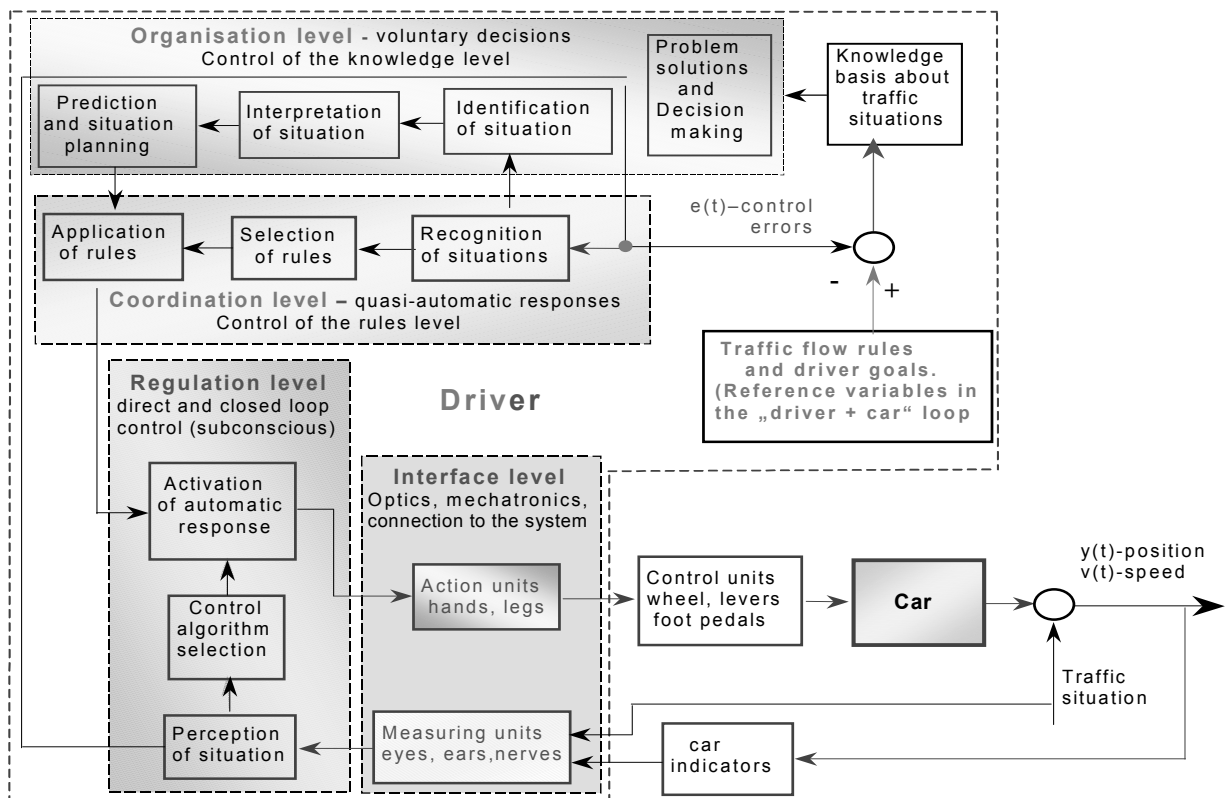


Fig. 1. Hierarchy and links in the driver decision-making response to the interpretation of the traffic situation.

- [1] Alexik M.: Modelling and Identification of Eye-Hand Dynamics. *Simulation Practice and Theory*, Vol. 8, Elsevier Science B.V., 2000, pp. 25-38
- [2] Alexik M.: Modelling and Identification of Interaction in Driver/Vehicle Dynamics. *Proceedings of 6th Vienna Conference on Mathematical Modelling (MATHMOD'09)*, February 11-13, 2009 Vienna University of Technology, Published by ARGESIM and ASIM, ARGESIM Report no.35, Full Papers CD Volume. pp. 500-510. ISBN 978-3-901608-35-3
- [3] Alexik M.: Measuring and Modeling the Dynamics Reactions of Car Drivers. *Proceedings of the 7th EUROSIM Congress on Modelling and Simulation*. Prague, Czech Republic, September 6 -10, 2010. Publisher: Czech Technical University in Prague, Faculty of Electrical Engineering, Karlovo náměstí 13, 121 35 Prague, Czech Republic. Vol. 2: Full Papers, pp. 1068-1077. ISBN 978-80-01-04589-3.

# STATE VARIABLES ESTIMATION OF FLEXIBLE LINK ROBOT USING VISION SENSOR DATA

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A vision sensor (camera) represents a contactless virtual movable measurement sensor, or a set of sensors working in the same time (i.e. getting a set of data from the camera), therefore visual servoing can be used effectively to control flexible manipulators. The research on flexible robots with vision based control was initiated in the early 1990s. The main inherent problem was the slow processing operation due to the limitations of the camera system in combination with the real time operation of the system. The state estimation of a single link flexible manipulator was studied in [1]; the vision system was used to estimate the state variables of the virtual joint model of a flexible link. Due to the slow image processing operation in comparison with the real time control several researchers used a two time scale control ([2], [3]) to overcome these problems. Due to the limitations of the sampling rate, and the resolution of the camera to detect all modes of the system; two different observers are designed to estimate the dynamical behavior of the system.

In this work the effect of time delay and noise in state estimation process of flexible robot arm are shown through the comparison between the states from different measured input data. The flexible link model used, is related to an elastic ship mounted crane. The system states are separated to slow and fast subsystems according to the frequencies of the system modes. The slow dynamics is chosen using assumed camera specifications. The states related to the slow dynamic are estimated by using the simulated signal of camera system. Two observers are designed, the first one to estimate the higher modes of the vibration using strain gauges, the second one represents an estimator using the camera as a sensor to estimate a modal set of slow dynamics based on the measurable frequencies of the modes. The states from the second estimator are combined with the same set of states, which are estimated using the full observer using the minimum mean-squared error. It can clearly be seen from the estimated tip point error in Fig. 1 that the slow and fast state estimator dynamics compensates the noise and delay from the estimated states. The observer and estimator which are designed in this work follow the states and remove the effects of noise and time delay very fast.

- [1] Yoshikawat, T., Ohta, A., and Kanaoka, K.: *State Estimation and Parameter Identification of Flexible Manipulators Based on Visual Sensor and Virtual Joint Model*. IEEE International Conference on Robotics and Automation, 2001, 2840–2845.
- [2] Bascetta, L., and Rocco, P.: *Two-Time Scale Visual Servoing of Eye-in-Hand Flexible Manipulators*. IEEE Transactions on Robotics, 22 (2006), 818–830.
- [3] Jiang, X., Konno, A., and Uchiyama, M.: *A Vision-Based Endpoint Trajectory and Vibration Control for Flexible Manipulators*. IEEE International Conference on Robotics and Automation, 2007, 3427–3432.

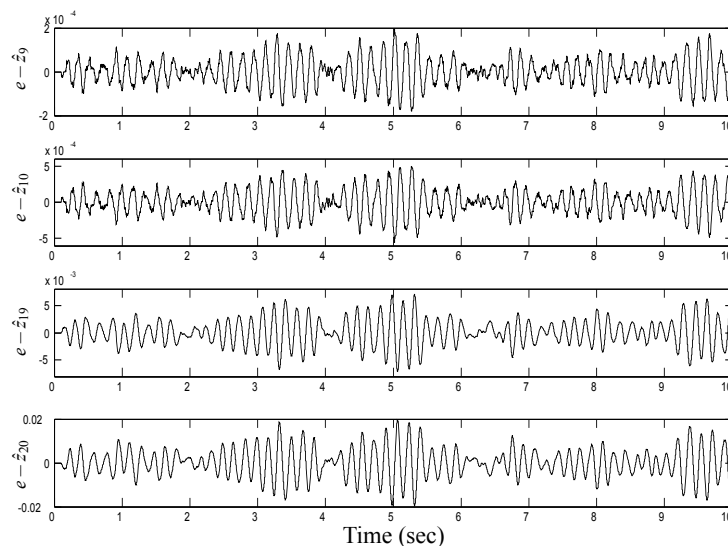


Fig. 1. Compensation of the effects of noise and time delay on the estimated states, sweep input

# OBSERVER BASED METHOD FOR JOINT TORQUE ESTIMATION IN ACTIVE ORTHOSES

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**Introduction.** For orthoses that enhance the user’s strength or reduce the user’s effort for a given task, several controllers have been proposed in the literature. The reference input to these controllers is the joint torque that the user applies to his body. This contribution presents a new approach of estimating the joint torques for an active orthosis. Electromyography, inverse dynamics [1], and calculating the joint torques from measured ground reaction forces [2] are three established methods of deriving the joint torques. The proposed approach combines inverse dynamics and the calculation of the joint torques using ground reaction forces.

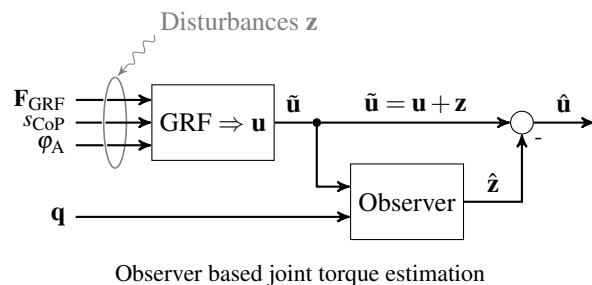
**Contribution** This paper focuses on the Sit-to-Stand (STS) movement. A model of the human lower extremity is derived by lagrangian mechanics and additional forces are introduced that simulate the seat. These forces fade after a certain height  $h_{SO}$ . This moment is called “Seat-Off” and describes the point where the body leaves the seat and all muscles have to carry the full body weight.

These seat forces are required for the estimation of the joint torques using inverse dynamics, but are not needed if the joint torques are calculated using ground reaction forces. Both methods, however, have significant drawbacks:

*Inverse Dynamics:* High resolution and low noise angular sensors are required since the angular value needs to be differentiated twice. Furthermore, the computed joint torques strongly depend on the accuracy of the model. A little error in the model causes large deviations in the joint torques.

*Ground Reaction Forces:* The computed joint torques strongly depend on the correct measurement of the ground reaction forces and the center of pressure. Also, the shear force component of the ground reaction forces must be measured for an exact estimation of the joint torques.

*Observer Based Approach:* An observer estimates the error in the joint torque calculation and adjusts the result. A mismeasurement of the ground reaction forces not only affects the forces themselves but also the center of pressure. Both signals have a considerable influence on the estimated joint torques. If the force sensors are placed in the shoe sole, some problems arise: The exact distance between the ankle joint and the center of pressure might be uncertain, and the foot might move within the shoe and therefore change these values, too.



That means the computed joint torques  $\tilde{\mathbf{u}}$  are flawed or disturbed. An observer can estimate these disturbances  $\mathbf{z}$  and the original signal can be restored if the estimated disturbances  $\hat{\mathbf{z}}$  are subtracted from the computed joint torques.

**Simulation Results** Simulation results show that the proposed approach has some advantage over the established methods. The estimation of the inverse dynamics method has a significant phase lag since a state variable filter is necessary to filter the joint angles prior to differentiating. The joint torques calculated using only ground reaction forces are non-zero in the sitting position if the shear force components are not measured. If the measured center of pressure is disturbed by a constant value, the joint torques are also non-zero in the standing position.

The new observer based approach produces zero torque in sitting and standing positions, regardless of missing shear force components or a disturbed center of pressure. However, the seat forces are required in order to compute the joint torques, and if the estimation of the seat forces is disturbed, the new approach also produces a non-zero torque in the sitting position.

- [1] H. Kazerooni, J.-L. Racine, Lihua Huang, and R. Steger.: *On the control of the Berkeley lower extremity exoskeleton (BLEEX)*. In: Proc. Int. Conf. on Robotics and Automation 2005, 4353–4360.
- [2] J.E. Pratt, B.T. Krupp, C.J. Morse, and S.H. Collins.: *The RoboKnee: an exoskeleton for enhancing strength and endurance during walking*. In: Proc. Int. Conf. on Robotics and Automation 2004, volume 3, 2430–2435.



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# NONLINEAR MODELING OF THE DYNAMICAL BEHAVIOR OF THE THREE-DIMENSIONAL ELASTIC BEAM

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The paper outlines a dynamic model of the nonlinear elastic beam. The investigated model in this paper based on a linear model with relevant geometrical nonlinear couplings is developed and considered up to the 3rd order. Furthermore, complex couplings between the guided motion of the beam in combination with external forces like the example given in [2] and the geometrical nonlinear relations of an elastic beam are considered. The coordinate systems used to analysis the rotating flexible beam are an inertial frame and a body-fixed frame. The three-dimensional finite beam element is modeled using Euler-Bernoulli beam theory as a model of 3<sup>rd</sup> order based on the formerly research in [1]. By using the description of geometric nonlinear beam kinematics, functions of the elastic variables are determined. The equations of motion of an elastic beam are derived based on the principle of virtual work with a state depending stiffness, damping and mass matrix-like structure. In addition to research of [1] more complex motions, the guided motions including external effects coupled with state as well as state dependences in the nonlinear matrices, are discussed and considered. Simulations of the flexible beam are used to show the coupling effects between the rotating motion and transverse deformations as well as the axial deformation with geometric nonlinear terms.

With this contribution, the dynamical behavior of a three-dimensional elastic beam undergoing a rotational motion is investigated. The coupling effect between the rotating motion and transverse deformations as well as the axial deformation is shown using a simulation example. From the results given in Fig.1, it can be concluded that the consideration of geometrical nonlinear terms of the flexible beam should be taken into account in the model, especially in the cases of the guided motion of the beam in combination with external forces. The developed model and the related dynamic system representation gives a good base for advanced study of the stability of the guided system in combination with external process forces resulting from the digging process of large excavator systems with long and slender booms.

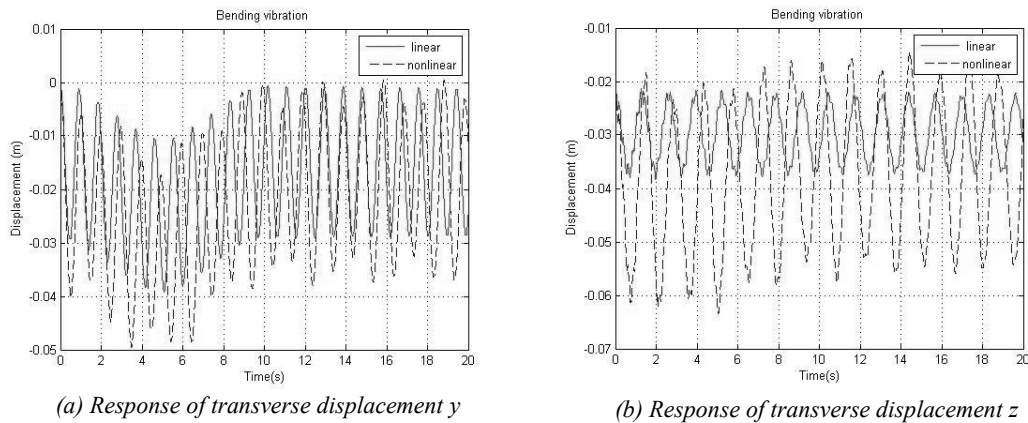


Fig. 1. Response of beam vibration with the applied transverse force according to y- and z-direction of the tip of the beam for a rotational beam

[1] Söffker D.: *Automatic generation of the equations of motion of the moving nonlinear elastic beam*. SAMS, (2)1999, 31-74.  
[2] Bošnjak S., Zrnić N., Oguamanam D.. *On the dynamic modelling of bucket wheel excavators*. FME Transactions, (34)2006, 221-226.

# TECHNIQUES FOR MODELING SIMULATION ENVIRONMENTS FOR MODULAR ROBOTICS

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In modular robotics, complex structures can be formed from basic modules to solve tasks which would be difficult for single robots. The development of techniques for adaptation and evolution of multi-robot organisms is the subject of Symbion project [2]. In the project, the bio-inspired evolutionary algorithms are massively simulated prior to run them on real hardware. It is crucial to evolve behaviors of the robots in simulation, that is close to a real world. Hence, accurate and efficient representation of an environment in the simulator is needed. Here, the environment is modeled using set of 3D objects (usually triangle meshes). The robots learn simple motion primitives or complex movement patterns during many runs of the evolution. The learned skills will be then used during the experiments with real hardware.

Important property of the models is thus amount of elements in the model which influences the speed of the simulation. To speed up the simulation, several models with different level of details can be used. Similarly as in nature, some simulated tasks require only rough approximation of the environment and sometimes details of selected objects in neighbors are needed.

In the paper, we describe a techniques for building the simulation environments for the purpose of Symbion project. To obtain such a model, the real arena is scanned using laser rangefinders. We describe method to remove noise from the scanned 3D point cloud. Then, two state-of-the art methods and also a novel method for 3D reconstruction will be described.

The first method is based on Growing self-reconstructions maps (GSRM) introduced by Rêgo et al. [3] that reconstructs a surface in the form of a triangular mesh. The method follows principles of growing neural gas (GNG), where the number of neurons and topology of the network change during the self-organization process. The second method – Growing grid (GG) – is another self-organizing feature map that adapts according to Hebbian rule [1]. Similarly to GSRM, GG is a growing structure, i.e., the number of neurons changes (increases) during learning. On the other hand (and in contrast to GSRM), GG has a fixed structure, which has a form of a rectangular grid. The process of adaptation has two distinct phases: a growth phase where the size of the network as well as raw estimate of neuron positions is determined and a fine-tuning phase which tunes the positions of the neurons.

We also propose a novel method for 3D reconstruction, which fits a set of plane through the input point cloud. The algorithm first randomly selects several hundred of clusters and examines, whether the points within these clusters lie on one plane. Planar clusters then compete for surrounding points until there is only one cluster per plane. After that, plane intersections are computed and the clusters are enlarged and triangulated. Using these several reconstruction methods, the environment can be modeled with various level of details.

In the experimental section, the reconstructed models will be used in a robotic simulator in two scenarios: a) a simple snake-like organism out-stepping a hole, where the models are used for physical simulation; and b) for simulation of robotics swarm exploring the environment. In the second scenario, the robots perceive the environment using laser rangefinders and the quality of the models influences the sensor simulation. The experimental results have shown, that a method for 3D reconstruction must be carefully chosen in order to allow fast and reliable simulation. It will be shown that the number of triangles in resulting 3D models does not influence the speed of physical simulation itself. However, the size of models significantly influences the speed of the laser rangefinder simulation. To simulate the sensor, collisions between rays and the 3D scene have to be determined, which is computationally intensive. To speed up the sensor simulation, a model with less number of triangles or a model consisting of a simple geometric objects (e.g. planes) is preferred.

- [1] Bernd Fritzke. Some competitive learning methods. Technical report, Ruhr-Universität Bochum, 1997.
- [2] P. Levi and S. Kernbach, editors. *Symbiotic Multi-Robot Organisms: Reliability, Adaptability, Evolution*. Springer-Verlag, 2010.
- [3] R. L. M. E. Rêgo, A.F.R. Araujo, and F.B. de Lima Neto. Growing self-reconstruction maps. *Neural Networks, IEEE Transactions on*, 21(2):211–223, February 2010.

# A DETAILED NONLINEAR DYNAMIC MODEL OF A 3-DOF LABORATORY HELICOPTER FOR CONTROL DESIGN

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**Introduction.** This work presents the derivation of a detailed nonlinear dynamic model of a commercial 3-DOF laboratory helicopter for subsequent control design. The equations of motion are derived from physical modeling and the engine characteristics are identified from measurements, yielding a coupled system of highly nonlinear differential equations. The system's kinematics and dynamics are thoroughly analyzed and validated using polynomial test trajectories. Linearized state space systems are derived for arbitrary operating points and a parameterized linear stability analysis is conducted. Finally, the model is successfully validated on the actual plant, and an outlook of closed-loop control performance, including gain-scheduled feedback and flatness-based feedforward controllers, is given.

**Content.** The studied tandem rotor helicopter is suspended via a linkage as shown in Fig.1 and has three angular degrees of freedom (DOF). The rigid-body components are described in local coordinates and assembled using homogeneous transformations, yielding a set of nonlinear coupled differential equations. In the onset of the present paper, all relevant geometric details are considered to obtain a high-fidelity nonlinear simulation model. Also, a parameterized family of linearizations is computed to support gain-scheduled, locally linear control design [1].



Figure 1: 3DOF helicopter, courtesy of Quanser Inc.

**Model.** The relation between the lift forces generated by the propellers and the input voltages were identified on the real plant and modelled using a quadratic onset. Lagrangian Mechanics were used to derive the system's equations of motion (EOM), which yields a nonlinear system representation. For subsequent controller design procedures, linearized models for stationary operating points in arbitrary elevation angles are obtained via MAPLE.

**Validation Results.** To evaluate the accuracy of the created nonlinear dynamic helicopter model, the actual system's responses are compared to the model-based Simulink simulations in an elevation-open-loop and a closed-

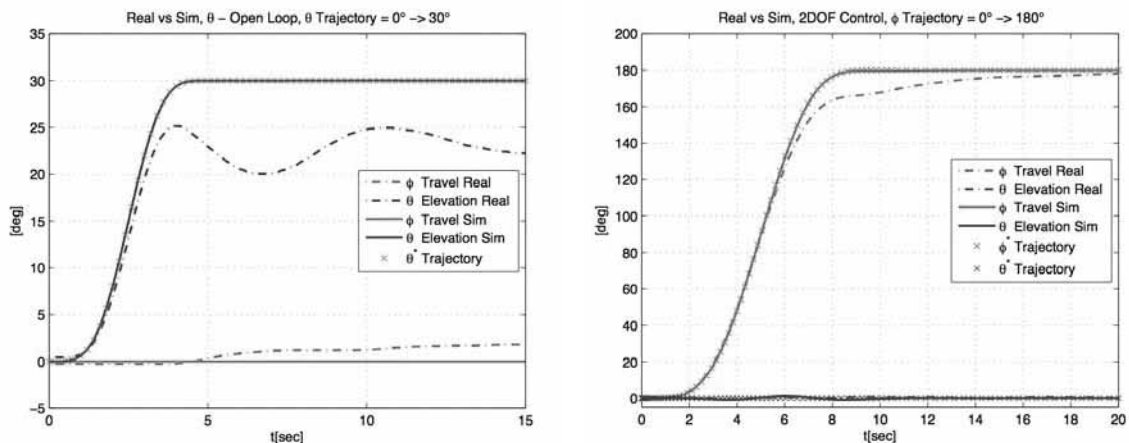


Figure 3 – left: open-loop validation; right: closed-loop validation

loop setting. Figure 3 (left) shows the responses of the system in simulation as well as in reality following an open-loop elevation trajectory. For the real plant, the Pitch DOF has been stabilized by a state vector feedback controller. The input signals are computed by a flatness-based approach [2] to obtain a prescribed polynomial trajectory in the elevation DOF. Figure 3 (right) shows the trajectory tracking performance of the closed-loop system utilizing a 2DOF control architecture with a gain-scheduled LQR feedback controller and a flatness-based feedforward controller.

[1] Rugh W. J., and Shamma J. S.: *Survey Paper – Research on gain scheduling*. Automatic 36 (2000) 1401-1425, 1998.  
 [2] Fliess M., Levine J., Martin P., and Rouchon P.: *Flatness and defect of nonlinear systems: introductory theory and examples*. Int. J. Control, 61(6): 1327-1361, 1995.

# SIMULATION OF NONHOLONOMIC MECHANICAL SYSTEMS USING ALGORITHMIC DIFFERENTIATION

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**Introduction** We consider mechanical systems with  $n$  degrees of freedom and  $p$  nonholonomic constraints. The system trajectories evolve on the  $n$ -dimensional smooth manifold  $Q$  with local coordinates  $q = (q^1, \dots, q^n)$ . The Lagrangian  $L$ , which is defined as kinetic minus potential energy, maps from the tangent bundle  $TQ$  to the real numbers, see [1] for details. The nonholonomic constraints are represented by a system of one-forms  $\omega^i \in T^*Q$ ,  $i = 1, \dots, p$ , in coordinates  $\omega^i = \sum_{k=1}^n \omega_k^i(q) dq^k$ , which restrict the solutions to a subbundle of the tangent bundle  $TQ$ . In coordinates this restriction reads as  $\omega^i \lrcorner \dot{q} = \omega^i(\dot{q}) = \sum_{k=1}^n \omega_k^i(q) \dot{q}^k = 0$ ,  $i = 1, \dots, p$ . Constraints of that type are called nonholonomic if they are not integrable. One way of dealing with this type of system is utilizing Lagrange multipliers. We pursue a different approach according to [3] here.

**Hamel's equations and quasi-velocities** *Hamel's* equations are a generalization of the *Lagrange* equations of motion. Since they also cover the special case of *Euler's* equations of rigid body motion, they originally had been called *Lagrange-Euler* equations by Hamel [3]. The crucial advantage of *Hamel's* approach is that so-called quasi-velocities  $\omega^i(\dot{q}) = \sum_{k=1}^n \omega_k^i(q) \dot{q}^k$ ,  $i = 1, \dots, n$  can be used, which are not necessarily a differential of a corresponding coordinate on  $Q$ . The change of velocity coordinates is required to be invertible:  $\dot{q}^k(\omega) = \sum_{i=1}^n \omega_i^k(q) \omega^i$ . Moreover, it is reasonable to choose the first  $p$  velocities according to the nonholonomic constraints. We can formulate the Lagrangian depending on the new coordinates:  $\tilde{L}(q^1, \dots, q^n, \omega^1, \dots, \omega^n) = \tilde{L}(q, \omega) = L(q, \dot{q}(\omega))$ .

The equations of motion can then be written as

$$\frac{d}{dt} \frac{\partial \tilde{L}(q, \omega)}{\partial \omega^k} - \sum_{j=1}^n \frac{\partial \tilde{L}(q, \omega)}{\partial q^j} \underbrace{\frac{\partial \dot{q}^j(\omega)}{\partial \omega^k}}_{\omega_k^j(q)} + \sum_{j=1}^n \sum_{l=p+1}^n \frac{\partial \tilde{L}(q, \omega)}{\partial \omega^j} \gamma_{l,k}^j(q) \omega^l = \tilde{f}_k, \quad k = p+1, \dots, n,$$

where  $\tilde{f}_k = \sum_{i=1}^n \frac{\partial \dot{q}^i(\omega)}{\partial \omega^k} f_i = \sum_i \omega_k^i(q) f_i$  and  $\gamma_{l,k}^j(q) = \sum_{v,\sigma=1}^n \left( \frac{\partial \omega_v^j(q)}{\partial q^\sigma} - \frac{\partial \omega_\sigma^j(q)}{\partial q^v} \right) \omega_l^\sigma(q) \omega_k^v(q)$ . These equations together with

$$\dot{q}^i = \sum_{k=p+1}^n \omega_k^i(q) \omega^k, \quad i = 1, \dots, n.$$

constitute a system of  $2n - p$  first order differential equations, which describes the motion of the mechanical system. Resolving the total derivative, the system contains plenty of partial derivatives, which can be efficiently calculated using algorithmic differentiation.

**Algorithmic Differentiation** In order to simulate the equations of motion, we have to compute first and second order derivatives. Numerical differentiation by divided differences is not well-suited for this task due to truncation and cancellation errors. Therefore, the derivatives occurring in these equations are usually computed symbolically with computer algebra packages or libraries.

We suggest the use of an alternative differentiation technique known as *automatic* or *algorithmic differentiation* [2]. Assume that the function under consideration is a sequence of elementary functions and operations. Derivatives of this function can be calculated by applying elementary differentiation rules to this sequence. In algorithmic differentiation, all intermediate values are floating point numbers instead of symbolic expressions. Thus, compared to symbolic calculations, this approach requires less memory for the exact calculation of the partial derivatives.

**Example** Finally, the presented approach is illustrated by the example of a nonholonomic robot.

- [1] Abraham, R. and Marsden, J. (1978). *Foundations of Mechanics*. Addison-Wesley Pub. Co.
- [2] Griewank, A. and Walther, A. (2008). *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. SIAM, 2nd edition.
- [3] Hamel, G. (1904). Über die virtuellen Verschiebungen in der Mechanik. *Mathematische Annalen*, 59, 416–434.

# AUTONOMOUS ROBOT PATH PLANNING ALGORITHM BASED ON NEURONAL NETWORK DISCRETE CHAOTIC DYNAMICS

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Path planning refers to determining and maintaining the most efficient path for a moving autonomous robot from its current location to the goal state. During the last decades heuristic methods had become dominant within the field of autonomous robot rational navigation. Although not guaranteeing to find an optimal solution, heuristic algorithms are simple and computationally efficient which makes them highly applicable to path planning.

Among the manifold of heuristics applied to the development of tools for robot path planning we can distinguish various noticeable approaches such as A\*, Fuzzy Logic, Potential Field, Cellular Automata and roadmap techniques like Cell Decomposition, Voronoi diagram and Probabilistic Roadmaps. Contribution of biologically inspired paradigms such as Neuronal networks and Genetic Algorithm to the development of heuristic tools for robot path planning should be especially mentioned. Algorithms employing chaotic dynamics play an important role in autonomous robot trajectory generation.

Chaotic dynamics existing within the biological neuronal networks are responsible for self-organized pattern formation represented by self-synchronized activated states of their composing neurons. According to our hypothesis, these neuronal patterns are the mechanism standing behind human creative behaviour – trajectories embedded within them could be used for rational path planning. Mathematical models based on neuronal networks consisting of interconnected chaotic oscillators provide self-organized and self-synchronized patterns similar to those observed within the biological neuronal networks [J. Kurths et al., 2007], [V. Gontar, 2004, 2007]. Based on the hypothesis, we intend to construct a mathematical model of robot's neuronal networks with embedded chaotic regimes and use patterns generated by it to autonomous robot path planning.

In the proposed model every neuron of the network is simulated by specific difference equations with chaotic regimes providing the neuron with chaotic dynamics. Spatially distributed over 2D or 3D space neurons' activated states lead to emergence of complex creative patterns. The patterns serve as a source of potential continuous trajectories for robot's path planning: for that purpose adjacent neurons with equal activated states are connected by straight lines, resulting in the formation of a trajectory. Based on robot's rational path planning criteria the best trajectory should be selected and translated into the robot's movement in physical space and time.

Within the current work we consider a goal-search mission performed by an autonomous robot in a known 2D environment with obstacles. Series of decisions need to be taken by the robot to succeed in performing navigation to the hidden goal state (goal-searching), avoidance of obstacles and selection of a rational trajectory minimizing a certain cost function.

Proposed heuristic method based on robot's chaotic neuronal networks with creative properties demonstrates some advantages over the methods not related to the biologically inspired paradigms (random search algorithms) and heuristics not justified by brain-functioning principles, such as Genetic Algorithm.

- [1] Kurths J., Zhou C. S., Zemanova L., Zamora-Lopez G. and Hilgetag C. C.: *Structure-Function Relationship in Complex Brain Networks expressed by Hierarchical Synchronization*. New Journal of Physics, 9 (2007), 178-200.
- [2] Gontar V.: *The dynamics of living and thinking systems, biological networks, and the laws of physics*. Discrete Dynamics in Nature and Society, 1 (2004), 101-111.
- [3] Gontar V.: *Some creative properties of the 2D and 3D lattice distributed interconnected chaotic oscillators and neuronal networks*. in Proc. Applied Mathematics and Mechanics, 7 (2007), 203007-203008.

# MODELLING OF THE MOON ORBITER FOR THE ESA PROJECT ESMO

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**Introduction.** This paper presents the simulator developed for the European Student Moon Orbiter (ESMO) project, which is planned to be the first European student mission to the Moon. During the ESMO project, student teams, supported by faculty staff, will produce a complete spacecraft from scratch. Its mission will be to fly towards the Moon, enter the Moon's orbit and execute scientific experiments while orbiting around the Moon. A Functional Engineering Simulator (FES) was produced as a part of the ESMO project and will allow the project teams to model the spacecraft's functions and performance at various stages of the mission and simulate the space environment. This paper focuses on the spacecraft's orbit and attitude propagation model. Finally, the overview of the FES simulator is presented along with the preliminary results produced with the simulator.

**Content.** The European Student Moon Orbiter (ESMO) is planned to be the first European student mission to the Moon. The ESMO represents a unique and inspirational opportunity for university students, providing them with valuable and challenging hands-on space-project experience in order to fully prepare a well-qualified workforce for future ESA missions in future decades [2].

ESMO student teams, supported by faculty staff, will produce a complete spacecraft from scratch. Its mission will be to fly towards the Moon, place itself into a stable Moon orbit, acquire images of the Moon with a narrow-angle camera and transmit them back to Earth for education outreach purposes. Additional measurements relevant to an advanced technology demonstration, lunar science and exploration will be executed as well [1].

A team from the University of Ljubljana entered the ESMO project with the aim to produce a Functional Engineering Simulator (FES) that will allow the project teams to model the spacecraft's functions and performance at various stages in the mission and simulate the operational environment, including ground-station contacts. Our work began on the foundations that were set by the teams of University Carlos III of Madrid, Polytechnic University of Madrid and Polytechnic University of Milano, which produced an early form of documentation and simulators. A Functional Engineering Simulator was then created that combines the propulsion, the power and the navigation subsystems and puts them into the virtual space around the Earth and the Moon, where experiments can easily be executed.

The article presents the spacecraft's dynamics with the major forces and torques effecting the orbit and the attitude of the spacecraft. This overview of the spacecraft's dynamics is encapsulated in the orbit and attitude propagation models, which are presented in the paper. These mathematical models were then used to produce the Simulink models of the spacecraft and its components. Together they form the Functional Engineering Simulator of the spacecraft. The simulator architecture, that was developed for this purpose, enables the execution of the predefined scenarios in various stages of the mission. After each simulation run, a mission report is generated automatically, based on the predefined scenario template.

**Results.** For the purpose of identifying the best solver for use in the simulator, the results of two tests are presented in the paper. In both tests, Earth and spacecraft were modelled as point masses with initial conditions of the spacecraft for the stable low Earth's orbit. To allow more transparent simulator validation process without the loss of generality, the effects of drag, gravity perturbations and solar radiation pressure were excluded. This enabled us to compare the results with analytically calculated orbit, based on Keplerian elements. In both tests, numerical stability and computational burden on the system were analyzed. Using a model with all on-board systems activated, the first test mainly focuses on differences in computational burden of the simulator using different solvers, while in the second test, only the spacecraft's dynamics was evaluated in the interval of one virtual Earth day and numerical stability of solvers was observed. The results show that the solvers ode45, ode23 and ode113 solvers are very similar in numerical stability with simulation execution times decreasing in the the same order as solvers were listed.

The third test was used to demonstrate the power budget analysis in the special use case scenario. As the spacecraft is an autonomous vehicle, the power budget analysis has a major importance in spacecraft design. In the simulated scenario, spacecraft is left spinning with some onboard components (e.g. communication equipment) turned on every 10 seconds with the 2 seconds duty cycle. Results of the simulation are two graphs, one showing the combined current of both solar panels and the second showing the battery charge state during experiment.

[1] ESA: *ESMO mission*. [http://www.esa.int/esaMI/Education/SEML0MPR4CF\\_0.html](http://www.esa.int/esaMI/Education/SEML0MPR4CF_0.html), 2007.

[2] Walker, R. and Cross, M.: *The European Student Moon Orbiter (ESMO): A lunar mission for education, outreach and science*. *Acta Astronautica*, 66 (7-8), 1995, pp. 1177–1188.



# NETWORK-BASED MODELING AND INDEX ANALYSIS OF COUPLED ELECTRO-MECHANICAL SYSTEMS

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**Introduction.** Modeling and simulation of multi-physics dynamical systems is an important issue in many industrial applications. In modern simulation packages such as DYMOLA or MATLAB/SIMULINK modeling of multi-physics systems is done in a modularized way, based on a network of subsystems for the different physical domains that again consists of simple standardized components which are coupled together via certain interface conditions. This approach is successfully used in circuit simulation and has become industrial standard in multi-body dynamics or mechatronics. This modeling of dynamical systems via a network of subcomponents leads to differential-algebraic equations (DAEs). In most simulation environments computer-algebra packages and symbolic differentiation are used on the whole flattened system of equations to identify and resolve the constraints and interface conditions in order to obtain a system in minimal coordinates. The disadvantage of this approach is that it produces formulas with bad numerical properties. Even worse the numerical solution can deviate from constraints and interface conditions since this information is no longer accessible in the underlying ODE system. This leads to physically questionable results (e.g. numerical damping or numerical dissipation). Also stabilization techniques used to avoid drift-off from the constraint manifold fail frequently, in particular for models with different time-scales or different levels of discretization accuracy. In order to get a grip on these problems, in this contribution a new remodeling approach for coupled electro-mechanical systems is introduced. At first each subcomponent is remodeled based on the strangeness-index concept [3] and index reduction by minimal extension [2]. Here, the special structure of the uni-physics component is incorporated to produce a minimally extended index 1 system using the system equations and some of its derivatives and introducing a minimal set of new variables. In this index 1 system all explicit and implicit constraints are available, such that the initialization process is easy and the numerical solution stays on its manifold. Furthermore, the variables keep their physical meaning. In a second step the index of the coupled system can be analyzed.

**Modeling of coupled electro-mechanical systems.** We consider coupled electro-mechanical systems, i.e., systems that are composed by interconnection of several subsystems that form either a mechanical multibody system or an electrical system. It is well-known that the equations of motion of constraint multibody systems form DAEs of index 3. For the electrical subsystems the dynamics can be described via the modified nodal analysis (MNA). The index of the MNA equations can be determined based on the topological structure of the electrical network. In particular, it is well-known that loops in the graph consisting only of capacitances and voltage sources or cutsets that contain only inductances and/or current sources lead to index-2 DAEs [1]. We consider coupled system where each subsystem  $\mathcal{S}_i$  is given by

$$F_i(t, x_i, \dot{x}_i, u_i, \dot{u}_i) = 0, \quad (1)$$

denoting a DAE describing the dynamical behavior of the subsystem with state  $x_i$  and input  $u_i$ . The coupling of subsystem  $\mathcal{S}_i$  with subsystems  $\mathcal{S}_{j_1}, \dots, \mathcal{S}_{j_k}$  is done via the coupling condition  $u_i = G_{i,j_1, \dots, j_k}(t, x_{j_1}, \dots, x_{j_k})$ , describing the connection of the outputs of subsystems  $\mathcal{S}_{j_1}, \dots, \mathcal{S}_{j_k}$  to the input of subsystem  $\mathcal{S}_i$ .

**Remodeling and index analysis.** Coupling of two subsystems can easily lead to high index DAEs, in particular to systems of index higher than 3. The proposed new remodeling approach basically consists of two steps. In the first step of the remodeling procedure we compute a minimally extended index 1 formulation for each subsystem using index reduction by minimal extension. Here, the special structure of the subsystem (i.e., electrical circuit or mechanical multibody system) is incorporated to decide which equations have to be differentiated and which new variables have to be introduced in order to extend the system size in a minimal way leading to a system of index 1. In a second step we analyze the index of the coupled system. We will present conditions that specify in which cases the coupled system is again of index 1, and in which cases an increase of the index due to coupling occurs.

- [1] D. Estévez-Schwarz and C. Tischendorf. *Structural analysis of electric circuits and consequences for MNA*. Int. J. Circuit Theory Appl., 2000, 28(2): 131-162.
- [2] P. Kunkel and V. Mehrmann. *Index reduction for differential-algebraic equations by minimal extension*. Zeitschrift für Angewandte Mathematik und Mechanik, 2004, 84:579-597.
- [3] P. Kunkel and V. Mehrmann. *Differential-Algebraic Equations — Analysis and Numerical Solution*. EMS Publishing House, Zürich, Switzerland, 2006.

# ADVANCED MODELING AND SIMULATION OF NANOWIRE FIELD-EFFECT TRANSISTORS

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**Introduction.** Nanowire field-effect transistors (NWFETs) are attractive sensing devices with a wide range of applications. In order to make NWFETs suitable for medical purposes the nanowire based on semiconducting materials is covered with a dielectric layer functionalized with immobilized probe molecules. In an electrolyte with target molecules, e.g., blood, the targets bind to the probes and in turn influence the charge in a boundary layer, which induces a field effect. Due to the high surface to volume ratio of the nanowire, high sensitivity and selectivity can be reached. Despite the experimental progress, many processes are not fully understood and hence modeling and simulation are crucial on the way to optimal sensing devices [1].

**Model.** To characterize such devices, two important issues need to be solved, which result in high computational cost: the charges of the molecules are in Ångström range and the nanowire is of micrometer length, leading to a multiscale problem. Furthermore, a simplification to smaller dimensions than 3d is not preferable due to the real-world boundary conditions. Fortunately, such multiscale problems can be solved with a homogenization method by splitting the charge into a nanowire and a boundary layer part [2]. The computational cost can be further reduced by a parallelization method.

The NWFET is modeled by three material dependent PDEs. The transport in the nanowire is described by the Poisson drift-diffusion system and the aqueous solution is modeled by the Poisson-Boltzmann equation. Models for the boundary layer can be of microscopic, macroscopic or empirical type. Recently we used Metropolis Monte-Carlo simulations to characterize the boundary layer charge of a DNA sensor [1]. The resulting system of PDEs with jump conditions at an interface  $\Gamma$  are expressed as

$$\begin{aligned} -\nabla \cdot (\varepsilon_{\text{liq}} \nabla V) &= -2\eta \sinh(\gamma V) & \text{in } \Omega_{\text{liq}}, & \quad -\nabla \cdot (\varepsilon_{\text{Si}} \nabla V) = q(p - n + C_{\text{dop}}) & \text{in } \Omega_{\text{Si}}, \\ -\nabla \cdot (\varepsilon_{\text{ox}} \nabla V) &= 0 & \text{in } \Omega_{\text{ox}}, & \quad \nabla \cdot J_n = R \\ V(x+) - V(x-) &= \alpha & \text{on } \Gamma, & \quad \nabla \cdot J_p = -R \\ \varepsilon_{\text{liq}} \nabla_{\nu} V(x+) - \varepsilon_{\text{ox}} \nabla_{\nu} V(x-) &= \beta & \text{on } \Gamma, & \quad J_n = D_n \nabla n - \mu_n n \nabla V \\ & & & \quad J_p = -D_p \nabla p - \mu_p p \nabla V \end{aligned}$$

which we solve for the electrostatic potential  $V$ , the electron density  $n$ , and the hole density  $p$ . The macroscopic dipole moment density  $\alpha$  and the macroscopic surface charge density  $\beta$  arise from the homogenization method. We proved existence and local uniqueness of this system around thermal equilibrium. In order to get accurate results it is important to solve the PDE system self-consistently with an enhanced Scharfetter-Gummel iteration scheme [3]. Due to 3d simulations we have to deal with a very large linear system and hence a parallelization method is inevitable.

**Parallelization.** Consequently we derived a novel finite-volume tearing and interconnecting (FETI) method based on the work of Farhat and Roux including the coupled heterogeneous system of the Poisson drift-diffusion equations, the linearized Poisson-Boltzmann equation, and jump conditions arising from the homogenization method as stated above.

This method works as follows: the system is discretized with a finite-volume method and then split into boxes. These boxes are glued together with Lagrange multipliers which are computed with a preconditioned conjugate gradient method. Within this glueing, the jump conditions are easy to implement in the discretized form and do not affect the usual condition number for FETI methods.

**Conclusion.** It is now possible to study such bio-functionalized NWFET devices from a physical and geometrical point of view. Our investigations help to understand devices based on NWFETs and can give a guideline on how to reach optimal sensitivity [1].

- [1] Baumgartner, S., Vasicek, M., Bulyha, A., and Heitzinger, C.: *Optimization of nanowire DNA sensor sensitivity using self-consistent simulation*. Nanotechnology, 22(42) 2011, 425503/1–8.
- [2] Heitzinger, C., Mauser, N., and Ringhofer, C.: *Multiscale modeling of planar and nanowire field-effect biosensors*. SIAM J. Appl. Math., 70(5) 2010, 1634–1654.
- [3] Baumgartner, S. and Heitzinger, C.: *Existence and local uniqueness for 3d self-consistent multiscale models of field-effect sensors*. Commun. Math. Sci., 10(2) 2012, 693–716.

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# INVERSE SIMULATION OF AN UNDERWATER VEHICLE MODEL USING FEEDBACK PRINCIPLES

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Inverse simulation is a technique used in the modelling of dynamic systems to find time histories of input variables that provide a set of required model output responses without the need for an analytically-derived inverse model. This has relevance for many engineering systems design problems, especially where nonlinearities are significant as, for example, in the case of actuators where amplitude and rate limits may be critically important in meeting given performance requirements. Examples of application areas in which inverse simulation methods have proved particularly useful include flight mechanics and agility investigations for fixed-wing aircraft and helicopters and much useful background information may be found in a review paper by Thomson and Bradley [1].

One method of inverse simulation that has received renewed attention in recent years involves the use of feedback principles [2]. In this approach, which can be traced back to methods of inverse function generation on analog computers, high gain feedback loops are applied around the model. The reference inputs for this feedback system represent the required outputs and the inverse solution is provided by the signal(s) applied as input(s) to the model. If the feedback design can be implemented successfully in simulation an inverse simulation solution can be generated for any desired form of output (subject to any relevant constraints). One important feature of this approach to inverse simulation is that it provides physical insight that can be missing with more traditional approaches to inverse simulation such as iterative gradient techniques [1].

The full paper describes an application of the feedback systems approach to inverse simulation studies involving a nonlinear dynamic model of an unmanned underwater vehicle (UUV). An outline of the nonlinear model of the UUV is provided. Feedback loops are designed around the model for selected sets of output variables, such as surge velocity, pitch rate and yaw rate. Inverse solutions are generated that provide the model inputs required for the specified manoeuvres and it is shown that the feedback approach provides accurate and useful inverse solutions for appropriate choices of feedback structure and associated gain factors.

One important feature of the feedback approach is that the design a feedback system for an inverse model is, in general terms, much less demanding than the design a feedback system for a control application involving a system of similar complexity. Issues relating to the response of the closed-loop system to external disturbances, insensitivity to measurement noise and robustness in terms of model uncertainties are all irrelevant for inverse simulation since disturbances and measurement noise are not present. The model is known so there are no issues of robustness (other than numerical robustness). Relatively simple methods of feedback design involving high-gain solutions and state-variable feedback can therefore be considered for the model inversion application. Although problems of numerical stiffness can arise, these should not create major difficulties with an appropriate choice of numerical integration algorithm.

It is concluded that inverse simulation methods can provide engineering design insight that is different from the understanding that comes from conventional modelling and simulation studies. Viewing the problem in terms of the inputs that are needed to achieve a defined pattern of outputs provides the investigator with information that is potentially important for use in design of the engineering system and it is believed that this understanding would not be so readily obtained using traditional modelling and simulation tools. It is also believed that the results included in the paper support the view that the feedback approach provides a viable alternative to other techniques for inverse simulation and model inversion.

- [1] Thomson, D. and Bradley, R.: *Inverse simulation as a tool for flight dynamics research- Principles and applications*, Progress in Aerospace Sciences, 42 (2006), 174-210.
- [2] Murray-Smith, D.J.: *Feedback methods for inverse simulation of dynamic models for engineering applications*, Mathematical and Computer Modelling of Dynamical Systems, 17 (2011), 515-541.

# NONLINEAR MODEL PREDICTIVE CONTROL OF A VAPOR COMPRESSION CYCLE BASED ON FIRST PRINCIPLE MODELS

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In 2010, refrigeration caused 14% of Germany's total electrical energy consumption. In other countries this number might even be higher. The majority of refrigeration systems is based on vapor compression cycles. It is well known that proper control of these systems provides a significant potential for energy savings.

Vapor compression cycles however are highly nonlinear systems. Modeling and control design for these systems is a nontrivial task. With the recent advance of electronic actuators like variable-speed fans, pumps, or compressors and electronic expansion valves, the number of possible control inputs has increased. On the one hand, this provides additional possibilities for efficient control algorithms, while on the other hand strong cross couplings of inputs and outputs lead to hard challenges for control design based on classical PID controller.

The principle of Model Predictive Control (MPC) seems to perfectly suit vapor compression cycles. Cross-couplings in multi-input-multi-output (MIMO) systems can be handled very efficiently and energy efficiency can be explicitly taken into account. The idea of MPC is to use a mathematical process model to formulate an optimization problem and determine appropriate control actions by repeatedly solving this optimization problem. One usually distinguishes between MPC, using linear process models, and Nonlinear Model Predictive Control (NMPC), using nonlinear models. A detailed description of this approach can e.g. be found in [3]. By now there are only few (N)MPC applications reported in literature that deal with the problem of controlling vapor compression cycles.

Elliott and Rasmussen [2] suggest an MPC scheme for multi-evaporator cycles. They use a local MPC controller for each evaporator and employ linear process models determined by system identification. Leducq et al. [4] use a nonlinear process model based on first principles such as energy and mass balance equations. Solving the resulting nonlinear optimal control problem takes considerable more computation time. The suggested NMPC scheme therefore required a comparably long sampling time of 20 seconds. Because expansion valves need much shorter sampling rates, it is controlled by an additional PID controller instead of NMPC. They use a single shooting discretization of the optimization problem with a time horizon of 80 seconds. The choice of integration algorithm and the resulting ODE discretization is not addressed.

In this contribution we present a new NMPC scheme for vapor compression cycles and demonstrate its applicability to real-time simulation experiments. The underlying process model is based on first principles and accurate fluid property data. A new method for efficient computation of fluid property data using bicubic spline interpolation is presented. In our NMPC scheme, the arising Optimal Control Problems (OCP) are solved by a fast structure exploiting Direct Multiple Shooting method, as first introduced by Bock and Plitt [1] and extended in a series of subsequent works, cf. [5] for a more recent presentation. This fast method allows us to use NMPC directly on all controls including expansion valve opening. In contrast to [4], we don't require local PID controllers to handle fast transients. The chosen sampling rate is only 0.5 s, and could be reduced further if required by the process dynamics.

- [1] Bock, H.G. and Plitt, K.J. (1984). A Multiple Shooting algorithm for direct solution of optimal control problems. In *Proceedings 9th IFAC World Congress Budapest*, 243–247. Pergamon Press.
- [2] Elliott, M.S. and Rasmussen, B.P. (2008). Model-based predictive control of a multi-evaporator vapor compression cooling cycle. In *American Control Conference*, state 3, 1463–1468. Ieee, Seattle.
- [3] Findeisen, R. and Allgöwer, F. (2002). An Introduction to Nonlinear Model Predictive Control. In *21st Benelux Meeting on Systems and Control*.
- [4] Leducq, D., Guilpart, J., and Trystram, G. (2006). Non-linear predictive control of a vapour compression cycle. *International Journal of Refrigeration*, 29(5), 761–772.
- [5] Leineweber, D.B., Bauer, I., Schäfer, A.A.S., Bock, H.G., and Schlöder, J.P. (2003). An Efficient Multiple Shooting Based Reduced SQP Strategy for Large-Scale Dynamic Process Optimization (Parts I and II). *Computers and Chemical Engineering*, 27, 157–174.

# EFFICIENT NONLINEAR WIND-TURBINE MODELING FOR CONTROL APPLICATIONS

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**Introduction.** Wind turbines are an attractive green alternative for power production, and this technology is presently experiencing widespread deployment. The growth of wind power production has spurred intensive research on all aspects of the technology.

The application of automatic control to wind turbines allows for greater power production and lessened aerodynamic loads. Active motion suppression is also being pursued. With the advent of floating wind turbines, the required analysis, modeling and control requires an increased level of sophistication. This also holds with respect to control engineering.

**Modeling the wind-turbine for control.** When applying automatic control, a simple but accurate model is usually required. The scope of the model must be chosen so as to capture the most important effects relevant for the desired control objectives. The model must also be put on an appropriate mathematical form. In control theory, a finite number of ordinary differential equations are most often used.

A wind turbine does not yield easily to a linear model, but is in fact highly nonlinear. This is particularly true in the aerodynamic modeling. Simple control models have hitherto been based mostly on local linearizations, or lookup-tables to generate a suitable system.

The rotor, as apart from its support structure, gives rise to the majority of effects in need of nonlinear modeling. The present work describes a simple nonlinear rotor model, which under some assumptions, yields a complete model for a wind turbine rotor. First principles are used where applicable, when developing the model. A vectorial form is used, yielding a compact and translucent model, composed of nine ODE's. The resulting model describes the dynamics of a rigid rotor, free to move in all six degrees of freedom, incorporating an unsteady aerodynamic model. This freedom is necessary for modeling a floating wind turbine, which does not have a fixed base. The model is shown to have several special properties relevant for control design.

A procedure is outlined, that describes how the parametric model may be fitted towards results from more sophisticated numerical wind turbine performance tools. The industry standard Blade-Element-Momentum (BEM) approach is used to calculate forces and moments on the rotor disk at a large set of operational states. These states cover the operational envelope of the turbine, as well as offsets caused by control action or a changing wind environment. The model parameters are subsequently adjusted by utilizing weighted nonlinear least squares to minimize the steady state model error with respect to the BEM. A Gauss-Newton iteration is used. Importantly, the weights are selected so that the cumulative weighted probability of wind speed is the same in the model data-set as at the turbine site. This probability is assumed to follow a Weibull-distribution. An ad-hoc data weighing is thereby avoided.

The structure of the model is quite simple, and very efficient in simulations, when compared to tools of similar scope. A simple nonlinear model will allow researchers to leverage the large field of nonlinear control towards wind turbine applications. The model is novel, due to its relaxed inflow treatment, the rigorous parameter estimation scheme, as well as its vectorial form.

The model replicates the steady state behavior simulated by more advanced tools with good accuracy, thus obviating the need for lookup tables. The transient performance is validated against experiment with excellent results. However, the present approach fails to model cyclical loads at yaw offsets properly, although the steady forces are captured well.

# OPTIMAL STRUCTURAL CONTROL UNDER STOCHASTIC UNCERTAINTY: ROBUST OPTIMAL OPEN-LOOP CONTROL

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**Introduction.** In practice, e.g. in active structural control [4], and in optimal control of robots [1], optimal control problems depend on several random variables, such as random initial values, random dynamic parameters, random environmental parameters, random applied loadings/payloads, etc.. In order to obtain optimal controls most insensitive with respect to random parameter variations, hence, robust optimal control, the problem is modeled in the framework of optimal control under stochastic uncertainty: Minimization of the expected total costs arising along the trajectory, at the terminal time/point and from the control input subject to the dynamic equation and possible control constraints. As is well known, e.g., from model predictive control [3], optimal feedback controls, e.g. of *PD*- and *PID*-type, can be approximated very efficiently by optimal open-loop feedback controls. Optimal open-loop feedback controls are based on a certain family of optimal open-loop controls. Hence, for practical purposes it is sufficient to determine optimal open-loop controls only. Extending the construction for the deterministic case, stochastic optimal feedback control laws are constructed by taking into account still the random parameter variations of the control system. Thus, corresponding to deterministic open-loop feedback controls, *stochastic optimal* open-loop feedback controls are obtained by computing first stochastic optimal open-loop controls on the *remaining* time intervals  $t_b \leq t \leq t_f$  with  $t_0 \leq t_b \leq t_f$ . Evaluating then these controls at the corresponding intermediate starting time points  $t_b$  only, the stochastic optimal open-loop feedback control law is obtained.

**Stochastic optimal open-loop control.** For the computation of stochastic optimal open-loop controls at each starting time point  $t_b$ ,  $t_0 \leq t_b \leq t_f$ , the stochastic Hamilton function  $H$  of the optimal control problem under stochastic uncertainty is introduced. Then a  $H$ -minimal control (law) can be determined by solving a finite-dimensional stochastic optimization problem [2] for minimizing the conditional expectation (with respect to the information  $\mathcal{A}_t$  up to time  $t$ ) of the stochastic Hamiltonian subject to the remaining deterministic control constraints at each time point  $t$ . Having a  $H$ -minimal control, the related two-point boundary value problem with random parameters is formulated for the computation of the stochastic optimal state and adjoint state trajectory. In case of a linear-quadratic control problem, which arises often in engineering practice, the state and adjoint state trajectory can be determined analytically to a large extent. Inserting then these trajectories into the  $H$ -minimal control, stochastic optimal open-loop controls are found. Having a stochastic optimal open-loop feedback control on each remaining time interval  $t_b \leq t \leq t_f$  with  $t_0 \leq t_b \leq t_f$ , the stochastic optimal open-loop feedback control law follows then immediately by evaluation each of the obtained stochastic optimal open-loop control on  $t_b \leq t \leq t_f$  just at the corresponding initial time point  $t = t_b$ .

**Approximations** Several approximations for solving the occurring two-point boundary value problem are discussed. A central problem is here the construction of suitable approximations of the fundamental matrices related to the occurring system matrix of the dynamic equation. In the linear-quadratic case the  $H$ -minimal controls can be determined explicitly. Moreover, depending on the properties of the (random) system matrix  $A = A(t, \omega)$ , solutions of the Hamiltonian system can be found explicitly and in real-time. Thus, appropriate approximations with corresponding error estimates are considered as follows: i) Approximation of the system matrix  $A(t, \omega)$  on each remaining time interval  $t_b \leq t \leq t_f$  by the matrix  $A(t_b, \omega)$ , being constant with respect to time  $t$ . Then the fundamental matrices of the system and the adjoint system can be determined by means of the matrix exponential function. Real-time computations are possible. Moreover, error estimates are found by means of the perturbation theory of systems of ordinary differential equations. Generalizing this approach, we consider also the ii) Approximation of the system matrix  $A(t, \omega)$  on each remaining time interval  $t_b \leq t \leq t_f$  by matrices being piecewise constant with respect to time  $t$ .

- [1] K. Marti, *Adaptive Optimal Stochastic Trajectory Planning and Control (AOSTPC) for Robots*. In: Dynamic Stochastic Optimization, (Eds.: K. Marti, K., Y. Ermoliev, G. Pflug), Springer-Verlag, Berlin-Heidelberg-New York, 2004, LNEMS Vol. 532, pp. 155-206.
- [2] K. Marti, *Stochastic Optimization Problems*, 2nd edition. Springer-Verlag, Berlin-Heidelberg-New York, 2008.
- [3] J. Richalet, A. Rault, J.L. Testud, J. Papon, *Model Predictive Heuristic Control: Applications to Industrial Processes*. Automatica, 1978, 14, 413-428.
- [4] T.T. Soong, *Active Structural Control: Theory and Practice*. Longman Scientific and Technical, J. Wiley, New York, 1990.



# STRUCTURE PRESERVING ITERATIVE SOLUTION OF PERIODIC PROJECTED LYAPUNOV EQUATIONS

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**Abstract:** Simulations and analysis of periodic systems can be unacceptably expensive and time-consuming when the systems are very large. Hence, model reduction is an efficient tool which helps the scientists and engineers to replace the large periodic models by smaller models which are amenable to fast and efficient simulation and which still preserve the input-output behavior of the original large models as good as possible.

We consider the linear periodic time-varying (LPTV) descriptor system

$$E_k x_{k+1} = A_k x_k + B_k u_k, \quad y_k = C_k x_k, \quad k = 0, 1, \dots, K-1, \quad (1)$$

where  $E_k, A_k \in \mathbb{R}^{n \times n}$ ,  $B_k \in \mathbb{R}^{n \times m}$ ,  $C_k \in \mathbb{R}^{p \times n}$ ,  $x_k \in \mathbb{R}^n$  is the state vector,  $u_k \in \mathbb{R}^m$  is the control input, and  $y_k \in \mathbb{R}^p$  is the output. The coefficient matrices are periodic with a period  $K \geq 1$ . The matrices  $E_k$  are allowed to be singular for all  $k$ . Analysis of LPTV descriptor systems and their applications to model reduction are strongly related to the generalized projected periodic discrete-time algebraic Lyapunov equations (PPDALEs), for  $k = 0, 1, \dots, K-1$ ,

$$A_k X_k A_k^T - E_k X_{k+1} E_k^T = Q_l(k) B_k B_k^T Q_l(k)^T, \quad X_k = Q_r(k) G_k Q_r(k)^T, \quad (2)$$

where  $X_K = X_0$ , and  $Q_l(k), Q_r(k)$  are the spectral projectors corresponding to the  $k$ -th left and right deflating subspaces of the periodic matrix pairs  $\{(E_k, A_k)\}_{k=0}^{K-1}$  corresponding to the eigenvalue at infinity [1,2].

The numerical solution of (2) has been considered in [2,1] for time-varying matrix coefficients. All these methods are not suitable for large scale problems, because the computational complexity for solving such a Lyapunov equation (2) using direct methods is at least of order  $\mathcal{O}(Kn^3)$ , and they require extensive storage. Here we discuss the structure preserving iterative solution of the PPDALEs (2). Two algorithms have been presented. The first one works with the cyclic lifted representation of the corresponding PPDALEs, and the second algorithm works directly with the periodic matrix coefficients. A low-rank version of this method is also presented, which can be used to compute low-rank approximations to the solutions of PPDALEs. Both the algorithms are efficiently implementable for large-sparse periodic systems. Numerical results are given to illustrate the efficiency and accuracy of the proposed methods.

## References

1. E.K.-W. Chu, H.-Y. Fan, W.-W. Lin, *Projected generalized discrete-time periodic Lyapunov equations and balanced realization of periodic descriptor systems*. In: SIAM J. Matrix Anal. Appl., 2007, 3(29): 982-1006.
2. P. Benner, M.-S. Hossain, T. Stykel, *Model Reduction of Periodic Descriptor Systems Using Balanced Truncation*. In: Model Reduction in Circuit Simulation, (Eds.: P. Benner, M. Hinze, and J. ter Maten) Lecture Notes in Electrical Engineering, Springer-Verlag, Heidelberg, 2011, (74): 193-206.

# STABILIZATION OF UNKNOWN NONLINEAR SYSTEMS USING A COGNITION-BASED FRAMEWORK

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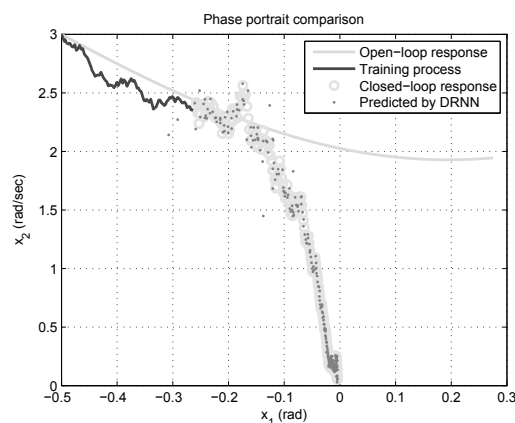
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This contribution considers an adaptive control method based on a cognition-based framework to stabilize unknown nonlinear systems in real time. Although important improvements have been made to deal with the control problem of unknown nonlinear system, the processes of both modeling and designing control input for different nonlinear dynamical systems are still mostly accomplished by humans. In order to solve this task, a cognition-based framework has been developed for the controller to stabilize the dynamical behavior of unknown systems. Using this framework, the controller requires neither the information about the systems dynamical structure nor the knowledge about system physical behaviors. The task is solved using only the system outputs, which are assumed as measurable.

The structure of the proposed framework is composed of four main elements: perception and interpretation, stability criterion, planning, and execution. The system to be controlled is as a part of the external environment. To realize this framework, a dynamic recurrent neural network (DRNN) has been selected in the element perception and interpretation, because it is able to identify system behavior in a predefined local time interval online without previously assumed knowledge about the systems and the environment [1]. The stability criterion is set up with data-driven quadratic stability criterion [2], which can establish a relationship between the system outputs and the stability of motion of the system in real time. In the framework above, state feedback control is utilized with the equation  $u(t) = -K(t)y(t)$ , which means that the procedure of defining actual system input  $u$  is the procedure of online searching a suitable state feedback gain  $K(t)$ . By using DRNN, the system outputs for the next predefined time interval can be predicted at the current time step, if the corresponding system inputs are known. That means, each possible state feedback gain can be used to generate control input and the corresponding control input can be judged whether it can lead the system stable during the predefined time interval using both DRNN and data-driven quadratic stability criterion. In this process, the most suitable state feedback gain can be determined using a suitable time-relevant criteria. With this control strategy, the system states for the next predefined time interval can always be planned at the current time step and the system stability is guaranteed by the stability criterion. The proposed controller is applied to the pendulum system described by

$$\begin{cases} \dot{x}_1(t) = x_2(t) \\ \dot{x}_2(t) = -10\sin(x_1(t) - \pi) - x_2(t) + u(t). \end{cases} \quad (1)$$

to demonstrate the successful application and performance of the method, as shown in the following figure.



Phase portrait of the pendulum system by using proposed controller

It is clear, that the desired control goal (the pendulum should be stabilized at its upper equilibrium point  $[0 \ 0]$ ) has been achieved by using the proposed method.

- [1] Parlos A.G., Rais O.T. and Atiya A.F.: *Multi-step-ahead prediction using dynamic recurrent neural networks*. Neural Networks, 13 (2000), 765–786.
- [2] Zhang F. and Söffker D.: *Quadratic stabilization of a nonlinear aeroelastic system using a novel Neural-Network-based controller*. Science in China Series E: Technological Sciences, 54 (2011), 1126–1133.

# A GEOMETRIC APPROACH OF THE CHEN'S SYSTEM

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The chaotic systems have been studied starting from the early 1960s by the help of Lorenz system. Since then, other chaotic attractors, such as the Chua's system, the Lü's system and so on, have been developed. In 1999, based on an engineering feed-back anti-control approach, Chen provided a new system, described by:

$$\begin{cases} \dot{x} = a(y - x) \\ \dot{y} = (c - a)x - xz + cy \\ \dot{z} = -bz + xy \end{cases} \quad (1)$$

$a, b, c \in R$ . The system is chaotic when  $a = 35, b = 3, c = 28$ . The question is if one can find other properties of this system which can give a different point of view from the old ones. The main goal of our work is to find a Hamilton-Poisson realization of the Chen's system and to point out some of its geometrical and dynamical properties from mechanical geometry point of view. Finding the Hamilton-Poisson realization for a given dynamical system could be a difficult problem; this consists in a space configuration, a constant of motion (the Hamiltonian,  $H$ ) and a Poisson structure ( $\Pi$ ), such as the system can be put into the following equivalent form:

$$\dot{x} = \Pi \cdot \nabla H \quad (2)$$

Being studied by different researchers, this realization has been made for a lot of dynamics in mechanics (the rigid body, the Lorenz 60 system, the Goryachev-Chapligyn top, the Rikitake system), in biology (the Lotka-Volterra system, the SIR system) or in economics (the Lagrange system). We are looking to find the specific conditions that produce a Poisson structure for the system (1). Since the phase portrait of the dynamics can hardly be found, establishing the Casimir's structure and considering the phase portrait as the intersection of the Hamiltonian and the Casimir of the structure is another important problem. Once the Poisson structure is established we can discuss stability problems (nonlinear stability of the equilibrium points) using energy-Casimir method, we can find the periodical orbits around the equilibrium states which are nonlinear stable (using Moser theorem) and we can make a comparison between the phase portrait obtained as the intersection between the Hamiltonian and the Casimir and some numerical integrators (Kahan's integrator and Runge-Kutta 4 steps one). Numerical simulations using MATHEMATICA 8.0 are presented, too.

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# A BOND GRAPH SWITCHING OBSERVER FOR SWITCHING LINEAR SYSTEMS

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**Introduction.** The investigation of dynamic hybrid systems is not motivated only because many real systems exhibit hybrid behaviours, but also because the control of many complex systems is only possible through a combination of classical continuous control laws with logic command. Among the issues to be addressed, building observers is particularly important for control. In this paper, we will consider the state estimation of the continuous part of switched systems assuming that the discrete state is always available. Using the bond graph tool, we proposed a graphical method to design a switched Luenberger observer. The bond graph is used for modelling (physical system and observer), for structural analysis (outputs redundancy, observability, stability) and for symbolic calculus of the observer gain matrices.

**Problem statement.** Switched linear systems, can be modelled by (1)

$$\begin{cases} \dot{X} = A_{q_i} \cdot X + B_{q_i} \cdot U \\ Y = C_{q_i} \cdot X \end{cases} \quad (1)$$

$X \in R^n$ ,  $U \in R^m$  and  $Y \in R^p$  are respectively state, control and output vectors.  $q_i, i \in \{1, 2, \dots, s\}$  represents the modes of the system.  $A_{q_i}$ ,  $B_{q_i}$  and  $C_{q_i}$  are respectively state, control, and output matrices in mode  $i$ .  $(q_i, x_i)$  is the hybrid state of the system in mode  $i$ . It is assumed that the switching law is known. The general structure of a hybrid observer consists of a discrete observer estimates the discrete mode and a continuous observer provided the state estimation of the continuous part of the hybrid system. In this work we assume that the discrete mode is available and we only estimate the continuous state and we propose the switched Luenberger observer. A full order Luenberger observer is a set of switched continuous observers, including the convergence of the global error. The observer and the error ( $e = x - \hat{x}$ ) are respectively given by (2) and (3).  $K_{q_i}$  is the matrix gain in mode  $i$ .

$$\begin{cases} \dot{\hat{x}}(t) = A_{q_i} \hat{x}(t) + B_{q_i} u(t) + K_{q_i} (y(t) - \hat{y}(t)) \\ \hat{y}(t) = C_{q_i} \hat{x}(t) \end{cases} \quad (2)$$

$$\dot{e} = (A_{q_i} - K_{q_i} C_{q_i}) e \quad (3)$$

The behaviour of the dynamics of the error is similar to that of a switching linear system. The stability of a switching system cannot be deduced from that of each mode. Indeed a switching system may be unstable, while all modes are stable and stable while all modes are unstable. This highlights the importance of the discrete part of the stability of the hybrid system. Indeed, its interaction with the continuous part can stabilize or destabilize the system. The bond graph approach has been used to study this problem based on energy considerations [2]

**Bond graph approach for hybrid observer design.** The bond graph approach was used for the synthesis of observers in the case of continuous linear systems [3], [1]. By using the results of [1] we propose a switched full order Luenberger observer for the reconstruction of the continuous state of the switching systems. Using the bond graph approach for the synthesis of an observer allows us to free ourselves of complex calculations, since it allows to use only the graph for analysis as well as for the symbolic computation of earnings. It also allows to use only one bond graph model of the switched observer to all modes. Only the gains change each switch. In the proposed switched bond graph Luenberger observer design, the bond graph is used for modelling (initial system and observer (step3)), for structural analysis (output redundancy (step 1), observability (step 2) and stability (step 5)) and for symbolic computation of observer gains (step 4). This method is based on graphical manipulations directly on the bond graph model without calculating and using only causality and causal paths. The proposed observer is tested on a physical example.

- [1] Pichardo-Almarza C., A. Rahmani, G. Dauphin-Tanguy et M. Delgado :Luenberger Observers for Linear Time Invariant Systems Modelled by Bond Graphs. *Journal of Mathematical and Computer Modelling of Dynamical Systems volume 12, n°2-3, avril-juin 2006, Ed taylor and Francis.*
- [2] Junco S, Rahmani A, Hihi H et Donaire A :On the stability of class of switched bond graphs. *ECMS2008, 3-6 June, NICISIA Cyprus, 2008*
- [3] Karnopp D :Bond graph in control: Physical State Variables and Observers. *Journal of the Franklin Institute, Vol.308 No.3, (1979), 221-234.*

# SYMBOLIC POLYNOMIAL TOOLS FOR NONLINEAR CONTROL SYSTEMS

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**Polynomial method in nonlinear control** Over the last decade the theory of non-commutative polynomial rings [1] has been frequently applied in the studies of nonlinear control systems. For that to be possible, the control system, or rather its 'tangent linearized model', has to be described by two polynomial matrices with their elements from the non-commutative ring of Ore polynomials that act on input and output differentials. Consider a multi-input multi-output nonlinear system, described by the set of higher order input-output differential equations, relating the inputs  $u_j$ ,  $j = 1, \dots, m$ , the outputs  $y_i$ ,  $i = 1, \dots, p$ , and their time derivatives:

$$y_i^{(n_i)} = f_i(y_r, \dots, y_r^{(n_{ir}-1)}, u_k, \dots, u_k^{(r_{ik})}, r = 1, \dots, p, k = 1, \dots, m), i = 1, \dots, p.$$

The above system can be represented in the form  $P\left(\frac{d}{dt}\right)dy = Q\left(\frac{d}{dt}\right)du$ , where  $P\left(\frac{d}{dt}\right)$  and  $Q\left(\frac{d}{dt}\right)$  are polynomial matrices, with their elements  $p_{ij}\left(\frac{d}{dt}\right)$  and  $q_{ij}\left(\frac{d}{dt}\right)$  in the Ore polynomial ring. Polynomial approach has been used to examine numerous modelling, analysis and synthesis problems of nonlinear control.

**Advantages of the polynomial method** Polynomial method has several advantages, if compared with the earlier method, based on the differential one-forms. The most powerful argument is computation speed - the programs taking advantage of the polynomial methods are able to produce the results remarkably faster than those based only on the approach of the vector spaces of the differential one-forms. Moreover, the program code of the polynomial solution is shorter and more compact, reflecting the fact that polynomial approach allows to express the solutions of the modelling problems via explicit formulas, whereas the approach of one-forms provides only the algorithms for the solution. What is also important, these explicit formulas coincide with the respective formulas used in the theory of linear systems, except that in linear case the coefficients of the polynomials are real numbers, the polynomials are applied to the variables  $u$  and  $y$  rather than their differentials and in the nonlinear case the integration is required, when coming back from the level of polynomials to the level of equations. This brings along the integrability restrictions, because integration is not always possible. This similarity makes the nonlinear system theory easier to understand to the people previously familiar (only) with linear systems.

**The developed software** We have developed a collection of *Mathematica* functions for solving the modelling problems of nonlinear control systems, based on the theory of Ore polynomial rings. The first part of the software includes the functions that implement the basic operations with Ore polynomials, since there is neither built-in functions nor supplement package available for *Mathematica*, addressing these operations. These basic functions include addition and multiplication, the left(right) quotient and remainder, the greatest common left(right) divisor and the least common left(right) multiple. Some functions are extended to the matrices with their elements from Ore polynomial rings. Rational expressions of Ore polynomials and the computations with them are also supported. The second part contains the programs for solving modelling problems by polynomial method. The function `Realization` checks whether the system given by the set of input-output equations can be transformed into the classical state-space form and in case of the confirmative answer finds the state equations. The function `Reduction` finds, if possible, for the system described by the set of input-output equations, a new, lower order representation, being transfer equivalent to the original set of equations. The transfer function/matrix of the nonlinear system may be found by using `TransferFunction`. The function `TransferEquivalent` allows to check the transfer equivalence of control systems described either by input-output or state equations. Finally, the model-matching problem is addressed, that is, for the given system  $F$ , the feedforward and feedback compensators can be found, such that compensated system coincides with the given system  $G$ , using respectively the functions `FeedForwardCompensator` and `FeedbackCompensator`. All functions are designed to work with both continuous- and discrete-time systems.

**Nonlinear control package and website** The above functions are part of our previously developed *Mathematica* package `NLControl`, devoted to modelling, analysis and synthesis problems of nonlinear control systems [2]. The developed programs are made partly available on `NLControl` web site and can be found at <http://webmathematica.cc.ioc.ee/webmathematica/NLControl/poly>. The main benefit of the web site is that one does not need *Mathematica* to be installed into local computer, only internet connection and browser are necessary.

- [1] Abramov S.A., Le H.Q., and Li Z. *Univariate Ore polynomial rings in computer algebra*. Journal of Mathematical Sciences, 131(5), 2005, 5885–5903.
- [2] Tönso M., Rennik, H., and Kotta Ü. *Webmathematica based tools for discrete-time nonlinear control systems*. Proceedings of the Estonian Academy of Sciences, 58(4), 2009, 224–240.



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## BIFURCATIONS IN MATHEMATICAL MODELS OF NICHE CONSTRUCTIONS

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A question of “how much overconsumption a renewable resource can tolerate”, which is related to a phenomenon known as “the tragedy of the commons”, is addressed using a mathematical model, where individuals in a population not only compete for the common resource but can also contribute to its restoration. The considered model can realize one of two pure strategies for interaction with the resource, namely using the resource to increase proliferation or to increase environmental capacity and become better competitors, with a full spectrum of possible intermediate strategies. Through bifurcation analysis a threshold of system resistance to over-consumers (individuals that take more than they restore) was identified, as well as a series of transitional regimes that the population goes through before it exhausts the common resource. We observe that just knowing the rules according to which the interactions occur is not enough to make accurate predictions about which strategy will come to dominate; one also needs to know the initial composition of the population. We also come to the conclusion that within the frameworks of the model there is no optimal strategy to avoid the tragedy of the commons.

- [1] Kareva I., Berezovskaya F., and Castillo-Chavez C.: *Niche Construction and Sustainability in Resource-Dependent Competition Models*. Journal of Mathematical Biosciences (in press).
- [2] Krakauer D.C., Page K.M., and Erwin D.H.: *Diversity, dilemmas, and monopolies of niche construction*. The American naturalist, 173 (2009), 26-40.
- [3] Karev G.: *On mathematical theory of selection: continuous time population dynamics*. Journal of Mathematical Biology, 60 (2010), 107-129.

# MATHEMATICAL MODELLING OF THE ANAEROBIC DIGESTION INCLUDING THE SYNTROPHIC ACETATE OXIDATION

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**Introduction.** Anaerobic digestion (AD) is an effective biotechnological process for treatment of different agricultural, municipal and industrial wastes. It combines environmental depollution (ecological aspect) with production of renewable energy – biogas (energy aspect). However, AD is known as a very complicated and unstable process in regard to the biogas reactors operation. This is due to the complicated interactions between different microbial species as well as of the complex transformations of the organic matter affected by a variety of environmental factors. In this context use of mathematical models is a powerful tool for investigations and optimisation of the AD [1, 2, 3].

In this paper a new mathematical model of the AD of activated sludge, including the syntrophic acetate oxidation process, is presented and verified both by laboratory experiments in continuously stirred tank reactor (CSTR) and by computer simulations. Parameters optimization, numerical simulations and analytical determinations of the static characteristics of the model were performed using Simulink, Optimisation and Symbolic Toolboxes of Matlab.

**Laboratory experiments.** A laboratory scale anaerobic CSTR with working volume of 2 dm<sup>3</sup>, equipped with system for automatic maintenance of constant stirring and mesophilic temperature (34 ± 0.5 °C) was used. The reactor was fed once daily. During the experiments samples for analysis of glucose, volatile fatty acids (VFA) and ammonia were taken out.

**Mathematical model.** The model consists of thirteen ordinary differential equations, describing the mass balances of the main stages of this process. Four new ODE, describing the acetate oxidation and the hydrogenotrophic methanogenesis, were developed. Additional parts, describing the acetate consumption from the acetate oxidizers and the dead cells lysis resulting in soluble organics, were included in the model equations. The model calibration was made using experimental data starting from known parameters values. For this purpose the changes in the concentrations of ammonia, glucose, propionate, acetate and biogas yield after pulse addition of ammonia (with amplitude corresponding to 0.5 g/L) to the feeding substrate were studied. A great number of optimisation procedures and computer simulations were performed in order to receive good coincidence between laboratory and computational data. After the calibration the model verification was performed, using pulse addition of ammonia with amplitude equal of 0.75 g/L. The comparison between laboratory and simulation data was shown that the calibrated model reflects well the process kinetics.

Analytical study of the model was performed obtaining the static characteristics of the process (Fig. 1).

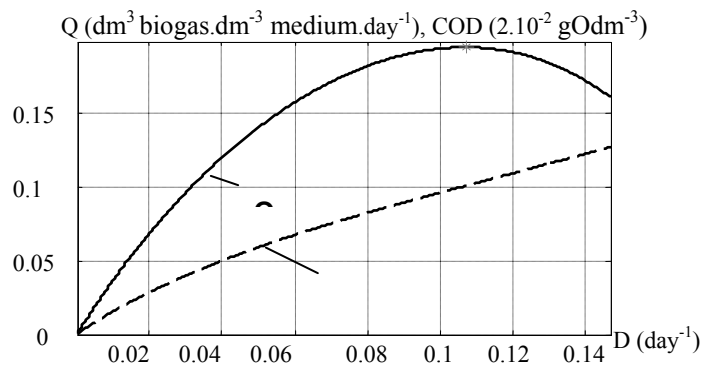


Fig. 1. Static input-output characteristics  $Q=Q(D)$  and  $COD = COD(D)$  of the model

It is evident that maximum of the function  $Q=Q(D)$  exists, which is in accordance with previously known results for simplest models [3]. The following important parameters were calculated:  $D_{sup}=0.147$  (day<sup>-1</sup>), above which the microorganisms will be washed out ( $0 < D < 0.147$  (day<sup>-1</sup>));  $D_{max}=0.1072$  (day<sup>-1</sup>) at which  $Q$  obtain maximal value  $Q_{max}=0.195$  (dm<sup>3</sup> gas.dm<sup>-3</sup> medium.day<sup>-1</sup>).

[1] Angelidaki, L., Ellegaard, L. E., Ahring, B. K. (1993). *Biotech.Bioeng.*, 42, 159-166.

[2] Dochain, D., Vanrolleghem P. (2001). *Dynamical Modelling and Estimation in Wastewater treatment Processes*. IWA Publishing, UK.

[3] Simeonov I. (2010). Chapter 2. Modelling and control of the anaerobic digestion of organic wastes in continuously stirred bioreactors. In Tzonkov S. (ed.), *Contemporary approaches to modeling, optimization and control of biotechnological processes*, 41-76. Prof. Marin Drinov Acad. Publ. House, Sofia.

# DISTRIBUTED MODELING AND PARAMETER ESTIMATION OF INFLUENZA VIRUS REPLICATION DURING VACCINE PRODUCTION

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In influenza vaccine production the use of permanent mammalian cell lines becomes more and more important. Besides sophisticated cell culture technologies and downstream processing methods, mathematical modeling plays a crucial role in improving production efficiency. Most notably for analysis, experimental design and optimization of the process, the benefit of combining extensive experiments with mathematical modeling approaches becomes apparent.

Heterogeneity of the cell population with respect to single cell characteristics gives rise to a distributed modeling approach. In the present contribution, a degree of fluorescence is introduced as an internal coordinate. It is proportional to the amount of viral NP protein in the cells and can be interpreted as degree of infection. The corresponding fluorescence distributions can be measured directly with flow cytometry. In our previous work, the replication of equine influenza A virus in Madin-Darby canine kidney (MDCK) cells was investigated in either deterministic [1] or stochastic [2] modeling frameworks. More recently, focus was on replication of human influenza A strains in MDCK cell cultures [3]. Interesting new phenomena in the distribution dynamics could be observed, like transient multimodality and reversal of propagation. In a first step, a model was derived that uses three hyperbolic partial differential equations describing the fluorescence distributions of uninfected, infected and apoptotic cells. Apoptosis is programmed cell death, which can be activated by a large variety of external and internal stimuli, in particular by viral infection. It invariably leads to cell lysis and has major influence on the process productivity. In addition, the system of PDEs is coupled to two ordinary differential equations that depend on integral quantities of the distributed species. These equations describe active and inactive virions in the medium, which is considered to be ideally mixed. The model includes the kinetic processes of infection, replication of virions, release of virions, apoptosis and cell death. The kinetic parameters were assumed to be constants or linearly dependent on the internal coordinate. In the present contribution a more detailed model is considered in which the kinetic parameters may also depend nonlinearly on the internal coordinate. In addition, the model is extended by a time-delay between the infection of the cells and the replication or release of the virions, respectively. This delay describes a lag period in which a cell changes its “mode” to virus production.

Kinetic parameters are determined from experimental data. Beside time resolved fluorescence distributions obtained by flow cytometry, the concentration of active virions and the total concentration of virus particles are monitored. In order to adapt the model to the measurements an infinite dimensional inverse problem has to be solved as the kinetic parameters depend on the internal coordinate. We follow the approach presented in [4] to translate the problem into finite dimension. Each fluorescence-dependent parameter is approximated by a hermite spline with a specific number of nodes. Hence the values of the constant kinetic parameters and the spline nodes can be obtained in a weighted least squares estimation framework. For a spline representation with two nodes a linear parameter function is obtained. In contrast to this, a spline representation with three nodes yields a non-linear parameter dependency. For more complex parameter functions with more than three nodes the parameter estimation became ill posed resulting in multiple local minima. Results of the estimation procedure for nonlinear dependencies of the parameters on the internal coordinate are compared to results for linear dependencies. It is shown that the model can be adapted adequately to the data in both cases. However, even a simple nonlinear approach using a three node representation of the distributed parameters improves the fit of the distribution dynamics particularly for late sampling instants.

- [1] T. Müller, J. Schulze-Horsel and Y. Sidorenko and U. Reichl and A. Kienle. *Population balance modelling of influenza virus replication during vaccine production*. In: Proc. 18st European Symposium on Computer Aided, 2008, 133-138.
- [2] Y. Sidorenko, J. Schulze-Horsel, A. Voigt, U. Reichl and A. Kienle. *Stochastic population balance modeling of influenza virus replication in vaccine production processes*. Chemical Engineering Science, 1 2008, (63): 157 - 169.
- [3] T. Müller, R. Dürr, B. Isken and J. Schulze-Horsel, U. Reichl and A. Kienle. *Population balance modelling of influenza virus replication during vaccine production - Influence of apoptosis*. In: Proc. 21st European Symposium on Computer Aided Process Engineering, 2011, 1336 - 1340.
- [4] T. Luzyanina, D. Roose and G. Bocharov *Distributed parameter identification for a label-structured cell population dynamics model using CFSE histogram time-series data*. Journal of Mathematical Biology, 5 2009, (59): 581 - 603.

# EMOTION IDENTIFICATION AND MODELLING ON THE BASIS OF PAIRED PHYSIOLOGICAL DATA FEATURES FOR COMPANION SYSTEMS

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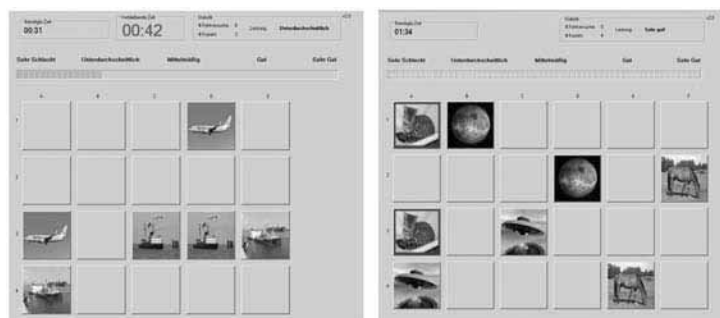
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**Introduction.** Emotion recognition on the basis of physiological data is a topic of great interest, especially in the research of adaptive Human-Computer Interfaces. There are many approaches and systems presented in numerous publications. Physiological responses that are typically assessed for this purpose are the cardiovascular system, by recording the electrocardiography (ECG) or the peripheral blood volume (BVP), the electrodermal system, by measuring the skin conductance (SC), the facial expressive system, by recording the electromyography (EMG) of the *corrugator supercilii* and the EMG of the *zygomaticus major* and the respiratory system, by measuring respiratory excursion. A technical companion system should be able to detect its user's emotion and model the user's emotional state in order to react to it accordingly. We have developed a novel method to determine a user's most significant emotional change in the two emotion dimensions of pleasure and arousal on the basis of paired data features of physiological data when comparing two events. An experiment was set up where participants first viewed blocked IAPS picture presentations and then took part in a memory training wizard-of-oz scenario. Six meaningful features from four physiological channels of the IAPS picture presentation data - containing two electromyography channels (*corrugator supercilii* and *zygomaticus major*), skin conductance and peripheral blood volume - were extracted. Three pairs of features were found to contain valuable information about emotional changes when comparing two situations with different emotional contents. The method was then tested on a new blocked IAPS dataset and on the wizard-of-oz interaction scenario dataset to verify its performance.

**Experiments.** First, blocked IAPS pictures were shown to 20 subjects. Then, a memory training wizard-of-oz-experiment was performed. In this experiment, the participants had to solve a memory training task. In each of the six experimental sequences (es 1-6) a number of hidden pictures was presented. The task was to uncover all matching card pairs. The whole interaction was controlled by voice. The goal of the manipulation was to induce certain emotions in certain parts of the experiment, such as the state of high pleasure and low arousal in the experimental sequence 6 and the state of low pleasure and high arousal in experimental sequence 4.

**Emotion Identification.** For all 20 subjects, after a feature extraction and baseline calculation and subtraction, the feature values of 'low arousal' were subtracted from the feature values of 'high arousal' to determine the feature tendencies of all six features when the dimension of arousal decreases. To determine the feature tendencies of all six features when the dimension of pleasure increases, the physiological data of 'low pleasure' was subtracted from the physiological data of 'high pleasure'. The tendencies of three feature pair changes were analysed analysed in those affect changes. On the basis of these empirical findings, a method was designed which will identify the strongest emotion out of the four emotional states 'relaxed', 'tensed', 'positive' and 'negative' with each of three modules. A majority voting of the three module decisions will determine the most significant emotional change. This approach derives, unlike the 'affective computing methods' like for example [1], from the 'basic research' approaches, as can be seen in [2].

- [1] K. H. Kim, S. W. Bang and S. R. Kim: *Emotion recognition system using short-term monitoring of physiological signals*. In: Medical and biological engineering, 2007
- [2] Sylvia D. Kreibig, Frank H. Wilhelm, Walton T. Roth and James J. Gross: *Cardiovascular, electrodermal and respiratory response patterns to fear- and sadness-inducing films*. In: Psychophysiology, 2004



The subject's screen in the experimental sequences 4 (es04) and 6 (es06) of the wizard-of-oz-experiment. The induced emotions were 'low pleasure, high arousal' in es04 (left) and 'high pleasure, low arousal' in es06 (right).

# DETERMINATION OF TIME DURATION OF POLYMER PARTICLE COLLISIONS IN FLUIDIZED BED USING DISCRETE ELEMENT METHOD

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**Introduction.** Collision behaviour of particles in the fluidized bed polymerization reactor and determination of the corresponding collision time duration were analysed using Discrete Element Method (DEM). Unwanted agglomerations and disintegrations of polymer particles cause various problems in gas- and liquid dispersion reactors for catalytic polymerization and in the down-stream processing of polymer particles. The description of collisions of polymer particles is based on the evaluation of the force interactions among individual particles belonging to the statistically characterized set and of the hydrodynamic conditions in the polymerization reactor.

**DEM representation of particle collision.** Colliding polymer particles in the DEM representation consist of individual mutually force interacting discrete elements. The trajectory of each discrete element is given by the numerical solution of the second Newton's law of movement. Binary force interactions between neighbouring discrete elements were assumed. The binary connection is established when the distance of discrete elements is less than or equal to the sum of their radii and is broken after the distance of discrete elements exceeds a prescribed value of maximum elongation. Collisions of two polymer particles result in three possible mechanisms: reflection, disintegration and agglomeration. The reflection occurs if the repulsive forces prevail the attractive ones. Then all inter-particle connections are broken after the connected discrete elements exceed prescribed maximum separation distance. In the case of particle disintegration some connections between discrete elements from the same polymer particles are broken as the consequence of the collision. The agglomeration proceeds in the case of the adsorption of the repulsive impulse by adhesive forces.

**Sub-algorithms needed for DEM.** The individual steps of the main algorithm of DEM are based on the following computational sub-algorithms: the algorithm for tracking positions and velocities of individual micro-elements, the algorithm for detecting particle pairs, and the algorithm for calculating micro-elements collision behaviour. It is apparent that the increasing complexity of these sub-algorithms results in the dramatic increase of computational time. For realistic simulations it is necessary to balance a complexity of the algorithms used and a reasonable duration of the simulation.

**Evaluation of the duration of the polymer particle collision.** The collision time was evaluated as the time period for which there exists at least one force connection between discrete elements from different colliding particles. The collision time for particles having the realistic size was determined by the extrapolation of the data obtained for smaller particles because of the limited number of discrete elements in the DEM simulation (due to the computational feasibility). The effects of the particle size, contact area between colliding particles and their mutual position on the time duration of the collision were investigated. The collisions of two-phase copolymers were also modelled. The copolymer particle was assumed to consist of discrete elements of 'hard' brittle and 'soft' sticky phases. The effect of various arrangements of both phases in the copolymer particle on the collision time was estimated.

**Comparison of the characteristic time scale of acting of adhesive forces with the collision time.** The agglomeration of polymer particles is caused by various adhesion forces (e.g. liquid-bridge force and the force reflecting entanglement of polymer chains) acting non-instantaneously, but at a characteristic time scale. Characteristic time of the liquid bridge formation and of the chain entanglement was compared to the collision time obtained by simulations of collisions of polymer particles. The result of the comparison is that the duration of the particle collision is long enough for application of these adhesive forces and thus for the formation of the particle agglomerate.

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## MULTISCALE MODELING OF BIOPOLYMER PRODUCTION IN MULTICELLULAR SYSTEMS

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Poly( $\beta$ -hydroxybutyrate) (PHB) is an organic polymer, which can be synthesized by many microorganisms. PHB serves as internal energy and carbon reserve material and provides an attractive source of bioplastics, that are biodegradable, biocompatible and do not depend on fossil resources. The production of PHB is favored under limitation of key nutrients such as nitrogen, phosphate or oxygen and can be degraded if these nutrients are available.

Homogeneity/heterogeneity of PHB production in multicellular systems is measured by means of flow cytometry and fluorescence microscopy. Depending on the organism different patterns of behavior are observed. For *Ralstonia eutropha*, which is an already established PHB producer, a homogeneous PHB distribution was measured. In contrast to that, *Rhodospirillum rubrum* shows interesting heterogeneous behavior. *Rhodospirillum rubrum* is a facultative photosynthetic microorganism and offers new perspectives for biotechnological biopolymer production. Experimental data from flow cytometry and microscopy for *Rhodospirillum rubrum* reveal transient bimodal population dynamics in a batch reactor indicating bistability on the single cell level. An initially homogeneous population is segregating into a first subpopulation with only little amount of PHB and a second subpopulation with relatively high amount of PHB. Both subpopulations are merging again at later time points to build a homogeneous population again.

To gain a deeper understanding of biopolymer production in multicellular systems a multiscale modeling approach is applied. In a first step single cell kinetics are described by a state of the art hybrid cybernetic model (HCM), which assumes optimal regulation in view of limited resources. The HCM allows a systematic derivation of the model equations from elementary mode analysis [3]. It is based on quasistationarity of internal metabolites, which are eliminated from the model equations. However, PHB is an internal metabolite. Hence, the HCM approach was extended to take dynamics of few internal metabolites explicitly into account, while for most of the internal metabolites the quasi-steady state approximation is still applied [1].

The single cell model is then used for nonlinear analysis and the occurrence of multiple states is discussed. Based on the single cell model a population balance model is developed, which includes cell internal regulation by means of cybernetic variables. However, since most state variables of the HCM will translate into internal coordinates of the population balance model the single cell model has to be reduced. This is done by using the lumped hybrid cybernetic modeling approach (L-HCM) [2] and by approximation of enzyme levels. Depending on available substrates and position in space of internal coordinates the population balance model is therefore able to switch between growth and PHB synthesis.

The application of the multiscale modeling approach is first demonstrated for *Ralstonia eutropha*. Good agreement between experimental data and theoretical results is shown.

Currently the multiscale modeling approach is extended to *Rhodospirillum rubrum*.

- [1] A. Franz, H.-S. Song, D. Ramkrishna, and A. Kienle. Experimental and theoretical analysis of poly( $\beta$ -hydroxybutyrate) formation and consumption in *Ralstonia eutropha*. *Biochem. Eng. J.*, 55(1):49–58, 2011.
- [2] H. S. Song and D. Ramkrishna. Prediction of metabolic function from limited data: Lumped hybrid cybernetic modeling (L-HCM). *Biotechnol. Bioeng.*, 106(2):271–284, 2010.
- [3] J. Stelling, S. Klamt, K. Bettenbrock, S. Schuster, and E. D. Gilles. Metabolic network structure determines key aspects of functionality and regulation. *Nature*, 420(6912):190–193, 2002.

# VIRTUAL-LAB OF A CEMENT CLINKER COOLER FOR OPERATOR TRAINING

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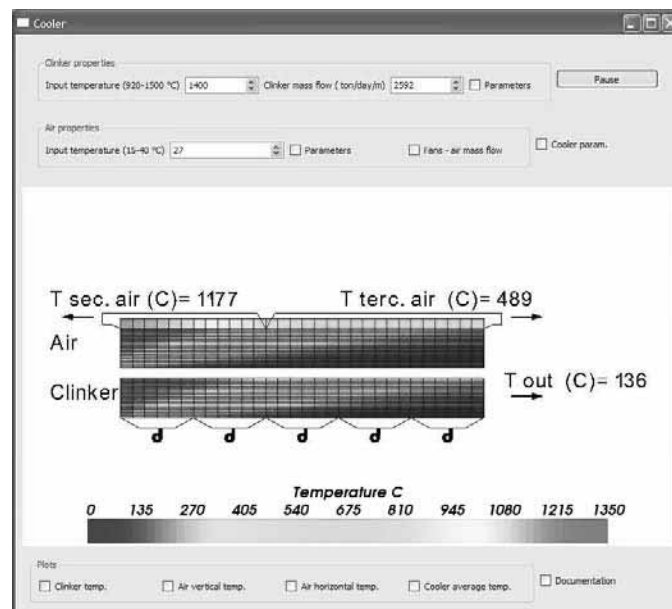
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Plant operator training plays a fundamental role in improving the energy efficiency of the the cement manufacturing process and reducing CO<sub>2</sub> emissions. In particular, proper operation of the clinker cooler is crucial in a cement industry. On one hand, the characteristics of the cooling process (e.g., residence time and temperature gradient of the clinker) strongly affect the clinker quality and, consequently, the properties of the produced cement. On the other hand, the energy efficiency of the clinker manufacturing process depends on how the cooler is operated.

A virtual-lab of a clinker grate cooler, intended for training of cement plant operators, has been developed. The grate cooler model, derived from first principles, is primarily based on the model described in [1]. The model, programmed in Modelica and simulated using Dymola, has been validated consulting cement industry experts, and comparing the simulated results with published data and available information from cement industries.

The applied procedure for virtual-lab implementation is based on the application of the following methodologies and software tools: (1) a systematic methodology [2] that facilitates to transform any Modelica model into a formulation suitable for interactive simulation; (2) a free Modelica library, named *Interactive* [3], that allows performing the object-oriented description of the virtual-lab view and the set up of the complete virtual-lab; and (3) the Dymola modeling environment, used to translate the Modelica description of the virtual-lab into an executable file. The *Interactive* Modelica library can be freely downloaded from <http://www.euclides.dia.uned.es/>

This approach, that facilitates the description of virtual-labs using only the Modelica language, has the following three main advantages. Firstly, existing Modelica libraries and models can be employed to develop virtual-labs. If new models need to be programmed, the use of Modelica reduces considerably the modeling effort. Secondly, as the complete virtual-lab is described in Modelica, virtual-lab developers don't need to use programming languages and the source code of the virtual-labs can be exchanged easily. Finally, the executable code of the virtual-lab can be easily distributed to the virtual-lab users, who don't need to install any additional software to run the virtual-lab. The main window of the virtual-lab is shown below.



Main window of the grate cooler virtual-lab.

- [1] K. Mujumdar and V. Ranade. *Modeling of rotary cement kiln*. VDM Verlag Dr. Müller, 2009.
- [2] C. Martín-Villalba, A. Urquía, and S. Dormido. An approach to virtual-lab implementation using Modelica. *Mathematical and Computer Modelling of Dynamical Systems*, 14(4):341–360, 2008.
- [3] C. Martín-Villalba, A. Urquía, and S. Dormido. Development of virtual-labs for education in chemical process control using Modelica. *Computers & Chemical Engineering*, doi:10.1016/j.compchemeng.2011.10.010, 2011.

## EXTENSION OF A THERMAL SIMULATION MODEL FOR A TRAM AND SIMULATION WITH ON-SITE MEASUREMENT DATA

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**Introduction.** Nowadays, HVAC systems are state of the art in buildings and cars. To compete with private transport, public transport operators have followed the trend and started to equip local public transport vehicles (like metros and trams) with HVAC systems. HVAC systems in trams can consume up to 10% of the whole electrical energy during the vehicle life cycle [1] and about one third of the total consumed energy during operation [2].

Only dynamic simulation models, where all relevant factors are considered, enable the simulation of energy consumption and passenger comfort [3]. An (existing) thermal simulation model of a tram is extended using on-site measurement data which were collected in Vienna by a tram.

**Existing Model** In the existing model various environmental conditions like outdoor air, radiation of the sun, wind speed and thermal load from passengers are considered [3]. The measured indoor air temperature is compared against the given set-point value by the controller and a control signal is calculated. The supply air is conditioned according to the control signal by the HVAC unit and blown into the vehicle body. With the supply air and environmental conditions a new indoor air temperature can be calculated. Therefore, the simulation model consists of three models: *a*) a controller, *b*) an HVAC and *c*) a vehicle model. The parameters of the model were achieved from climatic wind tunnel experiments. On-site measurement data was used to extend the existing simulation model.

**Model Extensions** The model is extended with the effect of the doorway during station stops and the indoor air temperature set-point is recalculated. The open doors have an effect on the indoor air, because indoor air is replaced with outdoor air. Explicit measurements are not possible due to security and vandalism concerns. The correction value was estimated using particle swarm optimisation.

The temperature set-point curve is derived from EN 14750-1. Closed loop simulation results of the indoor air temperature showed significant deviations from measurement results. An explanation is, that the actual set-point is modified by a further unknown effect. Parameters of the actual set-point function are estimated with a least-squares algorithm.

**Simulation** MATLAB is used as simulation platform. Measurement data were provided, sampling time is 10s. One measurement day lasts for about 20 hours. Simulation of a whole measurement day takes about 6-10 min (including pre- and post processing) on a single core processor.

- [1] Struckl, W. M. *Green Line - Umweltgerechte Produktentwicklungsstrategien für Schienenfahrzeuge auf Basis der Lebenszyklusanalyse des Metrofahrzeuges Oslo*. PhD thesis, Vienna University of Technology, 2007
- [2] Haller, G. and Kreitmayer, M. *Climatic wind tunnel test for higher energy efficiency*. In: Railvolution, M-Press plus, 38 - 40
- [3] Hofstädter, R. N. and Kozek M. *Holistic Thermal Simulation Model of a Tram*. Conference on Computer Modelling and Simulation, proceedings, Brno, 2011.



# CALIBRATION OF A DYNAMIC MODEL OF A FULL SCALE WASTEWATER TREATMENT PLANT FOR PREDICTION OF THE POTENTIALS OF COMBINED IN-LINE HYDROLYSIS WITH PREDENITRIFICATION

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**Introduction.** The Klagshamn municipal wastewater treatment plant (WWTP) in Sweden uses mechanical and chemical treatment as the primary treatment step. Thereafter, carbon is removed and ammonium is converted into nitrate in the activated sludge (AS) process. Nitrogen removal occurs in a subsequent moving-bed biofilm reactor (MBBR<sup>TM</sup>) with ethanol as an external carbon source. In 1998, a study predicted that the Klagshamn WWTP would reach its maximum capacity for nitrogen within 15 years due to the increasing number of connected households. A possible extension of the MBBR<sup>TM</sup> volume or carrier-filling degree was determined to be too costly. Converting the WWTP into a chemical-free plant that could provide the required capacity is a major challenge. Therefore, Jönsson et al. [1] investigated the predenitrification potentials by applying primary sludge hydrolysis. To reduce the nitrogen load into the MBBR<sup>TM</sup>, between 12.5% and 25% of the AS volume could be used for denitrification and 50% of the external carbon source could be saved. To determine the corresponding values in a full-scale application, dynamic variations such as flow, temperature and wastewater compound concentrations are needed.

Dynamic wastewater modelling was able to effectively evaluate the AS process on other full-scale WWTPs and applied to simulate possible scenarios for the Klagshamn WWTP. However, due to cost and time limitations, the characterisation of the wastewater compositions and variations are less satisfactory when modelling over a full year of operation. In addition, the Swedish Environmental Protection Agency stipulates that wastewater should be sampled on a 24 h flow-proportional basis, resulting in a limited number of samples that can be used for plant control. Therefore, the amount of analysed wastewater compounds can vary and lead to limited data on some of the main wastewater components. A method for generating reasonable estimates of the missing wastewater compound concentrations over the course of a year needs to be established.

**Methods.** The full-scale properties of Klagshamn WWTP were applied to the wastewater treatment simulation tool EFOR [2] based on the Activated Sludge Model (ASM) 2d [3]. To reflect the measured data (including hydraulic variations), the model was empirically calibrated to match the actual suspended solid (SS) measurements in the AS and the secondary settler. The wastewater treatment plant properties, process adjustments, and the wastewater treatment model that was implemented described as the reference scenario.

Linear regression was performed to estimate the missing values and establishing a complete annual time series of the incoming wastewater composition based on measured laboratory values is presented. The estimated values were compared with literature because some compounds appear in municipal wastewater in typical ratios.

**Results.** A reference scenario in the dynamic modelling tool reflecting the actual full-scale performance of Klagshamn was established. A complete annual time series of the incoming wastewater composition based on measured laboratory values was established and incorporated into the dynamic model. Furthermore, the implementation of primary sludge hydrolysis estimates into the reference scenario indicated a potential for removing a total nitrogen load of 25 tN·a<sup>-1</sup>, which corresponds to 3.1 gN·m<sup>-3</sup> less into the downstream process.

**Conclusion.** Dynamic wastewater treatment simulation was applied in this study and shown to be a valuable tool to quickly evaluate the potential operational changes without the risk associated with full-scale testing. Routine measurements made at most plants are not performed with the time resolution desired for modelling purposes.

- [1] Jönsson, K., Pottier, A., Dimitrova, I. and U. Nyberg. (2008). Utilising laboratory experiments as a first step to introduce primary sludge hydrolysis in full-scale. *Water Science and Technology*, 57, 1397-1403.
- [2] EFOR 2003.0. (2003). DHI Hørsholm, Hørsholm, Denmark; software available at <http://www.dhisoftware.com/efor>.
- [3] Henze, M., Gujer, W., Mino, T., Matsuo, T., Wentzel, M.C., Marais, G.V.R. and van Loosdrecht, M.C.M. (1999). Activated sludge model No. 2d, ASM2d. *Water Science and Technology*, 39, 165-182.



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## REQUIREMENTS ON EVOLUTION MANAGEMENT OF PRODUCT LINES IN AUTOMATION ENGINEERING

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**Introduction.** The initial investment costs for a production plant are enormous – in many cases up to 100 Mio. € and the entire life-cycle is up to 30 years [1]. In order to preserve existing investments and to retain the competitiveness of the production plant it continuously has to be developed and improved further.

**Challenges and state of the art.** During the conception of a new production plant it is possible to anticipate future product and production process innovations for some years. Considering the entire lifecycle of a plant up to 30 years however, it becomes obvious that the production plant has to be developed and improved further continuously. In consequence, parts of the software, the control hardware in combination with the electrical system and partly also mechanical components have to be upgraded during the life cycle. Otherwise the competitiveness of the production plant and thus also of the company running the plant is not assured anymore.

Therefore different procedures and methods have been established in the machine and plant manufacturing industry. A manufacturing plant owner, respectively an authorized system integrator, for example, does not develop a production plant from scratch. He rather uses existing application [3] modules from a module supplier. This illustrates that modularity is a key issue and a working variant and version management is needed.

The importance of Version and Variant Management was also demonstrated by the results of the research project BESTVOR [2]. Thereby 60% of the 60 surveyed companies from the machine and plant manufacturing industry stated new variants, versions and their configuration to be important, but 52% of these companies indicated that no interdisciplinary software tool for Version and Variant Management exists yet.

So two essential topics have to be considered: a) an integrated variant- and version management of basic modules, application modules based on product lines, and modules, which are part of production plants in the field and b) an interdisciplinary compatibility supervision technique to validate the compatibility of new module versions with respect to the various application contexts and the complex dependencies between software (software design), platform (electrical design) and/or context (mechanical design).

**Concept.** Both challenges can only be resolved with an appropriate tool support for variant and version management of modular models and for model validation to supervise the interdisciplinary compatibility. To provide this tool support a syntactic and semantic formal model is necessary. In this paper the requirements on a holistic mathematical modeling of evolution in automation engineering are proposed.

[1] T. Hauff, „Prozessleitsysteme: Lebenszyklus und Qualität.“, *atp - Automatisierungstechnische Praxis*, Bd. 48, Nr. 2, S. 34–42, 2006.

[2] BESTVOR, *Betriebliche Einführungsstrategie für ein anwendungsorientiertes Vorgehensmodell für die Entwicklung zuverlässigerer mechatronischer Systeme im Maschinen- und Anlagenbau (BESTVOR)*. 2011.

[3] U. Katzke, B. Vogel-Heuser, und K. Fischer, „Analysis and state of the art of modules in industrial automation“, *Automation Technology in Practice (atp) international*, Bd. 46, S. 23-31, 2004.

## SITUATIONAL SIMULATION IN SUPPLY CHAIN MANAGEMENT

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**Introduction.** The term industry-business processes (IBP) will here stand for flexible enterprises and technologies, regional business organisations, etc., functioning at an essential dependency on spatial features of their components and time.

Supply Chain Management (SCM) is a modern approach to coordination of resources and the optimization of activities across the value chain to obtain competitive advantages. The objective of supply chains (SCs) is to maximize the overall value generated. SCM focuses on an integration of suppliers and customers. Within the SCM, two problem classes can be distinguished: cooperation and coordination.

Cooperation decisions in the SCM can be divided in strategic (supply chain design), tactics (planning), and operations. As the term implies, strategic decisions are made typically over a longer time horizon. Supply chain planning considers a shorter time horizon (months, weeks) and deals with demand forecasting, production and logistics planning. Operational decisions are short term, and focus on activities over a day-to-day basis.

**Brief For Our Approach.** To acquire any practicable results, IBP have to be modelled as complex spatial dynamical systems with variable structure, multiple inner and outer links. Due to unavoidable knowledge incompleteness regarding IBP it is reasonable not to confine to classic analytic and simulating models only, but grant means for usage of experts' experience. So, any IBP modelling system ought to incorporate a geographical information system (GIS) and an expert system (ES), admit dynamical simulation and to be open for operative changes resulting from previous modelling stages. From the introduced point of view, we will describe IBP by using generalised logic-dynamical systems with controlled structure. Such systems can function and develop under changing conditions for goals, tasks, situations and criteria estimating efficiency and effectiveness of their performance.

So, this study introduces an integrated modelling environment (IME) developed according to the modern situational approach within the frames of Structured Analysis and Design Technology and intended for state analysis and prognosis of systems described according to General Systems Theory. An open for operative modification conceptual model of the subject domain is used as a core of the IME to maintain every stage of modelling. Combined processing of data coming from simulation modules of the object's structure components, embedded GIS and ES constitutes the main difference between the model and its prototypes. The IME provides using different methods for investigation of not-enough-formalized complex non-stationary spatial objects, ensures complex use of expert knowledge to form criteria and chose structural alternatives for more detail studying in the simulation mode.

Then we propose an extension of the mentioned IBP model to the problem of strategic management and comprehensive planning in a spatially distributed system of real enterprises in order to create virtual enterprises (VEs). This problem is considered within a class of IBP structure dynamics control problems and requires a multi-criteria optimization of IBP performance as well as reallocation of IBP control functions among nodes of the production network.

Operative management can be implemented by an incremental coordination technique developed by authors for multipurpose systems. The technique is based on the new necessary and sufficient conditions of coordinability for a locally organized hierarchy of dynamic systems.

**Conclusion** Two main up-to-date challenges in supply management are as follows: how to plan robust supply chains with maximal service level and minimal costs and how to control and adapt supply chains in case of different changes and disruptions? The paper presents a novel framework of SCM to integrate SCM, Agility, VEs, Coordinability and Sustainability. The main proposition of the approach is balancing agility (structural excessiveness), information sharing, and virtual structural-functional reserve to increase organizations' wealth by producing demand-corresponding products in the most cost-effective manner through increasing responsiveness and reaction speed to market changes on the basis of extended information coordination and continuous comprehensive improvements / adaptation of supply chains. We describe SCM from managerial and research prospects and present possible experimental environment and tools. In the course of supply management developments, new case studies should be learned and new methods and tools should be developed to strengthen the current state of the SCM approach.

# IN-PROCESS AGENT SIMULATION FOR EARLY STAGES OF HOSPITAL PLANNING

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**Introduction.** In the early stages of hospital planning, work processes are typically modelled in a static manner, using flow-charts or business process modelling notation as means. Diagrams of this kind are easily simulated, however, employed process engines lack possibilities for dealing with dynamic aspects of the process which depend on the building layout (e.g. elevators, behaviour of automatic delivery carts). If one could give planners the opportunity to employ dynamic entities without having to change their usual workflow, one of the benefits would be that they are not being forced to resort to naive assumptions (e.g. 15 seconds per floor) that are still commonplace in today's planning practice.

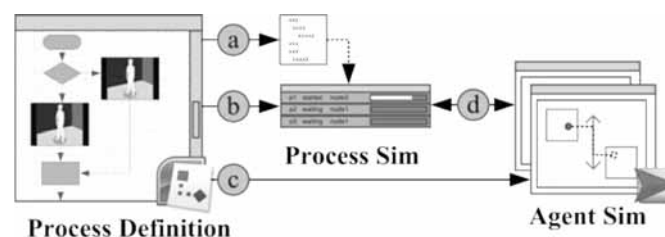
**Contributions.** Because processes are modelled in highly-formalized manner (e.g. as flow-charts), one might think that the application of simulation lies at hand from the very start of a building project. However, such static process descriptions lack the ability to also include aspects that depend on the building layout, such as the transition of persons and material from one space to the other, possibly using dynamic entities such as lifts as they move along. Resorting to naive assumptions (e.g. fixed passage times) might be inadequate (again taking the lift as example) and, furthermore, cumbersome to elaborate: In early planning, there are usually several variants of the spatial concept rather than only one for later phases.

Our work therefore focuses on overcoming the mentioned problems, by embedding dynamic entities into an otherwise static process model. Broken down into further detail, our contribution consists of: (1.) A thorough look at simulation needs in the early stages of process-driven building design. Such a survey is (surprisingly) novel, as the community has previously targeted hospital simulation problems but not their context within the planning process. (2.) An extension of static process simulation such that dynamic entities (acting in a spatial context) can be represented. Technically, this is achieved by invoking an agent-based simulation on behalf of the process simulation (i.e. a hybrid simulation).

**Overview of the simulation approach used.** Our central point of intervention lies in the introduction of a new type of activity in the process diagram that was coined as *agent node*, that acts as an injection point for dynamic behaviour inside the static process. Upon entering an agent node, the process execution is passivated and control is passed to an agent simulation, which performs a spatial simulation as required by the planning process. After finishing the dynamic simulation, control returns to the process simulation, which re-activates the process instance.

An overview of the implantation is given in the figure below: (a.) The process definition is done in Microsoft Visio, before being passed to a (b.) process simulation that can execute it. (c.) Furthermore, a set of agent simulations is opened, each one covering a different aspect of dynamic behaviour needed (e.g. movement simulation, simulation of elevators, etc.). Subsequent (d.) communication happens between the process simulation and the agent simulations.

**Audience and benefits of the approach.** Our work augments the now-common working style of planners in a non-intrusive manner, i.e. extending rather than reinventing design tools available. The choice of an agent-based simulation *on top of* a process simulation fits exactly this line of reasoning. We are convinced that our elaboration of the subject will impact not only the respective academic communities (simulation and architecture), but also gain a large interest in the everyday practice of hospital planning.



**Figure:** Overview. (left) Processes drawn in Visio are (a) written to a file, which is fed into a (b) process simulation that can execute them. Visio furthermore (c) opens a set of agent simulations, which are (d) then invoked by the process simulation for simulating dynamic aspects of the otherwise static process, based on the building's spatial concept.

# REPRESENTATION OF ACTION SPACES IN MULTIPLE LEVELS OF DETAIL

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**Motivation** In many domains human operators are working with complex dynamic systems. Working field examples are the supervision of industrial processes or power plants, air traffic control, or anesthesia. Human operators of complex dynamic systems should be able to predict future states of the system as well as the consequences of their actions to make good decisions, to avoid errors, malfunctions, and accidents. Thereby they have to deal with uncertainties when determining the current system state and especially when making predictions. Models of human planning processes suggest that one of many strategies to deal with uncertainties is to use flexible plans with an adaptable level of detail.

An assistance system imitating the human planning and proposing a flexible and adjustable plan could adapt to occurring disturbances and should be able to propose a plan according to the operator's mental model and thus make a better understanding of the plan possible. This could have a positive effect on the operator's performance and reduce the error rate. The prerequisite for such an assistance system is the ability to represent the action space in multiple levels of detail. This contribution will demonstrate how this can be achieved. The proposed method assumes that the task can be modeled by discrete events and thus by a Coloured Petri Net with the consequence that the action space can be described as a discrete state space.

**Method** The presented method uses the state space of the Petri Net (level 1) as input and identifies states representing possible intermediate goals of the human operator, which will constitute a more abstract state space (level 2). To identify the goal states, conditions are defined which these states must meet. These conditions can include specific characteristics of the goal state, of possible successor states, and of the states in the path on which this state is reached.

To generate a more abstract representation first the initial state of the detailed state space will also be defined as the initial state of the abstract state space. Because different goals can exist in a task environment, an activation function is needed which defines the currently active possible goals. The function is then used to determine the goals which are active at the initial state. After that an algorithm starting at the initial state searches for states which meet previously defined goal conditions. If a possible goal state is found, this state is added to the abstract state space together with an arc connecting it with the initial node. These steps are repeated starting from already identified goals. All goals found are added to the abstract state space. If this process is repeated until all goals are identified, a state space results which describes the action space, but does not specify the particular actions. The whole process can be repeated using the calculated state space (level 2) as input to calculate an even more abstract state space. The repetition of the method results in multiple representation of an action space with different levels of abstractions.

**Conclusion** The method described above is demonstrated at an example application. It is shown that the action space of a task can be described by state spaces with different levels of detail. The information is decreasing with every level and hidden in the lower levels. Further it is possible to combine the representations to describe the next steps in greater detail and to give only the goals for the next steps, similar to the mental model of the human operator.

This method could be used to develop assistant systems, which can propose plans with multiple levels of detail and thus would have to change the plan less often. A drawback of this method is that it requires a complete state space, which cannot be derived in many cases, especially if random effects like disturbances can occur in the task environment. It is also addressed how this method could be modified to be based on partial state spaces to allow for the use in environments with disturbances.

- [1] Jensen, K., and Kristensen, L.M.: *Coloured Petri Nets: Modelling and Validation of Concurrent Systems*. Springer, Berlin, Heidelberg, 2009.
- [2] Oberheid, H., Hasselberg, A., and Söffker, D.: *Know your options - analysing human decision making in dynamic task environments with state space methods*. In: D. de Waard, N. Gérard, L. Onnasch, R. Wiczorek, and D. Manzey (eds.), *Human Centred Automation*, Shaker Publishing, Maastricht, the Netherlands, 2011, 285–300.
- [3] Söffker, D.: *Systemtheoretische Modellbildung der wissengeleiteten Mensch-Maschine-Interaktion*. Logos Wissenschaftsverlag, Berlin, 2003.



# SCHEDULE OPTIMIZATION BASED ON COLOURED PETRI NETS AND LOCAL SEARCH

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**Introduction.** Petri nets compose a general modelling formalism suitable for description of systems with highly parallel and cooperating activities. Systems' specific properties, such as conflicts, deadlocks, limited buffer sizes, and finite resource constraints can be easily represented within a single formal model [5]. This motivated the investigation of Petri net based optimization of manufacturing planning and scheduling problems.

Our previous work dealt with a combination of Petri net modelling and simulation approach and local search optimization methods [2]. This paper focuses on Coloured Petri net (CPN) models of various classes of scheduling problems and explores the possibilities of use of CPN models in conjunction with local search algorithms provided a special type of parameterized conflict resolution strategy and neighbouring solution generation procedure are adopted. This improves the effectiveness of CPN based exploration of solutions compared to previous works.

**CPN representations of scheduling problems** Deterministic scheduling problems in manufacturing are classified according to machine environment structure, processing characteristics and constraints, and objectives [4]. Standard machine environment structures lead to standard scheduling problems, e.g., open shop, flow shop and job shop problems, which are commonly studied. The problems differ in restrictions on the job routings.

Petri nets can be used to effectively model all three standard problem classes. In particular, Coloured Petri nets enable to develop compact models with a chosen level of abstraction, which are functionally equivalent to basic Place/Transition model. To illustrate this, the paper shows simple examples of standard problem classes. The models are shown in three levels of abstractions, with initial common Place/Transition Petri net structure that is translated into two possible CPN models. The presented models can be used as modelling templates for modelling more complex problem instances where also automatic model generation can be applied.

**Neighbourhood solution generation strategy** In [2] the approach is presented, which extends the Petri net representation by predefined sequences and priorities. A sequence-supervised simulation run of the Petri net model from the prescribed initial to the prescribed final state yields a possible solution to the scheduling problem, i.e. the transition firing sequence represents a feasible schedule. The exploration of the solution space and the related search for the optimal schedule can then be driven by permutations of sequence index vectors. However, the resulting transition firing sequence can easily become infeasible, which results in a deadlock during simulation.

A possible way to avoid this is to use neighborhood generation operators that have been proposed in the operation research literature [1]. The described solution neighborhoods are based on moves of critical operations. These can be used in CPN based simulation-optimization if a correspondence of a critical path and the sequence index vectors is established. When the move is limited to swap of a pair of the adjacent operations in a block on the critical path this narrows down the set of allowed permutations. Every permutation from this set will result in a feasible firing sequence, i.e. a feasible schedule. The problem class specific constraints can be enforced as additional permutation constraints. E.g., permutation flow shop restrictions can be enforced by keeping all the sequence vectors in synchronization. The schedules generated in the proposed way belong to the class of semi-active schedules [4]. This is important in cases when the optimal solution can be missed unless some idle time is included in the schedule as shown in [3].

The described neighbourhood generation procedure was coded in Matlab and used in combination with a simple Simulated annealing (SA) search algorithm. Comparison of the minimum makespan for some standard open shop, flow shop and job shop problems calculated by the proposed algorithm and some other standard algorithms shows that the proposed algorithm performs well and is able to improve the initial solutions with a moderate effort.

- [1] J. Blazewicz, W. Domschke, and E. Pesch. The job shop scheduling problem: Conventional and new solution techniques. *European Journal of Operational Research*, 93:1–33, 1996.
- [2] T. Löscher, G. Mušič, and F. Breitenacker. Optimisation of scheduling problems based on timed petri nets. In *Proc. EUROSIM 2007*, volume II. Ljubljana, Slovenia, 2007.
- [3] M. A. Piera and G. Mušič. Coloured Petri net scheduling models: Timed state space exploration shortages. *Math.Comput.Simul.*, 82:428–441, 2011.
- [4] M. L. Pinedo. *Scheduling: Theory, Algorithms, and Systems*. Springer Publishing Company, Incorporated, 3rd edition, 2008.
- [5] G. Tuncel and G. M. Bayhan. Applications of Petri nets in production scheduling: a review. *International Journal of Advanced Manufacturing Technology*, 34:762–773, 2007.



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# MODELING THERMAL SHOCKS AND AIR COOLING USING THE FINITE DIFFERENCE METHOD

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For producing high-quality steel plates, it is of vital importance that the rolling takes place in the prescribed temperature range. Temperature models are thus needed to plan the roll passes and to schedule the whole process. These models have to take into account all producing steps influencing the temperature evolution. In this paper, two of them are dealt with, namely air cooling during transport and high pressure descaling.

Common temperature models for air cooling consider radiative heat transfer by means of the Stefan-Boltzmann law. In many cases, the radiative boundary conditions can be assumed to be symmetric. The emissivity of the plate can be constant or temperature dependent. Furthermore, convection heat transfer can be modeled either as natural or forced convection. Modeling the descaling process is a rather controversial issue, although it is mostly done by convective boundary conditions. Some approaches reported in the literature only use constant heat transfer coefficients, whereas others model the heat transfer coefficient as a function of the descaling pressure or the volume flow. The considered heat transfer coefficients vary over a wide range, as they are identified under specific experimental conditions and for different descaling times. Therefore, there is a need for a mathematical model of the temperature drop caused by descaling sprays that is validated by experimental data covering the whole operating range of hot rolling.

For modeling the temperature development of a plate, the heat conduction equation has to be solved. As the dimensions of the plate in the longitudinal and lateral directions are much larger than its thickness, the heat conduction along the thickness direction dominates and the one-dimensional heat conduction equation can be considered. The material properties, i.e., the specific heat capacity and the thermal conductivity, are regarded as temperature dependent. The boundary conditions are formulated depending on the respective production step.

For air cooling, the heat flow out of the plate consists of a radiative and a convective part. The re-radiation from the roller table is modeled by the net radiation method, see [1]. The required view factors are calculated by Hottel's crossed-string method [2]. As the interaction time of each roll with the hot plates is short, the temperature of the roller table is assumed to be constant as well as the temperature of the surroundings. For the convective part, forced convection is taken into account. For the descaling spray, a convective boundary condition is formulated that relates the heat flow out of the plate to the difference between the surface temperature and the water temperature. The heat transfer coefficients are identified on the basis of measurement data. The experiments show the influence of several parameters on the cooling effect of the descaler sprays, such as descaling speed, surface temperature and configuration of the descaling nozzles. Furthermore, the effect of the descaling on the radiation characteristics of the plate can be analyzed by the same experiments.

The heat conduction equation and the boundary conditions are spatially discretized by means of the finite difference method in order to obtain an ordinary differential equation. The numerical solver ode15s of Matlab<sup>®</sup> is used for solving the finite-dimensional approximation of the heat conduction equation. The identification of the heat transfer coefficients and the emissivities is done by minimizing a cost function, which sums up all squared deviations of the calculated temperatures from the respective measured temperatures.

The proposed model is suitable for calculating the temperature evolution of a plate during air cooling and high pressure descaling. The thermal shock caused by the impinging water spray can be accurately modeled. The model can be used for predicting the required waiting periods between the hot rolling passes and thus for scheduling the production process.

- [1] H. D. Baehr and K. Stephan, *Wärme- und Stoffübertragung*, 6th ed. Springer-Verlag, Berlin, Heidelberg, 2008.
- [2] R. Siegel and J. R. Howell, *Thermal radiation heat transfer*, 4th ed. Taylor and Francis, New York, London, 2002.

# A DYNAMIC MODEL OF PERCOLATING GAS IN AN OPEN WELL-BORE

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**Abstract.** The two-phase dynamics of a gas-kick percolating up a vertical well, drilled using a partly evacuated riser, is described by two ordinary differential equations and algebraic relations. We model the gas as bubbles distributed with a distribution function along the well. The simplicity of the model makes it well suited for estimation purposes and controller design. We present simulation results where an unscented Kalman filter is used to estimate the current location of the gas, distribution of the gas, and rise-velocity. These estimates can be used to predict when the gas will pass the blowout preventer and reach the drilling rig.

**Motivation.** After the Macondo incident, the need for automatic systems aiding the drilling crew in making the right decisions during critical events prior to possible blowouts has been highlighted. In this paper we address the modeling and handling of a gas-kick in a vertical well with a partly evacuated riser. We also use the model for estimation of the unmeasured states and two parameters. A gas-kick is an unwanted influx of gas from the reservoir, or the formation above the reservoir, into the well-bore. The influx is driven by a pressure difference between the well-bore and formation containing the gas. If no measure is taken to mitigate and handle the influx, the gas will expand as it rises upwards, thereby reducing the hydrostatic head in the well, which in turn will cause more gas to enter the well-bore. Such a situation can evolve into a blowout with disastrous consequences. The objective of this paper is to model gas percolating up a well-bore in a simple manner without resorting to the use of partial differential equations.

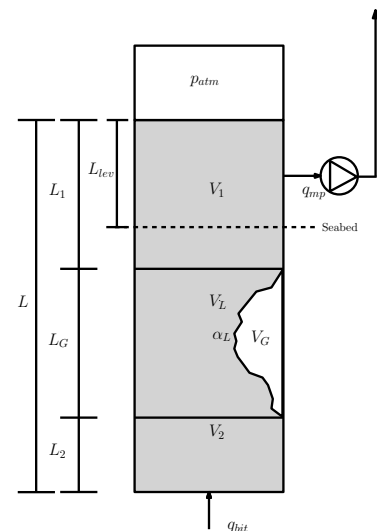
Well control for a partly evacuated riser is has some interesting benefits which are highlighted in [1]. For a small kick it is argued that the blowout preventer need not to be closed since the kick can be stopped by increasing the hydrostatic head in the well by shutting down the subsea mud return pump for a while and keeping the rig pump going. With this method the kick can be vented out in the riser.

**Modeling.** We intend to model a gas kick in a vertical well with a partly evacuated riser where the mud level is governed by a subsea mud pump. The low riser return system is thoroughly described in [2] and sketched in the figure to the right. We divide the well into control volumes portioned around the gas. The control volumes above and below the gas are pure liquid, while the mid control volume is viewed upon as a bubble structure. The distribution of the gas bubbles in this section is approximated with a triangle. These simplifications make it possible to develop a dynamic model of the percolating gas which is well suited for state estimation and parameter identification. We introduce the parameters  $\alpha_L$  and  $k_r$  which are the minimum liquid hold-up and rise velocity of the tail of gas, respectively, and the states  $V_G$  and  $V_2$  which are the volume of gas and volume of the lower control volume, respectively.

**Estimation.** We assume that the drillstring is equipped with pressure sensors every 300 m, as with a wired drillpipe. We also assume that a measurement of the liquid level in the riser is available. With use of the unscented Kalman filter, we are able to successfully estimate the two states and two parameters. The length of the upper control volume,  $L_1$ , is derived from the measurement of the liquid level and the estimated states and parameters, and gives the location of the front of gas.

**Conclusion.** The presented model is a simplification of the complex two-phase dynamics which occur during a gas-kick. We focus on capturing the qualitative behavior during such an event to gain insight to what is happening in the well. Using an unscented Kalman filter with the model, we estimate the dynamic states and two parameters and successfully determine the position of the bubble structure and its length. This information is useful for the driller, who must consider whether to close the BOP or vent the gas out into the riser.

- [1] K. Falk, B. Fossli, C. Lagerberg, A. Handal, and S. Sangesland. Well Control When Drilling With a Partly-Evacuated Marine Drilling Riser. In *IADC/SPE Managed Pressure Drilling and Underbalanced Operations Conference & Exhibition*, 2011.
- [2] Børre Fossli and Sigbjørn Sangesland. Managed pressure drilling for subsea applications; well control challenges in deep waters. In *SPE/IADC Underbalance Technology Conference and Exhibition, Proceedings*, Houston, Texas, USA, 11–12 October 2004. SPE/IADC.



Sketch of a low riser return system with control volumes and lengths.

# AN OBJECT-ORIENTED APPROACH TO THE DEVELOPMENT OF LIQUID CARGO HANDLING SIMULATORS IN TRANSAS

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**Introduction.** Proper training of ship crew in operational procedures, decision-making and emergency response is vital to avoid costly mistakes during liquid cargo transfer operations. Cargo handling simulators are the modern means of training qualified personnel of liquid cargo tankers and gas carriers to perform their functions safely and efficiently. Simulator can be used for system familiarization (arrangement of systems, instrumentation, local and remote controls), and for appropriate training in control procedures in normal conditions (cargo and ballast handling operations, auxiliary operations) and emergencies (system faults, malfunctions, accidents) [1].

The interactive mathematical models of ship systems are essential part of the marine technological simulator. Modern liquid cargo handling simulators include wide range of systems, such as cargo and ballast systems, tanks and cofferdams heating systems, tank stripping and washing systems, inert gas and nitrogen generation systems, gas detection and oil discharge monitoring equipment, deck wash and fire systems. Each of the listed systems may contain significant numbers (hundreds) of interconnected devices, changing their behaviour according to the actions of the trainee and their own operational conditions.

**Modelling approach.** Real time physical modelling of the specified systems is rather complicated task and requires specific approach. The dynamic behaviour of such systems is described by nonlinear differential-algebraic equations system of variable structure, consisting of thousands of equations. Attempts of the direct composition of such systems would require complex structures and extensive software code, requiring too much trial and error to create a working model. Another way of construction of such systems is the usage of “component-based modelling” methodology. In this approach, the object-oriented analysis of the application domain is conducted, and standard classes and inheritance between them are defined. Definitions of the classes comprise the libraries of standard components, represented as hybrid dynamic objects. Each particular model is constructed from standard components, connected by links. To incorporate the mathematical model into the simulator software, the source code is automatically generated from the mathematical description of the model by the designing software.

**Implementation.** The described technology has been implemented in mathematical models of Liquid Cargo Handling Simulators, developed by TRANSAS Technologies Company. The design environment, applied for the modelling, is the “RanD Model Designer” (previously named “Model Vision Studium”) [2]. The standard components library has been created, containing devices, which are typical for ship systems, modelled in the marine technological simulators [3]. The library contains hydraulic objects, such as tanks and reservoirs, pipes and ducts, valves, different pumps and compressors, heaters and vaporizers, etc. In addition, the library includes components of control systems, alarm and emergency shutdown systems. Library components are described by behaviour maps, representing different operational states of the devices (e.g. closed and opened valve), different physical conditions (e.g. laminar and turbulent flow in the pipe) and transitions between those states. Connections between the components are implemented by external variables of both directional (for control systems) and nondirectional (for physical connections in hydraulic systems) types. The developed standard components library has been employed for creation of mathematical models of Liquid Cargo Handling Simulators for Chemical Tanker, Product Tanker and LNG Tanker, and will be used for other ship types.

As the experience has shown, the real time operation of the models was one of the most challenging requirements for the modelling. To reach the sufficient calculation speed of numerical methods, simplification of compound system of equations, was required. The analysis and symbolic transformations of the equations system, allowed reducing number of nonlinear algebraic equations by excluding formulas, and separation of independent blocks. In the same time, the usage of “contact-flow” links leads to the necessity to rebuild of the system of equations in runtime, and therefore to the limited time for the equation system analysis. To overcome this contradiction, a suitable compromise has been found, allowing the real time operation of developed models within the simulator.

[1] *Transas Group. Products and Services. Liquid Cargo Handling Simulator (LCHS)* [online]. Available from World Wide Web: <[http://www.transas.com/products/simulators/sim\\_products/cargo/lchs/](http://www.transas.com/products/simulators/sim_products/cargo/lchs/)>.

[2] RanD Model Designer – high-performance visual environment for the modelling and simulation of multy-domain component models [online]. Available from World Wide Web: <<http://www.randservice.com/>>.

[3] D.V., Kiptily, Y.B. Kolesov, D.V. Lebedev, Y.B. Senichenkov, S.V. Tarasov. *An object-oriented approach to development of marine technological simulator*. In: International scientific-practical conference “Simulation and complex modelling in marine engineering and marine transporting systems” SCM MEMTS 2011. Proceedings of conference (Ed.: Plotnikov A.M, Sokolov B.V.), Russia, St. Petersburg, 2011, 70–76.

# DYNAMIC MULTIOBJECTIVE GLOBAL OPTIMIZATION OF A WASTEWATER TREATMENT PLANT FOR NITROGEN REMOVAL

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Optimal operation of industrial bioprocesses is crucial to ensure good performance and productivity. Such processes are usually carried out in a non-stationary regime, which implies that their associated mathematical models present dynamic nature and non-linearity. In this context, the optimization of such models can be a very difficult task thus robust (global) optimization methods should be used to address this problem.

As additional obstacles to satisfactory find the optimal operating conditions of such processes we should consider (i) the high computational time needed to run a single simulation due to the large systems of differential-algebraic equations defining the mathematical models, which requires optimization methods that use a low number of simulations to locate high quality solutions, and (ii) the presence of several conflicting objectives to be optimized at the same time, like e.g. productivity and sustainability, which advises the use of sophisticated formulations to locate the *Pareto* front.

In this work we have considered a challenging model describing a waste water treatment plant for nitrogen removal developed by European Cooperation in Science and Technology (COST) 624 work group [1]. This model was built to test different control strategies for the operation of this type of plants. The system dynamics is described by algebraic mass balance equations, ordinary differential equations for the biological processes in the bioreactors as defined by the ASM1-model [2] and the double-exponential settling velocity function [3], for a total number of around 100 differential algebraic equations.

Two manipulated variables, i.e., the aeration factor in the last anoxic reactor of the plant and an internal recirculation flow rate have been chosen to optimize two different performance indexes: the quality of the effluent (in terms of amount of pollutants) and the economy of the plant. The dynamic optimization problem has been formulated and solved using the control vector parameterization (CVP) approach, which divides the time horizon into a number of time intervals. The control variables are then approximated within each interval by means of basic functions, usually low order polynomials, with fixed or variable length along the time. This parameterization transforms the original (infinite dimensional) dynamic optimization problem into a non-linear programming problem where the systems dynamics (differential equality constraints) must be integrated for each evaluation of the performance index. For solving the multi-objective optimization problem (i.e., finding the solutions in the Pareto front), we have used the *epsilon*-constraint technique, in which one of the objectives is minimized and the rest are formulated as additional constraints.

The problem, which is highly computationally demanding (it takes around 30 s. per simulation in a standard workstation), has been solved using a multistart procedure with a sequential quadratic programming method and an advanced implementation of the scatter search metaheuristic which has successfully been applied to the solution of dynamic optimization problems. The application of such optimization techniques has revealed that the problem is highly multimodal and that only the robust global optimization technique (i.e., the scatter search method) is able to locate the best solutions).

The Pareto front obtained by the application of these techniques to the problem indicates that indeed, there is a conflict between the chosen performance indexes, and allows the designer to choose the best operation conditions according to different requirements. Further, the results obtained in this work not only generalize other that consider a single objective or a weighted sum of different objectives, but also outperform those obtained by the application of the control strategy proposed by the authors of the model, consisting on 2 PID's to control the same manipulated variables chosen in this work.

[1] J. Copp. *The COST Simulation Benchmark - Description and Simulator Manual*. Office for Official Publications of the European Communities. Luxembourg, 2002.

[2] M. Henze, C. P. L. Jr. Grady, W. Gujer, G. v. R. Marais, and T Matsuo. *Activated Sludge Model No. 1*. IAWPRC Scientific and Technical Reports No. 1. London, UK. 1987.

[3] I. Takács, G. G. Patry, and D. Nolasco. A Dynamic-Model of the Clarification Thickening Process. *Water Res.*, 1991, 25(10):1263-1271.



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**Bond Graph Modeling:**

**Theory and Practice**



## INPUT AND STATE OBSERVER FOR LTV BOND GRAPH MODELS

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**Abstract.** Linear Time Invariant (LTI) systems have been intensively studied since fifty years at different levels, from modelling to control. The design of controllers requires the integration of many kinds of information and a first step is often dedicated to the analysis of the model. LTI models have structural invariants which play a fundamental role and the structure of LTI models has been extensively studied in many papers and books. Note that among these structural invariants, the knowledge of zeros (decoupling zeros, transmissions zeros, invariant zeros) is often an important issue because zeros are directly related to some stability conditions of the controlled system. The infinite structure of LTI models is often related to solvability conditions and is often studied, either with an algebraic approach, a geometric approach or with a structured approach. The advantage of the geometric approach which is based on the concept of invariant subspaces is that this approach allows at the same time the study of the solvability conditions and the control synthesis. In case of LTV (linear time varying) models, and even non linear models, the algebraic approach, based on the module theoretic concept, seems to be useful for the above problems.

The unknown input and state observability problem (UIO) is a well known problem because for control design with a state space approach, the state vector cannot be entirely measured (an observer must be designed) and the system is often subject to unknown inputs (disturbance or failure...) which must be estimated. Different approaches give solvability conditions and constructive solutions. For LTI models, constructive solutions with reduced order observers are first proposed with the geometric approach [4] and [1]. Constructive solutions based on generalized inverse matrices taking into account properties of invariant zeros are given in [6] and then in [7] and [5] with observability and detectability properties. Full order observers are then proposed in a similar way (based on generalized inverse matrices) in [3], but with some restriction on the infinite structure of the model. The algebraic approach is proposed in [8] and in [2] for continuous and discrete time systems, without restriction on the infinite structure of the model.

The objective of this paper is the investigation of observers for linear systems modelled by bond graph when the system has two kinds of inputs: measured and unmeasured inputs. The first section deals with the problem statement. Conditions for the existence of an UIO are recalled in terms of the finite structure (invariant zeros) and of the infinite structure (invertibility). The solution proposed in [2] for the synthesis of an observer without restriction on the infinite structure is recalled, but with an extension in case of models with a known control input. In the following sections, procedures are proposed and solvability conditions are given for the UIO problem in case of bond graph models. In order to extend graphical procedures developed for LTI models, the algebraic approach is applied conjointly with the graphical approach. Notice that, at the analysis step, proposed methods on bond graph models do not require the knowledge of the value of parameters, because intrinsic solvability conditions can be given and that a formal calculus could be proposed at the synthesis level. An illustrative example of a DC motor is proposed. In this example, different choices for the unknown input variable (disturbance) illustrate the generic solvability. At the end, the module theoretic approach is justified by an extension to the LTV case, with some simulations.

- [1] Basile G., and G. Marro: *A new characterization of some structural properties of linear systems: Unknown-input observability, invertibility and functional controllability*. In: International Journal of Control, 1973, vol. 17(5), 931–943.
- [2] Daafouz J., and M. Fliess and G. Millerioux: *Une approche intrinsèque des observateurs linéaires à entrées inconnues*. In: CIFA 2006, Bordeaux, 2006.
- [3] Darouach M.: *Complements to full order observer design for linear systems with unknown inputs*. In: Applied Mathematics Letters, 2009, vol. 22, 1107–1111.
- [4] Guidorzi R., and G. Marro: *On Wonham stabilizability condition in the synthesis of observers for unknown-input systems*. In: IEEE Trans. Automat. Control, 1971, vol. 16, 499–500.
- [5] Hou H., and P.C. Muller: *Design of observers for linear systems with unknown inputs*. In: IEEE Trans. Automat. Control, 1982, vol. 37, 871–875.
- [6] Kudva P., and N. Viswanadham and A. Ramakrishna: *Observers for linear systems with unknown inputs*. In: IEEE Trans. Automat. Control, 1980, vol. 25, 113–115.
- [7] Miller B.J., and R. Mukunden: *On designing reduced-order observers for linear time-invariant systems subject to unknown inputs*. In: Internat. J. Control, 1982, vol. 35, 183–188.
- [8] Trentelman H. L., and A. A. Stoorvogel and M. Hautus: *Control theory for linear systems*. In: London, UK: Springer, 2001.

# FAULT INDICATORS AND ADAPTIVE THRESHOLDS FROM HYBRID SYSTEM MODELS

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**Introduction.** The bond graph approach has proven suitable for modelling especially multi energy domain systems and processes. As bond graph modelling starts from considering the exchange of energy between system components, initially, mainly continuous time models have been developed for the purpose of simulating the dynamic behaviour of a system or process. Furthermore, various approaches have been proposed in the literature to extend the bond graph methodology to *hybrid* system models including the convenient and common abstraction of instantaneous state transitions or discrete mode changes.

Beyond analysis and simulation, bond graph model-based quantitative fault detection and isolation (FDI) as a basis for fault diagnosis has received increased attention and remarkable progress has been achieved [1]. Again, so far the focus has been mainly on FDI in systems represented by continuous time models. Only recently, some work on bond graph model-based FDI of systems represented by *hybrid* models has been reported ([2, 3], Chapter 7 of [4]).

**Content.** This paper extends the *incremental* bond graph approach to FDI of systems represented by *hybrid* models. Incremental bond graphs introduced by the author [5] have been used for frequency domain parameter sensitivity of linearised time-invariant models or for the determination of parameter sensitivities of Analytical Redundancy Relations (ARRs) in symbolic form (Chapter 4 of [4]). Residuals of ARRs are used as fault indicators. The contribution of this paper is to show that incremental bond graphs can also be used to set up adaptive thresholds for ARR residuals that account for parameter uncertainties as well as for discrete mode changes. This is an issue of practical relevance because on the one hand, evaluation of ARRs should be robust with regard to parameter uncertainties, i.e. false indication of faults should be avoided. On the other hand, true faults must be detected. Moreover, hybrid systems operate in different modes and their continuous time behaviour in different modes may be quite distinctive. Therefore, different ARR thresholds adapted to different modes may be required.

The bonds of an incremental bond graph carry increments of power variables. Parameter variations are expressed by sources that are modulated by a power variable of a bond graph model with nominal parameters. From the latter bond graph the nominal part of ARRs can be derived while thresholds of ARR residuals are obtained by summing up increments of efforts or flows respectively at junctions of the incremental bond graph. The approach is illustrated by means of a boost converter as a simple example of power electronic systems incorporating switching devices. The approach, however, can be applied to hybrid models of multi energy domain systems.

**Results.** The results of the presented approach to FDI in *hybrid* system models are the following.

- One unique set of ARRs for all system modes can be derived from the bond graph.
- The nominal part of ARRs is obtained from a bond graph model of the system with nominal parameters.
- An incremental bond graph can be systematically constructed from an original bond graph. Bond graph elements are replaced by their incremental model.
- The uncertain part of ARR residuals with regard to parameter uncertainties is derived from the incremental bond graph. Resulting variations of ARR residuals give rise to the definition of adaptive thresholds that can be used to achieve robust FDI with regard to parameter uncertainties in order to avoid false alarms or disregarding faults.
- The Standard Causality Assignment Procedure (SCAP) can be applied and existing bond graph software can be used to establish model equations and ARRs.

- [1] A.K. Samantaray and B. Ould Bouamama. *Model-based Process Supervision – A Bond Graph Approach*. Advances in Industrial Control. Springer, London, 2008.
- [2] W. Borutzky. Analytical Redundancy Relations from Bond Graphs of Hybrid System Models. In A. Bruzzone, G. Dauphin-Tanguy, S. Junco, and M.A. Piera, editors, *Proc. of the 5th International Conference on Integrated Modelling and Analysis in Applied Control and Automation (IMAACA 2011)*, pages 43–49, Rome, Italy, 12-14 September 2011.
- [3] C.B. Low and D. Wang and S. Arogeti and J.B. Zhang. Causality Assignment and Model Approximation for Hybrid Bond Graph: Fault Diagnosis Perspectives. *IEEE Transactions on Automation Science and Engineering*, 7(3):570–580, 2010.
- [4] W. Borutzky, editor. *Bond Graph Modelling of Engineering Systems – Theory, Applications and Software Support*. Springer-Verlag, NY, NY, U.S.A., 2011.
- [5] W. Borutzky and J.J. Granda. Bond Graph Based Frequency Domain Sensitivity Analysis of Multidisciplinary Systems. *Proc. Instn Mech. Engrs, Part I, Journal of Systems and Control Engineering*, 216(1):85–99, 2002.

## BOND GRAPHS AND LAGRANGE EQUATIONS AS AIDS IN ANALYTICAL STUDIES OF ELECTRO-MECHANICAL SYSTEMS

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A well-known advantage of bond graph models of electro-mechanical systems is that they can be manipulated manually or with the aid of computer programs to yield first order state equations useful for numerical studies. A causal analysis can show in advance whether derivative causality will cause practical difficulties in the equation formulation which might be best circumvented by modification of the model.

Numerical studies are sometimes of limited use in preliminary investigation of the feasibility of a design because the large number of parameters involved precludes a general understanding of the limits of the concept being studied. Analytical studies of simplified models may find the existence of parameter combinations which are crucial to the successful operation of the system or fundamental limitations to performance not obvious in purely numerical studies.

Although the first order nature of the normal bond graph state equations are advantageous for numerical simulation, they are not necessarily the most convenient form for analytic studies using pencil and paper. In many cases, the use of Lagrange equations, based on energy state functions and degrees-of-freedom rather than state variables are advantageous for analytic work. Bond graph models and a special form of causality can be used to advantage, particularly when derivative causality is present, to yield sets of second order dynamic equations based on Lagrange equations, which are often easier to work with than their first order equivalents. This will be illustrated by an example by the analysis of the use of a rotary electric motor as an actuator in semi-active or active suspension element in a vehicle suspension.

*Keywords:* Bond graphs, Lagrange equations, mechatronic systems

# CANONICAL DECOMPOSITION OF MULTIPORTS REVISITED: PROPERTIES AND RELATIONS TO FUNDAMENTAL PRINCIPLES OF PHYSICS

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**Abstract.** Properties of decompositions of multiport models are discussed. In particular, it is shown that the congruent canonical decomposition of multiport storage elements or multiport resistors that is based on Choleski factorization of their Jacobians can be causally inverted without generating algebraic loops and that an arbitrary number of ports of such a multiport may be dualized without generating essential gyrators in its decomposition. As a result, it is argued that the congruent canonical decomposition is a preferred decomposition, in particular from a computational point of view.

**ABSTRACT FROM FULL PAPER**

## BOND GRAPH MODEL OF WIND TURBINE BLADE

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The design of the wind turbine system (sizing, control) according to specifications in terms of quality of produced electricity, maximization of power capture, regulation of power to the turbine's rated output, stability and safety, needs the use of performing simulation tools able to change from simple static calculations assuming a constant wind to dynamic simulation that, from the unsteady aerodynamic loads, models the aero elastic response of the entire wind turbine system, including blades, tower, drive train, rotor and control system.

In recent years, progress has been made both in Europe and the United States in developing and validating simulation codes for predicting wind turbine loads and response. Thus numerous, proprietary, black-box and one-of-a-kind modelling software/design codes have been produced. As a result, models are generally incompatible across simulation platforms and unavailable in some cases. They are also difficult to access, use and maintain. These design tools have been developed as specialized tools dealing with only structural part or aerodynamic part. Moreover, even the most recent papers in the literature dealing with control strategy for wind turbines take as model of the wind turbine only a mechanical power generator extracting power from the wind. Such approaches give simplified "representation models" well adapted for control designing, but they cannot be used as "knowledge models" or virtual test benches allowing the validation of the control strategies in terms of stability and reliability of the power system with high wind power penetration, vibration analysis, or simulation of faulty behaviours of the wind turbine system.

So, it is necessary to move towards a more unified approach for modelling wind turbine systems as a whole for understanding, analyzing and hence designing this multidisciplinary system. As an initiative to address the above mentioned problems, in this paper we present a bond graph model for wind turbine blade which correlates the wind inflow conditions to aerodynamic load and hence applies it on the flexible structural bond graph model of turbine blade. Bond graph methodology allows its further integration to bond graph model of drive train, tower and generator providing a common platform to access the whole turbine system and to deal with control problems (Dauphin-Tanguy et al, 1999).

The proposed bond graph model for the wind turbine blade to simulate the dynamic torque is capable of simulating the flexible blade and correlating the wind inflow conditions to the forces applied on blade accurately. The blades get deformed by these aerodynamic forces due to their inherent flexibility. So, while calculating the torque produced by the forces on the blades, the deformed shape of the blade needs to be considered. The bond graph simulates the torque as output response where wind flow is the input parameter for the model. The other parameters required are blade geometry and inertia properties.

The structural model of wind turbine blade is prepared based on Rayleigh beam model. The blade can be assumed as a twisted beam and is divided into finite number of elements where on each element aerodynamic forces due to the wind are acting. A generic bond graph sub model is proposed for a section of a blade; the complete bond graph model of the blade is obtained by connecting the sub models. The aerodynamic load for the blade is calculated using Blade Element Momentum (BEM) theory (Moriarty, Hansen, 2005).

The axial extension deformation and the Coriolis forces effect are not considered in the present model. Self weight of turbine blade is neglected.

Simulations are performed with data from NACA 4415 profile. Several results show the validity of the proposed model.

- [1] Dauphin-Tanguy G., Sueur C., Rahmani A.: *Bond graph aided design of controlled systems*, J. Simulation Practice and Theory, Elsevier Pub, Dekker Ed, 1999, volume 7, Issue 5-6
- [2] Moriarty P.J., A.C. Hansen: *AeroDyn Theory Manual*. National Renewable Energy Lab., Golden, CO (US), 2005

# BOND GRAPH MODELING OF MARINE VEHICLE DYNAMICS

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**Introduction.** The equations of motion for a marine vehicle in 6 DOF are derived using a Lagrangian approach. Utilizing the close relationship between the Lagrange method and the bond graph modelling method, the resulting equations of motion are consistently implemented into a bond graph framework for model representation and simulation. The bond graph implementation of the general rigid body equations of motion are shown and discussed. The added hydrodynamic forces occurring when a body moves in a fluid, forces from wind and current and propulsion and rudder forces are discussed and shown how to include into a bond graph representation. The purpose of a bond graph implementation of marine vehicle dynamics is to establish a selection of building blocks which supports the modelling process setting up marine mechatronic system models including the marine vehicle for complex system simulations

**Content.** Developing state-space models for time-domain simulations and design of control systems of ship dynamics has attracted a significant interest in recent years among researchers (Fossen, 1994). The study has traditionally however been separated into two main areas: maneuvering and seakeeping, where the first covers the study of the motion of the vessel in calm and confined waters while the latter refers to the study of motion, stability and control in the presence of wave excitation. Attempts to unify the description of these models have recently been added by Perez and Fossen (2006). In using the unified state-space model as an object in a marine mechatronic application we need to combine models of different disciplines or origins, hence the connection or causality problem needs to be observed when developing more complex models. The bond graph method does offer numerous attractive properties for model development and analysis.

The bond graph for the marine vehicle is developed using a Lagrangian approach. Using the *quasi-Lagrange equations* the equations of motion for the rigid body is stated in a general form including the inertia, centripetal- and Coriolis forces. The implementation of this general form in bond graphs is discussed and a new inertia-field with a second multibond representing the additional forces is proposed.

Finally the additional hydrodynamic forces such as added mass, hydrodynamic damping and restoring forces are shown how to include in bond graph form. Also environmental forces from waves and wind, plus propulsive forces such as truster and rudder forces are stated in bond graph form. Finally the complete bond graph for marine vehicle dynamic analysis is presented as shown in the Fig. 1 below.

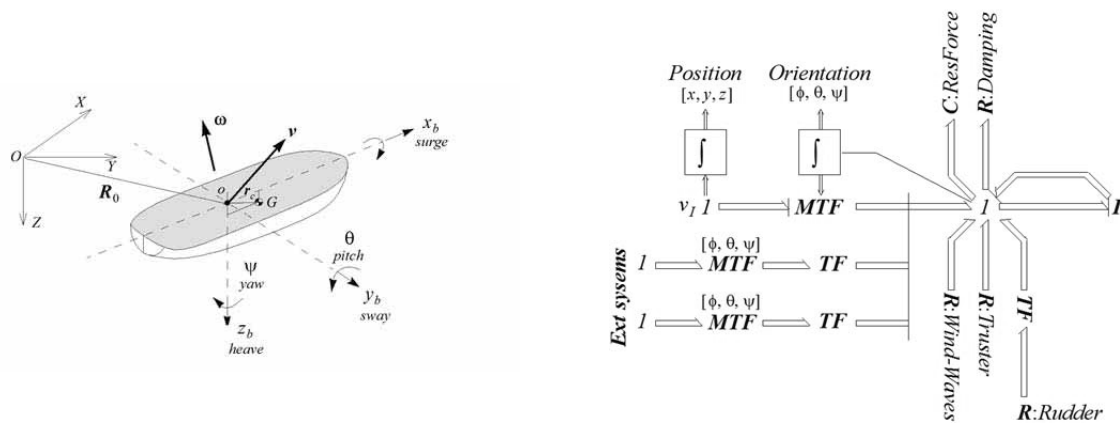


Figure 1: Bond graph model for marine vehicle dynamics.

[1] Karnopp, D. C., Margolis D. L., Rosenberg C., (2006). *System Dynamics: Modeling and Simulation of Mechatronic Systems*, 4th Ed., John Wiley & Sons.  
 [2] Fossen, T. I., (2005) A Nonlinear Unified State-Space Model for Ship Maneuvering and Control in a Seaway, *Journal of Bifurcation and Chaos*.  
 [3] Fossen, T. I., (1994). *Guidance and Control of Ocean Vehicles*, John Wiley&Sons Ltd., ISBN 0-471-94113-1.  
 [4] Pedersen, E. (2009). *Rotordynamics and bond graphs: basic models*, *Journal of Mathematical and Computer Modelling of Dynamical Systems*, Vol 15, Issue 4.



## BOND GRAPH MODELLING OF IN VIVO ROBOT FOR BIOPSY

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**Introduction.** Endoscopes have been in use for many procedures including limited surgery. A very common application of endoscopes been used in surgery is biopsy. However present Endoscopes has certain limitations such as restricted degrees of motion of tool leading to poor manipulation of tissues, limited visualization of surgical field, increased sensitivity to hand movement etc. Further reduced access reduces dexterity, limits perception, increases strain and likelihood of error in addition to increased procedural time. Biopsy of internal organ through natural opening involves two basic issues – insertion of biopsy tool and manipulation of tissues by tool. The proposed system will use one of the existing biopsy channels of the endoscopic tube for insertion of robotic arm. Endoscopic tube will be stationed at the end of the esophagus and robotic arm will be anchored in the leading face of the tube. The robotic arm will be actuated by servomotors kept outside the body through wires. The proposed robotic arm shall provide distinctly more degree of freedom and better maneuverability inside the stomach with respect to that of currently used biopsy tool. This will also enable the surgeon to access much greater area inside the stomach. The view of operating zone can also be improved by integrating vision system to the multiple arms of the manipulator. The robots used for surgery where the entire robot is placed inside the body are called as In Vivo Robot. Various configurations are being developed by the researchers around the globe and still the research is in infancy. The work presents bond graph model of a robot for taking a biopsy sample inside the stomach. To develop the bond graph model a kinematic analysis is carried out and various transformer modulli required for drawing of bond graph model are evaluated. The developed bond graph model can be used for trajectory or force control of in vivo robots. A CAD model of the proposed design was prepared using Solid works and is as shown in the Figure below. To ascertain the proposed design a 4 scaled model was prepared as shown in the Figure below. Then kinematic analysis of the proposed In-Vivo robot was performed and the Frame assignment can be seen in the Figure below. Based upon the equations obtained from the kinematic analysis the bond graph modelling of the In-Vivo Robot with the wired actuation was performed. Various transformer modulli were found from the kinematic relationships. And the tip trajectory was obtained by rotating the 1<sup>st</sup> joint and the up and down wire actuation was also simulated successfully.

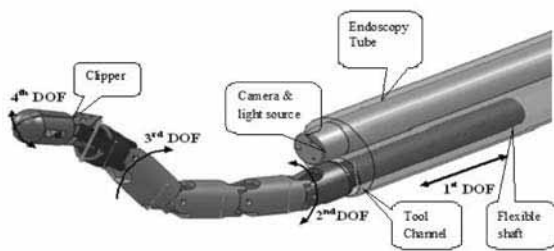


Fig. CAD Model of the In-Vivo robot



Fig. Fabricated 4 scaled model of proposed In-Vivo robot

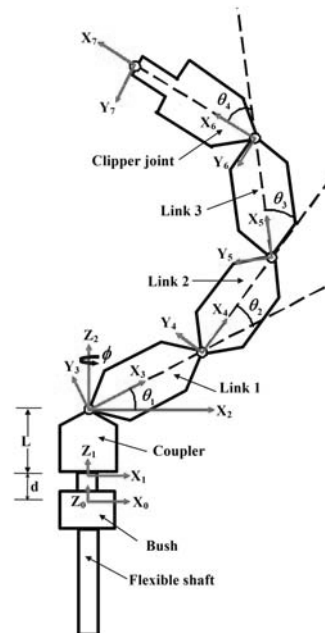


Fig. Frame assignments on In-Vivo robot for kinematic analysis

- [1] Chirkjian, G. S., Burdick, J. W. (1994). "A Model approach to Hyper redundant Manipulator Kinematics," *IEEE Conference on Robotics and Automation*, pp. 343-354,
- [2] Webster, R. J., Jones, B. A. "Design and Kinematic Modelling of Constant Curvature Continuum Robots: A Review," *The Journal of Robotics Research*, vol. 29, pp. 1661-1683, 2010.

## BOND GRAPH MODELING OF AUTOMOTIVE TRANSMISSIONS AND DRIVELINES

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In the last two decades there have been substantial advancements in design and application of automatic transmissions and drivelines, including new designs such as hybrid electric vehicle (HEV) transmissions, dual clutch transmissions, and torque vectoring differentials. The new transmission and driveline solutions have often imposed new requirements on the quality of power train control, which typically strongly depends on the fidelity of related transmission and driveline dynamics models. In the related previous publications [1,2], it has been demonstrated that the bond graph method can be an effective tool for unified, modular, and minimum-realization physical modeling of power train component and systems, and their insightful analyses. Since then, the work has been extended to modeling, analysis, and control of many new concepts of transmission and driveline systems, such as one-mode and two-mode HEV transmissions, V-belt continuously variable transmission (CVT), dry and wet dual clutch transmissions, active limited-slip and torque vectoring differentials, and four-wheel-drive (4WD) drivelines. This paper presents an overview of the bond graph models of these systems, including modeling of clutches and their actuators. It is illustrated that the bond graph method can be effectively used to gain valuable insights about the system dynamic behavior. Figure 1 shows an example of modeling a 4WD (Four Wheel Drive) driveline with passive front and torque vectoring rear differential (TVD). The model reflects the structure of the mechanical system, and can be readily transformed to system equations for computer simulations and further analyses.

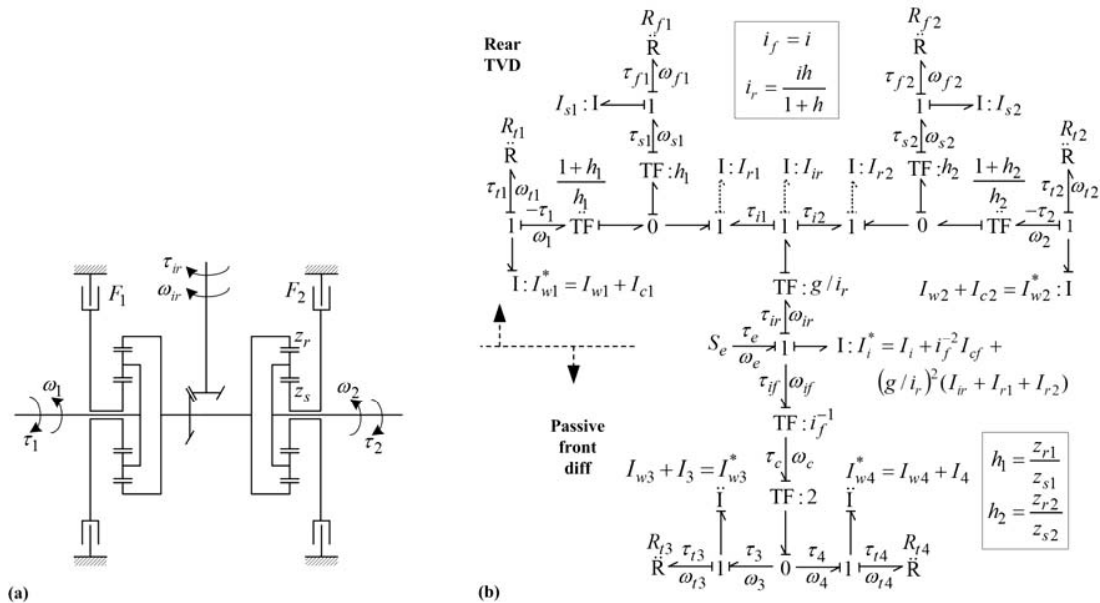


Figure 1. Kinematic scheme of rear TVD (a) and bond graph model of related 4WD driveline (b).

- [1] Hrovat, D. and Tobler, W.E.: *Bond Graph Modeling of Automotive Power Trains*. Journal of the Franklin Institute, Vol. 328, 1991, 623-662.
- [2] Hrovat, D., Asgari, J., and Fodor, M. G.: *Automotive Mechatronics Systems*. In Mechatronics Systems, Techniques and Applications, C. T. Leondes, Ed., Gordon and Breach Science Publishers, 200, 1-98.

# WHY PHYSICAL SYSTEM MODELING IS IMPORTANT TO INDUSTRY: BOND GRAPH MODELS THAT COULD HAVE PREVENTED SOME COSTLY MISTAKES

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In order to develop new concepts into prototypes and ultimately into products, physical system modeling is virtually a necessity. At the concept stage, low order models are needed to understand the interactive dynamics of complex systems, and, as development proceeds into prototyping and manufacture, more sophisticated models may be needed to size components, determine fatigue life, plus more.

As the product becomes more and more defined, the modeling depends more and more on special purpose software packages that evaluate stress and strain, magnetic circuit design, fluid flow fields, etc. These packages require that the product is near final form, as the input files for these programs require details about the system that would not be known in the concept development stage.

The modeling discussed in this paper is specifically directed to the concept development of mechatronic systems. These systems typically involve multiple energy domains where electro-mechanical, -pneumatic, and -hydraulic devices are involved. Since the device or system is not well defined at this stage, the modeling must be handled by the inventors using physical principles, and assembling the various pieces of the model into an overall dynamic model that can be simulated or analyzed.

Bond graphs are a pictorial representation of the interactive dynamics of all types of engineering systems and they are particularly well suited for concept development of multi-energy domain systems. This is demonstrated here using several examples from very real commercial applications where modeling at an early stage of development would have avoided some very costly mistakes.

One example is a hydro-mechanical tractor cab isolation device that was developed by a company and tested by 2 different truck manufacturers. One customer thought the resulting isolation was exceptional and bought the system while the other truck manufacturer thought the system provided little to no isolation. Understanding the physical system identified the problem and led to a simple solution.

A second example was a new backhoe that was developed by a company that manufactured backhoes for over 60 years. When the new design came off the assembly line it was determined to have a violent instability where the vehicle literally jumped off the ground. Physical system modeling was used to identify and correct the problem.

A third example is a fuel pump for a jet aircraft that was failing in hundreds of hours of operation rather than the anticipated thousands of hours of operation. This electro-mechanical, electro-hydraulic system was modeled using bond graphs and a very small part was identified as the source of the failure. A very inexpensive fix was introduced.

## MATHEMATICAL MODELLING OF PURELY ODE SYSTEMS BY USING THE BOND GRAPH TECHNIQUE AND TAKING THE INHERENT CAUSALITIES

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Simulation and especially computer simulation, is a basic tool since it enables engineers to understand how systems work without actually needing to see them. They can learn how they work in different circumstances and optimize their design with considerably less cost in terms of time and money than if they had to carry out tests on a physical system. One of the multi-domain techniques to represent a physical model is Bond Graph, which allows assimilating the model to an electric circuit made up of resistances (R), capacitances (C) and inductances (I), obtaining the results in a simple way by evaluating flows and efforts that join and connect the components of the model. Previously to obtaining the equations, a causal study is it necessary to do and, after do it, the resulting set of final equations is made up of as many differential equations “m” as there are type C or I ports with integral causality, and as many algebraic equations “n” as there are C or I ports with differential causality. That is, as many algebraic-differential equations exist as there are ports of one type or the other. This means that firstly a system formed by “m+n” equations needs to be resolved, and secondly for it to be done on a DAE system, with all the problems this involves. On the other hand, the resulting algebraic equations have emerged from a need to arbitrarily assign some or other causalities to different elements, such as R type ports or intermediate break variables, or as a result of the differential causality existing on different ports, since in both cases this is equivalent to introducing auxiliary variables. The ability possessed by causality for detecting algebraic loops and the relations presented by semi-state space variables in problems with DAE formulations has been studied by different authors with important differences about the correct procedure for resolving these systems.

The solution most frequently offered in the majority of cases is the introduction of highly rigid springs in order to eliminate loops between different ports of one or other type of causality. The problem arising from these elements being introduced is the appearance of stiff behaviour, it being necessary to use specific numerical methods. Another commonly used option for eliminating problems arising from the appearance of loops is the use of Lagrange multipliers. In both cases, the final number of equations is the same, their being equal to the number of inertias or springs initially existing, plus those corresponding to the introduction of new elements. Some proposals for opening algebraic loops established between resistor and storage ports with different causality are based on the introduction of flow or effort sources whose value is zero or the use of the zero residual value, which equations thus added are equivalent to those generated with the introduction of Lagrange multipliers. Other authors works with different sub-bond equivalencies before carrying out causal assignation, which is useful for simplifying Bond Graph models, but a modification of the initial model is required. Finally, other option is the use of break variables for opening arising causal loops, which generate a series of algebraic equations and the mathematical model thus obtained is a DAE one; the main advantage offered by this method is the non-modification of the initial bond graph model.

In most cases, when it is wished to simulate a BG model, the problem can usually be resolved by calculating the flows and efforts on the different bonds, at each step of the integration, thereby ignoring the equations represented by the BG. On other occasions, when the system of equations has been obtained for the model, the numerical values of the different variables and expressions are substituted. We can then resort to specific mathematical methods for operations such as a derivation or integration during the course of the simulation. This, when added, in some cases to the existence of a series of variable auxiliaries, excessively complicates the simulation, quantitatively as well as qualitatively.

In the presented work, an automatic procedure for reducing a system of algebraic-differential equations to a purely differential one, i.e. the minimum number of equations, within a simulation model carried out with a bond graph, and based only on causal assignation, is presented. Depending on the different types of Zero Order Causal Path (ZCP) and algebraic loops coexisting in a Bond Graph model, through a succession of algebraic operations carried out on matrices, the method is capable of obtaining a system of reduced equations. One advantage of this approach is the ease with which the matrix simplification can be programmed by means of a series of operations and derivations, which is especially interesting when it comes to generating symbolic equations for a bond graph model, once they have been reduced and simplified. In each ZCP case will firstly develop the different algorithms and it will then applied to a model, all of this using the Bond Graph technique.

## Stability analysis of a railway wheelset alongwith track structure using bondgraphs

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**Abstract:** The dynamics of railway vehicle on tangent track is dominated by motions in lateral plane commonly refereed as hunting. Vehicle running stability or hunting is a phenomenon associated with conically shaped wheels. The conical wheels provide a lateral guidance or centering action which tends to force the wheels into the tread region whenever the wheelset is displaced laterally from the centre. The friction or creep forces between the wheel and rail are a function of vehicle speed. As the speed increases, a value can be reached at which the vehicle rail system has zero effective damping and a sustained periodic oscillation is set up. This state is called hunting and the speed at which it occurs is called the critical speed. A railway vehicle becomes unstable beyond a critical speed. Assessment of the critical speed is important for safety and passenger comfort. The dynamics of a railway vehicle is essentially governed by the dynamics of a wheelset on track. Bond graph model of a wheelset system on flexible tangent track with tack structure has been created. Kalker's linear creep formulation has been used for rail-wheel contact forces. The model is simulated for a given set of nominal parameters value to study the lateral stability behavior of the wheel set on flexible tangent track.

This paper studies the dynamic behavior of a railway wheelset in different operating conditions, and investigates the effect of track structure on the stability and performance of the wheelset. The system studied combines the conventional wheelset along with the complete track structure including rail, sleeper, ballast, sub ballast etc. A comprehensive analysis is made to study characteristics of the wheelset and more importantly interactions between the wheelset and the track structure.

**Keywords:** Wheelset, Lateral Dynamics, Bond Graph, Conicity, Critical Speed

## **Analysis of Flexural Vibration of Cracked Rotating Shaft through Extended Lagrangian Formulation**

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### **Abstract**

This paper deals with the extended Lagrangian formulation for one-dimensional cracked continuous systems. The variational formulation for this system is similar to an internally and externally damped rotor driven through a dissipative coupling; however the umbra-Lagrangian density contributed by stiffness is different. Using such formulation, the invariance of the umbra-Lagrangian density is obtained through an extension of Noether's theorem.

The cracked rotor shaft is modeled as a Rayleigh beam. The dynamic analysis of the rotor shaft is obtained and validated through simulation studies. Results show an interesting phenomenon of limiting behaviour of the rotor shaft with internal damping beyond certain threshold speeds, which are obtained theoretically and affirmed by simulation. The results show that regenerative energy in the rotor shaft due to internal damping is dissipated through the external damping as well as the dissipative coupling between drive and the rotor shaft. With considering the stiffness variation of the cracked shaft, the amplitude of the rotor increases. In such case, with increase in the excitation frequency, the shaft amplitudes become huge, which further propagates the cracks.

*Key Words:* Umbra-Lagrangian density, Noether's theorem, Flexural vibration, cracked rotor.

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**Classical and Quantum Circuits**





# LAGRANGIAN AND HAMILTONIAN FORMULATIONS FOR CLASSICAL AND QUANTUM CIRCUITS

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Lagrange and Hamilton formulations yield powerful methodologies for the analysis of nonlinear circuits. In this contribution the application of Lagrange and Hamilton methods to classical electric circuits and to circuit quantum electrodynamics is discussed. The formulation of the Lagrangian and Hamiltonian equations for lossless electric circuits including linear and nonlinear circuit elements is treated.

The considered circuits are subdivided into a linear embedding circuit and the embedded nonlinear circuit elements. The linear lossless reciprocal embedding networks are represented by equivalent canonical Foster multiport circuits. The two kinds of canonical Foster multiport circuits are considered, i.e. the Foster admittance multiport circuits consisting of series resonant circuits coupled via ideal transformer networks to the ports and the Foster impedance multiport circuit consisting of parallel resonant circuits coupled by ideal transformer networks to the ports. The Foster multiports can be established also for distributed circuits, either by analytical electromagnetic full-wave analysis or by numerical full-wave analysis with subsequent system identification as described by [1] and [2].

In classical mechanics *Lagrangian* and *Hamiltonian* formulations provide a deeper insight and yield powerful methodologies for the analysis of complex systems, see for example [3]. Solving the Euler-Lagrange equations of a physical system yields the path for which the action functional is stationary. [4] has extended the application of Lagrangian formulations to electrical circuits. The embedding Foster circuits are represented as a Lagrangian or Hamiltonian system with port variables, where in the case of the Foster admittance representation the electric charges or in the case of the Foster impedance representation the magnetic fluxes are taken as the generalized coordinates. The complete Lagrangians and Hamiltonians for the circuits with embedded nonlinear capacitors or nonlinear inductors are derived.

Mesoscopic circuits in modern nanoelectronics can exhibit quantum behavior. On the basis of the of the classical Hamiltonian description of circuits a circuit quantum electrodynamic representation is introduced. As examples classical and quantum Josephson circuits are discussed. A quantum system does not follow a single path with stationary action, but the behavior of the system depends on a superposition of permitted paths. The time evolution of the quantum state is governed by the *Schrödinger equation* in which the system is described by the *Hamilton operator*, see for example [5]. For the treatment of circuits governed by quantum mechanics the Hamilton operator, describing the quantum mechanical system, is obtained from the classical Hamilton function of the lumped element equivalent circuit by substituting the classical state variables by the corresponding quantum mechanical operators.

As an example for a nonlinear circuit element the Josephson element is discussed. The Josephson effect is a macroscopic quantum effect, yielding a nonlinear dependence of the Josephson current on the integral of the applied voltage over time [6]. Its classical dynamic properties correspond to a nonlinear inductor. Mesoscopic Josephson structures can exhibit quantum dynamics, [7], [8], [9]. As a device dual to the Josephson element the Bloch wave oscillator is introduced.

- [1] P. Russer, *Electromagnetics, Microwave Circuit and Antenna Design for Communications Engineering*, 2nd ed. Boston: Artech House, 2006.
- [2] L. B. Felsen, M. Mongiardo, and P. Russer, *Electromagnetic Field Computation by Network Methods*. Berlin, Heidelberg, New York: Springer, 2009.
- [3] H. Goldstein, *Classical Mechanics*, 2nd ed. London: Addison Wesley, 1980.
- [4] D. A. Wells, "Application of the lagrangian equations to electrical circuits," *Journal of Applied Physics*, vol. 9, no. 5, pp. 312–320, May 1938.
- [5] A. Messiah, *Quantum Mechanics*. Amsterdam: North-Holland Publishing Company, 1964, vol. I.
- [6] K. K. Likharev, *Dynamics of Josephson Junctions and Circuits*, 3rd ed. Amsterdam, The Netherlands: Gordon and Breach, 1996.
- [7] F. X. Kaertner and P. Russer, "Generation of squeezed microwave states by a dc-pumped degenerate parametric Josephson junction oscillator," *Physical Review A*, vol. 42, no. 9, pp. 5601–5612, Nov. 1990.
- [8] P. Russer and J. A. Russer, "Nanoelectronic RF Josephson devices," *IEEE Transactions on Microwave Theory and Techniques*, vol. 59, no. 10, pp. 2685–2701, Oct. 2011.
- [9] A. Mátyás, C. Jiruschek, F. Peretti, P. Lugli, and G. Csaba, "Linear circuit models for on-chip quantum electrodynamics," *Microwave Theory and Techniques, IEEE Transactions on*, vol. 59, no. 1, pp. 65–71, 2011.

# MEMORY ELEMENTS: A PARADIGM SHIFT IN LAGRANGIAN MODELING OF ELECTRICAL CIRCUITS

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**Introduction.** Memristors, meminductors, and memcapacitors [1] constitute an increasingly important class of two-terminal circuit elements whose resistance, inductance, and capacitance retain memory of the past states through which the elements have evolved. All three elements are nonlinear and can be identified by their pinched hysteresis loop in the voltage versus current plane, current versus flux plane, and voltage versus charge plane, respectively. While there are many discovered experimental realizations and applications of systems that exhibit memristive behavior, ranging from applications in non-volatile nano memory to intelligent machines with learning and adaptive capabilities, the number of systems showing memcapacitive and meminductive behavior is still somewhat limited. Nevertheless, several applications of these concepts are foreseen in the field of logic and arithmetic operations using memristive and memcapacitive devices, and field-programmable quantum computation using meminductive and memcapacitive devices [2].

**Contribution.** In this paper we consider circuits made from memristors, meminductors, and memcapacitors and their conventional counterparts in the Lagrangian framework [3]. It will be shown that meminductors and memcapacitors do not allow a Lagrangian formulation in the classical sense since these elements are nonconservative in nature and the associated energies are not state functions. To circumvent this problem, a different configuration space is considered that, instead of the usual loop charges, consist of time-integrated loop charges. The Lagrangian is defined by the difference between two novel state functions in a fashion similar to the usual magnetic co-energy minus electric energy setup, but having the dimensions of energy times time-squared which is equivalent to action times time. As a result, the corresponding Euler-Lagrange equations provide a set of integrated Kirchhoff voltage laws in terms of the element fluxes. Memristive and resistive losses can be included via the introduction of a second scalar function that has the dimension of action. A dual variational principle follows by considering variations of the integrated node fluxes and yields a set of integrated Kirchhoff current laws in terms of the element charges.

Although integrated charge, which in SI units is measured in Coulomb times seconds, is a somewhat unusual quantity in circuit theory, it may be considered as the electrical analogue of a mechanical quantity called absement. Absement (a contraction of absence and displacement) is measured in meters times seconds and its rate of change coincides with position. One meter-second corresponds to being absent one meter from a reference point for the duration of one second. Based on this analogy, simple mechanical devices are presented that can serve as didactic examples to explain memristive, meminductive, and memcapacitive behavior.

- [1] Di Ventra, M., Pershin, Y., and Chua, L. (2009). Circuit elements with memory: memristors, memcapacitors and meminductors. *Proc. of the IEEE*, 97(10), 1717–1724.
- [2] Pershin, Y. and Di Ventra, M. (2011). Memory effects in complex materials and nanoscale systems. *Advances in Physics*, 60(2), 145–227.
- [3] Jeltsema, D. and Scherpen, J. (2009). Multi-domain modeling of nonlinear networks and systems: energy- and power-based perspectives. *IEEE Control Systems Magazine*, 29(4), 28–59.

# NOISE IN FREQUENCY-SENSITIVE ESR DETECTORS

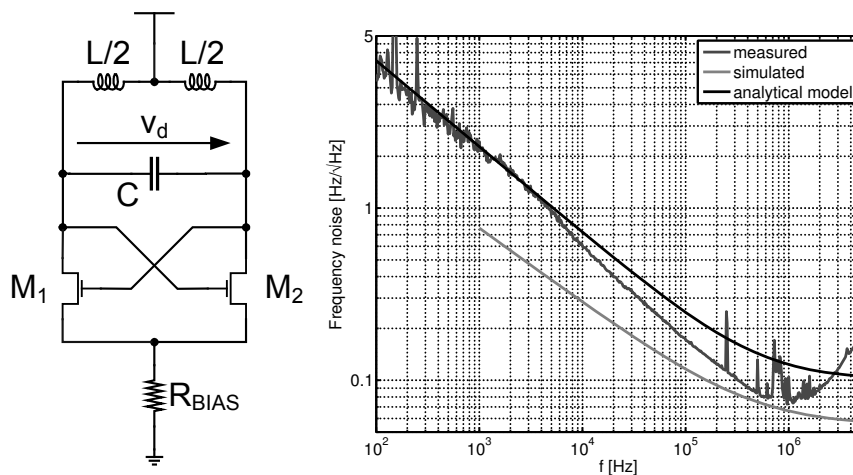
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In our talk, we discuss a method for computing analytical expressions for the phase, frequency and amplitude noise in LC tank oscillators using the stochastic averaging method proposed by Stratonovich in [1]. Our approach combines advanced MOS transistor modeling using the EKV model [2] with the solution of stochastic differential equations modeling the behavior of the noisy oscillator. We then apply our approach to the specific case of a frequency-sensitive electron spin resonance (ESR) detector as introduced in [3]. The circuit proposed there is of great interest, because it uses an intrinsically nonlinear circuit (the LC tank oscillator as shown schematically in Fig. 1(a)) to detect the resonance of an electron spin ensemble. Using our approach it becomes possible to investigate how the thermal noise associated with the loss of the tank inductance establishes a frequency noise floor for the frequency-sensitive detector and thereby sets the detection threshold. Combined with an energy-based approach for the signal calculation our noise models then allows us to estimate the achievable signal-to-noise ratio and thereby obtain an analytical expression for the limit of detection for this type of frequency sensitive ESR detectors. Finally, the theoretical results are verified against simulations performed in a commercially available circuit simulation tool as well as measured data obtained from a CMOS prototype of the frequency sensitive ESR detector. Fig. 1(b) shows such a comparison for the detector's equivalent frequency noise. From the figure it is clear that the proposed model provides results which are accurate enough to allow us to compute the noise floor in frequency-sensitive ESR experiments and thereby, together with the energy-based signal model, compute the limit of detection for frequency-sensitive ESR detectors.



(a) Schematic of an LC tank oscillator (b) Comparison of the measured frequency noise of the LC tank oscillator, a simulation performed using a commercially available circuit simulator and the proposed analytical model.

- [1] Stratonovich R.L.: *Topics in the theory of random noise*. Mathematics and its applications, Gordon and Breach, New York, rev. english edition, 1963.
- [2] Enz, C., Krummenacher F., Vittoz E.A.: *An Analytical MOS Transistor Model Valid in All Regions of Operation and Dedicated to Low-Voltage and Low-Current Applications*. Analog Integrated Circuits and Signal Processing Journal on Low-Voltage and Low-Power Design, 8:83-114, July 1995.
- [3] Yalcin T, Boero G.: *Single-chip detector for electron spin resonance spectroscopy*. Review of Scientific Instruments, 79(9), 2008.

# STOCHASTIC BEHAVIOR OF DISSIPATIVE HAMILTONIAN SYSTEMS WITH LIMIT CYCLES

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**Abstract.** The statistical behavior of complex physical systems can be discussed within the framework of statistical mechanics. However the most powerful tools of statistical mechanics are restricted to systems which are in the thermal equilibrium or near the thermal equilibrium where the Casimir-Onsager theory is available; see e. g. [1]. If we would like to consider systems that are far away from the thermal equilibrium only a few concepts are developed. The most prominent systems of this kind are electronic oscillators, lasers and some chemical reactions where so-called limit cycles arise. It is well-known that limit cycles are possible only if nonlinearity as well as energy supply and energy dissipation occur such that these systems are far away from thermal equilibrium. The deterministic behavior of this class of systems corresponds from a statistical point of view to the average behavior and the mathematical concept of dynamical systems based on nonlinear analysis can be used. Although a generalisation to stochastic dynamical systems is available a suitable relationship to the physical constraints of statistical mechanics does not exist.

On the other hand in classical mechanics of nonlinear systems the Hamilton's concept can be applied in a successful manner and there is a close relationship of Hamilton mechanics and the framework of statistical mechanics. Unfortunately Hamilton mechanics is restricted to systems with energy conservation. For this purpose some generalisations of Hamilton mechanics to systems with energy dissipation are known in the literature but these concepts are not close related to Hamilton mechanics if systems with limit cycles are considered. In this paper we will present an alternative generalisation of Hamilton mechanics that includes dissipation and allows limit cycles in a natural way. These so-called canonical dissipative systems (CD systems) [2], [3] which are described by  $((q, p) \in \mathbf{R}^n \times \mathbf{R}^n)$

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q} - g(H) \frac{\partial H}{\partial p}, \quad (1)$$

where Hamilton's function  $H = H(q, p)$  and a suitable function  $g(H)$  have to be prescribed. We assume that the zero set  $\mathcal{Z} := \{(q, p) \in \mathbf{R}^n \times \mathbf{R}^n | g(H(q, p)) = 0\}$  corresponds the set of all points of the limit cycle under consideration and where the CD system is a pure Hamilton system. In this case the trajectory remains in  $\mathcal{Z}$  if its initial point is an element of  $\mathcal{Z}$ . For the limit cycle behavior a stochastic variant of the corresponding CD system can be constructed where an ensemble concept from statistical mechanics can be applied. We illustrate the concept of stochastic CD systems for the stochastic analysis of a certain class of electronic oscillator circuits. Finally we study the statistical behavior of the so-called Cassini system where under certain conditions two limit cycles arise.

- [1] Kreuzer H. J.: *Nonequilibrium Thermodynamics and its Statistical Foundations*. Clarendon Press, 1981.
- [2] Ebeling W., and Sokolov I. M.: *Statistical Thermodynamics and Stochastic Theory of Nonequilibrium Systems*. World Scientific, 2005.
- [3] Thiessen T., and Mathis W.: *On Noise Analysis of Oscillators Based on Statistical Mechanics*. Intern. Journ. of Electronics and Telecommunications, 56 (2010), 357–366.

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## DESCRIBING HUMAN EMOTIONS THROUGH MATHEMATICAL MODELLING

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**Abstract** To design a companion technology we focus on the appraisal theory model to predict emotions and determine the appropriate system behaviour to support Human-Computer-Interaction. Until now, the implementation of emotion processing was hindered by the fact that the theories needed originate from diverging research areas. Due to this fact, divergent research techniques and result representations are used. Since this difficulty arises repeatedly in interdisciplinary research, we investigated the use of mathematical modelling as an unifying language to translate the coherence of appraisal theory. We found that the mathematical category theory supports the modelling of human emotions according to the appraisal theory and hence assists the implementation.

**Introduction** The correlation between human cognition, emotion and behaviour has been in the focus of research for several years. Historically these subjects were believed to be separate, and research on these different fields led to a good, basic understanding of each. However, the challenge of Human-Computer-Interaction (HCI) is to understand the interdependence of these fields, to combine the available knowledge and to use this interdisciplinary understanding to design human-adaptable and human-supportive systems.

Research in the field of HCI is not only challenging due to its interdisciplinary aspects, but it is also hindered by the fact that human cognition, emotion and behaviour are investigated by researchers from different disciplines. This has led to dissimilar research methods, goals, specifications and results.

Mathematics as an unifying modelling language can assist to combine research results of groups originating from different disciplines. This may lead to a better understanding of the interdisciplinary field of study and enhance research on the topic. We claim that the mathematical formalisation of emotion theories can support the study of emotions regarding origin, alteration and interaction with cognition and behaviour. We further claim that the mathematical description of research results from the area of emotion studies will support and facilitate the study and development of affective systems.

**Designing affective systems** For a system to be recognised by its users as affective, the system needs to have information and knowledge about the user's emotions.

For our task to design a companion technology (cf. [1]) we focus on the appraisal theory model (cf. [2]) to predict emotions and choose the appropriate system behaviour to support the HCI. The appraisal theory model allows both an understanding of when emotions arise and how emotions can be categorised.

To provide a system with information on emotions according to the appraisal model, the precise relation between user response patterns, appraisals and emotions must be known and feasible in technical terms.

Stating the appraisal theory in terms of category theory (cf. [3]) leads to the description of emotions as mathematical categories, consisting of appraisals as objects. Appraisals in terms are derivable from the observable response patterns, cf. [2, p.92-120]. Additionally, category theory establishes the links between objects of a category in terms of morphisms between the objects and in these terms allows further investigations regarding the correlations between categories.

**Summary** Category theory is a mathematical tool that allows a more formal description of appraisal theory. This facilitates the verification of derivations from the theory and promises a deeper understanding of the coherence of emotions. For the implementation of appraisal theory this is a tremendous advantage and may hence generally support the implementation of emotion processing.

- [1] A. Wendemuth, S. Biundo, *A Companion Technology for Cognitive Technical Systems*. COST 2012 Conference "Cross Modal Analysis of Verbal and Nonverbal Communication", February 21-26, 2011, Dresden, Germany
- [2] K. R. Scherer, A. Schorr and T. Johnstone, Eds., *Appraisal processes in emotion: Theory, Methods, Research*, Oxford University Press New York and Oxford 2001
- [3] Saunders Mac Lane, *Categories for the Working Mathematician*. Second Edition, Springer Verlag 1998

# A COGNITIVE ASSISTANT FOR SUPPORTING AIR TARGET IDENTIFICATION ON NAVY SHIPS

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During a simulation study a cognitive assistant (COGAS) is being developed for supporting the crew of a combat information centre (CIC) on Navy ships during air target identification. COGAS is a cognitive system that defines its own behaviour in its own natural or artificial environment (1, 2).

COGAS is based on Rasmussen's Decision Ladder (3), which describes the behaviour of well-trained and motivated operators controlling complex dynamic systems. The main activities modelled by the ladder are situation identification, goal determination, task selection and action accomplishment. These activities represent functional components of COGAS as well. Additionally, COGAS should configure the human machine interface (HMI) of the operator in charge. In order to carry out these activities both knowledge about the current situation and a priori knowledge about the domain of interest have to be applied. The current situation knowledge of surroundings is provided by sensors as tracks and their attributes like speed and altitude. The a priori domain knowledge will be stored by means of corresponding models which describe expected surroundings, relevant system goals, operator tasks and actions as well as display configurations. COGAS links the current situation knowledge with its own a priori knowledge, makes decisions and gives proposals for actions. The conceptual system description for COGAS is being developed through a simulation study and implemented by means of the Integrated Performance Modelling Environment (IPME).

The system description includes the surroundings model and functional relations between track relevant variables. In addition, it also includes models of goals, tasks, and actions with their hierarchical structures and their activation conditions. These conditions are specified by means of decision tables and implemented as boolean expressions. The content of the display configuration model will be defined through conducting further research. IPME is a simulation tool for modelling and simulating work processes of various operators by means of task networks. Parameters that describe work process are processing duration, system functions, performance failure, and various operator workload indices in order to determine workload of operators by means of multiple simulation runs.

This contribution describes the functional structure of COGAS and its various model components. Furthermore, the IPME task structure of COGAS and the crew members will be explained.

- [1] Onken R., Schulte A.: System-ergonomic design of cognitive automation. Studies in Computational Intelligence, Vol. 235, Springer, Berlin, 2010.
- [2] Putzer, H.J.: Ein uniformer Architekturansatz für kognitive Systeme und seine Umsetzung in ein operatives Framework. Wissenschaftliche Schriftenreihe Luft –und Raumfahrttechnik, Band 15. Berlin: Verlag Dr. Köster, 2004.
- [3] Rasmussen, J. (1976). Outlines of a Hybrid Model of the Process Plant Operator. In: Sheridan, T. B., Johanssen, G.: Monitoring Behavior and Supervisory Control. Plenum Press, New York., 1976, 371-391



# MODELING AND ANALYSIS OF HUMAN NAVIGATION WITH CROSSING INTERFERER USING INVERSE OPTIMAL CONTROL

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**Abstract.** The walking paths of humans in everyday life exhibit specific characteristics. Our investigation takes the well-established perspective that human locomotion approximately fulfills suitable optimality principles when walking from a starting position to a designated end position. Here, we address the special task of collision avoidance with a crossing interferer. While our model of the dynamics is quite simple, we focus on the task of determining the cost function out of a parametric family, that results in a best fit between the corresponding optimal control-based navigation and given recorded data of human navigation. The resulting bilevel optimization problem combines an optimal control problem on the lower level with a data fitting problem on the upper level. Our solution strategy uses the first-order optimality conditions of the (discretized) optimal control problem to transform the bilevel problem to a standard (one-level) optimization problem.

Modeling aspects concerning the walking process and especially the interfering person are discussed. Since human walking motions with a crossing interferer do not seem to be globally optimal, an MPC-like approach distinguishing between obstacle avoidance and free motion is introduced and optimization results using recorded human data are presented.

**Introduction.** The analysis of human motions is a long-standing research area and especially in the context of technical systems that mimic human strategies and cooperate with humans the interest in the underlying principles is still increasing. For human arm motions several cost functions were presented in the literature, but further research showed that each of the cost functions can only explain a limited range of motions. Thus, we consider a parameterized family of cost functions and search for the optimal parameters to explain the characteristics of a task at hand [1]. In the context of human locomotion the idea of determining the optimal cost function via inverse optimal control is introduced in [2]. There, obstacle-free paths are considered and the family of cost functions is given by the convex combinations of five basic cost functions. The bilevel problem is solved by nesting the individual solvers for the data fitting problem and the optimal control problem. It is reported that the characteristics of the human motion data are met and the results are used to control a humanoid robot.

The goal of our research is to extend the problem class to navigation problems with moving obstacles, e.g., crossing persons. Therefore, we consider additional cost functions and treat some of the modeling parameters as further optimization variables, which introduces additional nonlinearities with respect to the parameters of the family of cost functions. To solve this bilevel problem, we use a transformation approach based on the KKT-conditions of the discretized optimal control problem and solve the resulting nonlinear optimization problem with the interior-point code IPOPT [3].

**Structure of the Paper.** Our full paper starts with a description of the mathematical problem structure and a summary of our solution strategy. Followed by a section discussing details of the modeling process. First, a dynamical model of the walking person consisting of simple integrator chains is introduced, then several cost functions being the basis for the parametric family of cost functions are stated and finally, distance measures are discussed to suitably compute the differences between the computed trajectory of the optimal control problem and the recorded human data. Next, we state the experimental setup used to record human walking paths. In the numerical results section examples of the bilevel optimization results are presented including a task with a crossing interferer where the main characteristics of the observed avoidance maneuver are reproduced.

*This work is the result of a cooperation of the Chair of Mathematical Optimization (TUM), the Institute of Automatic Control Engineering (TUM) and the Center for Sensorimotor Research (LMU) partially funded by the cluster of excellence "Cognition for Technical Systems" (CoTeSys) within the Excellence Initiative of the DFG. Part of the numerical computations were performed on a Linux cluster supported by DFG grant INST 95/919-1 FUGG.*

- [1] S. Albrecht, M. Leibold, and M. Ulbrich. A bilevel optimization approach to obtain optimal cost functions for human arm movements. accepted by *Numerical Algebra, Control and Optimization (NACO)*, 2011.
- [2] K. Mombaur, A. Truong, and J.-P. Laumond. From human to humanoid locomotion - an inverse optimal control approach. *Autonomous Robots*, 28:369–383, 2010.
- [3] A. Wächter and L.T. Biegler. On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Math. Program.*, 106:25–57, 2006.

# PLANNING MODELS FOR TWO-WAY AVOIDANCE AND REVERSAL LEARNING

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The framework of reinforcement learning (RL), in particular temporal difference (TD) learning, is traditionally utilized to model Pavlovian and Instrumental Learning in animal and human subjects. Neurophysiological correlates' model parameters, on the level of both single cells and fMRI data, support this approach. Notably, most of these models are applied to appetitive learning, as their nature demands that reinforcement is directly related to an action. In aversive learning this is not the case, at least not for directly observable actions of the animal. Therefore RL models of avoidance learning are studied only relatively recently.

Previous work ([3]) has presented a study to investigate an extended RL model in the context of two-way avoidance and reversal learning in an animal experiment. It also found, that RL models can explain various aspects of two-way avoidance learning but do not provide a rationale for the relationship found between dynamics of initial learning and dynamics of reversal learning. However, the Artificial Intelligence (AI) paradigm of Automated Planning can provide a rationale for explaining such relationships.

AI planning offers the possibility to conceptualize the animal's cognitive processes by providing an explicit representation of and reasoning about internal processing stages. In a first step, the experiment is formalized in terms of an initial state that encodes the mental state of the (trained or untrained) animal subject and an abstract specification of the series of trials without the contingency reversal. We then make use of hierarchical, i.e., decomposition-based planning for implementing the abstract trial specifications: The planning system stepwise derives more and more concrete configurations of cognitive processes that are consistent with the specified subject's decision making procedure and with its knowledge about the world. Given a suitable planning strategy that minimizes negative feedback according to the predicted subject performance, this leads to a "best-case" reference plan of the animal for the trials in a non-contingency scenario.

Reversal learning can then be expressed by means of re-configuring the previously planned processes in order to meet the changes in the environment. An induced contingency reversal is consequently modelled as an instance of an execution failure of the reference plan that assumed a non-contingent scenario. The now failed reference plan is repaired accordingly by adding knowledge/behavior updates as explicit learning steps and by changing the implementation of complex sub-processes, respectively. We used AI plan repair techniques that try to address a failed plan in a way that only a minimal amount of change is introduced to the previous plan structure while causal consistency is restored and at the same time the observed failure is adequately taken into account. Please note that re-establishing the plan's causality focuses only on constructing a coherent view on the modeled subject and experiment. I.e., in some parts of the plan, it will be "easier" for the repair procedure to include a knowledge update process that fixes a number of wrong-based decisions of the subject, in other parts, minimal change translates into merely discovering and assessing that the subject made a wrong decision. Hence, the repair method does not necessarily prevent negative feedback for the subject. In this way, repairing the reference plan becomes a qualitative model for the effort it takes to re-establish a consistent cognitive process.

The AI planning model has two particularly interesting properties in this context: First, the repair strategy mimics the biological principle of minimal change, and secondly, the causal structure of the model takes explicitly into account all interdependencies of the subject's acquired knowledge. Our hybrid planning ([2]) and plan repair approach ([1]) thereby demonstrates that the empirically found relationships could be motivated from a consistent theoretical framework.

Future work aims at a more integrated model of RL and planning, as well as at investigating details of the conceptualization like the subject's feature selection mechanism's complexity and the granularity of actions in the knowledge update and decision-response processes.

- [1] Julien Bidot, Susanne Biundo, and Bernd Schattenberg. Plan repair in hybrid planning. In *Proceedings of the 31st German Conference on Artificial Intelligence*, volume 5243 of *Lecture Notes in Artificial Intelligence*, pages 169–176. Springer, 2008.
- [2] Susanne Biundo and Bernd Schattenberg. From abstract crisis to concrete relief – A preliminary report on combining state abstraction and HTN planning. In *Proceedings of the 6th European Conference on Planning*, pages 157–168, 2001.
- [3] A. L. Schulz, B. Schattenberg, M. L. Woldeit, A. Brechmann, S. Biundo, and F. W. Ohl. Reinforcement learning and planning models for two-way-avoidance and reversal learning. In *Proceedings of the Annual Meeting of the Society For Neuroscience*, Washington, USA, 2011.

# FORMAL MODELLING AND IDENTIFICATION OF OPERATING ERRORS FOR FORMAL USER INTERFACE RECONFIGURATION

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**Introduction.** Human error in human-machine interaction is frequently the source of catastrophic accidents. Research, especially in the field of psychology, has identified various reasons why such errors occur. One important example is the situation awareness model described by Endsley in [1], which measures human awareness of the current situation involving the machine, its state and the overall environment. Based on this information, humans decide the next step in controlling a machine. In [3], Parasuraman describes the converse situation: automated control, in which a number of state changes are made in the machine without the user's knowledge.

**Goals.** Our work seeks to include results from psychological research to generate formal models of human error that identify errors in interaction during runtime and reconfigure user interfaces [5]. The principal intention of the reconfiguration is to modify the user interface in such a way that in future interaction, the identified error occurs less frequently or is prevented completely. This study is motivated by positive results achieved in a 2010 case study at the University of Duisburg-Essen, which found user interface reconfiguration to have a highly significant impact on the number of errors made while controlling a complex process [8].

**Approach.** This paper introduces a new approach to the adaption of user interfaces by identifying input errors from a given user interface through modeled error automata. These error automata will also be used to generate reconfiguration rules for formal reconfiguration of a user interface on its logical layer paired with modeled patterns derived from psychological guidelines. These guidelines seek to describe concepts, such as enhancing situation awareness through physical rearrangement in certain control situations, or by increasing or decreasing the level of automation. The logical layer of a user interface describes the data processing of events occurring through input to the user interface or data sent by the system to be controlled. Furthermore, the logical layer models dependencies between interaction elements (button, sliders, text fields, etc.) on the user interface's physical representation. The whole process, starting with the generation of error automata and ending with reconfiguration of the user interface, is implemented based on a formal approach to user interface modeling and reconfiguration, as well as on formal description of deterministic finite automata (DFA).

The formal generation of error DFAs stems from the error classification introduced by Hollnagel in [9]. In combination with a given expert DFA describing correct interaction sequences using a certain user interface, error-class specific algorithms generate error DFAs automatically. Interaction sequences can be analyzed, and typical errors identified when those sequences serve as input to the error DFAs. The interaction sequence can be inputted from a file (offline analysis) or directly during interaction (online analysis).

Based on the identified error and its associated error automaton, formal reconfiguration rules can be automatically created to reconfigure the given user interface in such a way that the identified error in the current situation will be prevented in future interaction.

**Conclusion.** The final paper will present research on the modeling and generation of Hollnagel's error classification as DFAs. The choice of the specific formalism will be argued in accordance with a word problem describing the complexity of the decision as to whether or not an automaton accepts a specific task (here, an interaction sequence). Beside the classic type of DFAs, more general automata will be examined to deal with time-dependent errors regarding errors such as 'too early' or 'too late'. Furthermore, the use of formalisms such as non-deterministic finite automata and Petri nets will be discussed as a future work issue to extend the DFA-based approach to more general and more complex error pattern detection in a number of situations, including context-sensitive modeling. The generation of reconfiguration rules will be described in combination with the UIEditor framework, which was recently developed for formal modeling, simulation and reconfiguration of user interfaces.

- [1] Endsley, M. R.: *Measurement of situation awareness in dynamic systems*. Human Factors, 37(1), 1995, 65-84.
- [2] Parasuraman, R., and Riley, V.: *Humans and automation: Use, misuse, disuse, abuse*. Human Factors, 39(2), 1997, 230-253.
- [3] Weyers, B.: *Adaptive User Interface Design for Controlling and Observing Human-Machine Systems*. Dissertation, University of Duisburg-Essen, 2011.
- [4] Weyers, B., Burkolter, D., Kluge, A., and Luther, W.: *Formal modeling and reconfiguration of user interfaces for reduction of human error in failure handling of complex systems*. International Journal of Human Computer Interaction, accepted, 2011.
- [5] Hollnagel, E.: *Cognitive Reliability and Error Analysis Method*. Elsevier, Amsterdam, 1998.

# RATIONALITY THROUGH ANALOGY - TOWARDS A POSITIVE THEORY AND IMPLEMENTATION OF HUMAN-STYLE RATIONALITY

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**Introduction.** At times, human behavior seems erratic and irrational. Still, it is widely undoubted that humans can act rational and, in fact, appear to act rational most of the time, still making humans the gold standard for “natural” rational agents. Based on ideas from vernacular psychology, in many cases rational beliefs are interpreted as a foundation of rational behavior, making beliefs and knowledge, i.e. the epistemic aspects of rationality, one of the main concerns (and also main access points) when attempting to model and reproduce human rationality.

In the following, starting out from previous work on computational analogical reasoning, which resulted in the development of a theory for formal analogy-making, Heuristic-Driven Theory Projection, and the computational implementation HDTP (cf., e.g., [1]), we propose an architecture for a computational model that links rationality to basic cognitive capacities of humans, emphasizing the role of the human ability to establish analogical relations. On a very abstract level, the proposed architecture can functionally be subdivided into four steps: Given a problem description and domain, select and retrieve analogical situations from memory (**retrieval**). Use the problem as target domain for an analogy, the retrieved situation as base domain, and establish an analogy between both (**mapping**). Transfer solution-relevant knowledge from the base domain to the target domain via the analogical mapping (**transfer**). Apply the newly obtained knowledge in the target domain (i.e. the problem domain) for solving the problem (**application**).

One of the main advantages of such a cognitively-inspired architecture is the positive rather than normative character of the underlying theory of rationality, allowing for deviations from classical paradigms of rationality and seeming “rationality errors”, thereby also accounting for peculiarities of human-style rationality.

**Cornerstones of an Architecture for Human-Style Rationality.** In HDTP, base and target domains for analogy-making are represented as theories in a first-order logical language. Given the problem as target domain for the analogy, the *retrieval* problem comes down to selecting a fitting domain from memory as base domain. This can be done in different ways, for example by means of a separate module, or by forcing HDTP to construct analogies between all possible pairings of the target domain with a candidate base domain, subsequently taking the heuristics value HDTP computed when constructing the analogy as a measure for analogical distance between domains and proceeding e.g. with the analogically closest domain as base domain for the analogy. Of course, the outcome of the retrieval process does not have to be unique, and always strongly depends on the heuristics or distance measures used, thereby introducing a degree of uncertainty into the system (matching the uncertainty and irregularities humans exhibit in their decision and rationality behavior).

Once a base and target domain have been identified, HDTP constructs an analogical relation between both, *mapping* between elements from base and target domain. The construction of this mapping is based on a generalization mechanism, guided by a heuristics which tries to keep the analogy as simple (i.e. less general) as possible, whilst still maximizing the sub-theories of the sources which can be reinstated from the generalization (a trade off close in spirit to the precision/recall problem in pattern recognition and information retrieval). Also here, in most cases the mappings between elements of the respective domains do not have to be unique (e.g. different elements of the base could be mapped to one certain element of the target domain), again introducing a source of uncertainty. In the transfer phase, knowledge from the (with respect to problem solutions richer) base domain is transferred to the target domain (i.e. the problem at hand). Making use of the mappings established in the previous step, the concepts from the base domain are reinstated from the generalized theory into the target domain, enriching the latter and giving additional information needed for computing a solution to the problem.

In the last step, the newly added knowledge is *applied* in the target domain (e.g. used for reasoning and inference), yielding a solution to the problem. This step also includes a consolidation process, integrating the transferred knowledge into the target domain, giving an expanded or richer domain.

Of course, this type of architecture leaves ample space for uncertainty and deviating behavior: Apart of the already mentioned systemic influences, a certain chance of deviation from HDTP’s predicted outcome for a certain problem situation is automatically introduced by the use of logical theories as descriptive framework for situations and problems. As with every symbolic formalization, decisive information might accidentally be left out of considerations when formulating the domain descriptions. Nonetheless, we don’t see this as a major drawback, but rather as a natural constraint every system trying to predict a phenomenon as complex as human rational behavior has to face, and which even holds in the case where humans try to predict each others actions and decisions.

[1] A. Schwering, U. Krumnack, K. Kühnberger, and H. Gust. Syntactic principles of heuristic-driven theory projection. *Cognitive Systems Research*, 10(3):251–269, 2009.

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# FINITE ELEMENT APPROXIMATION OF THE STOCHASTIC LANDAU-LIFSHITZ-GILBERT EQUATION

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**Introduction.** The evolution of magnetization in ferromagnetic materials under the influence of thermal noise can be described by the stochastic Landau-Lifshitz-Gilbert (SLLG) equation

$$\begin{aligned} d\mathbf{m}(t, \mathbf{x}) &= \left[ -\alpha \mathbf{m}(t, \mathbf{x}) \times \left( \mathbf{m}(t, \mathbf{x}) \times \mathbf{H}_{\text{eff}}(t, \mathbf{x}) \right) - \mathbf{m}(t, \mathbf{x}) \times \mathbf{H}_{\text{eff}}(t, \mathbf{x}) \right] dt \\ &\quad + \nu \mathbf{m}(t, \mathbf{x}) \times \circ d\mathbf{W}(t, \mathbf{x}) \\ \partial_n \mathbf{m}(t, \mathbf{x}) &= 0 \\ \mathbf{m}(0, \mathbf{x}) &= \mathbf{m}_0(\mathbf{x}) \end{aligned} \quad \begin{aligned} \forall (t, \mathbf{x}) \in (0, T) \times D, \\ \forall (t, \mathbf{x}) \in (0, T) \times \partial D, \\ \forall \mathbf{x} \in D, \end{aligned}$$

where ‘ $\circ$ ’ denotes stochastic integration in the Stratonovich sense,  $\alpha$  is a damping constant and  $\nu$  is a temperature dependent parameter. The magnetization field  $\mathbf{m} = (m_1, m_2, m_3)$  satisfies a sphere constrain  $|\mathbf{m}| = 1$ . The vector valued Wiener process  $d\mathbf{W} = (W_1, W_2, W_3)$  models the effects of the thermal noise. The effective field  $\mathbf{H}_{\text{eff}}$  may include a number of terms derived from the free energy, such as, e.g., exchange, anisotropy and magnetic field, i.e.,  $\mathbf{H}_{\text{eff}} = \Delta \mathbf{m} + (\mathbf{m} \cdot \mathbf{p})\mathbf{p} + \mathbf{H}$ . The magnetic field  $\mathbf{H}$  introduces coupling with Maxwell’s equations and the vector  $\mathbf{p}$  is a material dependent (uniaxial) anisotropy direction.

**Numerical approximation.** We fix  $T > 0$  and denote by  $I_k$  an equi-distant partition of  $[0, T]$  into  $n$  sub-intervals of (local) size  $k = T/n$ ; we denote  $\varphi^{j+1/2} := \frac{1}{2}(\varphi^{j+1} + \varphi^j)$ . For simplicity we set  $\mathbf{H}_{\text{eff}} = \Delta \mathbf{m}$ . A finite-element based algorithm for the SLLG equation is given below.

**Algorithm A.** Let  $\mathbf{M}^j \in \mathbf{V}_h$  be given for some time level  $j \geq 0$ . The solution  $\mathbf{M}^{j+1} \in \mathbf{V}_h$  on the next time level is determined from

$$\begin{aligned} (\mathbf{M}^{j+1} - \mathbf{M}^j, \Phi)_h &= -\alpha k \left( \mathbf{M}^{j+1/2} \times [\mathbf{M}^{j+1/2} \times \tilde{\Delta}_h \mathbf{M}^{j+1}], \Phi \right)_h - k (\mathbf{M}^{j+1/2} \times \tilde{\Delta}_h \mathbf{M}^{j+1}, \Phi)_h \\ &\quad + \nu (\mathbf{M}^{j+1/2} \times \Delta \mathbf{W}^{j+1}, \Phi)_h \quad \forall \Phi \in \mathbf{V}_h, \end{aligned}$$

where  $\mathbf{V}_h$  is a finite element space of piecewise linear vector fields,  $(\cdot, \cdot)_h$  is a discrete (mass lumped) inner product, and  $\tilde{\Delta}_h$  is a discrete Laplace operator.

We consider two type of the noise: a noise uniform in space and a space-time white noise. For the space uniform noise we employ  $\mathbb{R}^3$ -valued Brownian increments with independent normally distributed components with zero mean and variance  $k$ , i.e.,

$$\Delta \mathbf{W}^{j+1} = \mathbf{W}(t_{j+1}) - \mathbf{W}(t_j) \sim \mathcal{N}(\mathbf{0}, k\mathbb{I}_3).$$

The space-time white noise is approximated as in [2].

It can be shown, c.f., [1, Lemma 4.1] that the solutions to Algorithm A, and satisfy a discrete sphere constraint, as well as an energy bound (for sufficiently regular noise) at finite times.

**Lemma 1.** *Suppose that  $|\mathbf{M}^0(\mathbf{x}_\ell)| = 1$  for all  $\ell \in L$ . Then the sequence  $\{\mathbf{M}^j\}_{j \geq 1}$  generated by Algorithm A satisfies for all  $j \geq 0$*

$$\begin{aligned} \text{(i)} \quad & |\mathbf{M}^j(\mathbf{x}_\ell)| = 1 \quad \forall \ell \in L, \\ \text{(ii)} \quad & \mathbb{E} \left[ \sup_{1 \leq j \leq J} \frac{1}{2} \|\nabla \mathbf{M}^j\|_{L^2}^2 + \alpha k \sum_{j=1}^J \|\mathbf{M}^{j+1/2} \times \tilde{\Delta}_h \mathbf{M}^{j+1}\|_h^2 \right] \leq C_{TJ}, \end{aligned}$$

where  $\mathbf{x}_\ell$ ,  $\ell = 1, \dots, L$  are the vertices of the finite element mesh.

We discuss efficient implementation strategies for Algorithm A and present a number of computational studies including: long-time behaviour of finite ensembles of magnetic spins, finite-time finite-energy blow-up behaviour of solutions, and thermal fluctuations in magnetic nanoparticles.

- [1] Bañas L., and Brzeźniak Z., and Prohl A.: *Convergent Finite Element Based Discretization of the Stochastic Landau-Lifshitz-Gilbert Equations*. Submitted.
- [2] L. Bañas, Z. Brzeźniak, A. Prohl, *Computational studies for the stochastic Landau-Lifshitz-Gilbert equation*. Submitted.

# AN EFFECTIVE INTEGRATOR FOR THE LANDAU-LIFSHITZ-GILBERT EQUATION

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The understanding and development of magnetic materials is of utter relevance for example in magneto-resistive storage devices. In the literature it is well-accepted that dynamic micromagnetic phenomena are described best by the Landau-Lifshitz-Gilbert equation (LLG). The non-dimensional formulation of this model reads

$$\begin{aligned}\mathbf{m}_t &= -\alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{H}(\mathbf{m})) + \mathbf{m} \times \mathbf{H}(\mathbf{m}), \\ \mathbf{m}(0) &= \mathbf{m}_0 \quad \text{in } H^1(\Omega; \mathbb{S}^2), \\ \partial_n \mathbf{m} &= 0 \quad \text{on } (0, \tau) \times \partial\Omega, \\ |\mathbf{m}| &= 1 \quad \text{a.e. in } (0, \tau) \times \Omega,\end{aligned}$$

where the ferromagnetic behavior of the body  $\Omega \subset \mathbb{R}^3$  is characterized by the vector valued magnetization  $\mathbf{m} : (0, \tau) \times \Omega \rightarrow \mathbb{R}^3$ . Here  $\mathbf{H}(\mathbf{m})$  denotes the total magnetic field, including exchange energy, anisotropy energy, stray-field energy, as well as Zeeman energy.

Numerical challenges for the time integration arise from the strong non-linearity, the non-convex side constraint  $|\mathbf{m}| = 1$  as well as from the non-local dependence of the demagnetization field  $\mathcal{P}(\mathbf{m})$  from the magnetization  $\mathbf{m}$ .

The great number of applications as well as the amount of numerical issues makes LLG of equal interest for both, physicists and mathematicians, and thus the scientific community benefits in many ways.

In our contribution we generalize the approach of ALOUGES, cf. [1], to the total magnetic field, i.e. including all four energy terms. Since the computation of the non-local demagnetization field is the most time and memory consuming part of the simulation, the proposed time integrator is split into an implicit part and an explicit part. The first one deals with the higher-order term  $\Delta \mathbf{m}$  stemming from the exchange energy, whereas the lower-order terms, collected in  $\mathbf{H}_{\text{low}}(\mathbf{m})$ , are treated explicitly. We derive the following time-splitting scheme by calling  $\mathbf{v} = \mathbf{m}_t$  and discretizing the weak form of an alternative but equivalent formulation of LLG according to  $P^1$ -FEM with piecewise affine and globally continuous functions, i.e. we use  $\mathcal{V}_h = \mathcal{S}^1(\mathcal{T}_h)^3$  to discretize functions in the spatial variable with  $\mathcal{T}_h$  a quasi-uniform and regular triangulation of  $\Omega$  into tetrahedra and  $\mathcal{N}_h$  the set of its nodes:

**Algorithm.** *Input:* Initial data  $\mathbf{m}_h^0 \in \mathcal{M}_h := \{\phi_h \in \mathcal{V}_h \mid |\phi_h(\mathbf{z})| = 1 \text{ for all } \mathbf{z} \in \mathcal{N}_h\}$ , damping parameter  $\alpha$ , parameter  $\theta$ .

(i) Compute  $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j} := \{\phi_h \in \mathcal{V}_h \mid \phi_h(\mathbf{z}) \cdot \mathbf{m}_h^j(\mathbf{z}) = 0 \text{ for all } \mathbf{z} \in \mathcal{N}_h\}$  by solving the (regular) linear system

$$\alpha \int_{\Omega} \mathbf{v}_h^j \cdot \boldsymbol{\Psi}_h + \int_{\Omega} (\mathbf{m}_h^j \times \mathbf{v}_h^j) \cdot \boldsymbol{\Psi}_h = - \int_{\Omega} \nabla(\mathbf{m}_h^j + \theta k \mathbf{v}_h^j) \cdot \nabla \boldsymbol{\Psi}_h + \int_{\Omega} \mathbf{H}_{\text{low}}(\mathbf{m}_h^j) \cdot \boldsymbol{\Psi}_h$$

for all test functions  $\boldsymbol{\Psi}_h \in \mathcal{K}_{\mathbf{m}_h^j}$ .

(ii) Set  $\mathbf{m}_h^{j+1}(\mathbf{z}) = \frac{\mathbf{m}_h^j(\mathbf{z}) + k \mathbf{v}_h^j(\mathbf{z})}{|\mathbf{m}_h^j(\mathbf{z}) + k \mathbf{v}_h^j(\mathbf{z})|}$  for all nodes  $\mathbf{z} \in \mathcal{N}_h$  and go to (i).

*Output:* Sequence of functions  $\mathbf{v}_h^j \in \mathcal{K}_{\mathbf{m}_h^j}$  as well as  $\mathbf{m}_h^{j+1} \in \mathcal{M}_h$  for  $j \geq 0$ .

In contrast to previous works, the most important benefit of our scheme is that only one linear system per time-step has to be solved. Finally, our analysis allows to replace the operator  $\mathcal{P}$  which maps  $\mathbf{m}$  onto the corresponding demagnetization field, by a discrete operator  $\mathcal{P}_h$ . Possible choices for  $\mathcal{P}_h$  are given by an extended convolution operator, the FEM-BEM coupling, or the hybrid FEM-BEM approach proposed in FREDKIN/KOEHLER, cf. [2], which is mostly used in the Physics literature. As the original algorithm, our extension guarantees the non-convex side constraint to be fulfilled as well as unconditional convergence.

- [1] Alouges F.: *A new finite element scheme for Landau-Lifchitz equations*. In: Discrete and Continuous Dynamical Systems Series S, Vol. 1, 2008, 187-196.
- [2] Fredkin D., and Koehler T.: *Hybrid method for computing demagnetizing fields*. In: IEEE Transactions on Magnetics 26, 1990, 415-417.
- [3] Goldenits P., Hrkac G., Page M., Praetorius D., Schrefl T., and Süß D.: *Effective Simulation of the Dynamics of Ferromagnetism*. Work in progress, 2012.



# NUMERICAL INTEGRATOR FOR THE LLG EQUATION WITH MAGNETOSTRICTION

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Ferromagnetic materials are utilized in a broad spectrum of devices and thus the understanding of the magnetic processes within such devices is essential for both industry and scientific community. In our work, we consider the Landau-Lifshitz-Gilbert (LLG) equation

$$\begin{aligned} \mathbf{m}_t &= -\alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{H}(\mathbf{m})) + \mathbf{m} \times \mathbf{H}(\mathbf{m}) \\ \mathbf{m}(0) &= \mathbf{m}_0 \quad \text{in } H^1(\Omega; \mathbb{S}^2) \\ \partial_n \mathbf{m} &= 0 \quad \text{on } (0, \tau) \times \partial\Omega \\ |\mathbf{m}| &= 1 \quad \text{a.e. in } (0, \tau) \times \Omega, \end{aligned}$$

which models the evolution of magnetization, coupled with the equation of elastodynamics

$$\rho \mathbf{u}_{tt} - \nabla \cdot \boldsymbol{\sigma} = 0 \quad \text{in } (0, \tau) \times \Omega$$

to include the magnetostrictive effects. Here,  $\mathbf{H}(\mathbf{m})$  denotes the total magnetic field and  $\boldsymbol{\sigma}$  denotes the so-called stress tensor.

We modify the approach of ALOUGES, cf. [1] to cover more general energy terms and combine it with the approach of BANAS and SLODICKA from [2] for the discretization of the second equation. As proposed by GOLDENITS ET. AL in [3], the LLG equation is integrated by a linear-implicit time-splitting algorithm. In addition, the two equations can be decoupled which makes the implementation easier, since one only has to solve two linear systems per timestep. Under some stability assumptions, we prove unconditional convergence to a weak solution of the coupled system, where we do not need any assumptions on the regularity of the exact magnetization  $\mathbf{m}$  but only on the regularity of  $\mathbf{u}$  and  $\boldsymbol{\sigma}$ .

- [1] F. Alouges, *A new finite element scheme for Landau-Lifshitz equations*. Discrete and Continuous Dynamical Systems Series S, Vol. 1, 2008, p.187-196
- [2] L. Banas, M. Slodicka *Error estimates for Landau-Lifshitz-Gilbert equation with magnetostriction*. Applied Numerical Mathematics, Vol. 56, 2006, p.1019-1039.
- [3] P. Goldenits, G. Hrkac, M. Page, D. Praetorius, D. Süss, *Effective Simulation of the Dynamics of Ferromagnetism*. work in progress, 2012.

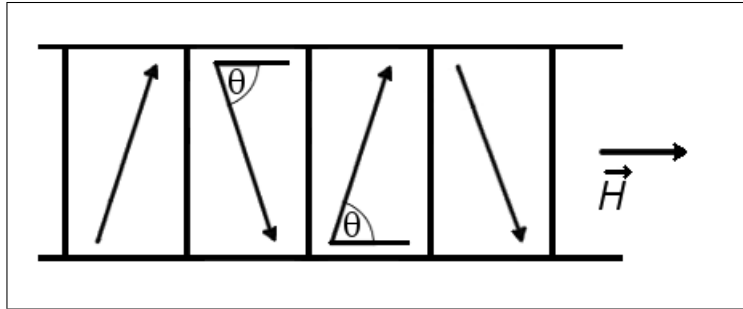
## MECHANICAL OSCILLATIONS OF MAGNETIC STRIPS UNDER THE INFLUENCE OF EXTERNAL FIELD

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By application of a magnetic field on an amorph metallic strip, the orientation of magnetisation of Weiss domains can be changed. We try to replicate this effect with finite elements to get a feasible model.

We solved the onedimensional wave equation for a metallic strip.



Orientation of magnetisation of Weiss domains on a metallic strip

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} E \left( \frac{\partial u}{\partial x} - \frac{3\lambda_s}{2} \left( \cos^2(\theta) - \frac{1}{3} \right) \right) \quad (1)$$

Here  $u$  is the displacement and  $E$  Young's modulus.

The right hand side of equation (1) contains the magneto-mechanical coupling. The angle of the magnetization is given by  $\theta$ , and  $\lambda_s$  is the magnetostriction constant.

This coupling is nonlinear as the magnetization angle depends on the external field  $H$  and the local stress  $\sigma(X)$  via the following set of equations:

$$\cos(\theta) = \frac{H}{H_{A\sigma}} \quad (2)$$

$$H_{A\sigma} = \frac{2K_u - 3\lambda_s\sigma}{J_s} \quad (3)$$

After discretisation with linear finite elements equations (1) to (3) build an differential - algebraic system, which we solve with the software code IDA.

- [1] L'ubomír Bañas: *On dynamical Micromagnetism with Magnetostriction*. PHD Thesis June 2005 University of Gent
- [2] J.D.Livingston: *Magnetomechanical Properties of Amorphous Metals*. phys. stat. sol. (a) 70, 591 (1982)

# DOMAIN CONFIGURATIONS IN SOFT FERROMAGNETIC FILMS UNDER EXTERNAL FIELD

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**Model problem.** We consider a cylindrical ferromagnetic sample  $\Omega = \omega \times (0, t)$  with diameter  $\text{diam}(\Omega) \sim 1$ . Its magnetization is, on a mesoscopic scale, a vector field  $\mathbf{M} : \Omega \rightarrow \mathbb{R}^3$  of constant length  $|\mathbf{M}| = 1$ . We assume *soft* material and apply a constant external field  $\mathbf{H}_{\text{ext}}$ . The micromagnetic free energy due to Landau and Lifschits [3], in an appropriately scaled form, reads

$$E(\mathbf{M}) = d^2 \int_{\Omega} |\nabla \mathbf{M}|^2 dx + \int_{\mathbb{R}^3} |-\nabla U|^2 dx - 2 \int_{\Omega} \mathbf{H}_{\text{ext}} \cdot \mathbf{M} dx, \quad (1)$$

cf. [2]. The stray-field  $\mathbf{H}_{\text{str}} = -\nabla U$ , which is induced by a potential  $U : \mathbb{R}^3 \rightarrow \mathbb{R}$ , is determined through the magnetostatic Maxwell equation. Local minimizers of the energy are (meta) stable states of the physical system, and the model is well accepted to reflect many relevant features of pattern formation in ferromagnetic material.

**Reduced model.** In [2], DeSimone, Kohn, Müller, and Otto derived a reduced model for the simulation of *thin, large, and soft* ferromagnetic samples. In the reduced model, the magnetization is an in-plane vector field  $\mathbf{m} : \omega \rightarrow \mathbb{R}^2$  that satisfies the constraints  $|\mathbf{m}| \leq 1$  in  $\omega$  and  $\mathbf{m} \cdot \nu = 0$  on  $\partial\omega$ . The reduced energy reads

$$e(\mathbf{m}) = \int_{\mathbb{R}^3} |-\nabla u|^2 dx - 2 \int_{\omega} \mathbf{h}_{\text{ext}} \cdot \mathbf{m} dx. \quad (2)$$

Analysis reveals that the energy is determined only by the (negative) divergence  $\sigma = -\nabla \cdot \mathbf{m}$  of the magnetization. In particular, minimizers of the reduced energy are not uniquely determined, but we can single out a relevant minimizer  $\mathbf{m}^*$ , which we call the *effective magnetization*.

**Domain pattern via viscosity solution.** Domain patterns are of major interest, and in [2] the authors give a heuristic approach to reconstruct a Landau-like structure from the effective magnetization: Given  $\mathbf{m}^*$ , one can compute the viscosity solution of

$$|(\mathbf{m}^*)^\perp + \nabla \psi| - 1 = 0 \text{ in } \omega \quad \text{with boundary condition } \psi = 0 \text{ on } \partial\omega. \quad (3)$$

The combined quantity  $(\mathbf{m}^* - \nabla^\perp \psi)$  is an admissible magnetization of unit length and has the same divergence, i.e. the same energy, as  $\mathbf{m}^*$  itself. This minimizer reveals a kind of domain pattern that coincides well with available data, at least for certain experimental set-ups. The reconstruction of the domain structure via the viscosity solution  $\psi$ , however, is not very well justified: First, interface energy, i.e. the cost of micromagnetic walls, is not measured. Second, hysteresis as observed experimentally in [1] cannot be simulated with this method.

**Wall energy driven pattern formation.** We enhance the reconstruction of domain patterns to overcome these two points of criticism while preserving numerical tractability. Given  $\mathbf{m}^*$ , we seek a stream function  $\psi^*$  that minimizes an Aviles-Giga type functional

$$G_\varepsilon(\psi) = \varepsilon \int_{\omega} |D^2 \psi|^2 dx + \frac{1}{\varepsilon} \int_{\omega} g(|(\mathbf{m}^*)^\perp + \nabla \psi|^2 - 1) dx. \quad (4)$$

The choice of the function  $g$  is delicate. Our goal is to obtain an asymptotically correct resolution of the wall energies as  $\varepsilon \rightarrow 0$ . Estimates of wall-energies, depending on the angles of the magnetization, are computed a priori by a different asymptotic model derived from the Landau-Lifschits energy (1), and these values enter the definition of  $g$ .

The fourth order Euler-Lagrange equation corresponding to (4) allows not only to prescribe the values of  $\psi$  at  $\partial\omega$ , but also the normal derivative  $\partial_\nu \psi$ . At the regions where  $|\mathbf{m}^*| < 1$  and no walls touch the boundary, we have  $(\nabla \psi^* + (\mathbf{m}^*)^\perp) \cdot \nu \in \{\pm 1\}$ . The viscosity solution of (3) corresponds to the fixed choice  $(\nabla \psi + (\mathbf{m}^*)^\perp) \cdot \nu = -1$ . In contrast, we can now model the pinning of boundary vortices at material defects—as observed in [1]—by a change of sign in the boundary data. In particular, the new approach allows us to model hysteresis, and hence observe the *formation of walls and other relevant patterns* apart from the Landau state.

- [1] H. van den Berg, D. Vatvani, *Wall Clusters and Domain Structure Conversions*, IEEE Transactions on Magnetics, Vol. 18(3), 880–887, 1982.
- [2] A. DeSimone, R. V. Kohn, S. Müller, and F. Otto, *A reduced theory for thin-film micromagnetics*. Comm. Pure Appl. Math., Vol. LV, 1408–1460, 2002.
- [3] L. D. Landau, E. M. Lifschits, *On the theory of the dispersion of magnetic permeability in ferromagnetic bodies*, Phys. Zeitsch. der Sow., 8:153–169, 1935.

## LOW RANK TENSORS AS POSSIBLE TOOL FOR MICROMAGNETICS

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In recent years, the use of low rank tensor structured formats have been recognized as an important concept for breaking the “*curse of dimensionality*“ in multidimensional numerics, [1, Khoromskij], related to material sciences, bio-science, stochastic modeling, signal processing, machine learning and data mining. These methods, which lead to a linear scaling in a given dimension, are strongly linked with the idea of separation of variables and fast evaluation of multilinear algebra operations of the structured function-related tensors, [2, 3, 4].

In [5, Goncharov et al.] the *canonical tensor format* was first used for an approximate representation of the demagnetizing tensor for the purpose of accelerating magnetostatic computations. Following pioneering works [2, Hackbusch and Khoromskij], the method introduced in [6] represents an analytically-based tensor representation approach for the computation of the magnetostatic scalar potential. Furthermore, recently developed optimization-based methods for low-rank tensor approximation, [7, 8, 9], make it possible to extend previous algorithmic developments for magnetostatics to (static) micromagnetics (minimization of the *total magnetic Gibb's free energy*).

We will present recent ideas in the field of low-rank tensor methods, which are promising for future applications in computational micromagnetics.

- [1] B. N. Khoromskij. Survey on Tensor-structured Numerical Methods in Scientific Computing. *Preprint 21/2010, Max-Planck-Institut für Mathematik in den Naturwissenschaften*, 2010.
- [2] W. Hackbusch and B. N. Khoromskij. Low-rank Kronecker-product approximation to multi-dimensional nonlocal operators. part i. separable approximation of multi-variate functions. *Computing*, 76(3-4):177–202, 2005.
- [3] B. W. Bader and T. G. Kolda. Efficient MATLAB computations with sparse and factored tensors. *SIAM Journal on Scientific Computing*, 30(1):205, 2008.
- [4] T. G. Kolda and B. W. Bader. Tensor decompositions and applications. *SIAM Review*, 51:455–500, 2009.
- [5] A. Goncharov, G. Hrkac, J. Dean, and T. Schrefl. Kronecker product approximation of demagnetizing tensors for micromagnetics. *Journal of Computational Physics* 229:2544–2549, 2010.
- [6] L. Exl, W. Auzinger, S. Bance, M. Gusenbauer, F. Reichel, T. Schrefl. Fast stray field computation on tensor grids. *Journal of Computational Physics*, submitted 2011. preprint: arXiv:1109.5878v2 (2011)
- [7] M. Espig, W. Hackbusch, T. Rohwedder, and R. Schneider. Variational Calculus with Sums of Elementary Tensors of Fixed Rank. *Preprint 52/2009, Max-Planck-Institut für Mathematik in den Naturwissenschaften*, 2009.
- [8] M. Espig and W. Hackbusch. A Regularized Newton method for Efficient Approximation of Tensors Represented in the Canonical Tensor Format. *Preprint 78/2010, Max-Planck-Institut für Mathematik in den Naturwissenschaften*, 2010.
- [9] E. Acar, D. M. Dunlavy and T. G. Kolda. A Scalable Optimization Approach for Fitting Canonical Tensor Decompositions. *J. Chemometrics* 25(2):67-86, 2011.

# ALGORITHMIC OPTIMIZATION OF STRAY-FIELD COMPUTATIONS

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**Introduction.** The numerical calculation of the magnetic stray field is the most time consuming part of micromagnetic simulations. The long ranged stray field takes into account the dipole-dipole interactions between all particles, which leads to a computational complexity of  $\mathcal{O}(N^2)$  for a naive implementation with  $N$  being the number of simulation cells. Several methods have been proposed to reduce this complexity.

We use a combined FFT–finite-difference method to calculate the stray field in the area of interest with a complexity of  $\mathcal{O}(N \log N)$ . Compared to the standard procedure which applies the demagnetization tensor, our method offers a speedup of approximately 1.5 and memory savings of up to 30%. The latter improvement is especially interesting in the context of GPU computing, since even modern GPUs offer only a small amount of memory as compared to the RAM used by CPU codes.

**Content.** The scalar potential  $\phi$  of the magnetic stray field  $H_{\text{st}}$  is the solution of a poisson equation

$$\Delta\phi = \nabla \cdot M \quad \text{and} \quad H_{\text{st}} = -\nabla\phi \quad (1)$$

A standard procedure for the fast computation of the stray field applies the demagnetization tensor  $\tilde{N}$  [1]:

$$H_{\text{st}}(r) = - \int \tilde{N}(r-r')M(r')dr' \quad (2)$$

On a regular grid this tensor–vector convolution can be numerically solved by applying the fast Fourier transform. The fast Fourier transform reduces the computational complexity of the convolution from  $\mathcal{O}(N^2)$  to  $\mathcal{O}(N \log N)$ .

However computing the scalar potential via the fast Fourier transform is still faster since the number of Fourier transforms is reduced.

$$\phi(r) = \int S(r-r')M(r')dr' \quad (3)$$

The stray field  $H_{\text{st}}$  can then be calculated as the gradient of the scalar potential, see (1). In order to gain a good accuracy of the stray field, care has to be taken on the discretization choice for the scalar potential. We propose to compute the scalar potential on the vertices of an equidistant cuboid grid [2]. In order to compute the convolution (3), we derive an analytical expression for the convolution kernel  $S$ .

**Implementation.** We implemented the demagnetization tensor method and the scalar potential with the micromagnetic simulation code MicroMagnum [3]. Both methods are implemented on the CPU as well as on the GPU. The scalar-potential method offers a platform independent speedup of up to 1.55.

- [1] Newell A. J., Williams W., and Dunlop D. J.: *A generalization of the demagnetizing tensor for nonuniform magnetization*. Journal of Geophysical Research, vol. 98, no. B6, pp. 9551–9555, June 1992.
- [2] Abert C., Selke G., Krüger B., and Drews A.: *A Fast Finite-Difference Method for Micromagnetics Using the Magnetic Scalar Potential*. IEEE Transactions on Magnetics, in press.
- [3] *MicroMagnum*. <http://micromagnum-tis.informatik.uni-hamburg.de/>

# COUPLING LLG WITH MAGNETOSTATIC MAXWELL EQUATIONS

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**Abstract.** Various applications ranging from spintronic devices, giant magnetoresistance (GMR) sensors, and magnetic storage devices, include magnetic parts on very different length scales. For example current storage devices consist of several macroscopic parts like magnetic shields or soft-underlayers, which have strong influence on their performance. Since using the Landau-Lifshitz-Gilbert equation (LLG) constrains the maximum element size to the exchange length within the media, it is not possible to simulate such macroscopic parts with this approach. On the other hand Maxwell's equations do not constrain the element size, but therefor cannot describe the short-range exchange interaction accurately. A combination of both methods allows to describe magnetic domains within the micromagnetic regime accurately using the LLG and also considers the macroscopic parts by a nonlinear material law using Maxwell's equations.

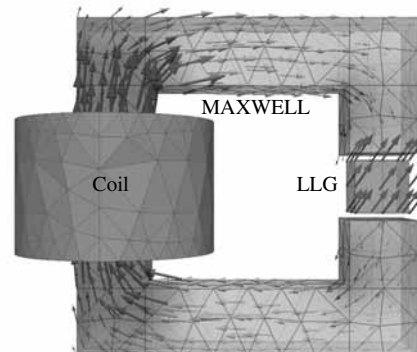
The LLG as well as magnetostatic Maxwell equations are solved using FEM/BEM algorithms for both regions (which are well separated). The strayfield interaction between the two models couples the micromagnetic part to the Maxwell part. For the time integration of the coupled system a variable-order, variable-step Backward Differentiation Formula (BDF) is used. The derived nonlinear problem is solved by a Newton-like algorithm which in turn applies a preconditioned generalized minimal residual method (GMRES) to the linear system of equations arising in each step.

A common method for strayfield calculation in the micromagnetic region is the hybrid Fredkin-Koehler FEM/BEM coupling [1], which consists of two consecutive steps. The first step uses finite elements to determine a potential inside of the micromagnetic part which describes the internal magnetic moments correctly. The second step then uses boundary elements to fulfill the proper boundary conditions at the surface of the magnetic parts. Finally both potentials are added and lead to a correct description of the strayfield of the micromagnetic part.

For the Maxwell part the situation is a bit more complex. Due to slightly modified boundary conditions it is no longer possible to use this two step approach. The Johnson-Nédélec FEM/BEM coupling [2] allows to handle arbitrary boundary conditions. This is achieved by combining FEM and BEM equations to one system of equations and solving them simultaneously. One drawback of the method is that it leads to non-symmetric matrices which require the use of a more general solver routine.

The algorithm is implemented using the open source solver suite SUNDIALS [3] which allows to solve implicit Differential-Algebraic-Equations (DAE) of the form  $F(t, y, y') = 0$ . For performance reasons H-matrix compression is used to handle the dense boundary element matrices. As a preconditioner only the next-neighbor interaction is considered, which can be described by sparse matrices and therefore be efficiently solved.

In order to validate the algorithm, simulation results of standalone micromagnetic problems, standalone Maxwell problems, as well as some combined problems are demonstrated.



Snapshot of an interacting example consisting of a coil which is driven by a square-wave signal (period  $3ns$ , risetime  $0.1ns$ ), a core described by Maxwell's equations (using a susceptibility of  $1e5$ ), as well as micromagnetic cube described by the LLG.

- [1] Fredkin D., and Koehler T.: *Hybrid method for computing demagnetizing fields*. IEEE Trans. Magn. 26 (1990) 415-417.
- [2] Johnson C., Nédélec J. C.: *On the coupling of boundary integral and finite element methods*. Math. Comp. 35 (1980) 1063-1079.
- [3] Hindmarsh A., et al: *SUNDIALS: suite of nonlinear and differential/algebraic equation solvers*. ACM Trans. Math. Softw. 31 (2005) 363-396.

# SILICON NITRIDE POTENTIAL FROM FIRST PRINCIPLES: REPARAMETERIZATION OF A TERSOFF POTENTIAL USING THE FORCE-MATCHING METHOD

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Optimization of high-performance solar cells depends largely upon the engineering of interfaces present in the device. Until now, modelling of solar cell devices has mainly been focused on modelling the electrical properties of the device, rather than the material properties. Usually cell parameters rely upon input of macroscopic properties such as band gap and empirical quantities such as contact resistance and carrier recombination. Modelling is normally done in 1-D, sometimes in 2-D and 3-D, using finite element programs.

We progress beyond the current state-of-the-art by utilizing atomistic simulation techniques based upon *ab initio* and classical potential models to provide non-empirical input for macroscopic models. We focus on two particularly important interfaces in the device, the electrical contacting interface, and the so-called passivation interface. The focus in our work is on the integration of modelling techniques to allow the simulation of properties over various time- and length-scales based on first principles techniques.

The passivation interface of a solar cell consists of a dielectric layer at the semiconductor surface, which acts to passivate defective geometries at the interface. We concentrate on the use of amorphous silicon nitride as a passivation layer. We use a Tersoff potential and simulated annealing to generate the amorphous structure.

Comparison of existing Tersoff potential models [1] for  $\text{SiN}_x$  to *ab initio* techniques revealed major differences in the topology of the amorphous networks generated with the different techniques, particularly in the presence of 4-ring structures in the network (figure 1). Thus we have re-parameterized the Tersoff potential for  $\text{SiN}_x$ .

We have parameterized our potentials using a force matching technique [2]. The basic concept of the force matching technique is to use the large amounts of data obtained from first principles calculations to fit the parameters for classical potentials. The computational fitting scheme allows for the derivation of better potentials with reduced human effort, whilst also addressing the problem of transferability of potential sets. The technique allows one to attack the traditional problem of transferability of potential sets at its very heart, by using *ab initio* data generated for a wide range of configurations and temperature.

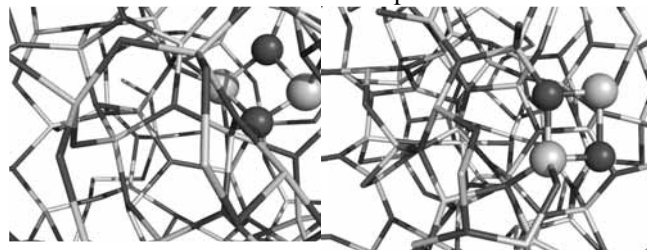


Figure 1 Snapshots from the full DFT MD simulation showing the presence of the 4-member Si-N-Si-N ring motif in the structure.

We improve the applicability of the Tersoff potential by re-fitting with a force-matching technique. However, as we will show, whilst the new parameterization yields improved structures, caution must be exercised in the transfer from classical potential to DFT simulations.

- [1] de Brito Mota, F., Justo, J. F. and Fazzio, A. (Structural properties of amorphous silicon nitride Phys. Rev. B ,1998, (58), 8323.
- [2] Ercolessi, F. Adams, J. B. *Interatomic potentials from ab initio simulations: The force-matching technique* , Europhys. Lett. 1994, (26) 583-588.

# COMPUTATION OF MAGNETIZATION NORMAL OSCILLATION MODES IN COMPLEX MICROMAGNETIC SYSTEMS

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The study of the normal oscillation modes of ferromagnetic nano-particle systems is a fundamental issue for its applications to the analysis of magnetization dynamics under microwave applied fields[1, 2]. In typical experimental situations, a small magnetic particle is saturated by applying a sufficiently strong DC magnetic field along a given direction. Small magnetization motions around this state are then excited by applying a small (compared to the DC component) radio-frequency (RF) applied field. In this condition, the ferromagnetic resonance curve is obtained by slowly varying either the frequency or the amplitude of the RF field and measuring the power absorbed by the particle. From the observation of the peaks in this curve, one determines the frequency values corresponding to the excitation of certain magnetization normal modes. This problem was theoretically analyzed by W.F. Brown and Aharoni [1, 3]. Their approach was based on the use of appropriate analytical techniques and was limited to particles of special shapes (spheres, ellipsoids).

Another scenario where the normal oscillations around an equilibrium play a fundamental role is in the modelling of thermal fluctuations. In fact, thermal agitation tends to slightly perturb the equilibrium magnetization and therefore, from the analysis of the resonant response of the micromagnetic system, one can retrieve insightful information about fluctuation and dissipation processes. For this reason, considerable research has been recently focused on numerical computations of normal modes for particles with generic shapes[4] and experimental observations involving spatially non uniform equilibrium magnetization configurations[5].

In this work, a general formulation of this problem is presented[6]. The small oscillation modes in complex micromagnetic systems around an equilibrium are numerically evaluated in the frequency domain by using a novel formulation, which naturally preserves the main physical properties of the problem. The Landau-Lifshitz-Gilbert (LLG) equation, which describes magnetization dynamics, is linearized around a stable equilibrium configuration and the stability of micromagnetic equilibria is discussed. Special attention is paid to take into account the property of conservation of magnetization magnitude in the continuum as well as discrete model. The linear equation is recast in the frequency domain as a generalized eigenvalue problem for suitable self-adjoint operators connected to the micromagnetic effective field. The generalized eigenvalue problem may be conveniently discretized by finite difference or finite element methods depending on the geometry of the magnetic system. The spectral properties of the eigenvalue problem are derived in the lossless limit. Perturbation analysis is developed in order to compute the changes in the natural frequencies and oscillation modes arising from the dissipative effects. It is shown that the discrete approximation of the eigenvalue problem obtained either by finite difference or finite element methods has a structure which preserves relevant properties of the continuum formulation.

This approach has several advantages as far as the numerical computation of the normal modes is concerned:

1. it may circumvent the problems of time-domain analysis for relatively low-frequency oscillations which are relevant, for instance, in magnetic vortex dynamics.
2. the discretized operator can be assembled by using the classical exchange and magnetostatic operators implemented in both finite differences and finite elements micromagnetic codes;
3. the discretized version of this problem is a standard self-adjoint matrix eigenvalue problem which can be solved with well-established techniques of numerical linear algebra.

The solution of this problem gives directly all the resonant frequencies and the normal modes. The results obtained by using this approach will be presented for several examples of complex micromagnetic systems.

- [1] W.F. Brown Jr, *Micromagnetics*, Interscience Publishers (1963).
- [2] H. Suhl, *Proc. IRE* 44, 1270 (1956); H. Suhl, *J. Phys. Chem. Solids* 1, 209 (1957).
- [3] A. Aharoni, *Introduction to the theory of ferromagnetism*, Oxford Press, New York (1996).
- [4] R.D. McMichael, M.D. Stiles, *Journal of Applied Physics* 97, 10J901 (2005).
- [5] K. Perzlmeier, M. Buess, C.H. Back, V.E. Demidov, B. Hillebrands, S.O. Demokritov, *Phys. Rev. Lett.* 94, 057202 (2005).
- [6] M. d'Aquino, C. Serpico, G. Miano, C. Forestiere, *Journal of Computational Physics* 228, 6130-6149 (2009).



PATH METHOD VS. STOCHASTIC THERMAL FIELD SWITCHING IN GRANULAR MEDIA-  
A MAGNETIC GRAIN STORY LOST BETWEEN LLG AND ENERGY-SPACE

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**Introduction.** A finite element micromagnetic[1] comparison study has been undertaken to describe the magnetization reversal dynamics of segregated CoCrPt-oxide perpendicular recording media as function of applied field angle. The effects of thermal activation (at T=150–350K) on  $H_{sw}$  were investigated by two different techniques: The nudged elastic band method (NEB) and a stochastic Landau-Lifshitz-Gilbert (LLG) approach were combined with the micromagnetic model to introduce the thermal activation in the system studied here. The results were compared to understand the quantitative and qualitative effect of the methods.

**Content.** The thermal stability calculation requires the information of the transition rates between the initial and final magnetization configuration of the magnetic grains. The NEB method [2, 3] initially guesses the minimum energy path (MEP) in the energy landscape between the two stable magnetization states. In order to obtain the MEP the energy is minimized until the energy gradient of the path points along the current path and the energy is constant along the path for any degree of freedom perpendicular to it. The MEP calculation provides an energy barrier  $E_b(\mathbf{H})$  of the transition in units of  $k_B T$  ( $k_B$  is the Boltzmann constant and  $T$  is the temperature) between the initial and final magnetic configurations of the grain at any given applied field and field angle. The energy barrier is directly associated with the thermal stability of the system.

In stochastic LLG approach the thermal activation is taken into account by expanding the LLG equation with the stochastic thermal field  $h_{th}$  term as follows [4, 5].

$$(1 + \alpha^2) \frac{dm}{d\tau} = -m \times (h_{eff} + h_{th}) - \alpha m \times [m \times (h_{eff} + h_{th})] \quad (1)$$

Where as in the equation  $m$  represents the normalized magnetisation vector,  $\alpha$  Gilbert damping constant,  $\tau$  is the time and  $h_{eff}$  is the normalized effective field. Here the thermal field accounts for the interaction effects of magnetization with macroscopic effects like conducting currents; nuclear spins etc. which leads to the fluctuation in the magnetization dynamics of the magnetic system under consideration [5]. As a result of effects posed by the interaction on the large number of degree of freedom the thermal field is described as Gaussian random distribution with the following statistical property:  $\langle h_{th}(t) \rangle = 0$ , which means that the average of the thermal field is taken over all realizations vanished in each direction space  $i \in \{x, y, z\}$  with the variance

$$\langle H_{th,i}(t); H_{th,j}(t') \rangle = 2D \delta_{ij} \delta(t - t') \quad (2)$$

Equation (2) is the similar to the fluctuation dissipation theorem and relates the strength of the fluctuation to the dissipation due to the damping. The different components of the system are uncorrelated and is expressed by the Kronecker delta  $\delta_{ij}$  whereas the Dirac  $\delta$  expresses the autocorrelation time of the thermal field is shorter then the response time of the system. The strength of the thermal fluctuation  $D$  is derived from the fluctuation dissipation theorem.

$$D = \frac{\alpha k_B T}{\gamma \mu_0 M_s V_i} \quad (3)$$

Where  $k_B$  is the Boltzmann constant,  $T$  is the temperature gyromagnetic ratio,  $M_s$  saturation magnetization and  $V_i$  surrounding the node of the finite element mesh.

- [1] T. Schrefl, G. Hrkac, G. Bance, D. Suess, O. Ertl, and J. Fidler, Handbook of Magnetism and Advanced Magnetic Materials, (Wiley, New York, 2007) **vol 2**, 765 (2007).  
 [2] R. Dittrich, T. Schrefl, D. Suess, W. Scholz, H. Forster, and J. Fidler, J. Magn. Magn. Mater. **250**, L12 (2002).  
 [3] D. V. Berkov, J. Magn. Magn. Mater. **186**, 199 (1998).  
 [4] W. Scholz, T. Schrefl, and J. Fidler, J. Magn. Magn. Mater., **233**, 296 (2001).  
 [5] G. Hrkac, T. Schrefl, J. Dean, A. Goncharov, S. Bance, D. Suess, and J. Fidler, J. Apl. Phys., **105**, 053901 (2009)



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# OPTIMAL CONTROL OF MOTION OF A ROBOT DRIVEN BY A MOVABLE INTERNAL BODY IN A RESISTIVE ENVIRONMENT

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A locomotion robot that can move in a resistive medium without special propelling devices (wheels, legs, caterpillars, etc.) due to the motion of internal bodies is considered. Such robots consist of the main body that interacts with the environment and auxiliary bodies that are movably connected to the main body, interact with it but do not interact with the environment. These auxiliary bodies will be referred to as the internal bodies, although it is not necessary that they are located inside the main body. The internal bodies interact with the main body by means of forces produced by the drives. The driving force applied to an internal body causes the reaction force applied to the main body. The reaction force changes the velocity of the main body relative to the environment, which leads to a change in the force of resistance of the environment to the motion of the main body. Therefore, by controlling the motion of the internal bodies, one can change the external force acting on the main body, thus controlling the motion of the entire system. This principle of motion seems to be reasonable to use for mini-sized locomotion robots. The main body of such robots can be made hermetic and smooth, without any protruding parts, which enables these robots to be used for nondestructive inspection of mini-sized engineering objects (e.g., thin-walled pipelines of small diameter), as well as in medicine.

The paper deals with the optimal control of a locomotion robot moving in a resistive medium due to the motion of an internal body. We consider a simple model of the robot with the internal body moving relative to the main body translationally along a straight line. The main body is assumed to move relative to the environment along the same line. For this model, it is required to find a periodic motion of the internal body relative to the main body that generates the motion of the main body relative to the environment with periodically changing velocity and provides a maximum for the displacement of the main body for the period. The period of the relative motion of the internal body is assumed to be prescribed and equal to the period of change of the velocity of the main body. The acceleration of the internal body relative to the main body or the force of interaction of these bodies is used as the control variable. Qualitative characteristics of the optimal motion, such as the number of switchings of the control function during the period, the absence or presence of a singular control mode, in which the control variable takes on an intermediate value between the minimum and maximum allowed values, the conditions for entering and leaving the singular mode, are investigated. It is proved that the singular mode necessarily occurs in the optimal motion in the environments, the law of resistance of which to the motion of the main body is characterized by a function of velocity that is odd and constant in convexity (upward or downward) when the argument is constant in sign. This fact is important, since such functions are widely used for modeling the resistance of viscous media to the motion of rigid bodies. For this class of resistance laws, the algorithms for calculating the optimal control are reduced to solving systems of finite equations for the control parameters.

# MODELING AND OPTIMIZATION OF CONTROL PROCESSES FOR COMPRESSIBLE LIQUID FLOW IN PIPELINE SYSTEMS

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**Summary.** Supplying buildings with water at desired pressure levels is an essential task for nowadays life. It requires reliable control of pipeline systems with numerous consumers to be supplied in a comfortable and safe way. Typical pipeline systems consist of several widespread elements, e.g. long tube sections transporting water with the help of some control pumps. Adequate mathematical models of the dynamics of pipelines, given in terms of partial differential equations (PDEs) have to take into account the distributed system characteristics, such as medium compressibility and variations of the fluid pressure and mass flow.

**Introduction.** The theoretical foundation for optimal control problems with linear PDEs and convex functionals was established by Lions [1]. Different approaches to the discretization of dynamical models with distributed parameters are being actively developed to reduce the original initial-boundary value problem to a system of ordinary differential equations (ODEs). In this context, variational and projection methods are powerful tools to solve control problems for elastic structures. The method of integrodifferential relations (MIDR) was proposed in [2] for the design of optimal control laws for dynamical systems with distributed parameters. A projection approach was developed as a modification of the Galerkin method in the frame of the MIDR for systems described by linear parabolic PDEs. In [3], control-oriented finite-dimensional system models have been derived for typical tree-style pipeline networks for pressure boosting systems in high-rise buildings. These models make use of a generalized network representation in which laminar and turbulent resistances of fluid flow, inertia properties and compressibility are mapped to lumped network parameters in the form of generalized nonlinear resistors, inductors and capacitors. These network models were used to design basic strategies for estimation of operating conditions on the basis of model-based state observers and for the development of novel sensitivity-based predictive control procedures.

Modeling and optimization of control processes for compressible fluid flow in pipeline systems are considered. A mathematical model of controlled elements with distributed parameters is proposed to describe the dynamical behavior of a long rigid tube with transported liquid supplied by a control pump. Functions describing effective displacements and linear approximations of fluidic resistances are used to reduce the original initial-boundary value problem to a variational formulation on the basis of the MIDR. Moreover, this approach makes use of a novel finite element technique. Optimal control procedures are derived for changing either the outlet pressure or the mass flow to desired operating points and to damp undesirable elastic oscillations at the end of the control process. A projection approach is implemented on the basis of a modification of the Galerkin method in combination with the semi-discretization of unknown functions over the spatial coordinate. This procedure is applied to reliable numerical modeling of a simple pipeline system and to the design of an efficient control procedure. Numerical results obtained for different system parameters and control objectives are analyzed and discussed.

**Conclusions and Outlook.** In this paper, a modeling and optimization algorithm has been derived for both pressure and mass flow control of distributed pipeline systems. Two feedforward control strategies have been developed based on the MIDR, a projection approach, and a novel finite element technique.

In future work, an offline identification of system parameters from measured data and design of a robust observer-based feedback control structure will be studied on the basis of the MIDR. Finally, we aim at performing an experimental validation of the proposed control strategies on suitable test rigs.

- [1] Lions J.L.: *Optimal Control of Systems Governed by Partial Differential Equations*. Springer-Verlag, New York, 1971.
- [2] Saurin V.V., Kostin, G.V., Rauh, A., and Aschemann, H. *Adaptive control strategies in heat transfer problems with parameter uncertainties based on a projective approach*. In: Rauh, A. and Auer, E. (eds.), *Modeling, Design, and Simulation of Systems with Uncertainties*. Springer-Verlag, Heidelberg, 2011, 309-332.
- [3] Rauh A., Dittrich C., Senkel L., and Aschemann H.: *Sensitivity analysis for the design of robust nonlinear control strategies for energy-efficient pressure boosting systems in water supply*. In Proc. of 2011 IEEE Intl. Symposium on Industrial Electronics ISIE2011, Gdansk, Poland, 2011, 1353–1358.

# AN INTEGRODIFFERENTIAL APPROACH TO ADAPTIVE CONTROL DESIGN FOR HEAT TRANSFER SYSTEMS WITH UNCERTAINTIES

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**Summary.** Open-loop and closed-loop control problems for distributed parameter systems, described by parabolic partial differential equations, are considered in this contribution. The goal of the study is the development of strategies for control and estimation of states, disturbances, and parameters. These strategies are based on the method of integrodifferential relations, a projection approach, and a suitable finite element technique. A real-time applicable control algorithm is proposed and its specific features are discussed. A verification of the control laws derived in this contribution is performed taking into account explicit error estimates resulting directly from the integrodifferential approach. The parameters, geometry, and actuation principles of a heat transfer system available at the Chair of Mechatronics, University of Rostock, are used for the numerical simulation and experimental validation. The test setup consists of a metallic rod equipped with a finite number of Peltier elements which are used as distributed control inputs allowing for active cooling and heating.

**The Method of Integrodifferential Relations for Control of Distributed Heating Systems.** The design of adaptive and optimal control strategies for dynamic systems with distributed parameters has been actively studied in recent years. Processes such as heat transfer, diffusion, and convection are part of a large variety of applications in science and engineering. The theoretical foundation for optimal control problems with linear partial differential equations (PDEs) and convex functionals was established in [2]. Furthermore, some common and efficient adaptive control approaches, including model reference adaptive control, adaptive pole placement, and adaptive backstepping were analyzed in related work. Typical fields of application, for which an adaptive control design of parabolic PDEs with unknown functional parameters can be applied, include reaction-convection-diffusion systems ubiquitous in chemical, thermal, biomedical, aerospace, and energy systems.

Different approaches to the discretization of dynamical models with distributed parameters have been developed in the past few years to reduce the original initial-boundary value problem to a system of ordinary differential equations (ODEs). Among these, variational and projection methods are of special importance to solve control problems for distributed parameter systems. The method of integrodifferential relations (MIDR) has been proposed by the authors in earlier work for the optimal control design of elastic beam motions.

The variational principle was applied in [1] on the basis of a MIDR formulation of a parabolic PDE system. This system describes an application from the field of heat transfer for which tracking control strategies are to be designed. Moreover, a projection approach, which is also based on the MIDR, has been developed in [3] for the same application.

One of the most important properties of the MIDR procedure is the fact that both local and global error estimates can be determined directly. For the heat transfer system under consideration, already Bernstein polynomials of the order  $M = 2$  in the developed finite element approach lead to relative integral errors of approx.  $\Delta = 1.5 \cdot 10^{-4}$ . A further increase of the approximation order  $M$  leads to a notable decrease of the integral error, which becomes equal to  $\Delta = 1.6 \cdot 10^{-6}$  for  $M = 3$  and  $\Delta = 1.1 \cdot 10^{-7}$  for  $M = 4$ .

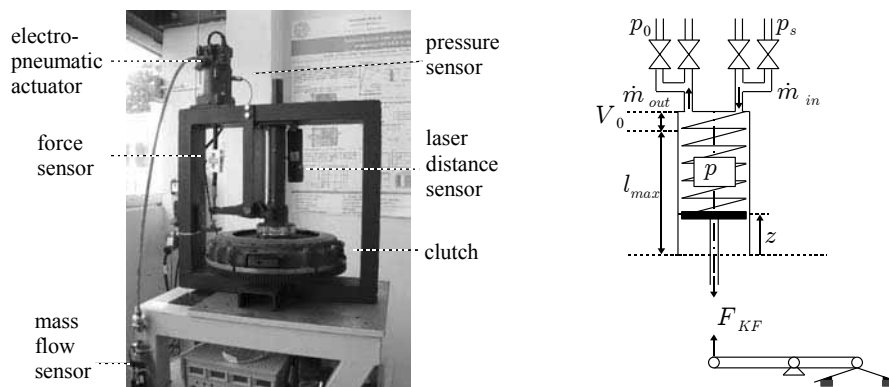
- [1] H. Aschemann, G. V. Kostin, A. Rauh, and V. V. Saurin. Approaches to Control Design and Optimization in Heat Transfer Problems. *J. Comp. Sys. Sci. Int.*, 49(3):380–391, 2010.
- [2] J. L. Lions. *Optimal Control of Systems Governed by Partial Differential Equations*. Springer Verlag, New York, 1971.
- [3] A. Rauh, G. V. Kostin, H. Aschemann, V. V. Saurin, and V. Naumov. Verification and Experimental Validation of Flatness-Based Control for Distributed Heating Systems. *Int. Rev. Mech. Eng.*, 4(2):188–200, 2010.

# NONLINEAR MODEL PREDICTIVE CONTROL OF AN ELECTRO-PNEUMATIC CLUTCH FOR TRUCK APPLICATIONS

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**Introduction.** This paper presents two nonlinear model predictive control designs for an electro-pneumatic clutch used in heavy trucks: a centralised approach and a cascaded one with a fast underlying pressure control. Clutches are needed in vehicle powertrains to decouple the angular velocities of the internal combustion engine from those of the driving wheels. Especially at start-up, when the velocity of the vehicle is zero, and during the gear shift process the clutch has to be employed. An automated actuator disburdens the driver and provides the necessary actuation force according to the large torque transmitted through the powertrain. Often, the clutch operation is automated using a combination of feedforward and feedback control, e.g. a model-based nonlinear control using extended linearisation techniques as presented in [1]. A test rig dedicated for the development and validation of sophisticated control approaches for an electro-pneumatic clutch is available at the Chair of Mechatronics, University of Rostock. The single disc clutch under consideration is driven by the piston rod of a pneumatic cylinder, which is actuated by pressurised air. Due to safety specifications, it is necessary to employ two inlet and two outlet valves, typically with different conductances. These electrically actuated valves operate in an on/off mode using a pulse-width-modulated signal. The corresponding control-oriented model developed in this paper accounts for the dynamic behaviour of the clutch piston as well as the internal pressure in the cylinder chamber.



**NMPC.** A problem with most of the MPC algorithms is that they are only suitable for systems with slow dynamics because they cannot be computed within very small sample times. One approach to deal with this problem is given in [2], where an explicit NMPC controller is proposed for an electro-pneumatic clutch actuator. In contrast, the NMPC approach considered here aims at reducing future state errors, see [3], and allows for relatively small computational effort as required in a real-time implementation. In this contribution, two different control approaches are compared: 1) a centralised control approach involving a NMPC controller for the clutch position as well as the internal pressure and 2) a cascaded approach involving a NMPC controller for the clutch position and a fast underlying controller for the internal pressure. As the internal pressure is usually not measured in truck applications, a nonlinear reduced-order disturbance observer estimates the internal pressure. Thereby, high tracking accuracy is achievable for the piston position as controlled variable without a pressure measurement. The efficiency of both proposed control structures are emphasised by experimental results from the test rig.

- [1] H. Aschemann, R. Prabel, and D. Schindele. Nonlinear control of an electro-pneumatic clutch for truck applications using extended linearisation techniques. *Proc. of 12th Scand. Intern. Conf. on Fluid Power, SICFP 2011, Tampere, Finland, 2011.*
- [2] A. Grancharova and T. A. Johansen. Design and comparison of explicit model predictive controllers for an electropneumatic clutch actuator using on/off valves. *IEEE Trans. on Mechatronics*, 16(4):665–673, 2011.
- [3] S. Jung and J.T. Wen. Nonlinear model predictive control for the swing-up of a rotary inverted pendulum. *ASME J. of Dynamic Systems, Measurement and Control*, 126(3):666–673, 2004.



# RELIABLE CONTROL AND DISTURBANCE REJECTION FOR THE THERMAL BEHAVIOR OF SOLID OXIDE FUEL CELL SYSTEMS

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**Summary.** Chemical energy can be converted directly into electricity and process heat with the help of solid oxide fuel cells (SOFCs). This type of fuel cells, moreover, allows for operating points with high efficiency and reasonable exploitation of the supplied gases at high temperature levels. However, the maximum admissible cell temperature is restricted by the properties of the materials contained in the fuel cell stack. For an application in a decentralized power supply grid, control strategies are essential which can cope with varying electrical load demands and prevent local over-temperatures leading to a decreased system reliability. To derive such control laws, mathematical models are required which represent the instationary thermal behavior of a fuel cell stack for the above-mentioned load variations. For that purpose, the spatial temperature distribution in the interior of the stack module is described by means of a finite volume discretization. This approach leads to a set of coupled nonlinear ordinary differential equations, where several parameters cannot be characterized exactly due to disturbances and an imperfect system knowledge. These uncertainties are taken into consideration in the thermal subsystem in terms of parameters which can be bounded by means of intervals.

**Reliable Control and Disturbance Rejection.** Control strategies for SOFC systems are required to ensure a high efficiency by a reasonable exploitation of the supplied gases and to increase the system reliability by considering the spatial temperature distribution in the interior of the SOFC stack module. Here, it is not only sufficient to design control strategies from a stationary point of view in such a way that the gas mass flows at the anode and cathode are stoichiometrically balanced. It is furthermore essential to guarantee robustness of the control strategies so that disturbances in the electrical load demands can be compensated with smallest possible additional load shaping devices such as additional battery buffers. Electric load variations may lead to changes in the internal temperature distribution of the SOFC stack and, therefore, may lead to mechanical strain on the stack components which limits life time and efficiency of the SOFC system. The spatial temperature distribution in the SOFC stack module results from a spatially distributed heat production process. This process is directly coupled with the local conversion rates of the chemical energy of the supplied gases along the anode and cathode gas channels into electricity and heat. Therefore, varying local over-temperatures, enthalpy flows of the fuel gas and air, heat conduction processes and Ohmic losses have to be taken into consideration for the development of suitable control-oriented system models [2].

The above-mentioned nonlinear system models are stabilized by robust nonlinear control laws in this paper. The main objective of controller design is the stabilization of the system in arbitrary operating points and to guarantee compensating disturbances which act on the system dynamics and can be described by interval parameters. In a first stage, the dominant nonlinear phenomena are compensated by the procedure of exact feedback linearization [1]. The resulting linearized thermal subsystem is asymptotically stabilized by a state feedback control. These feedback control procedures can be easily extended by a variable structure control part that can be designed by means of the sliding mode technique [3]. The sliding mode part in the control law is used to account for imperfect system knowledge that could not be considered in the stage of feedback linearization. The corresponding uncertainties can be introduced in the control law in terms of the suitably chosen interval variables.

The derivation of a scalable as well as control-oriented model for the instationary dynamics of the interior temperatures of a SOFC system has been performed by applying finite volume semi-discretization methods. Based on this modeling technique, a system model of the order  $n_x = 3$  has been derived and a feedback controller has been designed in such a way that all known nonlinear system characteristics are compensated. This leads to maximum control errors of  $|e| = 1.4\text{K}$  for the complete heat-up process. Additionally, the robustness of this control strategy has been improved by introducing a sliding mode controller to account for a-priori unknown disturbances in a desired operating range.

- [1] H.J. Marquez. *Nonlinear Control Systems*. John Wiley & Sons, Inc., New Jersey, 2003.
- [2] A. Rauh, T. Dötschel, and H. Aschemann. Experimental Parameter Identification for a Control-Oriented Model of the Thermal Behavior of High-Temperature Fuel Cells. In *CD-Proc. of IEEE Intl. Conference on Methods and Models in Automation and Robotics MMAR*, Miedzyzdroje, Poland, 2011.
- [3] V.I. Utkin. *Sliding Modes in Control and Optimization*. Springer-Verlag, Berlin, Heidelberg, 1992.

## TRAJECTORY PLANNING OF A REDUNDANT MANIPULATOR FROM INVESTIGATIONS OF UPPER LIMB MOTIONS OF HUMAN BEINGS

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**Introduction.** In recent years, developments of robotic systems are transiting from industrial applications to service applications. Therefore, a wide variety of service robots are proposed for different applications, including medical cares, home automations, security services, and so forth. In general, popular technologies developed for service robots consist of mechanical design, image capture and recognitions, intelligent controls, trajectory planning, mechatronics integrations, etc. From the viewpoints of robotics applications, the robotic manipulator plays an important role for service robots because the robotic manipulator provides the mechanical interface for the interactions with human beings and objects in application environments. Therefore, most of robotic manipulators developed for service robots are designed similarly to the structure of the human's upper extremities. With the human-like arm structure design concepts, the robot manipulators are capable of performing similar motions with humans.

This paper discusses the trajectory planning problem of a four-degrees-of-freedom (4-DOF) robotic manipulator with similar upper limb structures of human beings. The spatial motions of the end-effector (i.e., wrist) can be desired in terms of controlling four motors of the robotic manipulator; hence, such a configuration results in the redundancy problem. In general, Jacobian solutions [1], [2] perform linear approximations of inverse kinematics problems with redundancy conditions. With human beings, the same wrist position can be found from different limb postures, and these postures depend on different motion scenarios such as writing words, waving hands and shaking hands. Nevertheless, Jacobian solutions are hardly to realize specific limb motion scenarios of human beings. Therefore, this paper proposes a supervised neural network [3] based robotic manipulator trajectory planner which constructs limb motion characteristic models according to relative joint posture features with respect to different motion scenarios. The motion features are further used to provide an auxiliary condition for eliminating the redundancy problem of the inverse kinematics as well as to meet specific motion scenarios. Finally, several trajectory planning results were evaluated in terms of the Jacobian and neural network approaches respectively by using an optical motion capture system. Experiment results demonstrated that the proposed neural network based control system performs similar motion behaviors when compared to Jacobian approaches based on the same test trajectory and motion scenario.

- [1] Cheah, C.C., Liu, C. and Liaw, H.C.: *Stability of Inverse Jacobian Control for Robot Manipulator*. In: IEEE International Conference on Control Applications, 1 (2004), 321 – 326.
- [2] Tabaczynski, M.: *Jacobian Solutions to the Inverse Kinematics Problem*. In: Tufts University, Final Project Report, 2005.
- [3] Kuo, C.H., Yang, F.C., Wing, J.J. and Yang, C.K.: *Construction of 3D Solder Paste Surfaces Using Multi-Projection Images*. In: Journal of Advanced Manufacturing Technology, 31 (2006) 509 – 519.

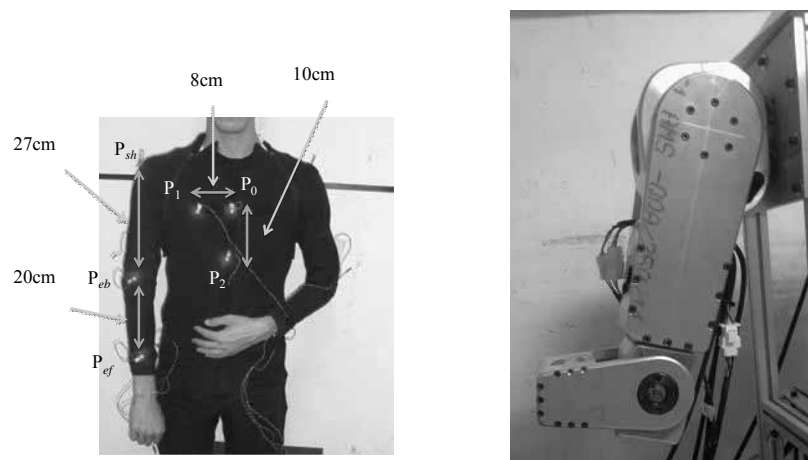


Figure: LED marker placements and 4-DOF robotic manipulator

# STABILITY AND OSCILLATIONS OF ELECTRICAL MACHINES OF ALTERNATING CURRENT

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**Introduction.** Stability is an important qualitative characteristic of an electrical machine of alternating current, providing the reliability of its work. In practice of operation of electrical machines sudden disturbances occur, for example line fault, changes of the external load, changes of supply voltage, etc. In this case damage of the electrical machine or even its failure requiring overhaul can arise. By this reason the investigation of stability is one of the major scientific and technological problems in the design of electrical machines.

By the stability of an electrical machine we mean the ability of the machine to re-establish a steady-state mode after disturbances of the initial mode. The process of pull into synchronism after asynchronous start-up is also a property of stability of the machine.

The stability problems may be divided into two kinds: steady-state, or static stability and transient, or dynamic stability. The problem of dynamic stability of an electrical machine consists of not only of checking whether the machine maintain synchronism after a given dynamic disturbances, but also finding the limit permissible disturbance, corresponding to the boundary of dynamic stability. Therefore, the problem of dynamic stability is closely related to the limit load problem.

**Limit load problem setting. Limit load estimations.** A typical situation for an electrical machine is as follows: the machine is started without load, then in transient process it is pulled in synchronism and only after that a load-on occurs. In this case the limit load problem is to find for what loads, after transient process, the electrical machine is pulled in a new synchronous operating mode.

In the work the limit load problem for induction motors with the cage rotor and synchronous motors with the quadrupole rotor is considered. Before this the new mathematical models of induction and synchronous motors with some simplifying assumptions are developed. Thus, the behaviour of these electrical motors may be described by the autonomous system of the form

$$\dot{z} = f(z), \quad z \in R^n.$$

In the work global stability of electrical motors under no-load condition is proved, so it is assumed that the motor operates in a synchronous mode. Let this operating mode correspond to the solution of the system  $z = z_0$ .

Further at time  $t = \tau$  the instantaneous load-on occurs. Thus, for  $t > \tau$  the moment of the external load is not already zero. Hence, the operating mode of the motor changes, that is a new synchronous operating mode of the motor under load condition corresponds to the solution of the system  $z = z_*$ . Thus, a mathematical setting of the limit load problem is the following: to find conditions, under which the solution  $z = z(t)$  with the initial data  $z = z_0$  is contained in the domain of attraction of the stationary solution  $z = z_*$ . The latter means that the following relations

$$\lim_{t \rightarrow +\infty} z(t) = z_*$$

must be satisfied.

In engineering practice for computing limit load the equal-area criterion is widely used. In 1958 A.A. Yanko-Trinitskii first applied the second Lyapunov method for analysis of stability of synchronous machines and also mathematically justified the equal-area criterion.

In 2006 G.A. Leonov proposed the non-local reduction method for analysis of the dynamics of electrical machines. An idea of the non-local reduction method is as follows: in studying stability of multidimensional systems of equations of electrical machines it is used Lyapunov-type functions, involving the information on solutions of equation of comparison, namely Tricomi equation, which describes the dynamics of synchronous machine in the simplest two-dimensional idealization. The non-local reduction method turns out highly effective for electrical machines.

In this work, the non-local reduction method and the equal-area criterion are applied to the solution of limit load problem for considered electrical machines. Analytical and numerical estimations of the limit load are obtained. In the case of non-local reduction method a substantially improved estimates of the limit load in comparison to the estimates, obtained by the equal-area criterion, are found.

# ENERGY TRANSFER IN PARAMETRICALLY DRIVEN SYSTEMS OF WEAKLY COUPLED OSCILLATORS

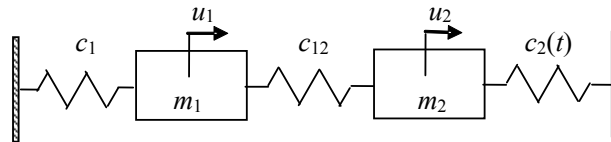
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The problem of energy transfer is currently a topic of intense research with a broad spectrum of applications, from multi-body systems and waves in fluids and plasmas, to semiconductors and quantum computers among other novel applications. Most of the results reported in the literature are related to energy exchange in systems with constant parameters. This work develops an analytical framework to investigate the dynamics of weakly-coupled oscillators with time-varying frequencies, with an attention to an analogy between energy transfer in this classical oscillatory system and quantum Landau-Zener tunnelling [1, 2]. For definiteness, we consider a model consisting of a linear oscillator with constant parameters weakly coupled with an oscillator with linear-in-time frequency modulation (Figure 1). However, the approach suggested in this paper allows a straightforward extension to multi-dimensional systems with a more complicated detuning law.



**Fig. 1.** Weakly coupled oscillators

Although a passage between two energy levels is an intrinsic feature of both classical and quantum processes, the evidence for a direct connection between energy transfer in a classical oscillatory system and Landau-Zener tunnelling is a recent development [3,4]. It has been shown that the equations of the adiabatic passage through resonance in a system of two weakly coupled oscillators with a slowly-varying frequency detuning are identical to the equations of the Landau-Zener problem. This paper is focussed on an explicit asymptotic description of the transient dynamics. A correctness of approximations is confirmed by numerical simulations.

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[1] Landau, L.D. *Zur Theorie der Energieübertragung*. Phys. Z. Sowjetunion 2 (1932), 46-51.

[2] Zener, C. *Non-adiabatic crossing of energy levels*. Proc. R. Soc. London, ser. A, 137 (1932), 696-702.

[3] Kovaleva, A., Manevitch, L.I., and Kosevich, Yu..A. *Fresnel integrals and irreversible energy transfer in an oscillatory system with time-dependent parameters*. Phys. Rev. E, 83 (2011), 026602.

[4] Kovaleva, A., Manevitch, L.I., *Classical analogue of quasilinear Landau-Zener tunneling*. Phys. Rev. E, (2012), 026602.

## CONTROL OF A MULTI-LINK INVERTED PENDULUM BY A SINGLE TORQUE

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**Introduction.** The goal of this study is to design a feedback control that brings a multi-link inverted pendulum from a small neighborhood of the upright equilibrium position to this position in a finite time by means of a bounded control torque applied to the first link.

A multi-link pendulum with deficient number of controls represents a great challenge for investigators. In recent decades, different control problems for pendulums have been intensively studied. The difficulty in controlling such mechanical systems is related to the fact that a multi-link pendulum has many degrees of freedom, the differential equations for its motions are substantially nonlinear, and the number of these equations exceeds the dimension of the vector of the control torque. Many investigations are devoted to the problem of stabilization of inverted pendulums, aiming to ensure the asymptotic stability of the pendulum in the upper equilibrium state. The goal of this study is to design a feedback control that brings a multi-link inverted pendulum from a small neighborhood of the upright equilibrium position to this position in a finite time by means of a bounded control torque applied to the first link.

**Problem formulation.** We consider a multi-link inverted pendulum that moves in a vertical plane actuated by a single control torque  $u$  applied to the first (lowest) link. We assume that the motions of the pendulum are limited within a neighbourhood of its upright equilibrium point. The problem is to find a control in the feedback form, that is as a continuous function of the angles and angular velocities, such that all the trajectories of the pendulum that begin inside a certain neighbourhood of the upright equilibrium point arrive to this equilibrium point in a finite time, and the control on these trajectories satisfies the inequality  $|u| \leq U_0$ ,  $U_0 > 0$ .

**Auxiliary control problem.** First, we consider an auxiliary control problem for the linearized system

$$\dot{x} = Cx + Du, \quad x \in \mathbb{R}^{2n}. \quad (1)$$

Using linear matrix inequalities techniques, we build a continuous bounded control function  $u(x)$  that would guarantee that the trajectories of system (1) arrive into the origin in a finite time.

It is shown in [1] that the proposed control meets imposed constraint in the small neighborhood of zero and, moreover, is locally applicable to a nonlinear control system

$$\dot{x} = Cx + f(x) + Du, \quad f(x) = O(|x|^2), \quad (2)$$

which can represent a multi-link pendulum in a small vicinity of the upright equilibrium state.

**Computer simulation of a triple-link pendulum motion.** We apply the approach described above for steering a multi-link inverted pendulum to the upright equilibrium position in a finite time. As one would expect, the control law designed is effective in a small neighbourhood of the equilibrium point. The computer simulation of the dynamics of pendulums subjected to the proposed control shows that the larger the number of pendulum links, the smaller the size of this neighbourhood.

- [1] I.M. Anan'evskii, N.V. Anokhin, and A.I. Ovseevich. *Synthesis of Bounded Controls for Linear Dynamical Systems by Using Common Lyapunov Functions*. Doklady Mathematics, 82(2), 1–4, Pleiades Publishing, Ltd., 2010.



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# DENDRITIC BRANCHING IN A CHEMOTAXIS MODEL WITH ATTRACTION AND REPULSION

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**NO ABSTRACT AVAILABLE**

# NONLINEAR DIFFUSION AND ADDITIONAL CROSS-DIFFUSION IN THE KELLER-SEGEL MODEL

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The Keller-Segel model [4] describes the chemotactic movement of cells towards certain chemicals in their environment, which are assumed to be emitted by the cells themselves. One possible consequence is the aggregation of cells resulting in a blow-up of solutions. In the two-dimensional case there exists a critical threshold for the mass, i.e. if the initial data is such that the mass is below this threshold, then solutions are globally bounded, whereas for masses above the threshold solutions may blow up in finite time. In three space dimensions the  $L^{3/2}$ -norm plays a similar role as the mass in the two-dimensional case in the sense that solutions are globally bounded under a smallness condition on the  $L^{3/2}$ -norm. However the situation is not as well understood, since no exact threshold is known.

We introduce a regularisation of the fully parabolic system by adding a cross-diffusion term to the equation for the chemical substance. This regularisation provides another helpful entropy dissipation term allowing to prove global existence of solutions for any initial mass in two space dimensions [3]. In the parabolic-elliptic case this model can be reformulated to the Keller-Segel model with nonlinear cell diffusion. Therefore solutions are known to be globally bounded, see e.g. [1], [5].

A generalisation of the model is obtained by replacing the cell diffusion and the regularising cross-diffusion by nonlinear versions. In particular global existence is obtained in the three-dimensional case for linear (or classical) cell diffusion if one uses a suitably chosen degenerate cross-diffusion. Moreover we investigate the parameters such that we can allow for fast cell diffusion. The corresponding parabolic-elliptic system can again be reformulated to a Keller-Segel model with nonlinear diffusion, which now exhibits an additional nonlinear growth term in the equation for the chemical substance. Careful estimations lead to uniform boundedness of solutions [2]. Numerical simulations illustrate the theoretical results.

- [1] V. Calvez and J.A. Carrillo. *Volume effects in the Keller-Segel model: energy estimates preventing blow-up*. J. Math. Pure Appl., 2006, 86: 155-175.
- [2] J.A. Carrillo, S. Hittmeir and A. Jüngel. *Cross diffusion and nonlinear diffusion preventing blow up in the Keller-Segel model*, submitted.
- [3] S. Hittmeir and A. Jüngel. *Cross-diffusion preventing blow up in the two-dimensional Keller-Segel model*. SIAM J. Math. Anal., 2011, 43: 997-1022.
- [4] E. Keller and L. Segel. *Initiation of slime mold aggregation viewed as an instability*. J. Theor. Biol., 1970, 26: 399-415.
- [5] R. Kowalczyk. *Preventing blow-up in a chemotaxis model*. J. Math. Anal. Appl., 2005, 305: 566-588.

# ON THE ASYMPTOTIC LIMIT OF A MODEL FRAMEWORK FOR FRICTION MEDIATED BY TRANSIENT LINKAGES

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**Abstract.** In this work we study a system of an integral equation of Volterra type coupled to an original renewal equation. This model arises in the context of cell motility: the integral equation describes the trajectory of a binding site which is connected via transiently remodelling linkages to the substrate and which evolves driven by a given force. The renewal model accounts for the remodelling process of linkages which attach and break with given probabilities. In the present paper we analyze existence and uniqueness issues for the coupled system of interest and provide a rigorous justification of the asymptotic limit of infinitesimally rapid turnover of linkages. The renewal model for the age distribution of linkages differs from more classical ones in that it describes competition between population size and birth and because it admits a new and specific Lyapunov functional. On the other side, using a comparison principle which applies to non-convolution linear Volterra kernels and the peculiar transport properties of the linkages, one establishes a convergence result when the turnover parameter  $\varepsilon$  tends to zero.

**ABSTRACT FROM REVIEW ABSTRACT**

# MIXED-MODE OSCILLATIONS IN BIOLOGICAL MODELS

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Oscillatory patterns with widely disparate amplitudes are often referred to as mixed-mode oscillations (MMOs). They appear in a wide variety of applications ranging from chemical oscillations, lasers, to virtually all fields of mathematical biology. Recently it has been established that large classes of MMOs are related to a multiple time scale structure of the underlying system. I will give an overview of basic theory for multiple time scales systems, MMOs and the related numerical analysis problems. Then two applications of these techniques in biology will be considered: the FitzHugh-Nagumo equation and a reduced version of the Hodgkin-Huxley model.

In particular, the basic classification of MMOs based on patterns of the form

$$\cdots L_{i-1}^{s_{i-1}} L_i^{s_i} L_{i+1}^{s_{i+1}} \cdots \quad (1)$$

of alternating  $L$  large and  $s$  small oscillations will be discussed. The relation of MMOs and bursting solutions will be clarified and an three-dimensional model example suggested by Koper will be used to introduce some of the mechanisms that generate MMOs. We shall also see that there is a nice interaction between direct numerical integration methods, boundary value solvers and the geometry of phase space.

Then we are going to discuss applications. The first example is a reduced version of the Hodgkin-Huxley model

$$\begin{cases} v' &= \bar{I} - m_\infty^3(v)h(v - \bar{E}_{\text{Na}}) - \bar{g}_k n^4(v - \bar{E}_K) - \bar{g}_l(v - \bar{E}_L), \\ h' &= \varepsilon \frac{k_h}{\tau_h} \frac{(h_\infty(v) - h)}{t_h(v)}, \\ n' &= \varepsilon \frac{k_n}{\tau_n} \frac{(n_\infty(v) - n)}{t_n(v)}. \end{cases} \quad (2)$$

The second example the spatially extended FitzHugh-Nagumo equation with diffusion

$$\begin{cases} \frac{\partial u}{\partial t} &= \delta \frac{\partial^2 u}{\partial x^2} + f_a(u) - w + p, \\ \frac{\partial w}{\partial t} &= \varepsilon(u - \gamma w). \end{cases} \quad (3)$$

where in both cases  $0 < \varepsilon \ll 1$  is a small parameter representing the separation of time scales. The main references for this talk are [1] and [4] with numerical methods developed in [2] and [3]. Further details on MMOs, bursting and the associated techniques from multiple time scale dynamical systems can also (soon) be found in [5].

- [1] M. Desroches, J. Guckenheimer, C. Kuehn, B. Krauskopf, H. Osinga, and M. Wechselberger. Mixed-mode oscillations with multiple time scales. *SIAM Rev. (to appear)*, 2012.
- [2] M. Desroches, B. Krauskopf, and H.M. Osinga. Numerical continuation of canard orbits in slow-fast dynamical systems. *Nonlinearity*, 23(3):739–765, 2010.
- [3] J. Guckenheimer and C. Kuehn. Computing slow manifolds of saddle-type. *SIAM J. Appl. Dyn. Syst.*, 8(3):854–879, 2009.
- [4] J. Guckenheimer and C. Kuehn. Homoclinic orbits of the FitzHugh-Nagumo equation: Bifurcations in the full system. *SIAM J. Appl. Dyn. Syst.*, 9:138–153, 2010.
- [5] C. Kuehn. *Multiple Time Scale Dynamics*. book in preparation, 2011.

## SLOW-FAST DYNAMICS IN THE CELL CYCLE

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**Abstract.** The cell cycle is the series of events that takes place in a cell leading to its division and duplication. This process is driven and controlled by complicated enzyme networks. The key elements this network are complexes of various cyclins and corresponding cyclin-dependent kinases. Mathematical modelling of these processes is a very active area in systems biology and has led to a large variety of models in the form of - often large - systems of ordinary differential equations. A common feature of many of the involved reactions are Michaelis-Menten type reactions with small Michaelis constants. We show that this leads to slow-fast dynamics which can be used to obtain a decomposition of the system into smaller sub-systems. To illustrate this point we analyse a relatively simple model due to A. Goldbeter, which describes oscillations caused by a single cyklin and cyclin-dependent kinase complex. We analyse its dynamics in the spirit of geometric singular perturbation theory and explain the observed periodic solutions as a new type of relaxation oscillations.



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**Fractal Conservation Laws – Hyperbolic**

**Conservation Laws Regularized by an**

**Anomalous Diffusion**





# CLASSICAL AND NON-CLASSICAL HYDRAULIC JUMPS IN TWO-LAYER FLUIDS

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**Summary.** Hyperbolic partial differential equations are central to many areas of science/engineering and the foundations of many modern technologies including semiconductors plasmas, fluids, environmental science. A general property of nonlinear hyperbolic wave equations is the eventual formation of discontinuities (shocks) in the evolving signal and a central issue in shock propagation is the identification of physically acceptable shock solutions. In this presentation we consider discontinuous solutions to hyperbolic systems of conservation laws that violate classical entropy criteria. The main focus is on hyperbolic systems which are not genuinely nonlinear and as a consequence have a much richer and complex structure. A key observation is that under-compressive shocks may arise in these systems where the number of characteristics entering the discontinuity is now smaller than that imposed by the classical Lax shock inequalities. Such shocks have been shown to be sensitive to the form of the dissipative-dispersive mechanisms present in the physical system.

- [1] A. Kluwick, S. Scheichl, E.A. Cox, *Near critical hydraulic flows in two-layer fluids*. J. Fluid Mech. 2007, 575: 187-219.
- [2] A. Kluwick, A. Exner, E.A. Cox, Ch. Grinschgl, *On the internal structure of weakly nonlinear bores in laminar high Reynolds number flow*. Acta Mech. 2010, 210: 135-157.

# ON NONLINEAR CONSERVATION LAWS WITH A NONLOCAL DIFFUSION TERM

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**Abstract.** Scalar one-dimensional conservation laws with a nonlocal diffusion term corresponding to a Riesz-Feller differential operator are considered. Solvability results for the Cauchy problem in  $L^{\infty}$  are adapted from the case of a fractional derivative with homogeneous symbol. The main interest of this work is the investigation of smooth shock profiles. In case of a genuinely nonlinear smooth flux function we prove the existence of such traveling waves, which are monotone and satisfy the standard entropy condition. Moreover, the dynamic nonlinear stability of the traveling waves under small perturbations is proven, similarly to the case of the standard diffusive regularization, by constructing a Lyapunov functional.

**ABSTRACT GENERATED FROM REVIEW ABSTRACT**

# A VARIATIONAL APPROACH TO THE INVISCID LIMIT OF FRACTIONAL CONSERVATION LAWS

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**NO ABSTRACT AVAILABLE**

# PROBABILISTIC PARTICLE APPROXIMATION FOR FRACTIONAL CONSERVATION LAWS

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We present a probabilistic interpretation and a numerical scheme for the one-dimensional conservation law with anomalous diffusion, namely the equation

$$\partial_t v(t, x) = \mathcal{L}v(t, x) - \partial_x(A(v(t, x))), \quad (t, x) \in ]0, \infty[ \times \mathbb{R}. \quad (1)$$

In (1),  $A : \mathbb{R} \rightarrow \mathbb{R}$  is some smooth function, and  $\mathcal{L}$  is a Lévy-type operator, defined for smooth bounded functions by

$$\mathcal{L}w(x) = aw'(x) + bw''(x) + \int_{\mathbb{R} \setminus \{0\}} (w(x+y) - w(x) - yw'(x)\mathbf{1}_{|y|<1}) v(dy). \quad (2)$$

In (2),  $a, b \in \mathbb{R}$ , and the measure  $v$  is some positive measure on  $\mathbb{R} \setminus \{0\}$ , satisfying  $\int_{\mathbb{R} \setminus \{0\}} 1 \wedge y^2 v(dy) < \infty$ . A particular example of Lévy operator is given by the fractional Laplace operator  $-(-\Delta)^{\alpha/2}$  corresponding to the case  $a = b = 0$  and  $v(dx) = |x|^{-1-\alpha} dx$ .

Lévy operators arise naturally in the study of some class of stochastic processes called *Lévy processes*, defined as processes whose increments are independent and stationary. Equation (1) thus has a natural probabilistic interpretation through space derivation, as first remarked by Jourdain, see [2]. Indeed, consider the space derivative  $u = \partial_x v$  of the solution to (1). The function  $u$  satisfies, if one denotes  $H = \mathbf{1}_{]0, \infty[}$ ,

$$\partial_t u(t, x) = \mathcal{L}u(t, x) - \partial_x(u(t, x)A'(H * u(t, x))). \quad (3)$$

Equation (3) is, at least formally, the evolution equation of the distribution of a stochastic process  $(X_t)$  driven by a Lévy process  $(L_t)$  with generator  $\mathcal{L}$  through the equation

$$dX_t = dL_t + A'(H * \tilde{P}(t, X_t))dt, \quad (4)$$

where  $\tilde{P}$  is the signed measure whose Radon-Nikodym density with respect to the distribution  $P$  of the process  $(X_t)$  is given by  $\gamma(X_0)$ ,  $\gamma$  being the Radon-Nikodym density of the signed measure  $u_0$  with respect to the probability measure  $|u_0| = |\partial_x v_0|$ . This means that  $H * \tilde{P}(t, \cdot)$  is a signed cumulative distribution function of  $X_t$  where each trajectory is given a sign  $\gamma(X_0) \in \{-1, 1\}$ .

One can naturally approximate the process (4) by an interacting particle system where each particle follows the dynamic (4) with the actual cumulative distribution function replaced by the empirical one. In the case where  $\gamma$  is not constant, one needs to take care for defining the particle system, since one requires colliding particles with opposite signs to disappear from the simulation. This can be done by discretizing time, and considering the Euler scheme associated to (4).

We prove the convergence of the signed cumulative distribution function of the particle system to the entropy solution of equation (1) defined by Alibaud in [1]. One can also prove an inviscid limit for the particle approximation: multiplying the diffusion term by a vanishing coefficient, the signed cumulative distribution function of the particle system converges to the entropy solution in the classical sense of Kruzhkov [5] for the conservation law with  $\mathcal{L} = 0$ . In both cases, the convergence holds with some conditions depending on the strength of the smoothing effects of the differential operator  $\mathcal{L}$ , see [3, 4].

From the numerical point of view, the particle system is easy to simulate, and the convergence rate is known in the Gaussian setting  $\mathcal{L} = \Delta$ , where it is given by  $N^{-1/2} + \Delta t$ ,  $N$  being the number of particles involved and  $\Delta t$  being the time step of the simulation. In our more general setting, the convergence rate is numerically the same, although no proof exists for the moment.

- [1] N. Alibaud. Entropy formulation for fractal conservation laws. *J. Evol. Equ.*, 7(1):145–175, 2007.
- [2] B. Jourdain. Probabilistic approximation via spatial derivation of some nonlinear parabolic evolution equations. In *Monte Carlo and quasi-Monte Carlo methods 2004*, pages 197–216. Springer, Berlin, 2006.
- [3] B. Jourdain, S. Méléard, and W. A. Woyczyński. Probabilistic approximation and inviscid limits for one-dimensional fractional conservation laws. *Bernoulli*, 11(4):689–714, 2005.
- [4] B. Jourdain and R. Roux. Convergence of a stochastic particle approximation for fractional scalar conservation laws. *Stochastic Process. Appl.*, 121(5):957–988, 2011.
- [5] S.N. Kruzhkov. First order quasilinear equations in several independent variables. *Mat. Sb.*, 81:228–255, 1970.

# DECAY STRUCTURE FOR SYMMETRIC HYPERBOLIC SYSTEMS WITH NON-SYMMETRIC RELAXATION

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The result of this article is based on a joint work with Professor Shuichi Kawashima from Kyushu University and Professor Renjun Duan from Chinese University of Hong Kong. In this article, we consider the Cauchy problem for the first-order linear symmetric hyperbolic system of equations with relaxation:

$$A^0 u_t + \sum_{j=1}^n A^j u_{x_j} + Lu = 0, \quad u|_{t=0} = u_0. \quad (1)$$

Here  $u = u(t, x) \in \mathbb{R}^m$  over  $t > 0, x \in \mathbb{R}^n$  is an unknown function,  $u_0 = u_0(x) \in \mathbb{R}^m$  over  $x \in \mathbb{R}^n$  is a given function, and  $A^j$  ( $j = 0, 1, \dots, n$ ) and  $L$  are  $m \times m$  real constant matrices, where integers  $m \geq 1, n \geq 1$  denote dimensions. When the degenerate relaxation matrix  $L$  is symmetric, Umeda-Kawashima-Shizuta [4] proved the large-time asymptotic stability of solutions. The key idea in [4] and the later generalized work [2] that first introduced the so-called Kawashima-Shizuta condition is to design the compensating matrix to capture the dissipation of systems over the degenerate kernel space of  $L$ . More precisely, taking the Fourier transform of (1) with respect to  $x$  yields  $A^0 \hat{u}_t + i|\xi|A(\omega)\hat{u} + L\hat{u} = 0$ . Here,  $\xi \in \mathbb{R}^n$  denotes the Fourier variable,  $\omega = \xi/|\xi| \in S^{n-1}$  is the unit vector whenever  $\xi \neq 0$ , and we define  $A(\omega) := \sum_{j=1}^n A^j \omega_j$  with  $\omega = (\omega_1, \dots, \omega_n) \in S^{n-1}$ . Then the following conditions for the coefficient matrices are needed:

**Condition (A):** For the coefficient matrices, it is assumed that  $\text{Ker}(L) \neq \{0\}$  and

$$(A^j)^T = A^j \quad \text{for } j = 0, 1, \dots, n, \quad A^0 > 0, \quad L \geq 0 \quad \text{on } \mathbb{C}^m.$$

Here, the superscript  $T$  stands for the transpose of matrices, and given a matrix  $X, X \geq 0$  means that  $\text{Re} \langle Xz, z \rangle \geq 0$  for any  $z \in \mathbb{C}^m$ , while  $X > 0$  means that  $\text{Re} \langle Xz, z \rangle > 0$  for any  $z \in \mathbb{C}^m$  with  $z \neq 0$ , where  $\langle \cdot, \cdot \rangle$  denotes the standard complex inner product in  $\mathbb{C}^m$ . Also, we use  $X_1 = (X + X^T)/2$  and  $X_2 = (X - X^T)/2$ .

**Condition (K):** There is a real compensating matrix  $K(\omega) \in C^\infty(S^{n-1})$  with the following properties:  $K(-\omega) = -K(\omega)$ ,  $(K(\omega)A^0)^T = -K(\omega)A^0$  and  $(K(\omega)A(\omega))_1 > 0$  on  $\text{Ker}(L)$  for each  $\omega \in S^{n-1}$ .

Under the conditions (A) with  $L^T = L$  and (K) one has:

**Theorem 1** ([4, 2]). *Assume that both the conditions (A) with  $L^T = L$  and (K) hold. Let  $s \geq 0$  be an integer and suppose that the initial data  $u_0$  belong to  $H^s \cap L^1$ . Then the solution  $u$  to the problem (1) satisfies the decay estimate:  $\|\partial_x^k u(t)\|_{L^2} \leq C(1+t)^{-n/4-k/2} \|u_0\|_{L^1} + Ce^{-ct} \|\partial_x^k u_0\|_{L^2}$  for  $k \leq s$ . Here  $C$  and  $c$  are positive constants.*

Unfortunately, when the degenerate relaxation matrix  $L$  is not symmetric, Theorem 1 can not be applied any longer. In fact, this is the case for some concrete systems, for example, the Timoshenko system [1] and the Euler-Maxwell system [3], where the linearized relaxation matrix  $L$  indeed has a nonzero skew-symmetric part while it was still proved that solutions decay in time in some different way. Therefore, our purpose of this article is to formulate some new structural conditions in order to extend Theorem 1 to the general system (1) when  $L$  is not symmetric, which can include both the Timoshenko system and the Euler-Maxwell system. More precisely, we formulate the structural conditions as follows.

**Condition (S):** For each  $\omega \in S^{n-1}$ , there is a real constant matrix  $S$  with the properties:  $(SA^0)^T = SA^0$  and

$$(SL)_1 + L_1 \geq 0 \quad \text{on } \mathbb{C}^m, \quad \text{Ker}((SL)_1 + L_1) = \text{Ker}(L), \quad i(SA(\omega))_2 \geq 0 \quad \text{on } \text{Ker}(L_1).$$

Under the above structural condition, we can state our main result on the decay property for the system (1).

**Theorem 2.** *Assume that the conditions (A), (S) and (K) hold. Let  $s \geq 0$  be an integer and suppose that the initial data  $u_0$  belong to  $H^s \cap L^1$ . Then the solution  $u$  to the problem (1) satisfies the decay estimate:  $\|\partial_x^k u(t)\|_{L^2} \leq C(1+t)^{-n/4-k/2} \|u_0\|_{L^1} + C(1+t)^{-\ell/2} \|\partial_x^{k+\ell} u_0\|_{L^2}$  for  $k + \ell \leq s$ . Here  $C$  and  $c$  are positive constants.*

- [1] K. Ide, K. Haramoto and S. Kawashima, *Decay property of regularity-loss type for dissipative Timoshenko system*, Math. Models Meth. Appl. Sci., **18** (2008), 647–667.
- [2] Y. Shizuta and S. Kawashima, *Systems of equations of hyperbolic-parabolic type with applications to the discrete Boltzmann equation*, Hokkaido Math. J., **14** (1985), 249–275.
- [3] Y. Ueda, S. Wang and S. Kawashima, *Dissipative structure of the regularity-loss type and time asymptotic decay of solutions for the Euler-Maxwell system*, preprint.
- [4] T. Umeda, S. Kawashima and Y. Shizuta, *On the decay of solutions to the linearized equations of electro-magneto-fluid dynamics*, Japan J. Appl. Math., **1** (1984), 435–457.



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# FRACTIONAL-ORDER FOURIER ANALYSIS OF HUMAN DNA

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**Introduction.** Phylogenetics is the study of the evolutionary relations between groups of organisms. With the advent of genome sequencing and genome databases, considerable information is available for computational processing, allowing worldwide research on decoding and understanding the informational structure present on DNA sequences.

In this paper is adopted the Fourier analysis and several approximations based on power law concepts. These ideas are usual in Fractional Calculus (FC) which is a paradigm that embodies the standard differential calculus a particular case.

**DNA Decoding and Fractional Order Analysis.** DNA is made up of two polymers forming a double helix and containing four nitrogenous bases, namely, {thymine, cytosine, adenine, guanine}, usually represented as  $\{T, C, A, G\}$ . Each base on one side bonds with just one type of base on the other side forming the base pairing  $A - T$  and  $C - G$ .

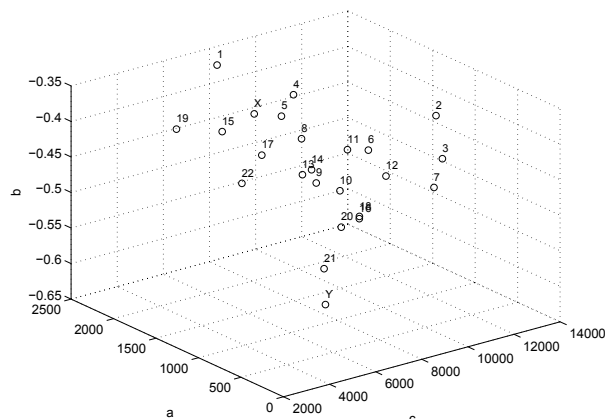
For processing the DNA information we need to convert the four symbols alphabet  $\{T, C, A, G\}$  into a numerical value. In fact, the available data includes a fifth symbol, represented by  $N$ , which is considered by DNA researchers to have no practical meaning for the decoding and, therefore,  $N$  is considered as “zero” during the calculations. In this paper is adopted the direct symbol translation  $A = 1 + i0$ ,  $C = -1 + i0$ ,  $T = 0 + i$ ,  $G = 0 - i$ ,  $N = 0 + i0$ . Note that the proposed translation follows the base pairing leading to  $A = -C$ ,  $T = -G$  and  $A$  “orthogonal” to  $T$ .

We consider that we move along the DNA strip, one symbol (base) at a time, and that the resulting values form a “signal”  $x(t)$  being  $t$  denoted loosely as the “time”. This signal can be treated by the Fourier transform (FT). In the present case we calculate the FT for 500 sampling frequencies in the interval  $10^{-7} \leq \omega \leq 10^0$ . Since the resulting plot has a significant level of noise, it is applied a median filter to the amplitude of the FT.

After performing several tests it was concluded that a power law using three parameters (PL3),  $|F(j\omega)| \approx a\omega^b + c$ ,  $a, c > 0$ ,  $b < 0$ , resulted in a good approximation. For adjusting the PL3 was adopted a standard genetic algorithm with elitism, crossover within all population and 5% mutation probability. Furthermore, was adopted a population of 20000 individuals and 5000 iterations of the genetic algorithm.

The parameters  $\{a, b, c\}$  of the PL3 approximation constitute a good tool for describing the characteristics of the chromosomes and to map their relationship. In fact, applying the PL3 to the twenty four chromosomes of the Human leads to the three dimensional locus represented in Figure 1. We verify the emergence of a graphical object including an ordering of the chromosomes, with 1 at one end and Y at the other. Rotating and zooming the graphical object we conclude that this locus reveals that some chromosomes have larger similarities (e.g., pair Hu3-Hu4, or pair Hu20-Hu21) while other are considerably distinct (e.g., pair Hu1-HuY, or pair Hu2-Hu20).

- [1] Machado J., Kiryakova V., and Mainardi F.: *Recent history of Fractional Calculus*. Communications in Nonlinear Science and Numerical Simulations, 16 (2011), 1140–1153.
- [2] Machado J., Costa A., and Quelhas M.: *Fractional dynamics in DNA*. Communications in Nonlinear Science and Numerical Simulations, 16 (2011), 2963–2969.



Locus  $\{a, b, c\}$  of the parameters of the PL3 approximations for the set of 24 chromosomes of the Human being

# DIFFERENTIAL EVOLUTION FOR TUNING FRACTIONAL ORDER CONTROLLERS APPROXIMATED BY PARTICLE SWARM OPTIMIZATION

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**Introduction.** A Fractional-Order Controller (FOC) is an extension of a standard PID controller because integral and derivative actions are of non-integer (e.g. fractional) order. In control systems application, FOC can increase closed-loop performance, enhance robustness to gain and parameter variations, and offer more design degrees of freedom, having positive impact on many industrial applications. Namely, FOC could replace PID in a high percentage of control loops. However, FOC design and tuning methods are still at their infancy. Despite many contributions in the literature, there are no established and systematic methods, or easy-to-use tuning rules as for PID controllers. Some authors attempt to generalize classical design approaches, some other apply optimization approaches based on performance error indexes. Even if optimization may result complex, in some cases it may provide more performing tuning methods. To this aim, the Differential Evolution (DE) optimization method is particularly useful when a powerful adaptive search mechanism is required, based on few search control parameters that are set constant.

**The tuning method.** We propose an approach that combines and extends the ideas presented in [1, 3]. We apply DE to tune parameters of FOC in a unitary feedback linear control system, for plants with a first order lag plus an integrator, namely  $G_p(s) = \frac{K}{s(1+\tau s)}$ . The FOC linearly combines two differintegrators at most for simplicity:  $G_c(s) = K_1 s^{\alpha_1} + K_2 s^{\alpha_2}$ , where  $-1 < \alpha_i < 1$  and  $K_i > 0$ , for  $i = 1, 2$ . We choose one or two fractional actions, but we can also have a more complex structure for achieving better results. The developed DE algorithm defines the most suited pair of derivative or integral actions for the known plant, given the closed-loop specifications. In particular, the desired peak value and settling time of the step response are translated in desired locations of dominant closed-loop poles.

The DE algorithm is run several times, each iterated for a certain number of generations on a population of candidate solutions to minimize an objective function  $J$  expressing the performance specifications. We assume  $J = \mathcal{R}^2 + \mathcal{I}^2$ , where  $\mathcal{R}$  and  $\mathcal{I}$  are the real and imaginary parts of the left-hand part of the characteristic equation  $1 + G_c(p_{1,2})G_p(p_{1,2}) = 0$ , that is computed in the desired pair of closed-loop dominant poles  $p_{1,2}$ . The DE algorithm minimizes  $J$ , then finds the best values of the FOC parameters  $K_1$ ,  $\alpha_1$ ,  $K_2$ , and  $\alpha_2$ .

**The approximation method.** The tuned FOC parameters yield an irrational transfer function, based on one or two differintegrators, that require an approximation by a rational transfer function for realization purpose. We use Particle Swarm Optimization with Constriction Factor (PSOCF) because it gives very reduced approximation errors also with respect to good existing approximation methods [2]. More specifically, we minimize  $\varepsilon = \min\{\max(|E_{mag,i}| \cdot P(\omega)) + \max(|E_{pha,i}| \cdot P(\omega))\}$ , then the magnitude and phase approximation errors with respect to the tuned fractional operators. The function  $P(\omega)$  penalizes errors outside the frequency range of interest.

The approximation is verified by plotting the frequency response diagrams, that show good matching with the response provided by the irrational operators, even if only 3 or 4 zero-pole pairs define the approximation. Obviously, the stability and minimum-phase properties are preserved in the approximation. Moreover, poles and zeros are interlaced along the negative real half-axis of the  $s$ -plane.

**Simulation results.** The proposed combined DE-tuning and PSOCF-approximation method is verified by simulation. Firstly, we specify a closed-loop performance that is better than in [3] for the same controlled plant. Secondly, we tune the FOC with one or two control actions by applying DE for 50 runs, that are iterated for 100 generations of a 50-dimensional population. Thirdly, we approximate the irrational operators with a rational transfer function by defining the search intervals that exploit values obtained by a method in [2] for zeros and poles. The magnitude and phase plots of the approximated rational controllers are in good agreement with the frequency characteristic of irrational operators in the chosen frequency bandwidth. Finally, we obtain the step responses determined by the two tuned FOCs in their realizations. The actual performance meets the specification quite well.

- [1] Biswas A., Das S., Abraham A., and Dasgupta S.: *Design of fractional-order  $PI^\lambda D^\mu$  controllers with an improved differential evolution*. Engineering Applications of Artificial Intelligence, 22 (2009), 343–350.
- [2] Maione G.: *Analog realizations of fractional-order integrators/differentiators: a comparison*. In: Filipe J., Andrade-Cetto J., and Ferrier J.-L. (eds.), Proc. 6th Int. Conf. on Informatics in Control, Automation and Robotics, Milan, Italy, July 2-5, 2009, 184–189.
- [3] Tenreiro Machado J. A.: *Optimal tuning of fractional controllers using genetic algorithms*. Nonlinear Dynamics, 62 (2010), 447–452.

## SYSTEM IDENTIFICATION OF THERMAL TRANSFERS INSIDE THE LUNGS USING FRACTIONAL MODELS

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**Abstract** - This paper is about fractional system identification of thermal transfers in the lungs. Most of the time during open-heart surgery, it is necessary to stop the heart from beating to allow the surgeon to operate properly. This is possible thanks to artificial heart/lung device. This device is called extracorporeal circulation (ECC). In order to connect the machine with the circulatory system, the heart and lungs are excluded from the blood stream. The lack of blood in the lungs during ECC is recognized as a potential cause of postoperative pulmonary dysfunction. Thus, anesthetists are developing methods to protect the lungs. One of these methods is to cool down the lungs by insufflating fresh gas inside it. This method has shown results but is based on the assumption that the thermal insulation of the lungs increases during ECC. This assumption has not been verified yet. A solution to verify it, is to design a thermal model of the lungs during ECC and during standard condition, and to compare both models. This paper presents the first step of this study. Different models of thermal transfer inside the lungs are identified.

Fractional transfer functions are especially appropriate to model thermal and biological systems and they are useful in system identification because they allow a few number of parameter (parametric compactness of the model). Among the fractional functions, the Havriliak-Negami function is rarely used, though it showed interesting results in system identification. Thus this paper studies the comparison between two fractional models, a classical one and another one using the Havriliak-Negami function. The results of these models are also compared with an integer model in order to emphasize the interest of fractional model with such application as biological system and/or thermal system.

This paper is composed of four parts. First, the approximations used for time simulation of fractional operator and Havriliak-Negami function are recalled. The second part deals with the experimental protocol. The results of the system identification and comparison of the models are presented in the third part. Finally, a conclusion considers the prospect.

Eight models of bronchial tubes thermal transfer are identified considering two different conditions ie with or without ECC. A significant variation in the parameters of the models is observed. For now, these variations are not linked with a physical meaning. Comparison between the fractional models show that the Havriliak-Negami is not very suited for this application. Nevertheless the comparison between an integer model and fractional models show the interest of the latter for black box system identification. The main focus of the followings works will be to link the parameter of the model with a physical or physiological meaning.

**Index Terms** - System identification, Bioengineering, Fractional model, Lungs model, Non-integer differentiation.

### References

- [1] Havriliak, S. and Negami, S. (1966). A complex plane analysis of alpha dispersions in some polymers. *Journal Polymer Science*, 14(B), 99–117.
- [2] Ionescu, C.-M., Machado, J.A.T., and De Keyser, R. (2011). Modeling of the lung impedance using a fractional-order ladder network with constant phase elements, *IEEE Transactions on Biomedical Circuits and Systems*, Vol. 5(1), pp. 83-89.
- [3] Magin R.L. (2010). Fractional calculus models of complex dynamics in biological tissues, *Computers and Mathematics with Applications*; 59: 1586-1593.
- [4] Pellet, M., Melchior, P., Petit, J., Cabelguen, J.M., and Oustaloup, A. (2010). Study of the peroneus digiti quarti muscle length effect on a motor unit fractional multi-model. In *IEEE/ASME International Conference on Mechatronics and Embedded Systems and Applications (MESA)*.
- [5] Sommacal, L., Melchior, P., Cabelguen, J.-M., Oustaloup, A., and Ijspeert, A.J. (2008). Fractional Multi-Models of the Gastrocnemius Frog Muscle, *Journal of Vibration and Control*, Sage Publishing, Vol. 14(9-10), pp. 1415-1430.
- [6] Sommacal, L., Melchior, P., Dossat, A., Petit, J., Cabelguen, J.-M., Oustaloup, A., and Ijspeert, A.J. (2007). Improvement of the muscle fractional multimodel for low-rate stimulation - *Biomedical Signal Processing and Control*, Elsevier, Vol. 2(3), pp. 226-233.
- [7] Victor, S., Melchior, P., Nelson-Gruel, D., and Oustaloup, A. (2008). Flatness control for linear fractional MIMO systems: thermal application, *3rd IFAC FDA'08*, Ankara, Turkey, 5-7 November.

## ROBUST PATH PLANNING FOR MOBILE ROBOT BASED ON FRACTIONAL ATTRACTIVE FORCE IN 3-DIMENSION SPACE

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**Abstract** - Path planning design is the elaboration of a strategy to define a trajectory which will reach a target by avoiding obstacles. The danger concept, which will modify smoothly the trajectory, is therefore of interest for the path planning of a mobile robot. For fixed polygonal obstacles, the connectivity of the robot free space can be captured in a network of nodes and arcs: the roadmap. A variety of methods can be used to obtain roadmaps for path planning. Local methods allowing a real time estimation of the trajectory have been introduced. The better known local methods in path planning are the fictitious potential methods. A fictitious force field is introduced to take into account the dynamics of the robot and to obtain realistic speeds.

The concept of a fictitious potential field in path planning is the following "The potential field concept considers the robot as a charged particle moving under the influence of repulsion potentials for the obstacles, and attraction potentials for the target". The attraction (negative) potential ( $U_{cible}(M)$ ) is associated to the target and the positive repulsive Coulomb type potential fields ( $U_k(M)$ ), are defined for each obstacle. The smoothness of the curve obtained with potential field methods makes practical steering and speed control possible. In previous works, a path planning design by fractional (or generalized) repulsive potential has been developed to avoid fixed obstacles: danger level of each obstacle was characterized by the fractional order of differentiation, and a fractional road was determined by taking into account danger of each obstacle. If the obstacles are dynamic, the method was extended to obtain trajectories by considering repulsive and attractive potentials taking into account position and velocity of the robot with respect to obstacles. The potential field method is a well-known tool to study and to drive the robot motion along a convenient trajectory. It allows an efficient control of the robot speed when it moves from its initial position to its goal. The main idea is to assume that the robot is attracted to the goal and is repulsed away from the obstacles. Then it is guided by a force field system generated by both the goal and the obstacle. Many formula dealing with the force applied on the robot to define its trajectory are found on the literature. Then, a 2-D space attractive force based on fractional potential was developed. The advantage of the generalized normalized force is the possibility to control its variation. The potential curve is continuously varying and depends only on one parameter, the non-integer order of the generalized attractive potential and robust in case of robot parameter variations.

This paper presents an extension of these fractional attractive forces in 3-D space for UAV application. This method allows obtaining robust and faster path planning in 3-D space despite UAV mass variations. The robustness of the obtained trajectories is studied. A comparison between a classical method and the proposed approach is presented. Section 1 is an introduction on path planning. Section 2 presents fractional mathematical background. Section 3 deals with the fractional attractive force definition and presents a dynamic analysis. Section 4 presents the robustness analysis in frequency domain and the comparison between a classical method and the proposed approach. Section 5 presents simulation results. Finally a conclusion is given in Section 6. Future works concern the use of this attractive force in 3D dynamic environment with mobile target and obstacles. The main application concerns UAV.

**Index Terms** - Robotics, Mobile robot, UAV, Robust Path planning, Fractional potential, Attractive force, Dynamic environment.

### References

- [1] A. Poty, P. Melchior and A. Oustaloup.: *Dynamic motion planning by fractional potential using Fast Marching optimisation*:. In First IFAC Workshop on Fractional Differentiation and its Applications (FDA'04), Bordeaux, France, July 19-20, 2004.
- [2] A. Poty, P. Melchior and A. Oustaloup.: *Dynamic path planning by fractional potential*:. In IEEE International Conference on Computational Cybernetics (ICCC'04), Vienne, Autriche, August, 30 August-1 September, 2004.
- [3] P. Melchior, B. Metoui, S. Najjar, A. Poty, M. N. Abdelkrim and A. Oustaloup.: *Attractive force based on fractional potential in dynamic motion planning for mobile robot*:. In ASME-MSND C IDETC/CIE'07, Las Vegas, Nevada, USA, September 4-7, 2007.
- [4] P. Melchior, B. Metoui, S. Najjar, M.-N. Abdelkrim and A. Oustaloup.: *Robust path planning for mobile robot based on fractional attractive force*:. IEEE American Control Conference (ACC'09), St. Louis, Missouri, USA, 10-12 Juin 2009.

# ON HILFER FRACTIONAL DERIVATIVES AND ITS APPLICATIONS

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**NO ABSTRACT AVAILABLE**

## SELF-SIMILARITY IN WORLD ECONOMY

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**Abstract.** Self-similarity is a property of complex networks, commonly observed in many distinct areas of science. Many real networks are said to be  $\checkmark$ scale-free $\checkmark$  since they show a power law behavior. In this paper, we focus in self-similarity of economical phenomena. For that purpose we analyze data and their corresponding statistical properties. We approximate data by trendlines, whose parameters are unequivocally related with each type of phenomenon.

**Self-similarity and power law behavior.** Self-similarity is a characteristic of complex nonlinear dynamical systems. It means that a system looks roughly the same, despite of the scale considered. A self-similar structure is infinite and is not differentiable in any point. Examples of self-similar systems are the fractals, observed in coastlines, turbulent flows, bacteria cultures and lungs. In music, structure and repetition are general features. A self-similar system,  $S(x)$ , obeys the scaling equation, given by:

$$S(\lambda x) = \lambda^s S(x) \quad (1)$$

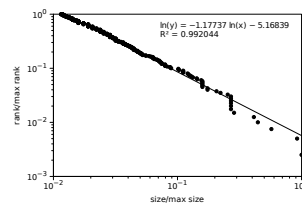
where  $s$  is the scaling factor, independent of  $x$ , and  $\lambda$  is a constant factor.

A power law (PL) tell us that the size of an event is inversely proportional to its frequency. Researchers usually represent a log-log plot of these quantities and verify if a straight line is obtained. The probability function of a discrete random variable following Pareto distribution is given by:

$$P(X = x) = Cx^{-\alpha} \quad (2)$$

A direct observation of equations (1) and (2), reveals that a PL satisfies the scaling condition.

**Power law behavior in economy.** The study of the Pareto's law validity for describing income or wealth distribution is very important. Though validity of PL behavior is restricted to a very small amount of income or wealth distribution, this amount can influence greatly the global economy. We analyzed the last fifteen years of the Forbes 400 list, from 1996 up to 2010. For each year the collected data was sorted, ranked, normalized, and represented in a log-log plot. A PL was adjusted to the data, using the least squares algorithm. Figure 1 depicts the result obtained for the year 2000. In that year the richest person was Bill Gates, with a fortune of 63 billions of dollars. At the bottom of the list were Christel Dehaan, Malcolm Glazer and Richard Haworth, with a fortune of 0.725 billions dollars. It can be observed that the distribution of wealth unveils a clear statistical regularity in a range of almost two orders of magnitude.



Rank/frequency log-log plot of the wealth of the 400 richest Americans in 2000

- [1] R. Gibrat. *Les inégalités économiques*. Paris, France, Librairie du Recueil Sirey (1931).  
[2] V. Pareto. *Cours d'Economie Politique*, Geneva, Switzerland: Droz (1896).

# FRACTIONAL ORDER MODEL AND CONTROL OF A HEAT PROCESS

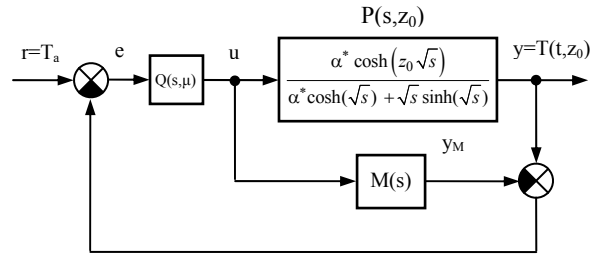
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**Introduction.** We consider the temperature control of a slab or long rod with given boundary conditions. Our aim is to control the temperature at a given point ( $z_0$ ) within a domain in spite of uncertainty in the process model. The physical model is given by a 2nd order parabolic partial differential equation and the process transfer function is of fractional order. Typical approach for the controller design of distributed parameter systems is to approximate the process and design the controller for the reduced-order model [3]. However, we now describe a robust internal model control (IMC) scheme which uses the exact (infinite dimensional) process model. The design procedure naturally leads to a fractional order controller. To tune the controller to satisfy design specifications we minimize the infinity norm of the robust performance index. We give a detailed example concerning the controller design and its properties.

**Internal Model Control scheme.** Internal model control (IMC) has been widely studied and applied for lumped parameter systems in the last decades. Recently, it has been extended to distributed parameter systems [1]. We apply it to a fractional order process and show how to design a robust controller. The IMC control scheme can be seen below. It consists of the process model  $P(s, z_0)$  which is not known exactly (the heat transfer coefficient  $\alpha^*$  is uncertain) and a nominal process model  $M(s)$ . For minimum-phase processes, the controller  $Q(s, \mu)$  includes the invertible part of the nominal model augmented with a low-pass filter:  $Q(s, \mu) = M(s)^{-1}F(s, \mu)$ . The filter  $F(s, \mu)$  is usually infinite-dimensional and must satisfy some conditions to guarantee zero steady-state error. The filter parameter  $\mu$  can be tuned to satisfy performance specifications.



IMC control scheme of the heat process.

**Fractional Order Controller.** Fractional order systems (FOS) have gained considerable attention in recent years. This is mainly due to the fact that many physical system naturally exhibits fractional order. Concerning theoretical background and application we refer to the extensive work of Tenreiro Machado [2]. As the nominal process model  $M(s)$  is strictly proper, consequently IMC controller will be improper. Therefore we augment it with a filter  $F(s, \mu)$  to make it proper. The resulting IMC controller have also fractional order and can be expressed as:

$$Q(s, \mu) = \frac{\alpha_N^* + \sqrt{s} \tanh(\sqrt{s})}{\alpha_N^* + \mu \sqrt{s} \tanh(\sqrt{s})}$$

where  $\mu$  is design parameter. One way to tune the  $Q(s, \mu)$  controller is by minimizing the infinity norm of robust performance index:  $\| |W_1 S| + |W_2 T_c| \|_\infty$  where  $W_1$  is a weighting function,  $W_2$  is the uncertainty weight,  $S$  is the sensitivity function and  $T_c$  is the complementary sensitivity function. Notice, that  $Q(s, \mu)$  can not be classified as a fractional order controller with fixed fractioner order. Rather, the fractional order is frequency dependent. It is interesting to note that if we replace the fractional order filter  $F(s, \mu)$  by a finite order low-pass filter  $F_n(s, \mu) = (1 + \mu s)^{-n}$ , then we can not find any value of  $\mu$  which satisfies the robust performance index. This is surprising but true! To simulate the "exact" process dynamics we applied Crank-Nicolson finite-difference scheme with grid size  $\Delta z = 0.02$  and time increment  $\Delta \tau = 0.01$  or smaller. To approximate  $Q(s, \mu)$  we used continued fraction expansion (CFE). We shall give a detailed example concerning th design procedure and optimal choice of tuning parameter  $\mu$ .

- [1] Kishida, M. and Bratz, R.D.: Internal Model Control of Infinite Dimensional Systems, *47th IEEE Conference on Decision and Control*, Cancun, Mexico, December 9-11, 2008, pp.1434-1441.
- [2] Machado, Tenreiro, J.A.: Application of Fractional Calculus in Engineering Sciences, *30th BENELUX Meeting on Systems and Control*, March 15-17, Lommel, Belgium, 2011.
- [3] Vajta, M. and Vajk, I.: IMC Based Boundary Control of a Thermal Process with Parameter Uncertainty, In: *The European Control Conference*, August 23-26, 2009, Budapest, Hungary, pp.2313-2318.

# A SCALABLE FRACTIONAL ORDER MODEL FOR IPMC ACTUATORS

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**Abstract.** New applications in a number of interesting fields, such as of bio inspired robotics, active prostheses, smart textiles, artificial tissues and organs, just to mention a few, will be possible, in the near future, largely because of new polymeric materials. These new materials are able to sense external stimuli and react to them, e.g. by changing their shape, so that they are not anymore passive tools but will be capable to cooperate to reach our objectives. A key role in the deep changes described above is played by Electro Active Polymers (EAPs), i.e. polymers that exhibit a mechanical reaction to an electrical stimulus. IPMCs belongs to the class of ionic EAPs, since transduction phenomena are due to ionic motion or ionic diffusion. IPMCs consist of a layer of ionic polymer, whose thickness is generally of the order of 100  $\mu\text{m}$ , interposed between two conductive layers to realize the electrodes. Nobile metals, such as platinum and gold, are used to this purpose. Electrodes are used both to impose the electrical stimulus when an IPMC is used as an electromechanical transducer, both to collect electrical signals, when the IPMC is used as a sensor. IPMCs models can be generally classified into black box, gray box, and first principle or white box models. A generally adopted scheme to model IPMCs consider the transducer as a pinned beam and applies the well know Eulero Bernoulli theory. Moreover the transduction phenomena are modelled by using suitable coupling terms in a similar way as for the case of piezoelectric devices.

In order to determine an IPMC model that could be parameterized according to the membrane dimension the following structure of the transfer function has been considered:

$$F(s) = \frac{k}{s^n (s^2 + 2as + \alpha^2 + \beta^2)^m}$$

where  $k$ ,  $\alpha$ ,  $\beta$ ,  $n$  and  $m$  are the system parameters to be determined. The characteristic of the proposed identification procedure consists in the fact that the obtained model is of fractional order, being  $n$  and  $m$  real numbers. The modelling phase has been applied to membranes of different lengths. For all the transfer functions the value of  $n$  is the same and equal to 0.756 and  $m$  is 1.15. In order to compare the models with the experimental data a series of laboratory test have been done. In the following figure are reported for the investigated cases, the real values of  $\alpha$  and  $\beta$  and their estimations obtained by using the linear and quadratic approximation respectively. In the same figure the real values of the IPMCs resonance frequency and the corresponding estimation is also reported.

[mm]	Experimental data			First order model			Second order model		
	[Hz]	$\alpha$	$\beta$	[Hz]	$\alpha$	$\beta$	[Hz]	$\alpha$	$\beta$
15	52,38	26	330	50	25,8	314,9	52,23	26,55	329,1
18	41,5	25	262	42,82	21,78	269,8	40,92	21,45	263,6
20	35,36	20	223	38,06	19,1	239,8	35,71	18,35	225
25	24,31	10	153	26,15	12,4	164,7	23,87	11,65	150,4
27	21	10	133	21,39	9,72	134,7	20,39	9,39	128,4
30	16,36	7	103	14,24	5,2	89,6	16,49	6,45	103,8

Fig. 1 Comparison between IPMCs actuator parameters and the corresponding estimation



# A RELATION BETWEEN THE FRACTIONAL DERIVATIVE AND THE HILBERT TRANSFORM

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**Introduction.** In past papers [2,3] two centred derivatives were presented. These are suitable for being used in problems where the causality is not important, like space problems. They are equivalent to the Riesz-Feller potentials but have a wider validity in the sense of being able to exist for any order excepting the negative integers. These derivatives were incorporated together with the Gr̃uwald-Letnikov derivatives into a unified fractional derivative that has the above referred derivatives as special cases [4]. This formulation uses 3 parameters: the derivative order, the causality parameter and the grid parameter. A very special result is obtained when we the derivative order is set to zero. We obtain an operator with an all-pass frequency response. In particular, we obtain the frequency response corresponding to the Hilbert transform (HT) [1]. This is confirmed from the integral representation of the unified derivative.

**A New Fractional Derivative Formulation.** Let  $f(t)$  be a real variable function. A general formulation of the fractional incremental ratio valid for any real or complex order leading to define the unified fractional derivative (UFD) is [4]

$$D_{\theta}^{\alpha} f(t) = \lim_{h \rightarrow 0} \frac{e^{-j\pi(\alpha-\theta)/2} \sum_{-\infty}^{+\infty} \frac{(-1)^k \Gamma(\alpha+1) f(t-kh+\gamma h/2)}{\Gamma[(\alpha+\theta)/2-k+1] \Gamma[(\alpha-\theta)/2+k+1]}}{h^{\alpha}} \quad (1)$$

where  $h$  is a positive real number,  $\alpha$  is the derivative order that can be any complex number,  $\theta$  is a parameter that sometimes is called skewness but we should call causality parameter and that determines the symmetry of the derivative (this can be viewed in the frequency response), and  $\gamma$  is a parameter that allows us to choose the used centred grid. This fractional derivative has an integral representation given by

$$D_{\theta}^{\alpha} f(t) = \frac{e^{j\pi \frac{\alpha-\theta}{2}}}{\Gamma(-\alpha) \sin(\alpha\pi)} \int_{-\infty}^{\infty} f(t-x) \frac{\sin[\alpha\pi/2+\theta\pi/2.\text{sgn}(x)]}{|x|^{\alpha+1}} dx \quad (2)$$

where the integral should be taken as the principal vale.

**A new Hilbert transform.** Put  $\alpha = 0$ ,  $\theta = 1$ , and  $\gamma = 1$  in the above formulae. We obtain after some manipulations

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(x)}{t-x} dx = - \lim_{h \rightarrow 0} \frac{1}{\pi} \sum_{-\infty}^{+\infty} \frac{f(t-kh+h/2)}{1/2-k} \quad (3)$$

that states a new way of computing the Hilbert transform.

- [1] Henrici, P. "Applied Computational Complex Analysis" Vol. 3, Wiley, 1993.
- [2] Ortigueira, M. D., "Riesz Potentials and Inverses via Centred Derivatives" International Journal of Mathematics and Mathematical Sciences, Volume 2006 (2006), Article ID 48391
- [3] Ortigueira, M. D., "On the Fractional Central Differences and Derivatives" Journal of Vibration and Control. 14(9–10): 1255–1266, 2008.
- [4] Ortigueira, M.D. and Trujillo, J., " On a Unified Fractional Derivative", Proceedings of the 2011 ASME/IEEE International Conference on Mechatronic and Embedded Systems and Applications (MESA2011), August 28-31, 2011 in Washington, DC, USA.

# ON PARTIAL DIFFERENTIAL EQUATIONS THAT EXHIBIT FRACTIONAL BEHAVIORS

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The link between fractional systems, recursivity and diffusion equations is now well known. If the following fractional system (fractional integrator) is considered.

$$H(s) = s^{-\gamma}, \quad (1)$$

with  $0 < \gamma < 1$ , its link with diffusion equation can be demonstrated through the system impulse response [1]. If  $u(t)$  and  $y(t)$  denotes respectively the system input and output, system (1) is equivalent to [2] [3]:

$$\begin{cases} \frac{\partial \phi(t, \zeta)}{\partial t} = \frac{\partial^2 \phi(t, \zeta)}{\partial \zeta^2} + u(t) \delta(\zeta) \\ y(t) = \int_{-\infty}^{\infty} m(\zeta) \phi(t, \zeta) d\zeta \end{cases} \quad (2)$$

This link should be used to implement fractional integration in software dedicated to numerical solving of differential equation such as for instance COMSOL Multiphysics software. However, the diffusion equation form of a fractional system requires the computation of an inverse Fourier transform,  $m(\zeta)$ , that is in most case impossible to compute analytically. This is why the paper proposes alternative differential equations that exhibits fractional behaviours in a given frequency band. Indeed, it is shown that transfer function (1) is equivalent to:

$$H(s) = \int_0^{\infty} \frac{\mu(x)}{p+x} dx, \quad (3)$$

and can be approximated in a given frequency band by:

$$H(s) = \int_{x_1}^{x_2} \frac{\mu(x)}{p+x} dx, \quad (4)$$

Let  $x(z, t)$  be a function of the space variable  $z$  of finite dimension ( $z \in [0..Z]$ ,  $Z \in \mathbb{R}^+$ ) and of the time variable  $t$ . This function satisfies the class of partial differential equations:

$$\beta(z) \frac{\partial x(z, t)}{\partial z} + \gamma(z) \frac{\partial^2 x(z, t)}{\partial t \partial z} = -u(t). \quad (5)$$

Also, let the system output  $y(t)$  be given by :

$$y(t) = x(0, t) - x(Z, t). \quad (6)$$

The input-output transfer function of this class of partial differential equations is defined by relation (4). These differential equations can be easily implemented to simulate a fractional real or complex integrator. As also shown, they also permit to represent real mechanical systems.

## References

- [1] Oustaloup A. (1983), Systèmes asservis linéaires d'ordre fractionnaire. Editions Masson, Paris.
- [2] Matignon D. (1998), Stability properties for generalized fractional differential systems, ESAIM: Proc. 5, pp 145-158.
- [3] Montseny G. (1998), Diffusive representation of pseudo-differential time-operators, ESAIM: Proc. vol 5, pp 159-175.

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**Mathematical Modeling for Decision  
Making in Epidemiology and Health  
Care**



## DATA, METHODS, MODELS AND RESULT INTERPRETATION: A MODEL BASED COMBINATION OF VARIOUS SKILLS TO THE IFEDH FRAMEWORK

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**Introduction.** As health care systems in all industrialized countries and newly industrialized countries have to deal with limited resources, growing demand and upcoming new technologies, high quality decision support and health technology assessment (HTA) based on dynamic and static modeling is getting more and more essential. In Austria the research project **Innovative Framework for Evidence based Decision support in Health care (IFEDH)** founded by The Austrian Research Promotion Agency is developing a framework addressing HTA questions.

The main focus of the project lies on the development of processes leading an interdisciplinary group of experts in the field of HTA, statistics, modeling, visualization and database analysts through the whole HTA production cycle, using infectious diseases simulation and vaccination as one example. The modeling process and the generation and design of adequate modeling methods are one core part. Besides this, the model and parameter validation as well as verification are in focus. The data quality assessments as well as the outcome interpretation are set up interdisciplinary, ensuring the necessary project quality and acceptance on the side of policymakers.

**Approach.** In the context of IFEDH a model based framework has to be implemented using detailed knowledge of the partners from different domains. The first step in the project is the analysis of model and structure know how as well as gathering the state of the art of modeling in HTA in Austria. Based on this information a specification of requirements regarding model structure and documentation of simulation outputs are set up. The third step, representing one of the core working tasks of the network is the development of adequate/reusable modeling structures and modeling methods. Therefore an evaluation table of methods in use as well as modeling and simulation strategies from other domains with a potential use in HTA is acquired. Furthermore modular model parts are developed and tested for their reusability. The analysis of data source depending to each module as well as the realization of usability tables and interface descriptions finalize this task, ensuring high flexibility and reusability. Based on exploratory work on

- different modeling techniques of infectious diseases [1],
- herd immunity effects of population groups using agent based modeling methods [2] and
- work of IFEDH members on serotype behavior modeling for infectious diseases and vaccination strategies [3]

recommendations for good practice are developed.

In act with the evaluation and integration of classical HTA methods, the development of methods for data preparation and analysis with respect to Austrian reimbursement data a "good practice" manual will be developed. The development of standardized visualization concepts for model parameters, model structures and the results, together with research on scenario set up and sensitivity analysis workflow is integrated and tested for practical use, by implementation of three real world HTA questions.

**Conclusion.** The description of the research project presented in the paper shows how different scientific domains can be joined to a joint overall approach in model based HTA. As decision support has to become faster because of legal obligations and the globalized interaction of people and therefore spreading of infectious diseases over borders and continents a predefined work plan, parameter sources and modular reusable model parts are developed. The theoretical work in the field of statistical methods, testing of adequate visualization methods and data quality assessment tools as well as a content management tool for the process guarantee that the boundaries regarding time span and quality can be observed.

- [1] G. Zauner, N. Popper, F. Breiteneker: *Evaluation of Different Modeling Techniques for Simulation of Epidemics*. in: Proceedings of the 7th Congress on Modelling and Simulation. ISBN: 978-80-01-04589-3
- [2] F. Miksch, N. Popper, G. Endel, I. Schiller-Frühwirth, F. Breiteneker: *Herd Immunity as a Result in Dynamic Agent-based Epidemic Models*. in: J. Wiley (Hrg.); Value in Health / Wiley-Blackwell, Vol. 13/ No. 7 (2010).
- [3] G. Zauner, N. Popper, F. Breiteneker, G. Endel: *Multi Agent Simulation Techniques For Dynamic Simulation of Social Interactions and Spread of Diseases with Different Serotypes*. in: "Public Health Decision Making - Program and Abstracts", U. Siebert, E. Fenwick, J. Pliskin (Hrg.); Target Conferences, (2010).

# A TOOLBOX FOR STATISTICAL VALIDATION OF HEALTH TECHNOLOGY ASSESSMENT PROCEDURES

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**Introduction.** When applying mathematical models to real-world problems, a central issue to address is the validation of results by comparing them to real-world data. In order to perform such a comparison, various statistical methods can be employed, ranging from visual comparison of results based on statistical graphics to parametric and non-parametric inferential methods.

Various outcome parameters of the mathematical models can be investigated and checked for their consistency with validation data. In each case, it is important to use an appropriate visualisation and/or test, taking into consideration factors like potential outliers in the data by using robust statistical methods.

When model outcome data for validation have been specified and the statistical methods for validation have been settled upon, there still remains the question of which validation data to use for comparison. A wide range of different options exist, and the researcher has a broad choice which data to use – yet there are important caveats to keep in mind when using them.

**Statistical Methods.** Outcome measures viable for validation of statistical model output include univariate statistics of some outcome values, most importantly measures for location and scale of these values, as well as multivariate measures such as association between different outcome variables.

For each of these outcome measures, different statistical methods for their validation are presented, with a particular focus on robust methods, as they are most appropriate in real-world datasets where outliers are encountered more often than not, as well as on graphical methods, emphasizing the need for exploratory analysis in the face of uncertainty about the nature of potential deviation of model output and real-world data.

**Validation Data.** A number of different sources of healthcare data are available that can be used for validation of model outputs. The most important validation data are presented, with a particular focus on Austrian social security data, and their possible applications for model validation are evaluated.

**Validation Standards.** When assessing a mathematical model's validity by qualitative and quantitative comparison of its results with validation data, some potential pitfalls must be kept in mind to avoid invalid or biased results.

An important consideration is to avoid overfitting a model to a specific dataset and, equally important, if overfitting occurs, to detect it at the level of validation. To this end, it is paramount that validation data are independent of the data on which the model has been fitted. Ignoring this principle invariably leads to overestimation of the model's fit to the real-world.

Furthermore, assessing variability of modeling can help gain important insights in reliability of a mathematical model. Techniques for quantifying this reliability, namely cross validation and bootstrapping, are often computationally intensive and involve multiple instances of model training on different training sets, but are necessary to get a sensible view on the quality of a model.

**Summary.** A set of tools to assess validity and reliability of model outputs based on independent sets of comparison data are described along with possible external data to be used for these analyses. Still, to employ them adequately, it is necessary to adhere to certain standards. The most important and necessary considerations are presented and the motivations behind them explained.

# MODELING HEALTH CARE SYSTEMS – AN APPROACH USING ROUTINE HEALTH CARE DATA

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**Introduction.** The use of dynamic models is already quite common in the field of health technology assessment. However, there has been less research on modeling and simulation addressing global questions of health care systems, for example which consequences a change of the reimbursement system could have. In health economics formal models do exist, but in most cases they provide just qualitative results without incorporating quantitative data. On the contrary, statistical methods are often used when analyzing large data sets. This approach is useful but cannot give insights into the behavior of the system at a different operating point where data do not exist, because its purpose is modeling the data and not the structure of the system.

In Austria there exist comprehensive routine health care data from reimbursement claims. Simulation models that can incorporate these data are therefore very beneficial. We present an approach that was used for building and parameterizing a model of extramural health care and its reimbursement system.

**Approach.** The model is agent-based and includes patients and medical service providers – physicians and other medical institutions of extramural health care – as agent types. Patients may develop one or many of several different chronic diseases that are incorporated into the model. These diseases provoke a certain service need in the patients. Therefore they consult the medical service providers in order to fulfill the service demand of all their illnesses. These providers get payment for the visits of the patients, where the actual reimbursement depends on the reimbursement system.

Some parts of the model are difficult to parameterize, especially what patients actually do if they have a certain disease (i.e. which treatment pathways they take and which services they get). This could be provided by expert opinion, but our approach tries to parameterize as much as possible from available routine health care data. The basis is probabilities for the association of medical diagnoses and prescribed drugs derived in [1], as the data in extramural care do not contain diagnosis codes. Thus it is possible to link patients and their medical claims to diseases.

The model uses prevalence of diseases (for determining how many patients have a certain disease at simulation start) and incidence rates (for determining at which rate patients get new diseases). Incidence rates are calculated from the data by counting patients that have a link to the corresponding diagnosis in one year but not before and dividing that by the time these patients were at risk. Prevalence is calculated by counting all the cases of a disease in one year, correcting it for the incidence of one year and dividing that by the total number of patients in the data.

The model input for the service need of the diseases is given by frequency distributions of services per quarter of year obtained from samples of patients with only one disease at a time. Every disease of a patient draws its service need from these frequency distributions every 90 days of simulation time. Each medical provider has their own portfolio of offered services. Probabilities for providers to offer a certain service, depending on specialty, equal the fractions of providers in the database who accounted the service at least once. When the medical problem has determined its new service need a provider search is performed. The chosen providers must be in a certain range of the patient, have acceptable waiting times (i.e. not too many patients in their queues) and must cover the service need in an optimal way – it has to be covered with as few providers as possible. Formally this is a minimum set cover problem with the service need as a universe and the subsets of offered services of each provider as the subsets from whom the covering family of sets is taken [2]. Patients consult the providers found regularly until their service need is fulfilled and thus treatment pathways emerge automatically.

**Conclusion.** The approach shows how analyses of routine health care data can serve as input for a complex and comprehensive model structure where it is not possible to do extensive literature searches and gathering of expert opinion as there are many different diseases to consider. Derivation of prevalence and incidence rates for diseases from the data is straightforward. For other parts such as treatment pathways additional assumptions are necessary, but for example the optimal selection of providers according to their service portfolio leads to at least plausible results.

[1] Weisser A., Endel F., Endel G. and Filzmoser P.: *Results of the project ATC-ICD – derivating ICD-codes from ATC-codes of prescription data*. In: Abstract Book of 26<sup>th</sup> PCSI Conference, Munich, 2010, 38.

[2] Vazirani V.: *Approximation algorithms*. Springer, Berlin, Heidelberg, New York, 2004.

## THE ONCOTYROL BREAST CANCER OUTCOME AND POLICY MODEL

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**Background.** Breast cancer is the most common malignant disease in Western women. Personalized medicine provides innovative technologies that promise more effective and efficient patient-targeted interventions and a decrease in adverse drug reactions. The overall goal of this project is to develop a comprehensive decision-analytic Breast Cancer Outcomes & Policy (BCOP) Model for the short- and long-term clinical and economic evaluation of patient-tailored treatment strategies. The project is part of ONCOTYROL - Center for Personalized Cancer Medicine.

The aim of the 1st project phase is to evaluate the cost-effectiveness of the new 21-gene assay that supports personalized decisions on adjuvant chemotherapy. The 21-gene recurrence score (RS) assay quantifies the likelihood of breast cancer recurrence and predicts the magnitude of chemotherapy benefit. However, the test costs around \$4000 per patient. It can be applied in conjunction with the Adjuvant Online! decision aid.

**Methods.** The model framework has been defined as follows. The target population for the evaluation of the 21-gene assay are women diagnosed with LN-negative HR-positive HER-2/neu-negative early-stage breast cancer. A hypothetical cohort of 50 year old woman is simulated for a lifetime period. For the economic analysis, a societal perspective has been adopted. Main model outcome parameters are expected life years, quality-adjusted-life years and costs. The BCOP model is a discrete event simulation model programmed using a process-oriented approach.

**Results.** Based on the BCOP model the application of modelling for Health Technology Assessment in personalized cancer medicine will be discussed. Within our presentation we will cover questions of selecting an appropriate modelling approach, discuss our model structure, challenges of the evaluation of multiple test and consequent treatment decision and model validation. New results and best practice recommendations of the ISPOR-SMDM Joint Modeling Good Research Practice Task Force will also be considered.

Within the process oriented simulation approach, the pathway of the patients is based on the natural history of the disease. Depending on the evaluated test-treatment strategy, the risk of cancer recurrence is determined by AOL or for specific subgroups by AOL and RS and a decision about adjuvant chemotherapy is made upon this risk classification. All patient characteristics, as well as information about adverse events, progression free survival, survival, cost etc. are tracked for each patient. Cost-effectiveness is calculated and risk group analysis is provided.

**Discussion.** Because personalized medicine takes into account that diagnostic and therapeutic health technologies should be based on individual characteristics such as risk profile and treatment response, a patient-level microsimulation approach is well suited in this decision-analytic context. The new 21-gene assay is an excellent example to demonstrate how sequential test-treatment combination can be evaluated using a discrete event simulation approach. The approach allows for subgroup analysis and because of the modular structure it provides the flexibility of further model extension e.g. additional information on new developed biomarker. However, main challenges in our evaluation of the 21-gene assay are data availability and limitations in the application of visual discrete event simulation software to incorporate HTA-specific analysis such as probabilistic sensitivity analysis.

**Conclusion.** Modeling in personalized medicine needs to provide the flexibility to evaluate sequential testing and subgroup specific targeting of treatment. Heterogeneity of individual characteristics and targeted treatment decisions call for microsimulation to evaluate personalized medicine.

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## R & GIS: GEOSPATIAL PLOTTING

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**Introduction.** Examples of spatial data within the R environment and the combination of R with data sets, spatial tools, libraries and other software products, which are common in real life environments, are provided in this paper.

R [1] is known as an upcoming statistical environment. Outlining various possibilities to utilize and display / plot spatial data using R is given. Not only an introduction to functionalities of R, but also the integration of different tools with the R environment will be discussed. Additionally ways to effectively develop a sophisticated report with R are outlined.

*Spatial* information can be found everywhere and often holds valuable details. Although there are methods to integrate spatial knowledge with data mining and analysis [2, chapter 8, page 191] procedures, displaying a meaningful map is in many cases necessary and very useful.

**Content.** Open source, platform independence, multilingualism and especially everyone's ability to utilize and contribute to the very rich environment of additional packages hosted mainly on "The Comprehensive R Archive Network" are good reasons to give R a try. More advanced userRs (spelling "user" and "developer" with capital 'R's is common in the R community) may use different extensions in addition to the variety of basic packages a normal installation offers.

Most of the more sophisticated packages provide worthwhile introductions and even extensive literature. Naturally these manuals concentrate on one or a few topics. As a result, easily reproducible examples and in-depth knowledge can be included while the degree of difficulty may still be manageable.

While these excellent resources are very useful concerning the targeting topic, the combination of different advanced packages within R and their integration with additional tools, data sources and even genuine productive working environments is quite complicated.

As this paper mainly discusses spatial data and R, a brief history and introduction to packages handling spatial information is provided. Because of recent developments, the `sp` package [2] became the preferred foundation and solution for most developerRs. Therefore possibilities, extensions and some technical background of `sp` is included. Since the official documentation covers the functionality of the entire package exhaustively, only chosen examples and necessary technical information is presented.

In addition to these fundamentals, the combination of `sp` with further packages targeting export and import of data structures, connection to databases, parallel usage of multiple processors, advanced or alternative plotting methods and also the linkage to cloud services will be explained. It should be obvious, that because of the vast amount of possibilities, only selected examples can be provided.

One great advantage of R - at least for advanced userRs - is the command line interface. Explorative investigations and playful experimentations using data and functionalities are possible, while the results can be combined in a script-file (batch-file) to document and automatically reproduce the entire work. Some projects tend to grow in size and several researchers contribute changes. Therefore the output of tables and plots has to be arranged in a document, refreshed or altered regularly. To deal with these common tasks, shared network drives and copy-paste procedures are quite common. A (better and) more sophisticated workflow based on different integrated development environments (IDEs),  $\LaTeX$ , Sweave and a distributed version management system is used to create the presented document.

**Summary.** The paper should provide a comprehensible and entertaining introduction to the practical usage of R and spatial data. Extensive technical details and theory are omitted in favor of a broader view and applicatory examples.

A combination of the presented technologies will be used to create the paper itself. Hence not only the content but also the applied methods creating the paper illustrate the conclusion of this work.

- [1] R Development Core Team: *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna Austria, 2008.
- [2] Roger S. Bivand and Edzer J. Pebesma and Virgilio Gomez-Rubio: *Applied spatial data analysis with R*. Springer, NY, 2008.

# ANALYSIS OF THE CHOLESTEROL BIOSYNTHESIS FEEDBACK CONTROL AND ITS CONSEQUENCES FOR THE HYPERCHOLESTEREMIA TREATMENT STRATEGIES

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**Introduction.** In the European Union 10-15% of the population has elevated levels of cholesterol. Elevated levels of cholesterol are known to be a risk factor for cardiovascular diseases. As a result, several treatment strategies and drugs have been developed to control these elevated cholesterol levels, but they are not always successful. A dynamic mathematical model of the cholesterol biosynthesis network was developed with aim to understand the key mechanisms of cholesterol biosynthesis.

**Cholesterol biosynthesis.** Cholesterol biosynthesis [2] is a complex system of metabolic pathways and control mechanisms that interact on many levels. The basis represents a metabolic pathway that starts at the Krebs cycle (cell breathing) and forms cholesterol in several steps. Some intermediates lead to other important substances, such as co-enzyme Q, vitamin D, corticosteroids, etc. To maintain the levels of many metabolites that are produced by the same metabolic pathway, a sort of cascade control with hierarchical arrangement must be used. The level of the most important metabolite has the highest priority in control action. The control mechanism for cholesterol biosynthesis operates mainly on two levels. One is the transcription level, where the rate of DNA transcription to mRNA is controlled. The other is degradation of enzymes involved in cholesterol biosynthesis. In case of elevated cholesterol levels cholesterol can mediate degradation of practically all cholesterologenic enzymes.

**Cholesterol regulation characterisation.** The developed model can be used for the analysis of the control mechanism of cholesterol levels through SREBF-2 expression and activation. The most important sterol that exists in homeostasis (the dynamical balance of concentrations) with SREBF-2 is cholesterol. At high concentrations of cholesterol, SREBF-2 is bound to the cell membrane and is, therefore, inactive. At low concentrations of cholesterol, SREBF-2 is released from the membrane and activated, which results in its migration to the cell nucleus where it can increase its own gene expression and that of the other cholesterologenic genes. The ratio of the total SREBF-2 (active and inactive) and cholesterol defines the concentration of the active SREBF-2. As the expression of all the cholesterologenic genes is regulated simultaneously, and since the reactions in the network are coupled through the metabolic flux, this can be modelled as a direct effect of SREBF-2 on the cholesterol metabolic influx. On the other hand, cholesterol is involved in numerous processes most of which are independent of the active SREBF-2 concentrations. The metabolic outflux of cholesterol can therefore be described as a constant outflux. The degradation of inactive SREBF-2 is rather slow as it is bound to the membrane and can be neglected, whereas active SREBF-2 is degraded faster and hence should be included in the model. Mathematical analysis of the developed model shows that the system operates similar to PI-control algorithm and can, therefore, precisely regulate the cholesterol levels.

**Conclusions.** We have shown that the added value of modelling and simulation in biological research is not necessarily in the development and simulation of large models but in their simplification [1]. The process of model simplification leads to the identification of the most important model mechanisms and thus indicates the key biological mechanisms of the researched process. The following can be concluded from the model analysis. To impair the presented control mechanism in a way that would produce elevated levels of cholesterol, a genetic disorder in several independently controlled pathways would have to occur simultaneously. However, high prevalence of hypercholesterolemia can not be explained by a genetic disorder as the frequency of the gene polymorphisms of the involved genes in the human population is much lower than the frequency of the hypercholesterolemia cases. The control mechanisms of cholesterol biosynthesis within the cell interact with a higher-level control mechanism that regulates the cholesterol production with regards to the global body needs for the cholesterol. It seems that in hypercholesterolemia liver is the organ that compensates for the metabolic disorders, while the origin of the disorder is located somewhere else. In this sense we need some radical changes in the current treatment strategies to improve the situation.

- [1] Belič, A., Ačimovič, J., Naik, A., and Goličnik, M.: *Analysis of the steady-state relations and control-algorithm characterisation in a mathematical model of cholesterol biosynthesis*. SIMPAT, doi:10.1016/j.simpat.2011.12.010 (2011).
- [2] Espenshade, P. J. and Hughes, A. L.: *Regulation of sterol synthesis in eukaryotes*. Annu. Rev. Genet., 41 (2007) 401–427.

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# DYNAMIC METABOLIC FLUX ANALYSIS FOR ONLINE ESTIMATION OF RECOMBINANT PROTEIN PRODUCTIVITY IN *Pichia pastoris* CULTURES

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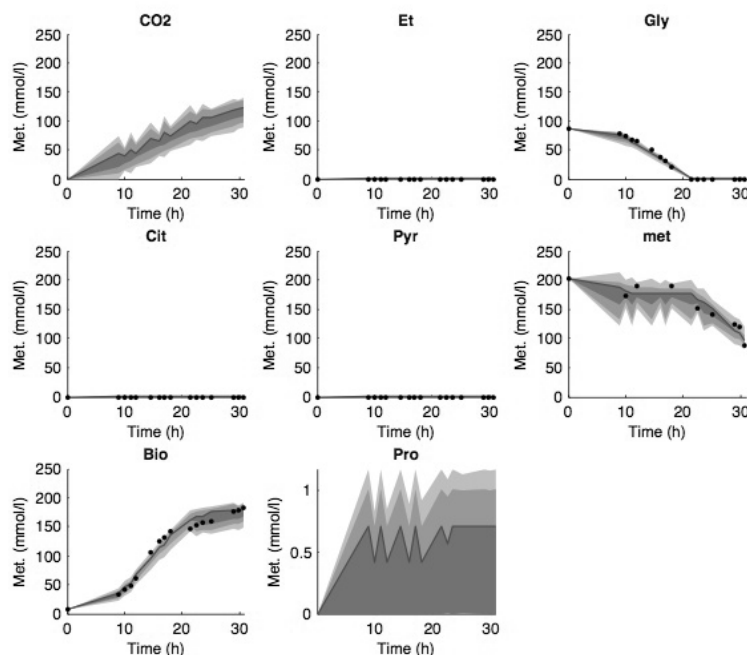
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**Introduction.** One approach to model living cells is based on successively imposing the (known) constraints –such as mass balances, thermodynamic laws, or enzyme capacities– that limit their behavior. This process results in a constraint-based model that encloses all the functional states that cells might exhibit. By combining the model with experimental measurements, it is possible to determine the particular cellular state at given conditions, an exercise that is generally referred to as Metabolic Flux Analysis (MFA).

**Results.** In this work we use a previously validated model [1] and an MFA-wise method [2] for on-line monitoring of industrial cultures of the yeast *Pichia pastoris*. Given a set of standard measurements –substrates, gases and biomass growth–, Possibilistic dynamic MFA provides estimates for unmeasured, time-varying extracellular metabolites and intracellular fluxes, while accounting for the imprecision and uncertainty common in an industrial settings. The production of the recombinant protein of interest can be estimated by means of a relationship among ATP consumption rate and specific growth rate, which is integrated into the model. To test the viability of the approach some preliminary experimental results are shown, using data from a set of batch cultivations performed in  $\tau$ -reactors.

The procedure is of great industrial interest because it can provide, not only a way to monitor the metabolic state of *Pichia pastoris* cultures during a running process, but also a direct online estimation of the protein production rate (see figure 1).



Metabolite concentrations and fluxes during a cultivation of a *Pichia pastoris* mutant producing a recombinant protein. Actual measurements are denoted with black dots; grey areas represent the possibilistic estimates of conditional possibility 1, 0.8 and 0.5.

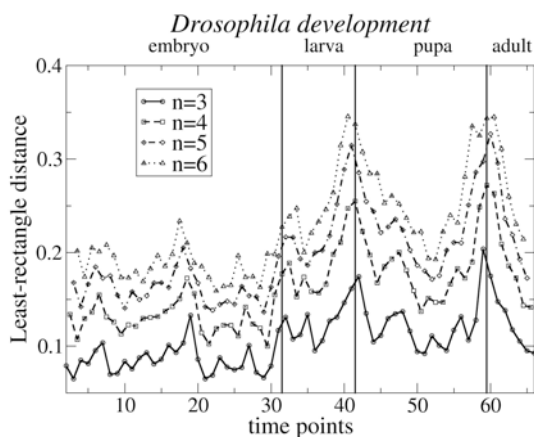
- [1] M. Tortajada, F. Llaneras, J. Picó, Validation of a constraint-based model of *Pichia pastoris* growth under data scarcity. *BMC Systems Biology*, Volume: 4:115 Pages: 1-11, 2010.  
[2] F. Llaneras, A. Sala, J. Picó, A possibilistic framework for constraint-based metabolic flux analysis, *BMC Systems Biology*, Volume: 3:79, 2009

# DETECTION OF DEVELOPMENTAL AND PERTURBATION STAGES FROM DNA MICROARRAY TIME SERIES AND ROBUST MODELING OF GENE EXPRESSION EVOLUTION

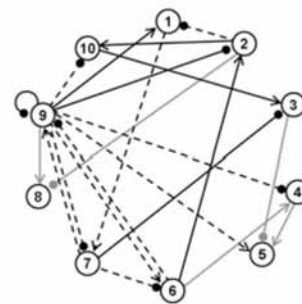
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We analyze DNA microarray time series describing gene expression in unicellular organisms subject to external perturbations or along developmental stages of higher eukaryotes. Using a translation-invariant and scale-invariant distance measure to compare the gene expression profiles, we show that peaks in the average distances are noticeable and are localized around specific time points. These coincide with the transition between developmental phases or follow external perturbations. This approach can be used to identify automatically, from microarray time series alone, the presence of such perturbations or transitions in arbitrary cell systems. Our results reveal the striking similarity between the gene expression responses to these very different phenomena. We set up a clustering method that uses the abovementioned distance to classify the genes within each stage and applied it to the development of the *Drosophila* embryo. The evolution of the average cluster expression levels was analyzed using coupled linear and non-linear differential equations. Different model structures and schemes for parameter identification and reduction were tested. The models obtained were compared on the basis of their abilities to reproduce the data, to keep realistic gene expression levels when extrapolated in time, to show the biologically expected robustness with respect to parameter variations, and to contain as few parameters as possible. A family of non-linear models reached all the objectives. It defined networks with an average of two connections per node.



Average distance between gene expression profile segments of length  $n$ , as a function of the time points, for the *Drosophila* DNA microarray time series; the vertical lines indicate the development stages.



Gene cluster regulatory network of the best solution obtained for the *Drosophila* embryo. The arrows and dots represent activation and inhibition, respectively.

[1] Rومان, M., Albert, J., Dehouck, Y., and Haye, A. (2011) Detection of perturbation phases and developmental stages in organisms from DNA microarray time series data. *PLoS One* 6, e27948.

[2] Haye, A., Albert, J., and Rومان, M. (2012) Robust non-linear differential equation models of gene expression evolution across *Drosophila* development. *BMC Res Notes*, in press.

# TOWARDS A NEXT GENERATION OF PREDICTIVE MODELS BASED ON SYSTEMS BIOLOGY TOOLS

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**Introduction.** In the area of predictive microbiology, most models focus on simplicity and general applicability, and can be classified as black box models with the main emphasis on the description of the macroscopic (population level) microbial behavior as a response to the environment. Their validity to describe pure cultures in simple, liquid media under moderate environmental conditions is widely illustrated and accepted. However, experiments have shown that extrapolation to more complex (realistic) systems is not allowed as such. In general, the applicability and reliability of existing models under more realistic conditions can definitely be improved by unraveling the underlying mechanisms and incorporating intracellular (microscopic) information [1]. Following a systems biology approach, the link between the intracellular fluxes and the extracellular measurements is established by techniques of metabolic flux analysis.

**Methodology.** Fundamental microbial research, in general, is conducted at three levels, i.e., the macroscopic, the mesoscopic and the microscopic level. At the *macroscopic level*, the overall population characteristics and behavior are studied. Macroscopic predictive models describe growth and inactivation dynamics of populations. As said in the introduction, macroscopic level models are able to accurately predict population dynamics under non-stressing conditions in liquid food model systems. For process control, monitoring and optimization purposes, macroscopic models are preferred as they have a rather simple structure, i.e., a limited number of model components and parameters. The *mesoscopic level* studies small populations, part of the population like subpopulations or colonies in structured environments. Due to environmental or population heterogeneity, differences in the microbial response are observed and all cells - or their dynamics - can no longer be assumed as identical. To completely unravel mechanisms underlying the specific microbial response to, e.g., stressing environments or environmental gradients, information is collected at a *microscopic level*, i.e., a cellular or even intracellular level.

In this methodology, the microscopic level is represented by a metabolic network. This is a graphical representation of (a subset of) the metabolic reactions that occur inside a cell. This information can equally well be described by the so-called stoichiometric matrix, which comprises the stoichiometric coefficients of the  $m$  metabolites in the  $n$  reactions. The number of metabolites and reactions in these networks can be very large, so first of all, these models have to be simplified. Different methods of model reduction for metabolic network-based models are presented in this paper.

A first simplification is the pseudo-steady-state assumption. Because intracellular dynamics are much faster than the macroscopic dynamics, a pseudo-steady-state can be assumed at the microscopic level. This assumption transforms the microscopic level model into an underdetermined system of linear equations, lowering the number of degrees of freedom significantly, i.e., from  $n$  to  $n - m$ .

Further model reduction is obtained by assuming that the cell has evolved to achieve optimal behaviour [2]. Mathematically, this quest for optimal behaviour is represented as an optimization problem via a technique called flux balance analysis (FBA). This technique is very popular, but has some important drawbacks. (i) After incorporating all available biochemical knowledge, it is possible that the solution of the FBA problem still results in multiple optima. (ii) The most important drawback is the fact that in some cases, the optimal solution does not correspond to the actual flux distribution. In this case, the assumption of optimal behaviour is not justified, and the FBA framework cannot be used. A solution to these drawbacks is the incorporation of a more generic objective function and more generic constraints. This is accomplished by introducing parameters into the objective function and the constraints, and estimating these parameters from experimental data.

**Case study.** The use of this methodology in a predictive modeling environment is exemplified for a theoretical case study. This methodology can prove very successful in describing different phenomena that occur during microbial growth, e.g., (induced) lag phases and stationary phases. Once this systems biology approach is successfully validated, it will be extended to develop next generation predictive models for more complex systems, such as co-cultures and structured environments.

- [1] Brul, S., Mensorides, F. I. C., Hellingwerf, K. J., Teixeira de Mattos, M. J.: *Microbial systems biology: new frontiers open to predictive microbiology*. International Journal of Food Microbiology, 128(1) (2008), 16–21.
- [2] Feist, A.M. and Palsson, B.O.: *The biomass objective function*. Current Opinion in Microbiology, 13(3) (2010), 344–349.

## MACROSCOPIC MODELLING OF OVERFLOW METABOLISM IN FED-BATCH CULTURES OF HYBRIDOMA CELLS

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Mammalian cell cultures are now well established as an industrial production platform for recombinant proteins, and with the recent PAT (Process Analytical Technology) initiative from the FDA, it now seems valuable to obtain a thorough metabolic characterization of cell lines and of the relationships between the cell environment and cellular behaviour.

This study aims at constructing a simple and identifiable macroscopic model of hybridoma cells that takes into account phenomena of overflow metabolism within glycolysis and glutaminolysis. These phenomena have been widely recognized in microbial biotechnology, e.g. in the case of ethanol production by *Saccharomyces cerevisiae* and acetate by *Escherichia coli*. In animal cell cultures cells convert a significant amount of glucose and glutamine to lactate and ammonia under high glucose and glutamine concentrations. Therefore, mathematically describing this phenomenon is important in order to control cells at the most desirable metabolism state without unnecessary overflow metabolism.

The macroscopic model proposed in this paper aims at simulating fed-batch cultures of hybridoma HB-58 cells. The model of central carbon metabolism is reduced to a set of macroscopic reactions describing three metabolism states: respiratory metabolism, overflow metabolism and critical metabolism. It is validated with experimental data of fed-batch hybridoma cultures and successfully predicts the dynamics of cell growth and death, substrate consumption (glutamine and glucose) and metabolites production (lactate and ammonia). Model parameters and confidence intervals are obtained via a non linear least squares identification. This model, on the one hand, allows quantitatively describing overflow metabolism in mammalian cell cultures and, on the other hand, will be valuable for monitoring and control of fed-batch cultures in order to optimize the process.

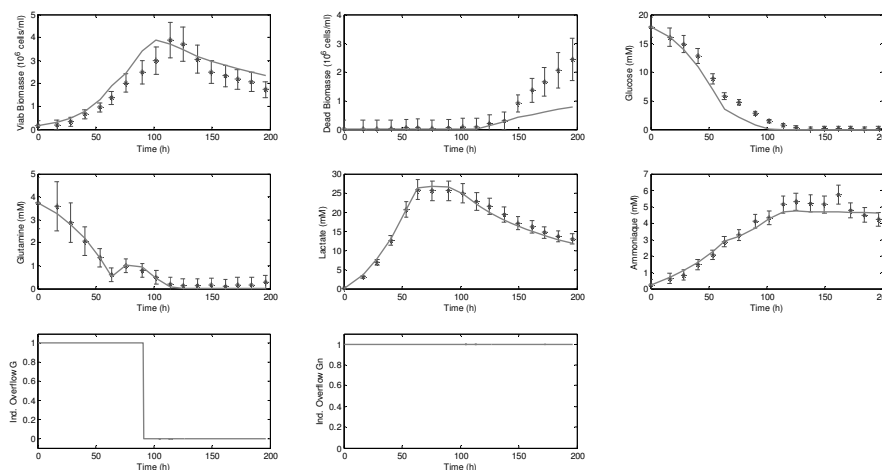


Fig. Comparison between model simulation and measurements of culture 4 after parameter identification with experiments 1, 2 and 3 (cross-validation).

- [1] Sonnleitner, B. and Käppeli, O.: *Growth of Saccharomyces cerevisiae is controlled by its limited respiratory capacity: Formulation and verification of a hypothesis*. Biotechnology and Bioengineering, 28(6) (1986), 927-937.
- [2] Doverskog, M., Ljunggren, J., Öhman, L. and Häggström, L.: *Physiology of cultured animal cells*. Journal of Biotechnology, 59 (1997), 103-115.
- [3] Friesewinkel, P., Niu, H., Drugmand, J.-Ch. and Bogaerts, Ph.: *Simple Metabolic Modelling of Vero Cell Growth on Glucose in Fixed-bed Bioreactors*. Proceedings of the 11th IFAC Symposium on Computer Applications in Biotechnology (CAB2010), Leuven (Belgium), 7-9/7/2010.



## A BACTERIAL INDIVIDUAL-BASED VIRTUAL BIOREACTOR TO TEST HANDLING PROTOCOLS IN A NETLOGO PLATFORM

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The choice of the basic modelling approach to study a bacterial system, either population-level (top-down, usually continuous with differential equations) or individual-based (bottom-up) is an important decision to be addressed according to the problem to be studied and the question to be answered. The two approaches are not incompatible or exclusive, but are complementary. Population-level approaches are mostly used for predictive purposes, due to their simplicity and computational efficiency. Moreover, they have been widely tested and, nowadays, many modelling frameworks exist. Individual-level models (IbMs) have also been used for some predictive purposes, but their strength is the means that they offer to disentangle and understand the dynamics of biosystems. They allow dealing with intra-population variability, with emergence of population behaviour from actions and interactions at the individual level and with those systems to which the continuum hypothesis is not applicable [1]. They also permit simulating different experimental protocols in labs and handling protocols in bioreactors in a simple manner, as IbMs are intrinsically discrete and take into account the individual behaviour adapted to internal and external conditions.

IbMs have been widely used and tested in the framework of ecology for more than 20 years, but their use in microbial systems began during the last decade. Despite the advantages they offer, IbMs are still far from being as readily accepted and widespread as continuous models in microbiology. Some of the reasons for this are: (i) the difficulty in determining the appropriate degree of complexity of the model, since models that become too complex fail to properly distinguish between causes and effects; and (ii) the difficulty in building, implementing, handling and analysing these computational models in a standard way, which complicates communication between specialists and with non-specialists. In recent years the scientific community has developed several strategies to overcome such difficulties, for instance, working with pattern-oriented modelling, establishing a standard protocol to describe IbMs (ODD protocol) [2] and developing specific open simulation environments such as NetLogo platform [3] to work with them, among others.

We present an IbM that simulates the dynamics of a bacterial bioreactor under different handling protocols, in an attempt to overcome the stated disadvantages with the above-mentioned strategies. The main objective is to provide a bacterial IbM simulator that will be easily understood and used by non-experts. The model has been designed on the same basis as INDISIM [4], and it is described with the ODD protocol. It has been implemented in NetLogo, so that it can be easily shared among the scientific community. This platform provides a user-friendly interface that can be managed by non-experts, and at the same time includes code that can be modified by any advanced user. The simulator allows the user to choose between three operating protocols (batch, fed-batch and continuous culture), to change some of the involved parameters, and to optionally take into account the inhibitory effect of an end product. The output of the simulation shows the evolution of bacterial population, nutrient and end product concentration, and biomass distribution. Different profiles in these outputs are clearly observed when the user changes the operating options and the involved parameters.

- [1] Hellweger L., and Bucci, V.: *A bunch of tiny individuals: Individual-based modeling for microbes*. Ecological Modelling, 220 (2009), 8-22.
- [2] Grimm V., Berger U., De Angelis D.L., Polhill J.G., Giske J., and Railsback, S.F.: *The ODD protocol: A review and first update*. Ecological Modelling, 221 (2010), 2760-2768.
- [3] Wilensky U. (1999). Netlogo. <http://ccl.northwestern.edu/netlogo/>. Center for Connected Learning and Computer-Based Modelling, Northwestern University. Evanston, IL
- [4] Ferrer J., Prats C. and López D.: *Individual-based modelling: an essential tool for microbiology*. Journal of Biological Physics 34 (2008), 19-27.

## ABOUT TRANSGRESSIVE OVER-YIELDING IN THE CHEMOSTAT

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**Introduction.** Recent investigations on the functioning of microbial ecosystems has revealed that combinations of certain species and resources enhance the functioning of the overall ecosystem, leading to a “transgressive over-yielding”. In the present work we show that spatialization can be a factor responsible for such a over-yielding, considering the usual framework of the chemostat splitting one volume into two tanks in parallel with different dilution rates.

Let consider a chemostat operated with constant volumetric flow rate  $Q$ , constant volume  $V$ , and constant input nutrient concentration  $S^{in}$ . We assume that the per capita growth rate  $f(\cdot)$  of each species is a smooth, concave and increasing function. Denote  $\lambda(\cdot)$  the break-even concentration and  $D^* = f(S^{in})$ .

**Configuration of two reactors in parallel.** We split the inflow channel to the chemostat in two channels, and the reactor volume in two parts. The first reactor is fed by the first channel with volumetric flow rate  $\alpha Q$  for some  $\alpha \in [0, 1]$  and it has volume  $rV$  for some  $r \in [0, 1]$ . Assume that we mix the outflows of both reactors (in the same proportions  $\alpha$  and  $1 - \alpha$  as the volumetric flow rates at their respective input channels).

The asymptotic value of the nutrient in the mixture is then given by the function

$$F(\alpha, r) := \alpha \lambda \left( \frac{\alpha}{r} D \right) + (1 - \alpha) \lambda \left( \frac{1 - \alpha}{1 - r} D \right), \text{ where } (\alpha, r) \in (0, 1)^2.$$

Define the subset of  $C = \{(\alpha, r) \in [0, 1]^2 \mid (\alpha/r)D \leq D^* \text{ and } ((1 - \alpha)/(1 - r))D \leq D^*\}$  and introduce the following “threshold” function  $T^{in}(D) = \lambda(D) + D\lambda'(D)$ .

The following Proposition shows that the performance of a single species chemostat can only be improved if  $S^{in}$  is small enough, and this is achieved by bypassing the second reactor with a unique, specific flow rate.

*Proposition 1.* The restriction of  $F$  to the convex set  $C$ ,  $F|_C$ , is convex. Moreover there holds that

$$\min_{[0,1]^2} F = \begin{cases} \lambda(D) = F(\alpha, \alpha), \forall \alpha \in [0, 1], \text{ for } S_{in} \geq T^{in}(D) \\ \min_{\alpha} F(\alpha, 0) < \lambda(D), \text{ for } S_{in} < T^{in}(D) \end{cases}$$

**Consideration of two species.** We consider two species with respective growth rate functions  $f_1$  and  $f_2$  and assume that there is a unique  $S \in (0, S^{in})$  such that  $f_1(S) > f_2(S)$  if  $S \in (0, S)$  and  $f_2(S) < f_1(S)$  if  $S \in (S, +\infty)$ . Let  $\bar{D} = f_1(S) = f_2(S)$  and  $D_i^* = f_i(S^{in})$  ( $i = 1, 2$ ). We assume that  $\bar{D} < \min(D_1^*, D_2^*)$ .

*Definition.* We say that a configuration  $(\alpha, r) \in (0, 1)^2$  corresponds to transgressive overyielding if

$$G(\alpha, r) := \alpha \lambda_1 \left( \frac{\alpha}{r} D \right) + (1 - \alpha) \lambda_2 \left( \frac{1 - \alpha}{1 - r} D \right) < \min(F_1(\alpha, r), F_2(\alpha, r))$$

The two next Propositions show that there always exist configurations of two parallel chemostats with only one of the species in each reactor volume that perform better than in the case in which for the same configuration, only one of the species is present in both reactors, regardless of the selected species.

*Proposition 2.* Let  $D = \bar{D}$  and fix  $\alpha \in (0, 1)$ . Then there always exist configurations  $(\tilde{\alpha}, \tilde{r})$  near  $(\alpha, \alpha)$  that correspond to transgressive overyielding.

*Proposition 3.* Let  $D \neq \bar{D}$ . Then there exist  $(\alpha, r) \in (0, 1)^2$  such that  $\frac{\alpha}{r} D < \bar{D} < \frac{1 - \alpha}{1 - r} D < \min(D_1^*, D_2^*)$  and this configuration  $(\alpha, r)$  corresponds to transgressive overyielding.

Finally we illustrate the benefit of the parallel configuration for different distributions of the volumes on numerical examples with the Monod growth functions.

# THE IDENTIFIABILITY OF BIOCHEMICAL MODELS

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**Introduction.** The aim of this paper is to discuss structural global identifiability of two recently proposed biochemical models: the first quantitatively describes a specific pathway, in two cell lines derived from two clinically different hematologic tumors, opening the possibility to guide the identification of therapeutic targets [4]. The second model investigates the receptor properties that critically determine processing of ligand-encoded information. The model provides important results on the information processing at the erythropoietin (EPO) receptor [1].

**Content.** Mathematical modeling of biological systems is becoming a standard approach to investigate complex dynamic, non-linear interaction mechanisms in cellular processes, like signal transduction pathways and metabolic networks. These are often modeled by ordinary differential equations involving parameters such as reaction rates, for example, Michaelis-Menten equation is often used to describe the internal structure of the biochemistry of the system. The system parameters contain key information but, in general, they can only be measured indirectly. The recovery of their values can then only be approached indirectly as a parameter estimation problem starting from external, input-output measurements. In this context, the first question is whether the parameters of the model can be determined assuming that for all observable variables continuous and error free-data are available. This is the subject of *a priori* or structural identifiability analysis of the model. Specifically, *global (unique) identifiability* is a necessary prerequisite for parameter estimation [5], [3]. It concerns the possibility of uniquely determining the model parameters from input-output data, under ideal conditions of noise-free observations and error-free model structure. Although necessary, global identifiability is obviously not sufficient to guarantee an accurate identification of the model parameters from real input/output data. However, if the parameters of the postulated model are not globally identifiable, the estimates which could, nevertheless, be obtained by some numerical optimization algorithms, will be totally unreliable and random. Identifiability analysis can be helpful also to provide guidelines to deal with non-identifiability, either providing hints on how to simplify the model structure or indicating when more information (measured data) are needed to allow unique identifiability. The recent bio-technological progress has provided the possibility of measuring many molecular species. To match these data and investigate the non-linear interaction mechanism in cellular processes, models of growing complexity have to be used and sophisticated identification techniques have to be adopted. Hence the need to investigate the identifiability properties of these nonlinear systems is therefore unquestionable.

In this paper it is shown how differential algebra techniques [5] can be used to test the identifiability of two important models which have been analyzed in the biological and biochemical literature. The software tool DAISY (Differential Algebra for Identifiability of SYstems) [2] is used, which automatically checks identifiability of (linear and) nonlinear dynamic models, by implementing a differential algebra algorithm.

**Conclusion.** In this paper we have analyzed global identifiability of two biochemical models: the first describes a specific pathway in two lymphoma cells, and the second describes the receptor properties that critically determine the processing of ligand-encoded information at the erythropoietin (EPO) receptor. We have analyzed and reduced these models to minimal form so that fundamental system theoretic properties, such as accessibility, hold and the reduced models are suitable to further mathematical investigations. For both of them, the differential-algebra based approach provides a direct check of global identifiability. The check shows a specific form of non-identifiability of two model parameters for the first model and global identifiability for the second. Both these examples bring up the relevance of testing global identifiability in biological studies, thus showing the advantages of the availability of a software tool able to check it in a fully automatic way, as DAISY does. Identifiability opens the avenue to the use of identification algorithms and eventually the way to therapeutic targets.

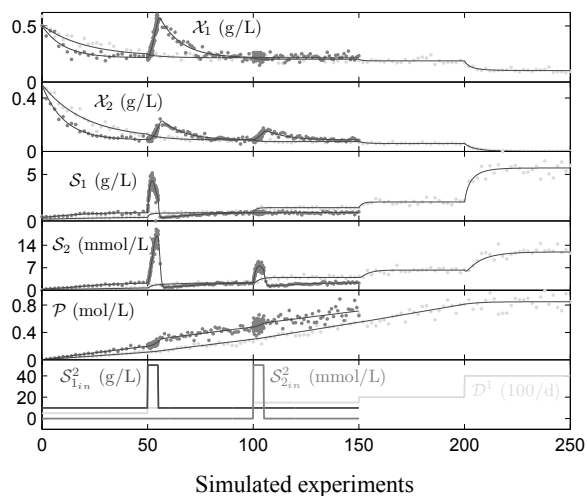
- [1] Becker V., Shilling M., Bachmann J., Baumann U., Raue A., Maiwald T., Timmer J., and Klingmüller U.: *Covering abroad dynamic range: information processing at the erythropoietin receptor*. Science, 328 (2010), 1404–1408.
- [2] Bellu G., Saccomani M.P., Audoly A., and D’Angiò L.: *DAISY: A new software tool to test global identifiability of biological and physiological systems*. Comp. Meth. Prog. Biom., 88 (2007), 52–61.
- [3] Ljung L., and Glad S.T.: *On global identifiability for arbitrary model parameterizations*. Automatica, 30, 2 (1994), 265–276.
- [4] Raia V., Shilling M., Böhm M., Hahn B., Kowarsch A., Raue A., Sticht C., Bohl S., Saile M., Möller P., Gretz N., Timmer J., Theis F., Lehmann W.D., Lichter P., and Klingmüller U.: *Dynamic mathematical modeling of IL13-induced signaling in Hodgkin and primary mediastinal B-Cell lymphoma allows prediction of therapeutic targets*. Cancer Res., 71 (2011), 693–704.
- [5] Saccomani M.P., Audoly S., and D’Angiò L.: *Parameter identifiability of nonlinear systems: the role of initial conditions*. Automatica, 39 (2004), 619–632.

# A SIMPLE PROCEDURE FOR THE IDENTIFICATION OF MACROSCOPIC BIOPROCESS MODELS: APPLICATION TO ANAEROBIC DIGESTION

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**Introduction.** The development of macroscopic models of bioprocesses from experimental datasets can be separated into two distinct problems. On the one hand, the stoichiometric identification problem deals with the determination of the reaction yields, while on the other hand, the kinetic identification problems aims at determining the structure and parameters of the reaction rates. This natural distinction in the modeling process has led us to develop a simple identification procedure that systematically attempts to a) assess the number of reactions required to represent the experiments at best, b) identify the unknown yield coefficients independently of the reaction rates, and c) determine the structure and the parameter values that characterize the reaction rates. Our identification procedure is illustrated with a simulated example of anaerobic digestion process.



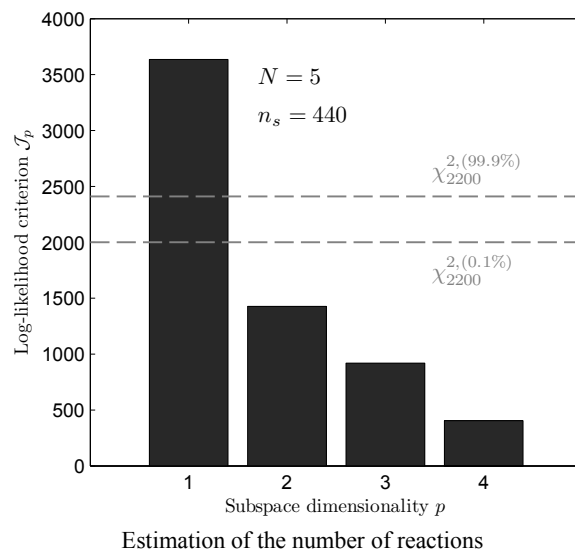
**Identification Procedure.** Both stoichiometric identification steps (i.e., assessment of the reaction number and determination of a yield matrix) use of the mathematical technique called Maximum Likelihood Principal Component Analysis [3] to estimate a vector basis of the best linear subspace that includes the concentration trajectory. The required number of reaction is equal to the dimension of this subspace, and each column of the yield matrix is expressed as a linear combination of the basis vectors.

During the kinetic identification step, reaction rates are expressed as a product of simple kinetic structures, each of which reflecting the influence of a particular species concentration. Kinetic structures are then classified into a set of decision trees, in which each branch represents a parametric condition to be tested by the statistical technique called Likelihood Ratio Test.

**Results.** Provided a good knowledge of the terms related to transport, our identification procedure is able to accurately estimate the reaction yields of the anaerobic digestion process and to determine the structure and parameters of its reaction rates. The identification results also stress the importance of designing informative experiments to avoid identifiability problems.

**Model and Data.** In this work, we consider that any bioprocess can be represented by the general dynamical model of [1], which expresses the evolution rate of the process concentrations as the product between a pseudo-stoichiometric matrix that contains the reaction yield coefficients, and a reaction rate vector, each element of which being expressed as a nonlinear function of the concentrations.

With the aim of illustrating the identification procedure on an example free of characterization error, two informative experimental datasets are simulated from a well-established model of anaerobic digestion [2]. Within these experiments, measurement errors are chosen as independent and normally-distributed, with known covariances.



Estimation of the number of reactions

- [1] G. Bastin and D. Dochain. *On-line Estimation and Adaptive Control of Bioreactors*. Elsevier Science Ltd, 1990.
- [2] A. Donoso-Bravo, J. Mailier, C. Martin, J. Rodríguez, C. Arturo A. L., and A. Vande Wouwer. Model selection, identification and validation in anaerobic digestion: a review. *Water Res.*, 45(17):5347–5364, 2011.
- [3] P. D. Wentzell, D. T. Andrews, D. C. Hamilton, K. F., and B. R. Kowalski. Maximum likelihood principal component analysis. *J. Chemom.*, 11:339–366, 1997.

# ROBUST OPTIMAL EXPERIMENT DESIGN: A MULTI-OBJECTIVE APPROACH

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**Introduction.** Optimal Experiment Design (OED) is an indispensable tool in order to reduce the amount of labour and cost intensive experiments in the modelling phase. The unknown parameters are often nonlinearly present in the dynamic process models, meaning that the Fisher Information Matrix also depends on the current guess for the parameters. These early estimates are often highly uncertain. So designing an optimal experiment without taking this uncertainty into account is troublesome. In order to obtain an informative experiment, a robust optimisation approach is necessary. In recent work, a formulation [1] using an implicit weighted sum approach is proposed where the objective function is split in a nominal optimal experiment design part and a robust counterpart. This weighted sum has well-known drawbacks as a Multi-Objective Optimisation approach. In this work these objectives are studied using advanced multi-objective optimisation methods like the Normal Boundary Intersection and the Normalised Normal Constraint [2].

**Content.** Optimal Experiment Design for nonlinear dynamic systems is a particular class of optimal control problems. In Optimal Experiment Design for parameter estimation, some scalar function of the Fisher Information Matrix is used as the objective function. In nonlinear dynamic models the elements of the Fisher matrix depend on the current estimate of the parameters. It is however possible that there is a large uncertainty with respect to these parameter values. This explains the need for *robust optimal experiment design*. This means that the information content is much less dependent on the current estimate of the parameters. Parameters are assumed to be normally distributed:

$$\mathbf{p} \sim N(\mathbf{p}_0, \Sigma) \quad (1)$$

where  $\mathbf{p}_0$  is the mean value and  $\Sigma$  the variance. The formulation used as robust optimal experiment design in [1] is a min-max optimisation problem of the following form:

$$\min_{\mathbf{x}(t), \mathbf{u}(t), t_f} \max_{\|p-p_0\|_{2,\Sigma^{-1}} \leq \gamma} \Phi(\mathbf{F}(\mathbf{p})) \quad (2)$$

where  $\gamma$  is a confidence quantile. In [1], this problem is solved by applying a Taylor expansion with respect to the parameters of the objective function, which leads to the following robust experimental design optimisation problem:

$$\min_{\mathbf{x}(t), \mathbf{u}(t), t_f} \Phi(\mathbf{F}(\mathbf{p})) + \gamma \left\| \frac{\partial}{\partial \mathbf{p}} \Phi(\mathbf{F}(\mathbf{p})) \right\|_{2,\Sigma} \quad (3)$$

It is clear that there are two parts in this objective function: the nominal Optimal Experiment Design objective,  $\Phi(\mathbf{F}(\mathbf{p}))$  and the robust objective,  $\left\| \frac{\partial}{\partial \mathbf{p}} \Phi(\mathbf{F}(\mathbf{p})) \right\|_{2,\Sigma}$ . The latter objective aims at having a cost surface which is flat with respect to the unknown parameters. An interesting thing about the formulation above is that this can be viewed as a *multi-objective optimisation* problem consisting of two different, possibly conflicting, objectives, which are subsequently solved using ACADO-Multi-Objective.

**Results.** The presented approach is applied to a predictive microbiological case study [3]. For obtaining the Pareto front, both the Weighted Sum and the more advanced Normal Boundary Intersection and Normalised Normal constraint are compared in this paper.

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- [1] S. Körkel, E. Kostina, H.G. Bock, and J.P. Schlöder. Numerical methods for optimal control problems in design of robust optimal experiments for nonlinear dynamic processes. *Optimization Methods and Software Journal*, 19(3-4):327–338, June-August 2004.
- [2] F. Logist, B. Houska, M. Diehl, and J.F. Van Impe. Fast pareto set generation for nonlinear optimal control problems with multiple objectives. *Structural and Multidisciplinary Optimization*, 42:591–603, 2010.
- [3] E. Van Derlinden, K. Bernaerts, and J. Van Impe. Simultaneous versus sequential optimal experiment design for the identification of multi-parameter microbial growth kinetics as a function of temperature. *Journal of Theoretical Biology*, 264:347–355, 2010.

## ON A THREE STEP MODEL OF ANAEROBIC DIGESTION INCLUDING THE HYDROLYSIS OF PARTICULATE MATTER

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**Summary.** Anaerobic digestion is a biological process in which organic matter is transformed into methane and carbon dioxide (biogas) by microorganisms in the absence of oxygen. The search for models simple enough to be used for control design is of prior importance today to optimize fermentation processes and solve important problems such as the development of renewable energy from waste. Within the studies of microbiology, biochemistry and technology, the anaerobic digestion is generally considered as a three step process: hydrolysis and liquefaction of the large, insoluble organic molecules by extracellular enzymes, acid production by an acidogenic microbial consortium and a methane production stage realized by a methanogenic ecosystem. Several mathematical models describing these phenomena have been proposed in the literature.

In this work, we focus on the mathematical analysis of the model of chemostat with enzymatic degradation of a substrate (organic matter) that can partly be under a solid form [2]. The study of this 3-step model is derived from a smaller order sub-model since some variables can be decoupled from the others. We study the existence and the stability of equilibrium points of the sub-model considering both Monod or Haldane growth rates and distinct dilution rates. In the classical chemostat model with monotonic kinetics, it is well known that only one equilibrium point attracts all solutions and that bistability never occurs [3]. In the present study, although (i) only monotonic growth rates are considered and (ii) the concentrations of input substrate concentration is less than the break-even concentration, it is shown that the considered sub-model may exhibit bistability. Hence, the importance of hydrolysis in the appearance of positive equilibrium points and the bistability is pointed out. If a non monotonic growth rate is considered, depending on the input substrate concentration, it is shown that at most four positive equilibrium points exist. Furthermore, for any positive initial condition, the solution converges towards one of the positive equilibrium points for which the washout is unstable. Finally, we study the case where the growth rate is density-dependent, such as the Contois kinetics, which may be of interest if we consider that we work in a non homogeneous environment [1]. Depending on the input substrate concentration, we show that the system can exhibit either a bistability or the global stability of the positive equilibrium point or of the washout.

- [1] C. Lobry and J. Harmand, *A new hypothesis to explain the coexistence of  $N$  species in the presence of a single resource*. CRAS série Biologie, 2006, (329): 40–46.
- [2] I. Simeonov and S. Stoyanov, *Modelling and dynamic compensator control of the anaerobic digestion of organic wastes*. Chem. Biochem. Eng. Q, 2003, 17(4): 285–292.
- [3] H.L. Smith and P. Waltman, *The Theory of the Chemostat, Dynamics of Microbial Competition*. Cambridge University Press, 1995.

# SIMULATION OF THE ANAEROBIC DIGESTION OF MICROWAVE PRE-TREATED WASTE ACTIVATED SLUDGE WITH ADM1

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The disposal of sludge originating from municipal waste water treatment is a major issue and represents up to 50% of the operating costs of wastewater treatment plants (WWTP) [1]. This sludge, a by-product of the treatment processes, however, has the potential to be converted into an energy rich biogas, i.e. a mixture of ca. 65% CH<sub>4</sub> and 35% CO<sub>2</sub>, which can be utilized for the sustainable production of heat and/or electricity. Additionally, the digestion improves the stability and dewaterability of the sludge, making incineration of the residue more sensible. Already, digestion of waste activated sludge is performed on a large scale. For instance, in the Flanders Region in 2010, more than 51% of the sludge was digested resulting in 7,000 MWh of electrical power [2]. Various pre-treatment methods have been suggested in literature for improving the solids reduction and biogas production rate by enhancing the digestion's rate limiting step, i.e. organic matter hydrolysis. They all induce the solubilization of complex particulate matter so this is more rapidly and completely consumed during the anaerobic digestion process. Methods that have been shown to have a positive effect on anaerobic digestion include chemical, mechanical, biological and thermal processes. An overview is presented in Appels et al. [1]. Microwave disintegration is one of the more recently applied pre-treatment methods. The disintegration is caused by the combination of thermal and athermal effects and may hence provide superior results compared to a heat treatment [3].

The application of mathematical models for the optimization of the digestion process is widely acknowledged. They, moreover, provide interesting and useful information regarding the phenomena occurring on micro-scale. Due to the complexity of the microbial process, accurate modelling of anaerobic digestion is, however, a daunting task. A major stride countering this problem was achieved by the development of the Anaerobic Digestion Model no 1 (ADM1) by the corresponding IWA task group [4]. This model is ever since, considered to be the state of the art in modelling of anaerobic digestion and has been the platform for further refinements and numerous applications [5]. In ADM1, both biochemical as well as physicochemical processes are included. All components except inorganics are expressed in terms of their COD. The biochemical reaction pathway includes: (i) an extracellular disintegration step converting composite particulate matter into carbohydrates, lipids and proteins, (ii) an extracellular enzymatic hydrolysis step converting the degradation products into monosaccharides, long chain fatty acids (LCFA) and amino acids (AA), (iii) acidogenesis or fermentation of these components into hydrogen, acetate and volatile fatty acids (VFA), (iv) acetogenesis of VFA to acetate, (v) acetoclastic and hydrogenotrophic methanogenesis. Additionally, the death of biomass is taken into account.

The main aim of this work is to investigate the ability of ADM1 to describe anaerobic digestion of microwave pre-treated sludge. Compared to untreated sludge, the composition and structure of the sludge is changed dramatically due to the treatment. The experimental results were obtained from a long-term pilot scale anaerobic digestion test using two parallel (one with untreated, the other with microwave-treated sludge) continuously mixed digesters, each having a volume of 50 L. For both digesters, several composition parameters of the feed and the digester liquid were measured on a frequent basis. The recorded data and digester performances were compared with the results of a modelling in ADM1 [4]. It was seen that the biogas production of the microwave enhanced sludge was increased significantly. Practically, the ADM1 implementation as described by Rosen & Jeppsson [6] is chosen as it effectively completes the mass balance for COD, carbon and nitrogen. It is investigated if the major dynamics can be accurately modelled based on the measured inputs and the used parameters. Also, the performance of ADM1 in modelling the digestion pre-treated sludge is compared to the digestion of untreated sludge.

[1] Appels, L., Baeyens, J., Degève, J., and Dewil R. (2008). Principles and potential of the anaerobic digestion of waste-activated sludge. *Progress in Energy and Combustion Science*, 34, pp 755–781.

[2] Aquafin (2010). Jaarverslag 2010 – Een integrale visie op waterzuivering, Aquafin (Luc Bossyns) (Belgium).

[3] Eskicioglu C., Terzian N., Kennedy K.J., Droste R.L. and Hamoda M. (2007). Athermal microwave effects for enhancing digestibility of waste activated sludge. *Water Research*, 41, pp 2457–2466.

[4] Batstone, D.J., Keller, J., Angelidaki, I., Kalyuzhnyi, S.V., Pavlostathis, S.G., Rozzi, A., Sanders, W.T.M., Siegrist, H. and Vavilin, V.A (2002). The IWA Anaerobic Digestion Model No 1 (ADM1). *Water Science and Technology*, 45(10), pp 65-73.

[5] Batstone, D.J., Keller, J. and Steyer, J.P. (2006). A review of ADM1 extensions, applications, and analysis: 2002-2005. *Water Science and Technology*, 54(4), pp 1-10.

[6] Rosen, C. and Jeppsson, U. (2005). *Anaerobic COST benchmark model description – Technical report*, Department of Industrial Electrical Engineering and Automation (IEA), Lund University, Lund, Sweden.

# SOME CONSIDERATIONS ABOUT CONTROL OF MULTISPECIES ANAEROBIC DIGESTION SYSTEMS

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**Motivation.** Anaerobic digestion is one of the most popular process for the biological treatment of wastewater, as it not only removes the pollutants but also allows the production of biogas. Compared to the aerobic treatment, the anaerobic digestion provides several advantages among which the higher energy production and the substantially lower sludge production are the most important ones. In terms of process stability, anaerobic digestion still lags behind aerobic biological treatment or physico-chemical processes. Substantial expertise is required to operate such a process properly, as the operational point is not globally stable. Thus a good understanding of process dynamics and an efficient start-up strategy are required to safely drive the reactor towards an optimal operating point.

Commonly, the models describing anaerobic digestion processes assume that only one species perform the transformation, while in reality the conversion is carried out by a consortium of microorganisms. Thus the model represents an approximation of the real system by averaging the dynamics of the species present in the reactor at a certain moment, which may substantially differ from the real dynamics. Hence, reactor start-up is an even more delicate problem, as not only it has to bring the system to an operational point but it has to lead to a consolidated ecosystem in terms of treatment efficiency and maximization of biogas production.

**Content.** This paper presents a simulation-based evaluation of a start-up strategy for multispecies anaerobic digestion systems modelled as two-step reaction systems, in which acidogenesis is described by Monod kinetics while the methanogenesis is described by Haldane kinetics. The start-up policy has been developed originally for single species systems with the aim of maximizing the biogas outflow rate [2, 3]. It is based on system convergence to an operational equilibrium point [1] and consists of switching the dilution rate from minimum to maximum and then to the optimal value in order to bring the system from an arbitrary initial condition to the optimal setpoint. This start-up strategy is applied to the multispecies system using an averaged model, which is usually the only model that can be identified for such a system, since measuring individual biomasses is quite difficult in practice. The averaged model is used to select the minimum ( $u_{min}$ ) and maximum ( $u_{max}$ ) dilution rates and to compute the optimal one ( $u_s$ ), as well as in determining the instants when the switchings in the dilution rate occur.

The investigations are carried out for two cases which respectively consider the availability of an accurate and inaccurate averaged models in order to evaluate to which extent the start-up procedure leads to a consolidated ecosystem in terms of biogas production maximization. The simulation results show that a meaningful steady state is reached, characterized by a higher biogas outflow rate and higher COD consumption than the ones predicted by the averaged model. It can be proved, using the analytical expressions of the equilibrium points, that the acidogenic and methanogenic species winning the competition for  $u = u_s$  are the most efficient ones at this dilution rate among the species present in the reactor. We conclude that the competitive exclusion is the best selection process of the most efficient species in generating the highest amount of biogas at the dilution rate  $u_s$ . However, a crucial condition is that these species are present in the reactor in the final stage of the control strategy, ie. they have not been washed out before switching the dilution rate to  $u_s$ . Hence, of particular importance is the estimation of the time span the species can coexist in the reactor, which may play a prominent role in some cases for the selection of the most efficient species.

- [1] Sbarciog M., and Loccufier M., and Noldus E.: *Determination of appropriate operating strategies for anaerobic digestion systems*. Biochemical Engineering Journal, 51 (2010), 180–188.
- [2] Sbarciog M., and Loccufier M., and Vande Wouwer A.: *On the Optimization of Biogas Production in Anaerobic Digestion Systems*. In: Preprints of the 18th IFAC World Congress, Milano, 2011, Italy, 2011, 7150–7155.
- [3] Sbarciog M., and Loccufier M., and Vande Wouwer A.: *An Optimizing Start-up Strategy for a Bio-methanator*. Bioprocess and Biosystems Engineering, DOI 10.1007/s00449-011-0629-5 (2011).

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## ADAPTIVE PORT REDUCTION IN STATIC CONDENSATION

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The reduced basis static condensation method recently introduced in [1] provides a computational framework for the solution of parameter dependent partial differential equations (PDEs) where the spatial domain is composed by a number of components attached to each other at predefined ports to form a global system. Attached to each component is a set of scalar parameters that may describe properties of the component related to for instance materials or geometry. The method is developed for linear elliptic problems, with applications to problems in, say, heat transfer or elasticity. It provides a tool for rapid solution of the global PDE both for different choices of the parameters as well as for different topological configurations of the components. Moreover, it allows treatment of problems in which the global system has *many* parameters since the reduced basis approximation is performed over the smaller parameter domain local to each component.

Within a standard static condensation framework it is necessary to solve a PDE local to each component for each of the degrees of freedom associated with the ports of the component. Within the reduced basis static condensation framework, each of these local solves is replaced by a reduced basis approximation [2]. Each component thus has a set of associated reduced basis models — one for each degree of freedom on its ports — that provide accurate approximation of the local solution for any value of the local parameters for any prescribed solution on the ports. Given any value of the *global* parameter, the global static condensation system for the unknowns associated with the degrees of freedom on all the ports may be assembled based on these reduced basis approximations.

In this work we are concerned with the representation of the solution on the ports. We demonstrate that if the solution is represented in certain ways, for example as an expansion in eigenfunctions on the ports, we may obtain rapid decay in the solution coefficients. In certain cases only the first few modes in this expansion suffice in order to represent the solution with minimal error, and hence only a few degrees of freedom are necessary on each port. In addition to eigenfunctions we may also represent the solution at the ports by *empirical* basis functions, that is, snapshots of the solution at the ports for selected values of the parameters. Ultimately, we may obtain in these cases a static condensation system of very small size, which thus results in additional computational speedup.

We present a procedure for adaptive truncation of the port expansions, and hence control of the size of the reduced basis static condensation system. The accuracy in this solution and hence the adaptive truncation procedure may be controlled through efficient evaluation of *a posteriori* error estimators.

- [1] DBP Huynh, DJ Knezevic, and AT Patera. *A Static Condensation Reduced Basis Element Method: Approximation and A Posteriori Error Estimation*. M2AN (submitted May 2011).
- [2] G Rozza, DBP Huynh, and AT Patera. *Reduced Basis Approximation and A Posteriori Error Estimation for Affinely Parametrized Elliptic Coercive Partial Differential Equations — Application to Transport and Continuum Mechanics*. Arch Comput Methods Eng 15(3):229–275, 2008.

# REDUCED BASIS *A Posteriori* ERROR BOUNDS FOR THE INSTATIONARY STOKES EQUATIONS: A PENALTY APPROACH

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In many engineering applications, it is crucial to understand the effects of geometry variations on a flow system. When the objective is to optimize, control, or characterize the system, classical discretization techniques such as finite element, finite volume, or finite difference methods are generally too expensive. As it can often capture the system behavior at significantly less cost, reduced order modelling for fluid flow has received considerable attention. Our particular approach is the certified reduced basis method, in which the emphasis is on rigorous *a posteriori* error bounds and adaptive sampling procedures to provide rapidly convergent and computationally efficient approximations.

The RB method exploits the parametric structure of the problem to construct rapidly convergent and computationally efficient approximations equipped with rigorous error bounds. Built upon a high-fidelity “truth” discretization, the RB approximation is defined as the Galerkin projection of the “truth” model problem onto a low-dimensional approximation space that focuses on the solution manifold induced by the parametrized partial differential equation.

We here investigate low-Reynolds number fluid flow in parametrized domains. Although reduced basis (RB) methods are well-developed for several classes of partial differential equations, incompressible fluid flow problems involving parametrized domains pose additional difficulties that have not been fully addressed: Parameter-dependent constraints in the Stokes and Navier–Stokes equations cause complications not only in the choice of stable RB approximation spaces [[3]] but also in the construction of rigorous and computationally efficient *a posteriori* error bounds [[1, 2]]. The analysis of the Stokes equations is often performed as a stepping stone for the more general Navier–Stokes equations but nevertheless remains relevant in many engineering applications. In [1], we introduced a penalty approach that circumvents the expensive computation of stability inf-sup constants. Geometry variations are admitted with relative ease but at the expense of an additional error in the “truth” approximation upon which the RB approximation is built.

In this paper, we extend the approach presented in [1] to time-dependent problems. We develop rigorous upper bounds for the errors in the RB approximations, which shall then be analyzed with respect to sharpness. As in the stationary case in [1], the introduction of the penalty term enables us to derive *a posteriori* RB error bounds that do not require the very expensive calculation of lower bounds to inf-sup stability constants. They only depend on comparably inexpensive lower bounds to coercivity constants associated with the diffusion and penalty terms and are thus computationally very efficient. However, the error bounds also depend on the penalty parameter  $\varepsilon$ : Effectivities increase as we approach the non-penalized problem ( $\varepsilon = 0$ ). Finally, RB approximation and error bounds are intimately linked through a POD greedy approach, in which the efficient error bounds are used to construct the subsequent approximation spaces more optimally.

The method is applied to a Stokes flow in a two-dimensional microchannel with a parametrized rectangular obstacle as illustrated as in [1]. Numerical results demonstrate that the RB approximations converge rapidly, the developed rigorous *a posteriori* RB error bounds are sharp, and that the effects of the penalty parameter on the effectivity of the error bounds are relatively benign.

- [1] A.-L. GERNER AND K. VEROY, *Reduced basis a posteriori error bounds for the Stokes equations in parametrized domains: A penalty approach*, Math. Models Methods Appl. Sci., 21 (2011), pp. 2103–2134.
- [2] D. J. KNEZEVIC, N.-C. NGUYEN, AND A. T. PATERA, *Reduced basis approximation and a posteriori error estimation for the parametrized unsteady Boussinesq equations*, Math. Models Methods Appl. Sci., 21 (2011), pp. 1415–1442.
- [3] G. ROZZA AND K. VEROY, *On the stability of the reduced basis method for Stokes equations in parametrized domains*, Comput. Methods Appl. Mech. Engrg., 196 (2007), pp. 1244–1260.

# EFFICIENT REDUCED BASIS SOLUTION OF QUADRATICALLY NONLINEAR DIFFUSION EQUATIONS

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Nonlinear diffusion problems appear in a large number of real world applications ranging from biology to ecology, heat radiation and fluid flows, see [4]. These equations often involve a large number of parameters such as viscosity constants or diffusion coefficients which, in general, have a strong influence on the behavior of the system. Hence, to analyze and understand a specific model many different combinations of parameters have to be investigated.

However, classical discretization techniques such as finite element methods and finite volume methods often prove prohibitively expensive if the system has to be evaluated at a large number of different parameters. Efficient techniques to solve these parametric problems are therefore important. Our goal here is development of a numerical technique that permits rapid yet accurate and reliable prediction of quadratically nonlinear parametrized diffusion equations of the type

$$\operatorname{div}(D(u)\nabla u) = f, \quad (1)$$

where  $u$  is the field variable,  $D(u) = \mu_0 + \mu_1 u$  is a linear function of  $u$ ,  $f$  is a source term, and  $\mu \equiv (\mu_1, \mu_2) \in \mathcal{D} \subset \mathbb{R}^2$  is the parameter which lies in the admissible parameter domain  $\mathcal{D}$ . This problem is particularly important in heat transfer applications with a temperature-dependent conductivity. To achieve this goal we pursue the reduced basis (RB) method. The reduced basis method is a model order reduction technique that has proven to admit efficient and reliable reduced-order approximations for a large class of parametrized partial differential equations; see [3] for a recent review. In this work we develop rigorous *a posteriori* error estimation procedures based on the Brezzi-Rappaz-Raviart theory [1] and present offline-online computational procedure to evaluate the reduced basis approximation and error bound. In the reduced basis context the BRR theory has already been successfully applied to the steady Navier-Stokes equation in [5]. Numerical results are presented to confirm the validity of our approach. We refer the interested readers to [2] for more details.

- [1] Caloz G. and Rappaz J.: *Numerical Analysis for nonlinear and bifurcation problems*. In Handbook of Numerical Analysis, Vol. V, Ciarlet PG, Lions JL (eds), Techniques of Scientific Computing (Part 2), Elsevier Science B.V.: Amsterdam, (1997), 487-637.
- [2] Rasty M. and Grepl M.A.: *A certified reduced basis method for generalized porous medium equations*. Preprint, (2012).
- [3] Rozza G., Huynh D.B.P., and Patera A.T. (2008) Reduced Basis approximation and a posteriori error estimation for affinely parametrized elliptic coercive partial differential equations: application to transport and continuum mechanics *Arch. Comput. Meth. Eng.*, 15(3), 229-275.
- [4] Vazquez Juan Luis. (2006) The porous medium equation, Mathematical Theory. *Oxford University Press*, 2006.
- [5] Veroy K. and Patera A.T.: *Certified real-time solution of the parametrized steady incompressible Navier-Stokes equations: rigorous reduced-basis a posteriori error bounds*. *Int. J. Numer. Meth. Fluids*, (2005), 773-788.

# SPACE-TIME REDUCED BASIS METHODS FOR TIME-PERIODIC PARTIAL DIFFERENTIAL EQUATIONS

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We consider parameter-dependent time-periodic parabolic problems of the following form: Let  $H$  be a Hilbert space,  $V \hookrightarrow H \hookrightarrow V'$  a Gelfand triple and  $\mathcal{D} \subset \mathbb{R}^p$  a parameter set. We are interested in outputs  $J(\mu) := \int_0^T \ell(u(t; \mu)) dt$ ,  $\mu \in \mathcal{D}$ , with a linear functional  $\ell : V \rightarrow \mathbb{R}$  and  $u(\cdot; \mu)$  being the solution over the time interval  $I := (0, T)$  of the time-periodic parametrized partial differential equation (PPDE)

$$\begin{aligned} u_t(t; \mu) + A(t; \mu)u(t) &= g(t; \mu) && \text{in } V', t \in (0, T), \\ u(0; \mu) &= u(T; \mu) && \text{in } H. \end{aligned}$$

Here,  $g(\cdot; \mu) \in L_2(I; V')$  is given and  $A(t; \mu) \in \mathcal{L}(V, V')$  is defined by  $\langle A(t; \mu)u, v \rangle_{V'} := a(t; u, v; \mu)$  for  $v \in V$ ,  $\mu \in \mathcal{D}$ ,  $t \in I$ , and a continuous and coercive bilinear form  $a(t; \cdot, \cdot, \mu) : V \times V \rightarrow \mathbb{R}$  with coercivity and continuity constants  $\alpha(\mu) \geq \alpha_0$ ,  $\gamma(\mu) \leq \gamma_0$  uniformly in  $\mathcal{D}$  and  $I$ .

Such problems are relevant e.g. for all kinds of rotators and propellers, with the parameter  $\mu \in \mathcal{D}$  modeling design or steering properties and  $J(\mu)$  representing the efficiency or some other time-averaged physical quantity.

Often, we are interested in the optimization of the output over the parameters  $\mu \in \mathcal{D}$ . Hence, e.g. in a numerical optimization scheme, the PPDE has to be solved for several values of the parameter. This is a typical *multi-query* situation where Reduced Basis Methods (RBMs) can be applied to construct a reduced model that can be solved highly efficiently and give rise to a-posteriori error control.

A standard approach to numerically solve such problems is a time-stepping (fixed-point) scheme. This approach, however, often suffers from some drawbacks, in particular within the RBM. First, there might be long transient phases before a periodic or steady state is reached, which is particularly disadvantageous in the online phase. Second, corresponding error estimates usually include sums over time-steps which might become inaccurate. Moreover, in case of time-variant operators, the construction of the RB basis requires either storage of additional information at each time point or additional computational effort to separate time and space.

Instead, we consider a space-time variational formulation using periodic basis functions in time, which avoids the need for fixed-point iterations. Based on this variational formulation, we develop a space-time RBM using wavelets in time and derive corresponding a-posteriori error estimates. We present numerical results indicating the efficiency of the method as well as the effectivity of the derived error bounds.

- [1] Martin A. Grepl and Anthony T. Patera. A posteriori error bounds for reduced-basis approximations of parameterized parabolic partial differential equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, 39(1):157–181, 2005.
- [2] C. Schwab and R. Stevenson. Space-time adaptive wavelet methods for parabolic evolution problems. *Mathematics of Computation*, 78(267):1293–1318, July 2009.
- [3] K. Urban and A. T. Patera. A new error bound for Reduced Basis approximation of parabolic partial differential equations. submitted to *C. R. Math. Acad. Sci. Paris*, 2011.

# AFFINE DECOMPOSITIONS OF PARAMETRIC STOCHASTIC PROCESSES FOR APPLICATION WITHIN REDUCED BASIS METHODS

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**Introduction.** We consider parameter dependent spatial stochastic processes in the context of partial differential equations (PDEs) and model order reduction. For a given parameter  $\mu$ , a random sample  $c(\mu, \omega)$  of such a process specifies a sample coefficient function of a PDE.

In the context of Reduced Basis Methods (RBM), it is essential that the differential operator is affine w.r.t. the (deterministic and stochastic) parameters, since this allows for an efficient offline-online decomposition. This is satisfied provided that  $c(\mu, \omega)$  allows for an affine decomposition of the parameters and the spatial variables. In general, however, this requirement is not fulfilled, in particular in the presence of stochastic influences. The objective here is thus (i) to find affine approximations of  $c(\mu, \omega)$  of the form

$$c(\mu, \omega) \approx \sum_{m=1}^M \theta_m(\mu, \omega) q_m \quad (1)$$

with so-called collateral basis functions  $q_m \in X$ ,  $m = 1, \dots, M$ , (ii) to construct efficient evaluation procedures for the coefficients  $\theta_m(\mu, \omega) \in \mathbb{R}$ ,  $m = 1, \dots, M$ , and (iii) the derivation of effective a-posteriori error estimators to choose  $M \in \mathbb{N}$  possibly small in order to guarantee a certain approximation.

Widely used methods for the construction of affine approximations of non-affine functions include the Empirical Interpolation Method (EIM) (cf. [1, 3]) for deterministic parametric functions and the Discrete EIM (DEIM) (cf. [2]) or the Operator EIM for discrete operator approximations. For stochastic influences in terms of random variables, the Karhunen-Loève (KL) expansion is used, which can also be seen as the stochastic counterpart of the Proper Orthogonal Decomposition (POD). The probability distributions of the KL expansion coefficients are modeled using Polynomial Chaos (PC) expansions.

**A Proper Orthogonal Interpolation Method (POIM).** The main observation is that the EIM is based on the  $L_\infty$  approximation error of previously chosen snapshot trajectories. Thus, for non-smooth trajectories, the basis will not be smooth either, and the method may be inappropriate due to the presence of singularities. Especially for stochastic processes, one can usually at most guarantee smoothness  $P$ -a.s., and even though the essential supremum is taken to determine the interpolation points (knots), it may be hard to distinguish between 'true' large deviations and singularities of measure zero.

We propose a Proper Orthogonal Interpolation Method (POIM) that is based on the EIM and POD. The main idea is to replace the  $L_\infty$ -error based basis selection by some  $L_2$ -'optimal' procedure. The method has similarities to the DEIM. In fact, we show that the POIM results in the same approximations, yet with reduced computational complexity. Furthermore, we show that the provided a-posteriori error estimates for the POIM can also be applied to the DEIM.

**A Least-Squares Empirical Interpolation Method (LSEIM).** Even using an 'optimal' basis for the approximation of non-smooth functions, errors occur due to insufficiently precise coefficients  $\theta_m$  in (1). Since the EIM is based only upon few interpolation points, these coefficients may also be strongly influenced by singularities.

We introduce a Least-Squares Empirical Interpolation Method (LSEIM) that uses more knots than basis functions and solves a least-squares problem to evaluate the coefficients. This can be combined with both EIM and POIM.

**Numerical Example.** We consider a Wiener process and apply a parameter dependent smoothing filter such that trajectories are continuous with increasing smoothness for larger  $\mu$ . We demonstrate that it is useful to add POD eigenfunctions instead of snapshots to generate the EIM basis. Furthermore, we show that using more knots than basis functions and solving least-squares problems improves the approximation quality and arrives at close to optimal results.

- [1] M. Barrault, Y. Maday, N. C. Nguyen, and A. T. Patera. An 'empirical interpolation' method: application to efficient reduced-basis discretization of partial differential equations. *C. R. Math. Acad. Sci. Paris*, 339(9):667–672, 2004.
- [2] S. Chaturantabut and D. C. Sorensen. Nonlinear model reduction via discrete empirical interpolation. *SIAM J. Sci. Comput.*, 32(5):2737–2764, 2010.
- [3] T. Tonn. *Reduced-Basis Method (RBM) for Non-Affine Elliptic Parametrized PDEs (Motivated by Optimization in Hydromechanics)*. PhD thesis, Ulm University, Ulm, Germany, December 2011.

# REDUCED BASIS MODEL REDUCTION OF PARAMETRIZED TWO-PHASE FLOW IN POROUS MEDIA

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Many applications, e.g. in control theory and optimization depend on time-consuming parameter studies of parametrized evolution equations. Reduced basis methods are an approach to reduce the computation time of numerical simulations for these problems. The methods have gained popularity for model reduction of different numerical schemes with remarkable results preferably for scalar and linear problems with affine dependence on the parameter [3]. Over the last few years, the framework for the reduced basis methods has been continuously extended for non-linear discretizations, coupled problems and arbitrary dependence on the parameter, e.g. [2, 4, 5].

In this presentation, we apply the framework developed in [5] on a problem that combines all these difficulties. The considered problem models two-phase flow in a porous medium discretized by the finite volume method like in [1]. The two-phase flow equation is of interest, e.g. in the context of oil recovery. An illustration of the solution at the final time can be found in the figure below.

For a first test, we concentrate on the development of an efficient reduced basis scheme without any parametrization. This reduced basis scheme is derived by two model reduction steps from the high dimensional finite volume scheme. Firstly, a Galerkin projection on the so-called reduced basis space — a function space spanned by snapshots of the high dimensional solution — is performed. Secondly, the non-linear operators are approximated by an efficiently computable empirical interpolant. We shortly introduce the main aspects of the reduced basis method including the concept of offline/online decomposition, empirical operator interpolation method and reduced basis generation by greedy algorithms.

The generalized formulation of the presented reduced basis scheme allows for a separation of the reduced basis space into function spaces for the three physical unknowns — saturation, velocity and pressure — and the approximation of the non-linear terms. It is discussed, how the coupling of the unknowns must be reflected in the generated reduced spaces. Furthermore, we compare the computational complexities of the high-dimensional to the low-dimensional computations theoretically and by numerical experiments. All the presented experiments are implemented with our reduced basis software package *RBmatlab* [6].

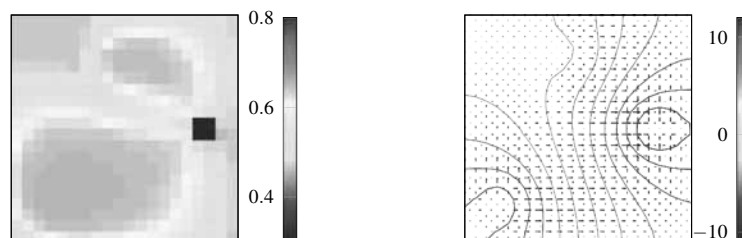


Illustration of saturation concentration, and contour plot of pressure field with velocity flux at final time instance  $t = 0.5$ . The snapshots are reconstructed from a reduced basis simulation.

- [1] A. Michel A finite volume scheme for two-phase immiscible flow in porous media. *SIAM Journal on Numerical Analysis*, 41(4), 1301–1317, 2004.
- [2] M. Barrault, Y. Maday, N.C. Nguyen, and A.T. Patera. An 'empirical interpolation' method: application to efficient reduced-basis discretization of partial differential equations. *C. R. Math. Acad. Sci. Paris Series I*, 339:667–672, 2004.
- [3] A.T. Patera and G. Rozza. Reduced Basis Approximation and a Posteriori Error Estimation for Parametrized Partial Differential Equations *Version 1.0, to appear in (tentative rubric) MIT Pappalardo Graduate Monographs in Mechanical Engineering* MIT 2006–2007
- [4] M. Grepl, Y. Maday, N.C. Nguyen, and A.T. Patera Efficient Reduced-Basis Treatment of Nonaffine and Nonlinear Partial Differential Equations *M2AN, Math. Model. Numer. Anal.*, pages 575–605, 2007
- [5] M. Drohmann, B. Haasdonk and M. Ohlberger Reduced Basis Approximation for Nonlinear Parametrized Evolution Equations based on Empirical Operator Interpolation Submitted to SISC, *SIAM Journal on Scientific Computing*, 2010
- [6] M. Drohmann, B. Haasdonk, S. Kaulmann and M. Ohlberger A software framework for reduced basis methods using DUNE-RB and RBmatlab Submitted to *Proceedings of the DUNE user meeting* 2010



# APPLICATION OF PROPER ORTHOGONAL DECOMPOSITION TO PARTICULATE PROCESSES

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Particle processes like crystallization or granulation are of great importance in chemical and pharmaceutical industry. The evolution of particle populations is strongly affected by the flow conditions in the fluid phase (aggregation, breakage, attrition etc.). Process models that account for the relevant physical effects in an adequate way comprise Navier Stokes equations, energy balances, and mass balances for the liquid phase, as well as population balance equations for the particle phase. They are distributed in several external (space) and internal (property) coordinates and are computationally very demanding. A direct application of such models to process control and process design problems is infeasible due to the enormous computational burden. Hence there is a need for reduced control oriented models of low system order.

In this contribution, a model reduction technique for population balance systems coupled with fluid dynamics is presented [1, 2]. Two examples are used to illustrate the reduction method. The first example is a model of a granulation process. The main challenge is to treat the integral term in the population balance, which results from particle aggregation. The example is also used to outline the reduction method. The second example is a laboratory scale crystalliser for the production of urea crystals. The process is growth dominated and the influence of the fluid flow is taken into account. This leads to a system with two external and one internal coordinate. For the model reduction by POD, a special difficulty arises from the nonlinearity of the growth term. This nonlinearity complicates the solution of integrals appearing when applying Galerkin's method of weighted residuals. Best point interpolation [3] is found to be a good solution for this problem.

## Literatur

- [1] M. Krasnyk and M. Mangold. Reduction of a urea crystallizer model by proper orthogonal decomposition and best point interpolation. *Industrial & Engineering Chemistry Research*, 49:9887–9898, 2010.
- [2] M. Krasnyk, M. Mangold, S. Ganesan, and L. Tobiska. Reduction of a crystallizer model with internal and external coordinates by proper orthogonal decomposition. *Chemical Engineering Science (accepted)*, 2011.
- [3] N.C. Nguyen, A.T. Patera, J. Peraire. A “best-points” interpolation method for efficient approximation of parametrized functions. *Int. J. Numer. Methods Eng.* 73:521–543, 2008.

# PARAMETRIC APPROXIMATION OF CONNECTED EULER-BERNOULLI BEAMS WITH VARIABLE BEAM LENGTHS

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**Introduction.** For the model order reduction of high-order lumped-parameter systems a variety of efficient techniques has been well-established both in theory and in application specific software tools. The underlying processes are in many cases mechanical systems with some kinematic degrees of freedom, so that it is often desired that the approximations depend on the geometric configuration in order to provide an acceptable approximation quality in the relevant operating range. Therefore, parametric model order reduction techniques have recently gained considerable attention. Several approaches are available that yield parametric approximations, which mainly are based on high-order finite-element (FE) models of the system. The well-known methods in [3] and [5] make use of the concept to determine local models at several operating points and to calculate a common reducing projection that is based on the merged local models. The contribution [1], using balanced truncation, proposes to reduce several locally valid models first and then to merge the reduced systems to a parametric reduced-order approximation. A Krylov subspace based approach is given in [4], where several local Krylov approximations of systems are suitably transformed by introducing new states and subsequently merged by interpolation.

**Proposed approach.** In this contribution an approach for parametric approximations of flexible beam systems are presented. In contrast to the mentioned FE-model based approaches the approximations are derived directly from the PDEs of the distributed-parameter systems, which is why this approximation paradigm can be regarded as *direct model order reduction*. The considered systems are built of several uniform Euler-Bernoulli beams with structural damping whose lengths are free parameters. This concept is motivated by the observation that many mechanical systems, such as, e.g., some construction vehicles, manipulators, and milling machines, can be considered to be composed of a number of flexible beams that are connected to a more complex structure. In this contribution the situation is considered where the beams are connected serially so that the overall composite system has the shape of a non-uniform cantilever beam whose parts with different stiffness and damping have varying lengths. It is assumed that the beam lengths are constant at runtime or vary only slowly so that Euler-Bernoulli beam models still can be used despite changes of the lengths. The Petrov-Galerkin projection is applied, which can be used to determine approximations that depend on the beam lengths explicitly. However, the resulting expressions are rather complex in general. Therefore, it is more efficient to use a suitable online-offline decomposition of the Petrov-Galerkin approximation scheme in order to adapt the approximation to the current beam lengths at runtime with tolerable computational efforts. To this end it is shown how the time-consuming parts of the Petrov-Galerkin approximation method, namely the computation of some integrations, can be carried out offline, while an adaptation of the approximation to changed beam lengths online requires only to solve some linear equations and scalar addition and multiplication operations. By applying the Krylov subspace method it can be assured that the approximations have a steady-state behavior that coincides with that of the distributed-parameter system.

- [1] Baur, U. and Benner, P. (2009). Model reduction for parametric systems using balanced truncation and interpolation. *at – Automatisierungstechnik*, 57(8), 411–419.
- [2] Harkort, C. and Deutscher, J. (2011). Krylov subspace methods for linear infinite-dimensional systems. *IEEE Transactions on Automatic Control*, 56(2), 441–447.
- [3] Leung, A.T. and Khazaka, R. (2005). Parametric model order reduction technique for design optimization. In *Proceedings of the IEEE International Symposium on Circuits and Systems*, 1290–1293.
- [4] Panzer, H., Mohring, J., Eid, R., and Lohmann, B. (2010). Parametric model order reduction by matrix interpolation. *at – Automatisierungstechnik*, 58(8), 475–484.
- [5] Peng, L., Liu, F., Pileggi, L.T., and Nassif, S.R. (2005). Modeling interconnect variability using efficient parametric model order reduction. In *Proceedings of the Design, Automation and Test in Europe Conference and Exhibition*, 958–963.

# MODEL ORDER REDUCTION OF NONLINEAR EDDY CURRENT PROBLEMS

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**Summary.** Conventional finite-element (FE) implementations for nonlinear eddy current problems employ an implicit time-stepping scheme together with some iterative technique, such as Newton's method [1], for solving a nonlinear boundary value problem (BVP) in the spatial domain. Even though such methods are unconditionally stable and, hence, allow for time steps of arbitrary length, they still tend to be computationally expensive, for the following reasons: First, there is no obvious way of re-using information from previous runs, even if the respective excitations do not differ much. In consequence, the whole nonlinear initial boundary value problem (IBVP) needs to be solved from scratch. Second, the IBVP requires solving a nonlinear BVP at each time step. Since the dimension of the corresponding FE discretization is large, this is costly. Finally, implicit time stepping itself is not cheap.

In the linear case, model order reduction (MOR) has become a well-established methodology for reducing computation times, and numerous methods are available. In the nonlinear case, however, only few reduction techniques are known, all of which have been developed in recent years.

One viable approach to nonlinear MOR is the trajectory piecewise linearization (TPWL) algorithm, which linearizes the system at multiple points along several training trajectories [2]. The resulting reduced order model (ROM) approximates the original system by a weighted superposition of linearized models. The TPWL method employs the proper orthogonal decomposition (POD) technique for generating a reduced basis for the linear models, by computing the singular value decomposition (SVD) of a matrix whose column vectors represent known system states of the nonlinear system. Numerical experiments have demonstrated that the method is sufficiently accurate provided that the system state does not differ too much from known training states.

The practical applicability of the classical TPWL method is limited by the high computational complexity and memory requirements of the ROM generation process. Both shortcomings result from the fact that the classical TPWL method uses a *global* basis for representing the reduced state space. In particular, it is the SVD that becomes overly expensive. As a remedy, locally reduced models were suggested in [3]. The local ROM matrices are of smaller size and cheaper to compute but cover only subspaces of the global state space. To obtain a global solution, adequate subspace transformation techniques are required.

**Present contribution.** This paper proposes a nonlinear time-stepping algorithm based on [3]. Its theoretical focus is on the computation of the state transformations needed for interpolating the global model and time integration. In addition, it presents a self-adaptive strategy for choosing linearization points, weighting functions, and projection matrices. In comparison to the classical TPWL method, the suggested approach achieves significant reduction in memory consumption and simulation time.

**Numerical Example.** The levitation system considered in this paper consists of a voltage-driven electromagnet with nonlinear ferrite core, suspending a hollow steel ball in the air. The computer simulation is based on an axisymmetric FE model for the electromagnetic subsystem, featuring 31597 degrees of freedom. The mechanical domain is not considered. While the standard TPWL algorithm takes 9.1 s to compute a trajectory of 1000 time steps and 92.8 s for 10000 time steps, the new, locally reduced approach solves the same problem in just 4.7 s and 13.4 s, respectively. With classical TPWL, the dimension of the global ROM is 353 whereas, with the new method, the size of the local ROM varies between 37 and 225.

- [1] E. Hairer, S. P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations I: Nonstiff Problems*. Springer, 2nd edition, 2009.
- [2] M. Rewienski and J. White, *Model order reduction for nonlinear dynamical systems based on trajectory piecewise-linear approximations*. Linear Algebra and its Applications, 2006, 415:426-454.
- [3] B. Lohmann and R. Eid, *Efficient Order Reduction of Parametric and Nonlinear Models by Superposition of Locally Reduced Models*. In: Methoden und Anwendungen der Regelungstechnik, Shaker Verlag, 2009.

# APPROXIMATION OF PARETO-OPTIMAL SYSTEMS USING PARAMETRIC MODEL-ORDER REDUCTION

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**Introduction.** Multiobjective optimization has been proven to be an efficient technique for computing optimal configurations of self-optimizing systems [1]. In most applications a multitude of objectives and parameters have to be considered. Hence, the use of multiobjective optimization is often a time-consuming task. Introducing a hierarchical structure and optimizing the resulting hierarchical system with optimization algorithms, known as hierarchical optimization, is one method to reduce optimization complexity. The hierarchical structure is used by restricting the optimization of a higher level to the results of the lower level [2].

Evaluation of the objectives is mostly effected by simulations of the system dynamics. A reduction of simulation time also accelerates the optimization and can be achieved by applying model-order reduction [3]. In this contribution we present a novel approach to combine the results of multiobjective optimization with parametric model-order reduction. To be more precise, we demonstrate how to parameterize the Pareto set, i.e., the solution of a multiobjective optimization problem, using piecewise matrix polynomials. This parameterization results in a finite set of parametric systems. Each system can be reduced by applying parametric model-order reduction. The reduced systems still represent the Pareto-optimal configurations and can be used as subsystems in an overlying optimization. However, we do not elaborate on that overlying optimization in this work. We compare three different types of parametric model-order reduction for an active suspension system.

**Parameterization of Pareto-optimal systems** In a multiobjective optimization problem several objectives are to be minimized at the same time. As the objectives typically contradict one another, the solution of a multiobjective optimization problem is a set of optimal compromises which is called the Pareto set. For the computation of such a Pareto set, a numerical set-oriented method, a subdivision algorithm, is employed in this work. It allows the computation of entire global Pareto sets.

The systems that correspond to the Pareto-optimal parameters are called Pareto-optimal systems. Our aim is to construct an approximation of these Pareto-optimal systems, in the case of two objective functions, that is at least continuous and can be reduced by means of model-order reduction. The first step is to compute a cubic smoothing spline to get a one-dimensional approximation of the Pareto set. Secondly, we create a second interpolation, not of the Pareto set but of the Pareto-optimal systems. This interpolation leads to a set of piecewise matrix polynomials which can be reduced by parametric model-order reduction. In this work we restrict ourselves to linear spline-interpolation. We present an algorithm that uses several results of classical spline interpolation to compute a good knot sequence. It is a modification of the Fortran algorithm *newnot* accomplished by an additional criterion to ensure convergence. In this way a satisfying linear piecewise matrix polynomial can be automatically computed.

**Parametric model-order reduction** Each piece of the piecewise matrix polynomial is reduced separately. We tested three different approaches which are all based on a particular interpolation of the (parametric) transfer function also known as (rational) Krylov methods: multi-moment matching, tangential interpolation and matrix interpolation.

By means of multi-moment matching an implicit matching of the moments also with respect to the parameter is possible. We implemented a two-sided Arnoldi-algorithm with deflation and multiple expansion points. Although we tried many combinations in the algorithm we were not able to compute satisfactory reduced systems.

The second method, tangential interpolation, interpolates the transfer function in certain tangent directions. We used a parametric version of the IRKA (iterative rational Krylov algorithm). In order to obtain good results two slight modifications as compared to literature are necessary: particular initial conditions and a modified common projection matrix for the parametric reduction.

We compare the results of the tangential interpolation with matrix interpolation. This method is also suitable for our approach as the piecewise matrix polynomial can be easily reformulated as a weighted sum. We also use the IRKA to compute non-parametric reduced systems and obtain the parametric reduced system by means of a reprojection to a common subspace.

- [1] Dellnitz, M.; Schütze, O.; Hestermeyer, T.: *Covering Pareto sets by multilevel subdivision techniques*. Journal of Optimization Theory and Application, 124 (1), 2005, 113–136.
- [2] Krüger, M.; Witting, K.; Trächtler, A.; Dellnitz, M.: *Parametric model-order reduction in hierarchical multi-objective optimization of mechatronic systems* In: 18th IFAC World Congress, Milano, Italy, 2011.
- [3] Antoulas, A.C.; Beattie, C.A.; Gugercin, S.: *Interpolatory model reduction of large-scale dynamical systems*. In: Efficient Modeling and Control of Large-Scale Systems, Springer, 2010, 3–58.

# A GOAL-ORIENTED DUAL LRFC-ADI FOR BALANCED TRUNCATION

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In this contribution we propose a more goal oriented stopping criterion for the ADI iteration employed in the computation of low rank Gramian factors for a system (1). In the case of balanced truncation the actual properties of interest are the Hankel singular values of the system since these are applied as the basis of the truncation. We develop a dual ADI iteration that solves the two dual Lyapunov equations (2) simultaneously and stops as soon as the Hankel singular are found to the desired accuracy, rather than relying on the two Lyapunov residuals.

**A Sketch of Balanced Truncation for Generalized Linear Time Invariant Systems** Consider the system

$$E\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t), \quad (1)$$

where  $E, A \in \mathbb{R}^{n \times n}$ ,  $E$  is symmetric positive definite and the pencil has only stable eigenvalues.

In BT-MOR the main task is to solve the generalized controllability and observability Lyapunov equations

$$APE^T + EPA^T = -BB^T, \quad A^T QE + E^T QA = -C^T C. \quad (2)$$

As the system is assumed to be stable and thus  $P$  and  $Q$  are positive semi-definite, there exist Cholesky factorizations  $P = S^T S$  and  $Q = R^T R$ . In the so-called *square-root* balanced truncation (SRBT) algorithms [3, 1] these are used to define the projection matrices  $T_l := \Sigma_1^{-\frac{1}{2}} V_1^T R$  and  $T_r := S^T U_1 \Sigma_1^{-\frac{1}{2}}$  determining the reduced order model as

$$\hat{\dot{x}}(t) = \hat{A}\hat{x}(t) + \hat{B}u(t), \quad \hat{y}(t) = \hat{C}\hat{x}(t), \quad \text{with} \quad \hat{A} := T_l A T_r, \quad \hat{B} := T_l B \quad \text{and} \quad \hat{C} := C T_r. \quad (3)$$

In the definitions of  $T_l$  and  $T_r$  the matrices  $\Sigma_1^{-\frac{1}{2}}$ ,  $U_1$  and  $V_1$  are determined via the singular value decomposition

$$S E R^T = U \Sigma V^T = [U_1 U_2] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}, \quad (4)$$

with decreasingly ordered singular values – the Hankel singular values of the system.

**Low Rank Gramian Factors and the Dual ADI Idea** In the case of large and sparse systems with  $B \in \mathbb{R}^{n \times m}$  and  $C \in \mathbb{R}^{p \times n}$  and  $m, p \ll n$ , the triangular Cholesky factors  $S \in \mathbb{R}^{n \times n}$  and  $R \in \mathbb{R}^{n \times n}$  are replaced by low rank Cholesky factors, i.e.,  $S \in \mathbb{R}^{n \times k_B}$  and  $R \in \mathbb{R}^{n \times k_C}$ , computed by a low rank Lyapunov equation solver. We are here focusing on the variant of LRFC-ADI (e.g., [2]) successively computing  $S$  as in

$$V_1 = \sqrt{-2 \operatorname{Re}(p_1)} (A + p_1 E)^{-1} B, \quad S_1 = V_1 \quad (5)$$

$$V_i = \sqrt{\frac{\operatorname{Re}(p_i)}{\operatorname{Re}(p_{i-1})}} \left[ I - (p_i + \overline{p_{i-1}}) (A + p_i E)^{-1} \right] E V_{i-1}, \quad S_i = [S_{i-1}, V_i]. \quad (6)$$

For  $R$  the same iteration is employed with  $A, E$  replaced by  $A^T, E^T$  and  $C$  instead of  $B$ . Thus when applying sparse direct solvers to the linear system solves, the LU-decompositions – being the most time consuming step – can be reused in the triangular solves for the dual equation. Thus we can efficiently formulate a dual iteration simultaneously computing both LRFCs. The two factors can then be employed to compute (4) and monitor the change of the singular values in  $\Sigma_1$ . Once these singular values stagnate we have matched the corresponding subsystem and thus get a good reduced order model evaluating (3). Thus we have a reliable criterion when to stop the iteration in contrast to the residual that may not tell us anything about the approximation. We will present numerical experiments substantiating both these observations.

- [1] A. J. Laub, M. T. Heath, C. C. Paige, and R. C. Ward. Computation of system balancing transformations and other applications of simultaneous diagonalization algorithms. *IEEE Trans. Autom. Control*, 32:115–122, 1987.
- [2] J. Saak. *Efficient Numerical Solution of Large Scale Algebraic Matrix Equations in PDE Control and Model Order Reduction*. PhD thesis, TU Chemnitz, July 2009. Available from <http://nbn-resolving.de/urn:nbn:de:bsz:ch1-200901642>.
- [3] M.S. Tombs and I. Postlethwaite. Truncated balanced realization of a stable non-minimal state-space system. *Internat. J. Control*, 46(4):1319–1330, 1987.

# IMPROVED SECOND-ORDER BALANCED TRUNCATION FOR SYMMETRIC SYSTEMS

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**Summary.** In this work we consider model order reduction for linear, time-invariant control systems of second order:

$$M\ddot{x}(t) + D\dot{x}(t) + Kx(t) = Bu(t), \quad y(t) = C_v\dot{x}(t) + C_p x(t) \quad (1)$$

with  $M, D, K \in \mathbb{R}^{n \times n}$ ,  $B \in \mathbb{R}^{n \times m}$  and  $C_p, C_v \in \mathbb{R}^{p \times n}$ . Such systems arise, for instance, through using a spacial finite element discretization of elastic mechanical bodies. For drastically decreasing the number of degrees of freedom, we employ balanced truncation [1] as model order reduction method to obtain accurate reduced order models. We mainly focus on a special class of symmetric second order systems whose properties turn out to be beneficial for our purposes from both a theoretical and computational point of view. Following the second order balanced truncation approach [2], the original second order structure can be preserved. For solving the occurring large-scale Lyapunov equation, an adapted version of the low-rank ADI method [3, 5] is used which has proven to be an efficient algorithm for this purpose.

**Balanced Truncation for Symmetric Second Order Systems.** By symmetric second order systems we refer to systems (1), where  $M, D, K$  are symmetric positive definite matrices and either  $B = C_p^T$ ,  $C_v = 0$  or  $B = C_v^T$ ,  $C_p = 0$  holds. These assumptions ensure that there is an equivalent generalized state space system

$$\begin{aligned} E\dot{z}(t) &= Az(t) + Gu(t), \\ y(t) &= G^T z(t) \end{aligned} \quad (2)$$

with symmetric matrices  $E, A \in \mathbb{R}^{2n \times 2n}$ ,  $G \in \mathbb{R}^{2n \times m}$  and  $z(t) := [x(t)^T, \dot{x}(t)^T]^T$ .

Balanced truncation model order reduction [1, 4] aims at the identification and truncation of states in (2) which are difficult to observe and to control. It can be directly applied to (2), where the main requirement is solution of the generalized Lyapunov equation

$$APE + EPA = -GG^T. \quad (3)$$

To preserve the second order structure a modified balanced truncation strategy [2] can be used. The main idea there is to partition  $P$  into two blocks corresponding to the position and velocity parts of the generalized state vector  $z(t)$  of (2). This leads to different possible reduced order models in second order form. We demonstrate that exploiting the symmetry of (1) (or (2)), yields some improvements compared to standard second-order balancing such as a guaranteed stability and symmetry preservation in certain cases.

Special emphasis is drawn to the efficient numerical solution of the associated generalized Lyapunov equation (3) which is the dominating computational task required in balanced truncation. We use a modified version of the low-rank ADI method [3, 4, 5] which computes a low-rank factor  $\hat{Z} \in \mathbb{R}^{n \times r}$ ,  $r \ll n$  such that  $\hat{Z}\hat{Z}^T \approx P$ .

- [1] B. C. Moore. *Principal component analysis in linear systems: controllability, observability, and model reduction*. IEEE Trans. Automat. Control, AC-26(1):17–32, 1981.
- [2] T. Reis and T. Stykel, *Balanced truncation model reduction of second-order systems*. Math. Comput. Model. Dyn. Syst., 14(5):391–406, 2008.
- [3] T. Penzl. *A cyclic low rank Smith method for large sparse Lyapunov equations*. SIAM J. Sci. Comput., 21(4):1401–1418, 2000.
- [4] P. Benner and J. Saak. *Efficient Balancing based MOR for Large Scale Second Order Systems*. Math. Comput. Model. Dyn. Sys., 17(2):123–143, 2011.
- [5] J. Saak. *Efficient Numerical Solution of Large Scale Algebraic Matrix Equations in PDE Control and Model Order Reduction*. PhD thesis, TU Chemnitz, July 2009. Available from <http://nbn-resolving.de/urn:nbn:de:bsz:ch1-200901642>.

# MODEL REDUCTION IN ELASTIC MULTIBODY SYSTEMS FOR LARGE INDUSTRIAL MODELS

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**Introduction.** In the modern development process elastic multibody systems (EMBS) are frequently used to describe the dynamical behavior of mechanical systems if large rigid body movements and additional elastic deformations have to be concerned. To enable the simulation of EMBS in industrial applications with large finite element models, often millions degrees of freedom have to be reduced by approximating the nodal displacements with the help of appropriate ansatz functions. Modern reduction methods, like Krylov-subspace based moment matching or Gramian matrix based reduction are used to find the ansatz functions.

**Main Calculation Step.** The main calculation step in modern reduction techniques is the solution of large sparse symmetric linear systems. There are two possibilities to solve these sparse linear systems, either to use a direct or an iterative solver. The iterative solver needs multiple steps to solve the system and is low in memory consuming. In contrast, the direct method solves the system by a decomposition, like LU-factorization, and a following forward elimination and backward substitution. For large right hand sides, which are common in using Krylov-subspace based model reduction, the LU-decomposition, in contrast to the iterative method, is calculated only once. However, the large memory consumption of the LU-decomposition is among the greatest numerical challenges in reducing large models.

**Solving Process.** At the Institute of Engineering and Computational Mechanics the software package Morembs [1] is developed to reduce the elastic degrees of freedom. In Morembs++, the C++ Version of Morembs, different numerical libraries for solving large linear sparse systems, like Umfpack [2] or Mumps [3], are tested in this contribution. Although using the most efficient direct solvers, the memory hardware limits the size of models which can be reduced in Morembs. One possibility to solve large systems with Morembs is using supercomputers. Therefore, the Cray XE6 supercomputer at the High Performance Computing Center Stuttgart is used. Unfortunately, the usage of supercomputers is expensive and not all users have access to such supercomputers. Therefore, some numerical direct solver packages, like Mumps, feature an Out-of-Core capability. This allows the solution of very large sparse linear systems with a standard computer by storing most parts of the matrices on the hard drive. With a fast solid-state-drive the reduction with the Out-of-Core solver Mumps is slower than reducing the model in-core but it is nearly four times faster than the serial reduction on the supercomputer. This allows the model reduction of large scale industrial models with millions degrees of freedom even on standard computers in a reasonable time. Some current developments are presented.

- [1] Fehr, J.; Eberhard, P.: Simulation Process of Flexible Multibody Systems with Non-modal Model Order Reduction Techniques. *Multibody System Dynamics*, Vol. 25, No. 3, pp. 313–334, 2011.
- [2] Davis, T.A.: Algorithm 832: UMFPACK, an unsymmetric-pattern multifrontal method. *ACM Transactions on Mathematical Software*, Vol. 30, No. 2, pp. 196–199, 2004.
- [3] Amestoy, P.; Duff, I.; Robert, Y.; Rouet, F.; Ucar, B.: On Computing Inverse Entries of a Sparse Matrix in an Out-of-core Environment. Technical report rt-apo-10-06, Institute National de Recherche en Informatique et en Automatique, 2010.

# A-POSTERIORI ERROR ESTIMATION FOR PARAMETERIZED KERNEL-BASED SYSTEMS

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**Introduction.** This work is concerned with derivation of fully offline/online decomposable efficient a-posteriori error estimators for parameterized, nonlinear kernel-based systems. The dynamical systems under consideration consist of a nonlinear, time- and parameter-dependent kernel expansion representing the system’s inner dynamics as well as time- and parameter-affine inputs, initial conditions and outputs. The estimators are established for an reduction technique originally proposed in [?] and are an extension of the estimators derived in [?] to the fully time-dependent, parameterized setting. Key features for the efficient error estimation are to use local Lipschitz constants provided by a certain class of kernels and an iterative scheme to balance computation costs against estimation sharpness. Together with the time- and parameter-affine system components a full offline/online decomposition for both the reduction process and the error estimators is possible. Some experimental results for synthetic systems illustrate the efficient evaluation of the derived error estimators for different parameters.

**Considered systems.** The class of dynamical systems we consider is given by

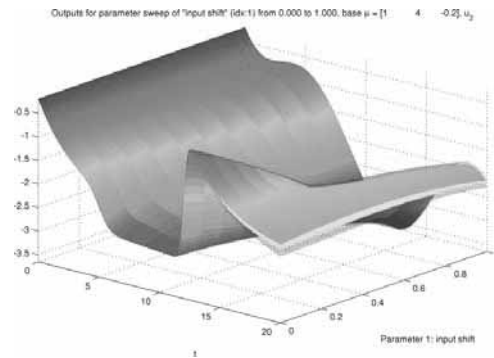
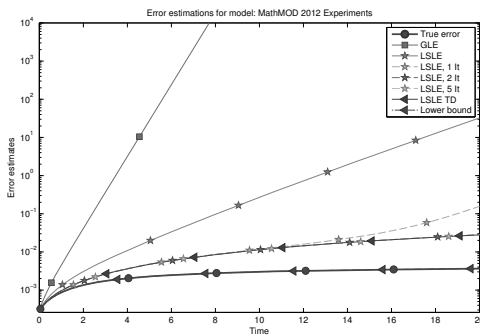
$$x'(t) = f(x(t), t, \mu) + B(t, \mu)u(t), \tag{1}$$

$$x(0) = x_0(\mu), \quad y(t) = C(t, \mu)x(t) \tag{2}$$

with  $x(t) \in \mathbb{R}^d$  denoting the system state,  $x_0$  initial condition,  $B, C$  input/output matrix, input/control  $u(t)$  and parameters  $\mu \in \mathcal{P} \subseteq \mathbb{R}^p$ . Further,  $f$  is a *kernel expansion*  $f(x, t, \mu) = \sum_{i=1}^N c_i \Phi_s(x, x_i) \Phi_t(t, t_i) \Phi_{\mathcal{P}}(\mu, \mu_i)$ , having scalar state, time and parameter *kernels*  $\Phi_s, \Phi_t, \Phi_{\mathcal{P}}$ , expansion centers  $x_i \in \mathbb{R}^d, t_i \in [0, T], \mu_i \in \mathcal{P}$ , and coefficient vectors  $c_i \in \mathbb{R}^d, i = 1 \dots N$ . The components  $B, C$  and  $x_0$  are time- and parameter-affine, e.g.  $B(t, \mu) = \sum_{i=1}^{Q_B} \theta_i^B(t, \mu) B_i$ , with  $Q_B \in \mathbb{N}$  small, constant matrices  $B_i \in \mathbb{R}^{d \times m}$  and low-complexity coefficient functions  $\theta_i^B : [0, T] \times \mathcal{P} \rightarrow \mathbb{R}$ .

**Reduction technique.** The system above is reduced applying a Galerkin projection with biorthogonal matrices  $V, W \in \mathbb{R}^{r \times d}, V^T W = I_r$ . For more general settings, the evaluation of the projected nonlinear term  $W^T f(V \cdot, t, \mu)$  would involve  $d$ -dimensional computations. Therefore, our key ingredient is to use translation & rotation-invariant kernels  $\Phi(x, x') = \phi(\|x - x'\|)$  induced by a so called *bell function*  $\phi$ . Their analytic properties allow lossless evaluation of complexity *independent* of  $d$  and to compute sharp and local Lipschitz constants for use in the error estimation.

**Error estimation.** An estimation of the error system and application of the comparison lemma yield the basic structure for our error estimators. The state space position of the reduced system is used to compute local Lipschitz constants using secant gradients in order to improve the estimation. Together with an a-priori bound an iterative scheme can be applied to further improve the estimation sharpness. Figure 1 shows improving estimation results for a synthetic system using global (square), local (star) and iterated local (star/triangle) Lipschitz constants. The right image shows a parameter sweep with system output and a-posteriori error bounds (transparent red).



Left: Estimation results using different (local) Lipschitz constants. Right: Parameter sweep with system output and error bounds



# SYLVESTER EQUATIONS AND THE FACTORIZATION OF THE ERROR SYSTEM IN KRYLOV SUBSPACE METHODS

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**Introduction.** This paper presents a factorization of the error system that arises in model reduction of linear time invariant systems by Krylov subspace methods. The factorization is introduced for reduced models that match moments and/or Markov parameters of the original system with multiple inputs and outputs. Furthermore, dual results are given for the reduction with input and output Krylov subspaces. To this end, this work constitutes a generalization of [3] where the factorization was first presented for a special case. The results emerge from an investigation of the Sylvester equations that arise in the context of Krylov subspaces. To that effect, previous results on Sylvester equations are revised and extended in this paper. The theoretic results on Krylov subspaces that are presented here can be useful in error analysis and in the selection of expansion points in Krylov-based model order reduction.

**Content.** In this work, linear time invariant systems (LTI) are considered

$$\begin{aligned} \mathbf{E}\dot{\mathbf{x}}(t) &= \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t), \\ \mathbf{y}(t) &= \mathbf{C}\mathbf{x}(t), \end{aligned} \quad (1)$$

where  $\mathbf{x}(t) \in \mathbb{R}^N$ ,  $\mathbf{u}(t) \in \mathbb{R}^m$  and  $\mathbf{y}(t) \in \mathbb{R}^p$  denote the states, inputs and outputs of the system, respectively. The dynamics of the system are described by  $\mathbf{E}, \mathbf{A} \in \mathbb{R}^{N \times N}$  and  $\mathbf{B} \in \mathbb{R}^{N \times m}$ ,  $\mathbf{C} \in \mathbb{R}^{p \times N}$ . It is assumed that  $\mathbf{E}$  is non-singular:  $\det(\mathbf{E}) \neq 0$ . The goal of model reduction is to approximate a large-scale system (1) by one of much smaller dimension  $n \ll N$ . In projection based model order reduction, this is carried out by finding appropriate projection matrices  $\mathbf{V}, \mathbf{W} \in \mathbb{R}^{N \times n}$ . Towards this aim,  $\mathbf{V}$  and  $\mathbf{W}$  can e. g. be chosen to span certain Krylov subspaces.

**Krylov subspaces and Sylvester equations.** In [2] it was already shown, that if a matrix  $\mathbf{V}$  spans a Krylov subspace, then it simultaneously solves a certain Sylvester equation. One scope of this paper is to reveal the correlations of Krylov subspaces and Sylvester equations. The connection is discussed for block Krylov subspaces due to multiple inputs and outputs. Both results from input and output Krylov subspaces are highlighted independently from each other. Moreover, the general case that  $\mathbf{E}$  is not identity is treated.

Characterizing Krylov subspaces as solutions of Sylvester equations as a starting point, it is straightforward to obtain different results available in the literature. Firstly, it is shown that with a given  $\mathbf{V}$  spanning a (block) Krylov subspace, all possible reduced systems (due to  $\mathbf{W}$ ) can be parametrized by the  $n \cdot m$  entries of the reduced input matrix, in contrast to the usual way of choosing the  $n$  directions of the projection matrix  $\mathbf{W}$ . Since the derivation of the parameterization is based on the projection of Sylvester equations, the result in the literature is generalized to multiple inputs/outputs as well as matching so-called Markov parameters in the reduced system is included.

Subsequent, it is shown that a second type of Sylvester equations can be associated with a matrix  $\mathbf{V}$  spanning a Krylov subspace, again by the help of projections. The authors of [1] have presented a similar result independently, which is based on the particular course of action in the Arnoldi and Lanczos algorithms, that are used to compute  $\mathbf{V}$ . On that account the second type of Sylvester equation was interpreted as Arnoldi and Lanczos-like equations.

The authors of this work, on the other hand, follow the projection-based view, where the only assumption is that  $\mathbf{V}$  has to span a Krylov subspace (whereas  $\mathbf{W}$  is almost arbitrary). This is why no constraints on the numerical implementation are necessary. Furthermore, the proof here is based on the first type of Sylvester equation, which eases the derivation of the second type and hence correlates the results.

**Factorization of the error system.** The theoretical results on Sylvester equations are used to factorize the error system which describes the error due to approximation in Krylov-based model order reduction. It is shown, that based on the second type of Sylvester equations, the error system can be factorized into two systems of order  $N$  and  $n$ , respectively. Furthermore, the particular state space representations can be given with negligible numerical effort. The scope of this work is only the presentation of the theoretical results in the most general case.

- [1] M. Frangos, and I.M. Jaimoukha: *Rational interpolation: Modified rational Arnoldi algorithm and Arnoldi-like equations*. In: Proc. 46th IEEE Conference on Decision and Control, New Orleans, December 2007.
- [2] K. Gallivan, A. Vandendorpe, and P. Van Dooren: *Sylvester equations and projection-based model reduction*. Journal of Computational and Applied Mathematics, 162 (2004), 213-229.
- [3] T. Wolf, H. Panzer, and B. Lohmann: *Gramian-based error bound in model reduction by Krylov subspace methods*. In: 18th IFAC World Congress, pages 3587-3592, Milano, Italy, August 2011.



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**Model-based Analysis and Control for  
Distributed-Parameter Systems**



## PORT-HAMILTONIAN SYSTEMS ON DISCRETE MANIFOLDS

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A large class of open distributed-parameter Hamiltonian systems can be defined with respect to the Stokes-Dirac structure [1]. This infinite-dimensional Dirac structure provides a theoretical account that permits the inclusion of varying boundary variables in the boundary problem for partial differential equations. From an interconnection and control viewpoint, such a treatment of boundary conditions is essential for the incorporation of energy exchange through the boundary, since in many applications the interconnection with the environment takes place precisely through the boundary. For numerical integration, simulation and control synthesis, it is of paramount interest to have finite approximations that can be interconnected to one another.

Most of the numerical algorithms emanating from the field of numerical analysis and scientific computing, however, fail to capture the intrinsic system structures and properties, such as symplecticity, conservation of momenta and energy, as well as differential gauge symmetry. Furthermore, some important results, including the Stokes theorem, fail to apply numerically and thus lead to spurious results.

Recently in [2], we have suggested a discrete exterior geometry approach to structure-preserving discretization of distributed-parameter port-Hamiltonian systems. The spatial domain in the continuous theory represented by a finite-dimensional smooth manifold is replaced by a homological manifold-like simplicial complex and its circum-centric dual. The smooth differential forms, in discrete setting, are mirrored by cochains on the primal and dual complexes, while the discrete exterior derivative is defined to be the coboundary operator. A discrete analogue of the Stokes-Dirac structure is a so-called simplicial Dirac structure defined over a space of primal and dual discrete differential forms.

In this paper, we address the issue of matrix representations of simplicial Dirac structures by representing cochains by their coefficient vectors. In this manner, all linear operator from the continuous world can be represented by matrices, including the Hodge star, the coboundary and a trace operator. Using these representations and discrete energy norms, we offer a general framework for the convergence analysis of the proposed scheme.

- [1] A.J. van der Schaft, B.M. Maschke, "Hamiltonian formulation of distributed-parameter systems with boundary energy flow", *Journal of Geometry and Physics*, vol. 42, pp. 166–194, 2002.
- [2] M. Seslija, J.M.A. Scherpen, A.J. van der Schaft, "A discrete exterior approach to structure-preserving discretization of distributed-parameter port-Hamiltonian systems," *Proc. 50th IEEE Conf. on Decision and Control*, Orlando, Florida, December 12-15, 2011

# MODELING AND SIMULATION OF LARGE-SCALE MANIPULATORS WITH HYDRAULIC ACTUATION

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**Problem description.** Due to the light-weight construction of modern large-scale manipulators used e.g., in concrete pumps or maritime crane systems, the elasticity of the construction elements plays a significant role in the dynamic behaviour of the overall system. These systems are vulnerable to vibrations caused by external disturbances like the pumping of wet concrete or the wave motions on the sea. Therefore, current research is concerned with control strategies for active damping of elastic vibrations, trajectory planning and the computation of the inverse kinematics. For the development of such control methods, tailored mathematical models are required. In the considered applications, the inhomogeneous distribution of mass and of the geometrical moment of inertia over the length of the segments of the boom has to be explicitly considered in the model which makes the problem more involved. Furthermore, it is known that stick-slip effects of the hydraulic cylinders can be a major problem in the design of a control strategy, so that this effect has to be taken into account in the model, too.

**State of the art.** For the modeling of flexible multi-body systems well developed methods exist in the literature, see, e.g., [6] and [2]. Most investigations in this field are related to flexible robot systems with electromechanic actuators. In large-scale applications like mobile concrete pumps, hydraulic actuators comprising hydraulic cylinders and valves are commonly used, which have a different dynamic behaviour and assembling. The combination of flexible multi-body systems and hydraulic actuators has been studied, e.g., in [1], [5] and [4]. Therein different strategies for modeling the elasticity of the boom have been used. In [1] and [5] the elastic beam elements are approximated by a number of rigid bodies which are connected by joints and spring elements. This leads to a well known procedure for the derivation of the equations of motion as it is common in robot applications. The position of the additional joints and the spring rates have, however, no direct relation to real physical parameters. Another different approach is to model the elastic segments in form of Euler-Bernoulli beams. Due to their distributed parameter characteristics, a finite-dimensional approximation, e.g., by means of the Ritz-method, is typically performed in order to obtain a system of ordinary differential equations, see, e.g., [3] and [4]. In order to obtain fast simulation times of the model and to simplify the controller design, the dimension of the model should be kept as small as possible. In this context the right choice of the basis functions for the Ritz-method turns out to be the crucial point to achieve a high model accuracy. E.g., in [3] the eigenfunctions of the homogeneous Euler-Bernoulli beam equation are chosen as basis functions whereas [4] recommends the use of Legendre polynomials. Both approaches are feasible, but due to the inhomogeneous structure of the beam elements of the considered application a lot of basis functions are required to accurately describe the beam deflection dynamics. The choice of the degrees of freedom has also an important influence on the complexity of the resulting equations, which describe the interconnection between the mechanical and the hydraulic part. E.g. the model of [1] results in a simple relationship between piston force, joint torque and the rigid body angle while in contrast, the approach of [4] leads to a complex relationship of the generalized forces depending on the elastic deformations.

**Proposed approach.** This paper proposes a systematic procedure for the modeling of large-scale manipulators with hydraulic actuation. The derivation of the equations of motion is based on Ritz's method and the Euler-Lagrange formalism. The static bending profile of each beam and an orthogonal polynomial are used as the first and the second basis function. This ensures a more accurate approximation of the beam deflection. It is shown that the suggested selection of the degrees of freedom results in a cylinder piston position which is solely a function of the rigid body angle. This is of special interest, since this enables a simple modeling of the static friction of the hydraulic cylinders. A mathematical model of an industrial concrete pump is derived based on the proposed procedure. The model is evaluated by means of simulation and measurement results.

- [1] Aschemann H., Sawodny O., Bulach A., Hofer E.P., *Model based trajectory control of a flexible turntable ladder*. In: Proceedings of the American Control Conference, Anchorage, 2002, 921 - 926 vol. 2.
- [2] Bremer H., Pfeiffer F., *Elastische Mehrkörpersysteme*. Teubner Taschenbücher: Mechanik, Stuttgart, 1992.
- [3] De Luca A., Siciliano B., *Closed-Form Dynamic Model of Planar Multilink Lightweight Robots*. In: IEEE Transactions on Systems, Man and Cybernetics, vol. 21, no. 4, 1991, 826 - 839.
- [4] Gerstmayr J., Diebold M., Irschik H., *Dynamik geregelter flexibler Mehrkörpersysteme unter Berücksichtigung hydraulischer Aktorik*. In: e&i Elektrotechnik und Informationstechnik, vol. 129, 2004, 307-312.
- [5] Lambeck S., Sawodny O., Arnold E., *Trajectory Tracking Control for a new Generation of Fire Rescue Turntable Ladders*. In: Proceedings of the 2nd IEEE Conference on Robotics, Automation and Mechatronics, Bangkok, 2006, 847 - 852.
- [6] Shabana A. A., *Dynamics of Multibody Systems*. Cambridge University Press, 2005.

# ENERGY-BASED CONTROL OF SPATIALLY-DISCRETIZED DISTRIBUTED PORT-HAMILTONIAN SYSTEMS

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This paper illustrates a novel procedure for the control by energy shaping of distributed port-Hamiltonian systems [10]. In recent works [3, 4, 7], this task has been accomplished by looking at or generating a set of Casimir functions in the closed-loop system that robustly (i.e. independently from the Hamiltonian function) relates the state of the infinite dimensional port-Hamiltonian system with the state of the controller. The controller has been usually modelled as a finite dimensional port-Hamiltonian system which has to be interconnected in a power conserving way to the boundary of the distributed parameter system. The shape of the energy function of the closed-loop system can be changed by properly choosing the Hamiltonian function of the controller in order to introduce a (possibly global) minimum in a desired configuration. This procedure is basically the generalization to the distributed parameter case of the control by interconnection via Casimir generation developed for finite dimensional port-Hamiltonian systems, [5, 6, 9].

In case of plants modelled as distributed parameter systems, it is relatively easy to shape the energy function. The main difficulties arise in proving that the new minimum of the closed-loop Hamiltonian function corresponds also to an asymptotically stable equilibrium point. Only stability can be verified by means of relatively simple techniques, as reported in [8]. This because, even if the extension to distributed parameter system of La Salle's Invariance Principle exists, its application is not immediate due to several technical problems mostly related to the analysis of the solution of linear or nonlinear PDEs, [2].

Instead of working on the *full-order* (i.e. infinite dimensional) dynamics of the plant, the idea is to rely on a finite dimensional approximation provided by the spatial discretization procedure presented in [1]. In particular, given a distributed parameter system in port-Hamiltonian form, from the analysis of its geometric structure (i.e. of its Stokes-Dirac structure, [10]), a finite dimensional approximation still in port-Hamiltonian form can be obtained. The main contribution of this paper is to show how the control by energy shaping via Casimir generation, developed for finite dimensional systems [5, 6, 9], can be applied to the finite element approximation of a distributed parameter port-Hamiltonian system. In this way, standard tools for studying the stability of finite dimensional port-Hamiltonian systems can be used to prove the validity of the (boundary) controller. On the other hand, these well-established techniques cannot be applied *as is*, not only because of the intrinsic difficulties related to the large number of state variables of the finite dimensional approximation, but also because the finite element model is completely *a-causal*. This means that the plant dynamics is not given in standard input-state-output form, but as a set of DAEs. Consequently, the classical energy-Casimir method has to be extended in order to deal with dynamical systems with constraints, usually appearing in the form of Lagrangian multipliers.

- [1] G. Golo, V. Talasila, A. J. van der Schaft, and B. M. Maschke. Hamiltonian discretization of boundary control systems. *Automatica*, 40(5):757–771, 2004.
- [2] Z. H. Luo, B. Z. Guo, and O. Morgul. *Stability and stabilization of infinite dimensional systems with applications*. Springer-Verlag, London, 1999.
- [3] A. Macchelli and C. Melchiorri. Modeling and control of the Timoshenko beam. The distributed port Hamiltonian approach. *SIAM Journal on Control and Optimization*, 43(2):743–767, 2004.
- [4] A. Macchelli and C. Melchiorri. Control by interconnection of mixed port Hamiltonian systems. *Automatic Control, IEEE Transactions on*, 50(11):1839–1844, Nov. 2005.
- [5] R. Ortega, A. J. van der Schaft, I. Mareels, and B. M. Maschke. Putting energy back in control. *Control Systems Magazine, IEEE*, pages 18–33, Apr. 2001.
- [6] R. Ortega, A. J. van der Schaft, B. M. Maschke, and G. Escobar. Energy-shaping of port-controlled Hamiltonian systems by interconnection. In *Decision and Control (CDC 1999). Proceedings of the 38th IEEE Conference on*, volume 2, pages 1646–1651, Dec. 1999.
- [7] H. Rodriguez, A. J. van der Schaft, and R. Ortega. On stabilization of nonlinear distributed parameter port-controlled Hamiltonian systems via energy shaping. In *Decision and Control (CDC 2001). Proceedings of the 40th IEEE Conference on*, volume 1, pages 131–136, Dec. 2001.
- [8] G. E. Swaters. *Introduction to Hamiltonian fluid dynamics and stability theory*. Chapman & Hall / CRC, 2000.
- [9] A. J. van der Schaft. *L<sub>2</sub>-Gain and Passivity Techniques in Nonlinear Control*. Communication and Control Engineering. Springer-Verlag, 2000.
- [10] A. J. van der Schaft and B. M. Maschke. Hamiltonian formulation of distributed parameter systems with boundary energy flow. *Journal of Geometry and Physics*, 42(1-2):166–194, May 2002.

# CONTROLLER CANONICAL FORMS AND FLATNESS BASED STATE FEEDBACK FOR 1D HYPERBOLIC SYSTEMS

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Flatness based controllability analysis and closed loop control design for networks of spatially one-dimensional boundary value problems (b.v.p.) involving several second order hyperbolic partial differential equations (p.d.e.'s) with constant coefficients is considered. The main idea is the transformation of the b.v.p. under consideration into an equivalent system of functional differential equations (f.d.e.'s). This is achieved using the explicit representation of the solution of the Cauchy boundary value problems associated with the p.d.e.'s. Regarding the system of f.d.e.'s as linear convolution equations over the ring  $\mathcal{E}'(\mathbb{R})$  of compactly supported Schwartz distributions algebraic techniques can be used to introduce a flat output [6]. The latter can be used to parametrize arbitrary smooth solutions of the model under consideration.

In the single input case the flatness based parametrization of the system variables can be directly used for the analysis of the state space controllability. The parametrization of the input appears as a single scalar f.d.e. the controllability of which in an appropriately chosen state space is not difficult to show. In accordance with [4] the abstract evolution equation associated with this f.d.e. is called the controller canonical form (c.c.f.) of the system under consideration. This evolution equation comprises a chain of integrators that is attached to the output of a single unperturbed transport system. Moreover, up to an unbounded state feedback, the control input corresponds to the boundary value at the boundary where the matter enters the domain. State space controllability of the original system cannot be deduced immediately from the flatness of the system. However, on the basis of the flatness based parametrization of the state variables a map that relates the state of the c.c.f. to the original state coordinates can be established. This map can be used to identify the controllable subspace of the originally given state space description.

Based on the f.d.e. associated with the c.c.f. a feedback that stabilizes the closed loop system can be given. As a feedback of the flat output trajectory this control law involves explicit but well defined predictions. Using the state of the c.c.f. such control laws appear simply as an unbounded state feedback. They can be easily given w.r.t. the original state coordinates by means of the derived state transform. The proposed method is illustrated by means of a nontrivial example modelling a simple network of interconnected strings with boundary loads. This example, which is known from the previous publication [5] is shown to be approximately controllable. A feedback law that achieves a finite spectrum assignment is proposed.

The contribution involves and generalizes several ideas known from literature. Stabilizing by flatness based predictive control laws has been originally used for linear wave equations with linear and nonlinear boundary conditions in the context of  $\delta$ -flatness of linear delay systems [2]. Moreover, for the transformation into the c.c.f. two different approaches are known from the literature. The first one, which goes back to ideas presented in [1], makes use of the theory of characteristics to obtain the desired f.d.e. while the second one, established in [3] and further detailed in [4], rather relies on the spectral properties of the b.v.p. under investigation. Note that these results have been originally formulated only for b.v.p.'s involving one p.d.e., only. Moreover, the equivalence to a simple transport equation and the notion of a c.c.f. was established only in the latter contribution.

- [1] K. L. Cooke and D. W. Krumme. Differential-difference equations and nonlinear initial-boundary value problems for linear hyperbolic partial differential equations. *J. Math. Anal. Appl.*, 24:372–387, 1968.
- [2] H. Mounier and J. Rudolph. Flatness based control of nonlinear delay systems: A chemical reactor example. *Internat. J. Control*, 71:871–890, 1998.
- [3] D. L. Russell. Canonical forms and spectral determination for a class of hyperbolic distributed parameter control systems. *J. Math. Anal. Appl.*, 62(1):186–225, 1978.
- [4] D. L. Russell. Neutral FDE canonical representations of hyperbolic systems. *Journal of Integral Equations and Applications*, 3(1):129–166, 1991.
- [5] F. Woittennek. On flatness and controllability of simple hyperbolic distributed parameter systems. In *Proc. 18th IFAC World Congress*, pages 14452–14457, Milano, Italy, 2011.
- [6] F. Woittennek and H. Mounier. Controllability of networks of spatially one-dimensional second order p.d.e. – an algebraic approach. *SIAM J. Control Optim.*, 48(6):3882–3902, 2010.



# AN EFFICIENT IMPLEMENTATION OF BACKSTEPPING OBSERVERS FOR TIME-VARYING PARABOLIC PDES

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The need of state estimation algorithms for distributed-parameter systems occurs in many applications, ranging from advanced control schemes to process monitoring and diagnostics (see, e.g., [2] and references therein). Thereby, when dealing with the state estimation problem for systems governed by partial differential equations (PDEs), an early or late lumping approach can be used. In the last decade, the backstepping method, see, e.g., [3] has emerged as a promising and in particular systematic approach for the design of exponentially convergent distributed-parameter observers for systems governed by PDEs. One of the essential and computationally most expensive part of the backstepping approach is concerned with the determination of the kernel of a Volterra integral equation, which is governed by a higher-dimensional PDE. Its solution is required for the determination of the output injection weights of the state observer to ensure the exponential stability of the observer error dynamics. A classical solution of the kernel-PDE traces back to [1], where the kernel is obtained in terms of a series expansion by means of the method of integral operators followed by a successive approximation. Herein, the main drawback is the recursive way of the determination of the series coefficients, which significantly increases the computing time. In [3], the Ablowitz-Kruskal-Ladik scheme is suggested for the direct numerical solution of the kernel-PDE in the case of spatially varying parameters. However, since in the case of spatially and time varying parameters so far no direct numerical methods are known for the solution of the resulting kernel-PDE characterized by a hyperbolic spatial operator and a first order derivative with respect to time defined on a triangular spatial domain, it is desirable to construct a new computationally efficient solution approach for such PDEs.

The proposed solution method is based on the implicit integral formulation of the kernel-PDE. For this, following an appropriate change of coordinates a formal integration over the triangular domain is applied. Subsequently, the kernel integral equation is discretized in space and the involved integral terms are approximated by means of the composite trapezoidal rule. As a result, a system of first-order ordinary differential equations (ODEs) is obtained governing the pointwise explicit-in-time evolution of the backstepping-kernel. Consequently, for the numerical solution of the resulting time-varying kernel-ODE the absolute stable backward Euler method is applied. Finally, observer gains based on the numerical solution of the kernel-ODE are employed in the state observer scheme and the impact of the method on the computing time and on the observer error convergence is evaluated by means of numerical simulations.

- [1] Colton, D. (1977). The solution of initial-boundary value problems for parabolic equations by the method of integral operators. *Journal of Differential Equations*, 26, 181–190.
- [2] Meurer, T. and Kugi, A. (2009). Tracking control for boundary controlled parabolic PDEs with varying parameters: Combining backstepping and differential flatness. *Automatica*, 45(5), 1182–1194.
- [3] Smyshlyaev, A. and Krstic, M. (2004). Closed-form boundary state feedbacks for a class of 1-D partial integro-differential equations. *IEEE Transactions on Automatic Control*, 49(12), 2185 – 2202.



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# APPLICATIONS OF MATHEMATICAL MODELS OF ROAD CYCLING

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Mathematical models are at the core of much research in sport science. They provide the means to simulate individual athletic or team sport performance, to analyze human movement in game sports, to predict and improve performance, to name just a few. In this paper, we provide an introduction and overview of our recent research on applications of mathematical modeling for road cycling.

Our work is oriented towards two primary and one auxiliary goals. The first one is the development of an indoor simulator. The physical setup is based on a programmable ergometer measuring power output of a cyclist. Together with measurements of bike/rider parameters and distances/altitudes along a real-world track we apply a mechanical model for road cycling to control the ergometer which delivers an accurate simulation of a particular athlete's ride on the measured track. Such simulators can be used for realistically training and acquainting athletes with unfamiliar tracks, e.g., for some upcoming racing event at a location too far away for traveling. Moreover, such simulators bring studies in training and sport science, that must be carried out in a lab environment, a step closer to reality. Field studies may not be possible for some experiments because they may require, e.g., regularly taking blood probes to measure lactate concentration.

The second main goal is to optimize rider performance for an uphill time trial, assuming the track has a varying slope profile along the course. For that purpose we propose to additionally apply a simple physiological model of athlete performance that relates the rider's exhaustion to the energy consumed so far. The objective then is to prescribe a strategy to optimally distribute the rider's available energy such that the rider is completely exhausted at the finish line of the time trial and such that the required time is minimal. Our preliminary study indicated that indeed a small performance increase is possible in practice using our simulator for an evaluation.

Our third application of modeling lies in the estimation of parameters of the models. For example, coefficients specifying aerial drag and rolling resistance are required for our applications for simulation and optimization. Typically, such parameters are obtained by linear regression, i.e., in our case by making field measurements of output power while cycling on a known flat track with constant speed and then determining the model parameters such that the predicted power best matches the measured data. However, not all physical parameters can be determined in this way. In our method we propose appropriate compound parameters all of which can be estimated. Moreover, the method allows to make the measurement on tracks that need not be perfectly flat and even significant variations in speed along the measurement rides do not invalidate the experiments.

In case of road cycling in mountainous terrain the dominating factor determining the required power to overcome the forces of gravity and to reach a desired speed is the slope of the track. Thus, together with the mechanical cycling model and the rider and bike parameters an accurate road height respectively slope profile is required. We found that current standard GPS measurements of elevation do not provide sufficient accuracy for our application. This can be attributed to the amplification of measurement errors that takes place when numerically differentiating height profiles to compute road gradients. Differential GPS devices are based on correcting ordinary GPS measurements using a reference signal of a fixed base station. With current technology, altitudes measured by differential GPS are exact up to just a few centimeters. However, such devices are prohibitively expensive when compared to other devices required for cycling studies like bicycle computers and even power meters. Moreover, with our differential GPS device, we encountered the disadvantage that common obstacles like trees and houses along the roadside may deteriorate the signal quality to the point that it becomes useless. To fill in such gaps and to generally improve the quality of measured height profiles, we propose to extend the standard procedure for parameter estimation by linear regression of model predictions to measurement data to also approximate entire road slope profiles. Of course, the resulting geometrical road model is incorporated in the computations for the simulation and optimization mentioned previously.

For this exposition and review we partially follow our previous publications on the road cycling simulator [1], performance optimization [3], and calibrating model parameters [2].

- [1] T. Dahmen, R. Byshko, D. Saupe, M. Röder, and S. Mantler. Validation of a model and a simulator for road cycling on real tracks. *Sports Engineering*, 14:95–110, November 2011.
- [2] T. Dahmen and D. Saupe. Calibration of a power-speed-model for road cycling using real power and height data. *International Journal of Computer Science in Sport*, 10(2):18–36, December 2011.
- [3] S. Wolf and T. Dahmen. Optimierung der Geschwindigkeitssteuerung bei Zeitfahrten im Radsport. In D. Link and J. Wiemeyer, editors, *Sportinformatik trifft Sporttechnologie*, pages 235–239. dvs-Sektion Sportinformatik, September 2010.

## LOAD OPTIMIZATION IN ENDURANCE SPORTS BY MEANS OF ANTAGONISTIC DYNAMICAL MODELS

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**Introduction.** Prediction of performance dynamics as well as planning and control of corresponding optimal load profiles are difficult tasks in endurance sports. The reason is that fatigue and recovery are effective with delays. I. e. a small overload in the start phase can cause a collapse long time later. Such interaction between load and performance can be modelled by means of antagonistic models like PerPot [1] and then can help to optimize performance together with avoiding overload.

**State-of-the art.** Based on a lot of positive results, extensions of PerPot have been developed, which are now able to determine the individual anaerobe threshold (IAT) by simulation, giving heart rate oriented load scheduling a new quality [2]. Also an extension DoMo has been developed that demonstrates that the concept of PerPot also works if two or more types of load are concurrently effective [3]. Finally an internet-based approach is being developed by the Vienna working group of Arnold Baca, which allows online checking and control of marathon runners during the run.

**Method.** The major problem that arises with modelling a system like human physiology is that of complexity. The huge amount of interacting organ components of a body makes it extremely difficult to decide what to take into account principally – and what to use for simulation. The Per-Pot-approach demonstrates the way of abstraction from the original physiologic system over a structural description down to a most simple model with mainly two parameters [1]:

Briefly spoken, the meta-model PerPot describes physiological adaptation on an abstract level as an antagonistic process: A load input flow is feeding identically a fatigue potential as well as a recovery potential. From the recovery potential the performance potential is increased by a positive flow, while the fatigue potential reduces it by a negative flow. All flows show specific delays modelling the time that components of the modelled system need to react.

In particular, reserve and load overflow play an important role in calculating optimal performance. If the reserve is reduced to zero an overflow of fatigue reduces the performance potential with small delay, possibly causing a sudden break down, which cannot be compensated by the slow recovery flow. This particular dynamics can be taken for calculating the individual anaerobe threshold, which then can be used for planning optimal speed schedules and finishing results in endurance sports.

- [1] Perl J.: *Dynamic Simulation of Performance Development: Prediction and Optimal Scheduling*. International Journal of Computer Science in Sport, 4 (2005), 2, 28-37.
- [2] Perl J., and Endler S.: *PerPot: Individual Anaerobe Threshold & Marathon Scheduling*. To appear in International Journal of Computer Science in Sport, 2012.
- [3] Perl J., and Pfeiffer M.: *PerPot DoMo: Antagonistic meta-model processing two concurrent load flows*. International Journal of Computer Science in Sport, 10 (2011), 2, 85-92.

# CREATING A CONTINUOUS TOPOGRAPHY OF PERFORMANCE FROM DISCRETE SPORTS ACTIONS

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**Introduction.** Often in sports, discrete data describing actions of athletes are collected in order to analyze performance. The data usually consist of information about the location of an athlete's action and the quality or quantity of the action. Performance analysis using these data usually involves creating categories by which the quality of the performance of athletes in a certain sport can be described [1],[2]. The definitions of these categories often only take a few circumstances or just the most important one into account which influence the performance of an athlete. The aim of the study was to develop a mathematical model with which this method of classifying performances can be broken up and performances are put in context of the place where they occurred, in context of the internal and external circumstances which influence the athlete's performance, with respect to the performance of other athletes in that area. This is realized by calculating a continuous topography of the performance of the field based on the collected discrete data which includes information about internal and external circumstances that influenced an athlete performing an action [3].

**Method and Results.** The topography of the performance of the field is calculated in three steps. First, a grid is assigned to the field of play for the respective sport. At the grid nodes a representative performance of the field is calculated out of the discrete data by an exponential smoothing algorithm. Finally, a continuous, three dimensional topography is generated based on the smoothed representations of the performance using a spline interpolation (figure 1.a)). In an additional fourth step, contour levels of the topography can be plotted on a two dimensional map of the field of play to visualize performance and characteristics of this performance which should be analyzed (figure 1.b)).

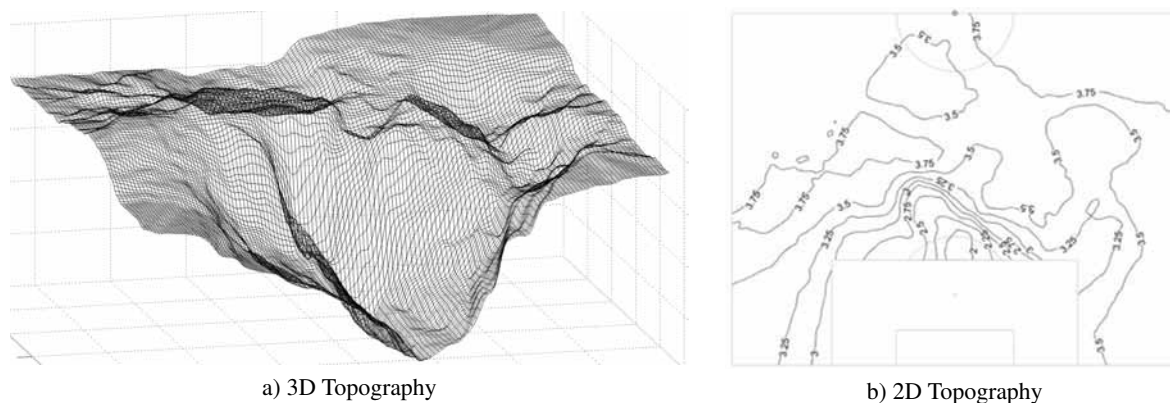


Figure 1: Three dimensional (a) and two dimensional (b) Topographies of danger zones of direct free kicks ( $n = 117$ ) in women's FIFA World Cup 2007

**Conclusion.** Calculating continuous topographies of performances from discrete sport actions is a reasonable method to break up the classifying methods which are commonly used in performance analysis. The method presented in this paper provides three dimensional and two dimensional topographies of a representative performance of the field. These can be used to analyze performance with respect to other athletes's performance in different sports. Furthermore, in future studies, performance indicators for individual performance should be derived from this method by comparing an athlete's performance to the values of the topography and hence by comparing the performance to the representative performance of the field.

- [1] James N.: *Performance analysis of golf: Reflections on the past and a vision of the future*. International Journal of Performance Analysis in Sport, 9(2) (2009), 188–209.
- [2] Alcock A.: *Analysis of direct free kicks in the women's football World Cup 2007*. European Journal of Sport Science, 10(4) (2010), 279–284.
- [3] Stöckl M., and Lames M.: *Modeling Constraints in Putting: The ISOPAR Method*. International Journal of Computer Science in Sport, 10(1) (2011), 74–81.

# IDENTIFYING TIBIO-FEMORAL JOINT KINEMATICS: INDIVIDUAL ADJUSTMENT VERSUS NUMERICAL ROBUSTNESS

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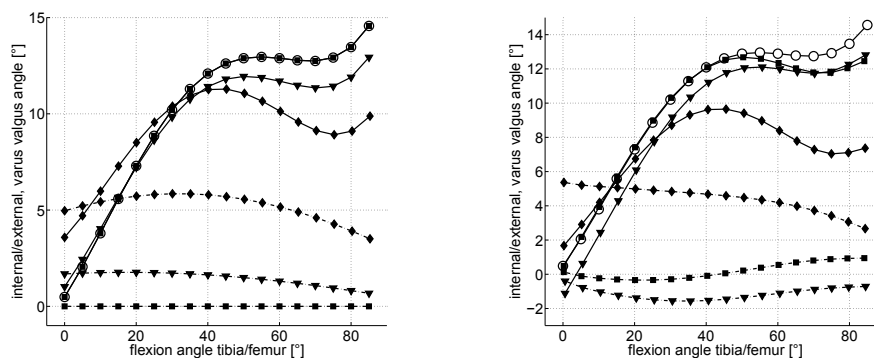
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**Introduction.** The interpretation of joint kinematics data in terms of displacements is sensitive to the type of movement, the measurement technique and the reference axes where rotations and translations are associated with. Misaligned knee joint axes do not only lead to a misinterpretation of knee joint kinematics but, additionally, have a general impact on lower body kinematics. Therefore, several groups independently propose to *a posteriori* replace empirically palpated axes by functionally calculated axes. Flexion is the most dominant motion of the knee joint. Thus, the flexion axis has the largest effect on the kinematical calculation. The large angular flexion range facilitates the mathematical procedure of axis determination. The second rotation of importance is the internal/external rotation which is sometimes controlled by mathematical optimization techniques.

**Aims.** This contribution focuses on the evaluation of the concepts of *symmetrical axis of rotation approach* (SARA, [1]) and *finite helical axis* (FHA, [2]) regarding their applicability in axis reorientation procedures, and to explore which of the underlying algorithms performs most robust and convenient under typical data perturbations.

**Methods and results.** Numerical implementation of the algorithms underlying the axis determination for given measurement data is not straightforward. In the SARA approach, special care has to be taken in selecting an appropriate solution obtained via the SVD of the system matrix of the underlying least squares problem. The FHA approach makes use of local (instantaneous) IHA axes defined via differential geometric arguments. Basically, this is defined for smooth movements and needs to be discretized. It is shown how this is to be performed in a natural way, avoiding discretization artefacts as far as possible.

Both approaches are tested using fictive data sets, also involving perturbations as typically inferred in a clinical setting (soft tissue artefacts). As basis for a healthy knee joint model, the approximation as a compound hinge joint exhibiting flexion-extension and tibial rotation was taken. For kinematics data of a squat movement, functional flexion axes are determined via both, the SARA and FHA approaches, and the results are represented in the joint coordinate system due to [3]. Comparison with a given reference axis allows the evaluation of the accuracy and robustness of the underlying algorithms. The figure displays results for a typical example. Apparently, the FHA approach is less robust, especially in the presence of perturbations.



Rotations represented in joint coordinates: Data for flexion and tibial rotation ( $\circ$ ). Displacements are computed for different flexion axes, namely, first the true axis used to generate the fictive kinematic data ( $\blacksquare$ ), the SARA axis ( $\blacktriangledown$ ), and the FHA ( $\blacklozenge$ ). Solid lines depict ie-rotation (tibial rotation), dash-dotted lines depict vv-rotation (adduction/abduction). The first plot shows a case without perturbation, the second one a case with a maximum deviation of a marker from its true position by estimated 8 mm.

- [1] Ehrig, R.M., Taylor, W.R., Duda, G.N., and Heller, M.O. (2007). A survey of formal methods for determining functional joint axes. *Journal of Biomechanics*, 40, 2150–2157.
- [2] Woltring, H., de Lange, A., Kauer, J., and Huijskes, R. (1987). Instantaneous helical axis estimation via natural, cross-validated splines. In *Bergmann G, Kölbel R, Rohlmann A (eds.). Biomechanics: Basic and Applied Research. Springer*, 121–128.
- [3] Grood, E.S. and Suntay, W.J. (1983). A joint coordinate system for the clinical description of three-dimensional motions: Application to the knee. *Journal of Biomechanical Engineering*, 105(2), 136–144.



# A MATHEMATICAL MODEL OF THE RELATIVE AGE EFFECT (RAE) IN SPORTS TALENTS

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**Introduction.** In selections of young athletes especially in soccer it is frequently observed that their birth days show a bias towards the beginning of the year. This bias of the birth dates is called the Relative Age Effect (RAE) and is attributed to the selection of early maturers (Augste & Lames, 2011). This paper suggests a mathematical model for the selection process leading to a RAE based on one parameter, a selection threshold consisting of the physical maturation of the selected athletes ahead of the average of the population. It provides two indices that characterize the underlying selection process leading to the respective RAE. STA (Selection Threshold Applied) is an estimate for the percentage of the population eligible to the sample, and MLA (Maturity Level Applied) is the corresponding biological age expressed in years ahead of the maturation level of the population.

**Method.** The probability of being selected is assumed to be proportional to having a certain maturity level or biological age at time of selection. Biological age may be assumed to be normally distributed with chronological age as mean value and a standard deviation  $s_{pop}$  that is typical for the population the sample is drawn from (Sherar et al., 2007). From these assumptions one may calculate the probability of having a certain biological age (BA):  $P(BA > x) = \int_{-x}^{\infty} \mathcal{N}(CA_{pop}, s_{pop})$ . The probability of being selected is proportional to having a certain biological age. As the sample is composed of athletes born at the  $k^{th}$  of  $n$  time intervals the probability of being in class  $k$  is:  $P(k) = \frac{\int_{-x}^{\infty} \mathcal{N}(k, s_{pop})}{\sum_{i=1}^n \int_{-x}^{\infty} \mathcal{N}(i, s_{pop})}$ . MLA is the  $x$ -value that gives the best approximation of the sample's empirical distribution. STA is the probability of having MLA as biological age..

**Results.** The model was applied to four different samples in youth football of different selection level and sample size. RMSE as goodness-of-fit indicator varied from 0.49% in the largest ( $n=22,238$ ) to 3.25% in the smallest ( $n=26$ ) sample. Correlations between observed and expected values ranged from 0.917 to 0.986. Processes employed to select German national youth team players are characterized by a MLA of 2.58 years ahead of population that corresponds to 0.5% of the population being eligible.

**Discussion.** Modeling the RAE based only on the assumption that a biological threshold is applied has turned out to be successful in terms of conceptual considerations and the goodness of fit results in different samples. Although problems of prediction grow with decreasing sample size even results for small samples give a valid description of the underlying selection process.

- [1] Augste, C. & Lames, M. (2011). The Relative Age Effect and Success in Elite U17 Soccer Teams. *Journal of sports sciences*, 29(9), 983-987.  
[2] Sherar, L. B., Baxter-Jones, A. D. G., Faulkner, R. A. & Russell, K. W. (2007). Do physical maturity and birth date predict talent in male youth ice hockey players. *Journal of Sports Sciences*, 25 (8), 879-886.



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**Modeling of Dry Friction**



## THEORETICAL AND EXPERIMENTAL MODELLING OF THE COMBINED DRY FRICTION EFFECTS

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It is presented a new approach for dry friction modelling under conditions of combined kinematics. The main distinguish feature of this approach is building of the multi-component dry friction models [1-8] which are suitable for using in differential equations of motion templates.

The procedure of the models constructing consists of the two parts. In the first part, the exact integral expressions for the net vector and torque are formed with the assumption that Coulomb's friction law in classical [1-5, 7] or generalized [6, 8] differential forms is valid at each point of the contact area. In addition, in process of the exact integral models construction there are used well known results from the theory of elasticity that tangent stresses lead to shift in the symmetric diagram of the normal contact stresses in the direction of the instantaneous sliding or rolling velocities [9]. To use the theory of elasticity results in the dynamics problems, it is proposed the simple asymptotic representations for the contact stresses distributions based on their general properties known from the theoretical results of the theory of elasticity [4-8].

In the second part the exact integral models are replaced by appropriate Pade expansions or Zhuravlev [7] approximations. These replacements substantially simplify the combined dry friction modeling, making the calculation of double integrals over the contact area unnecessary. Another advantage of proposed models is obviating a necessity to solve the problem of the theory of elasticity and exactly define the boundaries of area of contact. Unlike available models, the proposed dry friction models enables as well to describe the relationship between force and kinematical characteristics by smooth analytical functions over the entire range of angular and linear velocities as to take into account the more realistic representation about normal contact stresses distribution. The approximate models preserve all properties of the models based on the exact integral expressions and correctly describe the behaviour of the net vector and torque of the friction forces and their first derivatives at zero and infinity. Moreover, the models coefficients are numbers that can be identified from experiments. Consequently, these models may be considered as phenomenological models of the combined dry friction.

It is presented experiments on the verification of the sliding and spinning dry friction models [10]. It is described the experimental stand developed for the checking of these models. Installation allows to measure simultaneously both friction force components and friction torque at rectilinear sliding of rubbing solids at the presence of spinning for the various contact areas forms. The installation parameters permit to make experiments for a wide range of the kinematics parameters changing at the various values of the normal pressure. It is described the procedure of the experiments carrying out and the received results which are brightly demonstrate correctness of the theoretically developed multi-component dry friction theory.

- [1] Zhuravlev V.Ph., *The Model of Dry Friction in the Problem of the Rolling of Rigid Bodies*. Prikl. Mat. Mekh., 62(5) (1998), 762–767.
- [2] Kireenkov, A.A. *On the Motion of a Homogeneous Rotating Disk along a Plane in the Case of Combined Friction*. Izv. Akad. Nauk. MTT. 1 (2002), 60–67.
- [3] Zhuravlev, V.Ph.; Kireenkov, A.A.: *Pade Expansions in the Two-Dimensional Model of Coulomb Friction*. Izv. Akad. Nauk. MTT. 2 (2005), 3–14.
- [4] Kireenkov, A.A.: *Coupled Models of Sliding and Rolling Friction*. Doklady Physics, 53(4) (2008), 233–236.
- [5] Kireenkov A.A. *Combined model of sliding and rolling friction in dynamics of bodies on a rough plane*. Izv. Akad. Nauk. MTT. 3 (2008), 116-131.
- [6] Kireenkov, A.A. *Generalized two dimensional model of the sliding and spinning friction*. Doklady Physics. 55(4) (2010), 186–190.
- [7] Andronov, V.V.; Zhuravlev, V.Ph.: *Dry Friction in Problems of Mechanics*. R&C Dyn., Mosc.-Izhev., 2010.
- [8] Kireenkov, A.A.: *Coupled Model of Sliding and Spinning Friction*. Doklady Physics, 56(12) (2011), 626–631.
- [9] Goryacheva, I.G.: *Mechanics of friction interaction*. Nauka, Moscow, 2001.
- [10] Kireenkov A., Filatov V. *Experimental investigation of the three-dimensional dry friction*. In: Dynamical Systems. Nonlinear Dynamica and Control. Lodz, December 5-8, 2011, 441-446.

## REGULARIZATION OF A DISK IN A FRICTIONABLE WEDGE

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**Introduction.** We consider, in two dimensions, a disk placed between the two walls of a fixed V-shaped wedge. We suppose that there is friction between the disk and the wedge. Let  $\mu$  be the coefficient of static friction between the disk and the wedge (at both walls).

We apply forces to the disk, and wish to know what happens. It turns out that if the coefficient of friction is small, then this can be determined, but if it is large, then for large forces one cannot determine whether the disk will continue to remain at rest or not.

This ambiguity is related to the fact that there are four unknown contact forces (a normal contact force and a frictional force at each wall), but only “three modes of motion” (horizontal, vertical, and rotational).

In this paper, we approach the problem by means of contact regularization—that is, treating the regions in contact as not completely rigid but just very stiff. More precisely, we regularize the wedge, while keeping the disk rigid.

**Relation to work done so far.** Examples of setups involving friction where “existence and uniqueness” of possible motions becomes problematic date back to Jellett [1] and Painlevé [2]. Some general theory has been formulated for such problems since then, but relatively little work has been done specifically on a disk in contact with two frictionable walls.

McNamara et al. [3] considered the disk-in-a-wedge problem, viewing it as a prototype for granular packing problems. They approached the problem by means of contact regularization, as in this paper. One of the main tasks of their paper was to demonstrate that, when switching from the rigid case to the regularized case, the indeterminacy of the rigid case is replaced by memory-dependent determinacy. In order to make this point, it was sufficient for them to use as simple a model as possible. One of the properties of this model was that the “normal stiffness” (governing the normal contact forces) and the “tangential stiffness” (governing the frictional forces while in the sticking state) were equal to each other.

Now in order to gain clearer insight into the seemingly indeterminate behaviour of the disk, we would ideally like to observe *uniformity* in the behaviour of the disk across some *variation* of the regularization of the wedge. Accordingly, in this paper, we use much the same regularization that McNamara et al. used, except that we do *not* restrict the two stiffnesses to being equal. Nonetheless, under certain conditions, we obtain formulae for how the contact forces vary over time while in the sticking state, and these formulae make no reference to any regularization parameters but only to concepts which make sense in the rigid case. (This said, we still do need, for our study, that the ratio of the larger stiffness to the smaller stiffness is not *too* extreme.)

**Findings.** We work with a “linear” regularization of the wedge. This means that, while in the sticking state, the normal contact forces and frictional forces acting on the disk behave like Hookean springs. We also need that the two walls of the wedge are made of the same material as each other, i.e. have the same regularization.

Perhaps our strictest requirement is that the forces which we apply to the disk have a vector total that is *perpendicular* to the axis of symmetry of the wedge. We also require that, as functions of time, they are bounded and sufficiently regular.

The regularized case must approximate the rigid case. This fact gives us three (approximate) equalities for the four unknown contact forces. We cannot find a further constraint on the contact forces themselves, but (as the paper by McNamara et al. suggests) if we know the *initial values* of the contact forces, then it is sufficient to find a further constraint on the *changes* in the contact forces. The symmetry of wedge and the “antisymmetry” of the applied forces about the axis of symmetry of the wedge turn out to provide this further constraint.

[1] Jellett J. H.: *A Treatise on the Theory of Friction*. Hodges, Foster, and Co., Dublin, 1872.

[2] Painlevé P.: *Sur le lois du frottement de glissement*. Comptes rendus de l’Académie des Sciences (Paris), 1895, 121: 112–115.

[3] McNamara S., García-Rojo R., Herrmann H.: *Indeterminacy and the onset of motion in a simple granular packing*. Physical Review E, 2005, 72: 021304.

# INFLUENCE OF KELVIN-VOIGT DAMPING ON THE EXISTENCE AND STABILITY OF TRAVELLING WAVE SOLUTIONS

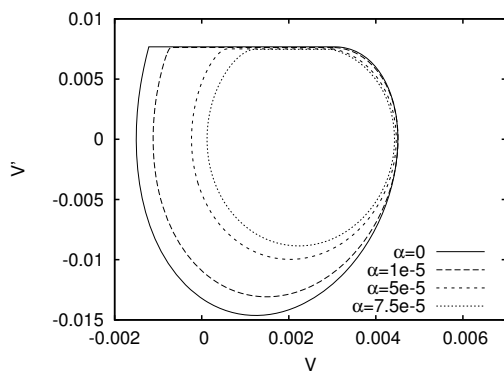
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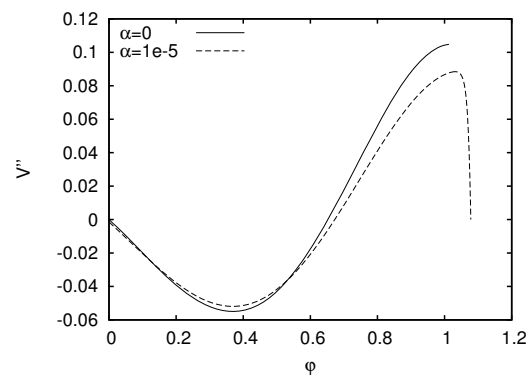
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**Introduction.** We consider a simple model of a brake, a rigid shaft rotating in an elastic cylinder. Due to the frictional contact between these bodies stick-slip travelling waves occur; also separation zones are possible, if the pressure between the bodies is small. Numerical investigations show, that these travelling waves are mostly unstable, which causes quasiperiodic and chaotic dynamics.

In this talk we investigate the influence of viscous damping on the existence, shape and stability of the travelling wave solutions more closely. Preliminary calculations indicate, that the smoothing effect may stabilize the travelling waves against the Hopf bifurcation, but it also can destroy the travelling waves in a grazing bifurcation and force steady state solutions.



Phase portraits of 4-mode stick-slip waves with and without damping.



Tangential acceleration of 4-mode solutions with and without damping.

The presence of the damping terms also changes the structure of the differential equations for the travelling waves by introducing a small leading coefficient. This singular perturbation also has smoothing effects at the transitions between the different solution regimes.

- [1] Nguyen, Q. S., Oueslati, A., Lorang, A. (2004): Brake Squeal: A Problem of Dynamic Instability and Stick-Slip-Separation Waves? *Proceedings of the EUROMECH 457, S. Bellizzi et al (eds.) Press of the ENTPE, Lyon, 99-102*
- [2] Nguyen, Q. S., Oueslati, A., Steindl, A., Teufel, A., and Troger, H. Travelling interface waves in a brake-like system under unilateral contact and Coulomb friction. *COMPTES RENDUS MECANIQUE*, 336:203-209, 2008.
- [3] Steindl, A.: Bifurcations of Stick-Slip-Separation Waves in a Brake-like System *Proc. Appl. Math. Mech.* 6, 337-338 (2006), DOI 10.1002/pamm.200610150

# STICK-SLIP TRANSITION APPEARING IN A DISK-BALL SYSTEM

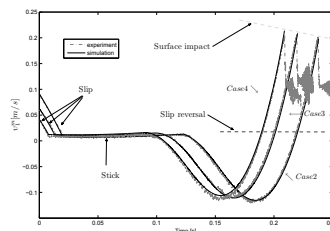
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**Introduction.** General features of systems with multiple frictional contact/impacts are the strongly non-linear nature of the dry friction, multi-scale effects coupled in systems, and the singularities induced by simplified models. In general, the process of modeling such systems is related to developing an appropriate way of properly dealing with the nonlinearity of friction, efficiently reckoning the effects from the coupled multiple scales, and reasonably avoiding the singularities appearing in the model. In this paper, an experimental apparatus relating a disk-ball system is established for providing experimental observation. The measurements for the motion of the system are implemented by two laser vibrometers. In terms of the theory proposed for dealing with the problems of mechanical systems with multiple frictional contact/impacts points, numerical analysis are carried out to obtain the initiated states for the motion of the disk after impacts, and then to track the time history of the instantaneous velocities at two measured points on the disk surface. Good agreements between numerical results and experimental observation present a powerful support for the theory of multiple impacts, in which the multi-scale process involved in impacts is analyzed in an impulse-energy level, and the intrinsic discontinuity of dry friction relating the stick-slip transition is not smoothed artificially.

**Basic idea for the theory of multiple impacts with friction.** The problem of Multiple impacts refers to the situation where several contact points take simultaneously part into impacts. Basically speaking, it belongs to a singular problem in rigid body dynamics, partly because the post-velocities of the system after impacts cannot be uniquely determined only by combining the momentum theorem with a simple impact law, something like the coefficient of restitution conventionally used in shock dynamics. The main idea relating the theory of frictional multiple impacts is summarized as follows:

- Adopting a compliant model to represent the transformation between the kinetics and potential energies at contact points, such that the normal contact force at each contact point can be expressed as a function with respect to the potential energy accumulated during impacts.
- Combining with Coulomb's friction law, the dispersion of energy during impacts is reflected by ratio matrices, both of them are functions relative to the potential energy accumulated at contact points
- Introducing the basic assumptions of shock dynamics, the multiple impacts dynamics are converted into a set of impulsive differential equations with respect to a unique normal impulse, which is an independent time-like variable adopted to drive the numerical simulation.
- The potential energy are updated dynamically based on the relative normal velocities at contact points, and modified by using a coefficient related to the transformation efficiency between the potential energy and the work done by the normal contact forces.
- The end of an impact is distinguished by the potential energy, and multiple impacts finish when no potential energy exists at all contact points.



The horizontal velocities of the disk at the gauged point

**Conclusion.** With the help of the disk-ball system, this paper propose a general theory for dealing with the problem of a mechanical system with multiple contact/impacts. By setting the impacting position spanning the symmetry axis of the disk surface, a comprehensive investigation for the various states of the disk initiated by impacts indicates that the results from numerical analysis can be fully accordant with the experimental observation, as shown in the figure for the part of the results relating the horizontal velocities at a gauged point near to the contact point.



## FRICTION IN CURLING GAME

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**Introduction.** There exist different approaches to determination of friction forces, acting on moving bodies. Straightforward “physical” methods are based on certain equipment: dynamometers, sensors etc. On the contrary, “dynamical” methods use the simplest devices only, such as a clock and a ruler. Starting from Newton-Euler equations, one measures distances, (angular) velocities and accelerations and thus calculates acting forces, including friction. For instance, Euler used (1748) this idea to measure the coefficient of friction in the problem of rigid body, sliding downwards an inclined plane. Equations of motion in this example are

$$\ddot{s} = g(\sin \alpha - \mu \cos \alpha), \quad (1)$$

where  $s$  is driven distance,  $\alpha$  is the inclination angle, and  $g$  is acceleration of gravity; the coefficient of friction  $\mu$  to be determined. Measuring  $s(t)$ , we can determine  $\mu$  from eq. (1). Euler found that  $\mu = \text{const}$ , but further investigations of Stribeck (1902) showed that in the presence of lubrication (which may be caused by melting of micro-juts at high velocity)  $\mu$  depends on  $v = \dot{s}$ . In this paper, we discuss more general case where a body with flat base slides with rotation (spinning) upon a horizontal plane. .

**Idea of dynamical consistency.** In the case of planar motion, simple collinear system (1) is substituted by the following three-degree of freedom system:

$$m\ddot{x} = X + T_x, m\ddot{y} = Y + T_y, (J\omega)^\bullet = M + M_T + M_N, \quad (2)$$

where  $m, J$  are the body mass and inertia tensor,  $X, Y$ , and  $M$  are components of active forces and their momentum,  $T_x, T_y$ , and  $M_T$  are components of friction forces and their torque,  $M_N$  is the torque of normal stresses,  $\omega$  is angular velocity. To calculate friction terms in eqs. (2), one should specify local law of friction in the form

$$\vec{T}(A) = -\mu(A) \frac{\vec{v}(A)}{v(A)} N(A) \quad (3)$$

with point  $A$  belonging to contact area  $D$ ; function  $\mu(A)$  might be constant or depend on kinematical and/or dynamical quantities. The global values  $T_x, T_y$ , and  $M_T$  are calculated by integration of formula (3) through the contact area  $D$ . To implement this integration, it is necessary to set the distribution of normal stresses  $N(A)$  in area  $D$ . We adopt linear dependence

$$N(A) = p_0 + p_1 x(A) + p_2 y(A) \quad (4)$$

where the coefficients are determined uniquely by the condition that  $v(A)$  is parallel to the basement for any  $A \in D$ . This is idea of dynamical consistency: given local friction law (3), we can uniquely determine global values  $T_x, T_y$ , and  $M_T$ .

**Deviation of the trajectory of cylinders.** If the body is axial symmetric, the following properties are proven.

*Proposition 1.* In the absence of external forces (except gravity) i.e.  $X = Y = M = 0$ , for any local friction law the following relation is valid:

$$\vec{M}_N = h(-T_y, T_x) \quad (5)$$

where  $h$  is the distance between the base plane and the mass center.

*Proposition 2.* In case  $\mu = \text{const}$  the trajectory deviates to the right (for anti-clockwise rotation of the body).

*Proposition 3.* If coefficient  $\mu(A)$  is any function of  $v(A)$ , and spinning is not too fast (i.e. the instant centre of velocities lies outside the base), then the trajectory deviates to the right. For fast spinning and ring contact area, deviation to the left is possible.

The curling stone has a ring base and moves upon ice. It is known that this device deviates (curls) to the left for angular velocities being not too fast. According to Prop.1-3, this means that the coefficient of friction must depend on some additional characteristics. Numerical analysis was performed which shows satisfactory explanation of deviation phenomena with the help of Hersey-Gümbel number which is proportional to the sliding velocity and inversely proportional to the normal load.

# GAUSS' PRINCIPLE AND PRINCIPLE OF LEAST CONSTRAINTS FOR DISSIPATIVE MECHANICAL SYSTEMS

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The aim of this work is to formulate the Gauss' principle and the principle of least constraints for dissipative systems. For dynamics, where the evolution requires the determination of the accelerations of the system, it is shown that in the presence of dissipative force laws a similar principle holds, which requires the augmentation of the optimization problem of least constraints by the time rate of change of the total dissipation. The principle of Gauss has been published in (3) by Gauss and provided a variational criteria on admissible accelerations of bilaterally holonomically constraint mechanical systems. The principle of maximal dissipation was introduced by Moreau in (4) solely for single point frictional contacts. The principle considers the friction as maximizing dissipation over all feasible friction forces at a contact. In this work, for mechanical systems with tresca-type of friction following extended problem of least constraints is proposed:

$$\min_{\dot{\mathbf{q}}^+} \frac{1}{2} \langle \dot{\mathbf{q}}^+, M\dot{\mathbf{q}}^+ \rangle - \langle \mathbf{h}, \dot{\mathbf{q}}^+ \rangle + \dot{P}_D, \quad (1)$$

with  $M$  being the symmetric and positive-definite mass matrix and  $\mathbf{h}$  a continuous function of the generalized positions and velocities of the mechanical system and  $\dot{P}_D$  is the total time rate of change of the total dissipation function. Here  $\dot{\mathbf{q}}^+$  is the right-continuous generalized acceleration, which is the acceleration in the imminent future. Though the distinction between Tresca and Coulomb type dry friction is made regularly in literature, there is no common view on how these friction laws differ from each other. In this work, Tresca type dry friction is seen as a friction law of which normal contact force is independent of future generalized accelerations at a given position and generalized velocity of the system contrary to Coulomb friction. Already in (1) by Pozharitskii the spatial friction force model of tresca-type on acceleration level as well as friction acceleration potentials are used without definition, in order to extend the principle of Gauss to systems with dry friction.

The principle of Gauss for mechanical systems with tresca type of dry friction is shown to be related to the time-rate of change of the total dissipation. The new principle can be extended to include general dissipative force laws, which derive from convex potentials. This relation is accomplished by making use of the most general definition of dissipative forces and applying the methods and techniques of nonsmooth analysis. The relation of  $\dot{P}_D$  to the dual principle of least constraints is presented in (2).

- [1] Pozharitskii, G. K.: *Extension of the Principle of Gauss to systems with dry (Coulomb) friction*. Journal of Appl. Math. and Mech. , 25 (3) (1961), 586–607.
- [2] Yunt K.: *On the Relation between the Dual Principle of Least Constraints and the Principle of Maximal Dissipation*. In: Proc. of the 7th WSEAS Int. Conf. on Applied and Theoretical Mechanics, Montreux, 2011, 75–80.
- [3] Gauss, C. F.: *Über ein neues allgemeines Grundgesetz der Mechanik*. J. Reine Angew. Math., 4 (1829), 232–235.
- [4] Moreau, J. J.: *On unilateral constraints, friction and plasticity*. In: New variational Techniques in mathematical Physics, 1973, 172–322.

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# MODELING OF ETHERNET AVB NETWORKS FOR WORST-CASE TIMING ANALYSIS

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**Introduction.** Ethernet is currently explored as the upcoming network standard for distributed control applications in many different industries such as automotive, avionics and industrial automation. It offers higher performance and flexibility over traditional control bus systems such as CAN and ProfiBus. For distributed control applications, predictable communication timing is highly important which can be problematic using standard Ethernet. The new Ethernet AVB standard aims to improve this by a new scheduling algorithm based on priorities and traffic shaping. However, the current AVB standard lacks formal latency guarantees which are required for safety-critical control applications. As a solution to this, we present a model for Ethernet AVB networks and a transformation into a timing model. Based on the timing model, we apply a compositional performance analysis (CPA) approach known from the analysis of distributed real-time systems (see e.g. [2]) to derive worst-case timing properties and hence latency guarantees for the original Ethernet AVB network, similarly to [1] for classical Ethernet. Our extension is the derived formalism which covers the scheduling properties of Ethernet AVB.

**Models and Model Transformation.** For the modeling of Ethernet AVB networks, we use a domain-specific model. The main components are *switches* and *nodes*, which are interconnected through *ports* to form the network topology. *Targets* describe traffic streams by source and destination nodes and the parameters of the worst-case packet injection behavior (e.g. minimum period and maximum packet size). The compositional performance analysis relies on a timing model, which consists of a set of *tasks* processed by *resources*. For the tasks, formal and conservative characteristics are assumed, such as bounds on the task execution time. Tasks are activated by events which can originate from an external source, such as a timer interrupt, from other tasks via inter-task communication. Events are modeled using arrival curves which capture all possible event arrival sequences. The domain-specific Ethernet AVB model can be transformed into a CPA timing model. To model the dynamic delay due to contention on the output ports of Ethernet switches, we map each output port to a scheduling resource. The transfer of a frame over multiple hops is then captured by a chain of tasks mapped to the resources corresponding to the output ports passed by the frame. Event models are derived from the parameters of the packet injection. The model transformation is unidirectional, but the analysis results from the timing model can be back-annotated into the Ethernet AVB model. The transformation process covers all possible Ethernet AVB network configurations.

**Worst-Case Timing Analysis of Ethernet AVB.** With the model transformation described above, we have obtained an analyzable timing model of an Ethernet AVB network. However, no existing resource analysis matches the behavior of Ethernet AVB, so we require new formulas to compute e.g. the upper bounds on the worst-case response time. In principle, the AVB switch follows a static-priority non-preemptive schedule (SPNP) for which analysis formulas exist. However, the traffic shaping applied in Ethernet AVB requires an extension of the standard SPNP analysis. Furthermore, Ethernet allows different streams with the same priority being scheduled in FIFO ordering which requires an extension similar to the analysis of earliest-deadline-first (EDF) scheduling. In order to derive the worst-case delay observed by a specific frame, we decompose the possible delays by their originators: The *transfer time* is determined by the network speed only and includes no blocking. *Blocking* can occur from other frames of *lower, same or higher priority*, for which individual upper bounds can be derived. Further blocking originates from the *traffic shaper* which occurs if previous transfers have used up the credits for a specific traffic class. The paper includes a detailed formulation of the individual terms.

**Experimental Evaluation and Conclusion.** We have implemented the presented Ethernet and CPA models, the model transformation and the analysis in Python. For evaluation, we have modeled a simple industrial automation network. We compare the latency bounds for the system assuming (a) standard Ethernet (only priorities) and (b) Ethernet AVB with additional traffic shaping. We observed that standard Ethernet allows tighter latency bounds than Ethernet AVB for high-priority streams due to the added latency of traffic shaping. Nevertheless, we demonstrate that our approach is capable of deriving worst-case bounds on the latency of Ethernet AVB. This way, formal guarantees on the timing of Ethernet AVB streams on the system level can be obtained which enables the use of such networks in real-time critical embedded systems.

- [1] Jonas Rox and Rolf Ernst. Formal timing analysis of full duplex switched based ethernet network architectures. In *SAE World Congress*, volume System Level Architecture Design Tools and Methods (AE318). SAE International, Apr 2010.
- [2] Simon Schliecker, Jonas Rox, Mircea Negrean, Kai Richter, Marek Jersak, and Rolf Ernst. System Level Performance Analysis for Real-Time Automotive Multi-Core and Network Architectures. *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, 28(7):979–992, July 2009.

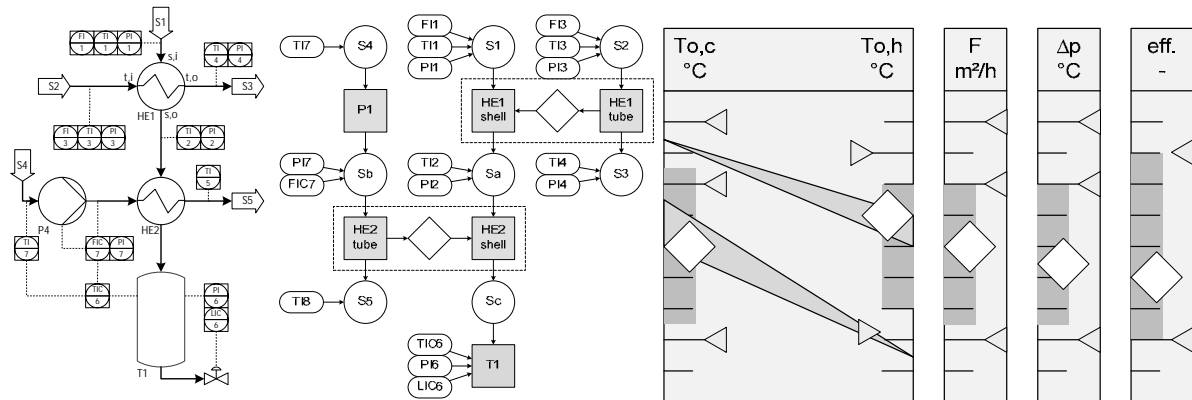
# FORMAL MODELS FOR HIGH PERFORMANCE HMI ENGINEERING

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Engineering of Human Machine Interfaces for supervisory control in process industries can be characterized as an information integration task. This is particularly true for configural displays that are the core element of high performance HMI. Design and parameterization of these display units requires a large amount of data, usually readily available in the process design databases but missing in the engineering systems for the automation systems. This class of displays also requires further information that is not yet made available in any database or is not formal enough to provide a base for model driven HMI engineering approaches. Unfortunately the research area of ecological interface design did not address the aspect of engineering efficiency up to now.

To overcome this shortcomings, we designed a formal graph-theoretic model of chemical process plants that makes it possible to automate the before mentioned information integration task for predefined templates. The model is an extension of a previously developed model for the automated generation of simple mimics displays from P&ID data [1]. Besides the topology and mereology of the process design, the model addresses the abstraction-decomposition space of ecological interfaces by a simple hierarchical HMI level model.



This allows for task specific assemblies of process data and provides basic means to integrate standard mimics and complex displays. However, because the information integration is the core feature of configural displays, the formal basis for model based HMI engineering needed to be enhanced substantially. This paper presents the resulting core model and a graph-based search algorithm. The algorithm makes it possible to parameterize a certain set of configural displays directly from engineering data.

- [1] Urbas, L. and Doherr, F. autoHMI: a model driven software engineering approach for HMIs in process industries. In Proc. IEEE Int. Conf. Computer Science and Automation Engineering, 3, 627–631. 2011

# EVALUATING DOMAIN SPECIFIC LANGUAGES FOR THE DEVELOPMENT OF OPC UA BASED APPLICATIONS

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The OPC Unified Architecture (OPC UA) [2] is becoming more and more important for industrial automation products. It is a central component to modern industrial applications. The classic OPC (OLE for Process Control) specification is successfully applied for accessing and distributing data in industrial systems. With the more recent OPC Unified Architecture, new facilities like a unified address space, service oriented interfaces and an extensible information model have been introduced. This allows OPC UA to be used from small embedded systems, industrial controllers, Distributed Control Systems (DCS) up to Manufacturing Execution Systems (MES) and Enterprise Resource Planning (ERP) systems. OPC UA defines platform- and programming-language independent access to server-defined address spaces providing an object-oriented information model, based on a client-server-model.

The development of OPC UA components is currently supported by the use of special software development kits (SDKs) for OPC UA (for clients and servers). These SDKs provide APIs for developing code that deals with the creation and navigation in the OPC UA address space, registration of monitors for value changes, calling of defined methods as well as connection and session handling. However, one of the largest drawbacks of working directly with these APIs is the poor type safety support. Code that accesses the address space has to deal with node identifiers or browse names that are mostly passed as string variables. During design time it is therefore not checked if the specific nodes and/or variables that code accesses actually exist in the used address space. Furthermore, code that e.g., builds up queries or filters against the address space is very lengthy and not clearly structured. This leads to error prone code and thus additional test effort that needs to be spent while developing these central components.

The OPC specification already proposes that higher level languages such as a graphical address space modelling language [4] may be used to efficiently develop OPC UA applications. With current Domain Specific Language (DSL) tools it is possible to create extensive editor support for such a language. This includes - e.g., for textual languages - syntax highlighting, error recognition, code completion and many other productivity enhancing features. However, apart from the already mentioned graphical modelling of address spaces no DSL support is given by currently available OPC UA SDKs.

The contribution of this paper is to evaluate the feasibility of creating productivity enhancing development tools based on DSL engineering for the use with OPC UA. The use of such tools would improve developer productivity and reduce test efforts when developing OPC UA based applications. We identify use cases in OPC UA application development in which DSLs might unfold their strengths. Based on these use cases, another key question that is answered by this paper is whether internal DSLs or external DSLs [1] are more suitable for the given task. Internal DSLs are based on a host language and add additional language constructs to that language which are in a compile step mapped towards structures of the host language. Language Integrated Queries (LINQ) [3] in MS Visual Studio are an example for such an internal DSL. On the other hand there are external DSLs where the DSL is a standalone language. Based on this language then also lower level constructs can be generated.

Creating an OPC UA based application may consist of several tasks, starting from the definition of an address space up to the creation of subscriptions to events including complex event filters. Many of these tasks deal with the underlying semantic model [4] of OPC UA, i.e. the specific metamodel that it defines. Hence, making it a good target for DSLs to support the development of these tasks.

We identify the type of language along two dimensions: Whether they are considered to be internal or external (cf. [1]) and what kind of concrete syntax they would provide (graphical, textual, tabular, etc.). Additionally, we mark those use cases where view-based modeling seems reasonable to reduce the clutter within the language. Furthermore, we rate the potential impact on development efficiency of the DSL. This estimate is based on discussions with experienced OPC UA developers/users. To be able to relate the creational effort to the benefits for each language we also rate the effort for defining and implementing the respective DSL.

[1] Martin Fowler. *Domain-Specific Languages*. Addison-Wesley Professional, 2010.

[2] W. Mahnke, S.H. Leitner, , and M. Damm. *OPC Unified Architecture*. Springer Press, 2009.

[3] Microsoft. LINQ: .NET Language-Integrated Query. <http://msdn.microsoft.com/library/bb308959.aspx>, 2007.

[4] OPC Foundation. OPC UA Specification: Part3 - Address Space Model. <http://opcfoundation.org/>, 2010.

## TEST-CASE GENERATION FOR THE VALIDATION OF INTEGRATED AUTOMATION SYSTEMS ENGINEERING ENVIRONMENTS

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Nowadays large-scale engineering projects (such as e.g., power plants or car manufacturing plants) typically involve a broad range of engineering disciplines, which rely on their specific engineering tools and engineering systems to manage their specific engineering processes. For realizing and managing such complex projects a cooperation of all disciplines is required to form an integrated engineering system. However, error-prone and time-consuming human work, such as manually copying information from one tool to another, is often needed to handle integration concerns at the interfaces of engineering disciplines and to configure the integration platform on the technical detail level, which is typically focused on a single technology or vendor. The configuration of such system integration technologies is a complex task requiring high manual effort and only doable by designated integration experts (IEs) or with appropriate domain knowledge. Manual work is needed to write scripts for transformations and connection purposes with existing integration solution in case engineering tools are added to or updated in this solution, resulting in high efforts to check whether an engineering tool is compatible with running engineering processes. Consequently, as knowledge regarding the overall system is captured in non-machine understandable documents, the outcome of the integration is only known at the end of the integration process. Biffi and Schatten proposed a platform called Engineering Service Bus (EngSB) [1] which integrates not only different tools and systems but also different steps in the software development lifecycle. The EngSB platform introduces the concept of tool domains that provide interfaces for solving a common problem, independent of the vendor-specific tool used. This is possible since different tools, developed to solve the same problem often provide at least similar interfaces [2]. This concept allows the EngSB to interact with a tool domain without knowing which specific tool instances are currently available. Tool domains do not implement tool instances but provide the abstract description of events and services, which have to be provided by concrete connectors of tool instances to the EngSB.

This paper describes a model-based concept which facilitates the derivation of test cases for introducing test methods at an early stage of the integration process. System integrators capture domain expert knowledge in ontologies which describes data models and functionalities of tool instances, tool domains, and restrictions regarding data model elements. Based on these captured information, system integrators are capable of deriving configurations and source code artefacts to create an overall technical integration solution by using a semi-automated model-driven configuration approach. The process derives a) tool connector source code templates with implementations of checks to verify whether all restrictions regarding the described data elements are fulfilled; b) tool domain interfaces and method calls; c) data model transformation instructions to translate data models of tool instances to the data model of the tool domain and between data models of tool domains; c) tests cases derived for tool instances by deriving test cases using the signature (e.g., method name, parameters, parameter types) of the tool domain. We evaluate the proposed concepts in an industrial use case in the context of manufacturing hydro power plants. First results show that the effort for the initial configuration of the integration solution is higher due to the need to capture domain expert knowledge in ontologies in comparison to manual configuration. However, in case of adaptations the effort is significantly lower as updates effects only the models. Furthermore, the validation of the integration solution is already performed during modelling and through the derived test cases executed immediately after the execution of the model-driven system configuration process. Nevertheless, the derived test cases are only capable to check the correct handling of data based on provided input and retrieved output values, rather than based on the real semantics of the method. Plausibility checks, which may be modelled in the ontology as well, are open to future research to address this limitation.

- [1] Biffi, S. and A. Schatten. *A Platform for Service-Oriented Integration of Software Engineering Environments*. in *Eight Conference on New Trends in Software Methodologies, Tools and Techniques (SoMeT 09)*. 2009.
- [2] Biffi, S., R. Mordinyi, and T. Moser, *Automated Derivation of Configurations for the Integration of Software(+) Engineering Environments*, in *1st International Workshop on Automated Configuration and Tailoring of Applications (ACoTA 2010)* 2010, IEEE Computer Society: Antwerp Belgium.



# INTEGRATED GRAPH TRANSFORMATIONS IN AUTOMATION SYSTEMS

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**Introduction.** A big part of the automation system engineering consists of the reconciling of engineering models. Hence, information from a source model is used to generate instances of a target model. For example, for each element in the plant and instrumentation diagram (P&ID) a corresponding representative is generated on the operator screen of the human machine interface (HMI). Most of those reconciliations follow simple rules. Nevertheless, due to the lack of tool support, most of the reconciliation is done manually. On the other hand, well studied transformation techniques exist. The main application of those techniques is the field of model driven development which is exactly the target application of automation system engineering. The paper combines the concept of model transformation with the help of triple graph grammars (TGGs) and the approach of an integrated rule-based system to gain a formal background for the model transformation at runtime of an automation system. It will be demonstrated that TGGs are suitable to formulate the transformation rules in automation system engineering and that the rules can be generated by the system engineer without additional knowledge. Further, the paper proposes the adaption of the existing rule-based system ACPLT/RE to the concepts of bidirectional TGG rules to benefit from the possibilities of the TGG concept for model transformation at runtime.

**Content.** As already demonstrated by [1] the availability of rule-based model transformation at runtime enables a set of new application fields for automation systems. Also if the rule-based model transformation inside of the automation system runtime environment could already demonstrate its feasibility (e.g. as introduced by Schmitz and Epple [2]) for those application fields, current approaches lack a formal background. Hence, formal requirements such as traceability, correctness and completeness can not be investigated. Due to this, the rule-based systems are not reliable enough for real-world applications. The paper closes the gap between model transformation at runtime and a formal description of the model-interrelationships by the use of the well-studied Triple Graph Grammar (TGG) approach. Introduced in [3], TGGs are an extension of Pratt's pair grammar approach from 1971. TGGs are a convenient way to integrate two domain-specific languages (DSLs) on a metamodel level.

Based on the TGGs concept the paper introduces a rule-based system for model transformation in an automation system runtime environment. We demonstrate that the rules are straight-forward adaptable to IEC-61131 function blocks. Due to limited space on automation system runtime environments the parametrization without additional space consumption is an important property. We reach this goal by taking advantage from the executability of function blocks. Instead of using an additional interpreter or even compiled rules for model transformations, the TGG rules themselves are parametrized and hence be executed as forward graph translators, backward graph translators and more.

On the one hand, the formal background to the model transformation in automation system runtime environments by the use of TGGs provides the foundation for a formal analysis of the transformation rules. This is a first step towards a certified consistency mechanism for automation system engineering based on the involved models. On the other hand, the integration of the TGG approach to model transformation into the runtime of an automation system can be used to engineer automation functions on the fly. This is of special interest where information needed for engineering is not available at the engineering phase yet. One example of such dynamic adaption of the automation system is the flow analysis, presented in the paper.

- [1] Tina Krausser, Gustavo Quirós, and Ulrich Epple. An IEC-61131-based Rule System for Integrated Automation Engineering. In *INDIN 2011*. IEEE, 2011.
- [2] Stefan Schmitz and Ulrich Epple. Automatisiertes Engineering leittechnischer Funktionen durch integrierte Regeln. In *EKA 2008*, pages 241–252. ifak, 2008.
- [3] A. Schürr. Specification of Graph Translators with Triple Graph Grammars. In G. Tinhofer, editor, *WG'94*, volume 903 of *LNCS*, pages 151–163. Springer, 1994.



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**Modelling and Simulation in and for  
Education**



# MMT – AN E-LEARNING SYSTEM BASED ON COMPUTER NUMERIC SYSTEM FOR TEACHING MATHEMATICS AND MODELLING

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**Introduction.** The MMT system constitutes a tool enabling e-learning of modelling and simulation in a user-friendly and unique way. It is a server with a collection of examples in many fields of mathematics and modelling being arranged in a variety of topics and offered in certain courses. The abbreviation MMT stands for Mathematics, Modelling and Tools.

The name implies that one of the things taught with the help of the MMT system is basic mathematics. In lectures for students of electrical engineering and geodesy and geomatics engineering the MMT environment is used to enable students the experimentation with examples out of Analysis and Linear Algebra to strengthen their understanding of the current subject in their lecture, see the impacts of the calculation in a graphical output wherever it makes sense and compare the computed results with their own ones.

The most important use of the MMT server lies in the support of teaching modelling and simulation for students of technical mathematics and computer sciences. To cover a wide field of modelling, the MMT examples concerning modelling and simulation are implemented using many different modelling approaches. By varying the input parameters of models students can find out in which way they affect the output of the simulation. To enable profound understanding of the models, all source codes are offered to be downloaded from the MMT and possibly modified and tried out on the student's own personal computer.

**Content.** This paper focuses on the new possibilities of modelling and simulation on the MMT server. To become acquainted with the MMT interface we give a short overview of the system before addressing certain examples. The first example shows a model implemented in Matlab consisting of one m-file. Since the MMT server has to interact with Matlab, the description of this MMT example concerns mostly the extraction of the input variables from the MMT system into the Matlab function and the creation of graphical and textual output on the MMT server.

One of the latest achievements within the MMT system has been the successful inclusion of examples accessing more than one m-file. This allows models to be way more complex and therefore students can be taught high-level modelling via the MMT system. To reach different fields of modelling like *physical modelling*, MMT examples using Simulink models have recently been embedded into the MMT system. The communication between the MMT server and the Simulink model is realised in a m-file exchanging the parameters and the output among the Simulink model and the corresponding MMT example.

The last part of the paper discusses the use of the MMT system in exams. This is realised by another e-learning platform, the moodle based TUWEL (Technische Universität Wien E-Learning System). Via this tool students are asked questions concerning the MMT examples already shown in the respective lecture. Then they have to follow a link to a certain MMT example and find out some specific data coordinates or input values for a given problem.

**Summary.** Apart from being a tool for teaching basic mathematics in lectures for students of electrical engineering and geodesy and geomatics engineering the MMT system has become important to enable e-learning of modelling and simulation and is used in various lectures about modelling and simulation offered by the Institute for Analysis and Scientific Computing. The variety of examples goes from simple models with only one Matlab function over complex ones with several m-files to models implemented in Simulink. All in all e-learning at Vienna University of Technology would not be possible in the way it is without the MMT system.

- [1] Andreas Körner, Irene Hafner, Martin Bicher, Stefanie Winkler, Felix Breitenecker, *MMT - A Web Environment for Education in Mathematical Modelling and Simulation*. ASIM 21. Symposium Simulationstechnik - Grundlagen, Methoden und Anwendungen in Modellbildung und Simulation, Winterthur, 2011.
- [2] Stefanie Winkler, Andreas Körner, Irene Hafner, *MMT – A web-based e-learning System for Mathematics, Modeling and Simulation using MATLAB*. In: 7th EUROSIM Congress on Modelling and Simulation, Prag, 2010, paper 231.
- [3] Andreas Körner, Günther Zauner, Günther Schneckenreither, *Ein e-learning System für MMT – Mathematik, Modellbildung und Tools, Systemerweiterung und Einbindung von graphischer Modellbildung*. 20th Symposium Simulation Techniques, Cottbus, 2009, 87-94.

# A MATLAB BASED PETRI NET TOOL FOR E-LEARNING: EXAMPLES FOR TIMED SIMULATION AND SCHEDULING

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**Introduction.** The MMT-web server is a part of the E-learning infrastructure at Vienna University of Technology, which enables students to get basic insight into the field of simulation and modelling in a user-friendly way. Main model parameters of examples can be adjusted and the parameter effects can be observed. Most examples on the MMT server are implemented in Matlab and recent developments include the ability to implement complex examples by various Matlab modelling and simulation toolboxes, including Simulink and Simscape.

An increased interest in discrete-event and hybrid systems motivated the investigation of possible implementation of Petri net based examples on the MMT server. Petri nets are widely used modelling formalism for description of discrete-event systems with highly parallel and cooperating activities. Therefore an object oriented Matlab based Petri net kernel was implemented that can be used to implement simple examples within MMT server environment.

**Petri nets and Petri net classes** Petri nets were initially introduced in the form of Condition/Event Systems with only binary markings and simple arcs. Later a number of modifications of the basic system model was introduced, including integer markings and weighted arcs. The resulting Place/Transition Petri nets became a central model, which is well explored in terms of analysis and synthesis techniques [3]. The basic Place/Transition Petri net model can be extended in different ways, leading to other Petri net classes.

The concept of time is not explicitly given in the original definition of Petri nets. For many practical applications, execution times have to be considered. Therefore various authors extended Petri nets with time representation, e.g. firing durations, holding durations and enabling durations. Coloured Petri nets enable to distinguish among tokens based on an assigned attribute, which is called colour. This way the structurally complex P/T Petri net models can be represented in a compact form, while preserving the model behaviour. A definition of simple Coloured Petri nets (CPN) without transition guards can be derived by folding places and transitions of the P/T Petri net [1]. If a token count of a place is replaced by a token quantity, firing of a transition only removes a fraction of the token quantity from its input places. The token flow through firing transitions becomes continuous. Much of the research deals with basic timed continuous Petri nets (CCPN) where maximal firing speeds are constant [2].

**Matlab implementation** The previously developed PetriSimM Petri net toolbox [4] is based on Matlab graphical user interface with callbacks to a number of m-script functions. The specifics of MMT server environment as well as improved object oriented programming support in recent versions of Matlab motivated the development of a new object oriented toolset, which can be used to build, analyze and simulate Petri net models in a script based manner without a dedicated user interface.

Different Petri net classes naturally map to object classes in the software implementation of the developed toolset. All classes are based on an abstract APetriNet object class in order to standardize basic Petri net properties and methods. Two basic sub-classes are PTPetriNet, which implements Place/Transition Petri net class and CPetriNet, which implements simple coloured Petri net class. HDPetriNet and EDPetriNet represent two classes of timed Petri nets, with implementation of holding duration and enabling duration time principle, respectively. CCPetriNet implements a version of continuous time Petri nets, and CTPetriNet implements a timed version of Coloured Petri nets, also applying holding duration time principle.

**Examples** A set of testing examples was implemented to check the performance of the developed toolset in combination with MMT server. Due to limited interaction with the user and the lack of animation capabilities the examples were chosen, which result in a series of markings that can be simply plotted in a Matlab figure.

The timed simulation example tends to illustrate the simulation of a Petri net employing holding duration time principle. It also illustrates the notion of conflict in Petri nets, possible conflict resolution strategies and corresponding effects on marking evolution of the timed Petri net. The scheduling example illustrates a classical job-shop scheduling problem. The goal is to optimize the processing order of a number of jobs on a number of machines in a way to minimize the total processing time, i.e., the makespan.

- [1] F. Basile, C. Carbone, and P. Chiacchio. Simulation and analysis of discrete-event control systems based on Petri nets using PNetLab. *Control Engineering Practice*, 15:241–259, 2007.
- [2] R. David and H. Alla. *Discrete, Continuous and Hybrid Petri Nets*. Springer, 2005.
- [3] T. Murata. Petri nets: Properties, analysis and applications. *Proc. IEEE*, 77:541–580, 1989.
- [4] G. Mušič, T. Löscher, and D. Gradišar. An open Petri net modelling and analysis environment in Matlab. In *Proc. of the International Mediterranean Modelling Multiconf.*, pages 123–128, Barcelona, Spain, 2006.

# AN E-LEARNING COURSE OF MODELLING FOR CONTROL DESIGN PURPOSES

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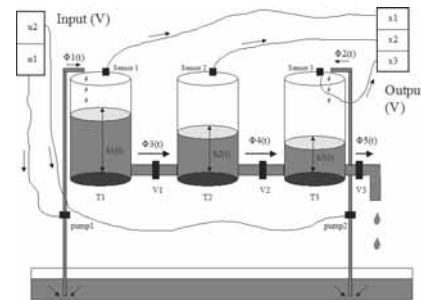
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**Introduction.** The great majority of EU countries are introducing the so called Bologna study (common studies structure in EU), where Slovenia and Austria are no exception. The results of such study organization are also a comparable studying programs where students', as well as teaching staff mobility are encouraged. Taking into account developing technologies also the aspects of e-learning are becoming more and more important. Intensive efforts have already resulted in effective solutions regarding individual institutions [1-4], but now attention is directed also to the possibilities of sharing teaching lectures, devices and/or experimenting systems. In this way studying efficiency can be improved while in the same time also the cooperation among different scientific and educational institutions can be intensified. Modelling for control design purposes of three tank system (Fig. 1) is a result of a close cooperation between the Faculty of Electrical Engineering, University of Ljubljana (Laboratory of Modelling, Simulation and Control and Laboratory of Autonomous Mobile Systems) and the Vienna University of Technology (Institute of Analysis and Scientific Computing). The goals of the project were: further development and extensions of the MMT-System, development of remote and virtual experiments and projects in E-CHO Learning Management and Content Management System, analysis of system properties regarding the development of virtual and/or remote experimenting environment, analysis of cooperation possibilities through (mixed) student projects.

**Modelling Process.** The system under consideration is schematically presented in Fig. 1.

The process, which is located at the Faculty of Electrical Engineering, University of Ljubljana, consists of three plexiglass cylindrical tanks and beyond them a collecting water pond is located. Out of this basin water can be pumped into the left or the right tank. Two water pumps which can be controlled using voltage signal in the range of  $\pm 10V$ , are therefore system's actuators. Water levels can be measured in all three tanks by corresponding sensors. These signals are also in the same voltage range. The system is equipped with six manual valves with which different operation conditions can be realized. As this process is also highly nonlinear one it enables the development of different model presentations suitable for simple and more demanding control design purposes.



**Fig. 1:** Three tanks system - Amira DTS 200

**MMT platform.** At Vienna University of Technology, Institute of Analysis and Scientific Computing the so called MMT - a web-based e-learning system for mathematics, modelling and simulation is developing. It is using MATLAB and SIMULINK which means it is very suitable also for developing education experiments for presented process. Experiments can be developed in such manner that first only one tank is included into observation (by closing valve  $V_1$ ). When using only the first pump such process is operating as single - input, single - output system. If later on also the second and the third tank are included, multi - input, multi - output (MIMO) design control problem with cross couplings can be observed.

- [1] Atanasijević-Kunc M., Logar V., Karba R., Papič M., Kos, A. *Remote multivariable control design using a competition game*. IEEE Trans. Ed., Feb. 2011, Vol. 54, No. 1, 97-103.
- [2] Logar V., Atanasijević-Kunc M., Karba R., Papič M., Bešter J. *E-learning game using virtual and remote laboratory environment*. In: Preprints of the 6th Vienna Conference on Mathematical Modelling, 2009, Vienna University of Technology, Austria. MATHMOD Vienna 09 : proceedings, (ARGESIM Report, no. 35). Vienna: ARGESIM, cop. 2009, 2100-2105.
- [3] Körner A., Hafner I, Bicher M., Winkler S., Breitenecker F. *MMT- A Web Environment for Education in Mathematical Modelling and Simulation*, ASIM 2011.
- [4] Winkler S., Körner A., Hafner I. *MMT - A web-based e-learning System for Mathematics, Modeling and Simulation using MATLAB*, In: Preprints of EUROSIM Congress, Prague, Czech Republic, 2010, paper 231.

# BCP - A BENCHMARK FOR TEACHING STRUCTURAL DYNAMICAL SYSTEMS

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**Introduction.** Since 2000, the relatively old CSSL standard (Continuous System Simulation Language) for simulation of continuous systems has become obsolete and new standards and techniques for system simulation are arising. At *modelling level*, object-oriented modelling or component-based modelling has introduced a new era for multi-domain modelling of physical systems (physical modelling). With Modelica [1] and with competitive VHDL-AMS, modelling languages with a certain standard have emerged using component-based modelling with acausal relations.

From a *mathematical viewpoint*, instead of classical explicit state space descriptions with an ODE system, physical modelling techniques very often result in (semi-) implicit differential-algebraic equation systems (DAE). The additional algebraic equations emerge new problems, which relate to the *simulation level*. As a consequence, the simulator must either be capable of automatic symbolic 'extension' of the system (index reduction) or the model description has to be split into different models where algebraic conditions control switching between these models, leading to handling a structural dynamic system and requiring features for state event handling [2].

Three case studies allow investigation of new approaches and modelling techniques for hybrid or structural dynamic systems with emphasis on physical modelling techniques and state event modelling [3]. These examples are also well suited to be used in education for teaching event handling, hybrid and structural dynamic systems.

**Case Study 1: Bouncing Ball.** The classical example of a ball bouncing on a surface allows various modelling approaches and incorporates events. A first modelling approach for the bouncing ball dynamics recognizes two different phases: the free falling phase (flying phase) with or without air resistance, and a '*timeless*' *contact phase*, where the ball hits the ground and changes direction of movement. A more realistic model takes into account the *elasticity in the contact region* by modelling the deformation with a spring-damper-element (Kelvin-Voigt model). The contact phase in this case is not an isolated event anymore, it consumes time. Beginning and end of the contact phase are controlled by state events.

**Case Study 2: Switching RLC Circuit.** The second case study defines an extension of a class-E amplifier including a diode. It aims for investigation of modelling techniques and efficient calculation of switching elements (i.e. time events and state events) and for physical modelling of circuits or similar methods. One switching element is represented by a *time-variant resistor*, which switches continuously via a fast transition between high and low resistance values. Modelling such a variable resistor seems to be a trivial task, although some variants are possible. The chosen approach may have advantages or disadvantages in combination with event handling.

Switching in a circuit may also be designed by a *diode* as an active switch with dynamic behaviour. Simple diode models mimic the dynamic behaviour as an *ideal switch*, possibly with threshold voltage, other (more realistic) diode models use e.g. the *Shockley* equation defining nonlinear algebraic conditions.

**Case Study 3: Rotating Pendulum with Free Flight Phase.** The third example discusses an idealized rotating pendulum on a rope with damping. It has to be distinguished between two different states: The *rotation phase* where the mass is moving along a circular path and the *flying phase* where the rope is loose due to gravitation and the mass is free falling. Additional state-dependent algebraic equations define switching conditions for transition between the models. Since the two states have different numbers of degrees of freedom, i.e. the state space dimension changes cyclically as the pendulum alters its state, this model represents a structural dynamic system.

- [1] Fritzson P.: *Principles of Object-Oriented Modeling and Simulation with Modelica 2.1*. John Wiley and Sons, 2004.
- [2] Breitenecker F., Zauner G., Popper N., Judex F., and Troch I.: *Development and New Concept for External and Internal State Events*. SNE Simulation News Europe, 17/2, 2007.
- [3] Körner A., Heinzl B., Rößler M., Zauner G., Breitenecker F., and Ecker H.: *Comparison of Hybrid Modelling Approaches: ARGESIM-comparison BCP - Bouncing Ball, Circuit with Diodes, Rotating Pendulum*. ASIM 2011 - 21. Symposium Simulationstechnik, 2011.



## SIMULATION OF HEAT RADIATION ASYMMETRY WITH MAPLE

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**Introduction.** Former calculation procedures of the radiation temperature asymmetry are only of approximate validity because of the fixed, i.e. vertical or horizontal position of the plane separating the two hemispaces and because of the fact, that in practical calculations the room terminating surfaces beyond those being thermally active and their temperatures are taken into account with their average values.

**Simulation of heat radiation asymmetry.** A novel method was developed for the determination of radiated temperature asymmetry giving a result more closer to the reality, where the plane dividing the two hemispaces of the surface element at the test point separates the thermally active (coldest and warmest) surfaces in all cases and determines the irradiation factor through drawing.

This novel method of asymmetry calculation enables a more accurate calculation of the “one side radiation asymmetry” parameter defined by us and being a further characteristic parameter of the comfort of rooms in case of cold and warm surfaces being within the same plane.

**Visualisation of the results with help of computer algebra system.** Using the Maple computer algebra system there are several possibilities to simulate the radiation asymmetry values in space.

Three different cases were simulated:

- Thermally active surfaces in orthogonal arrangements – a.) warm (heating) ceiling and cold (cooler) window (winter period), or b.) cold ceiling and warm window (summer period).
- Thermally active, parallel surfaces – cold glass wall and wall-heating on the opposite side (winter time).
- Thermally active surfaces in the same plane – radiator under the window.

**Conclusion.** With help of this new way of simulation there are possibilities to determinate the comfort zones, where we feel “thermally well” ourselves.

- [1] Vajda J., and Perjési-Hámori I.: *Two dimensional mathematical model of heat-transmission of one- and double-layer building* Pollack Periodica Vol. 2, No.3, 2007, 25-34.
- [2] Vajda J.: *Keine Alternative zur Passivhaustechnik*, HLH, 59. (2008)
- [3] Frohner I., Perjési-Hámori I., Bánhidi L.: *Lassen sich die Diskomfortzonen bei Passivhauser zurückgewinnen?* Internationale Passivhaustagung 2005 Ludwigshafen

## Short Remark on Lateral Vibration of Functionally Graded Beams

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The Euler-Bernoulli differential equation for the lateral vibrations of FG beams has the form

$$\frac{\partial^2}{\partial x^2} \left( E(x) J \left( \frac{\partial^2}{\partial x^2} w(x, t) \right) \right) + \rho A \left( \frac{\partial^2}{\partial t^2} w(x, t) \right) = 0 \quad (1)$$

where  $\rho$  is the density,  $A$  is the cross sectional area,  $w$  is the transverse deflection,  $J$  is the moment of inertia and  $E$  is the elasticity modulus of the beam and  $t$  is the time. In [1] Aydogdu supposes that the vertical displacement  $w(x, t)$  is supposed to have a special form  $w(x, t) = W_m \sin(x\beta) \sin(\omega t)$  and points out that the substitution of this form into the Euler-Bernoulli differential equation above transforms it into DE which depends on the axial coordinate only. In this paper we generalize the method used by Aydogdu and determine the largest function class of the form  $w(x, t) = F(x) \cdot G(t)$  for which the same method is applicable.

### Proposition 1.

For arbitrary function  $F(x)$  and for the functions  $G(t) = A \cdot \sin(\omega \cdot t) + B \cdot \cos(\omega \cdot t)$  the choice

$$w(x, t) = F(x) \cdot (A \cdot \sin(\omega \cdot t) + B \cdot \cos(\omega \cdot t))$$

results in a differential equation, which does not depend on variable  $t$ .

### Proposition 2.

The general solution of DE resulted by the substitution of  $w(x, t) = F(x) \cdot (A \cdot \sin(\omega \cdot t) + B \cdot \cos(\omega \cdot t))$  in (1)

$$E(x) = \frac{-C_2 + -C_1 x + \frac{\rho A \omega^2}{J} \left( \iint F(x) dx dx \right)}{\frac{d^2}{dx^2} F(x)}.$$

### Proposition 3.

If the function  $w(x, t)$  is of the form  $w(x, t) = F(x) \cdot G(t)$  so that its substitution into DE (1) results in a differential equation which does not depend on variable  $t$ , than  $G(t)$  must have the form

$$G(t) = -C_1 \sin(\omega t) + -C_2 \cos(\omega t).$$

### Acknowledgement

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### References

- [1] Aydogdu, M., Semi-inverse Method for Vibration and Buckling of Axially Functionally Graded Beams, Journal of Reinforced Plastics and Composites, Volume 27 2008, online version <http://jrpsagepub.com/content/27/7/683>
- [2] Maróti, Gy., Finding Closed-Form Solutions of Beam Vibration, Pollack Periodica, Volume 6, Number 1, 2011
- [3] Maróti, Gy. Elishakoff, E., On Buckling of Axially Functionally Graded Beams, Pollack Periodica, Volume 7, Number 1, 2012
- [4] Maróti, Gy., Klincsik, M., Maple, Livermore, Békéscsaba, Hungary 2006

## USING SYMBOLIC CAPABILITIES OF MAPLE STATISTICS PACKAGE FOR ENHANCING THE CONCEPTS OF PROBABILITY THEORY AND STATISTICS

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The symbolic manipulations now are available not only for the expressions or functions however also for the random variables by using “Statistics” package of Maple Computer Algebra System (CAS). These facilities are unique among the CAS programs. Such an implementation of the random variables is a similarly hard task as to realize symbolic manipulations with algebraic expressions.

We use these capabilities of the Maple CAS in order to better understand the mathematical concepts of the randomness by the students. These are useful tools for students to

- manipulate symbolically with different random variables and asking from the Maple CAS to answer for specific features of them
- experiment with the random variables to obtain some new results

We can demonstrate theoretical results of the probability and statistics by symbolically using only the CAS program without proving the theorems algebraically or/and analytically.

What is the appropriate ratio between the rigorous mathematical verifications and the computer demonstrations? The answers are varying from course to course and from topic to topic. In this lecture we examine the usability of the random variables of the Maple “Statistics” package throughout examples.

In the first example we are looking for the parameter “n” from the binomial distribution on the basis of a given side condition. We can write the side condition in a “strongly” nonlinear equation form. This equation can be set up by using the built-in functions of the Statistics package. On the basis of this demonstration the students can realize the problem and try to solve the equation (i) analytically, (ii) numerically or/and (iii) graphically. The CAS “solve” command doesn’t give the desired result in this case therefore we have to calculate a numerical sequence to obtain the value of the parameter of the binomial distribution. Thinking about the concept of the cumulative distribution function we can draw a step function where the independent variable is the parameter “n”. This function is not the cumulative distribution however we use it when plotting the graph. So the visualization helps to understand and solve the problem and the concepts about the random variables.

In the second example we investigate a system consists of two components which are connecting in series form. Knowing that the distributions of the lifetime of the two components are exponential with different parameters and independents from each other then we want to verify that the lifetime of the whole system is also has an exponential distribution. We get this result if we consider the minimal value of the two lifetime’s variable. These well known theoretical results are “proving” by the symbolic facilities of the CAS. When the students are motivated by these manipulations then we can follow the ideas of rigorous proving.

[1] T. T. Soong: *Fundamentals of probability and statistics for engineers*, John Wiley and Sons Ltd, 2004.

## MAPLE T.A. IN ENGINEERING EDUCATIONS

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**Introduction.** The department for modelling and simulation of the Institute for Analysis and Scientific Computing deals with education in mathematics and modelling. There are many lectures and exercises held by this department. Most of these lectures are supported by an e-learning system. In some of these lectures an e-learning system called MMT, Mathematics Modelling and Tools, is used. Courses where the students have the possibility to learn with the MMT system focus on modelling and simulation.

Lectures containing basic and advanced mathematics are supported by an e-learning system called Maple T.A.. Maple T.A. stands for Maple Testing and Assessment. This system makes an easy creation of tests possible. In addition the automatic grading allows the tutors to concentrate on the compilation of examples and enables the lecturers to offer extra oral exams.

**Maple T.A.** Maple T.A. is based on Maple, a computer algebra system. Maple supports analytic and algebraic calculations. The programming language Maple is often used by the students of the Vienna University of Technology which was one reason for using this e-learning system. This Software focuses on the creation of examples and the arrangement of tests.

Maple T.A. offers its own programming commands for the coding but it is not necessary to know the commands of Maple T.A., because it is possible to programme with devices from Maple. On the other hand it is helpful to know some of the short devices of Maple T.A., because using the commands of Maple leads to a call of Maple, so it needs more capacity.

Concerning the examples a great advantage of Maple T.A. is the one-time creation of the examples. Because of the randomised variables, every time the example is opened the numbers are changed. The designers of the Maple T.A. examples developed an additional library. This library supports the creation of randomised vectors, matrices and eigenvalues. For instance, for the examples of differential calculus one single question rotates between the trigonometric, exponential and logarithmic functions. The new library not only includes commands for the creation of examples but also supports the higher level of grading.

**Courses.** The aim of the modelling and simulation department of the Institute for Analysis and Scientific Computing by inventing **the refresher course of mathematics** is to ease the entrance to university for students. It starts before the normal daily routine of lectures and exercises begins and supports the students by reminding them of their mathematical skills and knowledge they had at school.

The modelling and simulation department is responsible not only for the refresher course of mathematics but also for **basic mathematical courses**. These courses are held for students of electrical engineering. Mathematics 1 and 2 are scheduled in the first and second semester of the study. Both courses consist of lecture and exercises. During the semester there are three tests in Maple T.A. of which each takes 30 minutes and consists of four examples. A necessary condition to pass the course is to get two of the three tests positive.

The third semester of the students of electrical engineering contains an advanced mathematical course, called **Mathematics 3**. Since this year the lecture is supported by Maple T.A. as well. An advantage of using Maple T.A. for e-learning is that the students are used to this tool. There is no time loss due to learning new commands or getting used to the new interface.

**Summary.** Apart from being a tool for teaching basic mathematics in lectures offered by the Institute for Analysis and Scientific Computing for students of electrical engineering the Maple T.A. system has become important to enable automatical grading of exams to support the lecturers. All in all Maple T.A. is used since 2008. In the last four years the examples and their grading were improved to embrace the requirements of students, tutors and lecturers. The routine in creating examples had saved time which we could spend to update the version of Maple T.A. and to equip the old questions with the new commands. Despite of some problems at the beginning the use of Maple T.A. it is now appreciated by students and lecturers.

- [1] A. Körner, S. Winkler, V. Urbonaite *E-Learning Einsatz im Auffrischkurs Mathematik an der TU Wien* Proc. 4th International eLBa Science Conference, Rostock, 2011, 145-154.
- [2] A. Zimmermann, V. Urbonaite, A. Körner *Advanced randomization and grading in the E-learning system Maple T.A.* EUROSIM 7th Congress on Modelling and Simulation, Prague, 2010
- [3] A. Körner, A. Zimmermann, F. Breitenecker *Blended-Learning mit Maple T.A. in der Lehre für Mathematik und Modellbildung* Extended Abstracts 20th Symposium Simulation Techniques, Cottbus, 2009, 62-64.

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# MODELLING METABOLIC PATHWAYS INVOLVED IN THE PATHOGENESIS OF NON-ALCOHOLIC FATTY LIVER DISEASE

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Non-alcoholic fatty liver disease (NAFLD) is the most common chronic liver disease in Western populations affecting 25-30% of the general population and 70-80% of obese populations. It is a complex disorder arising from the close interaction of genetic predisposition factors, lifestyle and the environment. The progression of steatosis, the benign form of NAFLD, characterised by the hepatic accumulation of lipids, to non-alcoholic steatohepatitis (NASH), which additionally involves the activation of inflammation, and ultimately to cirrhosis and hepatocellular carcinomas, is poorly understood [1]. Systems biology tools provide an efficient, cheap and rapid methodology to dissect biological systems, which are essentially non-linear in nature. Although systems biology has been utilised at a large scale in understanding the physiology of prokaryotes, the complex, compartmentalised and multi-cellular nature of eukaryotes has proved to be major hindrance for using modelling approaches to study profoundly interconnected pathways in higher organisms.

This article aims to provide a description of the generation of a metabolic and signalling model of the pathways that have been implicated or hypothesized in the pathogenesis of NAFLD. An object-oriented modelling and simulation programme, Dymola, has been utilised to generate the network of reactions utilising a systems biology library of components, with evidence from literature searches ( $n=470$ ), the Kyoto encyclopaedia of genes and genomes and the Reactome databases. The reversibility and stoichiometry of the reactions were maintained only in the presence of evidence from the literature. The flux through reactions at pathway branch points have been assigned approximate values from the metabolic flux analysis using labelled glucose in the HepG2 human carcinoma cell line [2]. The completed model represents multi-tissue interactions between the liver, adipose tissue, pancreas, macrophages and the peripheral tissues, while focussing on intra-tissue metabolite biosynthesis and transport regulation at the transcriptional and post-translational levels.

The model validation procedure involved comparing model simulations of experimental situations with published data from the literature to ensure correspondence. The lack of correlation of the model simulation with the data suggests errors or missing components in the network, which were identified by a close inspection of the model and further data mining. The model has been validated to simulate fasting conditions [3] and data from a mouse model with a target disruption of stearoyl CoA desaturase-1 (SCD-1), a crucial lipogenic enzyme that is involved in the conversion of saturated fatty acids to unsaturated fatty acids [4].

Testing model simulations by varying flux parameters indicated a stiffness of reactions involving  $\geq 2$  substrates. This limited tolerance can be explained for reactions whose substrates are generated via separate network branches, as the reaction depends on reaching equilibrium between different pathway branch flux values. Hence, enzymes catalysing these reactions may be identified as intolerant focal points within the network, thus suggesting novel molecular mediators that may play a crucial role in the pathogenesis of NAFLD. Interestingly, a majority of the multi-substrate reactions are catalyzed by highly-regulated enzymes, thus providing a mechanistic explanation of the molecular mediators in maintaining the flux through these reactions within narrow limits. This observation also suggests that NAFLD may be a disease with a flux-disruption to such an extent that the regulators of the network fail to bring the system to a nominal steady state.

The NAFLD metabolic model thus aims to identify novel mechanisms of disease initiation and progression and perhaps suggest novel regulatory mechanisms that are yet to be identified by experimentation. Further model validation and simplification is required to increase the robustness of the network and visual transparency whilst maintaining the functionality and precision of the model. On completion, the model can be utilised by the wider scientific community to test experimental hypotheses in a rapid and cheap manner prior to experimentation.

- [1] de Alwis, N.M. and C.P. Day, *Non-alcoholic fatty liver disease: the mist gradually clears*. J Hepatol, 2008. **48 Suppl 1**: p. S104-12.
- [2] Hofmann, U., et al., *Identification of metabolic fluxes in hepatic cells from transient  $^{13}\text{C}$ -labeling experiments: Part I. Experimental observations*. Biotechnol Bioeng, 2008. **100**(2): p. 344-54.
- [3] Kersten, S., et al., *Peroxisome proliferator-activated receptor alpha mediates the adaptive response to fasting*. J Clin Invest, 1999. **103**(11): p. 1489-98.
- [4] Ntambi, J.M., et al., *Loss of stearoyl-CoA desaturase-1 function protects mice against adiposity*. Proc Natl Acad Sci U S A, 2002. **99**(17): p. 11482-6.

## EFFECTS OF DIFFERENT BLOOD FLOW MODELS ON THE DETERMINATION OF ARTERIAL CHARACTERISTIC IMPEDANCE

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**Introduction.** Cardiovascular diseases are the major cause of death in many developed countries. Due to the effects of an aging society and a hopefully increasing prosperity in now underdeveloped regions, the diagnosis and treatment of these diseases doubtlessly will be of special importance in the future. Within the concept of pulse wave analysis, arterial pressure and flow curves over a whole cardiac cycle are analyzed. Preferably aortic measurements or calculated aortic pulse waves gained via a transfer function from peripheral measurements are used.

A possibility to characterize the arterial system is to relate pressure and flow via a linear time-invariant transfer function. The transfer function can be expressed as the ratio of output to input in the frequency domain. This ratio of pressure to flow is called impedance. The characteristic impedance ( $Z_c$ ) is obtained when pressure and flow waves are not influenced by wave reflection. This situation will never occur in the arterial tree, therefore the characteristic impedance can be approximated only, usually with the help of a calculated input impedance.

**Methods.** Since the measurement of blood flow in the aorta is cumbersome, models are used to generate flow curves for the determination of vascular impedance. The aim of this work is to evaluate the effects of different blood flow models on the determination of the characteristic impedance compared to flow curves gained from ultrasound measurements. The simplest model to approximate aortic blood flow is a curve of triangular shape during systole. Another approach is to use an averaged flow curve from readings of different subjects. Recently a new blood flow model based on Windkessel theory was developed (ARCSolver flow model). By optimizing the left ventricular work using the calculus of variations a personalized flow curve can be obtained.

In a study population of 148 patients, pressure and flow curves were measured non-invasively using tonometric and ultrasound techniques. For the evaluation of the different models the input impedance and subsequently the characteristic impedance will be calculated in the frequency domain. For a fair comparison all flow curves are scaled in such a way that the maximal value is at the level of 100 arbitrary units (AU).

**Results.** The mean characteristic impedance using flow curves from ultrasound images is 0.22 (0.08 SD) AU. For the triangular flow a mean difference to the ultrasound flow for  $Z_c$  of -0.148 (0.097 SD) is found. For the averaged flow a mean difference for  $Z_c$  of 0.027 (0.036 SD) AU and for the ARCSolver flow a mean difference of 0.016 (0.039 SD) AU compared to the ultrasound flow is obtained. In a Bland-Altman analysis small trends of underestimation for higher values can be seen for the averaged and the ARCSolver flow, whereas for almost all subjects the values for  $Z_c$  are higher using the triangular flow curve.

**Conclusion.** These results indicate that the characteristic impedance strongly depends on the accuracy of the used flow model. While the averaged and the ARCSolver flow provide good estimates for impedance, the triangular flow curve seems to be too simplistic for getting accurate values. These findings are helpful because the characteristic impedance is not just an important parameter on its own, but is furthermore a key parameter for pulse wave separation and in a newly developed model for the estimation of aortal pulse wave velocity. Since the ARCSolver flow model provides estimates for impedance with sufficient accuracy compared to those gained from ultrasound measurements, this new model offers an easy way to perform pulse wave separation and furthermore to calculate pulse wave velocity based on information from a single blood pressure measurement.

- [1] Kips J., Rietzschel E., De Buyzere M., Westerhof B., Gillebert T., Van Bortel L., and Segers P. Evaluation of Noninvasive Methods to Assess Wave Reflection and Pulse Transit Time From the Pressure Waveform Alone. *Hypertension*. 2009;53(2):142–149.
- [2] Nichols W. and O'Rourke M.: *McDonald's Blood Flow in Arteries*. Arnold, London, 4th edition, 1998.
- [3] Weber T., Haiden A., Hametner B., Mayer C., Kropf J., Wassertheurer S., and Eber B.: Aortic pulse wave velocity, estimated with a simplified method based on radial waveforms and body height, predicts cardiovascular events. *Artery Research*. 2011;5:178.



# IDENTIFICATION OF THE LONG-TERM EFFECTS OF MILD TO MODERATE NEONATAL CEREBRAL HYPOXIA BASED ON EEG SIGNALS ANALYSIS

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**Introduction.** Hypoxic-ischemic encephalopathy (HIE) during perinatal period is the most common cause of neonatal seizures and is associated with an increased risk of epilepsy in the later life. Among newborns affected by perinatal brain injury 20-50% die during the newborn period, and 25-60% of the survivors suffer from permanent neurodevelopmental handicap, including cerebral palsy, seizures, mental retardation, and learning disabilities. Long-term neurological sequelae in children after HIE can be attributed to both disturbed brain development and functioning as well as tissue loss after hypoxic-ischemic insult. Although delivery can be a critical point, since it presents a shock to a child's organism that can be accompanied with several complications, hypoxia can occur also prior the delivery due to many causes such as: prolapsed or compressed cord, ruptured uterus, incidents during delivery, etc. Despite the improved pre- and perinatal health care, neonatal encephalopathy still occurs with the incidence of 1-6/1000 [2]. As brain is a very complex organ there are no models to predict the long term effects of perinatal hypoxia on the basis of the hypoxia duration and severity. In our study we analysed data from the long-term observations of children with mild to moderate HIE.

**Measurement of EEG.** EEG signals are measurements of electrical activity of brain obtained by using electrodes on the scalp surface. The magnitude of the measured EEG signal varies with the position of the electrodes and their distance from the electrical source. The measured activity represents the sum of the repetitive and periodic electrical activity, and most likely originates from the sum of the excitatory and/or inhibitory postsynaptic potentials in large populations of pyramidal cells in the neocortex. Local postsynaptic potentials along the pyramidal cell membranes cause an electrical gradient, and the sum of all the gradients results in an electrical current, which is reflected in an electrical potential that can be measured on the surface of a human scalp [1]. In the presented case the signals on standard 19 EEG electrode sites and ear lobes were recorded at 256Hz sampling rate, using a bipolar longitudinal montage. We used a set of recording conditions after whole night sleep deprivation using: eye movements and alpha blocking followed by eyes closed resting; eyes open resting; hyperventilation; and photic stimulation. Data were exported and further analysed. Numerical analysis was performed in Matlab 2009b. Eleven subjects were enrolled in the study with mild or moderate HIE.

**Analysis methods.** There are two important aspects that can be analysed by PCA: dimensionality of the signals, linear dependency of the signals. When the result are reviewed in the context of the observed system, the dimensionality and linear dependence can be interpreted in the frame of system's properties. The dimensionality of the EEG signals is directly linked with the number of most active synchronous groups of neurons which are considered as signal sources. We performed spectral analysis on the first principal component and compared it to the clinical findings. In parallel, EEG signal complexity was assessed by fractal dimension calculation (Higuchi) and sample entropy, and compared to the clinical findings as well.

**Conclusions.** The interesting correlation between power spectrum of the first principal components of the EEG signals and learning difficulties of the subjects was an important finding. Although alpha spectrum brain waves are associated with resting, their function, although sometimes controversial, is not irrelevant for the higher functions of the brain. It is known that our memories consolidate during resting, since severe disruption of resting cycle, such as prolonged sleep deprivation, can cause memory problems. Alpha waves are also associated with the long range synchronisations of brain areas that requires good connectivity between several brain regions. Considering hypoxic-ischemic encephalopathy it would be reasonable to expect that HIE can cause connectivity problems in brain that can have different effects on the brain functioning. The size of the brain structures seems to have no direct effect on the connectivity, however, systemic analysis of the brain rhythms can show reduced connectivity through reduced power densities at the frequencies of the major brain rhythms. Surprisingly, the connectivity does not seem to correlate with any of the complexity measures used in this study.

[1] Nuñez, P. L. and Srinivasan, R.: *Electric Fields of the Brain: The Neurophysics of EEG*. Oxford University Press, Oxford, second edition 2006.

[2] Volpe, J.: *Neurology of the newborn*. Saunders, Chicago, USA 2001.

## BURDENS OF OBESITY - MULTI-MODEL DESCRIPTION

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**Introduction.** Unhealthy life style very frequent consists of inactivity, stress, improper and/or too rich or abundant nutrition resulting in a number of problems among which the first one is usually overweight. Overweight and obesity are defined as abnormal or excessive fat accumulation that may impair health (WHO 2011). Obesity was in 1997 by World Health Organization recognized as disease. It has reached epidemic extensions and as such it has become an important social and economic burden because it is an important risk factor for developing diabetes type 2, hyperdislipidemia and hypertension. These four chronic diseases are also known as deadly quartet because they are essentially increasing the development of cardiovascular diseases which have already become the main reason for mortality.

**Methods.** In the paper the modeling structure is proposed with which it is possible to evaluate the burdens important for certain country or population and eventual healing influences and/or life style improvement which are notable also for disease economics. In the same time it enables the observation of different dynamic processes connected with the observed disease. It consists of four main levels which indicate problem observation from the population perspective. In addition also some other important dynamical processes or modeling results of complementary models can be combined with the results of the main structure.

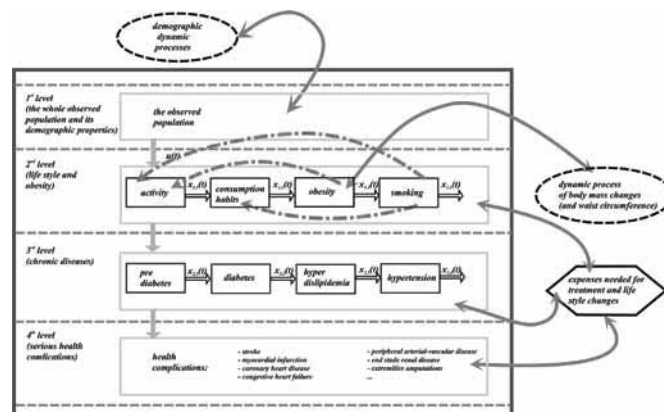


Fig. 1. Proposed modeling structure.

**Results.** In the paper some of direct expenses regarding overweight and obesity are identified, evaluated and compared for Slovenia and Austria. The same methodology can be used for both countries. Regarding the efforts for body mass reduction over 325 million € is used in Slovenia and over 1.5 billion € in Austria each year. But, unfortunately these are not complete costs. Chronic diseases and serious health complications are more frequent among obese population. For diabetes type 2, for example, additional 56 million € is needed in Slovenia and 230 million € in Austria each year. As populations are growing older the effective burden will become for future generations even higher. It is also important to mention that indirect expenses of obesity are comparable with direct ones.

**Conclusions.** It seems that in everyday life people are not enough aware of the burdens (economic and social) of overweight and obesity. It is obvious that both societies Austrian and Slovenian (and this is true also for other EU countries and USA) should do something to reduce these tremendous burdens with increased prevention programs, and also with intensive and integrative programs provided by medical specialists, where motivation is of central importance.

WHO - World health organization (2011). Obesity and overweight, *Fact sheet No. 311*, <http://www.who.int/mediacentre/factsheets/fs311/en/>.

# MODELING ELASTIC WALLS IN LATTICE BOLTZMANN SIMULATIONS OF ARTERIAL BLOOD FLOW

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**Introduction.** An essential part in the simulation of blood flow in arteries is the incorporation of the arterial elasticity by modeling the vessel wall and its interaction with the fluid inside the vessel. Common numerical methods for blood flow simulations with elastic walls are complex. We suggest a simple approach for modeling elastic walls in lattice Boltzmann (LB) simulations of arterial blood flow. Our model fulfills the essential properties of an elastic wall and respects the basic conservation laws.

**Modeling elastic walls in lattice Boltzmann simulations.** In simulations of blood flow, it is important to consider the compliance of the vessel. Therefore, a model for the vessel wall is needed that describes its spatial displacement as it interacts with the flow dynamics. Based on [1], we have developed a model which does not need a parametrization of the wall. The method acts strictly locally, like the LB method, so that the complexity of the algorithm is low.

The model uses a lattice of nodes that can have two different states: *fluid*, representing the blood inside the vessel, and *solid*, describing the vessel wall. The compliance of the wall is modeled by changing the type of a node - from solid to fluid in the case of expansion and vice versa in the case of contraction of the vessel. This change of node type is dependent on the local pressure of the surrounding fluid nodes. Pressure thresholds are assigned to each node, increasing with the radius of the vessel segment (based on a linear relationship between the pressure and the radius).

**Improved method to model elastic vessel wall.** In our model, contrary to [1], the wall of the vessel is not situated on the solid nodes but is imagined to be located between last fluid and first solid node in a given direction. All nodes that are not fluid are by default solid. Thus, the problem of rupture of the vessel wall does not occur and our approach does not require the use of cellular automata. Created fluid nodes need to be initialized, which is done by averaging the LB populations from the fluid nodes surrounding the new fluid node. Compared to the method of [1], where new fluid nodes are initialized with an equilibrium distribution function, this approach includes also the non-equilibrium part of the populations, which is not negligible for nodes in proximity of the wall.

Furthermore, mass is a priori not conserved when the total number of fluid nodes increases or decreases (its circumvention is not detailed in [1].) In order to ensure mass conservation, we developed two methods that rescale the LB populations when a node type change occurs. The method of *local rescaling* takes into account only the nearest neighbors of the node changing its state. It redistributes mass between nodes that change state and their neighboring nodes. The method of *rescaling 'by columns'* takes into account the whole column of nodes - the vessel can be considered as a sequence of 'rings' adjoint to each other - in which a node type change occurs. When a node changes its state, mass is redistributed along all nodes in the same column.

**Simulation and preliminary results.** We implemented a simulation software for the lattice Boltzmann algorithm in two dimensions combined with our elastic wall model using the programming language C. The program includes the rescaling methods and the pressure threshold algorithm described in the full paper. Using our software program, we conducted numerical experiments to show the feasibility of our approach.

First, we compared the computed velocity profile in a straight channel to the analytical solution of a Poiseuille flow showing that both velocity profiles coincide. Second, we tested our modeling of elasticity using local rescaling, showing that mass is properly conserved and initial values of the density and the velocity are recovered after one cycle of expansion and subsequent contraction. Third, we tested the modeling of elasticity using rescaling 'by columns' which minimizes local perturbations but exhibits the drawback that node type changes at one wall boundary affect the flow field within the whole channel, which does not correspond to real fluid dynamics.

**Outlook.** The aim of the future work is the simulation of blood flow in stented arteries. The approach for the modeling of elastic walls presented in this work has the advantage that it can also be extended to include stents. This enhanced model will be implemented in our simulation software and further elaboration of our approach will be reported in a later work.

[1] Leitner D.: *Simulation of Arterial Blood Flow with the Lattice Boltzmann Method*. Ph.D. thesis, Vienna University of Technology, 2007.



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## MEASUREMENT OF ENZYME AND MICROBIAL ACTIVITY ON-LINE FOR IMPROVED PROCESS CONTROL

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Enzyme activity is the most important variable to control in all microbial processes, and so also for activated sludge processes. The enzyme activity relates to different compounds like  $\text{NH}_4$ ,  $\text{PO}_4$ ,  $\text{NO}_3$  and COD/BOD/TOC. What we see from our research is that the overall enzyme activity was higher in some wastewater treatment plant basins compared to others, but we don't have an exact value for the specific enzyme activity. This would be very interesting to determine to make it possible to control all lines to the same good level and hopefully also reduce  $\text{NO}_3$  and  $\text{PO}_4$  as well. We also know that there are changes in activity between seasons and over the day, as well as depending on how the plants are operated, which is no news as such. Still, the conclusion is that we need to adapt the performance of the microorganisms both short term over the day and long term over the season. To do this we need to have some indication of the total enzyme activity as well as the specific enzyme activity (that is activity per kg sludge).

The enzyme activity can be measured in different ways. By filtering a certain volume of sludge from the process, wash it and then feed with a surplus of a specific substance the activity can be measured by e.g. measuring the concentration of the same substance after passing the microorganisms. This can be done directly by using ion selective electrodes for the ions we are interested in.

As an alternative the temperature evolution can be measured giving an indication also of the reactions. For example the microbial activity can be estimated by measuring how heat is evolved as different substances like  $\text{NH}_4$ ,  $\text{NO}_2$ ,  $\text{NO}_3$ ,  $\text{PO}_4$  are added to a batch of microorganisms sampled from the process. By having two separate sets of the same microorganisms and having a blank without the addition of the studied chemical, the difference in activity can be measured.

Another alternative is using the actual process as a large scale reactor by measuring the air flow and follow the DO (dissolved oxygen) as well as specific substances before and after the activated sludge step. If we dose the same amount of oxygen and have the same amount of organic material entering the plant, the DO level will go up in the far end of the basin as the organic material has been mainly decomposed. If the DO level changes as we run under steady state conditions, the change will be an effect of changing enzyme activity in the microorganisms.

The enzyme activity has been modeled using a Dymola model that is used inside Matlab/Simulink as an object, which is communicating with the process data base. In this way an on-line simulation can be achieved. The model is compared to measured data to follow the activity and this in turn is used for feed forward control of dosage of different control variables like air flow, chemical additions and carbon source. The model is containing the reactions for a number of important reactions and how these are affected by the control variables. It has a base in the ADM1 model, but is including also process dynamics to be useful also for control purposes.

## A LabVIEW-BASED SIMULATOR FOR THE ACTIVATED SLUDGE PROCESS

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**Abstract:** Activated sludge process is the main process in most urban wastewater treatment systems. It is considered complex in nature, and building its mathematical model in practice becomes difficult. A simple and easy way to build the simulation models for the system is needed. In this paper, a LabVIEW based simulator for this system is presented. LabVIEW offers a highly efficient, simple and flexible platform for simulation and control. Building applications in LabVIEW require less coding, and debugging is easy and fast. The proposed simulator utilizes the Benchmark Simulation Model no.1 (BSM 1) for the biochemical reactor and clarification processes. The operation of the simulator is via a graphical user interface (GUI) built in the LabVIEW environment. The simulation results can be displayed in digital and graphical forms. Simulation results obtained were compared with the results from other software simulation packages in which the COST/IWA Simulation Benchmark has been implemented. The developed simulator is very useful due to its efficiency and accuracy in simulating the wastewater process model. The simulator can serve as a training tool for plant operators/students to provide them with better knowledge and understanding of the process.

**Introduction.** Modelling and simulation plays an undisputable role in the development of the activated sludge wastewater treatment process due to its highly complex nature coupled with needs to reduce pollutants in the effluent and minimize production rate of sludge at a lower cost [1]. Mathematical models are mostly used for description of process performance, prediction and process design and control [1;2]. Several models to describe the biological processes taking place in the activated sludge process exist, but the International Water Association models such as Activated Sludge Model No.1 (ASM1), ASM2, ASM2d and ASM3 are the internationality accepted models. The models serve as a guide for research, and valuable tools for better understanding of the biological processes and interactions. ASM1 is considered as reference model for many research and practical applications and has been used for developing the simulator platform in this work.

**Simulation Software Platform.** Based on the ASM1 modelling techniques, many simulation software packages have been used to develop and implement the simulation platform BSM1 [3]. Some of the simulators developed in line with BSM1 require much coding, debugging and are less user friendly [4]. In LabVIEW, it is easy and faster to build applications compared to scalar languages due to large extensive libraries of several functions. This helps to solve most of the programming difficulties. Therefore, it is one of the objectives of this paper to describe the development of a more user friendliness simulator namely a LabVIEW-based simulator for the activated sludge process, which will give more insight to plant operators or for student laboratory teaching.

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- [1] Jeppsson, U.. *Modelling of Wastewater Treatment Processes*, PhD thesis, ISBN 91-88934-00-4, 1996, Lund University, Lund, Sweden
- [2] Henze, M., Grady, C.P.L., Gujer, W., Marais, G.v.R. and Matsuo, T. *Activated sludge model no.1*. Scientific and Technical report no. 1, IWA Publishing, 1987, London, UK.
- [3] Copp, J.B. (ed.), *The cost simulation benchmark: description and simulator manual*. ISBN 92-894-1658-0, 2002, Office for Official Publications of the European Communities, Luxembourg.
- [4] Morgenroth, E. Arvin, E. and Vanrolleghem, P. *The use of mathematical models in teaching wastewater treatment engineering*, Water Science and Technology, 45 (6), 2002: 229-233



# EVALUATING THE POTENTIAL FOR PROCESS CONTROL IN PULP MILL WASTEWATER TREATMENT PLANT BY SIMULATION

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**Introduction.** More advanced instrumentation, control and automation are necessary to meet the tightening standards for effluent quality from wastewater treatment plants (WWTPs) treating pulp and paper mill wastewater. Although the methods and equipment necessary for implementing process control at WWTPs have been developed, there is not much prior experience of their application in industrial WWTPs making the plant operators hesitant to make the necessary investments. Modeling and simulation is an inexpensive method to evaluate the benefits of improved process control. This paper presents the development of a simulator for evaluating the potential for process control in an activated sludge process (ASP) treating pulp mill wastewater. The principles of WWTP benchmarking introduced with the Benchmark Simulation Model 1 (BSM1) [1] are applied in the simulator. A simple control strategy developed to improve the operation of the pulp mill ASP and to decrease operating costs is evaluated with the simulator. The benefits of process control are evaluated based on effluent quality and costs of operation.

**Materials and Methods.** The WWTP under study is an aerobic activated sludge plant designed for the removal of suspended solids and organic carbonaceous material from bleached kraft pulp mill wastewater. Concentration of nitrogen in the pulp mill wastewater is low, and nitrogen has to be added to the process in order to avoid nitrogen limitation problems in the removal of carbonaceous material.

Aeration basin of the pulp mill ASP was modeled with an Activated Sludge Model no. 1 (ASM1) modified to be more feasible in modeling the biological treatment of nutrient deficient wastewaters. Activated sludge model parameters have to be calibrated for each application. Calibration of the ASMs consists of choosing a subset of model parameters and identifying values for parameters in the subset. The modified ASM1 was calibrated according to the calibration procedure described by Keskitalo and Leiviskä [2].

A simple control strategy was developed to improve the operation of the pulp mill ASP and to decrease operating costs. In the control strategy, dissolved oxygen (DO) concentration in the aeration basin of the ASP is kept at a predefined setpoint of 2.0 mg l<sup>-1</sup> by a PI feedback controller. DO concentration measurement is provided by a DO probe in the aeration basin and the controller output is the airflow rate. Nitrogen is dosed in proportion to the influent chemical oxygen demand (COD) load by a feedforward controller. COD load is measured by an online COD analyzer and a flow rate sensor.

**Results and Discussion.** The proposed control strategy was implemented in the calibrated simulator and evaluated in terms of effluent quality and costs of operation. The simulation results show, that introducing the DO control reduces aeration energy consumption significantly, by 41.1%. Control of nitrogen nutrient dosing results in 5.6% increase in chemical consumption, but as nitrogen is dosed according to the influent organic load, the soluble nitrogen effluent load is reduced by 22.0%. The soluble phosphorus effluent load can also be expected to be reduced due to avoiding nitrogen deficient conditions and having more stable operation overall.

**Conclusions.** A simulator was developed to evaluate the potential for process control in a pulp mill ASP. The proposed control strategy is simple and can be implemented with standard sensors and actuators. The simulation results show that the control strategy is beneficial in terms of operating costs and effluent quality. In future work, the simulator can be used to evaluate more advanced control strategies. In addition, disturbances and faults, such as changes in influent wastewater composition and sensor faults, can be taken into account.

The simulator developed in this work is not an alternative to the BSM1 but rather a tool which applies the principles of WWTP benchmarking introduced with the BSM1 to evaluate the potential for process control in a specific pulp mill ASP. However, the simulator can be applied to other pulp and paper mill WWTPs by calibrating the process model with appropriate process data.

[1] Copp J.B. (ed.): *The COST simulation benchmark: Description and simulator manual*. Office for Official Publications of the European Communities, Luxembourg, 2002.

[2] Keskitalo J., and Leiviskä K.: *Application of evolutionary optimisers in data-based calibration of Activated Sludge Models*. Expert Systems with Applications, in press, 2012.  
<http://dx.doi.org/10.1016/j.eswa.2011.12.041>

## DATA AND TREND ANALYSIS OF WASTEWATER TREATMENT IN PULP AND PAPER INDUSTRY

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In activated sludge plant, which is a complex biological process, several physical, chemical, and microbiological mechanisms simultaneously affect purification results. A lot of process measurements are available, but measurement sets do not include sufficient information on special features of the influent nor on microbial composition of the sludge. Dynamic models should be adapted to the condition of the biomass, which changes slowly. Temporal reasoning is a very valuable tool to diagnose and control slow processes. For control system software it is a difficult problem to detect such patterns including trend extraction and similarity analysis.

Modelling and simulation of the treatment plant in pulp and paper industry requires hybrid models. Linguistic equation (LE) modelling based on advanced data analysis is useful in biological wastewater treatment [1]. Compact dynamic simulation models consist of two parts: interactions are handled with linear equations, and nonlinearities are taken into account by membership definitions, which are generated with generalised norms and moments. The same scaling approach is used in trend analysis and modelling. The LE based trend episodes and deviation indices provide good tools for detecting changes in operating conditions [2] [3]. Triangular episodes are classified with the trend index and the derivative of it. Severity of the situations is evaluated by a deviation index which takes into account the scaled values of the measurements. This index has its highest absolute values, when the difference to the set point is very large and is getting still larger with a fast increasing speed.

In this study, an intelligent trend index is developed from scaled process and laboratory measurements of the Stora Enso Fine Paper wastewater treatment plant in Oulu. Data set consists of measurements on period of one year and eight months. On-line process data is averaged to one day data and combined with laboratory measurements. The trend analysis was used for short time periods to develop advanced control solutions. By choosing specific time periods and weight factors the intelligent trend analysis can be done parallel in several time scales, which are needed for control, fault diagnosis and performance monitoring. Working point variables, load/nutrition balance and treatment results are analysed to detect changes in operating conditions of an activated sludge plant. Efficiency of wastewater treatment process is analysed by comparing the chemical oxygen demand (COD) and diluted sludge volume index (DSVI) values. Deviation index should be high for COD reduction and low for the DSVI. Early warning of the changes of operation conditions, nutrients balance and treatment results is provided by the trend episodes and the deviation indices.

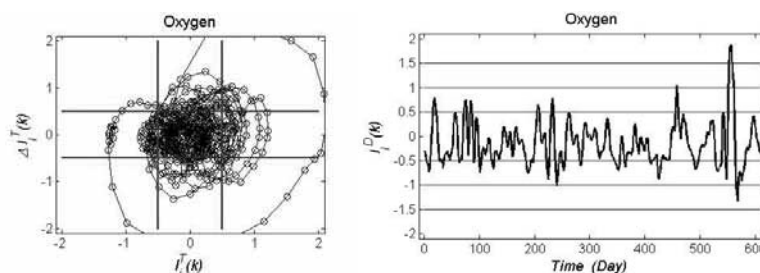


Fig. Trend episode (left) and deviation indice (right) for the working point variable oxygen.

- [1] Juuso, E.K. (2009). *Hybrid models in dynamic simulation of a biological water treatment process*. In J. Kunovsky, P. Hanacek, F. Zboril, Al-Dabass, and A. Abraham (eds.), *Proceedings First International Conference on Computational Intelligence, Modelling and Simulation*, 7- 9 September 2009, Brno, Czech Republik, 30–35. IEEE Computer Society.
- [2] Juuso, E.K. and Laakso, I. (2011). *Trend analysis in dynamic modeling of water treatment*. In *SIMS 2011 Proceedings, The 52nd Conference on Modelling and Simulation*, Västerås, 29-30 September, 2011, 10 pp.
- [3] Juuso, E.K. (2011). *Intelligent trend indices in detecting changes of operating conditions*. In *2011 UKSim 13th International Conference on Modelling and Simulation*, DOI 10.1109/UKSIM.2011.39, 162–167. IEEE Computer Society.

# CHARACTERIZATION OF ALUM FLOC BY IMAGE ANALYSIS IN WATER TREATMENT PROCESSES

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**Introduction.** In surface water treatment plants, flocculation is the key unit concerning the performance of water treatment. For this reason, monitoring the flocculation (i.e. floc size) is important in water treatment plants, and it is usually performed manually by visual scanning or using complex, sample based methods. This is expensive and laborious, however, and should be either automated or alternative methods for estimating the floc quality should be developed if possible. One interesting approach to characterize the floc formation is the image analysis of the forming floc. The main advantage of this approach is that we can measure the most essential features of the floc such as the size and the form of the floc. Previously, there have been some studies of the image analysis in ex-situ or in-situ considering for water treatment [1], or waste water treatment cases [2]. However, the referred applications are laboratory or pilot scale studies, which is necessary if the purpose is to validate the results of image analysis. In real-world processes, such applications would be complex and expensive.

In this paper we present a low-cost online characterization system for estimating the size and other features of the floc in the flocculation unit. The system consists of an ordinary systems camera which is automated to snap images over the flocculation pool. The images are then analyzed to calculate characteristics which indicate the size of the floc and other features such as eccentricity, and the number of floc particles.

**Image data and analysis.** Images were taken from the flocculation pool of a water treatment plant automatically by the system during one month in the summer of 2011. The stages for determining the floc properties using the digital images are as follows: **1)** Upload colour image to analysis, **2)** Convert image to grayscale, **3)** Adjust contrast, **4)** Convert to binary image by using a fixed threshold, **5)** Find connected components (objects) using 4-neighborhood, **6)** Calculate object properties, which in this case are: the average surface area, the number, the average equivalent diameter and the eccentricity of floc particles. In addition, we make interpretations of the image analysis by comparing the calculated floc quality parameters to process parameters.

**Conclusions.** The results show that especially the average surface area and eccentricity of the floc seem to be the most interesting quality parameters in this case. The source of the raw water (i.e. ground or lake water) treated seems to have an effect on the size of the floc particles. The changes in the surface area can be explained using five variables, two of which are variables describing lime feed. The results also suggest that the eccentricity of the floc particles seems to provide an indicator of the changes in the process. Especially the lime feed seems have an influence on the formation or breaking of the floc particles. The main conclusions from testing the industrial camera system in the flocculation unit and analyzing the data are:

- Image analysis enables the monitoring of different floc properties and therefore indirect estimation of floc quality.
- The system enables both online and long-term monitoring, because it provides online information on the process, and trend lines can be used to monitor changes occurring during a longer period of time.
- The system can be programmed to alarm in case there are unwanted trends in any of the quality parameters. A warning signal could be delivered to process operators, so that they could check the condition of the floc by naked eye.
- Based on the preliminary results of data analysis it seems that there are dependences between the surface area of the floc and certain process measurements, which suggests that it is possible to create data-based models for floc quality.
- Quality models can reveal interesting factors affecting flocculation and help in studying physical phenomena behind the complex process.

[1] Chacrabarti R. K, Atkinson J.F., and Benschoten, J. E. *Characterization of Alum Floc by Image Analysis*. Environ. Sci Technology, 34 (2000), 3969-3976.

[2] Perez Y.G., Leite S.G.F., and Coelho M.A.Z. *Activated Sludge Morphology Characterization Through an Image Analysis Procedure*. Brazilian Journal of Chemical Engineering, 23 (2006), 319-330.



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## LOW-COST CAMERA SYSTEM FOR ONLINE ESTIMATION OF GRAIN SIZE IN FLUIDIZED BED

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**Introduction.** Monitoring the condition of the bed is increasingly important in fluidized bed combustion of biomass. Short- and long-term changes in the properties of the bed material, such as coarsening, may lead to incomplete combustion, decreased efficiency, an increased level of emissions and even to agglomeration of bed material. The possibilities for performing sampling and measurements in industrial-scale CFB combustors are generally rather restricted, however [1]. Monitoring the quality of the bed material in fluidized beds, for example, has to be performed manually by sieving the bottom ash, which has been transferred out of the combustion chamber. This is expensive and laborious, and should be therefore automated if possible.

Data-based soft sensors have been developed for estimating the fluidized bed quality [2], but they have certain limitations, which include the need for example data (i.e. manually acquired sieving data) and the demands for the quality of data. On the whole, it seems that there is not a widely-recognized method for monitoring the grain size of the bed material in utility- and industrial-scale CFBs online. In this paper we present a low-cost online inspection system for estimating grain size of the bottom ash in a large-scale circulating fluidized bed boiler fired by biomass using a methodology which can be fully automated. The system consists of an ordinary systems camera which is automated to snap images over the bottom ash conveyor of the boiler. The images are then analyzed to calculate an index which indicates the grain size in the ash. The index offers a tool for estimating the coarseness of the bed indirectly, without the manual sieving work.

**Process and data.** The case process is a 385 MW<sub>th</sub> large-scale industrial boiler. The boiler is fired by biomass or a mixture of biomass and peat. The biomass consists of forest residue (bark, branches, crowns, stumps etc.). The plant produces steam and electricity for a pulp and paper plant and electricity and district heat for an energy company. Images were taken from the process automatically by the system during one month in the spring of 2011. After the measurement period the system had collected 843 digital images of good quality, which yields approximately 27 images per day on an average.

**Methods.** The purpose of the study was to develop an index which would indicate the coarseness of the bottom ash. The stages for determining the grain index are as follows: **1)** Upload digital colour image to analysis, **2)** Convert image to grayscale, **3)** Adjust contrast, **4)** Convert to binary image by searching for a global threshold based on histogram shape, **5)** Find connected components (objects) using 4-neighborhood, **6)** Calculate object areas in pixels, **7)** Find those areas ( $A$ ) corresponding to particle size  $d$ , **8)** Calculate grain index:  $\sum(A \text{ particles over } d) / \sum(A \text{ all detected objects})$ .

**Conclusions.** The results show that the index indicates both short- and long-term changes in the coarseness of the material during the measurement period. On the other hand, the lack of real problems such as severe coarsening of the bed makes it difficult to draw any conclusions on the operation of the system in a problematic situation. By inspecting the trend line it becomes evident, however, that there are both periods in which the bed gets coarser and periods in which the fine material becomes more abundant. The main conclusions from testing the industrial camera system in the industrial CFB boiler are:

- An ordinary digital camera can be used for getting quality images from the ash flow.
- Image analysis enables the monitoring of grain size in the bottom ash and therefore indirect estimation of bed quality.
- The system provides online information on the process, and trend lines can be used to monitor changes occurring during a longer period of time.
- The system can be programmed to alarm in case there is a growing trend in the grain index (i.e. the bed is coarsening), which could serve as a warning signal for the process operators to either perform sieving to verify the coarsening or, alternatively, verify the coarsening straight from the online image.
- The system has several other possible future applications such as monitoring the amount of unburned fuel particles or quality control of solid fuels before combustion.

[1] Redemann K., Hartge E.-U., and Werther J. *Ash Management in Circulating Fluidized Bed Combustors*. Fuel, 87 (2008), 3669-3680.

[2] Liukkonen M., Hälikkä E., Hiltunen T., and Hiltunen Y. *Adaptive Soft Sensor for Fluidized Bed Quality: Applications to Combustion of Biomass*. Fuel Processing Technology (in press).

## KEY VARIABLE BASED DETECTION OF SENSOR FAULTS IN A POWER PLANT CASE

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Good quality of sensor data collected from an industrial process is an essential factor to reliable operation of the process. Sensor faults are almost inevitable even with the most advanced design of instruments especially in harsh industrial environments. Roughly speaking, sensor faults can be categorized as “hard faults” with abrupt changes and as “soft faults”, which are slowly developing failures. In real environments, sensor noise, deterioration, system dynamics, and changing conditions bring challenges to detection of sensor faults. In addition, it is important to distinguish sensor faults from process changes.

A physical system that involves several sensors monitoring the operating state has usually certain relationships between the sensor values. The expected value of one sensor might be obtained from the remaining sensor values involved in the same relationship. The verification of sensor values with other information is called sensor validation, which is often based on redundancy of several sensors. Physical redundancy involves redundant sensors measuring the same parameter of the system. Analytical redundancy, on the other hand, utilizes a functional relationship between the sensors that are of different types or positioned at different locations. In addition, categorization into spatial redundancy, temporal redundancy and knowledge-based redundancy is presented in literature [1], [2]. Some sensor validation methods produce sensor health information from a single sensor [3].

In this study, an approach for detection of sensor faults is presented. It is based on an identification principle, which takes into account linear relationships between process variables and a key variable. Variables without strong linear relationship to the key variable are rejected. Simple linear regression models are formed between the key variable and the identified process variables. The identified variables are then proportioned to the key variable using the response variables from the linear models. The approach defines relative limits, which are taken as quantiles from the cumulative distribution function of the proportioned data. The limits are then used to scale the identified variables and to monitor exceptionally high and low values. Scaling is linear between the relative limits and the used slope is defined based on the range, in which a data point falls.

A coal-fired power plant is used as a case to test the approach. In identification of process variables, real process data of nearly one hundred days is used. The functionality of the approach is tested with simulation of sensor faults. Electric power output is chosen as the key variable, and data from two different power output levels are used in simulations. The sensor values are artificially deflected from the actual values to cause anomalous sensor values for the studied operating states. The approach is not proper for a quickly and significantly changing operating state in the process, and therefore, such a state is seen as an anomaly in the identified variables. In addition to detection of exceptionally high and low values, trends can be checked from the scaled values. Most of the data is scaled close to zero. To mark out exceptionally low or high values, those values are scaled closer to the lower limit -2 or the upper limit 2, respectively.

According to the results, the approach can be used in systems with strong linear relationships between variables and with similar dynamic behaviour. Considering future development, building of a graphical user interface to choose the key variables and identify the related variables based on the proposed approach is encouraged. With this approach, an insight into the process characteristics is gained and the new parameters for monitoring can be quickly put into operation.

- [1] Frank P.M.: *Fault diagnosis in dynamic systems using analytical and knowledge-based redundancy – a survey and some new results*. Automatica, vol. 26 (3), 459-474, 1990.
- [2] Lee S.C.: *Sensor value validation based on systematic exploration of the sensor redundancy for fault diagnosis KBS*. IEEE transactions on systems, man, and cybernetics, vol. 24 (4), 594-605, 1994.
- [3] Ma J., Zhang J.Q., and Yan Y.: *Wavelet transform based sensor validation*. In: IEEE Colloquium in intelligent and self-validation sensors, Oxford, UK, pp. 10/1-10/4, 1999.



# MODELLING AND SIMULATING ENERGY CONVERSION PROCESSES USING MODELICA.

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This paper describes the ongoing work on modelling and simulation of energy conversion processes. The models have been implemented in Modelica language and simulated in Dymola environment. The studied processes are a biomass fired Circulating Fluidized Bed (CFB) boiler and an anaerobic digester for biogas production. The models were validated towards real process data. The models have been running on-line and off-line respectively. The aim of the paper is to demonstrate the potentials and limitations of the simulation approach proposed as well as highlight the possibility of reusing the designed libraries in other energy conversion systems. The proposed approach has shown acceptable results for process diagnostics and can be used for the study of other energy systems.

In recent years simulation of energy conversion systems has achieved a big relevance, in particular for system design, diagnostics, process optimization and operator training. Energy conversion systems models are usually complex models which required a high structured programming language and prefer dynamic models in order to reach a deeper understanding of the process. Many works have point out Modelica as straightforward object oriented language developed for modelling of large physical systems. There are several Modelica libraries for different domains, electrical, hydraulic, thermodynamic and chemical systems. However, this wide range of libraries is not always suitable for the modelling purpose.

Modelica component libraries with process components for a biomass fired CFB boiler and an anaerobic digester for biogas production were developed. The component models were represented graphically and stored in the designed Modelica libraries. Once the model components were defined the physical connection was established. Both models were validated towards real process data and run afterwards on-line and off-line.

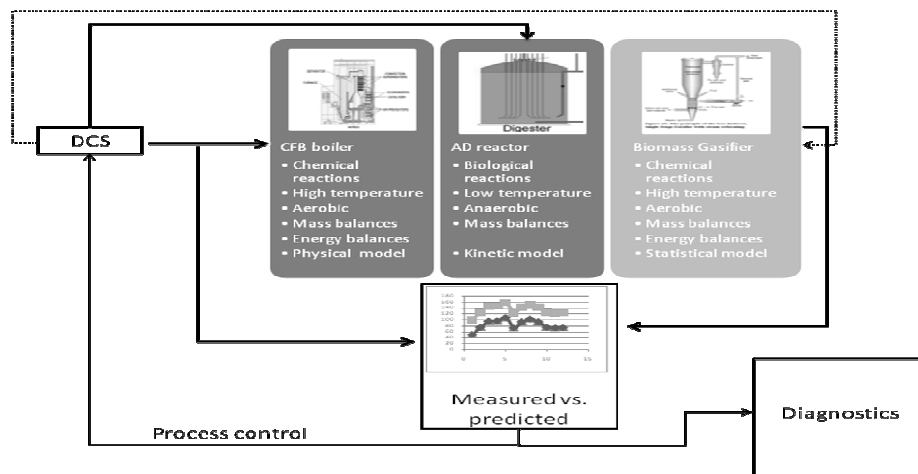


Fig. 1. Common simulation approach

This work focuses in the development of comprehensive Modelica libraries to meet the requirements of the process models. The models are based on temperatures, flows, chemical reactions, mass and energy balances and kinetic reactions. Figure 1 shows the similarities and differences between three energy conversion processes that can be considered as completely different processes but many synergies when modelling can be found. The difference between the simulation results and measured values for the studied variables are analyzed and used in diagnostic tools and to establish strategies for improved process control. In many occasions conversion processes are based on the same physical laws and can be therefore modelled in similar ways. The construction of a Modelica energy conversion library, allows reuse of the designed classes.

## MODEL-BASED ADAPTATION OF INTELLIGENT CONTROLLERS OF SOLAR COLLECTOR FIELDS

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Solar power plants should collect the available thermal energy in a usable form within a desired temperature range. The collection is controlled by the flow of oil pumped through the pipes during the plant operation. The control system consists of a nonlinear linguistic equation (LE) controller with predefined adaptation models, some smart features for avoiding difficult operating conditions, and a working point controller to adapt the setpoint to the operating conditions. The intelligent LE control activates special features when needed. Fast start-up, smooth operation and efficient energy collection is achieved even in variable operating condition. [1]

Nonlinear LE controllers are based on scaling with two second order polynomials, whose parameters are obtained with a data-driven approach introduced in [2]. The approach is based on generalised norms, which increase with increasing order, and the arithmetic mean, the harmonic mean and the standard deviation are special cases of the norms between the minimum and the maximum, which correspond to the orders  $p = -\infty$  and  $p = \infty$ , respectively [3]. In this paper new state indicators are introduced to analyse fluctuations of irradiation, temperature and oil flow: the fluctuations are obtained as moving differences of the high and the low values, which are calculated by generalised norms of orders 30 and -30, respectively, for one minute periods. The indicator is obtained in each sample time as an average of 25 latest values. The smart indicators react well to the changing operating conditions and can be used in smart working point control to further improve the operation for cloudy conditions and load disturbances. Fast changes, disturbances and oscillations increase the corrected limits, which then decrease the acceptable setpoint levels.

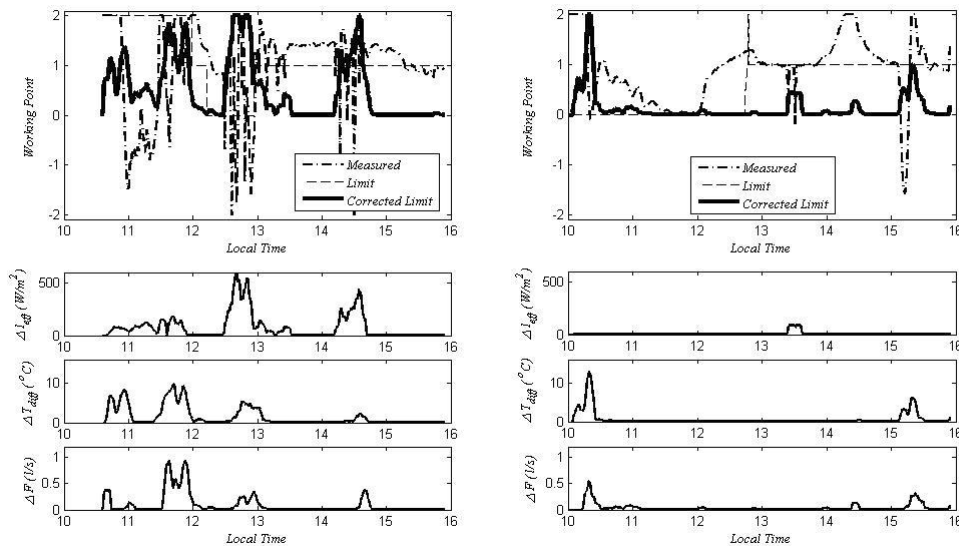


Fig. Working point and state indicators in a case on a cloudy day (left) and on a clear day with load disturbances (right).

- [1] Juuso, E.K. (2011). Recursive tuning of intelligent controllers of solar collector fields in changing operating conditions. In S. Bittani, A. Cenedese, and S. Zampieri (eds.), *Proceedings of 18th IFAC World Congress, Milano, Italy, August 28 - September 2, 2011*, 12282–12288. IFAC.
- [2] Juuso, E. and Lahdelma, S. (2010). Intelligent scaling of features in fault diagnosis. In *Proceedings of the 7<sup>th</sup> International Conference on Condition Monitoring and Machinery Failure Prevention Technologies, 22-24 June, 2010, Stratford-upon-Avon, UK*, 15 pp. BINDT.
- [3] Lahdelma, S. and Juuso, E. (2011). Signal processing and feature extraction in vibration analysis, Part 1: Methodology. *The International Journal of Condition Monitoring*, 1(2), 46–53.

# SMART ENERGY NETWORKS IN THE NORTHERN PERIPHERY: DEVELOPMENT OF AN END-USER ORIENTED PROFILED HYBRID MICRO-GRID SIMULATOR

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**Introduction.** The expression smart energy network indicates an energy production, transmission and distribution network based on a two-ways communication between suppliers and consumers; a real time monitoring of the network condition (i.e. energy production, consumption and distribution) allowing for a more prominent position on the market of those renewable energy resources characterized by a discontinuous and irregular generation [1, 2].

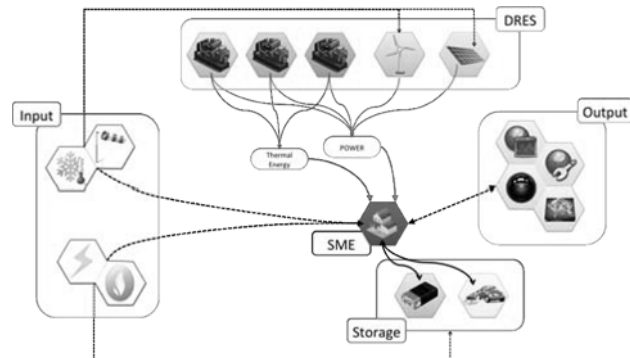
In the presented study we have been addressing the potential and the adaptability of a smart energy network based system within the Northern Periphery. A hybrid micro-grid simulator has been developed, which makes use of the available renewable energy resources on a demand-response logic principle ([3] and references therein). In this report, we present our preliminary analysis results concerning the system performance.

This project has been funded by the EU's MicrE (Micro Energy to Rural Enterprises) project and the Pohjoista voimaa Ympäristötili grant.

**System architecture** The developed simulator, built in the Matlab® Simulink environment, has been developed maintaining a modular structure in order to guarantee the highest level of scalability and adaptability. A schematic representation of the system architecture is shown in the figure below. Thought to eventually operate in real-time managing on-line data, its performance has been insofar tested on the base of predetermined signal (i.e. power consumption profile) and historical weather and environmental data (i.e. weather and energy prices data) over one year time window.

The micro-grid system can be schematically described as made of five main blocks.

- The *SME* block contains all the necessary information and operational units necessary for a basic modeling of the built environment.
- The *Input* block includes all the necessary environmental and system information.
- The distributed renewable energy sources (*DRES*) block includes a number of selectable energy production systems, some of which directly dependent onto the environmental data.
- The *Storage* block includes the electrical energy storage device and a sub-block considering the possibility of a plug-in hybrid electric vehicle (PHEV).
- The *Output* block includes all the metering and monitoring components.



Schematic representation of the developed simulator system architecture.

**Results and future developments** Our preliminary results showed that the developed system is capable to perform the required tasks and to respond to the changes in the system and environmental conditions. Thermal and electrical energy requirements were properly monitored and system requirements fulfilled.

We are currently working on the development the system able to efficiently build, monitor and manage clusters of hybrid micro-grids. Our ultimate goal is to build a tool capable of rapidly build a complex structured local or regional network, monitoring and effectively improving its performance.

- [1] International Energy Agency World energy outlook. OECD/IEA, Report. Academic Press, Paris, 2009.
- [2] U.S: Energy Information Administration International energy outlook. DOE/EIA Report-0484(2010), Office of Integrated Analysis and Forecasting, U.S: Dept. of Energy, Washington, 2010.
- [3] Caló A. Assessing the potential for smart energy grids in the Northern Periphery. Master Thesis University of Oulu, Oulu, 2011.

## EFFICIENT SOLUTION OF EQUATIONS ARISING FROM SMART ENERGY NETWORKS INCLUDING PRODUCTION AND STORAGE

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**Introduction.** The development of sustainable energy solutions, both from domestic and industrial perspective, require efficient evaluation tools that are able to produce full year scenarios of the dynamic behaviour of the energy systems based on estimated weather conditions, energy consumption rates, wind and solar energy production rates, and the flexibility of other energy resources available. Both distributed and central energy storages need to be considered in this kind of evaluations. In addition, the possibility for such long term evaluation of the economic issues, the reliability of the energy supply for consumers, and the feasibility for isolated operation in smaller islands, e.g. a smart house or smart village, are of high importance. Smart energy systems are considered as very heterogeneous whence they are including components with very different dynamics and granularity. They can be very extensive and are accordingly very challenging.

**Different propagation speeds.** The modelling approach in each analysis case depends on its scope of view. For instance, if only the behaviour of the electrical equipment used by a grid-tie photo voltaic solar cell or wind mill is studied, the rest of the grid can be considered by boundary conditions and the equipment itself can be studied with say 1  $\mu$ s time step. This step allows also for studies of harmonic noise introduced by the applied type of inverter. However, if it is a part of a large grid, its internal dynamics can be neglected. Then the model reduces to an algebraic efficiency correlation. Looking at the dynamics of a large grid, say with 1 s time step, also the study of travelling electromagnetic waves resulting e.g. from switching surges, can be neglected. However, the frequency of each grid island needs to be calculated thoroughly. The electric grid itself can be modelled with algebraic equations. In addition the dynamics of the rotating masses in the grid, the controls of the production plants and energy storages as well as the adaptability of the consumption need to be considered. Looking at district heating and cooling networks, the pressure transients moving with the speed of one kilometre per second are out of scope for the one year long studies. The heat convection flow in the range of metres per second in the pipes, and the heat diffusion proceeding with millimetres per second, are of course of interest. The accumulation of heat in fluids and structures, and the relevant condensing/boiling or solidification/melting energy, are well within the scope.

**Different sizes of control volumes.** It is of large importance to find a suitable spatial discretisation of the process for a specific dynamic study. Courant [1] has noted that the phenomena under a dynamic study not should proceed further than between two control volumes during one time step. For instance, pipe networks should accordingly be discretized into pipe sections of different lengths, depending on if the phenomenon under study is the propagation of pressure or temperature transients. Sometimes, the detailed studies of a part the process require smaller control volumes. Accordingly, it might be required to solve different parts of the process with different time steps, as well as different phenomena of the same part of the process with different time steps.

**Efficient semi-implicit solution.** Dynamic studies of smart energy networks include solution of the load flow in electrical networks and the relevant frequencies of the network islands, the pressure distribution in pipe networks as well as the energy convection, diffusion and accumulation, and also the relevant control system algorithms. After the spatial discretisation of the original partial differential equations we can consider a heterogeneous differential algebraic system. The nonlinearities and the discontinuities of the system need to be treated as well to enable the use of efficient implicit solution methods. The nonlinear coefficients originating from fluid material properties are linearized and iteratively corrected at the end of each time step. The discontinuity instances, for example the time for complete filling up of a control volume, are predicted for instant adaption of the time step. There are efficient solvers for equations arising from such sparse networks [2]. Also, specific challenges that arise from the need to speed up the solution, making use of many multi core computers in parallel, are dealt with.

**Applications and conclusions.** Experiences from example studies of selected parts of smart energy networks are presented. The Apros [3] process simulation software was used. Its new graphics interface will make it easier to specify large network models. Further developments are needed for connections to CAD and GIS databases. The feasibility to include cost calculations in this kind of dynamic simulations will be evaluated.

- [1] Courant R., Friedrichs K.O. & Levy H.: *On the Partial Difference Equations of Mathematical Physics*. IBM Journal of Research and Development 11. 1967, pp. 215-234.
- [2] Juslin K.: *A Companion Model Approach to Modelling and Simulation of Industrial Processes*. VTT Publications 574. Espoo 2005. 155 p. + app. 15 p.
- [3] Apros 2012. *Apros Process Simulation Software*. Web site <http://www.apros.fi>.

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IDENTIFICATION OF FLUX PROFILES AND KINETIC EQUATIONS FROM DYNAMIC LABELING  
EXPERIMENTS: THEORY AND COMPUTATIONS

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**Introduction.** A dynamic model for the regulation of metabolism is an essential tool for design-based metabolic engineering, and a better understanding of robustness of metabolic function. Three major challenges need to be tackled for in-vivo kinetic modeling: (1) computational limitations, since kinetic models are highly non-linear; (2) measurement limitations: the available data set contains only few observations of noisy data; and (3) distinctive experimental setup: a high excitation is required.

**Content.** In this work we propose a two-stage, sequential approach. In the first step a time-dependent flux identification is performed, which is based on concentration and labeling time series data. In the second step the outcomes are used for the identification of the kinetic functions and their parameters.

For the first step we resort to a class of dynamical models known as piecewise affine (PWA). PWA models are characterized by dynamics that are piecewise-linear-with-offset (hence, piecewise affine) over their domain of definition. PWA models are worth investigating since they are prone to formal mathematical analysis. Furthermore, there exist developed approaches and software tools to study the system identification problem for PWA models. We approximate the dynamic fluxes with time-dependent PWA functions by solving an optimization procedure. The optimization employs a sequential approach, so that a good PWA matching of the actual non-linear flux is achieved. Both concentration and labeling data are used for the identification procedure.

For the second step the estimated time-dependent dynamic fluxes are embedded onto the concentration space, based on the available observations. By integrating two existing hybrid identification software toolboxes, a concentration dependent PWA kinetic equation is reconstructed.

We have developed a number of algorithms and an overall software tool to (1) approximate a dynamic flux by a time dependent PWA function and to (2) reconstruct the concentration-dependent kinetic functions by PWA models.

- [1] Abate, A. Hillen, R.C. and Wahl, S.A.: *Piecewise affine approximations of fluxes and enzyme kinetics from in vivo  $^{13}C$  labeling experiments*. Int. J. Robust Nonlinear Control, in print, 2012.

# IDENTIFICATION OF FLUX PROFILES FROM DYNAMIC LABELING EXPERIMENTS: *S. CEREVISIAE* CULTIVATION UNDER FAST FEAST/FAMINE CONDITIONS

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**Introduction.** A dynamic model for the regulation of metabolism is an essential tool for (1) design based metabolic engineering, and (2) a better understanding of robustness of metabolic function. Three major challenges need to be tackled for in-vivo kinetic modeling: (1) Computational limitations, kinetic models are highly non-linear (2) Measurement limitations: the available data set contains only few observations of noisy data, (3) Experimental setup: a high excitation is required.

**Content.** An experimental platform based on a dynamic, cyclic feeding regime (20s feed in 400s cycle) is performed. The cycles are highly reproducible, enabling to sample first for concentrations and in a following cycle switch to a labelled substrate and sample the labelling enrichment. Thus labelling and concentration data for a dynamic analysis is obtained. A dynamic flux profile is estimated using a hybrid modelling approach [1]. This profile is integrated with the concentration data to obtain in-vivo enzyme kinetics. An aerobic culture of *S. cerevisiae* at an average growth rate of 0.1h<sup>-1</sup> is analysed and the flux profile is compared to results obtained under continuous cultivation conditions. Under dynamic conditions, storage metabolism (glycogen and trehalose) are interacting with glycolysis and seem to reduce the dynamics of flux changes.

- [1] Abate, A. Hillen, R.C. and Wahl, S.A.: *Piecewise affine approximations of fluxes and enzyme kinetics from in vivo 13C labeling experiments*. Int. J. Robust Nonlinear Control, accepted.
- [2] van Kleeff B.H.A., Kuenen, J.G., and Heijnen, J.J.: *Heat Flux Measurements for the Fast Monitoring of Dynamic Responses to Glucose Additions by Yeasts that were subject to different Feeding Regimes in Continous Culture*, Biotechnol. Prog. 1996, 510-518



## COMPUTING COMPLEX METABOLIC INTERVENTION STRATEGIES USING CONSTRAINED MINIMAL CUTSETS

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An important application of stoichiometric models of metabolic networks is the identification of targeted modifications and rational redesigns of microorganisms for the production of fuels or chemicals. One theoretical approach is based on Minimal Cut Sets (MCSs) which are minimal sets of reactions whose knock-out will abolish a given (target) function in the network. MCSs can be computed from the set of elementary modes (EM) enabling the target function and are useful for target identification, robustness analysis or diagnosis. However, in their original definition, MCS may induce undesired side effects (e.g. biomass synthesis becomes infeasible) limiting its practical use for designing intervention strategies. We, therefore, generalize MCSs to Constrained MCSs (cMCSs) and adapted the algorithm for computing MCSs accordingly. With the additional definition of a set of desired modes, of which a minimum number must be preserved, the cMCSs approach allows systematic enumeration of all equivalent gene deletion combinations and also helps to determine robust knockout strategies for coupled product and biomass synthesis. Moreover, many existing methods (even those based on mixed integer linear programming) can be reformulated as special cMCS problems. Case studies will illustrate the applicability and enormous flexibility of the proposed approach in defining and solving knockout problems.

- [1] Hädicke O., and Klamt S.: *Computing complex metabolic intervention strategies using constrained minimal cutsets*. *Metab. Eng.*, 13 (2011), 204-213.
- [2] Klamt S.: *Generalized concept of minimal cut sets in biochemical networks*. *BioSystems.*, 83 (2006), 233-247

## VISUALLY-ASSISTED MODELING OF KINETIC METABOLIC NETWORKS – FROM OMX TO MODELICA AND BACK

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**Background.** Kinetic-based modeling of intracellular processes is an emerging field in systems biology [1]. Here, mechanistic models base on components and interactions between them, the *metabolites* the *reactions* and their *regulation*, respectively. The related quantitative information, i.e. metabolite concentrations, reaction rates and regulatory strength, usually stipulate the appropriate model structure and the participating kinetic parameters. By integration of the metabolic network backbone, the component interactions and a diversity of measured multi-omics data the unknown kinetic model parameters are identified.

**Challenges.** The accompanying modeling approach involves several challenges:

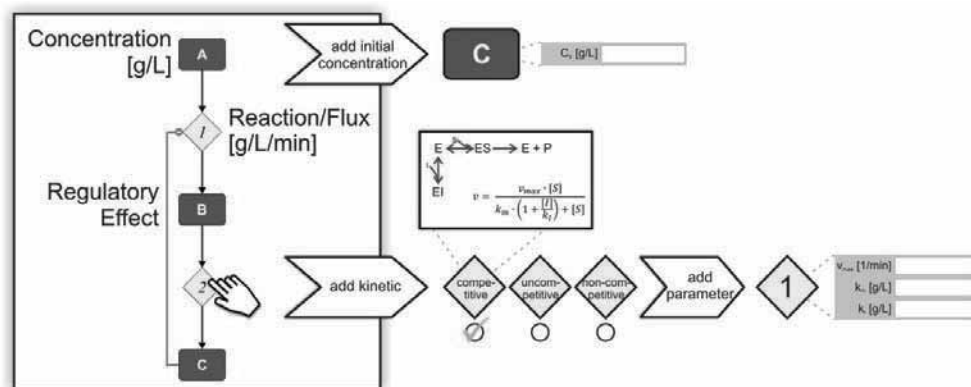
- Countless types of catalytic mechanisms for the enzyme-driven transformation of substrates into products are referred to in literature and public databases. These types may be nearly arbitrarily complex.
- The choice of the kinetic mechanism depends intimately on experimental data and may vary from organism to organism. Moreover, in many cases the selection is driven by educated guesses driven by the background knowledge of experts.
- Sometimes, the enzymatic mechanism is not clear at all and several possibilities have to be hypothesized.
- Even if the mechanism is known, available data may not be sufficient to identify the kinetic parameters. Thus, approximate enzymatic rate laws with fewer unknowns have to be applied.

Summarizing, the model composition procedure as well as the subsequent simulation and evaluation workflow particularly for large-scale kinetic models is iterative, time-consuming, and typically error-prone.

**Modeling Workflow.** We propose a flexible framework to set up kinetic models in a visually-assisted manner. After model assembly, efficient source code is generated that is compiled and used for simulation and model analysis:

1. As graphical modeling front-end the network editor and visualization tool OMX is used, a software developed to draw customizable network diagrams [2].
2. For simulation the multi-domain modeling language MODELICA and the software environment DYMOLA are chosen [3].

This combination allows for object-oriented modeling, i.e. the setup of easily extensible kinetic libraries, a drag-and-drop like assembly of large-scale models from kinetic mechanisms deposited in these libraries and, finally, the automatic generation of very fast simulation code. Finally, the simulation results are visualized in the original network diagram. The simplification potential of our graphical-based modeling workflow is demonstrated with a realistic example.



Adding kinetic mechanisms and concentration values to a network diagram drawn in OMX

- [1] Steuer, R.: *Exploring the Dynamics of Large-Scale Biochemical Networks: A Computational Perspective*. The Open Bioinformatics Journal, 5 (2011), 4-15.
- [2] Droste, P., et al., *Visualizing multi-omics data in metabolic networks with the software Omix-A case study*. BioSystems, 105(2011), 154-161.
- [3] Elmqvist, H., *Object-Oriented Modeling and Automatic Formula Manipulation in Dymola*, 1993.

## MULTI-OBJECTIVE EXPERIMENTAL DESIGN OF LABELING EXPERIMENTS – REVISITING OPTIMALITY CRITERIA

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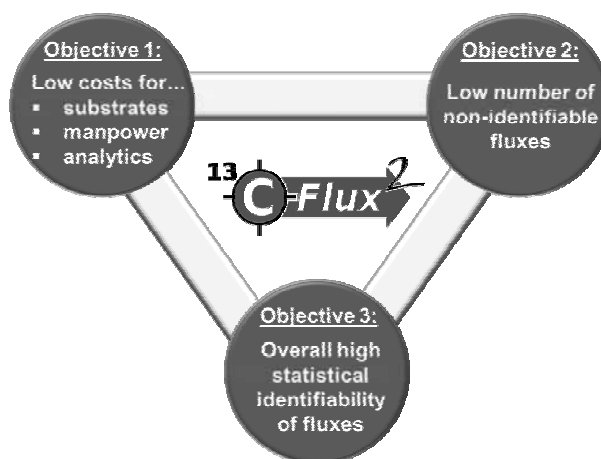
**Abstract.** In systems biotechnology costly carbon labeling experiments are the methods of choice to estimate otherwise non-measurable reaction rates, or synonymously the metabolic fluxes, within living cells [1]. The quality of the rate estimation, i.e., the final metabolic flux map, strongly relies on the combination of specifically labeled substrates used and the measurements (in type, quantity, and quality) at hand.

In our contribution we investigate the application of multi-objective evolutionary algorithms in the identification of the pay-off characteristic between total experimental cost, information content of measurements, and reliability of flux maps. Therefore, a decision maker is formulated that accounts for the conflicting objectives involved:

- (1) costs of labeled substrate species and efforts of analytic sample processing,
- (2) model-related structural flux non-identifiability, and
- (3) measurement accuracy-related practical flux non-identifiability.

The resulting multi-objective problem is high-dimensional, non-linear and highly constrained.

The JAVA framework jMetal [2], which contains several state-of-the-art algorithms, is used to identify a set of Pareto optimal experimental designs. We compare the algorithms SPEA2 and SMPSO to find D-optimal designs for a realistic scenario. Results are compared amongst alternative information criteria, i.e., A- and E-optimal designs [3]. The derived methodology is used to plan economic whilst informative labeling experiments for a yeast model organism.



- [1] Zamboni N., Fendt S. M., Rühl M., Sauer U.: *<sup>13</sup>C-based metabolic flux analysis*. Nature Protocols, 4 (2009), 878-892.
- [2] Durillo J. J. and Nebro A. J.: *jMetal: A Java framework for multi-objective optimization*. Advances in Engineering Software, 42 (2011), 760-771.
- [3] Pukelsheim F.: *Optimal Design of Experiments*. Wiley, Philadelphia, 2006.

## THE IDEAL MODEL OF CHROMATOGRAPHY AS A TOOL FOR PROCESS DESIGN

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Production scale chromatographic separation is widely applied in pharmaceutical and fine chemicals industry, food and sweeteners industry, as well as in biotechnological applications. Simulation of chromatographic separation units is interesting from the mathematical modelling point of view because the separation columns are operated in a non-steady state mode. The separation is based on differences in the velocities at which the various compounds travel through the separation column. Velocity differences originate from distribution of the compounds between the mobile (liquid or gas) phase and the stationary phase, which is governed by thermodynamics.

Various mathematical models of different degree of complexity and detail are often used to describe the process. The relevant physical phenomena include hydrodynamics, mass transfer rates, and phase equilibrium thermodynamics. In some cases, complex formation kinetics in the adsorbed phase or speciation equilibrium in the liquid phase need to be taken into account. On the other hand, the simplest of all models – the “ideal model of chromatography” – has become a powerful tool for designing chromatographic separation processes. This is because it can in certain important cases be solved analytically. The ideal model neglects all kinetic and dispersive effects, and thus reduces to a coupled system of quasilinear first order PDEs. The solution procedures around the ideal model are often referred to as the Equilibrium Theory of chromatography.

This contribution focuses on the recent developments in application of the Equilibrium Theory in design and analysis of various chromatographic separation processes. The process modes discussed include batchwise operated single column [1] and continuously operated multicolumn systems, systems with internal recycling [2], and integrated chromatographic and membrane separation units [3].

It is shown that such a heavily simplified (and thus unrealistic) mathematical model is useful also for practical process design. For example, it may give the upper limit of process performance with given operating parameters or approximate values of operating parameters to satisfy given design constraints. Moreover, analytical solutions of the governing equations enable analysis of process behaviour (e.g., the feasible range of operating parameters) and performance (e.g. sensitivity of performance for certain operating parameters).

- [1] Siitonen, J., Sainio, T., *Explicit equations for the height and position of the first component shock for binary mixtures with competitive Langmuir isotherms under ideal conditions*, J. Chromatogr. A., 1218(2011), 6379-6389.
- [2] Sainio, T., Kaspereit, M., *Analysis of steady state recycling chromatography using equilibrium theory*, Sep. Purif. Technol., 66(2009), 9–18.
- [3] Siitonen, J., Sainio, T., Kaspereit, M., *Theoretical analysis of steady state recycling chromatography with solvent removal*, Sep. Purif. Technol, 78(2011), 21-32.

## SIMULATION OF NON-ISOTHERMAL REACTIVE CHROMATOGRAPHIC PROCESSES

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This work is focused on modelling and simulation of non-isothermal reactive liquid chromatography. The model is formed by a system of convection-diffusion-reaction partial differential equations. The corresponding systems have to be solved numerically because analytical solutions are usually impossible to derive or available only in simple (ideal) situations. The simulation of non-isothermal reactive chromatography is generally a challenging task for a numerical scheme due to the nonlinearity of the convection dominated mass and energy balance equations and because of stiffness of the reaction terms. A high resolution finite volume scheme is implemented to solve the model equations. The scheme is a flux-limiting scheme in which fluxes are limited by using a nonlinear minmod limiter. This limiting procedure guarantees the positivity of the scheme and hence suppresses the numerical oscillations, usually encountered in the numerical schemes of second and higher orders. In the semi-discrete form, the scheme has a third order accuracy in space. The scheme is robust and gives high order accuracy on coarse grids, resolves sharp discontinuities, and avoids numerical dispersion which may lead to incorrect solutions. Thermal effects are typically neglected in reactive liquid chromatography. In this work, reactive liquid chromatography is investigated theoretically considering thermal effects that originate from heats of reaction and adsorption enthalpies. The results of systematic parametric studies demonstrate that temperature gradients can significantly influence conversion and separation in reactive liquid chromatography. To validate the results, several consistency tests and evaluations of trivial studies are carried out. The results prove the accuracy of the numerical scheme and agree well with theoretical predictions for limiting cases. The key parameters that influence the reactor performance are systematically investigated. It was found that the heats of reaction and the enthalpies are the reason for complex concentration and temperature profiles. It is important to mention, that higher conversion can be achieved under non-isothermal conditions as compared to isothermal chromatographic reactor operation. It was observed, that in particular an exothermic heat of reaction can be source for the development of a positive thermal waves leading to significant improvements in conversion and separation. The simulation results acquired in this study emphasize the necessity to account in more detail for thermal effects in reactive liquid chromatography.

- [1] Rhee, H.-K., Aris, R., Amundson, N.R., *First-order partial differential equations. Theory and Application of Hyperbolic Systems of Quasilinear Equations*, vol. II. Prentice-Hall, New Jersey, 1989.
- [2] Lieres, E.V., Andersson, J.: *A fast and accurate solver for the general rate model of column liquid chromatography*, Computers & Chemical Engineering, 34, (2010), 1180-1191.
- [3] Javeed, S., Qamar, S., Seidel-Morgenstern, A., Warnecke, G.: *Efficient and accurate numerical simulation of nonlinear chromatographic processes*, Computers & Chemical Engineering, 35, (2011), 2294-2305.
- [4] Javeed, S., Qamar, S., Seidel-Morgenstern, A., Warnecke, G.: *A discontinuous Galerkin method to solve chromatographic models*, Journal of chromatography A, 1218, (2011), 7137-7146.
- [5] B. Medi, M. Amanullah, *Application of a Finite-Volume Method in the Simulation of Chromatographic Systems: Effects of Flux Limiters*, Ind. Eng. Chem. Res. 50 (2011), 1739-1748.
- [6] Koren, B. *A robust upwind discretization method for advection, diffusion and source terms. In C. B. Vreugdenhil, B. Koren (Eds.), Numerical Methods for Advection- Diffusion Problems*, Volume 45 of Notes on Numerical Fluid Mechanics, 117-138, Vieweg, Braunschweig 1993.

## SIMULATION OF CONTINUOUS PREFERENTIAL CRYSTALLIZATION PROCESSES

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An attractive process for gaining pure enantiomers from racemic mixtures is the so-called preferential crystallization (PC) which has been realized up to now in a discontinuous operation mode. For elucidating the principle of a continuous enantioselective process one might consider a suspension crystallizer revealing MSMPR characteristics, i.e. a perfectly mixed tank (concerning both phases), which is continuously fed with a solution possessing a racemic composition of two enantiomers. Solid particles and liquid phase are continuously withdrawn. By a continuous supply of homochiral seed crystals of the preferred target enantiomer the preferential crystallization (PC) of only this enantiomer is initialized, i.e. growth of the seed crystals and possibly secondary nucleation of crystals of the seeded enantiomer, provided the crystallization takes place within the metastable zone where spontaneous, uncontrolled primary nucleation is kinetically inhibited. During a starting-up period, which strongly depends on the properties of the system as well as on the process parameters, the concentration of the target enantiomer is decreasing until a steady state is reached where the composition is determined by the mean residence time. Due to different kinetic mechanisms and their inherent different time constants, a different depletion of the supersaturation for each enantiomer can be realized by an appropriate choice of the process conditions. As long as a critical mean residence time, where primary nucleation may appear, is not exceeded, the concentration of the undesired counter enantiomer remains constant during the whole time. This fact reveals a benefit of this continuous process in comparison to the batch one. An optimal selection of the process conditions allows a constant production of the goal enantiomer at a high purity level. This contribution investigates the effects of different seeding strategies and residence time characteristics on the dynamics of a Mixed Suspension Mixed Product Removal (MSMPR) crystallizer equipped with a fines dissolution unit. For the first time continuous preferential enantioselective crystallization is investigated. The fines dissolution is included as recycle streams around the MSMPR crystallizer. Moreover, primary heterogeneous and secondary nucleation mechanisms along with size-dependent growth rates are taken into account. Different seeding and operating strategies are numerically investigated. The high resolution finite volume schemes and evolution Galerkin finite element methods are employed to solve the model equations. Several numerical case studies are carried out. To judge the quality of the process some goal functions are used such as product purity, productivity, yield and mean crystal size of the preferred enantiomer. These goal functions give detailed information about the success and potential of continuous preferential crystallization. The results obtained could be used to find the optimum operating conditions for improving the product quality and for reducing the operational cost of continuous preferential crystallization. Altogether, the process appears to possess large potential and deserves practical realization which is currently in progress.

- [1] Elsner, M.P., Ziomek, G., Seidel-Morgenstern, A.: Simultaneous preferential crystallization in a coupled, batch operation mode—Part I: Theoretical analysis and optimization, *Chemical Engineering Science*, 62, (2007), 4760-4769.
- [2] Elsner, M.P., Ziomek, G., Seidel-Morgenstern, A.: Efficient separation of enantiomers by preferential crystallization in two vessels, *AIChE Journal*, 55, (2009), 640-649.
- [3] Qamar, S.Elsner, M.P.; Angelov, I., Warnecke, G., Seidel-Morgenstern, A. : A comparative study of high resolution schemes for solving population balances in crystallization, *Computers & Chemical Engineering*, 30, (2006), 1119-1131.
- [4] Qamar, S., Hussain, I., Seidel Morgenstern, A.: Application of discontinuous Galerkin scheme to batch crystallization models, *Industrial and Engineering Chemistry Research*, 50, (2011), 4113–4122.

# NUMERICAL ANALYSIS OF MODEL UNCERTAINTIES AS A RESULT OF EXPERIMENTAL UNCERTAINTY — AN EXAMPLE FROM PREPARATIVE CHROMATOGRAPHY

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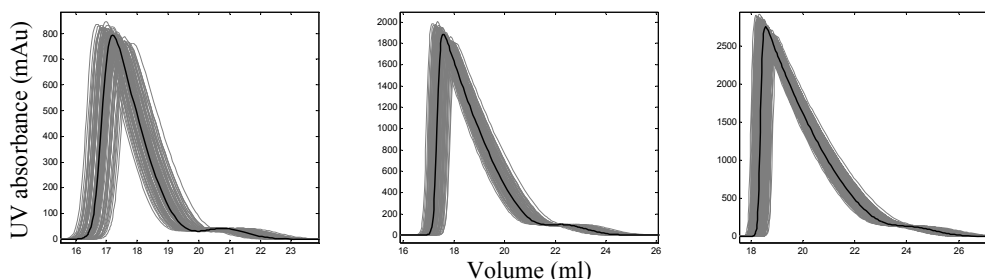
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Preparative chromatography of biological products is well suited for model-based process design and mechanistic, nonlinear models have been used for design of separations [1] and for analysis of the performance and robustness of the process under selected operating conditions [2]. For a complete model-based analysis the effect of the model uncertainty should also be taken into account. Model uncertainty is the combined uncertainty of the model structure and of the model parameters. Experimental error can be assumed to be normally distributed whereas errors due to model structure are thought to be systematic. The assessment of model parameter uncertainty caused by experimental errors, and how this uncertainty can be taken into account in the model-based design methodology, are the focus of this work.

Chromatographic processes are nonlinear, small errors in experimental conditions may cause large error in the process output. Moreover, when the process output is measured by an in-line UV detector the measurement error is small. Therefore common methods to estimate model parameter uncertainties that assume a normally distributed error on the experimental measurements are not suited for when chromatographic models are fitted to this data. Instead, a version of the Monte Carlo simulation method was used where the calibrated model was used to generate a large number of new data sets where a random error  $\varepsilon$  was added on the experimental conditions  $x$  instead of the measurement data  $y$ :

$$y^k = f(x + \varepsilon, \hat{p}) \quad (k = 1, 2, \dots, K)$$

where  $f$  and  $p$  are the model and model parameters calibrated to the original experimental data. New model parameter sets  $p^k$  were found by recalibrating the model to the data sets  $y^k$  and the model parameter covariance estimated from these.



An example of the simulated experimental chromatograms (grey) together with the nominal simulation (black).

The proposed methodology is showed for a case study of robust design of a chromatographic separation. Modelling had been used to design the product pooling strategy, based on the UV absorbance measurements during the processing, so that the quality is robust to process disturbances in a previous study [2]. By recalibrating the model to Monte Carlo simulations with experimental errors the model parameter correlations to eachother and to the process conditions were found. It is shown that this methodology can be used also in the presence of model parameter uncertainty since the qualitative effects of the process variance stay the same independent of the actual values of the model parameters.

- [1] Degerman, M., Jakobsson, N. and Nilsson, B.: *Constrained Optimization of a Preparative Ion-Exchange Step for Antibody Purification*. In: Journal of Chromatography A, 1099 (2006), 157-166.
- [2] Westerberg, K., Borg, N., Andersson, N. and Nilsson, B.: *Supporting Design and Control of a Reversed Phase Chromatography Step by Mechanistic Modeling*. In: Chemical Engineering & Technology, 35 (2012), 169-175.

## DISTRIBUTED PORE SURFACE MODEL

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**Introduction.** It is not uncommon to separate aggregates and impurities from monomers of antibodies with ion exchange chromatography. For this kind of system the components clearly have different sizes. For an ion exchange resin with a wide pore distribution and differently sized proteins, the described problem is likely to appear. A way to analyse and deal with this problem was developed based on a work by Gu et al. (1991). The difference in apparent particle porosity for all proteins, with the assumption that the ligand concentration in the particle is homogeneous, can then be used to determine the competitive effects.

**Distributed Pore Surface Model.** the difference in apparent porosities can be used to determine how the competitive effects can be described. The pore surface can be divided into porosity fractions,  $\theta_f$ :

$$\theta_f = \begin{cases} \varepsilon_{p,f} - \varepsilon_{p,f-1}; & f \geq 2 \\ \varepsilon_{p,f}; & f = 1 \end{cases}$$

The apparent porosities in the model are numbered ascending and without duplicates. For the fractions of pores smaller than the specific component the ligands cannot be reached, and the component is therefore excluded from participating in the displacement, described by the size exclusion factor,  $\delta$ :

$$\delta_{f,i} = \begin{cases} 1; & \varepsilon_{p,i} \geq \varepsilon_{p,f} \\ 0; & \varepsilon_{p,i} < \varepsilon_{p,f} \end{cases}$$

Large proteins therefore cannot displace smaller proteins completely even if they bind harder, since they do not bind to participate in the competition in all fractions.

The adsorption source term for the desorbed concentration with discretized pore surface competitive adsorption isotherms is the product of a volumetric ratio and the sum of the components' desorption rates.

$$a_i = -\frac{V_{c,i}}{V_{q,i}} \sum \frac{\theta_f}{\varepsilon_{p,i}} \frac{\partial q_{i,f}}{\partial t}$$

**Method.** Isotherm parameters and operation conditions were chosen to give reasonable, but not complete, separation. The isotherm parameters are assumed to be a result of a single component inverse method calibration. To look at how different apparent porosities affect the process, a capacity estimation that does not depend on the apparent porosity is needed.

The volume of packed bed was used as countable for the capacity or shielding factor, under the assumption that they were determined on a column with known packing void but unknown apparent particle porosity.

A set of apparent porosities was simulated with a kinetic-dispersive model with and without distributed pore surface. This way the cases where the distributed pore differs most from conventional displacement models can be found.

**Results.** Most effect of the distributed pore model can be seen for the cases when the weaker binding component has the largest apparent particle porosity and the component with higher concentration, in this case the aggregate, has the smallest apparent particle porosity. When this happens, the smaller protein is displaced less than for the other cases.

**Conclusions.** A general model structure for handling different apparent porosities in chromatography has been proposed. It adapts known isotherms to give better displacement effects without adding extra parameters. The implemented model structure works with different mass transfer models and isotherms.

As can be expected the greatest difference appears when a hard binding components has much lower apparent porosity than a weaker binding component.

This model can be used to describe separations where experimental competitive effects are smaller than predicted by standard models. The distributed pore surface model always predicts the same or less displacement than a standard isotherm model.



## SPATIAL HOMOGENEITY ANALYSIS OF PACKED BED CHROMATOGRAPHY

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**Abstract.** Packed bed chromatography is usually modeled in one or two spatial dimensions, for example by the general rate model. Such models assume that fluid flow and solute molecule concentrations are homogeneously distributed over column cross sections. Moreover, concentration gradients within the beads are at most considered along the radial coordinate.

These homogeneity assumptions are studied with a three-dimensional model of the involved convection, diffusion and adsorption processes. Due to the complex geometry only bed sections with up to several hundred spheres can be computed on personal computers. Simulation studies are performed for random packings that present sections of small columns with volumes on the micro-liter scale.

Complex flow profiles and dominant wall effects are observed in the interstitial volume. The resulting concentration profiles in the interstitial column volume and within the porous beads can vary as strongly along the radial coordinate as along the axial coordinate of the column.



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# MULTISCALE COMPUTATIONAL MODELING OF COMPOSITE NANOMATERIALS IN TISSUE ENGINEERING SCAFFOLDS AND PROTECTIVE SHIELDS

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**Abstract.** Traditional experimental and computational techniques are inadequate for the development and analysis of nanocomposite based materials as they are either too expensive (e.g. experimental methods) or are unable to capture the properties of the advanced materials (e.g. using conventional computational techniques). Multiscale analysis strategies are therefore required for the analysis of these nanocomposites based materials. In the first part of the talk, determination of material properties of nano-composites using a multiscale model is presented. In these multiscale models, analysis is performed at the atomistic scale using MD simulations, and the properties are scaled-up using various linear and nonlinear homogenization techniques. Material properties are derived at the macroscale for scaffolds in a bioreactor and for shields to protect soft tissues during impact with a projectile. Use of nano-polymeric scaffolds for tissue engineering applications has gained attention recently due to the enhanced mechanical properties of the nano-structures. The effective property of the nanofiber scaffold estimated from this study was compared with experimental data and was found to be in good agreement. Similarly, the effectiveness of nanocomposite shields is energy dissipation thereby mitigating some of the severe effects of projectile impact is presented. To maintain optimal growth environments for the tissue growth in a bioreactor, it is necessary to provide adequate nourishment of nutrients and removal of waste materials from the scaffolds. Computational modeling of nutrient transfer is complicated as the mass transport equations should be concurrently solved in the fluid and scaffold/fiber domain. In the second part of this talk, a theory of mixtures based finite element model for nutrient transfer in the fluid and porous domain is presented. The model considers the open channel-porous domain as a single continuous domain with the momentum and mass transfer occurring at the interface. The nutrient transfer in the bioreactor is then studied by incorporating convection-diffusion equations into the theory of mixture framework. The developed finite element model developed in this work would be a great tool in the study of both fluid flows through the porous-open channels as well as optimizing the nutrient distribution in a HFMB.

**ABSTRACT GENERATED FROM REVIEW ABSTRACT**

## CHANGES ON THE ARCHITECTURAL AND MATERIAL SCALE OF LIVING BONE

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**Introduction.** The structure of living bone changes continuously due to the processes of bone remodeling and mineralization. The network-like trabecular bone is remodeled by resorption and deposition of small bone packets from and to the surface. The typical shape of such a bone packet is a roughly semi-cylindrical “trench” running along a rod-like trabecula. The remodeling is rather slow with resorption taking a few weeks, while new bone deposition even takes months. The newly deposited bone initially only consists of an organic collagen matrix. Only with time, mineral particles are incorporated into the matrix, which increases the stiffness of the bone material. This incorporation of mineral occurs over years. As a result of bone remodeling and mineralization, the structure of bone is a patchwork of bone packets of different mineral content. In bone remodeling the behaviour of cells is decisively controlled by mechanical stimuli. How mechanical stimulation regulates in detail cell behavior is very challenging to study in animal experiments. Computer experiments are an alternative approach to test our understanding of the mechanobiological control of these processes in bone. In a phenomenological computer model different hypotheses of cell reaction can be implemented, and the resulting consequences on the bone structure and its time evolution can then be compared with experiments.

**Models.** Two models for bone remodeling will be presented. The Markov chain model [1] is simplified enough so that the model allows concluding from architectural parameters on the remodeling rules controlling the process. In the more sophisticated cellular lattice model [2, 3, 4], the research strategy is inverted. Now, different remodeling rules are implemented and their effect on the time evolution of the trabecular architecture is studied. On a submillimeter length scale, the third model approach describes the time-dependent material heterogeneity of trabecular bone in the form of a partial differential equation [5, 6]. The material heterogeneity is characterized by the bone mineralization density distribution (BMDD), which describes how likely it is to find bone with a given mineral content in a bone sample.

**Results and Discussion.** In the cellular lattice model of bone remodeling we chose as candidates for remodeling rules “generic” functions like a linear or step-like increase of the bone deposition probability as a function of the mechanical stimulus. The different remodeling rules are then implemented into the model and the resulting time evolution of the trabecular architecture is compared with experimental data. The simulations showed that the effect of different remodeling rules can best be distinguished when the system is perturbed. As perturbations, standard therapies against osteoporosis were “mimicked”, i.e., physical exercise was modeled by an increase of the external loading, and an antiresorptive therapy was modeled by a reduction of the probability of bone resorption. A step-like remodeling rule showed the best agreement with experimental evidence [3]. This control of bone remodeling via a threshold of the mechanical stimulation is also in reasonable accordance with results obtained with the Markov chain model.

The model for the material heterogeneity of bone was employed to predict the time evolution of the BMDD for important clinical scenarios. Bone diseases and pharmaceutical therapies often cause a change in the rate of bone turnover. For example, in postmenopausal osteoporosis the rate of remodelling is increased, while an antiresorptive treatment with bisphosphonates decreases the bone turnover.

- [1] Rusconi M., Valleriani A., Dunlop J.W.C., Kurths J., Weinkamer R. (2012). Quantitative approach to the stochastics of bone remodeling, *Europhysics Letters*, in press.
- [2] Weinkamer R., Hartmann M.A., Bréchet Y., Fratzl P. (2004). Stochastic lattice model for bone remodeling and aging. *Physical Review Letters*, 93, 228102.
- [3] Dunlop J.W.C., Hartmann M.A., Bréchet Y.J., Fratzl P., Weinkamer R. (2009). New suggestions for the mechanical control of bone remodelling. *Calcified Tissue International*, 85, 45-54.
- [4] Hartmann M.A., Dunlop J.W.C., Bréchet Y.J.M., Fratzl P., Weinkamer R. (2011). Trabecular bone remodeling simulated by a stochastic exchange of discrete bone packets from the surface. *Journal of the Mechanical Behavior of Biomedical Materials*, 4, 879-887.
- [5] Ruffoni D., Fratzl P., Roschger P., Klaushofer K., Weinkamer R. (2007). The bone mineralization density distribution as a fingerprint of the mineralization process. *Bone*, 40, 1308–1319.
- [6] Ruffoni D., Fratzl P., Roschger P., Phipps R., Klaushofer K., Weinkamer R. (2008). Effect of temporal changes in bone turnover on the bone mineralization density distribution: a computer simulation study. *Journal of Bone and Mineral Research*, 23, 1905–1914.

## MICRO AND NANO SCALE ANELASTIC PHENOMENA IN HUMAN DENTIN

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**Introduction.** Dentin is a complex hydrated biological composite consisting of about 50 vol% mineral in the form of apatite, 30 vol% organic matter, which is largely type I collagen, and about 20 vol% fluid. Other non-collagenous proteins and organic components are also present in small amounts.

On a macro scale dentin can be modelled as a continuous fibre-reinforced composite, with the intertubular dentin forming the matrix and the tubule lumens forming the cylindrical fibre reinforcement. On a meso scale intertubular dentin is formed by fibres randomly oriented in a plane perpendicular to the direction of dentin formation. On a nanoscale the characteristic features are collagene fibrils, apatite crystals and water. Each fibre consists of several fibrils (50-100 nm in diameter) which exhibit periodically spaced gaps. Three polypeptide chains are wound together in a triple helix. A triple-helical molecule is cylindrically shaped (diameter of  $\sim 1.5$  nm, length of  $\sim 300$  nm). The molecules are all parallel, but their ends are separated by holes of about 35 nm, they pack together to form a single fibril. The mineral is either within the fibrils (intrafibrillar) or between the fibrils (interfibrillar). The shape of apatite crystals is needle-like near the pulp and progressively becomes plate-like near the enamel, the thickness,  $\sim 5$  nm, does not change with location. Water is the third major component and is located within and between the fibrils, between fibres and between triple-helical molecules.

This work focuses the attention on damping phenomena occurring from 100 K to 673 K. The samples have been subjected to Mechanical Spectroscopy experiments using the method of frequency modulation. Damping ( $Q^{-1}$ ) has been determined from the logarithmic decay of flexural vibrations and dynamic modulus  $E$  from the resonance frequency  $f$  [1].

**Results above room temperature.** As temperature increases a broad and asymmetric  $Q^{-1}$  maximum at 523 K has been observed; it is no more present during the successive cooling to room temperature testifying the occurrence of an irreversible transformation. TGA shows a remarkable weight loss in the same temperature range of the maximum and two stages have been identified, which basically correspond to the ascending (stage 1) and descending (stage 2) parts of the maximum. The results have been related to loss of fluids and degradation of collagen.

Another set of MS tests have been carried out vs. strain amplitude at room temperature. In each strain ramp  $Q^{-1}$  progressively increases while modulus decreases. Recovery of original anelastic properties occurs when strain decreases to the initial value. The phenomenon has been ascribed to the breaking of weak H-bonds between polypeptide chains forming the triple-helix in collagen with consequent increase of the mean length of vibrating chain segments.

**Results below room temperature.** Repeated cooling-heating cycles in the range 300-100 K have been carried out on the same samples. In the cooling stage of the first cycle  $Q^{-1}$  exhibits a very broad maximum due to a series of phase transformations involving water present in the pores, in the interstices between fibres, between fibrils and inside collagen triple helix. The formation of ice  $I_h$  produces permanent damages to the dentin structure (rupture of fibres and fibrils) leading to a decrease of maximum intensity in the following cycles.

In the heating stage of all the cycles two maxima, M1 and M2, have been observed around 155 K and 178 K. M1 is due to the transformation of low-density amorphous (LDA) ice into ice  $I_C$  while M2 to that of ice  $I_C$  to ice  $I_h$ . Above 200 K,  $Q^{-1}$  progressively increases with lower damping values in the cycles after the first one. Dehydrated samples do not exhibit the aforesaid anelastic phenomena confirming that their origin is connected to water and its transformations.

[1] Amadori, S., Campari, E.G., Fiorini, A.L., Montanari, R., Pasquini, L., Savini, L., and Bonetti, E. *Automated resonant vibrating-reed analyzer apparatus for a non-destructive characterization of materials for industrial applications*. Materials Science and Engineering A, 442 (2006), 543-546.

# MULTISCALE MODELLING ON BONE MECHANICS - APPLICATION TO TISSUE ENGINEERING AND BONE QUALITY ANALYSIS

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**Introduction.** One of the main functions of bone is to provide support to soft tissue and protect the organs of the body. This structural function of bone is enhanced by the characteristics of bone tissue. In fact, bone is a natural biological material that can adapt its structure depending on diverse factors including the mechanical environment. The structural arrangement of bone tissue can be observed at different scales. At a first level (macroscale) a non-homogeneous distribution of apparent density leads to different type of bone, the compact bone and spongy bone; at a second level the trabecular architecture of bone characterizes the mechanical properties such as bone anisotropy, and at the lowest levels we can distinguish different stages of mineralization and arrangements of the collagen fibres, among others. A mathematical description of the behaviour of bone at these different scales is essential not only to understand the bone adaptation but also to evaluate the bone quality helping on the diagnosis of bone disease such as osteoporosis and to build models that are able to support the design of new bone implants and scaffolds for bone tissue engineering.

**Methods.** In this work the multiscale model proposed by the authors [1,2] is explored to study its capabilities as a design tool for bone substitutes as well as to analyse the bone behaviour in case of disease. The bone adaptation is modelled as a two-scale material distribution problem where not only the apparent density is determined but also the trabecular structure of bone is characterized. The solution is obtained assuming that bone adapts itself to maximize stiffness and to satisfy biological driven constrains such as the cost of bone formation, the relation between volume fraction and bone surface area density and the permeability necessary for mass transport (nutrients, blood supply, etc). The model is compared with some clinical data obtained by DXA enabling to understand the influence of the parameter in the model that controls the bone formation. Furthermore, the multiscale model is applied to design bone substitutes presenting a microstructure with properties equivalent to the actual bone.

**Results.** The bone density distribution on the macroscale is equivalent to the one obtained by models which work with a single design scale only. The microstructure for each bone site has properties that are equivalent to bone anisotropic properties and it respects the bone surface area and permeability constraints when that information is included in the model (figure 1). The distribution of bone density is comparable with the data obtained by DXA and the microstructure evolution predicted by the model as bone becomes osteoporotic shows that there are preferential directions that tend to maintain its structural strength.

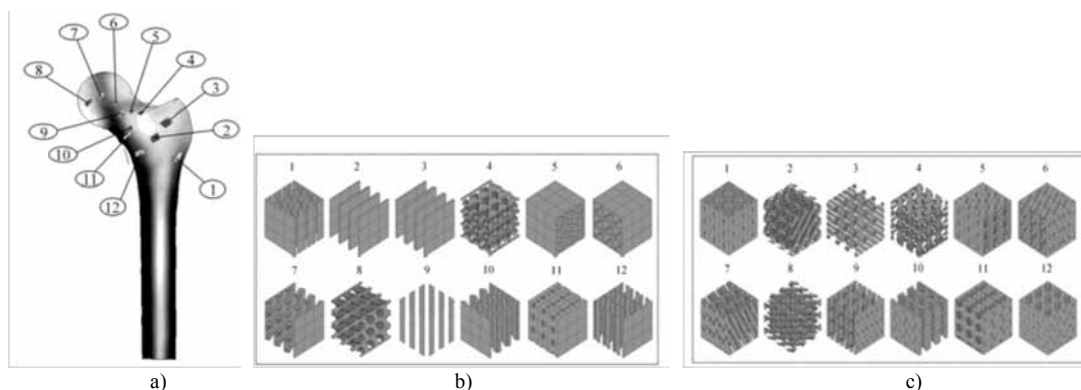


Figure 1. Results of the multiscale model for bone adaptation. a) Bone apparent density distribution on a proximal femur. b) bone microstructure obtained without permeability control c) bone microstructure obtained with permeability control (adapted from [2]).

**Conclusion.** The multiscale approach to model bone tissue presented in this work is a useful tool to gain insight into the bone behaviour as well as to design new orthopaedic devices.

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- [1] Coelho P.G., Fernandes P.R., Rodrigues H.C., *Multiscale Modeling of Bone Tissue with Surface and Permeability Control*, Journal of Biomechanics, 44 (2011), 321-329.
- [2] Coelho P., Fernandes P. R., Rodrigues H. C., Cardoso J.B., Guedes J. M., *Numerical Modeling of Bone Tissue Adaptation – A Hierarchical Approach for Bone Apparent Density and Trabecular Structure*, Journal of Biomechanics, 42 (2009), 830-837.



# SUBJECT-SPECIFIC BONE FRACTURE RISK PREDICTION: MODELLING A MULTISCALE PROBLEM

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**NO ABSTRACT AVAILABLE**

## INTEGRATED MECHANICAL MODELS FOR COLLAGENOUS BIOSTRUCTURES AT DIFFERENT LENGTH SCALES

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**Introduction.** Biological collagen-rich structures (such as tendons, vessels and cornea) share a peculiar histology, characterized by a hierarchical organization from the nano (molecules), through the micro (fibers made up of bundles of fibrils) up to the macroscale (tissues and organs) [1, 2]. The mechanical behaviour of soft collagenous tissues is strictly related with the one of its constituents (especially of collagenous bio-structures) and affects several micro (e.g., mechano-regulated tissue remodeling) and macro (e.g., mechanics of joints or vessels) physiological aspects. In the recent specialized literature, the mechanical response of soft collagenous tissues is addressed by both phenomenological [3] and structural multiscale approaches [4, 5, 6, 7, 8], eventually accounting for damage mechanisms [9].

**Model.** A multiscale model for the elasto-damage response of soft collagenous tissues is proposed, accounting for geometrical and constitutive non-linearities. Starting from the structured organization of biological tissues, models at very different length scales are developed and integrated. The damage onset and propagation is described by an internal-constrained approach employing convex analysis, and allowing to account for damage at the molecular level. The model depends on few parameters measurable by means of standard experimental techniques, and tissue inhomogeneities occurring in real biological tissues for nano or microscale features can be easily incorporated.

**Results.** Stress-strain constitutive relationships are obtained, predicting the failure response of soft collagenous tissues. The proposed model reproduces the well-known experimental evidence [10] that the occurrence of microscopic alterations may result in a reduced strength of soft collagenous tissues, and thus, place them at increased risk of ruptures. Interestingly, even if a brittle behavior for molecular damage is assumed, the ultimate tissue response appears to be characterized by yielding mechanisms when a microscopic alteration occurs.

- [1] Fratzl P. *Collagen: structure and mechanics*. Springer-Verlag, Berlin, 2008.
- [2] Humphrey J.D. *Cardiovascular Solid Mechanics. Cells, Tissues, and Organs*. Springer-Verlag, New York, 2002.
- [3] Fung Y.C. *Biomechanics – Mechanical properties of living tissues*. Springer, New-York, 1981.
- [4] Holzapfel G.A., Gasser T.C., and Stadler M. *A structural model for the viscoelastic behavior of arterial walls: Continuum formulation and finite element analysis*. Eur J Mech A-Solid 21 (2002), 441-63.
- [5] Maceri F., Marino M., and Vairo G. *A unified multiscale mechanical model for soft collagenous tissues with regular fiber arrangement*. J Biomech 43 (2010), 355-363.
- [6] Maceri F., Marino M., and Vairo G. *From cross-linked collagen molecules to arterial tissue: a nano-micro-macroscale elastic model*. Acta Mech Solida Sinica 23(S1) (2010b), 98-108.
- [7] Marino M., and Vairo G. *Stress and strain localization in stretched collagenous tissues via a multiscale approach* Comput Meth Biomech Biomed Eng, accepted (2011).
- [8] Tang H., Buehler M.J., and Moran B. *A constitutive model of soft tissue: from nanoscale collagen to tissue continuum*. Ann Biomed Eng 37 (2009), 1117-1130.
- [9] Holzapfel G.A., and Gasser T.C. *Computational stress-deformation analysis of arterial walls including high-pressure response*. Int J Card 116 (2007), 78-85.
- [10] Järvinen T.A.H., Järvinen T.L.N., Kannus P., Józsa L., and Järvinen M. *Collagen fibres of the spontaneously ruptured human tendons display decreased thickness and crimp angle*. J Orth Res 22 (2004), 1303-1309.

## MULTISCALE MODELLING OF MICROTUBULES AND ACTIN FILAMENTS

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Microtubule (MTs) and Actin Microfilaments (MFs) are cytoskeleton filaments which play important roles in a wide range of biological and mechanical phenomena including cell migration, structural stability, mitosis, and intra-cellular processes [1, 2]. At the molecular level, mechanical properties of these supramolecular assemblies depend on both the mechanical properties of their building blocks (tubulin and actin monomers), and on the intermolecular interactions holding monomers together in the filament lattice. While several experimental studies with atomic resolution have been carried out to better understand the relationship between monomer structure and the monomers' organization in the filament lattice, there is still uncertainty over a number of issues, concerning mechanics of MTs and MFs. From a computational point of view, subcellular structures as large as MTs or actin MFs, with dynamics occurring at timescale of microseconds, require to be investigated by multiscale approaches. In this study, multiscale models of MTs and MFs have been developed to investigate how their mechanical properties (e.g., persistence length, bending stiffness and Young's modulus) depend on the rearrangements of their molecular structures. All-atom MD simulations are coupled with coarse grained (CG) stochastic dynamics (SD) simulations. First, MD simulations are performed in order to compute the energetic properties of MTs and MFs with contour lengths up to tens of nm. The evolution of their molecular rearrangements is detected for time scales of hundreds of nanoseconds.

Then, a coarse grained strategy (CG) is adopted to increase the length and the time scales. In particular, the combination of MD with SD simulations is performed through a CG approach used to parameterize a specific force field, based on the so-called Boltzmann inversion method [3].

The CG models here employed is based on an expression of the potential energy function, that is simplified with respect to the potential energy functions used in all-atoms MD simulations. Each monomer of the MT and of the MF is coarse-grained in few beads (representing the atomistic domain in terms of centre of mass, radius of gyration and total mass). Five beads are used to represent each tubulin monomer (while the atomistic representation consists of about 4,000 atoms) and four beads are used to represent the actin monomer (while the atomistic representation consists of about 3,000 atoms).

BD simulations on the coarse-grained models of MTs and MFs with length up to 1.5  $\mu\text{m}$ . The results for each MT and for MF are obtained in terms of persistence length and bending stiffness, calculated on the basis of the fluctuations of the filament at the equilibrium during the simulation.

Results of MTs and MFs bending stiffness show to be in agreement with experimental findings. These properties are related with the rearrangements induced by thermal fluctuations at the molecular scale. The potential of this multiscale modelling approach relies on combining the thermal effects on the molecular conformation of the protein systems with their overall mechanics.

The size of the simulated MTs and MFs is several order of magnitude higher than the dimension of proteins usually simulated by MD simulations (few nm). SD simulations were able to reproduce the dynamics of MTs and MFs with lengths up the micrometer and for time scales of the order of microseconds. By combining MD simulations with SD simulations, the time step is enhanced from 0.001 ps up to 5 ps.

This multiscale modelling approach could be further extended to investigate the dynamics of protein systems with contour lengths of several micrometers and scales of the order of microseconds.

- [1] Howard, J.: *Mechanics of motor proteins and the cytoskeleton*, Sunderland, Mass.: Sinauer Associates, Publishers, 2001.
- [2] Pfaendtner, J., Lyman, E., Pollard, T. D. and Voth, G. A.: *Structure and Dynamics of the Actin Filament*, J Mol Biol, 2010, 396(2), 252-63.
- [3] Reith, D., Putz, M. and Muller-Plathe, F.: *Deriving effective mesoscale potentials from atomistic simulations*, J Comput Chem, 2003, 24(13), 1624-36.

# CONTINUUM ELASTICITY OF HYDRATING COLLAGEN: A MULTISCALE APPROACH

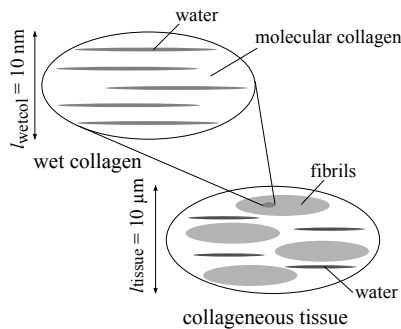
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**Introduction.** Collagen is an abundant protein in biological tissues, playing an important role in maintaining the architecture of multicellular organisms. However, despite a large number of contributions in the collagen properties, the continuum elasticity of this protein remains an open topic. By combining "polymer-in-a-box"-type hexagonal packing considerations with multiscale micromechanics, we here provide triple evidence that the continuum elasticity of collagen at different hydration states stems from the interaction of a contiguous molecular collagen phase with water inclusions, at the intermolecular as well as at the fibrillar level.

**Methods.** Due to the hierarchical organization of collagen, a two-scale micromechanical model is developed to account for its mechanical behavior:

- Within a representative volume element (RVE) of 10 nm size, called wet collagen, collagen molecules are multiply interconnected, forming, from a mechanical viewpoint, a contiguous matrix with water-filled pores being embedded.
- Within an RVE of 10  $\mu\text{m}$  size, representing collageneous tissue (with straightened fibers), fibrils of wet collagen and water pores are embedded in a self-consistent matrix.



Two-scale model of collageneous tissue.

In this theoretical framework, hydration is reflected by different volume fractions of the aforementioned phases (molecular collagen, water, fibrils). At the level of wet collagen, the volume fraction of molecular collagen follows from a "polymer-in-a-box"-type hexagonal packing model [2],

$$f_{col} = \psi \left( \frac{d_{dry}}{d} \right)^2, \quad (1)$$

with  $d$  as the equatorial X-ray diffraction spacing at the considered hydration state,  $d_{dry}$  as the tissue-independent limiting dry-state diffraction spacing ( $d_{dry} = 1.09 \text{ nm}$ ), and  $\psi = 0.88$  according to the spatial organization of collagen molecules with gap and overlap zones. The volume fractions at the tissue scale follow from mass density considerations.

**Results.** Predictions of this hierarchical model agree very well with results from absorption-drying experiments (cf., e.g., [3]) and Brillouin light scattering-based elasticity experiments [1]. This agreement concerns multiple quantities, namely: (i) the hydration level corresponding to air-dried collagen, i.e. to the start of the diffraction spacing increase; (ii) the maximum hydration level of the fibrils; (iii) the evolution of the diffraction spacing with water content; (iv) the transversely isotropic elasticity of collageneous tissues at very different hydration states.

- [1] S. Cusack and A. Miller, Determination of the elastic constants of collagen by Brillouin light scattering. *Journal of Molecular Biology* 135:39-51, 1979.
- [2] C.A. Miles and M. Gheslshvili, *Polymer-in-a-box mechanism for the thermal stabilization of collagen molecules in fibers*. *Biophysical Journal*, 76 (1999), 3243-3252.
- [3] M.H. Pineri, M. Escoubes and G. Roche, *Water-collagen interactions: calorimetric and mechanical experiments*. *Biopolymers*, 17 (1978), 2799-2815.

# MODELING TISSUE PERFUSION USING A HOMOGENIZED MODEL WITH LAYER-WISE DECOMPOSITION

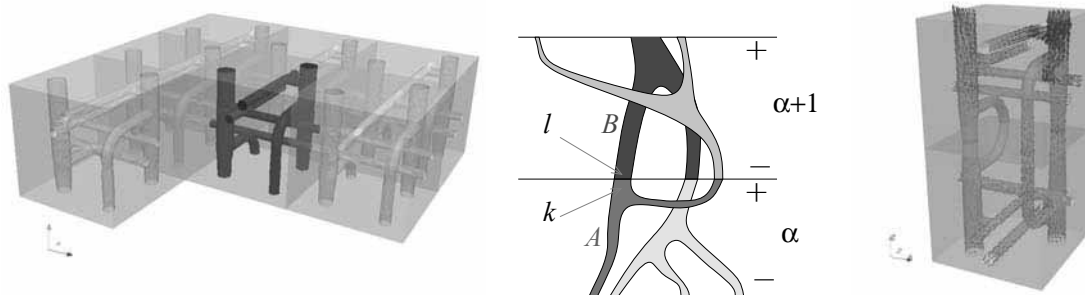
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**Introduction.** Our aim is to develop a microstructurally-oriented and computationally efficient modeling tool which will allow for simulations of tissue perfusion. We focus on modeling the perfusion of tissue parenchym, being motivated by medical applications: a) the assessment of the local cerebral blood flow and b) the liver segmentation (to associate given a point within the liver with one of the hepatic and portal veins). At the level of small vessels and microvessels, the perfusion can be described using the Darcy flow in double porous structure consisting of 3 compartments: two mutually disconnected channels (small arteries and veins) and the matrix (microvessels and capillaries), represented as the dual porosity, where the permeability is decreasing with the scale parameter, i.e. the size of the microstructure, cf. [2].

**Homogenized model with layer-wise decomposition.** The model of perfusion is constituted by several transversely periodic layers, which enable us to approximate flow through different hierarchies of the porosity. A 3D layered structure occupying a 3D volume can be replaced by a finite number of 2D “homogenized layers” [1] coupled by conditions governing the fluid exchange between them. Each layer is assumed to have a locally periodic “3-compartment” structure generated by the reference periodic cell, see the Figure (left). Using this cell, homogenized coefficients relevant to the macroscopic level can be calculated.



Left: A periodic structure of the layer with the highlighted reference cell comprising two channel systems A and B. Middle: schematic expression of the coupling conditions. Right: illustration of flow reconstruction in the channels at two attached microscopic cells belonging to two neighbouring layers.

**Model of N-coupled layers.** In each layer the perfusion is described by the homogenized model involving macroscopic pressures. Flows between the layers are respected by coupling conditions, see the Figure (middle). In the simplest case, we assume perfect-matching microscopic cells of two attached layers, so that, at the microscopic level, the pressures at the “channel junctions” must equal and the fluxes must be opposite. Analogous conditions express coupling for the pressures and fluxes at the interface in the dual porosity. This approach allows us to approximate the hierarchical structure of the perfusion tree: in each layer the periodic microstructure can be different.

**Applications.** The model is being developed for an approximate description of blood perfusion in brain or liver tissues. Due to the 3D-to-2D reduction and the two-scale decomposition it leads to computationally feasible problem which is now implemented in our in-house developed code *Sfepy*, see <http://sfepy.org>. The solution of the macroscopic problem can be used for the flow reconstruction at the microscopic level. Using the computed velocities we can solve a transport equation describing redistribution of a contrast fluid, to mimic the output of enhanced CT perfusion investigation.

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- [1] E. Rohan. *Homogenization of the perfusion problem in a layered double-porous medium with hierarchical structure*. 2010. Submitted.
- [2] E. Rohan, R. Cimrman. *Two-scale modelling of tissue perfusion problem using homogenization of dual porous media*. *Int. Jour. for Multiscale Comput. Engrg.*, 8:81–102, 2010.

## HISTO-MECHANICAL MODELING OF THE WALL OF ABDOMINAL AORTA ANEURYSMS

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Proteolytic degradation of elastin and collagen in the aortic wall may result in an Abdominal Aortic Aneurysms (AAAs), i.e. a local dilation of the infrarenal aorta that eventually ruptures. Ruptured AAAs are a frequent cause of death in elderly male population and clinical trials indicated that a maximum diameter of 55 mm appears to be the best indication for elective (surgical or endovascular) AAA repair in a larger cohort. However, a single threshold diameter is not appropriate for every patient, and the decision to perform elective AAA repair should be individualized. Specifically, the biomechanical rupture risk assessment allows for an individual analysis using indices like Peak Wall Stress (PWS) and Peak Wall Rupture Risk (PWRR). Computing these parameters involves a nonlinear biomechanical analysis, which to some extent depend on the constitutive description of the AAA wall. The late stage of AAA disease is characterized by irreversible pathological remodeling of the aortic wall connective tissue, which, amongst many others, involve degradation of the elastin and compensatory increased collagen synthesis and content. Consequently, the passive mechanical response of a larger AAA can be modeled as fibrous collagenous tissue with negligible contribution from the degraded and fragmented elastin. Specifically, collagen fibrils are the basic building blocks of fibrous collagenous tissues, and their hierarchical organization into suprafibrillar structures determines the tissue's macroscopic mechanical properties. This is confirmed by biomechanical and clinical studies that invariably show that the mechanics of the arterial wall essentially relies on fibrillar collagens in media and adventitia.

For vascular tissues numerous constitutive models have been reported, where specifically histomechanical approaches aim at integrating collagen fiber density and orientations. This presentation follows such a histomechanical method and assumes that the tissue's macroscopic mechanical properties being entirely governed by interlinked collagen fibrils. According to this approach, the spatial orientation and undulation of collagen fibrils are the most influential micro-histological parameters and macroscopic properties are derived through two integrations, i.e. once over the undulation and twice over the spatial orientation of fibers. Specific assumptions regarding the constitution of the collagen fibril proteoglycans-complex (CFPG-complex) and the undulation of collagen fibrils allowed us to derive a piece-wise continuous relations for the stress-stretch property of a collagen fiber. This leads to a numerically efficient multi-scale concept and facilitates a biomechanical analysis of an entire AAA within reasonable computational times. The orientation density of collagen in the AAA wall was taken from polarized light microscopy measurements and the model captures its macroscopic properties over a large range of biaxial deformations. Finally, the model was enriched by a description of collagen turn-over and implemented in a finite element environment, such that the enlargement of patient-specific AAAs until rupture can be computed.

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## HYBRID MODELLING AND PROCESS OPTIMIZATION OF BIOLOGICAL SYSTEMS

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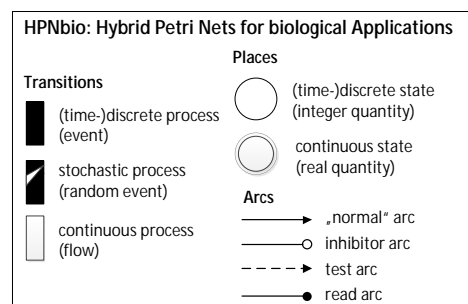
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**Introduction.** Modern computer techniques and large memory capacities make it possible to produce an enormous amount of biological data stored in huge databases. These data are indispensable for the scientific progress but they do not lead necessarily to insight about the functionality of biological systems. Hence, an approach is needed to achieve usable information from this huge data amount. A *mathematical model* provides a means for summarizing and structuring experimental data in order to *simplify the communication* of knowledge progresses with other researchers. Additionally, it improves the *understanding* of the living system and allows the *directed design of experiments* by predicting the system behaviour under specific conditions and proving it by experiments.

**Petri-nets.** Petri-nets with their various extensions are a *universal graphical modelling concept* for biological systems in nearly all degrees of abstraction. They provide an intuitive and generally comprehensible way to represent and communicate experimental data and knowledge of biological systems. The biological processes can be modelled discretely as well as continuously and, in addition, discrete and continuous processes can also be combined within a Petri-net model to so-called *hybrid Petri-nets* (cp. [1]). Despite several works and publications with Petri-net approaches, there is a serious problem according to the lacking unity of concepts, notations, and terminologies. The definition of Petri-nets are not standardized; every author has own definitions which are partly not precisely enough, not common, or contradictory. Hence, to show the research community the power of Petri-nets, a formalism has been developed which is able to represent nearly all kinds of biological processes. It is called *Hybrid Petri-Nets for biological applications (HPNbio)*.



**Modelica.** To use Petri-nets as a graphical modelling concept for biological systems, the Petri-nets, for their part, have been modelled by the object-oriented modelling language *Modelica*. Modelica, developed and promoted by the Modelica Association since 1996 for modelling, simulation, and programming primarily of physical and technical systems and processes, has become the de-facto standard for hybrid, multidisciplinary modelling. Each Petri-net element, places and transitions, is described by a model in the Modelica language defined on the lowest level by *discrete* (event-based), *algebraic*, and *differential equations*. The developed Petri-net element models are structured in a Modelica library called *PNlib* (*Petri Net library*, cp. [2]). An appropriate Modelica-tool enables then graphical hierarchical modelling, hybrid simulation, and animation.

**Wrapping Technique.** An additional Modelica library, called *PNproBio* (*Petri Nets for process modelling of Biological systems*), provides wrapped HPNbio which offer on the one hand an easy-use-model at the top level with an intuitive and familiar adapted biological view and on the other hand the flexibility and generality of the HPNbio concept at a lower level. Several wrappers have already been implemented to model: kinetic effects/laws, stochastic effects, cell growth and death, substrate uptake and product formation, activation and inhibition mechanisms, and fermentation processes, in a simple and biological adapted way.

**Process Optimization.** Moreover, an established model can be used to control biological processes which plays an important role in the industrial biotechnology. There, organic substances are converted by microorganisms such as bacteria, fungi, or animal cells to specific products used in foods or pharmaceuticals; this procedure is called *fermentation*. The industry is mainly interested in achieving a maximum product yield from the organisms at minimum costs. Thereby, a process optimization procedure applied on an established model can achieve an *open-loop control* for the biological process, i.e. the process parameters are calculated based on the model representing the state of the biological system; no feedback is used to determine if the output has yielded the intended purpose of the adapted process parameters. Possible process parameters are temperature, pH-value, stirrer speed, or feeding parameters. This process optimization procedure is performed by means of *hybrid optimization methods*, i.e. a global method is combined with a local method by use of a specific switching strategy.

[1] David R, Alla H (2001) *On Hybrid Petri Nets*. Discrete Event Dynamic Systems: Theory and Applications (11), 9-40.

[2] Proß S, Bachmann B (2011a) *An Advanced Environment for Hybrid Modeling of Biological Systems Based on Modelica*. In: Journal of Integrative Bioinformatics (8), 1–34.

## FLUID FLOW MODELLING WITH MODELICA

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**Abstract** This work shows how the problem of modelling fluids motion can be addressed in Modelica. This innovative approach makes possible to face such a problem in a multi-physic modelling language as Modelica is. In this way it is possible to simulate together the fluid and the system that interact with it, without any additional effort and taking advantage of the Modelica libraries representing buildings, power plants, water treatment systems, HVAC and so forth.

**Introduction** Modelling fluid flows is extremely important in simulating many engineering processes. When the fluid is constrained to move in ducts or pipes strong assumptions/simplifications can be taken into account without affecting the description of the fluid properties (e.g. temperatures, pressures, densities,...) and their distributions. The mentioned simplification for such cases where a spatial coordinate prevails the others leads to zero or one dimensional models where the spatial dependence is respectively disregarded or limited to just one coordinate (e.g. pipes). However there are elements like tanks (in the context of hydraulic systems) or rooms (in the context of HVAC systems) where zero or one dimensional models are not appropriate. The standard practice when simulating such more complicated scenery, is to employ CFD codes. Despite this approach is capable of representing in a very detailed way the fluid thermal dynamics, it has some drawback. The main one is in its modularity. CFD cannot be easily integrated with other models in order to represent the entire system, the only way for doing such a task is to employ the so called co-simulation techniques, that introduce a communication overhead and some non trivial convergence problem [3].

The aim of this work is to provide a general methodology for modelling 2D or 3D fluid flows with Modelica. Modelica is a multi-physic Object-Oriented modelling language [1]. In Modelica several modelling libraries, representing a variety of systems are already available ([2]), and new ones can be developed. Thanks to the modularity of the language and the definition of standard interfaces, models belonging to different physical domains can be coupled together. Providing a way for modelling fluid flows in such an environment is a step ahead in the direction of a real integrated multi-domain simulation tool, thus avoiding co-simulation and its drawbacks [3]. The proposed modelling approach aims at representing simple scenery in cases where the powerful capabilities of CFD software are not needed. More precisely, complex geometries and high velocities are not taken into account, however a wide range of application like rooms, portion of buildings, storage tanks can be modeled. As consequence, despite the apparent simplicity of the proposed approach a widespread set of relevant cases can be investigated.

**Content** The paper is structured in the following way, after an introductory section where the modelling approach is presented and the constitutive equations are shown, the discretisation of the set of equations as well as the numerical methods employed are presented. In the validation section a comparison between experimental data (that ensure the correctness of the approach) is reported. Some conclusions as well future works complete the paper.

- [1] S.E. Mattsson, H. Elmqvist, and M. Otter. Physical system modeling with Modelica. *Control Engineering Practice*, 6:501–510, 1998.
- [2] Modelica Association. Modelica home page. <http://www.modelica.org/>.
- [3] Marija Trčka, Jan L.M. Hensen, and Michael Wetter. Co-simulation for performance prediction of integrated building and hvac systems - an analysis of solution characteristics using a two-body system. *Simulation Modelling Practice and Theory*, 18(7):957 – 970, 2010.

# ANAEROBIC DIGESTION MODELS: A COMPARATIVE STUDY

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**Introduction.** Modelling of anaerobic digestion process is of fundamental importance not only in order to design wastewater treatment and biogas power plants, but also to study the sensitivity of the plant behavior to operational parameters, to monitor and control the plant performance and to assess to feasibility of the use of new substrates, with varying characteristics, biodegradability and operational conditions.

In the literature, many anaerobic digestion models have been proposed for specific applications or fermenters, fed with a very specific substrate, which can be roughly grouped into three main categories. The simplest ones [5] are single-step models involving a single bacterial population, endowed with a limited description of inhibition effects. Models of intermediate complexity [2] consider a higher number of processes and bacterial populations, as well as a more accurate description and implementation of inhibition factors. Finally, complex models [1, 7] take into account a large number of processes and specific bacterial populations, along with an in-depth description of the inhibition effects and of relevant chemical equilibria.

The best known and the most sophisticated model, able to describe the anaerobic degradation of various substrates (even if designed considering activated sludge as substrate), is the Anaerobic Digestion Model no. 1 (ADM1) [1], developed by the IWA Task Group for Mathematical Modelling and later modified by several authors [3, 4] to improve accuracy and robustness, and to fit the model to other specific applications. While being very detailed in the description of the anaerobic digestion processes, it can be hardly used for design and control purposes. In fact, a large number of parameters (about a hundred) depending on the specific substrate needs to be estimated, which is particularly difficult in complex plant operations and also because of the scarce data available in the literature. This fact has motivated the research of simpler models, focused for example on a few number of processes or specifically designed for particular substrates. Among them, the most important is the AMOCO model [2], which reaches a good compromise between simplicity and accuracy. The AMOCO model has been developed mainly as a tool to monitor and control the anaerobic digestion process rather than as a tool for accurate numerical simulation.

In this paper, a comparison between the ADM1 and the AMOCO model is investigated, mainly in order to assess the performance of the AMOCO model as a control design tool. First, the ADM1 model has been calibrated with reference to the degradation of waste activated sludge, considering data reported in [6], and assumed as the reference model. Then, in order to compare the outputs of the two models, some variables of the ADM1 models have been lumped to match the relevant aggregated AMOCO variables.

The parameters of the AMOCO model have been then calibrated by assuming the steady-state outputs of the ADM1 model as a reference. Since the values of the concentrations of the two biomass families considered in the AMOCO model, not measurable in normal operations, were available from ADM1 simulations, a different (and simpler) identification procedure has been followed with respect to the one proposed in [2].

The AMOCO model however failed in predicting the steady state values relevant to the inorganic carbon species and alkalinity. The reason for this failure has been detected in the lack of description of the balance of the inorganic nitrogen species. Consequently, a new version of the AMOCO model has been developed, accounting for the dynamics of the inorganic nitrogen concentration. Steady-state and dynamic simulations based on this new model version showed an improvement with reference to simulation obtained with ADM1 model.

- [1] Batstone, D.J., Keller, J., Angelidaki, I., Kalyuzhnyi, S.V., Pavlostathis, S.G., Rozzi, A., Sanders, W.T.M., Siegrist, H., Vavilin, V.A.: The IWA Anaerobic Digestion Model No. 1 (ADM1). *Water Science and Technology* **45**(10), 65–73 (2002)
- [2] Bernard, O., Hadj-Sadok, Z., Dochain, D., Genovesi, A., Steyer, J.: Dynamical model development and parameter identification for an anaerobic wastewater treatment process. *Biotechnology and Bioengineering* **75**(4), 424–438 (2001)
- [3] Blumensaat, F., Keller, J.: Modelling of two-stage anaerobic digestion using the IWA Anaerobic Digestion Model No. 1 (ADM1). *Water Research* **39**(1), 171–83 (2005)
- [4] Galí, A., Benabdallah, T., Astals, S., Mata-Alvarez, J.: Modified version of adm1 model for agro-waste application. *Bioresource Technology* **100**(11), 2783–2790 (2009)
- [5] Graef, S.P., Andrews, J.F.: Stability and control of anaerobic digestion. *Journal of the Water Pollution Control Federation* **46**(4), 666–683 (1974)
- [6] Rosen, C., Vrecko, D., Gernaey, K., Pons, M., Jeppsson, U.: Implementing ADM1 for plant-wide benchmark simulations in Matlab/Simulink. *Water Science and Technology* **54**(4), 11–19 (2006)
- [7] Sötemann, S.W., Ristow, N.E., Wentzel, M.C., Ekama, G.A.: A steady state model for anaerobic digestion of sewage sludges. *Water SA* **31**(4), 511–528 (2005)

# A PARAMETRIZATION SCHEME FOR HIGH PERFORMANCE THERMAL MODELS OF ELECTRIC MACHINES USING MODELICA

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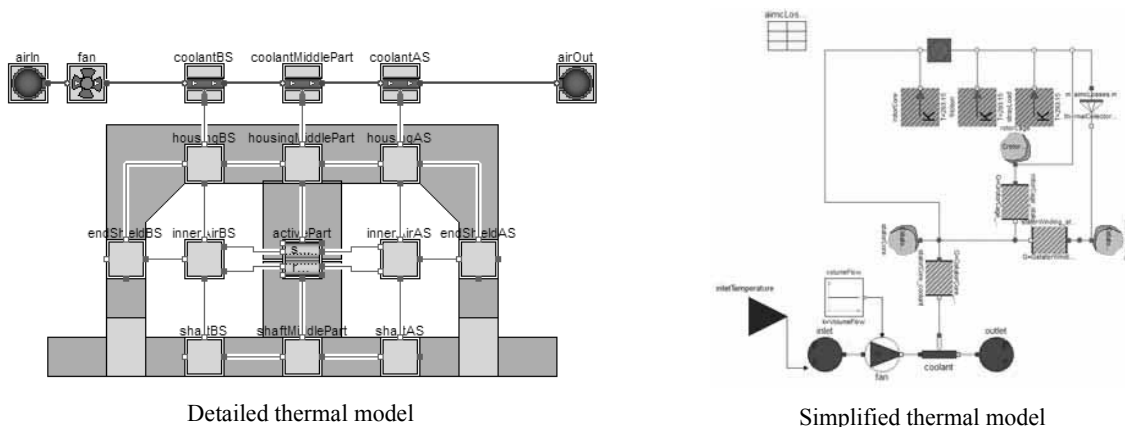
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**Introduction.** For many applications of electric drives it is desired to have a thermal model of the electric machine. Being able to simulate the relevant temperatures allows to take advantage of the thermal inertia during non-steady duty cycles, cooling down the machine during a period of low load condition after overload operation. However, such detailed thermal models require detailed geometric data of the machine to calculate the parameters of the thermal model. In many cases, such a detailed thermal machine model is not performant enough, or detailed geometric data is not available from the manufacturer. In both cases a simplified thermal model is desired.

An application of a simplified thermal model is checking whether a chosen machine is sufficient for a given duty cycle with varying speed and load during an early design stage of the drive. Another application is the thermal protection of the machine during such load cycles, without using too many thermal sensors. A third case is represented by high precision inverter control of an asynchronous induction machine with squirrel cage rotor.

For both the thermal model and the drive model, the modeling language Modelica<sup>®</sup> is used. Modelica<sup>®</sup> is a non-proprietary, object-oriented, equation based language to conveniently model complex physical systems containing, e.g., mechanical, electrical, electronic, hydraulic, thermal, control, electric power or process-oriented subcomponents.



Detailed thermal model

Simplified thermal model

**Parameterization.** Thermal conductances are calculated from temperatures and losses obtained by measurement or simulation with a detailed thermal model. Having temperature characteristics versus time, it is possible to vary the thermal capacitances and compare simulated with measured temperature characteristics. Using an aggregating criterion it is possible to utilize optimization methods to determine best-fit thermal capacitances.

**Validation.** The thermal model of an asynchronous induction machine with squirrel cage is coupled with an electrical model of the drive. For validation, simulation results of an optimally parameterized simplified model are compared with temperatures obtained by simulation of a detailed thermal model, which in turn has been validated against measurement results, both for continuous duty S1 and intermittent duty S6 (6 minutes no-load followed by 4 minutes of 140% nominal load). The deviations are not more than 4 K which is quite satisfying.

[1] Kral, C. and Haumer, A. (2011). Object Oriented Modeling of Rotating Electrical Machines. INTECH.

[2] Haumer, A., Bäuml, T., and Kral, C. (2010). Multiphysical simulation improves engineering of electric drives. 7<sup>th</sup> EUROSIM Congress on Modelling and Simulation.

[3] Haumer, A., Kral, C., Kapeller, H., Bäuml, T., and Gragger, J.V. (2009). The AdvancedMachines library: Loss models for electric machines. Proceedings of the 7<sup>th</sup> Modelica Conference, 847-854.

# OBJECT-ORIENTED MODELING OF SWITCHING MOVING BOUNDARY MODELS FOR TWO-PHASE FLOW EVAPORATORS

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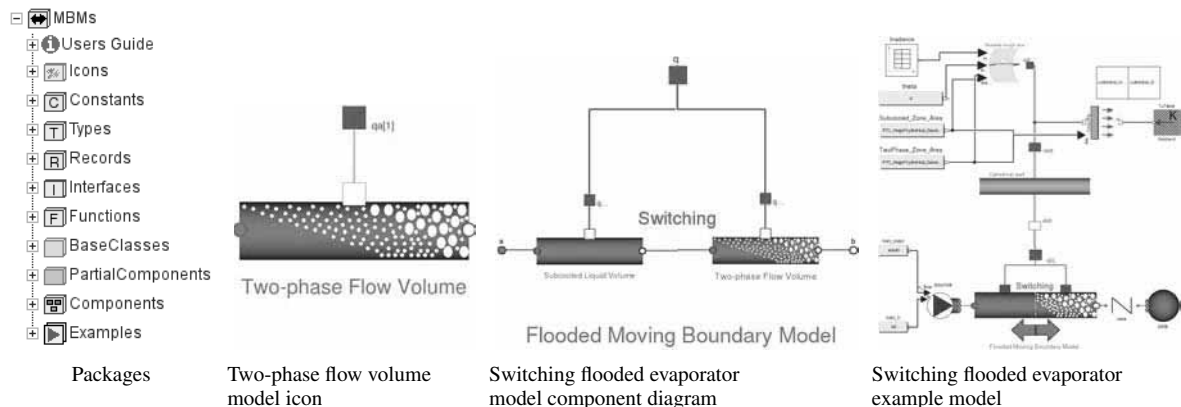
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**Summary.** The most common approaches used in fluid dynamic and heat exchange modeling are the finite-volume distributed-parameter method [3] and the moving-boundary lumped-parameter method [2]. Dynamic modeling is always a challenging task in which the trade-off between accuracy and speed must be evaluated. In [1], both methods for a centrifugal chiller system were studied and analyzed. The conclusion is that the moving boundary method is much faster although not as accurate and robust as the finite volume method. Despite of the loss of accuracy of the moving boundary method, in the context of real-time simulation, dynamic system optimization and model-based control, where fast computation is required, the moving boundary method seems to be the appropriate one.

The moving boundary method divides the evaporator in different regions, also called Control Volumes (CVs), depending on the fluid phase. In each CV, the lumped thermodynamic properties are average in some way, the barrier is not fixed and it may move between the CVs. This paper describes and compares briefly the current boundary models for two-phase flows showing its features. However, none of them includes all the desirable features.

This paper also presents the design of switching moving boundary models (MBMs) for two-phase flow evaporators and the development of a still-under-development object-oriented equation-based library written in the Modelica language. The main idea is to design basic models for each flow state: subcooled liquid, two-phase flow and superheated steam models, applying the conservation laws. The design must be done in order that the basic models can be interconnected to create complete, flooded or dry-expansion evaporators depending on the particular case. The basic models should consider the balances of mass, energy and momentum, meanwhile the evaporator models should include mechanisms to switch between them, for example from a complete to a flooded evaporator in case that the superheated region becomes extinct. The following figures show the different packages which compose the library, the two-phase flow volume model icon, the component diagram of the switching flooded evaporator model and an example model to test the switching flooded evaporator model.



Moving boundary models library for two-phase flow evaporators (MBMs Library)

[1] S. Bendapudi, J. Braun, and E. Groll. A comparison of moving-boundary and finite-volume formulations for transients in centrifugal chillers. *International Journal of Refrigeration*, 31(8):1437–1452, December 2008.

[2] M. Dhar and W. Soedel. Transient analysis of a vapor compression refrigeration system. In *Proceedings of the 15th International Congress of Refrigeration*, pages 1031 – 1067, Venice, Italy, 1979.

[3] S. V. Patankar. *Numerical heat transfer and fluid flow*. Hemisphere, Washington, D.C, 1980.

## A REFERENCE-BASED PARAMETERIZATION SCHEME FOR OBJECT-ORIENTED MODELING LANGUAGES

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**Motivation.** An ever increasing complexity of equation-based modeling has led to the creation of increasingly larger systems that contain a vast number of components. Such systems raise the demand for elaborated parameterization schemes. It is no longer sufficient to regard parameters simply as real numbers or values of any other base type. Instead, whole components or component classes become subject to parameterization. For instance, the gear box of a vehicle needs to be changed, or the class of medium-models within a fluid system shall be replaced.

In Modelica, one of the most prominent object-oriented modeling languages, several language constructs have been added in order to support such advanced parameterization tasks. Unfortunately, they revealed to be conceptually flawed and are the origin of many intricate problems. The publication “*Towards Improved Class Parameterization and Class Generation in Modelica*” [3] outlines the current deficiencies and contains a concrete proposal for a redesign. The cited paper remains, however, on a conceptual level since the proposed solutions have not been validated by a corresponding test-implementation.

**Summary.** Meanwhile, such a prototype implementation has become available by the design effort of the experimental language Hornblower. This language represents an attempt to embrace the core ideas of Modelica while reorganizing the higher-level modeling tasks that evolved during time. In contrast to Modelica, Hornblower is based on a reference-based parameterization scheme. This enables to handle whole components or classes of models as simple parameters in a simple unified concept. In addition to simplicity, the concept of Hornblower incorporates many further particular advantages such as:

- Models, model classes and even annotations are elements of first-class status [1].
- The handling of attributes or annotations can be integrated into the process of parameter evaluation with virtually no effort.
- Sharing objects as for the case of world models is now easily possible. Complicated concepts such as inner/outer [2] can be abandoned.
- Large parameter arrays can be handled more efficiently in the translation process.

This paper will present the language Hornblower with its parameterization scheme. The key concepts of the language design will be outlined and their feasibility will be demonstrated by the prototype implementation. Many examples clarify the ideas behind

**Conclusions.** Modelica 3 contains many diverse language constructs: there is a separate syntax for normal parameters and component parameters. In addition, the concept of outer models is part of the language specification. The specification is further enlarged by the description of various annotations.

In Hornblower, all these different concepts can be expressed by a much smaller and consistent set of language constructs. By introducing a reference-based parameter scheme, object-oriented, equation-based languages can be significantly simplified while increasing their level of expressiveness. The modeller can profit from the flexibility of dynamic typing for the higher-level modelling task. On the other side, the resulting modelling code is statically typed and hence leads to the generation of efficient simulation code.

We hope that the research undertaken in the Hornblower project may influence the future development of Modelica.

[1] Burstall R., and Strachey C. *Understanding Programming Languages*. In: Higher-Order and Symbolic Computation 13:52, 2000.

[2] Fritzson P.: *Principles of Object-oriented Modeling and Simulation with Modelica 2.1*. John Wiley & Sons, 897p. 2004.

[3] Zimmer D.: *Towards Improved Class Parameterization and Class Generation in Modelica*. In: Proc. of the 3rd International Workshop on Equation-Based Object-Oriented Languages and Tools (EOOLT), Oslo, Norway, 2010.

# MODIM - A MODELICA FRONTEND WITH STATIC ANALYSIS

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**Abstract.** We present ModIM, a Modelica front-end library written in Java. ModIM is designed to not only support the development of Compilers/Interpreters but also tools that are currently underrepresented in the Modelica ecosystem. This includes (but is not limited to) advanced editors, documentation generators and model checkers. For that purpose ModIM offers a static environment generation and type inference algorithm. Both algorithms are adaptations of standard techniques to the characteristics of Modelica. Environment generation is rather complex, but specified intensely. The type system is straight forward, but lacks a formal specification and thus is an *interpretation* of the Modelica specifications' intents. Additionally it is extended to also cover some unique features of Modelica. This extension consists of a formalization of the four kinds of variabilities and the introduction of a new type for unknowns.

**Introduction.** Modelica [1] is a modeling language for physical systems. The need for complementary tools and software grows, as the language becomes more and more successful in research as well as industrial application. Usually such software does not implement the complete model-compile-simulate workflow (which is already covered quite well). Instead, it focuses on a single task in or next to this workflow (e.g. version control [2]). Since Modelica is currently usually interpreted just prior to the generation of simulation code, there is little to no available support for the development of such tools. Especially there is currently no library that one could use for *static analysis* of Modelica models.

ModIM is designed to allow easy integration in any use-case (interpreters, compilers, integrated development environments etc.). Therefore the library sacrifices the extensibility of data structures for the ease of implementing operations on those. ModIM is not meant as a base for developing a new language but as a platform for tools that support standard Modelica.

**Static Analysis** ModIM extends classical type systems (as discussed e.g. in [3]) by *variabilities* and *the variable type*. Informally, variabilities describe, when the result of evaluating an expression might change (never, at initialization, during events or with every time step). The variable type describes expressions that are evaluated to *unknowns*. This is a new concept which is a conclusion from the interpretation of Modelica's Specification.

```

1  model example
2      Real x,y;
3      discrete Boolean b(start = false);
4
5      equation
6      when time > 1 then
7          b = true;
8      end when;
9
10     x = time;
11     y = if b then y else x;
12 end example;
```

In the example model listed above, the expression `if b then y else x` has the type  $\langle d, \text{var}\langle t, \mathbb{R} \rangle \rangle$ , i.e. it yields an unknown, which can be evaluated to a continuous real value. But *which* unknown it yields, depends on a discrete-time expression. Such structural dynamics can easily be specified by the combination of variability and the type for unknowns.

## References

- [1] Modelica - a unified object-oriented language for physical systems modeling, 2010.
- [2] Peter Harman. Effective version control of modelica models. In *Proceedings of the 8th International Modelica Conference, March 20th-22nd, Technical University, Dresden, Germany*, Linköping Electronic Conference Proceedings, pages 650–656. Linköping University Electronic Press, Linköpings universitet, 2011.
- [3] Benjamin C. Pierce. *Types and Programming Languages*. MIT Press, 2002.

# A PYTHON PACKAGE FOR SIMULATING VARIABLE-STRUCTURE MODELS WITH DYMOLA

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## Abstract

In the field of modeling and simulation of physical systems, it becomes increasingly important to raise the level of detail and to simulate faster. One way to deal with these contradictory targets is to use variable-structure models. In such models, variables as well as the set of equations can change during simulation. A model can therefore have different modes, whereas each mode has its own set of equations. This is highly useful when the behavior of a model changes during runtime (variable-behavior), as e.g. a rope-pendulum does when becoming a falling mass. Furthermore, such models can be used to create models with different levels of detail (variable-detail). These variable-detail models enable the user to create models, which are as complex as necessary and as simple as possible at all times. Therefore, such models can make a simulation faster and sometimes at the same time even more accurate.

Currently, simulation tools like Matlab/Simulink<sup>®</sup> and Dymola<sup>®</sup> do not support the modeling of variable-structure models since a change of the set of equations is not allowed. Different works of variable-structure modeling have been made such as the tool MOSILAB<sup>®</sup> [2] which is a Modelica based tool that supports the modeling and simulation but does not support index reduction and is so far not suitable for complex models. Another solution is SOL [3] which is an experimental language that enables the user to create variable-structure models. The language has many similarities to Modelica. For both approaches it is not possible to reuse existing Modelica models, they have to be modeled anew in the chosen tool/language. Furthermore, MOSILAB is still in development and SOL is an experimental language, which means they are not easily accessible and usable for common users.

In our paper we present an approach that reuses existing Models and handles the mode switches through a script. In the approach a variable-structure model consists of modes and transitions which describe the change from one mode to another. Each mode is an independent model that can be simulated on its own in the tool it was implemented in. In [1] the general idea was presented. There Matlab-scripts were used to simulate Simulink and Dymola variable-structure models. It was shown that the approach does work, but it did only work for two modes and when using Dymola it is also necessary to have Matlab which makes the approach depended on two commercial tools. To overcome this drawback a Python package for the simulation of variable-structure models in Dymola is introduced. All functionality like compiling Dymola models, starting a simulation, reading simulation data, storing simulation data and plotting results is integrated in the presented package. A template to describe the variable-structure models guides the user through the necessary steps to simulate the desired model. The user can also specify which simulation data should be observed and in what fileformat it should be saved. To enable the user to postprocess the observed data in a preferred tool the data can be exported to different file types. The package is designed so the variable-structure models can be described through object-oriented means and that the package is extensible to other simulation engines. To use this package no Python programming knowledge is necessary to describe new variable-structure models.

Various examples from different physical domains are used to explain the template and the functionality of the Python package. The examples are also used to present the advantages of simulating variable-structure models with the introduced package. With the gained knowledge from the modeling and simulation of variable-structure models, it is discussed which information is needed to create such models. Furthermore, it is explained which requirements a model needs to fulfill to be used in a variable-structure model. The introduced package allows a user to use a template to specify variable-structure models for existing Dymola models and use the Dymola simulation engine to simulate these models. Therefore, the user is now able to test if variable-structure models are feasible for his particular work.

- [1] Mehlhase A.: *Varying the level of detail during simulation*. In: 21. Symposium Simulationstechnik, ASIM Pub., Winterthur/CH, 2011.
- [2] Nytsch-Geusen C., Ernst T., Nordwig A., et al.: *Mosilab: Development of a modelica based generic simulation tool supporting model structural dynamics*. In: Proceedings of the 4th International Modelica Conference, Hamburg, 2005.
- [3] Zimmer D.: *Equation-Based Modeling of Variable-Structure Systems*. PhD thesis, Swiss Federal Institute of Technology, 2010.



## EFFICIENT DEBUGGING OF LARGE ALGORITHMIC MODELICA APPLICATIONS

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**Abstract.** A large amount of time of modelers are spent in finding the source of errors and fixing them. Often modelers use print statements or asserts to locate the root cause. These techniques are handy at times but are mostly time consuming, and can lead to wrong results in some cases. In this paper we present a new efficient debugger for debugging of large algorithmic Modelica code.

This replaces our earlier work in debuggers for the algorithmic subset of Modelica which used trace-based techniques. These have the advantages of being very portable, but turned out to have too much overhead for very large applications.

The new debugger is the first Modelica debugger that can operate without trace information. Instead it communicates with a low-level C-language symbolic debugger, the Gnu debugger (GDB), to directly extract information from a running executable, set and remove breakpoints, etc. This is made possible by the new bootstrapped OpenModelica compiler which keeps track of a detailed mapping from the high level Modelica code down to the generated C code compiled to machine code.

We developed and integrated this debugger as part of Modelica Development Tooling (MDT). MDT is molded in such a way that the new symbolic debugger and the old trace-based debugger can be used simultaneously by the user.

The debugger is operational, supports browsing of both standard Modelica data structures and tree/list data structures, and operates efficiently on large applications such as the OpenModelica compiler with more than 100 000 lines of code. To address debugging of full Modelica models, we plan to integrate this debugger with debugging mechanisms that support equation-based part of models.

**Keywords.** Modelica, Run-time Debugging, Modeling and Simulation, Algorithmic code, Eclipse.

- [1] Adrian Pop and Peter Fritzson (2005). A Portable Debugger for Algorithmic Modelica Code. In Proceedings of the 4th International Modelica Conference, Hamburg, Germany.
- [2] Adrian Pop, Peter Fritzson, Andreas Remar, Elmir Jagudin, and David Akhvlediani (2006). OpenModelica Development Environment with Eclipse Integration for Browsing, Modeling, and Debugging. In Proc of the Modelica'2006, Vienna, Austria.
- [3] Adrian Pop, David Akhvlediani, and Peter Fritzson (2007). Towards Run-time Debugging of Equation-based Object-oriented Languages. In Proceedings of the 48th Scandinavian Conference on Simulation and Modeling (SIMS'2007), available at [www.scan-sims.org](http://www.scan-sims.org) and <http://www.ep.liu.se>. Göteborg, Sweden.
- [4] Martin Sjölund, Peter Fritzson, and Adrian Pop (2011a). Bootstrapping a Modelica Compiler aiming at Modelica 4. In Proceedings of the 8th International Modelica Conference (Modelica'2011), Dresden, Germany.
- [5] Martin Sjölund and Peter Fritzson (2011b). Debugging Symbolic Transformations in Equation Systems. In Proceedings of the 4th International Workshop on Equation-Based Object-Oriented Modeling Languages and Tools, (EOOLT'2011), Zürich, Switzerland.
- [6] Peter Bunus and Peter Firtzson (2003). Semi-Automatic Fault Localization and Behavior Verification for Physical System Simulation Models. In Proceedings of the 18th IEEE International Conference on Automated Software Engineering, Montreal, Canada.
- [7] Peter Bunus (2004). Debugging Techniques for Equation-Based Languages. PhD Thesis. Department of Computer and Information Science, Linköping University.
- [8] Peter Fritzson (2004). Principles of Object-Oriented Modeling and Simulation with Modelica 2.1, 940 pp., ISBN 0-471-471631, Wiley-IEEE Press.
- [9] Peter Fritzson, Peter Aronsson, Håkan Lundvall, Kaj Nyström, Adrian Pop, Levon Saldamli, and David Broman (2005). The OpenModelica Modeling, Simulation, and Software Development Environment. In Simulation News Europe, 44/45.
- [10] Richard Stallman, Roland Pesch, Stan Shebs, et al. (2011). Debugging with GDB. Free Software Foundation. [online] Available at: < <http://unix.lsa.umich.edu/HPC201/refs/gdb.pdf> > [Accessed 30 October 2011].

## FUNCTION INLINING IN MODELICA MODELS

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**Introduction.** Equation-based, Object-Oriented Modelling Languages (EOOMLs) are increasingly being used for the modeling of complex dynamical systems. The key idea of EOOMLs is to describe systems declaratively in terms of differential-algebraic equations, which can then be symbolically processed to bring them in a form suitable for efficient solution. Among these languages, Modelica [2, 3] has received much attention, both from an academic and from an industrial perspective.

A notable feature of Modelica, which is lacking in most other EOOMLs, is the possibility to define custom *functions*, beyond the built-in mathematical functions such as  $\sin()$  or  $\exp()$ . Informally (see [4] for details), Modelica functions are defined by declaring the input variables, the output variables, optional local protected variables, and an algorithm to compute the protected and output variables from the inputs. The algorithm is written using statements typical of procedural programming languages: assignments, conditional statements, loops. A Modelica model using such functions has therefore a mixed semantics, in part declarative and in part procedural.

This approach is convenient in many applications, where parts of the model are better described in a procedural way; for example, consider the model of a vehicle running on a test track, whose shape in 3D space is described by a suitable algorithm. On the other hand, many symbolic analysis and optimization techniques which are commonly used in EOOMLs require the model to be formulated in terms of equations only: symbolic differentiation, symbolic index reduction, symbolic solution of implicit equations, handling of overconstrained connection equations, and so forth. Furthermore, there might be cases (e.g., optimization applications) in which the Modelica model needs to be translated into some other intermediate modelling language which is purely equation-based and does not allow to define custom functions, e.g., AMPL. It is then worth investigating how and to which extent a Modelica model using custom functions can be transformed into an equivalent one using only equations.

In the context of programming languages, a technique named *inlining* is often used by optimizing compilers, which substitute the call to a function in the code with a suitably adapted copy of the function body; this eliminates the overhead of a function call at the expense of an increased memory usage. Similar techniques can be devised in the context of EOOML, though the task is made harder by the fact that the body of a function algorithm is procedural, while the rest of the code is declarative.

In fact, the concept of *inlining* is well-known in the Modelica community, to the point that some parts of the Modelica Standard Library (e.g., the Multibody and Media libraries) can only be dealt with efficiently if some functions are inlined. Surprisingly, to the authors' knowledge, there is no published paper or technical document that clearly explains how inlining should be performed. Experimental evidence demonstrates that the Dymola tool inlines functions only in the special case when the function has no protected variables and the algorithm is given by a single assignment computing the output as an expression using the inputs. In this case inlining is trivial: it is sufficient to replace the function call with the right-hand-side of the assignment, changing the formal input variable names into the actual names. All functions in the Modelica Standard Library that need to be inlined belong to this special class, even though this requirement is not explicitly stated.

The goal of this paper is then to outline algorithms to transform Modelica models using custom-defined functions into purely equation-based models, going beyond the current state of the art. The proposed techniques will be demonstrated by a prototype implementation in the JModelica.org<sup>1</sup> platform. Optimal control problems where Modelica code is exported to XML format and then in turn imported into the CasADi [1] package for efficient solution will be used as a demonstrator in the final paper.

- [1] J. Anderson, B. Houska, , and M. Diehl. Towards a computer algebra system with automatic differentiation for use with object-oriented modelling. In *Third International Workshop on Equation-based Object-oriented Modeling Languages and Tools - EOOLT 2010*, Sept. 2010.
- [2] P. Fritzson. *Principles of Object-Oriented Modeling and Simulation with Modelica 2.1*. Wiley, 2003.
- [3] S. E. Mattsson, H. Elmqvist, and M. Otter. Physical system modeling with Modelica. *Control Engineering Practice*, 6(4):501–510, 1998.
- [4] The Modelica Association. Modelica - A unified object-oriented language for physical systems modeling - Language specification version 3.2. Online, Mar. 24 2010. URL: [https://www.modelica.org/news\\_items/documents/ModelicaSpec32.pdf](https://www.modelica.org/news_items/documents/ModelicaSpec32.pdf).

<sup>1</sup>[www.jmodelica.org](http://www.jmodelica.org)

# A LIMITER FOR PREVENTING SINGULARITY IN SIMPLIFIED FINITE VOLUME METHODS

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System simulation with object-oriented modelling languages has become an important tool for system and control design of vapour compression cycles. A common approach of modelling one-phase and two-phase fluid flow is 1-D spatial discretisation according to the Finite Volume Method.

In order to avoid stiff systems and to speed up simulation, pressure loss and momentum balance are usually handled in a simplified way. At low mass flow rates and in case of mass or heat flow reversal in a heat exchanger, the systems of equations of these simplified models often are not solvable. E.g. this is the case for simulation of vapour compression cycles with heat exchangers that are only part time activated.

To allow a simplified transient simulation of those vapour compression cycles under all boundary conditions the system of equations must be modified. Although the overall evaluation of those cycles is hardly influenced by the critical system states, the termination of the simulation impedes the evaluation process. This contribution presents a way to modify the system of equations to enable the simulation even under critical system states.

$$V \frac{dp}{dt} \frac{\partial \rho}{\partial p} + V \frac{dh}{dt} \frac{\partial \rho}{\partial h} = \dot{m}_A + \dot{m}_B \quad (1)$$

$$m \frac{dh}{dt} = \dot{m}_A (h_A - h) + \dot{m}_B (h_B - h) + \dot{Q} + V \frac{dp}{dt} \quad (2)$$

$$0 = p_B - p_A \quad (3)$$

Based on the mass balance (1), the energy balance (2) and the momentum balance (3) a tube or heat exchanger can be described. As the pressure is part of the mass and energy balance in every control volume at the same pressure, an algebraic system of equations is created. This system of equations can be described by a set of linear systems.

$$A \cdot x = b \quad (4)$$

$$x = A^{-1} \cdot b = \frac{\text{adj}(A)}{\det(A)} \cdot b \quad (5)$$

A linear system can generally be written in the form of equation (4). The matrix  $A$  multiplied by the vector of unknowns  $x$  is equal to the vector  $b$  on the right hand side. To solve that equation for  $x$ , it is necessary to calculate the determinant of matrix  $A$  as shown in equation (5). If the determinant is zero the system is singular and cannot be solved.

$$\psi_i = \left( \frac{\partial \rho}{\partial p} + \frac{\partial \rho}{\partial h} \frac{1}{\rho_i} \right) \quad \gamma_{i,A} = \left( 1 - \frac{\partial \rho}{\partial h} \frac{1}{\rho_i} (h_{i,A} - h_i) \right) \quad \gamma_{i,B} = \left( 1 - \frac{\partial \rho}{\partial h} \frac{1}{\rho_i} (h_{i,B} - h_i) \right) \quad (6)$$

$$\det(A) = \sum_{i=1}^n \left[ \psi_i \cdot \prod_{j=2}^n (\gamma_{j,A}) \cdot \prod_{k=1}^{i-1} (\gamma_{k,B}) \right] \quad (7)$$

If  $\psi$  is always positive, a simple approach to avoid the singularity of each linear system is to prevent zero-crossings of the  $\gamma$  terms. The approach that is presented allows to eliminate the singularity with only information on the control volume and the two neighbour control volumes.

As the density  $\rho$  is always positive and the partial derivative  $\frac{\partial \rho}{\partial h}$  always negative, the  $\gamma$  term can only cross zero if the difference of the specific enthalpies is negative. So for a given fluid state  $p_i, h_i$  in the control volume it is possible to determine the specific enthalpy  $h_{i,A}$  at the control volume's surface causing  $\gamma_{i,A} = 0$ .

$$h_{\text{limit},i} = h_i + y_{\text{limit}} \frac{\rho_i}{\frac{\partial \rho}{\partial h}} \quad (8)$$

$$h_{i-1,B,\text{modified,outflow}} = \max \{ h_{i-1}, h_{i,\text{limit}} \} \quad h_{i+1,A,\text{modified,outflow}} = \max \{ h_{i-1}, h_{i,\text{limit}} \} \quad (9)$$

Based on the zero crossing of  $\gamma$  the minimum specific enthalpy flowing out of the control volume can be calculated and hence a constraint for this specific enthalpy formulated (see equations (9)). The factor  $y_{\text{limit}} \in ]0, 1[$  is used to define how close  $\gamma$  can approach zero and should be set close to 1.

The presented limiter is an effective way to enable the simulation under those critical boundary conditions. It can easily be implemented in the object oriented modelling language Modelica using the stream connector concept.

## REALISATION-PRESERVING MODEL REDUCTION OF MODELS IN MODELICA

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The central guideline in modelling is that a model should not be more complex as necessary for a given purpose. Models satisfying this requirement, i.e., having proper complexity, are often designated as *proper models* [1].

However, contemporary component-based modelling approach often yields very detailed models from the beginning and the obtained models can be too complex for many intended tasks. Therefore, automatic model reduction techniques are active research topic and so far numerous automatic model reduction methods have been developed [2]. In some fields, e.g., integrated circuits design, they reached a stage of becoming an indispensable part of system analysis and hence provided as part of domain-specific modelling environments [3].

The most successful methods, for example, those based on projection techniques, are not realisation-preserving [2] – the reduced model retains input-output behaviour of the system, but loses physical interpretability of its structure and parameters. In some cases it may be no longer possible to simulate the reduced model with the simulator of the modelling environment which was used to design the full model.

Although preservation of realisation is a very desirable property, realisation-preserving reduction methods are mostly neglected in the literature due to their bad efficiency. Furthermore, most of the existing methods are limited to a certain type of models, e.g., RC circuits. There are no realisation-preserving model reduction methods known to the authors that could adequately handle multi-domain models implemented in contemporary object-oriented modelling languages such as Modelica.

Models in Modelica are usually decomposed into several hierarchical levels. At the bottom of the hierarchy, differential-algebraic equations are used for the component description, while on higher levels, model is described by connecting acausal objects (components). This is often done graphically and resulting schematics are called *object diagrams* [4]. In order to preserve the organisation of original model combinations of model reduction methods are needed. Moreover, for some tasks, e.g., model verification [5], only a part of the model might be desired to be reduced.

A framework consisting of methods for reduction of schematics (Modelica's object diagrams) and set of equations is proposed whereby some existent methods were adapted to cover also more diverse models in Modelica. For reduction of object diagrams, energy-based model reduction techniques developed for bond graphs [6, 7, 2] were adapted. Reduction of a system of differential-algebraic equations was done using method of [8, 9].

- [1] B. H. Wilson and J. L. Stein, "An algorithm for obtaining proper models of distributed and discrete systems," *ASME Journal of Dynamic Systems, Measurement and Control*, vol. 117, pp. 534–540, 1995.
- [2] T. Ersal, H. K. Fathy, D. G. Rideout, L. S. Louca, and J. L. Stein, "A Review of Proper Modeling Techniques," *Journal of Dynamic Systems, Measurement, and Control*, vol. 130, no. 6, p. 061008, 2008.
- [3] M. V. Ugryumova, *Applications of Model Order Reduction for IC Modeling*. PhD thesis, Eindhoven University of Technology, 2011.
- [4] *Modelica Specification, version 3.2*, 2010. <http://www.modelica.org/documents/-ModelicaSpec32.pdf>.
- [5] A. Sodja and B. Zupančič, "On using model approximation techniques for better understanding of models implemented in modelica," in *Proceedings of 8th International Modelica Conference*, (Dresden, Germany), 2011.
- [6] R. Rosenberg and T. Zhou, "Power-based model insight," in *Proceedings of the ASME WAM Symposium on Automated Modeling for Design*, (New York, USA), pp. 61–67, 1988.
- [7] L. S. Louca, *An Energy-based Model Reduction Methodology for Automated Modeling*. PhD thesis, University of Michigan, 1998.
- [8] T. Wichmann *et al.*, "On the simplification of nonlinear dae systems in analog circuit design," in *Proceedings of CASC'99*, (Munich, Germany), 1999.
- [9] T. Wichmann, "Transient ranking methods for the simplification of nonlinear dae systems in analog circuit design," *Proceedings in Applied Mathematics and Mechanics*, vol. 2, pp. 448–449, 2003.

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# A MPC SCHEME WITH GUARANTEED STABILITY FOR THE CONTROL OF BLOCH SYSTEMS

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**Abstract.** Optimal control strategies are of paramount importance in applications that range from microscopic to macroscopic. In the microscopic world, control schemes are being used to steer atomic systems. In this paper, we focus on Bloch systems that model the dynamics of an ensemble of atomic spins in an external magnetic field:

$$\frac{d}{dt} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix} = \gamma \begin{bmatrix} 0 & -B_z & B_y(t) \\ B_z & 0 & -B_x(t) \\ -B_y(t) & B_x(t) & 0 \end{bmatrix} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix},$$

where  $B_z$  is large static magnetic field and  $(B_x, B_y)$  are time-dependent magnetic control fields to be constructed in such a way to steer the Bloch system to the equilibrium configuration while an admissible maximum control amplitude is given at any time as follows

$$B_x^2 + B_y^2 \leq B_{max}^2.$$

These models are at the core of nuclear magnetic resonance (NMR) technology where there is the need to design optimal magnetic pulses with limited energy. For this purpose, we consider the optimal control of Bloch systems and develop a model predictive control (MPC) strategy that accommodates nonlinearity and constraints on the control while guaranteeing stability of the controlled system.

We discuss a state-space model predictive control scheme and the corresponding quasi-infinite horizon approach for controlling Bloch systems. This control procedure requires to choose a finite time horizon  $T < \infty$  and to solve a finite horizon open-loop optimal control problem with the measured state of the system as the initial value. We apply the resulting control function  $\bar{u}(\cdot|t)$  until the next state measurement becomes available. We then repeat the finite horizon open-loop optimization procedure taking this new measured state of the system as the initial value.

Let the Bloch system be denoted with  $\dot{x} = f(x, u)$ , where  $x$  denotes the state variables and  $u$  denotes the controls. The finite horizon open-loop optimal control problem to be solved at every sampling instant  $t$  is described as follows

$$\left\{ \begin{array}{l} \min_{\bar{u}(\cdot|t)} J(\bar{u}(\cdot|t); \bar{x}(\cdot|t)) \\ \dot{\bar{x}}(r|t) = f(\bar{x}(r|t), \bar{u}(r|t)) \\ \bar{x}(t|t) = x(t) \\ \bar{u}(r|t) \in \mathcal{U} \\ \bar{x}(r|t) \in \mathcal{X} \\ \bar{x}(t+T|t) \in \Omega \end{array} \right.$$

where  $r \in [t; t+T]$ , and the objective  $J$  becomes

$$J(\bar{u}(\cdot|t); \bar{x}(\cdot|t)) = \frac{1}{2} \int_t^{t+T} [\bar{x}(\tau|t)' Q \bar{x}(\tau|t) + \bar{u}(\tau|t)' R \bar{u}(\tau|t)] d\tau + E(\bar{x}(t+T|t)).$$

It has been shown that under appropriate conditions, for any sampling time  $0 < \delta < T$  the nominal closed-loop system is asymptotically stable.

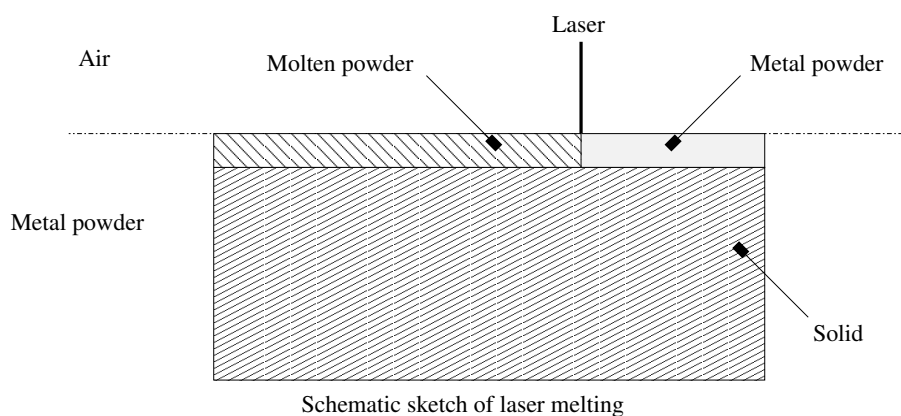
Results of numerical experiments demonstrate the ability of the proposed algorithm to robustly control Bloch systems while satisfying given control constraints.

# STATE-CONSTRAINED OPTIMAL CONTROL PROBLEMS IN THE MODELLING OF LASER MELTING TECHNOLOGIES FOR THE PRODUCTION OF COMPLEX METALLIC COMPONENTS

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A new innovative industrial laser technique called laser melting enables the efficient limited-lot production of complex metallic structures from metal powders. In the laser melting process a thin layer of metal powder is locally fused by a moving laser beam. The components are built up layer by layer by successively applying new powder and melting. In recent years several models for the simulation of this production process were derived (e.g. [1]), where the energy input and the velocity of the laser beam were considered as constant parameters.



The locally limited input of energy by the laser results in high temperature gradients in the workpiece. Consequently, the so called temperature gradient mechanism causes residual stresses and deformations. However, there are various situations, e.g. when reaching the boundary of a workpiece, in which a strategy of keeping the power and the velocity of the laser beam constant generates unnecessary large energy input and avoidable deformations.

Therefore, in a first step the power of the laser should be controlled in such a way, that on the one hand a melting of the relevant regions is guaranteed but on the other hand the occurring temperature gradients are as low as possible. From a mathematical point of view this leads to an optimal control problem with a partial differential equation (PDE), where the heat distribution is modeled via the heat equation. The melting condition for the relevant powder is modeled by a threshold for the temperature in the regions next to the current laser position. Thus, this model also involves state constraints, which are in the focus of current research in PDE constrained optimization.

In a second step alternatively, resp. additionally the motion of the laser beam shall be controlled in an optimal way, which is motivated by a reduction of the production time. Consequently, the model has to be enhanced by the equations of motion of the laser. An optimal control problem with a coupled system of ordinary and partial differential equations arises, which is also in the focus of current research. The crucial problem in this model is the melting condition. The position of the laser, and thus the position, where the threshold for the temperature is enforced, is no more known a priori. Indeed, this position is dynamic and depending on the control during the optimization procedure. Herewith another new type of state constraints arises.

Although there are a lot of new aspects in this model, several links to existing work concerning laser hardening and laser material treatment can be found (cf. [2, 3]).

Since the model presented is currently work in progress, only first numerical results according to a *First-Discretize-Then-Optimize* Ansatz for a simplified model problem as well as an outlook at the future line of action conclude the talk.

- [1] Branner G.: *Modellierung transientser Effekte in der Struktursimulation von Schichtbauverfahren*. iwv-Forschungsberichte, 246, Herbert Utz Verlag, München, 2011.
- [2] Hömberg D., and Sokolowski J.: *Optimal control of laser hardening*. Adv. Math. Sci., 8 (1998), 911–928.
- [3] Hömberg D., Steinbrecher A., and Stykel T.: *Optimal control of robot guided laser material treatment*. Preprint 1405, WIAS Berlin, 2009.



# ADAPTIVE FINITE ELEMENT METHODS FOR OPTIMAL CONTROL OF ELASTIC WAVES

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**Introduction.** In this talk we present the dual weighted residual method (DWR, cf. Becker & Rannacher [1]) for finite element methods for optimal control problems of the following type

$$\text{Minimize } J(u, y), \quad u \in U, \quad y \in X, \quad \text{s.t. } y_{tt} - A(u, y) = f, \quad y(0) = y_0(u), \quad y_t(0) = y_1(u) \quad (1)$$

governed by a hyperbolic partial differential equation of second order. Thereby,  $U$  denotes the control space,  $X$  the state space,  $f$  a given force,  $A$  an operator depending on the control  $u$  and the state  $y$ , and  $y_0$  and  $y_1$  denote the initial data which may also depend on the control. The results presented here are an extension of Meidner & Vexler [4] and Schmich & Vexler [5], where parabolic equations are considered. The optimal control problem (1) is discretized by space-time finite elements. Let  $(u, y)$  be the solution of the continuous problem and  $(u_\sigma, y_\sigma)$  of the discretized one. Then the aim is to estimate the error  $J(u, y) - J(u_\sigma, y_\sigma)$  in the cost functional by separating the influences of time, space, and control discretization. This allows to set up an efficient adaptive algorithm for local mesh refinement of the space and time discretizations to improve the accuracy of the error in the cost functional. A numerical example for optimal control of the dynamical Lamé system is presented. For a discussion of these methods in detail we refer to Kröner [2, 3].

**Discretization.** The state equation and the corresponding adjoint equation are reformulated equivalently as first order systems in time and are discretized by space-time finite elements. We apply a  $cG(r)cG(s)$  method. The state equation is discretized in time by a Petrov-Galerkin scheme, i.e. we use continuous ansatz functions and discontinuous test functions. Then we discretize the equation in space using conforming finite elements. Finally, we discretize the control space by choosing a finite dimensional subspace of  $U$ . We assume, that the corresponding control problems on the different levels of discretization admit a locally unique solution and denote them by  $(u_k, y_k)$ ,  $(u_{kh}, y_{kh})$ , and  $(u_\sigma, y_\sigma)$ , respectively.

**A posteriori estimate.** To derive an a posteriori error estimate we split the error in the cost functional in the parts arising from time, space and control discretization

$$J(u, y) - J(u_\sigma, y_\sigma) = (J(u, y) - J(u_k, y_k)) + (J(u_k, y_k) - J(u_{kh}, y_{kh})) + (J(u_{kh}, y_{kh}) - J(u_\sigma, y_\sigma)) =: e_1 + e_2 + e_3$$

where the arguments of the functional are the solutions of the control problems on the continuous level as well as on the different levels of discretization. The errors  $e_1$ ,  $e_2$ , and  $e_3$  in the cost functional are estimated by first derivatives of a corresponding Lagrangian up to terms of higher order resulting in an a posteriori error estimate. This estimate leads to an adaptive algorithm for local mesh refinement improving the accuracy of the error in the cost functional and equilibrating the errors arising from time, space, and control discretization.

**Numerical example - Control of the dynamical Lamé system.** The approach described above is applied to an optimal control problem governed by the dynamical Lamé system. This system describes the propagation of elastic waves in solid materials. It can be seen as a model for seismic waves in the earth and acoustic waves in solid materials. An optimal control problem governed by the dynamical Lamé system with time-dependent control entering the right hand side of the system is considered. The components of the control act on different parts of the spatial domain. The numerical results confirm that the considered approach leads to a speedup with respect to computational time as well as with respect to the number of degrees of freedom in comparison to uniform mesh refinement.

- [1] Becker R., and Rannacher R.: *An optimal control approach to a-posteriori error estimation*. Acta Numerica, (2001), 1–102.
- [2] Kröner A.: *Numerical Methods for Control of Second Order Hyperbolic Equations*, Ph.D. thesis, Technische Universität München, (2011).
- [3] Kröner A.: *Adaptive finite element methods for optimal control of second order hyperbolic equations*, Comput. Methods Appl. Math., 11 (2011), 214 – 240.
- [4] Meidner D., and Vexler B.: *Adaptive space-time finite element methods for parabolic optimization problems*. SIAM J. Control Optim., 46 (2007), 116–142.
- [5] Schmich M., and Vexler B.: *Adaptivity with dynamic meshes for space-time finite element discretizations of parabolic equations*. SIAM J. Sci. Comput., 30 (2008), 369 – 393.

# ENERGY MINIMIZERS OF THE COUPLING OF A COSSERAT ROD TO AN ELASTIC CONTINUUM

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In this article we analyze the coupling of a three-dimensional elastic continuum model to a geometrically exact one-dimensional rod with an orthonormal director frame (Cosserat rod). We assume that both objects are governed by hyperelastic material laws, and consider the static case only. We then propose two different coupling conditions and show that the coupled problem has solutions for both of them. Existence of more than one set of plausible coupling conditions is a general feature of heterogeneous models (cf. [1]). The proof uses the direct method of the calculus of variations. For each coupling condition we also obtain the corresponding dual conditions, which we interpret as coupling conditions for the forces and moments.

The coupling of mechanical models of differing dimensions has been treated both in the engineering and the mathematical literature ([4, 3, 2]). We would like to point out the work of [1], where a systematic treatment for coupling linear models (without directors) of different dimensions is given. In particular, they provide existence and uniqueness of solutions for their coupled problems. To the knowledge of the authors, coupling conditions for a reduced model with director variables has only been treated in [5]. Additionally, in that work, an algorithm based on fixed-point iteration was proposed to numerically solve coupling problems of the type considered here. Our variational approach instead suggests to treat the problem as a global minimization problem with nonlinear constraints. A detailed treatment may appear in a separate article.

We proceed as follows. First, we formally introduce the rod and continuum models in a variational framework. The rod is modelled as an element of an infinite dimensional manifold, based the special orthogonal group. The continuum is taken from a class of hyperelastic models, including polyconvex nonlinear elasticity. Then we propose two sets of coupling conditions for the displacement and director variables. The first coupling condition enforces a pointwise coincidence of the cross section of the rod with the coupling interface of the continuum. The second condition only enforces this coincidence in an integral sense. Next, we formulate the coupled problem as an energy minimization problem, which amounts in an optimization problem on an infinite dimensional manifold with the coupling condition as an equality constraint. Finally we give existence results of global minimizers and optimality conditions for solutions for both coupling conditions. This leads to corresponding conditions for the dual variables, i.e., the coupling forces and moments.

- [1] Blanco, P.J., Discacciati, M., and Quarteroni, A. (2011). Modeling dimensionally-heterogeneous problems: analysis, approximation and applications. *Numer. Math.*, 119(2), 299–335.
- [2] Ciarlet, P., LeDret, H., and Nzengwa, R. (1989). Junctions between three-dimensional and two-dimensional linearly elastic structures. *J. Math. Pures Appl.*, 68, 261–295.
- [3] Lagnese, J., Leugering, G., and Schmidt, E. (1994). *Modeling, Analysis and Control of Dynamic Elastic Multi-Link Structures*. Birkhäuser.
- [4] Monaghan, D.J., Doherty, I.W., Court, D.M., and Armstrong, C.G. (1998). Coupling 1D beams to 3D bodies. In *Proc. 7th Int. Meshing Roundtable*. Sandia National Laboratories.
- [5] Sander, O. (to appear). Coupling geometrically exact cosserat rods and linear elastic continua. In *Proc. of DD20*.

## MODELING AND SOLVING MIXED-INTEGER ODE/DAE CONSTRAINED OPTIMAL CONTROL PROBLEMS IN AMPL

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Modeling languages and systems for simulation and optimization of continuous ODE/DAE systems are commonly available. For the most part, they focus on convenience of user interaction, and are tightly coupled to one or a few selected numerical methods.

Control problems with discrete and hybrid controls, called mixed-integer optimal control problems (MIOCPs), have recently gained increased attention as the potential for optimization is high, e.g. [6, 5]. The mixed-integer optimization community however most often considers static problems such as MI(N)LPs, and relies on symbolic modeling languages such as AMPL [2]. Access to many advances MI(N)LP codes is provided by the NEOS Server for Optimization [3] through the AMPL modeling language.

Addressing this gap, we describe a set of extensions to the AMPL modeling language to conveniently model mixed-integer optimal control problems for ODE or DAE dynamic processes. These extensions are easily realized and do not require intrusive changes to the AMPL language standard or implementation itself. We provide TACO, the publicly available “Toolkit for AMPL Control Optimization” that addresses developers of existing and new MI(N)LP and MIOCP solvers who wish to process such extended AMPL models.

An example of such a solver is the “multiple shooting code for optimal control” MUSCOD-II [1, 4], a direct and simultaneous method for ODE/DAE-constrained optimal control, and its extension MS-MINTOC [6] for mixed-integer optimal control. We use the AMPL extensions to model exemplary control problems and obtain solutions to these problems by using MUSCOD-II and MS-MINTOC inside the AMPL environment.

A collection of further AMPL control models is now available on the web site [mintoc.de](http://mintoc.de). MUSCOD-II and MS-MINTOC are now available on the NEOS Server for Optimization, using the presented toolkit to enable the efficient solution of AMPL models for optimal control problems.

- [1] H.G. Bock, K.J. Plitt. A multiple shooting algorithm for direct solution of optimal control problems. In: Proceedings of the 9th IFAC World Congress, Pergamon Press, Budapest, 1984, pp. 242–247.
- [2] R. Fourer, D. Gay, B. Kernighan. A modeling language for mathematical programming. *Management Science* 36:519–554, 1990.
- [3] W. Gropp, J. Moré. Optimization environments and the NEOS Server. In: M. Buhmann, A. Iserles (Eds.) *Approximation Theory and Optimization*, Cambridge University Press, 1997, pp. 167–182.
- [4] D.B. Leineweber, I. Bauer, A. Schäfer, H.G. Bock, J.P. Schlöder. An efficient multiple shooting based reduced SQP strategy for large-scale dynamic process optimization (Parts I and II). *Computers & Chemical Engineering* 27:157–174, 2003.
- [5] C. Kirches. Fast numerical methods for mixed-integer nonlinear model-predictive control. In: H.G. Bock, W. Hackbusch, M. Luskin, R. Rannacher (Eds.) *Advances in Numerical Mathematics*, Vieweg+Teubner, Wiesbaden, 2011.
- [6] S. Sager. *Numerical methods for mixed-integer optimal control problems*. Der andere Verlag, Tönning, Lübeck, Marburg, 2005.

# DISCRETIZATION BASED CONVERGENCE RESULTS FOR EULER APPROXIMATIONS OF BANG-BANG CONTROLS

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**Introduction.** We consider Euler discretizations to a class of linear-quadratic optimal control problems. Assuming that the discrete controls are of bang-bang type and define switching functions with a uniform structure independent of the discretization we show, that the discrete controls converge to a bang-bang control, which is a solution of the original problem.

**Problem Statement and Related Results.** Mathematical modelling of many problems from technical applications or economics results in optimal control problems with control appearing linearly. In this case the optimal control is often of bang-bang type, and numerical methods are needed which are able to detect such a structure. We consider a general class of linear-quadratic optimal control problems with control appearing linearly. In [1] we derived error estimates for Euler approximations for such control problems assuming that the optimal control is of bang-bang type and the switching function has a stable structure. Here we investigate the question if conversely a sequence of discrete bang-bang-controls converges to a bang-bang solution of the original problem provided the discrete controls are of bang-bang type. Related results have been obtained in [2] and [3] (see also the papers cited therein) assuming that a certain second-order optimality condition is satisfied uniformly for the discretized problems. Since such a second-order condition is not satisfied for bang-bang controls, we use a different proof technique based on structural assumptions for the discrete controls and switching functions.

**Main Result.** We assume that the discrete optimal controls obtained by Euler discretization are of bang-bang type and that the discrete switching functions have finitely many zeros, which are stable under perturbation. This is guaranteed by the assumption, that the directional derivative of the switching functions in the zeros is uniformly positive. Then we show that the discrete controls converge to a bang-bang solution of the original problem. This theoretical result is also of practical interest, since the assumptions for the discrete control problems can be checked numerically. Therefore, we can conclude from numerical checks that the original problem has a bang-bang solution.

## References.

- [1] Alt W., Baier R., Gerdt M., and Lempio, F.: Error Bounds for Euler Approximation of Linear-Quadratic Control Problems with Bang-Bang Solutions. NACO(2012), to appear.
- [2] Dontchev, A. L.: An a priori estimate for discrete approximations in nonlinear optimal control. SIAM J. Control Optim. 31 (1993), 569–603.
- [3] Felgenhauer, U.: Numerical optimality test for control problems. In: Guddat, J., Jongen, H. Th., Nozicka, F., Still, G. Twilt, F. (eds.) Parametric Optimization and Related Topics IV, Enschede 1995, Peter Lang Publ. House, Frankfurt (1996), 85–101.

# MODELLING AND OPTIMAL CONTROL OF A DOCKING MANEUVER WITH AN UNCONTROLLED SATELLITE

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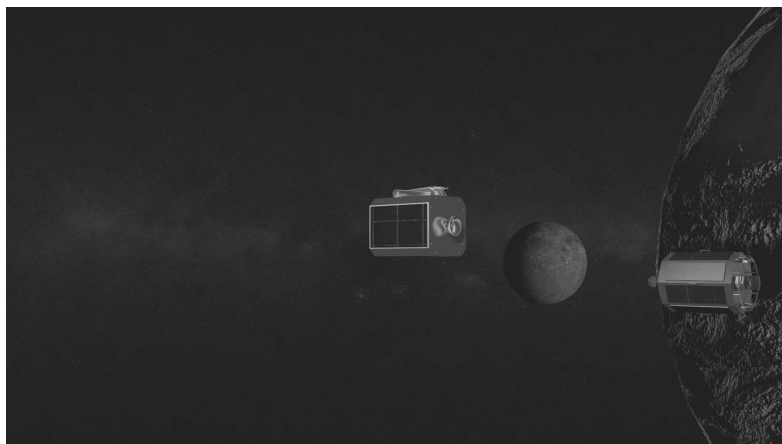
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**Introduction.** Even in space the space is limited. The orbits around earth are populated with disused satellites, propulsion stages and space debris. Every piece poses a possible threat to working projects like communication satellites or the international space station. Additionally, the reentry of such objects endangers the population as the place of impact cannot be controlled anymore. In 2011 the german satellite Rosat crashed uncontrolled on earth. Even only hours before impact it was not sure if fractions will strike populated areas. To reduce this threat the German Space Operations Center (GSOC) is planning to develop a satellite which is able to dock at disused satellites and force the target to reenter the atmosphere in a predefined entry corridor. A technology demonstration mission called DEOS (Deutsche Orbitale Servicing Mission) is supposed to take the first step towards this goal. It consists of two separate spacecraft, one acting as uncontrolled target and one as active servicer. Different docking and berthing maneuvers and finally a controlled reentry in coupled constellation shall be tested to gather data for future space debris removal.

**Content.** This paper is dedicated as a feasibility approach for the DEOS mission, i.e. it demonstrates the modelling and optimal control of a rendezvous scenario between a controlled service satellite and an uncontrolled target. The results can be used to distinguish whether a docking maneuver is possible. Here, we present a model which consists of the following subsystems: The first subsystem represents the relative position of the service spacecraft and the uncontrolled target. These dynamics are given by the so called Clohessy-Wilshire equations. The second subsystem defines the dynamics for the orientation. Since in aerospace engineering the rotation is most commonly described by quaternions instead of Euler angles, a quaternion differential equation is added to model the rotation. Last, as the derived system is able to describe not only stable but also tumbling motion of the target, the gyroscopic equation is included to model the angular velocities. In total, the obtained model consists of twenty state and six control variables. All equations of motion are presented as first order ordinary differential equations.

To prevent the collision of the two spacecraft a state constraint is included in the optimal control problem. As the terminal time is to be minimized as well, a time dependent rendezvous condition is added to ensure a docking position at the end of the maneuver. In the Bolza type cost functional weight parameters can be chosen to distinguish between cost and time optimal control strategies or any wanted combination of these.

The derived optimal control problem is solved using a full discretization approach. To this end, the modeling language AMPL is used together with the interior point optimizer IpOpt. The results for a flyaround maneuver with a rotating target are presented and a 3D simulation of the model is shown.



Rendered picture of the satellites

- [1] Alfriend, K., Gurfil, P., and Vadali, S. (2009). *Spacecraft Formation Flying: Dynamics, Control, and Navigation*. Elsevier Astrodynamics Series. Elsevier Science & Technology.
- [2] Sellmaier, F., Boge, T., Spurrmann, J., Gully, S., Rupp, T., and Huber, F. (2010). On-orbit servicing missions: Challenges and solutions for spacecraft operations. In *SpaceOps 2010 Conference*. German Space Operations Center (GSOC), Huntsville, Alabama, USA.

# FLIGHT PATH OPTIMIZATION SUBJECT TO INSTATIONARY HEAT CONSTRAINTS

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## Summary

We consider a flight path optimization problem in the hypersonic flight regime. The aerothermic heating requires the use of innovative lightweight materials and a sophisticated thermal protection system (TPS). Therefore advanced mathematical approaches are needed, to compute and optimize the thermal load in hypersonic flight regimes. Mathematically this leads to a trajectory optimization problem s.t. an instationary heat equation. The model of the hypersonic plane is based on the lower stage of the German Sänger II concept, which may be also considered for intercontinental hypersonic flight. The thermal protection system consists of different insulated layers of suitable materials and thicknesses. For simplicity we consider only the most critical stagnation point.

The model of the hypersonic space vehicle used here is based on [4], see also [2, 1]. The complete formulas of the model used in the code are given for the first time in [5]. The aim of the paper is to describe in a detailed mathematical way the modelling of the coupling between a complicated but standard trajectory optimization problem with an instationary heat equation (partial differential equation) in order to investigate in future the observed numerical difficulties in more detail. The presented numerical results are based on a revised Fortran code [5] using a direct collocation method [3] for the solution of the ODE constrained optimal control problem. The resulting nonlinear program is solved by SNOPT.

- [1] K. Chudej, H.J. Pesch, M. Wächter, G. Sachs, F. Le Bras: *Instationary heat constrained trajectory optimization of a hypersonic space vehicle by ODE-PDE constrained optimal control*. Preprint IOC-11, Feb 2008, International Doctorate Program: Identification, Optimization and Control with Applications in Modern Technologies, Univ. Bayreuth, Univ. Erlangen-Nürnberg, Univ. Würzburg, Germany.
- [2] M. Dinkelmann, M. Wächter, G. Sachs: *Modelling and simulation of unsteady heat transfer effects on trajectory optimization of aerospace vehicles*. *Mathematics and Computers in Simulation* 53 (2002) 389–394.
- [3] O. von Stryk: *User's Guide for DIRCOL. A Direct Collocation Method for the Numerical Solution of Optimal Control Problems*. Version 2.1, Lehrstuhl M2 Höhere Mathematik und Numerische Mathematik, Technische Universität München (1999).
- [4] M. Wächter: *Optimalflugbahnen im Hyperschallflug unter Berücksichtigung der instationären Aufheizung*. Dissertation, Lehrstuhl für Flugmechanik und Flugregelung, Technische Universität München (2004).
- [5] M. Witzgall: *Optimale Steuerung eines Hyperschallflugzeugs mit Beschränkung der instationären aerothermischen Aufheizung*. Diplomarbeit, Lehrstuhl für Ingenieurmathematik, Universität Bayreuth (2009).

# OPTIMAL REAL-TIME CONTROL OF FLEXIBLE RACK FEEDERS USING THE METHOD OF INTEGRODIFFERENTIAL RELATIONS

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**Summary.** Rack feeders are of high practical importance as automated conveying systems. In this paper, control-oriented models are derived for an experimental setup representing the structure of a typical high bay rack feeder. On the basis of these models, feedforward control strategies are designed. The rack feeder is a viscoelastic structure consisting of two identical flexible beams which are attached to a horizontally movable carriage. The beams are rigidly connected at their tip by a pulley block which is necessary for the vertical positioning of a payload. To develop a real-time applicable control algorithm, a frequency analysis is performed for the original double-beam structure. As a consequence, a simplified Bernoulli beam model is derived with specific boundary conditions. The control objective under consideration is the positioning of the flexible beam structure at a desired position in such a way that the terminal mechanical energy stored in the beam is minimized. A modification of the Galerkin method which is based on an integrodifferential approach and a suitable finite element technique are employed to describe the viscoelastic structural vibrations and to design optimal control strategies. Results of numerical simulations are presented and compared with measured data.

**Introduction.** The design of control strategies for dynamic systems with distributed parameters has been actively studied in recent years. Processes such as oscillations, heat transfer, diffusion, and convection are part of a large variety of applications in science and engineering. The theoretical foundation for optimal control problems with linear partial differential equations (PDEs) and convex functionals was established by [1]. Different approaches to the discretization of dynamical models with distributed parameters are developed to reduce the original initial-boundary value problem to a system of ordinary differential equations (ODEs). In this context, variational and projection methods are powerful tools to solve control problems for elastic structures. The method of integrodifferential relations (MIDR) was proposed in [2] for the design of optimal control laws for dynamical systems with distributed parameters. A projection approach was developed as a modification of the Galerkin method in the frame of the MIDR for systems described by linear parabolic PDEs. In the current paper, this approach is combined with a suitable finite element method and extended to modeling and optimal control of rack feeder structures. This application has already been considered in [3] by using an alternative system representation.

**Conclusions and Outlook.** In this paper, a Fourier technique has been applied to derive a control-oriented model of a typical high bay rack feeder. A modeling and optimization algorithm has been developed for feedforward control of distributed viscoelastic structures based on the MIDR, a projection approach, and a novel finite element technique. A numerical verification and experimental validation on a test rig has been performed for the proposed control strategy. In future work, an offline identification of system parameters from measured data and the design of a robust observer-based feedback control structure are planned on the basis of the MIDR.

- [1] Lions J.L.: *Optimal Control of Systems Governed by Partial Differential Equations*. Springer–Verlag, New York, 1971.
- [2] Saurin V.V., Kostin, G.V., Rauh, A., and Aschemann, H. *Adaptive control strategies in heat transfer problems with parameter uncertainties based on a projective approach*. In: Rauh, A. and Auer, E. (eds.), *Modeling, Design, and Simulation of Systems with Uncertainties*. Springer–Verlag, Heidelberg, 2011, 309-332.
- [3] Aschemann H., Schindele D., and Ritzke J. *State and disturbance estimation for robust control of fast flexible rack feeders*. In: Rauh, A. and Auer, E. (eds.), *Modeling, Design, and Simulation of Systems with Uncertainties*, Springer–Verlag, Heidelberg, 2011, 333-351.





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# VIBRATIONS OF A PARAMETRICALLY EXCITED MEMS-STRUCTURE WITH TWO MASSES

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**Background.** Microelectromechanical systems (MEMS), see Fig. 1, are becoming more and more important for all kinds of industrial applications. One of them are filters in communication devices, due to the growing demand for efficient and accurate filtering of signals [1]. In recent developments single degree of freedom (1-dof) oscillators that are operated at a parametric resonances are employed for such tasks. Typically vibration damping is low in such MEM systems. While parametric excitation (PE) is used so far to take advantage of a parametric resonance, this contribution suggests to also exploit parametric anti-resonances in order to improve the damping behavior of such systems [2]. Modeling aspects of a 2-dof MEM system, see Fig. 1, and some first results are the focus of this paper.

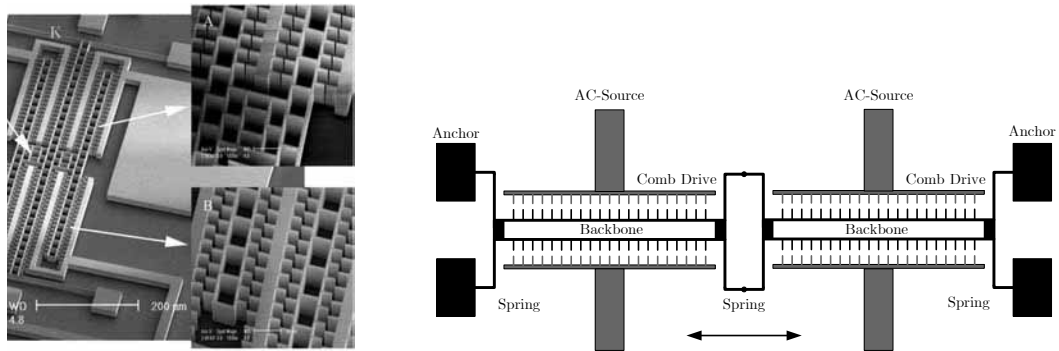


Figure 1. Left: Image of a MEM structure. Right: Sketch of the mechanical model of the 2-dof system as investigated.

**Modelling the mechanical system.** In principle the system is an oscillating mechanical system with two degrees of freedom  $\mathbf{x} = [x_1, x_2]^T$  that can be described by

$$\mathbf{M}\ddot{\mathbf{x}} + \mathbf{C}\dot{\mathbf{x}} + \mathbf{K}_1\mathbf{x} + \mathbf{K}_3\mathbf{x}^3 + \mathbf{F}_{\text{es}}(\mathbf{x}, t) = 0, \quad \mathbf{F}_{\text{es}}(\mathbf{x}, t) = V_0^2(\mathbf{R}_{10}\mathbf{x} + \mathbf{R}_{30}\mathbf{x}^3) + V_A^2(1 + \cos(\omega t))(\mathbf{R}_{1A}\mathbf{x} + \mathbf{R}_{3A}\mathbf{x}^3). \quad (1)$$

The system is inherently non-linear because of the cubic mechanical stiffness  $\mathbf{K}_3$  of the structure, but also because of the electrostatic forces  $\mathbf{F}_{\text{es}}(\mathbf{x}, t)$  that act on the system. Electrostatic forces are generated by so-called *comb drives* (see Fig. 1) and are proportional to the applied voltages  $V_0^2$  and  $V_A^2$ . These drives also provide the means to introduce time-periodic coefficients, i.e. parametric excitation  $(1 + \cos(\omega t))$  with frequency  $\omega$ .

For a realistic MEM system the coefficients of the non-linear set of differential equations need to be scaled for efficient numerical treatment. So the final mathematical model is a set of four non-linear time-periodic homogeneous differential equations of first order.

**Solution method and numerical results.** Numerical results are obtained from two different methods. The linearized time-periodic (LTP) system is studied by calculating the Monodromy matrix of the system. The eigenvalues of this matrix decide on the stability of the LTP-system. To study the unabridged non-linear system, numerical simulation in the time domain is employed.

Stability maps are calculated and show the frequency ranges for which the 2-dof system becomes unstable due to parametric resonances. Moreover, the existence of frequency intervals where enhanced damping for the system is observed, is shown for the first time for MEMS. The results from the stability studies are confirmed for the non-linear system by numerical simulation in the time-domain. It is shown that the nonlinearities of the system have no negative consequences for the exploitation of the parametric anti-resonance effect and hence the linear stability analysis is an appropriate method of investigation.

- [1] Rhoads J., Shaw S. W., Turner K., and Baskaran R.: *Tunable Microelectromechanical Filters that Exploit Parametric Resonance*. Journal of Vibration and Acoustics, 127 (2005), 423–432.
- [2] Ecker H.: *Suppression of Self-excited Vibrations in Mechanical Systems by Parametric Stiffness Excitation*. Argesim/ASIM, Vienna, Austria, 2005.

# IDENTIFYING STRUCTURAL DAMAGE IN A CRACKED PLATE USING A MODEL-BASED BAYESIAN METHODOLOGY

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**Abstract.** In this paper a new approach is proposed for detecting a single crack in a simply supported plate undergoing free vibration. This approach uses Bayes theorem along with Markov Chain Monte-Carlo (MCMC) methods. To generate the required time series of the damaged plate, a semi-analytical free response is calculated using an FEM based eigen-solution. To speed up the simulations, modified elements are used at the crack tips; this permits a more course mesh without sacrificing accuracy. There are several significant advantages to this Bayesian/MCMC approach to structural health monitoring (SHM). First, unlike many approaches there is no need for reference data on a healthy structure. Second, very little experimental data is needed; moreover, only free response data is needed, which is easy to generate in an experimental setting. Third, very few sensors are required. Three arbitrarily located sensors are used throughout this work and prove to be satisfactory. Finally, the Bayesian/MCMC approach identifies all of the parameters associated with the crack: its location, orientation and its length. Furthermore, a natural by-product of this method is that it also provides a confidence interval for each of these parameters. The results show the utility and accuracy of this method for signals with various levels of experimental noise superimposed.

## ABSTRACT FROM FULL PAPER

## ACCELERATION OF UNBALANCED ROTORS

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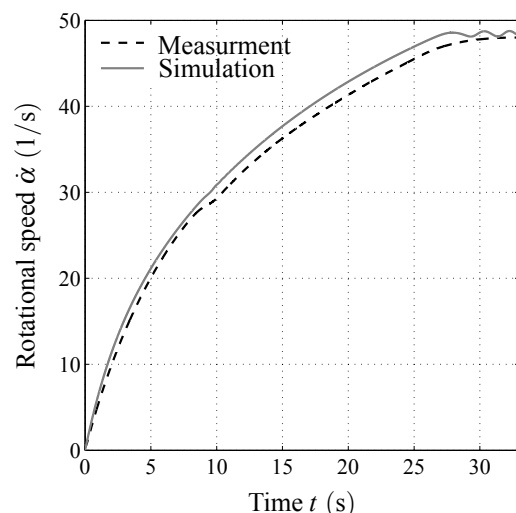
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The basic mechanisms describing the highly nonlinear phenomenon of the sticking of rotors in the natural frequencies, also called critical speeds, can be found in e.g. [1]. Unfortunately these authors only deal with the laval rotor. In the case of multisteped and multidisc rotors the laval model is not applicable and different approaches have to be used. One possibility is the Finite Element Method (FEM). The disadvantage applying FEM is the use of a high number of local shape functions for the discretization of the system. This type of shape functions is highly unsuitable for the description of large rigid body translations and velocities, as required in the field of rotordynamics. However using this method results in very small time steps during the system's numerical time integration and furthermore in huge calculation times. On the other hand the classical multibody approach is unusable for calculating small elastic deformations. Hence a floating frame of reference formulation is worked out to combine the large rigid body rotation and the small bending and torsional vibrations as well as the longitudinal displacement of the rotors.

The Projection Equation, see e.g. [2], is used to derive the dynamical equations of motion for spinning Timoshenko beams, leading to Partial Differential Equations (PDE). The Transfer-Matrix-Method is an analytical technique to calculate the eigenfrequencies and eigenmodes for arbitrary beam systems with diverse boundary conditions. In this paper the eigenfrequencies and eigenmodes are calculated, using the linearized PDEs, for free-free beams, implying the shear force and bending moment to be zero at the boundaries of the beams.

**Experiment.** The test bench consists of a circular shaft, two discs including asymmetric masses and a motor for the acceleration of the shaft. The mounting is realized by two self-aligning ball bearings. A simple tooth belt realizes the connection between the motor and the rotor shaft. This type of mounting was chosen to minimize the influence of parameter excited vibrations which could occur when using a gear system for the coupling. A single screw thread hole in the face of the larger disc acts as eccentricity. Additional masses, for example lining discs, can easily be applied by a screw to vary the mass of the eccentricity.

A Bernecker & Rainer automation system is used for measurement and acceleration of the rotor. It is assumed that damping and friction, in particular the friction of the driving belt and in the bearings, will play a major role when accelerating the rotor. To proof this assumption the rotor was driven at different rotational speeds and the motor torque was measured. Different run ups with variable but fix driving torques are measured and calculated.

Acceleration with constant motor torque  $m_x = 0.055\text{Nm}$ 

- [1] Gasch, R., Nordmann, R., and Pfützer, H.: *Rotordynamik*. Springer, 2005. 2. Auflage.
- [2] Bremer, H.: *Elastic Multibody Dynamics*. Springer, 2008.
- [3] Hubinger, S., Gatringer, H., Bremer, H., and Mayrhofer, K.: *Nonlinear Vibration Analysis of Discontinuous Coupled, spinning Timoshenko Beams*. In: Proceedings of the 8th IFToMM International Conference on Rotor Dynamics, Seoul, 2010, 948–955.

# REDUCTION OF SELF-EXCITED, TIME-PERIODIC SYSTEMS USING PROPER ORTHOGONAL DECOMPOSITION

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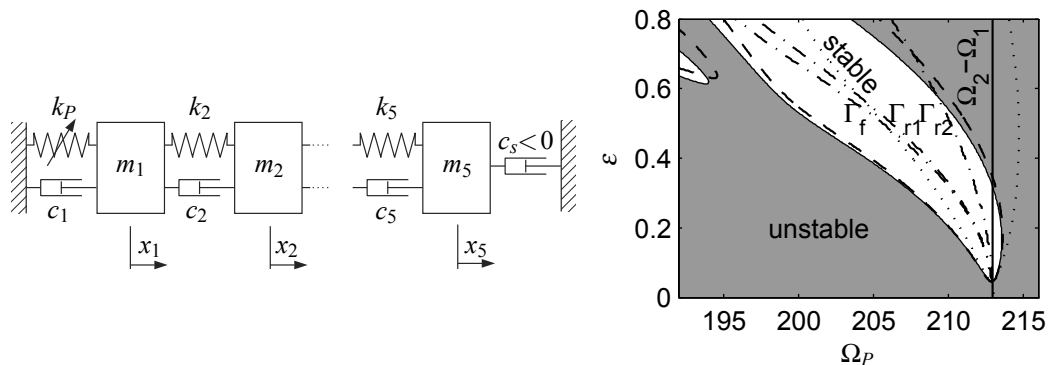
In almost all fields of mechanical engineering, the mathematical models of dynamical systems become more and more computationally expensive, and therefore, the necessity of providing reduced models, reflecting the principal system dynamics is growing continuously. The reduction of the equations of motion of the mechanical system depicted in the figure below (left) is investigated in this contribution. Time-periodic coefficients are introduced by the stiffness  $k_P(t) = k_1(1 + \varepsilon \cos \omega_P t)$ , and self-excitation by a negative damping  $c_s < 0$ . The equations of motion, non-dimensionalized and modally transformed are written in the form

$$\eta'' + (\alpha\Theta + C_{s,\dot{\phi}})\eta' + (\Theta + \varepsilon \cos(\Omega_P \tau) \mathbf{K}_{P,\dot{\phi}})\eta = \mathbf{0}. \quad (1)$$

A dynamical system with time-periodic coefficients possesses principle parametric resonances and parametric combination resonances. As it was shown in [1], self-excited vibrations can be suppressed if  $\Omega_P$  is near certain combination frequencies, e.g.  $\Omega_2 - \Omega_1$ . Hence, the trivial solution, which is unstable due to self excitation is stabilized by parametric excitation. The stability of time periodic systems is investigated using the Floquet theory. The maximum absolute value  $\max|\Lambda|$  of the eigenvalues of the monodromy matrix decide on the stability, where  $\max|\Lambda| < 1$  indicates a asymptotically stable,  $\max|\Lambda| > 1$  a unstable trivial solution, and  $\max|\Lambda| = 1$  represents the stability threshold. In the vicinity of  $\Omega_2 - \Omega_1$ , a significant drop of the stability parameter to a minimum value, denoted by  $\Gamma_f$ , is observed. A reduced model of Eq. (1) is set up using the method of Proper Orthogonal Decomposition (POD) which requires numerical solution of the full order system equations. It is proposed to use a parameter set  $[\varepsilon, \Omega_P]$  corresponding to a minimum  $\Gamma_f$  of the Floquet stability parameter  $\max|\Lambda|$ , for reduction. Numerical solution of (1), leads to the modal-displacement histories  $\eta_i = [\eta_i(\tau_1), \eta_i(\tau_2), \dots, \eta_i(\tau_j), \dots, \eta_i(\tau_m)]^T$ ,  $i = 1, 2, \dots, n = 5$ , which are collected in the ensemble matrix  $\mathbf{N} = [\eta_1, \eta_2, \dots, \eta_n]$ . The  $n$  orthogonal eigenvectors  $\zeta_i$  of the covariance matrix  $\mathbf{R} = \mathbf{N}^T \mathbf{N} / m$  are termed *Proper Orthogonal Modes* (POMs) and the  $n$  eigenvalues are denoted as *Proper Orthogonal Values* (POVs), see [2], for example. Applying the reduction-transformation  $\eta = \mathbf{V}\xi = [\zeta_1, \zeta_2, \zeta_3]\xi$  to Eq. (1), where the  $\zeta_i$ ,  $i = 1, 2, 3$ , represent the POMs related to the largest POVs, leads to the time-periodic equations of motion of the reduced system

$$\xi'' + (\alpha\Theta_r + C_{s,r})\xi' + (\Theta_r + \varepsilon \cos(\Omega_P \tau) \mathbf{K}_{P,r})\xi = \mathbf{0}. \quad (2)$$

The figure below (right) gives a comparison of the stability maps of the original model, the POD reduced model, and for the sake of comparison, a modal truncated model of the same size, in the vicinity of the parametric antiresonance frequency  $\Omega_2 - \Omega_1$ . The POD-reduced model approximates the stability limit in a very good way, whereas the modal truncated model shows good agreement only if  $\varepsilon$  is small. The same behaviour is shown by the minimum curve of the stability parameters  $\Gamma_{r1}$  of the POD-reduced model, and  $\Gamma_{r2}$  of the modal truncated one, compared to  $\Gamma_f$  of the original model. Also in the timedomain (omitted here for brevity), the POD-reduced model approximates the original model much better than the modal truncated model.



Schematic diagram of the investigated mechanical system (left). Stability maps of the original model (solid), the POD reduced model (dashed) and the modal truncated model (dotted), and minima  $\Gamma_f$ ,  $\Gamma_{r1}$  and  $\Gamma_{r2}$  of the stability parameter  $\max|\Lambda|$  of original and reduced models (dashed-dotted), (right).

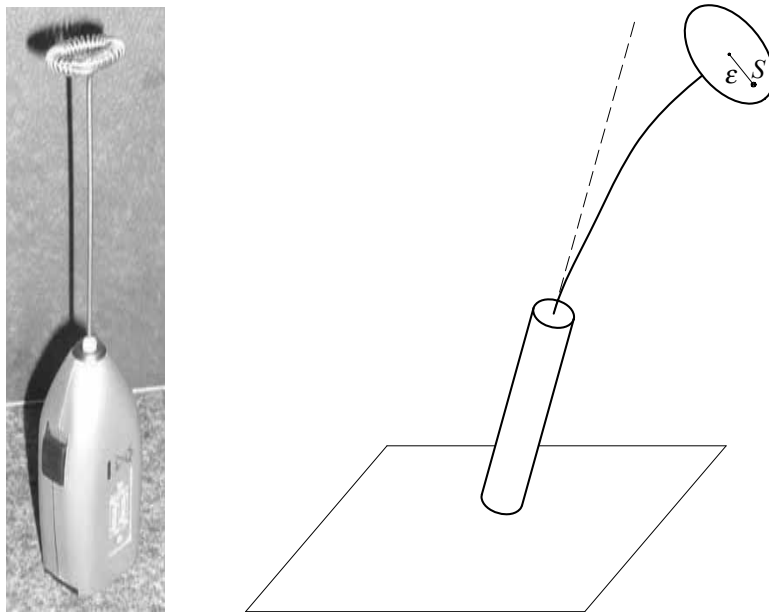
[1] Tondl A.: *To the problem of quenching self-excited vibrations*. Acta Technica ČSAV, 43, 1998, 109–116.  
[2] Feeny B.F., Kappagantu R.: *On the physical interpretation of proper orthogonal modes in vibrations*. Journal of Sound and Vibration, 211(4), 1998, 607–616.

# DYNAMICS OF A MILKSHAKER – PASSAGE THROUGH RESONANCE AND FREQUENCY TRANSFORMATION

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Rotor dynamics is a fascinating subject both from an experimental and a theoretical point of view. Most often experiments on various phenomena require more or less sophisticated test rigs, either because the experiments are dangerous or because the effects are difficult to reproduce. In teaching it is, however, beneficial to have experiments that are simple and can be performed by the students themselves. One of these examples is a standard milkshaker, which at a closer look, exhibits rich dynamical phenomena. The first phenomenon that can be observed and studied is the passage through resonance. Depending on the eccentricity  $\varepsilon$  of the rotor the driving torque of the motor is strong enough or not to reach supercritical speeds. If for a given torque the eccentricity is too large, the system



Milkshaker and rigid body model

gets stuck in the resonance with a rather large amplitude. A second phenomenon that can be observed is the following: When the milkshaker is placed on an even surface it starts to move on the surface. The movement is caused by a wobbling motion of the system caused by the eccentricity. Although the angular velocity of the rotor is high, the motion on the surface is quite slow in comparison. This is an interesting phenomenon that can be related to mechanical frequency transformation which occurs in the contact between the milkshaker and the ground. Depending on whether the rotor is running in a supercritical range or stuck below the resonance frequency, different motions can be observed. The system can be analyzed with a relatively simple nonlinear rigid body model, which is shown in figure 1. In this paper we study both phenomena mentioned above from a theoretical point of view. The equations of motion are derived in analytical form and their nonlinear behavior is investigated. Due to its relatively simple nature, the system has been used in lectures as a demonstrator and for student tutorial projects.

## 1:3 INTERNAL RESONANCE OF AN ELASTIC FLUID-CONVEYING TUBE

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**Problem description and governing equations.** Motivated by the article [3], we consider the planar motion of a slender elastic tube of length  $l$ , which is assumed to be inextensible at the centerline, and having a point mass  $m$  fixed to its lower end. The fluid being carried has a constant relative velocity  $U$  relative to the tube tangent to the centerline. Two springs with constants  $c$  are fixed to the tube at the position  $s=l\xi$  (with  $0 < \xi < 1$ ) and exert forces only in horizontal direction. A coefficient  $\alpha$  describes the internal material damping of the tube.

We adopt the model equations for the tube system from previous works, see [1, 2]. With  $m_T$  and  $m_F$  denoting the masses per unit length of the tube and the fluid, respectively,  $EJ$  denoting the flexural rigidity of the tube, and  $g$  denoting the gravity acceleration, the model equations may be non-dimensionalized according to the following change of variables and definitions of parameters:

$$\beta := \frac{m_F}{m_T + m_F}, \quad \gamma := \frac{m_T + m_F}{EJ} l^2 g, \quad \Gamma := \frac{m}{(m_T + m_F)l}, \quad \rho := \sqrt{\frac{m_F}{EJ}} Ul, \quad (1)$$

the dimension-free governing equations and boundary conditions read in the standard form of a dynamical system:

$$\mathbf{w} = (w_1, w_2) = (u, \dot{u}), \quad \lambda = (\rho, \Gamma, \alpha, \xi), \quad (2)$$

$$\dot{\mathbf{w}} = \mathbf{A}(\lambda)\mathbf{w} + \mathbf{g}(\mathbf{w}, \lambda), \quad \mathbf{A}(\lambda) = \begin{pmatrix} 0 & 1 \\ -C & -B \end{pmatrix}, \quad (3)$$

$$Cw_1 = w_1'''' + \rho^2 w_1'' - \gamma[(1 + \Gamma - s)w_1']', \quad Bw_2 = \alpha w_2'''' + 2\sqrt{\beta}\rho w_2', \quad (4)$$

$$s=0: \quad w_1 = w_1' = 0, \quad (5)$$

$$s=\xi: \quad w_1'''(\xi+) + \alpha w_2'''(\xi+) - w_1'''(\xi-) - \alpha w_2'''(\xi-) = -cw_1(\xi), \quad (6)$$

$$s=1: \quad w_1''' + \alpha w_2''' = \Gamma(\gamma w_1' + \dot{w}_2), \quad w_1'' + \alpha w_2'' = 0, \quad (7)$$

where the parameters  $\lambda$  are the distinguished parameters of the problem. The conditions (5)-(7) represent the clamping at the upper end of the tube, the intermediate force jumping due to the elastic support, the force due to the fixed point mass and the zero bending moment at the free end of the tube, respectively.

**Linear stability analysis.** Performing a linear stability analysis of the straight downhanging equilibrium position of the tube ( $u = 0, \dot{u} = 0$ ) leads to a three-point boundary-value inverse eigenvalue problem of two fourth-order ordinary differential equations, which can be solved numerically. The numerical values for the parameters were taken from measurements of [3].

**Non-linear stability and low-order resonance.** Including the non-linear terms in equation (3), the techniques of dimensional reduction and the transformation to normal form can be applied. An analysis of the resonance condition following from normal form theory for  $(\omega_1 : \omega_2) = (1 : m)$ -resonances shows that  $m=3$  is the lowest-order resonance leading to additional terms in the bifurcation equations. The case  $m=2$  does not affect the bifurcation behaviour due to the symmetry properties of equations (3)-(7). The bifurcation equations in polar coordinates are given by

$$\dot{r}_1 = ar_1 + \text{Re}[(A_1 r_1^2 + A_2 r_2^2)r_1 + R_1 r_1^2 r_2 e^{-i(3\varphi_1 - \varphi_2)}], \quad (8)$$

$$\dot{r}_2 = br_2 + \text{Re}[(A_3 r_1^2 + A_4 r_2^2)r_2 + R_2 r_1^3 e^{i(3\varphi_1 - \varphi_2)}], \quad (9)$$

$$\begin{aligned} (3\varphi_1 - \varphi_2)' &= 3\omega_1 - \omega_2 + \text{Im}[(3A_1 - A_3)r_1^2 + (3A_2 - A_4)r_2^2 + \\ &\quad + (3R_1 r_1^{-2} e^{-i(3\varphi_1 - \varphi_2)} - R_2 r_2^{-2} e^{i(3\varphi_1 - \varphi_2)})r_1^3 r_2^3], \end{aligned} \quad (10)$$

where  $a$  and  $b$  are the unfolding parameters. The (complex) parameters  $A_i$  ( $i=1$  to 4),  $R_1$  and  $R_2$  are related to the parameters in equation (1) within normal form theory.

In this talk we consider the dynamics caused by the internal low-order resonances of the two-dimensional motions of the tube, and we focus on the 1:3 resonance.

- [1] B. Albrecht, *Dynamische Verzweigungen eines rotationssymmetrischen, flüssigkeitsdurchströmten Schlauches mit einer punktförmigen Masse*, diploma thesis, TU Wien (1997).
- [2] M. Paidoussis, *Fluid-structure interactions*, Vols. 1 and 2, Academic Press (1998).
- [3] M. Ghayesh, M. Paidoussis, and Y. Modarres-Sadeghi, *Three-dimensional dynamics of a fluid-conveying cantilevered pipe fitted with an additional spring-Support and an end-mass*, JSV **330**, p. 2869–2899 (2011).



## AN OVERVIEW OF THE RECEPTANCE METHOD IN ACTIVE VIBRATION CONTROL

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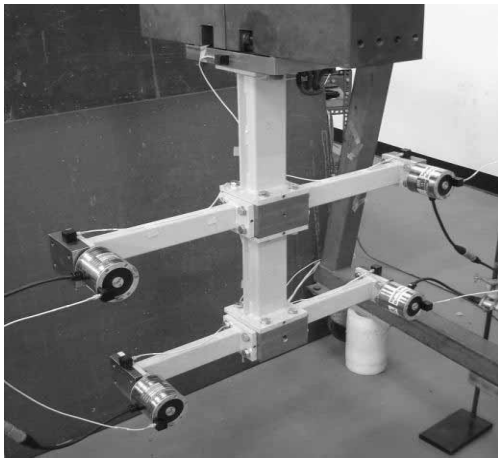
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**Abstract.** In this paper the practical implementation of the receptance method [1] in active vibration control of real structures is presented. The method uses in general the measured transfer function between the input/output data including the dynamics of the actuators and sensors. Therefore, it does not require knowledge or evaluation the system matrices  $\mathbf{M}$ ,  $\mathbf{C}$ ,  $\mathbf{K}$  which usually contain modelling errors. This would be the main advantage over conventional matrix-based approach such as state-space.

A modular test structure is considered for partial pole placement using single input state feedback [2]. The structure can have different configurations, in which two of these configurations in the form of a 'T' and an 'H' are presented in this paper. For the T-configuration two actuators and two sensors are used to control the first two flexural, bending and torsional, modes. For the H-configuration, four actuators and four sensors control four flexural modes, two bending modes and two torsional modes. The control force distribution is chosen so that it excites certain modes easily while the other modes remain unchanged. The method is also developed for robust pole placement using the sensitivity of the closed-loop poles with respect to the measured receptance terms. Sequential multi-input state feedback is also applied to assign all the modes simultaneously. It is shown that multi-input state feedback is inherently more robust than the single-input state feedback [3].

The method is also applied to an AgustaWestland W30 helicopter airframe in the vibrations test house at Yeovil. In the experiments, we measured the transfer function between the input voltage to the electro-hydraulic actuators, built into the airframe structure and the accelerations. The poles of the system are assigned to the prescribed values in the complex s-plane using active control [4].



Modular test structure



W30 helicopter airframe

- [1] Ram, Y.M., and Mottershead, J.E.: *Receptance Method in Active Vibration Control*, AIAA Journal, 45(3), 2007, 562-567.
- [2] Ghandchi Tehrani, M., Mottershead, J.E., Shenton, A.T., and Ram, Y. M.: *Robust pole placement in structures by the method of receptances: Mechanical Systems and Signal Processing*, 25(1), 2011, 112-122.
- [3] Ghandchi Tehrani, M., Elliott, R.N.R., and Mottershead, J.E.: *Partial Pole Placement in Structures by the Method of Receptances: Theory and Experiments*, Journal of Sound and Vibration, 329(24), 2010, 5017-5035.
- [4] Mottershead, J.E., Ghandchi Tehrani, M., S. James and P. Court, *Active Vibration Control Experiments on an Agusta-Westland W30 Helicopter Airframe*, Proceedings of the IMechE Part G: Journal of Aerospace Engineering, 221, (3), 2011, 313-325.



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# A 3-D POTENTIAL BASED BOUNDARY ELEMENT METHOD FOR MODELLING AND SIMULATION OF MARINE PROPELLER FLOWS

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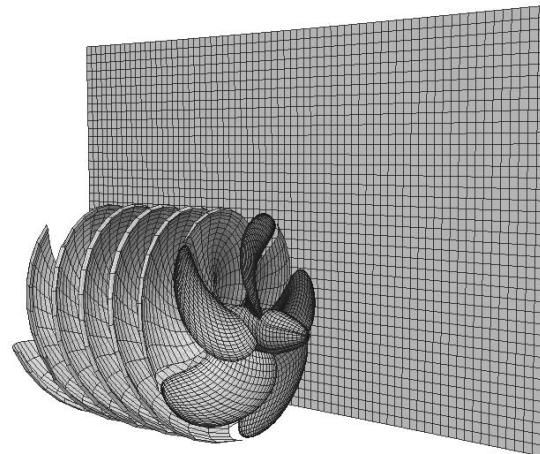
**Introduction.** The present article focuses on the modelling and simulation of marine propeller flows in port basins. In spite of the low ship motion velocities in port basins, high local fluid velocities and high changes of velocity gradients can occur in the flow. These phenomena mainly appear in propeller's area of influence when the ship is close to harbour facilities. The employed numerical method aims to accurately predict operational loads induced by marine propeller flows on quay walls in ports.

The numerical method used in this work is a three-dimensional potential based panel method which is implemented into the in-house simulation tool *panMARE*. The novelty of the presented calculation method refers to the partial sheet cavitation model which has been developed and implemented in *panMARE*. Cavitation is a physical effect where the pressure in the flow falls below the vapour pressure such that a vapour region develops on propeller blades. Cavitation has a significant influence on propeller's performance and will also influence the magnitude of the unsteady loads generated by a propeller flow on quay walls.

**Numerical Method.** For the numerical investigation of propeller flows and their effects on quay walls the three-dimensional boundary element code *panMARE* is used. The mathematical model employed in this code is based on potential theory where the flow is assumed to be irrotational, inviscid and incompressible. The numerical scheme is derived by means of a first-order panel method. Hereby, the propeller surface is discretised into flat quadrilateral elements and the governing equations of the potential flow problem are applied on the midpoint of each panel element [1]. The advantage of the developed panel code is its short computation time, compared to e.g. viscous methods, which allows for a wide range of parameter variations during the design procedure of a propeller. Moreover, the model includes a sheet cavitation model for the determination of cavitation effects on the induced pressure fluctuations. The sheet cavitation model consists of two additional boundary conditions on the cavitating parts of the body. By means of these conditions the cavity length and cavity thickness are calculated. The numerical sheet cavitation model is based on the partially non-linear approach where the boundary conditions are applied not on the exact cavity shape, which is not known a priori, but on the known body panels [2].

**Simulations.** The capabilities of the presented simulation tool are demonstrated by validation studies on two- and three-dimensional foils with respect to the implemented cavitation model. Hereby, the pressure distribution as well as the cavity shapes are evaluated for the investigated validation cases and the results are compared to those obtained by other authors.

In addition, a marine propeller is studied both in cavitating and non-cavitating conditions. The propeller is located close to a quay wall and the flow is considered during several propeller rotations. The simulations are performed in order to analyse the loads induced by propeller's slipstream on quay walls. The calculated pressure values are evaluated on different monitoring points of the wall and plotted against the time. Moreover, the results of the cavitating and non-cavitating propeller are compared and the influence of sheet cavitation on the computed pressure pulses on the quay wall is outlined.



Simulated marine propeller and quay wall

- [1] J. Katz, A. Plotkin, *Low-Speed Aerodynamics*. Cambridge University Press, Cambridge, (2001).
- [2] G. N. V. B. Vaz, *Modelling of Sheet Cavitation on Hydrofoils and Marine Propellers using Boundary Element Methods*. Aerospace Engineer of Instituto Superior Tecnico, Lisbon, Portugal, (2005).

## CONCEPTUAL DESIGN OF A TWO-LEVEL SERVER ARCHITECTURE FOR MATLAB-JAVA COUPLING

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In previous research an efficient MATLAB Java coupling was implemented [1] by using a server architecture. A well-known MATLAB problem is the non-existent thread-safety in its API. Therefore this contribution suggests the concept of a two-level server architecture (see Fig. 1) to further improve the MATLAB Java coupling performance. A single master server is responsible for the distribution of the requests of the clients to several worker servers. This novel architecture allows a parallel execution of MATLAB requests.

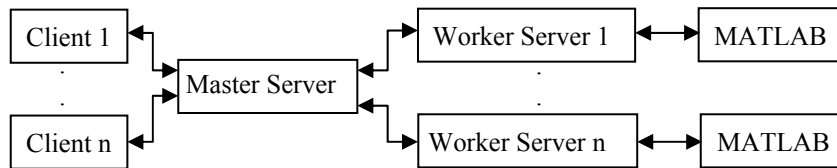


Fig. 1. Two level server architecture

The "Efficient Airport 2030" Cluster of Excellence project [2] aims at identifying and investigating new technological approaches for the improvement of airport ground processes. In the sub-project, which represents the background for this contribution, the essential task is to describe the processes at an airport on the basis of estimated passenger numbers for the year 2030 by using simulation models. This chain of processes starts at the passenger's front door and ends at the ground-handling, including the boarding and baggage loading, taking into account expected technical and organizational developments. Special emphasis is put on the coupling of MATLAB/Simulink simulation models, to map the continuous flow of passenger [3] and baggage in the airport terminal - from the processes at the counter to the transport to the respective aircraft, including freight handling.

The coupling of models is based on a pipelining concept, which is realized with a freely available Java framework. Since a majority of the models have been implemented in MATLAB, it is required to determine an efficient MATLAB-Java coupling. MATLAB offers different interfaces to that kind of programming language. There are two efficient MATLAB interfaces to Java, one uses JNI (Java Native Interface) and the other uses JMI (Java MATLAB Interface). In previous research activities, a Java-MATLAB Server [1] was implemented to allow the simulation models the access to a MATLAB environment running in the background on a single machine. Therefore input data including for example the name of the simulation model, is sent from a client to the server. This data executes the simulation in the running MATLAB environment, and sends the output data back to the client, which implies that the corresponding simulation models are available on the computer. The Java-MATLAB Server was implemented in Java and uses the Transmission Control Protocol (TCP) for communication. The server has been implemented with both JNI and JMI.

Because MATLAB lacks any kind of multi-threading capability, a first conceptual design of a two-level server was made (see Fig. 1). This architecture uses a master server for the communication with clients and is furthermore responsible for the equal distribution and forwarding of requests to the worker servers, by using the FIFO principle for example. The worker servers are responsible for the execution of the simulation models on their machines. The structure of the worker server is based on the aforementioned Java MATLAB server. However, in contrast to it, it can only accommodate one request, because the master server already has a queue. After the execution, the output data will be returned to the master server, and forwarded to the client. The implementation of the master and worker server will be done by using Java. The communication between master and worker server or master server and client uses TCP/IP. The worker servers should run on separate environments, like a separate server or just a virtual machine. This depends on the computing speed of the used machine. Statements about the efficiency of this architecture can be given during the upcoming implementation and validation. The main goal of this two level server architecture would be that several clients would be able to send their requests to the master server and these requests could be run simultaneously by distributing the request to several worker servers.

- [1] Y. Farschtschi, M. Widemann, K. Himstedt, J. Wittmann, and D.P.F. Möller. *Zusammenstellung von Alternativen zur MATLAB-Java-Kopplung*. in Simulation in den Umwelt- und Geowissenschaften. 2011 Shaker Verlag: Berlin. p. 179-192.
- [2] A. 2030. *Airport 2030*. 2011; Verfügbar in: <http://www.airport2030.de/>.
- [3] Y. Farschtschi, D. Formella, K. Himstedt, and D.P.F. Möller. *Macroscopic modelling of passenger streams on the airport and its adaptation in MATLAB Simulink*. in EUROSIM 2010. 2010 CSSS: Prague. p. 159.

## COMPARISON BETWEEN AUTO-TUNING OF PID, PFC AND MODIFIED-PFC CONTROLLERS

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**Introduction.** This paper presents a comparison between the auto-tuning of PID, PFC and modified-PFC controllers. Auto-tuning is a modern approach to tuning controllers, which helps us to tune controllers more quickly than standard tuning methods. The auto-tuning of PID, PFC and modified-PFC controllers is performed by using the relay-feedback method. After sustained oscillation of the process output, an identification of the process model can be made. The PFC and modified PFC controllers are then tuned and the PID parameters are calculated. The advantages and disadvantages of both approaches are discussed. Some experiments and results on real devices are shown in the end, where the modified-PFC controller gives better results than the other two controllers.

**Content.** Several PID tuning methods have been proposed over the years. However, most of them were developed for manual tuning, which is time-consuming and requires experienced operators. These drawbacks can be avoided by employing modern approaches to controller tuning, such as auto-tuning. This is a method where the controller is tuned automatically on demand from the user. By building such methods into the control scheme, we can drastically simplify its use. Such an approach to controller-tuning allows even operators with less knowledge about control theory to tune the controller accurately.

Auto-tuning of the PID controller based on relay feedback belongs to the closed-loop tuning methods. It is a frequency response method and is very effective in determining the ultimate gain  $K_u$  and the ultimate frequency  $\omega_u$  [1]. The distinct advantage of relay feedback is that it identifies process information around an important frequency (ultimate frequency). As it is a closed-loop test, processes will not drift away from the nominal operating point; hence, it can also be used online. For processes with long time constants, it is a more time-efficient method than conventional step- or pulse-testing, as described in [2].

Model predictive control is a wide area of control algorithms, some of which are: Model Predictive Heuristic Control, Richalet et al. (1978), Dynamic Matrix Control (DMC) [3] and Predictive functional control [4]. The basic idea of model predictive control is computing the control signal based on some sort of plant model. This could be a parametric model, a step-response matrix, an impulse response matrix or even a fuzzy model. In this paper only predictive functional control (PFC) and modified predictive functional control (mPFC) will be used for the comparison.

In this paper performance of the PID, PFC and mPFC controllers is compared. First the algorithm determines  $K_u$  and  $\omega_u$ , calculates the PID parameters and identifies the process-model. After identification the model is used for PFC and mPFC tuning. The reference tracking and disturbance response is tested.

**Conclusions.** The main aim of this paper was to draw a comparison between the auto-tuning PID, PFC and mPFC controllers. We obtained some good results, which show that the mPFC gives better performance than the PID and PFC controllers, especially during a reference-tracking test. The paper also shows that the mPFC operates much faster and with less overshoot than the PFC controller during disturbance response. The PID settling time during the disturbance response is comparable to the mPFC, but gives a larger OS than the mPFC.

**Acknowledgements.** We would like to thank Competence Center for new technologies of control (KC STV) and the European Union, European fund for regional development, for funding the research.

- [1] Åström, K. and Hägglund, T. (1995). *PID controllers: Theory, Design, and Tuning*, 2<sup>nd</sup> edition, Instrument Society of America, USA.
- [2] Yu, C. (2006). *Autotuning of PID Controllers, A Relay Feedback Approach*, pp. 23-25, 2<sup>nd</sup> Edition, Springer, Germany.
- [3] Cutler, C.R. and Ramaker, B.L. (1980). Dynamic matrix control-A computer control algorithm, *JACC Proceedings, Paper*, WP5-B.
- [4] Richalet, J., Rault, A., Testud, J.L. and Papon, J. (1978) Model predictive heuristic control: Application to industrial processes, *Automatica*, vol.14, pp. 413-428.

## A COMBINED CELLULAR AUTOMATA AND DEVS SIMULATION

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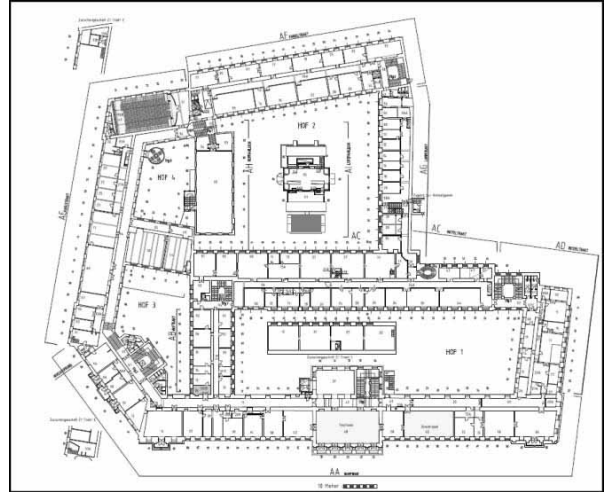
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**Summary:** In autumn of 2006, at the Vienna University of Technology the project TU University 2015 was launched, which includes the modernization of the buildings and the concentration of the faculties on maximum two locations. In the context of this project, the Institute for Analysis and Scientific Computing developed a model to optimize the classroom assignment and simulate the processes in place at the university. This model called MoreSpace was realized mostly in the simulation language Enterprise Dynamics (ED), with exception of the part that calculates the time that the students need to change between lecture rooms. This outsourced part of the simulation is the main topic of this paper. The model is implemented in the object-oriented programming language Java and connected via TCP/IP with Enterprise Dynamics. To model the dynamic behavior of single individuals an agent-based system was chosen in which the individuals move on a discrete grid. The cell size is  $0.125 \times 0.125\text{m}$ , so that one  $\text{m}^2$  consists of 64 cells. Each student takes  $4 \times 4$  cells, or  $0.5\text{m} \times 0.5\text{m}$ . The forward movement of people in a building depends on several interrelated factors. Some of these e.g. are the density of people in a group, the maximum speed which varies for each individual. Of course these factors are conditioned by the environment; For example moving into a room area or a staircase makes a noticeable difference. It is also of crucial importance, whether a person is facing multiple other individuals. All this is relevant for the speed and thus for the required time which the students need to switch from location A to another location B.



**The Model:** Basically, this simulation consists of two simulators: On the one hand Enterprise Dynamics, a commercial Simulation Software from INCONTROL based on the DEVS (Discrete Event System Specification) formalism in which the optimization of the room utilization is modeled. On the other hand a proprietary development in JAVA which provides the time needed by students to changed between lecture rooms. This part is designed to ensure that the time between two teaching units that may be held in different buildings, is sufficiently dimensioned. In order to implement the task a cellular automats (CAs) model was used [1, 2]. The main components of this model is a discrete plane and the individual agents, or as in our case, the individual students who are moving on this grid, and whose decision on their further action depends on the behaviour of the surrounding agents. Because of the fact that the university area is too big to display on only one of such grids, the buildings are divided in logically coherent parts that are connected at several points to give the agent the possibilities to change between these discrete planes. In order to allow the students to move through the huge number of planes in the shortest possible way a combination of graph theory and a kind of scalar field is used

**The Elevator:** An Important Part of this simulation was the implementation of the Elevators. This component creates a lot of problems for example the elevator controller for grouped elevators and the decision making for the students to find her best (with consideration of way length and walking time) personal way.

**Persons with physical handicap:** This Program also regards the needs of people with physical handicap. This means that it is possible to adjust the probability that a random generated person is physical handicapped and is rely on a wheel chair. Some consequences of this are the inability of using stairs, an increased required space, and a special speed distribution and so on.

This project is supported by “ZIT – Die Technologieagentur der Stadt Wien GmbH”.

- [1] Victor J. Blue, Jeffrey L. Adler. *Cellular automata microsimulation for modeling bi-directional pedestrian walkways*. Transporation Research Part B 2001
- [2] Fang Weifeng, Yang Lizhong, Fan Weicheng. *Simulation of bi-direction pedestrian movement using a cellular automata model*. Physica A 2003



# A CONCEPTUAL APPROACH FOR A SOFT COMPUTING FRAMEWORK TO DETERMINE CORRELATIONS IN HIGH-DIMENSIONAL DATA

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**Abstract.** Based on previous results from the “Efficient Airport 2030” cluster of excellence project, we will present a conceptual approach for a Soft Computing Framework which is focused on analyzing high-dimensional data for possible correlations. The data to analyze consists of various (in some cases fuzzy) input parameters that are expected by Web Service based simulation models; the delivered results are taken into account as well. The input can be considered to be an element of the Cartesian product of the sets containing the respective input parameters possible values. Even though the data can be generated by using the simulation models, it is not viable (due to the complexity) to compute the data as a whole. Being capable of working on fuzzy or incomplete data, Soft Computing provides an interesting approach that we expect to lead to a suitable solution to find correlations without the need to compute the data for all possible inputs.

Due to our design choice to realize the overall simulation as a Web Service [1, 2], the whole Soft Computing Framework is designed such that it implicitly supports the usage of Web Services. This allows the Soft Computing Framework to be embedded within Service Oriented Architectures and to be used within the Cloud.

The presented framework is separated into several parts: We will provide appropriate structures as a wrapper for the generation of the data to gain independence from the actually used data source. We will further provide the needed data structures to be able to represent several input parameters with arbitrary data types as a tuple. Furthermore we will provide a possibility to use user-defined (complex) data types.

We will present an initial selection of Soft Computing methods we intend to use, alongside with their integration in the framework. We will also give a first idea on how to use Soft Computing methods to find correlations in high dimensional data. It is based on a combination of genetic algorithms and fuzzy logic.

## References

- [1] K. Himstedt, J. Wittmann. *Modellkopplung und Szenarioanalyse am Beispiel des Projektes ‘Effizienter Flughafen 2030’*. Simulation in Umwelt- und Geowissenschaften, Aachen, 2010, 91-104.
- [2] J. Wittmann, K. Himstedt, D. P. F. Möller, *Ein Pipeliningkonzept zur Modellierung der Passagier und Gepäckbearbeitung am Flughafen*. Simulationstechnik/Simulation Techniques 20. Symposium in Cottbus. Aachen, 2009, 404-414.

# A LINEAR FEM BENCHMARK FOR THE HOMOGENIZATION OF THE EDDY CURRENTS IN LAMINATED MEDIA IN 3D

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**Introduction.** An efficient and accurate simulation of eddy current losses in laminated iron cores is of great interest in designing of electrical machines. Modeling each lamination individually by the finite element method (FEM) leads to large equation systems. Brute force methods applying anisotropic material properties in finite element models [1] yield losses, which are too small, because the losses caused by the main magnetic flux parallel to the lamination are neglected. Therefore, the solution obtained by this method is frequently corrected in a second step exploiting different approaches, i.e. [2]. Homogenization methods, where the main magnetic flux is considered directly, have been proposed for instance in [3]. Contrary to [3] the present method [4] is based on a multi-scale finite element method. An approach for a two-scale finite element method (TSFEM) has been derived for the magnetic vector potential  $\mathbf{A}$  describing eddy currents in laminated iron cores and capable to treat a laminated core efficiently as a bulk without the necessity to model the laminates individually. The accuracy and the computational costs of the TSFEM are evaluated by a reference solution of a linear FEM Benchmark.

**Two-Scale FEM.** The weak form of the eddy current problem in the time harmonic case

$$\int_{\Omega} \mu^{-1} \operatorname{curl} \mathbf{A} \operatorname{curl} \mathbf{v} \, d\Omega + j\omega \int_{\Omega} \sigma \mathbf{A} \mathbf{v} \, d\Omega = \int_{\Omega} \mathbf{J} \mathbf{v} \, d\Omega \quad (1)$$

using the magnetic vector potential  $\mathbf{A}$  is considered. The two-scale approach

$$\mathbf{A} = \mathbf{A}_0 + \phi (A_1, A_2, A_3)^T + \nabla(\phi w) \quad (2)$$

has been derived. In (2)  $\mathbf{A}_0$  stands for the mean value,  $\phi$  times the vector with the entries  $A_1$ ,  $A_2$  and  $A_3$  models currents parallel to the lamination, and the last term takes account of the normal component of the current density. The quantities  $A_1$ ,  $A_2$ ,  $A_3$  and  $w$  are scalar functions. The micro-shape function  $\phi$  is a periodic saw shaped function perpendicular to the lamination and constant in the plane of the lamination.

**Linear FEM Benchmark.** The *Linear FEM Benchmark* consists of a laminated stack with the dimensions of 0.2x0.1x0.3m, (see Fig.1), arranged symmetrically in the center of the race track coil. The thickness of the laminates is 0.35mm, which leads to 556 laminates in the stack. A fill factor of  $f = 0.9722$ , a relative permeability of  $\mu_r = 30,000$ , a conductivity of  $\sigma = 2 \cdot 10^6 \text{S/m}$  and a frequency of 50Hz were selected. The gap between the laminations was assumed to be air. The height of the race track coil is 0.4m, the straight sections are 0.2m long and thickness equals to 0.05m, respectively. The inner and the outer radius of the four hollow cylinder parts in the corners are 0.01m and 0.06m, respectively. A current density of  $10^6 \text{A/m}^2$  was chosen. To study the accuracy of TSFEM and the anisotropic solution (AS) the eddy current losses are compared with those obtained by a reference solution (RS) in which the laminates are modeled individually. The results are summarized in Table I. A fairly good agreement between TSFEM and RS can be observed. The computational costs for TSFEM are essentially smaller than that for RS.



Fig.1: One eighth of the lamination stack (dark) and the race track coil (bright).

Tab.1: Comparison of Eddy Current Losses.

RS	AS	TSFEM
Losses in W		
0.952	0.677	1.011
No. of Unknowns		
14 313 242	411 930	597 597

- [1] V. C. Silva, G. Meunier, A. Foggia. *A 3D finite element computation of eddy currents and losses in laminated iron cores allowing for the electric and magnetic anisotropy*. IEEE Trans. Magn., May 1995, vol.:31, no. 4, pp. 2139-2141.
- [2] K. Hollaus, O. Bíró. *A FEM formulation to treat 3D eddy current in laminations*. IEEE Trans. Magn., Sep. 2000, vol.: 36, no. 5, pp. 1289-1292.
- [3] P. Dular et al. *A 3-D magnetic vector potential formulation taking eddy currents in lamination stacks into account*. IEEE Trans. Magn., May 2003, vol.: 39, no. ?, pp. 1147-1150.
- [4] K. Hollaus, J. Schöberl. *Homogenization of the Eddy Current Problem in 2D*. In: Proc. 14th Internat. IGTE Symposium on Numerical Field Calculation in Electrical Engineering, Sept. 2010, Graz, Austria, pp. 154-159, ISBN: 978-3-85125-133-3.

## BALANCE GROUP MODEL WITH SMART GRID ELEMENTS

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Rising demand for electrical power and environmental awareness has triggered new types of electrical power producers like solar and wind power plants. They cause a problem in electrical power systems because of their stochastic nature of energy production. Smart grid technology offers a solution to these problems. In this paper a smart grid solution made for balance group's responsible party is presented. It includes model of balance group, concept of balance group internal market and scheduling algorithm developed by evolutionary algorithms method called Cell based Genetic Programming (CGP).

Balance group is a group of measuring points on the grid that connects consumers and producers under one group which is called balance group responsible party (BRP). Purpose of balance group is to provide balance between production and consumption of electrical energy. To balance energy BRP must predict its consumption and production of electrical energy and purchase difference on the external market. Because predictions aren't accurate new imbalances are produced that has to be balanced with energy purchased on external market [1]. With higher rate of renewable energy sources especially solar and wind power plants the balance group energy production predictions are more inaccurate which leads to higher imbalances.

Smart grids implements active distributed energy producers and consumers. They represent household consumers, small power plants and small electrical storage facilities distributed among the grid that can produce or consume energy by demand. Household consumers can shift in time their energy consumption (instead running washing machine at 3 pm it can work also at 5 pm). Small power plants like biomass power plants, small hydro power plants can produce energy by demand. Energy storage facilities like hydrogen fuel cells, electrical cars, pumping hydro power plants can consume energy by filling up their storage tanks and produce energy from stored energy by demand. With their help BRP can lower the predicted imbalances. To include them into energy market a balance group internal market is implemented (BGIM). BGIM insures competition between all active distributed energy producers and consumers and energy that can be purchased on external market.

BGIM uses scheduling algorithm to optimize expenses of balancing the predicted imbalances. Fast scheduling algorithms are more efficient in cost reduction of imbalances because energy prices are higher closer to the point of real energy flows. In this paper a scheduling algorithm that can calculate schedule analytically with usage of mathematical mapping is presented. It was developed by CGP method and tested in simulation environment of small balance group.

- [1] Z. Marinšek, G.Černe. Roles and processes model for electricity market trading processes in Europe. 6<sup>th</sup> International Workshop on Deregulated Electricity Market Issues in South-Eastern Europe, Bled, Slovenia, 2011
- [2] M. Corn, M. Atanasijević-Kunc. Cell based Genetic Programming Toolbox (CGP - Toolbox). Proceedings of the 20<sup>th</sup> ERK 2011 Conference, Portorož, Slovenija, IEEE Region 8, iss. A, pp. 295-298, 2011.

## BOUNDARY INTEGRAL METHOD IN THE DYNAMICAL THEORY OF THERMOELASTICITY WITH MICROTEMPERATURES

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In recent years several mathematical models of continua with microstructure have been formulated in which the deformation is described not only by the usual displacement vector field, but by other vector or tensor fields as well.

The mathematical model of the linear theory of thermoelasticity with microtemperatures for materials with inner structure whose particles, in addition to the classical displacement and temperature fields, possess microtemperatures was presented by Iesan and Quintanilla [1]. The fundamental solutions of the equations of the theory of thermoelasticity with microtemperatures were constructed by Svanadze [2]. The representations of Galerkin type and general solutions of equations of dynamic and steady vibrations in this theory were obtained by Scalia and Svanadze [3]. In [4], the basic boundary value problems (BVPs) of steady vibrations were investigated using the potential method and the theory of singular integral equations. Recently, the basic theorems in the equilibrium and steady vibrations theories of thermoelasticity with microtemperatures were proved by Scalia et al. [5].

This paper concerns with the mathematical model of the linear dynamical theory of thermoelasticity with microtemperatures. The basic initial-BVPs are formulated. The corresponding BVPs in the Laplace transform space are investigated. The existence, uniqueness and representation of the classical solutions of these BVPs are proved by virtue of boundary integral method (potential method) and theory of singular integral equations. Finally, the uniqueness and existence of regular (classical) solutions of the basis initial-BVPs are proved and these solutions are obtained in the inverse Laplace transform form.

- [1] Iesan D., and Quintanilla R.: *On the theory of thermoelasticity with microtemperatures*. J. Thermal Stresses, 23(2000), 199-215.
- [2] Svanadze M.: *Fundamental solutions of the equations of the theory of thermoelasticity with microtemperatures*. J. Thermal Stresses, 27(2004), 151-170.
- [3] Scalia A. and Svanadze M.: *On the representation of solutions of the theory of thermoelasticity with microtemperatures*. J. Thermal Stresses, 29(2006), 849-864.
- [4] Scalia A. and Svanadze M.: *Potential method in the linear theory of thermoelasticity with microtemperatures*. J. Thermal Stresses, 32(2009), 1024-1042.
- [5] Scalia A., Svanadze M. and Tracinà R.: *Basic theorems in the equilibrium theory of thermoelasticity with microtemperatures*. J. Thermal Stresses, 33(2010), 721-753.

# CALCULATING ELLIPSOIDAL APPROXIMATION OF REACHABILITY TUBES FOR CONTROL SYSTEMS OF HIGH DIMENSIONS

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**Abstract.** We consider a feedback control problem for a linear system with set-membership uncertainty. A common approach to this problem is to express the feedback control in terms of solvability (backward reachability) tube. Since calculating the exact tube for systems of higher dimensions is computationally unfeasible, one usually uses its inner ellipsoidal. An attempt to apply known ellipsoidal approximation formulae to oscillating systems of high dimensions with scalar control revealed that the matrix of ellipsoid is ill-conditioned. This presents a serious problem for practical computations. In this paper we propose a modification to ellipsoidal approximation formulae that help to overcome the indicated difficulty. This is achieved by calculating a set of approximations which are then mixed by an additional term in the approximation ODE.

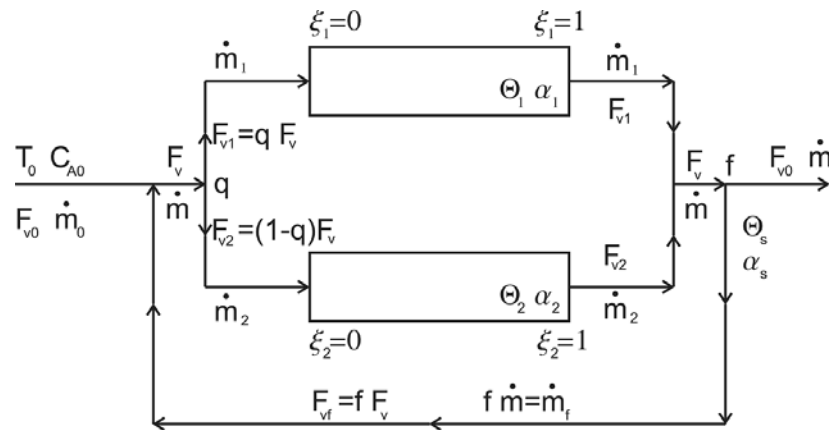
**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

## CHAOTIC DYNAMICS OF CHEMICAL REACTORS SYSTEM WITH MULTIPLE DELAY

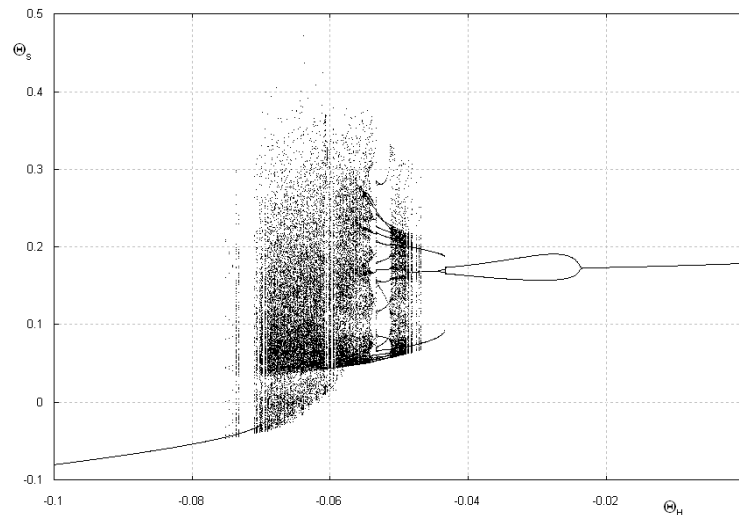
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In processing it is possible to find systems parallel jointed reactors with recycle of mass, as well as different types of systems generating delays [1]. The presented system includes both of this cases (*Presented system*). It concerns two parallel tubular homogeneous chemical reactors, which causing multiple delays. This delays are resulting from time, required on flow string through reactors. From mathematical view point, model of this system is a discrete model. The results of the analysis were illustrated by numerical example in the form of Feigenbaum's diagram where we can see stationary, periodic, multiperiodic and chaotic solutions (*Feigenbaum's diagram of presented system*) [2].



Presented system.



Feigenbaum's diagram of presented system.

- [1] E.W.Jacobsen, M.Berezowski: *Chaotic dynamics in homogeneous tubular reactors with recycle*. Chemical Engineering Science, 53 (1998), 4023-4029.
- [2] M.Berezowski, E.Fudała: *Bifurcation analysis of the statics and dynamics of a logistic model with two delays*. Chaos, Solitons&Fractals, 28/2 (2006), 543-554.

# CONVENIENT MODEL INVERSION BY MEANS OF OBJECT-ORIENTED MODELING FOR A PARALLEL KINEMATIC ROBOT

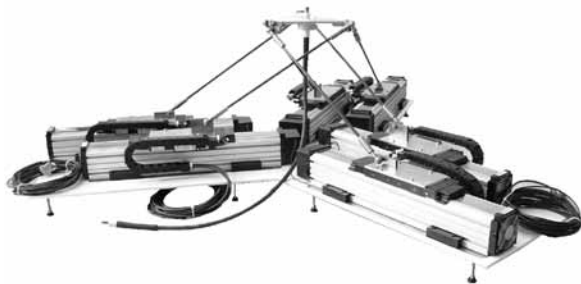
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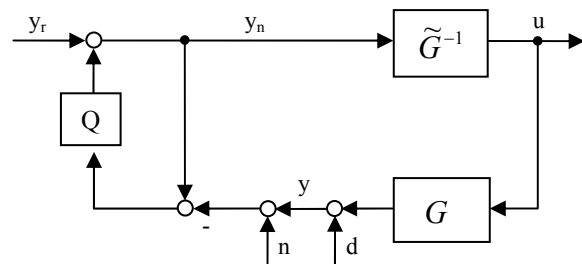
**Summary.** The paper presents the capability of object-oriented modeling languages to obtain inverse plant models almost automatically by means of Modelica and the simulation tool Dymola. Based on an available plant model in Modelica the construction of its inverse model is shown with focus on new blocks from the free Modelica Standard Library (Version 3.2). This method is applied to a model of a six degrees of freedom (DOF) parallel kinematic robot that should be implemented in a so called inverse disturbance observer (IDOB) control architecture.

**Inverse Models.** A lot of modern control structures include inverse plant models as a core part of the controller. In general it is difficult to create the required inverse plant model with signal flow based modeling tools (e.g. Simulink) as the inverse model can not be derived directly from the plant model. A promising approach for solving the task of dynamic model inversion is given by object-oriented modeling languages like Modelica and modern simulation tools as Dymola that are based on it. Here the inverse plant model can be obtained almost automatically by exchanging the meaning of input and output variables. In consequence the plant model (and its inverse) can be analyzed and tested in various control architectures at an early stage of the development process.

Latest major updates in the Modelica language specification included not backward compatible changes that also have an impact on model inversion as described in [1]. A new standard component (“InverseBlockConstraints”) for dynamic model inversion has been introduced in order to meet the new requirement of balanced modeling. The paper points out the usage of this new block in a complex mechatronics system as kind of a parallel kinematic robot that is controlled by an IDOB control loop.



Parallel kinematic robot “Black Beetle”



IDOB control scheme [2]

**Application.** The method of dynamic model inversion is applied to a model of an experimental prototype as a kind of parallel kinematic machine (PKM) with 6 DOF. This experimental robot was developed and realized in cooperation between the Fraunhofer Institute of Machine Tools and Forming Technology Chemnitz and Leipzig University of Applied Sciences. The resulting model contains single-input/single-output inversion problems in terms of drive position control of each linear direct drive as well as multi-input/multi-output tasks when using the model in an IDOB control scheme. Purpose of this control structure is optimal tracking control of the tool center point by considering the non-ideal and load-sensitive tracking behaviour of the linear drives (contouring errors) as well as the elastic dynamics of the whole PKM structure. As the inverse plant model is generated automatically the shape of the filter in the feedback path of the IDOB loop is the only remaining design parameter. The bandwidth of the filter is limited by the resonance frequency of the single axis controller and the whole mechanical structure of the robot. It is shown that the simulation environment of Dymola is capable to find a reasonable cut-off frequency of the filter.

- [1] M. Thümmel, G. Looye, M. Kurze, M. Otter, J. Bals. Nonlinear Inverse Models for Control. In 4th International Modelica Conference, pages 267-279, Hamburg-Harburg, March 2005. Hamburg University of Technology, The Modelica Association
- [2] N. Bajcinca and T. Bünte: A novel control structure for dynamic inversion and tracking. IFAC World Congress 2005
- [3] M. Krabbes and Ch. Meißner: Dynamic modeling and control of a 6 DOF parallel kinematics. In 5th International Modelica Conference, pages 385–390. Arsenal Research, The Modelica Association. Vienna, September 2006

## DIAGNOSIS OF TECHNOLOGICAL SYSTEMS BASED ON THEIR COLOURED PETRI NET MODEL

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Model-based techniques [1] are widely used and are very popular in control and diagnostic applications because of their efficiency and good performance both for systems with continuous and discrete range spaces. The appropriate models in the discrete range space case are built using the tools and techniques of discrete event systems, and these are mainly in the form of Petri nets. When used for model-based fault detection and isolation, one not only needs a model for the normal operation of the system, but also other models are required that describe the considered faulty modes. This gives the possibility to isolate the actual faulty mode using measured data and the structurally different faulty models the comparison of which is the subject of the present paper.

Starting from these results the aim of our work is to develop diagnostic methods for the following purposes:

- investigation of the models describing both the normal, faultless operational mode and different faulty operational modes;
- diagnosis of the faults during a given course of the technological system;
- analysis of the work of the investigated system based on several courses using process mining tool.

To achieve these goals several problem has to be solved. The first is to develop a suitable modeling method for the simulation both faultless and faulty operational modes. At the recent stage of our research models are used both as a reference model for normal operation and for the simulation of the real process. As a further step we plan to use data coming from the investigated system instead of simulation.

The next step is to elaborate on the method for transforming data resulting either from the simulation or from the technological system into suitable form for process mining. For this a converter software is needed which transforms the output data of the simulation software and the structure of the model into the necessary form.

The analysis of the resulted data, i.e. the diagnosis is performed both with simulation and in theoretical way. The latter method is based on the comparison of graphs coming from process mining and our goal is to develop a suitable metrics to determine the distance between them.

The model of the investigated system was defined in hierarchical colored CP-net form. Both normal reference model describing the faultless operation and the extended model containing the different faults were developed. For the fault simulation we used the arc and transition inscriptions.

The visualization of net was performed by ProM. In order to get the files having the appropriate form and extension a converter program has been developed. The main task of this tool is to convert the structure of the model described in the form of multi level colored Petri net into low level net and is to take into account the user defined faults to its structure. Comparing the structures of the faultless reference model and of the model reconstructed from the log files one can conclude to work of the investigated system.

The proposed procedure was illustrated on a simple manufacturing process with three faulty modes.

[1] Blanke, M., Kinnaert, M., Lunze, J., Staroswiecki, M. (2006). *Diagnosis and Fault-tolerant Control*, Springer-Verlag, Berlin.



# EFFICIENT USE OF SPACE OVER TIME – DEPLOYMENT OF THE MORESPACE-TOOL

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**Motivational Idea.** The debate around global warming and necessary consequences is still far from being settled; nevertheless it has become clear that the ecological footprint has to be reduced drastically. Massive investments in new technology can only be a part of this effort. The question arises what to do with existing buildings, as it is unrealistic to rebuild (all of) them with state of the art-technology.

A simple but elegant solution for this is to increase utilization-efficiency. This directly leads to a better footprint/ utilization ratio and also features positive economic side-effects (e.g. reduced “costs per unit” or savings of resources). As proposed in a study carried out at the ETH Zürich [1] educational facilities hold a high potential yield with respect to such improvements.

**State of the Art.** Extensive literature search shows that the problem of university course timetabling is still not solved satisfactory (at large scale). Various attempts and algorithms for scheduling and timetabling exist, although there are only very few course timetabling papers that actually report that the (research) methods have been implemented and are used in an institution. Methods for the simulation of room utilization are - to the authors’ knowledge - not in use at all.

**Approach.** Within the research project “MoreSpace” such a model for simulation of room utilization (primarily of university buildings) is being developed. It is based on discrete event simulation, cellular automata, agent-based techniques and business process modeling (see [2, 3] for further reference). In order to successfully deploy this model within the intended peripheral real-life system, its preconditions and requirements have to be met. Thus an analysis - and eventually a transformation - of that peripheral system is necessary for the successful introduction of the simulation model. While still in progress, this analysis and its findings are covered within the paper.

At first three possible *modes of operation* (of the model) are identified. Next the model’s preconditions are derived and split into structural preconditions and necessary input-data. For the latter an entity relationship model (ERM) is developed which describes the model’s database. The ERM is then mapped onto the peripheral system, which requires an assessment of disposable data-sources and their (quantitative and qualitative) content. This subsequently leads to the necessity of a *stakeholder analysis*, investigating their interconnecting relationships. Based on the stakeholder analysis the processes surrounding the space management (e.g. room reservation) are explored and described with business process models (BPM).

Further a *deployment matrix* is set up, which puts the mode of operation into context with met preconditions and required depth of system-integration. Thus it becomes possible to estimate whether a model can be deployed as intended or not; with alternatives being either a transformation of the system, reformulation of the question(s) towards the model or – in the worst case – abortion of the deployment process.

**Outlook.** As with all simulation results the data needs post-processing which requires data mining and visualization techniques to draw sensible conclusions. Since stakeholders’ interests differ so do their perspectives upon simulation outcome. Subsequently post-processing and visualization need “individual” fitting to meet those demands. For this an automated but customizable visualization-tool is currently under development.

The methods applied for system analysis seem fairly adequate to prepare the model deployment within a real-life system. Motivated by the positive insights gained, further investigation on utilization of techniques for efficient model deployment (also in other areas of simulation) seems rewarding.

- [1] D. Wiegand, P. Mebes, V. Pichler, *Event based simulations: enabling improved development planning and partnerships*. In: Proceedings of Real Corp 007, (Eds.: M. Schrenk, V.V. Popovich, J. Benedikt), CORP, 2007, 17-23.
- [2] S. M. Tauböck, *Integration of Agent Based Modelling in DEVS for Utilisation Analysis: The MoreSpace Project at TU Vienna*. Vienna University of Technology, 2010.
- [3] M. Bruckner, *Modellierung der Fußgängerdynamik im universitären Betrieb mit Hilfe von Zellulären Automaten in der Programmiersprache JAVA*. Vienna University of Technology, 2009.

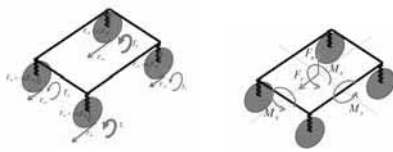
# ELECTRIC VEHICLE LATERAL DYNAMICS CONTROL BASED ON INSTANTANEOUS CORNERING STIFFNESS ESTIMATION AND AN EFFICIENT ALLOCATION SCHEME

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**Introduction.** Beyond the establishment of a pollution free mobility, Electric Vehicles (EVs) show attractive features as far as vehicle motion control is concerned. As particularly advantageous for the purpose of motion control can the integration of In Wheel Motors (IWMs) in each wheel be considered. Together with Active Front and Rear Steering (AFS and ARS) six degrees of freedom are available in order to determine an advantageous vehicle behaviour as far as longitudinal and lateral dynamics, as well as roll and pitch motion is considered. This contribution focuses on the modelling issues and implications for the controller design of a 4 IWMs driven EV with AFS and ARS with regard to lateral dynamics and roll motion control. At the core of this approach is a vehicle model that takes into account the particularities of the 4 IWMs driven EVs with consideration of the anti lift and anti dive forces (vertical forces generated by the IWMs) as introduced in [1]. A linear parameter variant model is used for the controller design. Nonlinear effects due to reaching the lateral tire force saturation (e.g. by heavy steering command and/or low  $\mu$  road) are counteracted by a robust control approach and the determination of the lateral tire force saturation which is detected with an Instantaneous Cornering Stiffness (ICS) estimator which differs from [2] as far as no particular mass distribution of the vehicle is assumed but lateral tire force sensors (nowadays available at a reasonable price) are used. Simulation results show the effectiveness of the modelling and control approach.

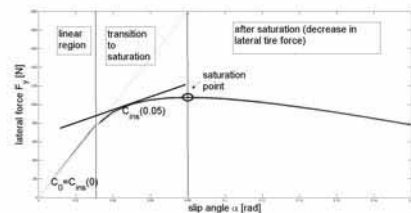
**Modelling.** The vehicle model used is a linear state space model with two slowly time variant parameters (the front and rear cornering stiffness) and six inputs. The torque  $T_i$  applied at a wheel of the EV



Principal sketch of the forces acting in longitudinal and vertical direction due to In-Wheel-Motor traction of the electric vehicle without cornering (left) and possible forces and moments generated by IWMs (right)

does not lead only to a driving force  $F_{x,i}$  in the longitudinal direction but also to a remarkable vertical force  $F_{z,i}$ . In that point IWM driven EVs differ from conventional vehicle with a powertrain (different position of the instantaneous center of rotation). Since the 4 wheels can be controlled independently either one force  $F_x$  and three moments  $M_z, M_x, M_y$  can be determined or two forces  $F_x, F_z$  and two moments  $M_x, M_z$  (figure left) acting on the vehicle. The linear model cannot reflect the behaviour of the EV approaching lateral tire force saturation. Instead of enhancing the vehicle model the model uncertainty in this region is overcome by a robust control approach that achieves its target regardless of some model deficiencies the controller is based on. However surpassing the saturation threshold should be avoided in order to prevent the control system to become unstable. This is achieved by using the ICS as an indication for the lateral saturation point of the tires (figure bottom right).

**Control design.** The robust controller generates virtual control signals by comparing the relevant vehicle signals with the reference signals generated by a reference model from the drivers input. This virtual signals have to be translated into the six actuator inputs by using the vehicle model (control allocation). Since this allocation is under determined (4 virtual control signals versus 6 actuator inputs), additional criteria like the minimization of wheel load can be integrated [3]. In order to avoid reaching tire force saturation, front and rear steering angles are limited. This limits are computed by modelling the tire force saturation as a result of a drastic decrease in the instantaneous cornering stiffness value computed with an appropriate estimation scheme.



Definition of Instantaneous Cornering Stiffness (ICS)

- [1] E. Katsuyama, *Decoupled 3D Moment Control by In-Wheel Motor*. In: Proc. JSAE Annual Congress (Spring), Vehicle Dynamics and Control II, 2011, 1–6.
- [2] W. Sienel, *Estimation of the tire cornering stiffness and its application to active car steering*. In: Proc. 36th Conference on Decision & Control, 1997, 4744-4749.
- [3] O. Haerkegard, *Backstepping and control allocation with applications to flight control*. Ph.D. dissertation, Linköping University, 2003.

## EXEMPLARY INDUSTRIAL SYSTEM AND NETWORK PERFORMANCE MODELING IN POLAND

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**Abstract.** The paper presents the exemplary industrial system models from the event-driven simulator up to Approximate network analytical performance evaluation system tool (Anapest). The basic approximations assumed in Anapest are roughly discussed together with the basic network configuration for which the tool was developed. The two basic ways of Anapest validation, i.e. the internal network measuring tool Sitwa and event-driven simulation are depicted. In addition, the major network performance evaluation projects run till now described, together with the basic outcome from Anapest.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

## EXPLICIT AND IMPLICIT TAYLOR SERIES SOLUTIONS OF STIFF SYSTEMS

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The paper deals with stiff systems of differential equations. To solve this sort of system numerically is a difficult task. Generally speaking, the stiff system contains several components, some of them are heavily suppressed while the rest remain almost unchanged. This feature forces the used method to choose an extremely small integration step and the progress of the computation may become very slow. However, we often need to find out the solution in a long range. It is clear that the mentioned facts are troublesome and ways to cope with such problems have to be devised.

There are many (implicit) methods for solving stiff systems of ODE's, from the most simple such as implicit Euler method to more sophisticated (implicit Runge-Kutta methods) and finally the general linear methods. The mathematical formulation of the methods often looks clear, however the implicit nature of those methods implies several implementation problems. Usually a quite complicated auxiliary system of equations has to be solved in each step. These facts lead to immense amount of work to be done in each step of the computation.

In spite of the fact that we come across stiff systems quite often in the common practice, a very interesting and promising numerical method of solving systems of ordinary differential equations (ODE) based on Taylor series has appeared. The question was how to harness the said "Modern Taylor Series Method" (MTSM) for solving of stiff systems.

An important part of the MTSM is an automatic integration order setting, i.e. using as many Taylor series terms (*ORD*) as the defined accuracy requires. Thus it is usual that the computation uses different numbers of Taylor series terms for different steps of constant length. On the other hand, for a pre-set integration order, the integration step length may be selected.

The potential of the Taylor series has been exposed by many practical experiments and a way of detection and explicit solution of large systems of ODE has been found. Detailed analysis of stability and convergence of explicit and implicit Taylor series is presented and the algorithm using implicit Taylor series - based on recurrent calculation of Taylor series terms and Newton iteration method (ITMRN) is described. ITMRN proved to be useful for our experimental examples.

The MTSM has been implemented in TKSL software.

## FUZZY MODELING OPTIMIZATION

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**NO ABSTRACT AVAILABLE**

# GRAPH-THEORETIC MODELING AND DYNAMIC SIMULATION OF AN AUTOMOTIVE TORQUE CONVERTER

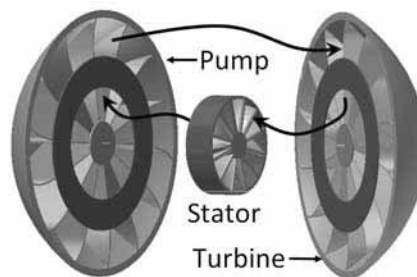
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**Introduction:** Torque converters are used as coupling devices in automobile powertrains involving automatic transmissions. Efficient modeling of torque converters capturing various modes of operation is important for powertrain design and simulation, [1]. In this paper a linear graph model of a torque converter is presented and analyzed. The presented model accounts for the dynamic behavior of the mechanical components, i.e. the pump, the turbine and the stator, and that of the hydraulic fluid used in a torque converter.

**Motivation:** Conventional modeling methods, [1], require manual derivation of equations, which can be tedious and prone to errors. By employing linear graph theory to model the behavior of the torque converter, it is possible to generate the governing equations in an automated fashion, [2]. Also, using graph-theoretic methods makes it easier to extend the model to include other powertrain components from different physical domains. Our ultimate goal is to develop tools for automated generation of real time simulation codes for complete automotive systems. Currently, very efficient graph-theoretic methods are available that can perform accurate simulations of multibody vehicular systems. However, graph-theoretic models of certain key components of the transmission system are not available at this point. This is precisely the motivation behind the current research.

**Model background:** The operation of a torque converter can be described as that of a hydraulic pump driving a hydraulic turbine. The torque from the engine drives the pump which imparts energy to the hydraulic fluid in the system, the hydraulic fluid flows through the vaned construction of the turbine and makes it rotate thereby transmitting the torque coming from the engine towards the rest of the transmission system. From the standpoint of energy transmission, the pump converts mechanical energy into hydraulic energy and the turbine converts it back to the mechanical domain. A linear graph can be used to represent the flow of power across different domains of the system and account for the storage and losses incurred in the process, [2]. Figure below shows a schematic diagram for a typical torque converter.



Schematics of a torque converter

**Paper organization:** We start by introducing the objective of modeling a torque converter. We try to explain why it is important to use linear graphs to model the dynamics of a hydro-mechanical device. We explain the way a torque converter functions and outline the general methodology for a graph-theoretic model of the same.

In the next section, we briefly cover the basics of graph-theoretic modeling, [2], Using a simple system as an example, we explain key terminologies and demonstrate how governing equations can be generated directly from the graph representing the system.

Next we present the linear graph for the torque converter and explain its structure. We demonstrate how it captures the topology of the system and how various physical phenomena are encapsulated into components. By discussing the nature of the constitutive equations we explain how a torque converter can be described to be made of a few inertia elements, energy dissipators, external sources of torques and energy transducers. We present the generated set of governing equations and simulated them with predefined input conditions. The results are evaluated against that available from existing literature, [1].

- [1] D. Hrovat and W. E. Tobler, *Bond-graph modeling and computer simulation of automotive torque converters*. Journal of the Franklin Institute, Vol. 319, pp 93-114, 1985
- [2] John J. McPhee, *On the use of linear graph theory in multibody system dynamics*. Nonlinear Dynamics, Vol. 9, pp. 73 - 90, 1996.

# HYBRID COMBINATION AND MODULAR MODELLING TECHNIQUES IN HEALTH TECHNOLOGY ASSESSMENT - AN EXAMPLE BASED EXPLANATION FOR COMMUNICABLE DISEASES

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**Introduction.** Modelling and simulation of communicable diseases is an important field of interest in HTA. There are different approaches to simulate epidemics but they have one characteristic in common: The more details the modeller considers, the more complex models become. But standards are getting stricter and requirements of stakeholders in the field of HTA are getting higher so there is a need for complex models.

A concept to deal with the increasing effort and complexity is to split up models into single parts, so called modules. The intention is to make development easier, increase the efficiency of teamwork, make models more flexible and reuse modules in other projects. In this work we concentrate on two different modular approaches for simulation of epidemics.

**The agent based approach.** The first approach is agent based modelling. It deals with single persons with attributes and individual behaviour. They have contacts in an environment, can get infected upon contacts, run through individual sickness states, infect others and eventually recover. So an epidemic emerges. Additionally people may require resources for prevention and treatment that sum up to economical evaluations. This structure was further developed and improved within IFEDH (Innovative Framework for Evidence-Based Decision-Making in Healthcare), a project funded by FFG. We underline this concept with three examples:

- A model for influenza where people move in different environments that look like lattice gas cellular automata [1]
- A model for Streptococcus Pneumoniae that deals with complex infection rules [2]
- And another influenza-model with an extensive social environment where people move and meet each other [3].

These examples are models in different projects but still they are able to share some of the modules while others need to be developed separately.

**The top-down approach.** Top-down models for epidemics are a different approach than agent based models. They do not consider single persons, instead they calculate the fractions of the population that are in certain states. Common techniques are Markov models and differential equations. Since this approach works on a different basis it splits up into three parts. It starts with the epidemiological part, where infections and incidences are calculated in a general way. In the next step the demographical part maps the results from the first part on a real population of a country. It ends with the economical part that calculates costs and other outcome values and evaluates economic aspects. A model for HPV serves as an example [4]. The epidemiological module uses an adopted model that has been developed in Britain to receive epidemic outcome parameters. The demographic and the economic module match these results on Austria's situation to estimate the total costs caused by HPV in the long term.

**Conclusions.** The examples show that it is possible to split up models into the proposed modules. In general we can conclude that modular modelling helps to structure modelling process and that reusability of tested and validated modules makes projects more efficient and reliable.

- [1] Emrich S., Breiteneker F., Zauner G., Popper N.: "Simulation of Influenza Epidemics with a Hybrid Model - Combining Cellular Automata and Agent Based Features." Proceedings of the ITI 2008 30th Int. Conf. on Information Technology Interfaces, (2008), ISBN: 978-953-7138-13-4; S. 709 - 714.
- [2] G. Zauner, F. Miksch, N. Popper, G. Endel, I. Schiller-Frühwirth, F. Breiteneker: "Long-Term Effects of Children Pneumococcus Vaccination: An Agent Based Approach"; Value in Health - The Journal of the International Society for Pharmacoeconomics and Outcomes Research" J. Wiley (Hrg.); Value in Health / Wiley-Blackwell, Vol. 13/ No. 7 (2010), ISSN: 1098-3015; S. 383 - 384.
- [3] F. Miksch, C. Urach, N. Popper, G. Zauner, G. Endel, I. Schiller-Frühwirth, F. Breiteneker: "News Insights on the Spread of Influenza Through Agent Based Modeling"; Value In Health, 14 (2011), 7.
- [4] Zechmeister I, Blasio BF, Garnett G, Neilson AR, Siebert U. "Cost-effectiveness analysis of human papillomavirus-vaccination programs to prevent cervical cancer in Austria.", Vaccine. 2009 Aug 13;27(37):5133-41. Epub 2009 Jun 28.

# IDENTIFICATION OF AN IMPULSE DIFFERENTIAL INCLUSION FOR THE BEHAVIOR OF A MECHATRONIC SYSTEM

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**Introduction.** The behavior of mechatronic systems consists of discrete jumps between continuous states linked to mechanical laws. This type of behavior is typically that of hybrid dynamic systems. An impulse differential inclusion is a tool which can be used for modeling hybrid phenomena. Our researches relate to the influence of parameters' variations on systems' behavior and are based both on differential inclusion and impulse differential inclusion. We present an example in which we use differential inclusion to show the impact of variation of parameters includes in a system modeled by hybrid automaton.

**Parameter variations.** Tolerancing is based on the idea that each parameter of the model of a system is affected by an uncertainty. The behavior of a dynamic system depends on the value of its parameters. By modeling the system by differential equation, each variation of one component is traduced by a variation of its corresponding coefficient on the differential equation. We talk about tolerancing when we have small variation and we have a sizing problem when we have big one. A mathematical tool to model the temporal behavior in continuous domain is differential inclusions.

**Differential inclusions.** Differential Inclusions represent an important generalization of differential equations for parameter variation. It is known as a differential equation with a multivalued right hand side. The solution to a DI is a reachable set, instead of a single trajectory [2]. The general forum of a DI is as follow:

$$\frac{dx}{dt} \in F(t, x(t)), \quad x(0) \in X_0$$

With  $x \in R^n$  and F is an application from  $R \times R^n$  to subsets of  $R^n$  and  $X_0$  the initial set

$$F(t, x(t)) = \{z = f(t, x, v) \mid v \in C(t, x)\}$$

v is a variable element of variation field C. This variable may be the control or a parameter of the system. We have developed our approach which uses variable step to explore all the interval of variation and deliver the reachable set that includes all possible solutions.

**Impulse differential inclusions.** An impulse differential inclusion (IDI) is a collection  $H = (X, F, R, J)$  consisting of a finite dimensional vector space X, a set valued map  $F : X \rightarrow 2X$ , which corresponds to differential inclusion [1]. A run of an impulse differential inclusion  $H(X, F, R, J)$  is a hybrid trajectory  $(\tau, x)$  which consists on hybrid time trajectory  $\tau = \{\tau_i\}_{i=0}^N$  and an application  $x : \tau \rightarrow X$  that satisfies:

- Discrete Evolution: for all i,  $x(\tau_{i+1}) \in R(x(\tau_i))$
- Continuous Evolution: if  $\tau_i < \tau_i'$ ,  $x_i(\cdot)$  is a solution of differential inclusion  $\dot{x} \in F(x)$  over the interval  $[\tau_i, \tau_i']$  starting at  $x_i(\tau_i)$ , with  $x_i(t) \notin J$  for all  $t \in [\tau_i, \tau_i']$

**Example of application.** We consider a mechatronic system composed by a DC motor, a threaded rod and a threaded mass to test out our approach. The mass is powered by a controller module which delivers the DC motor supply voltage (U or -U) according to the position x of the mobile which moves between two stops. We show the influence of small and big variation of the resistance "r" and the screw's step "p". We simulate the result using Mathematica.

We model the system by hybrid automaton. The variation of the resistance of the motor is modeled with differential inclusion in the state.

In the result we have the identification of the different sets of the impulse differential inclusion and a scheme of them.

[1] Aubin J.-P., Lygeros J., Quincampoix M., Sastry S. & Seube N. : *Impulse Differential Inclusions : A Viability Approach to Hybrid Systems*, IEEE Transactions on Automatic Control 2002, 47, 2-

[2] Raczynski S. : *Modeling and simulation: The Computer Science of Illusion*, Wiley, England, 2006 p115-116

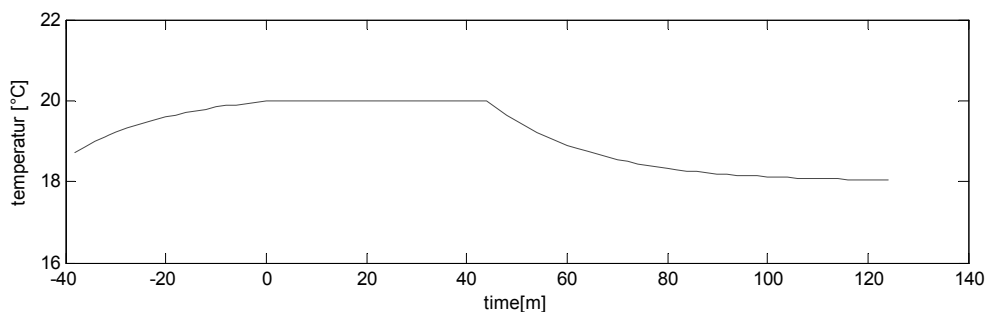


## IDENTIFYING SIMPLIFIED MODELS FOR LOAD SHIFTING CONTROL

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**Introduction.** In industrialized countries, the buildings stock consumes about 40 per cent of the overall final energy, and is responsible for over a third of the CO<sub>2</sub> emissions. Out of these 40 per cent, approximately half in turn is used for the operation of the building, with most of it going into the HVAC systems, as well as room lighting. In the 20/20/20 goals of the European Union [1] – reducing the consumption of primary energy by 20 per cent by 2020 – buildings are therefore major focus. Due to the parallel increase of electric generation renewable energy sources, especially photovoltaic and solar power [2], demand-response-management (DR) will also play major role, as their stochastic behaviour has to be met at the consumer side. Considering those two approaches, DR using building HVAC systems is a promising strategy.



**Figure 1: Intended operation of the building for DER, assuming a peak in the electrical grid from  $t=0$ .**

**Methodology.** To reduce the manpower during building modelling and the computational power during building operation, a combination of tools was used to arrive at auto generated models, which only have to be properly parameterized for the building controller.

Taking only characteristic values from the “Energieausweis”, the mandatory Austrian implementation of [1], a rough geometrical model of the building for the use in TRNSYS is generated and parameterized, with the critical thermal zone being identified using rules of thumb from building physics.

Using MATLAB, parameter variations of the model with respect to inner loads, air exchange rate and outside temperature are the run in TRNSYS, giving the thermal behaviour of the critical zone for each of the runs. The results of these simulations are then fit to simple exponential equations, which originate in the solution of the simplest physical model of the thermal process, again using MATLAB.

Using these models, the energy demand for heating can be determined, and in combination with a simple tank model for thermal storage tanks, the controller can guide the HVAC system through the three phases of the load shifting process. As seen in (Fig. 1), the intended operation of the building is to reach the upper limit of the room temperature right before the peak, holding this temperature as long as possible using storage and then letting the building cool down. In the ideal case, the peak is over before the critical zone reaches the lower end of the thermal comfort zone.

**Field testing for validation:** To test the approach presented in this paper, 10 objects in the Salzburg federal state in Austria are equipped with building management systems. The buildings were chosen for a mix with respect to use and thermo-electric systems present in the buildings. Systems present include direct electric heating, heat pumps, and combined heat and power (CHP) plants. Some of the systems also include storage tanks, which add to the load shifting capacity. On the other hand, in some of the building no information about the room temperature will be available. Those will either be controlled over the temperature levels in the storage tanks, or using the models and only using feedback from the tenants to adjust the controllers.

Load shifting load shedding will be performed manually under the supervision of representatives of building owners and operators (the local multiutility and a local profit housing cooperative). In case of large deviations, models will be re-calibrated using the monitoring data. Afterward, a control logic using the models and parameters will control the building HVAC systems.

[1] “DIRECTIVE 2010/31/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 19 May 2010 on the energy performance of buildings (recast),” Official Journal of the European Union, vol. 31, 2010.

[2] “EU energy and transport in figures”, European Commission, Luxembourg: Publications Office of the European Union ISBN 978-92-79-13815-7, 40ff.

# IMPLEMENTATION OF THE TOOLS OF FUNCTIONS' ALGEBRA: FIRST STEPS

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**Algebra of functions.** The mathematical approach, called the algebra of functions, has been recently developed as an alternative to differential geometric methods for handling the modeling, analysis and synthesis problems for nonlinear control systems [1]. Compared with the conventional methods, the new approach allows to address also the non-smooth systems. In this approach the computations are not linearized by applying the differential operators and therefore, there is no need to solve the specific partial differential equations or to integrate the sets of differential forms to find the solutions to modeling problems. Though it is too early to evaluate the advantages/disadvantages of the new approach compared to differential geometric methods, it is obvious that one may hardly expect to find the solutions manually, except for the very simple cases and for the new approach to be applicable, one has to develop the specific symbolic software.

**The developed software.** The Mathematica-based package NLControl, see [2], developed in the Institute of Cybernetics at Tallinn University of Technology, consists of functions that assist the solution of different modeling, analysis and synthesis problems for nonlinear control systems, described either by state or by input-output equations, both discrete- and continuous-time and is based either on the approach of differential forms or non-commutative polynomial methods. The package has been made partially available over the internet using web-Mathematica tools [2].

A number of new Mathematica functions have been developed related to the mathematical approach, called the algebra of functions in order to expand the functionality of the package NLControl. The elements of algebra of functions are vector functions and its main ingredients are:

- relations of partial preorder and equivalence,
- binary operations on functions, denoted by  $\times$  and  $\oplus$ ,
- binary relation, denoted by  $\Delta$ ,
- operators  $\mathbf{m}$  and  $\mathbf{M}$ .

The first two elements are defined on the arbitrary set  $S_X$  of vector functions whereas the last two are defined for the set of vector functions with the domain being the state space of the control system. In this paper we only deal with the first two elements. In the smooth cases one may develop many algorithms/Mathematica functions to address these tasks whereas in the non-smooth cases the number of tools will be limited. The most interesting non-smooth functions for practical applications are those describing such phenomena as saturation, hysteresis, Coulomb friction and backlash.

We have implemented two separate Mathematica functions for every functions' algebra relation/operation under consideration: generic version and strict version. The generic standpoint is what we have used in NLControl package so far. Usually generic version of the function is simpler and works faster than its strict counterpart. The strict version of the function mostly finds first the generic solution of the problem, and then tests whether the necessary strict partial preorder relations are valid and finally checks the existence of singular points. The strict version also allows to specify the domain of the functions, thus it can be used to check whether the properties/relations are valid locally.

In order to simplify the computations, one is advised to replace the components by equivalent but more simple functions. In our implementation we use certain replacement rules. These rules are based on the theoretical justification and do not necessarily apply the definitions directly.

**The website.** The developed programs are made partly available at <http://webmathematica.cc.ioc.ee/webmathematica/NLControl/FuncAlg>. The main benefit of the web site is that one does not need Mathematica to be installed into local computer, only internet connection and browser are necessary.

- [1] A.N. Zhirabok and A.Ye. Shumsky. *The algebraic methods for analysis of nonlinear dynamic systems (In Russian)*. Dalnauka, Vladivostok, 2008.
- [2] M. Tönso, H. Rennik, and Ü. Kotta. Webmathematica-based tools for discrete-time nonlinear control systems. *Proceedings of the Estonian Academy of Sciences*, 58(4):224–240, 2009.

# IN-SILICO MODELLING OF TUMOUR-IMMUNE SYSTEM INTERACTIONS FOR GLIOBLASTOMAS

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**Introduction.** Glioblastoma is the most aggressive and most common primary brain tumour in adults. These highly vascular and invasive tumours exhibit a large degree of cellular heterogeneity that account for their resistance to standard multi-modal therapies consisting of surgical resection, radiotherapy and chemotherapy. Immunotherapy may represent an alternative strategy [1], however, the role of immune cells in glioma biology is still controversial. Clinical observations and in vitro studies [2] indicate that microglia and macrophages that infiltrate the brain tumour tissue in high numbers play a tumour-supportive role. With the help of our current in silico study, we intend to introduce a mathematical model to approach and evaluate the role of these cells and validate our results by in vitro studies.

The main contribution of this work is the development of a novel model that describes the immune response to tumour growth in the brain.

**Methods.** For a realistic in silico study, the simulations are obtained by incorporating tumour-related factors: The extracellular matrix (ECM), nutrients (as oxygen, glucose) and signals emitted by tumour cells (TS), which activate the MG.

The resting microglia in primary brain tumours are activated and attracted by TS, which is described by a partial differential equation. The secretion of matrix degrading enzymes from amoeboid immune cells can be modelled with the help of an additional term for the degradation of the ECM. This supports a more invasive migration of tumour cells.

**Results.** The simulated tumour depicts a distribution that can typically be observed in vivo [2, 3]: A big necrotic core surrounded by a rim of quiescent cells and an outer rim of strongly diffusive glioma cells surrounded by microglia.

**Conclusion.** In agreement with published observations, comparison of our in silico data with in vitro data indicates that resting microglia/macrophages are tumour-supportive. This demonstrates the validity of our in silico approach and its relevance for further use to undermine the interactions between tumour and immune cells.

- [1] M.B. Graeber, B.W. Scheithauer, and G.W. Kreutzberg. Microglia in brain tumors. *Glia*, 40:252–259, 2002.
- [2] Kees, T., Lohr, J., Noack, J., Mora, R., Gdynia, G., Tödt, G., Ernst, A., Radlwimmer, B., Falk, C., Herold-Mende, C., and Régnier-Vigouroux, A. (2011). Microglia isolated from patients with glioma gain antitumor activities on poly (i:c) stimulation. *Neuro-Oncol.*, doi:10.1093/neuonc/nor182.
- [3] D. Marković. *The role of microglia in glioma invasiveness*. PhD Thesis, Medizinische Fakultät der Charité, Universitätsmedizin Berlin, 2007.

# INTEGRATING AIR-POLLUTION DISPERSION SIMULATION MODELS AND GIS FOR URBAN AIR-POLLUTION EMERGENCY MANAGEMENT

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**Introduction.** A system for management and control of incident air pollution events should integrate several key subsystems such as: a) Geographical Information System (GIS), b) System for monitoring contamination in the case of accidents, c) Hydro-meteorological monitoring and prognosis system, d) Simulation system for air pollution dispersion and, e) Emergency response service system. An estimate of air pollution dispersion can only be properly estimated by the application of simulation models. It is of prime importance that such models are available for emergency situations with state of the art input-output, user-friendly networked interfaces. Since the processes influencing air pollution dispersion are fast, the final system should incorporate near real-time data collection.

**Methodology.** There are several approaches to model air-pollution dispersion: Gauss model [1, 2], Ermak model [3] regression models, box model, multiple cell model and other new approaches. For the purpose of the proof of the concept the Gaussian model was implemented in MATLAB® [4]. Gaussian model has several assumptions: a) the smokestack emission is constant and continuous b) terrain which is observed is flat, c) the wind speed is constant. Here, one considers, that in main wind direction ( $x$ ), advection dominates over diffusion and dispersion. If diffusion in horizontal direction is neglected the following differential equation is obtained which describes the dispersion process:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial y} D_y \frac{\partial c}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial c}{\partial z} - v \frac{\partial c}{\partial x} - \lambda c \quad (1)$$

where  $D_y$  and  $D_z$  represent the diffusivity in  $y$  and  $z$  direction and  $\lambda$  represents the decay rate of the process. On the Gaussian solution of the Eq. 1 further development was performed in order to implement the complete Ermak model of air pollution process [3], which considers the deposition and settling:

$$C(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} e^{-\frac{y^2}{2\sigma_y^2}} e^{-\frac{W_s(z-H)}{2K_z} - \frac{W_s^2 \sigma_z^2}{8K_z^2}} \times \left[ e^{-\frac{(z-H)^2}{2\sigma_z^2}} + e^{-\frac{(z+H)^2}{2\sigma_z^2}} - \sqrt{2\pi} \frac{W_0 \sigma_z}{K_z} e^{\frac{W_0(z+H)}{K_z} + \frac{W_0^2 \sigma_z^2}{2K_z^2}} \operatorname{Erf}\left(\frac{W_0 \sigma_z}{\sqrt{2} K_z} + \frac{z+H}{\sqrt{2} \sigma_z}\right) \right] \quad (2)$$

where  $W_0 = W_d - \frac{1}{2} W_s$  i.e. determined by settling and deposition. Results gained by the implemented models were put into the GIS system from the MATLAB by the kml format [5]. In order to evaluate accuracy of the developed models, the results were with ALOHA [6] software which can be considered as reference in this field.

**Results and Discussion.** The applied Gaussian model as well as the Ermak modification proved to be sufficient for the test of concept. MATLAB was applied as the tool for rapid development of the system. An important aspect was GIS representation, which was successfully provided by the application of a Google Earth component. In this respect, the results of the simulation run could be widely distributed to the response team and local population. Since the processes of air pollution dispersion are fast, the final system should incorporate near real-time data acquisition. The development of the system requires air-pollution dispersion models that should be validated and tested. In our case the ALOHA system was successfully used for validation.

- [1] E. Holzbecher, *Environmental Modeling using MATLAB®*, Springer-Verlag Berlin Heidelberg, 2007.
- [2] G. M. Masters G.M. *Introduction to Environmental Engineering and Science*, Prentice Hall, 1997.
- [3] D. L. Ermak, An analytical model for air pollutant transport and deposition from a point source, *Atmos. Env.*, 1977, Vol. 11, No. 3, pp. 231–137.
- [4] MATLAB version R2008a. Natick, Massachusetts: The MathWorks Inc., 2008.
- [5] Google-Earth-Toolbox, <http://code.google.com/p/googleearthtoolbox>, Accessed 11.11.2011.
- [6] U.S. Environmental Protection Agency, National Oceanic and Atmospheric Administration, ALOHA User's Manual. Washington D.C. Seattle, WA, 2007.
- [7] Google Earth, <http://www.google.com/earth>, Accesed, 11.11.2011.

# MATHEMATICAL ASPECTS OF THE IMPLEMENTATION OF PARTICLE FILTERS ON FPGA

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Particle filters are a type of Bayesian filters commonly used for system state estimation such as tracking and localization applications. Tracking and localization are important tasks for autonomous robots, and particle filters are particularly well suited to deal with such tasks, as demonstrated by many RoboCup-Teams. Tracking and localization are also of growing importance in the automotive field and in airport environments to build intelligent sensors. However the computational complexity of particle filters lead to a high load of the Central Processing Unit (CPU) resulting in a high clock and a high energy usage. This limits the use of particle filters in small autonomous robots or intelligent embedded sensor for traffic surveillance.

Since the algorithm is well suited for parallel execution on customized hardware architectures, a hardware-software solution has been developed where task like data association, track management and data normalization are done in software while the computationally more expensive execution of the particle filter algorithm is done on customized hardware. Such architectures can be realized using an embedded PC and Field Programmable Gate Arrays (FPGA). The feasibility of the implementation of particle filters on FPGAs has been shown [2, 1]. This approach allows the system to be placed in embedded sensors and small autonomous robots.

The parallel execution of the particle filter algorithm leads to a significant reduction of clock and therefore of energy, making embedded high performance particle filters possible, relieving the CPU from a computational expensive task while providing high performance tracking capabilities. For reasons of logical cell usage the use of fixed point representations of the numbers involved in the computation of the algorithm is used. This poses a bigger problem than one might expect, as the original theory of the particle filter is based on continuous representations, and the algorithm won't work without modifications to counter the effects resulting from the limited precision of the fixed point number representation.

A fixed point based particle filter for tracking of an object in six dimensions, 2D-translation, rotation, and 2D-translation and rotation speed has been implemented on a FPGA. Some mathematical aspects of the implementation are introduced and the feasibility of some treatment approaches is shown for a RoboCup scenario and a simulated airport traffic surveillance scenario.

- [1] Sangjin Hong, M. Bolic, and P.M. Djuric. An efficient fixed-point implementation of residual resampling scheme for high-speed particle filters. *Signal Processing Letters, IEEE*, 11(5):482 – 485, May 2004.
- [2] Binli Ye and Yunhua Zhang. Improved fpga implementation of particle filter for radar tracking applications. In *Synthetic Aperture Radar, 2009. APSAR 2009. 2nd Asian-Pacific Conference on*, pages 943 –946, October 2009.

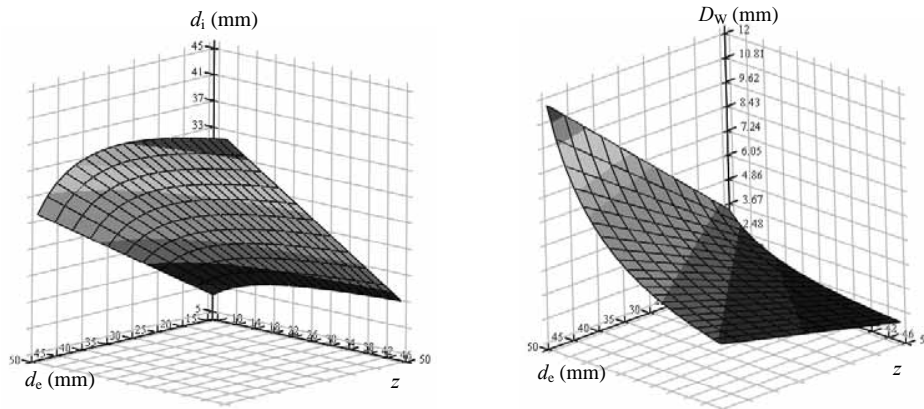
## MATHEMATICAL BACKGROUND OF U-JOINT REPAIR

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**Introduction.** The universal joint – U-joint (also called Cardan or Hook’s joint) is a type of the oldest flexible mechanical coupling designed to compensate for the misalignment between connected shafts. The U-joint is commonly known for its use on vehicles. The failed U-joint is the most common vehicles driveline problem. The U-joint consists of shaft yokes, cross and four needle rolling bearings. When the operational ability of U-joint is lost due to intensive wear, it has to be replaced by a new one or to be repaired. The repair implies additional machining of worn out needle bearing parts. It means that damaged surface layers of material have to be removed. Due to remanufacturing, dimensions of U-joint parts are changed, but appropriate relations between dimensions have to be unchanged [1]. So, appropriate geometrical relations, primarily based on limited radial and circular internal clearance, must not be disturbed by repair process. Hence, it is necessary to establish a mathematical model of the needle bearing internal geometry and the corresponding algorithm for determining appropriate dimensions. It was carried out in this paper.

**Dimensions of U-joint bearing.** The main dimensions of U-joint needle rolling bearing are journal diameter ( $d_i$ ), cap raceway diameter ( $d_e$ ), needle roller diameter ( $D_w$ ). The dependence of journal diameter and needle diameter on both cap raceway diameter and number of needles ( $z$ ) according to functions given in the paper is shown in the figures below. The internal radial clearance ( $e = d_e - d_i - 2 D_w$ ) is significant geometrical and functional characteristic of U-joint rolling bearing. Too large radial clearance causes unequal load distribution between rollers [2,3], impact loads, increased vibrations and noise. Too small radial clearance causes increased friction and heating and, finally, bearing failure. Because of that, bearing internal radial clearance has to be in appropriate recommended limits. The nominal value of the internal radial clearance is zero, and its positive deviation depends on combination of deviations of all relevant needle rolling bearing diameters ( $(d_i, d_e, D_w)$ ).



**Conclusion.** To ensure proper reassembling, as well as functionality and operational ability of the U-joint bearing, appropriate internal radial clearance need to be achieved. It depends on proper determination of diameters of bearing parts (cross journal, cap raceway and rollers), as well their tolerances. The procedure for determining these dimensions is presented in this paper. This is the basis for further mathematical modelling of U-joint needle bearing dimensions, mechanical behaviour and load distribution, in order to optimize internal geometry, increasing load carrying capacity and service life of U-joint.

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- [1] Köttritsch H., Wagner K.: *Remanufacturing of rolling bearings*. In: Proc. ÖTG Symposium 2009, Vienna, 2009, 5-13.
- [2] Marinkovic A., Lazović T.: *Modelling and simulation of rolling bearings using advance software tools*. In: Proc. 6th Vienna Conference on Mathematical Modelling – MATHMOD 09, Vienna, 2009, 2580-2583.
- [3] Lazovic T., Ristivojevic M., Mitrovic R.: *Mathematical model of load distribution in rolling bearing*. FME Transactions, 36 (4) (2008), 189-196.

# MATHEMATICAL MODELING FOR INVISIBILITY DEVICES

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Recently, the application of geometry and conformal mappings to artificial materials (metamaterials) has attracted the attention in various research communities. These materials, characterized by a unique man-made structure, have unusual optical properties, which materials found in nature do not exhibit. By applying the geometry and conformal mappings theory to metamaterial science, it may be possible to realize so-called “Harry Potter cloaking device”. Although such a device is still in the science fiction realm, several works have shown that by using such metamaterials it may be possible to control the direction of the electromagnetic field at will. We could then make an object hidden inside of a cloaking device. Here, we will explain how to design invisibility device using differential geometry and conformal mappings. Furthermore, we plan to apply our modeling to moving metamaterial devices.

In [8,9], we propose a novel method that uses a combination of positive and negative refraction indices, called plus-minus construction, that enables us not only to enclose the trajectory of light, but also to achieve perfect invisibility in isotropic media, without both phase delay and reflection.

In particular, we introduce a new construction of cloaking devices by performing three successive conformal maps on the space defined by a trivial flat metric [9]. This operation results on a physical space  $R^2$  with a non trivial refractive index. A technical advantage of using first a flat space metric is that the trajectory of light is trivial in the mathematical space and can be easily derived in the physical space through the conformal mappings. Hence, it is unnecessary to consider the motion equation for light rays a priori. As we show here, the trajectory is readily obtained as the result of operating three successive conformal mappings that rotate the space. Interestingly, the proposed dielectric media leads to perfect invisibility with absence of both phase delay and reflection. These findings strongly highlight the role of the negative refraction in material sciences. Although currently the application of negative refraction is confined to the construction of perfect lens, our results show that a device consisting of alternating positive and negative refraction (plus-minus construction) exhibits extraordinary properties like the perfect cancelation of reflection phenomena.

It was reported that the moving media of metamaterial realizes the event horizon for light [10]. It is called “artificial black holes”. After the light enters the event horizon, it never comes back. Interestingly, moving media of metamaterial realizes such a horizon. On the other hand, it is known that a combination of plus and minus refractive index enables us to truncate the space [11]. However, as far as we know, the effect is unknown when the combination of plus-minus refractive index is moving in space. We are currently exploring this issue using space-time geometry-based mathematical tools.

- [1] Pendry, J.B., Schuring, D. and Smith, D.R. (2006). *Controlling Electromagnetic Fields*, Science 312, 1780.
- [2] Schurig, D., Mock, J. J., Justice, B. J., Cummer, S. A., Pendry, J. B., Starr, A. F., and Smith, D. R. (2006). *Metamaterial Electromagnetic Cloak at Microwave Frequencies*, Science 314, 977.
- [3] Leonhardt, U. and Philbin, T. G. (2009). *Transformation Optics and the Geometry of Light*, Prog. Opt. 53, 69.
- [4] Leonhardt, U. (2006). *Optical Conformal Mapping*, Science 312, 1777.
- [5] Leonhardt, U. (2006). *Notes on conformal invisibility devices*, New. J. Phys. 8, 118.
- [6] Nachman, I. (1998). *Reconstructions from boundary measurements*, Ann. Math. 128, 531.
- [7] Wolf, E. and Habashy, T. (1993). *Invisible bodies and uniqueness of the inverse scattering problem*, J. Mod. Opt. 40, 785.
- [8] Ochiai, T., Leonhardt, U., and Nacher, J. C. (2008). *A novel design of dielectric perfect invisibility devices*, J. Math. Phys. 49, 032903.
- [9] Nacher, J.C., Ochiai, T. (2011). *Plus-minus construction leads to perfect invisibility*, J. Math. Phys.52, 012903.
- [10] Philbin, T. G., Kuklewicz, C., Robertson, S., Hill, S., Konig, F., and Leonhardt, U. (2008). *Fiber-Optical Analog of the Event Horizon*, Science 319, 1367-1370.
- [11] Pendry, J. B. and Ramakrishna, S. A. (2003). *Focusing light using negative refraction*, J. Phys. Condens. Matter 15, 6345.

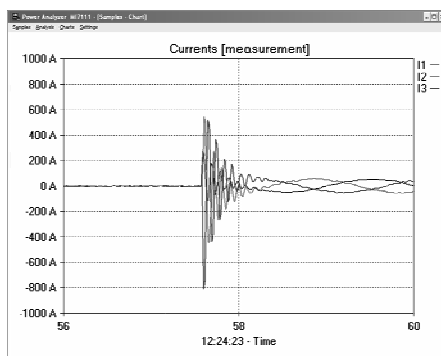
## MEASUREMENT, MODELING AND SIMULATION OF CAPACITOR BANK SWITCHING TRANSIENTS

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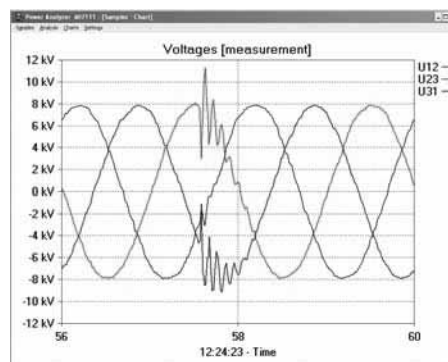
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This paper presents the results of experimental and simulated investigations of electromagnetic transient phenomena during energizing of industry capacitor banks. Experimental and simulated investigations based on the electrical network model having the nominal voltage of 6 kV are carried out.

**Experimental measurements:** Waveforms of phase currents and phase to phase voltages resulting from experimental measurements during energizing of a 500 kVAr capacitor bank at the 6 kV network with isolated neutral point, are presented in the next Figures.

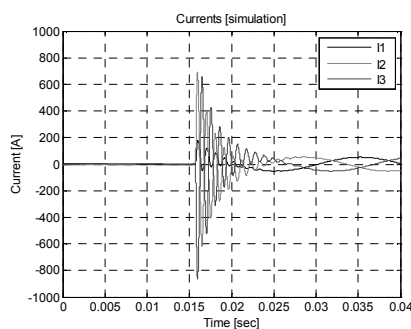


Measured phase currents during energizing of capacitor bank

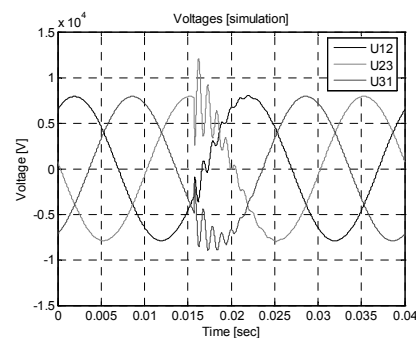


Measured phase to phase voltages during energizing of capacitor bank

**Modeling and simulations:** Waveforms of phase currents and phase to phase voltages as a result of simulations during energizing of a 500 kVAr capacitor bank at the 6 kV network with isolated neutral point, are presented in the next Figures.



Simulated phase currents during energizing of capacitor bank



Simulated phase to phase voltages during energizing of capacitor bank

**Sensitive analysis of the system parameters:** The sensitive analysis of influential parameters within a three phase system by observing characteristic parameters of phase transient currents and phase to phase transient voltage waveforms (amplitude, duration, frequency) are performed.

### References:

- [1] Math H. J. Bollen, Irene Y. H. Gu, *Signal Processing of Power Quality Disturbances*, IEEE Press, Wiley, New York, 2006.
- [2] C. E. McCoy, B. L. Floryancic, *Characteristics and Measurements of Capacitor Switching at Medium Voltage Distribution Level*, IEEE Transactions on Industry Applications, Vol. 30, No. 6, November/December 1994, 1480-1489.
- [3] R. A. Adams, S. W. D. Middlekauff, *Solving Customer Power Quality Problems Due to Voltage Magifications*, IEEE Transaction on Power Delivery, Vol.13, No. 4, October 1998, 1515-1520.



## MINIMUM TIME PATH CONTROL OF REDUNDANT PLANAR CABLE-SUSPENDED ROBOTS

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**Abstract.** Due to the fact that industrial automations require manipulators performing tasks in the smallest time to raise productivity, the ability of manipulators to perform a task in minimum time is desirable. Cable-driven parallel manipulator is a special class of parallel manipulators in which the moving platform is driven by cables, instead of rigid links. As regards lightweight structure, low inertial properties, and large reachable workspace of this type of manipulators, cable-actuated manipulators are suitable case for applications requiring high speed, high acceleration, and high payload but with moderate stiffness and accuracy. Hence, many researchers have extensively studied cable-suspended manipulators in recent years, thereby scrutinizing kinematics, dynamics and control of these robots. However, optimal control of this group of parallel manipulators has not been explored in many works. In particular, time optimal control of redundant cable-suspended manipulators along a specified path has been rarely discussed, unless the ones which have been based on solving redundancy regardless of time-optimality.

In this paper, time optimal trajectory planning of redundant planar cable-based parallel manipulators is studied for a predefined geometric path, subject to cable tension limits. The dynamic equations of these robots are generated and parameterized by non-dimensional path parameter. Proposed scheme, which is founded upon phase-plane analysis and linear programming technique, manages the full use of redundancy to increase the path-tracking velocity. In the end, some computer simulations are executed, the effects of the number of redundant cables on the value of minimum time and the amount of consumed energy are examined, and the improvement of applied method, in comparison with previous works, is presented.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

## MODEL OF STATE AND MOVING OF WORKFORCE IN THE REGION

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**Abstract.** It is known that education of optimal number of workers with certain speciality is a relevant object for many counties. Economic of the country or some region can not effectively develop without appropriate workforce supply, which generally formed by graduates from educational institutions of professional education. The model of state and moving of workforce in the region aimed at forecasting the condition of labor market in alignment with system of education, which can provide sensible information to governments concerning the current situation in system of education and labor market and what it leads to. Moreover, model provides the scenario analysis with possibility to regulate admission quotas and collate the optimal number of students with certain speciality.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

# MODEL-BASED ROBUST ENGINEERING DESIGN FOR THE QUALITY IMPROVEMENT OF ELECTRON BEAM MELTING AND REFINING

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**Abstract.** The requirements for the quality of model design and automatic control in the process industries and at the same time the available computing power increased significantly in recent years. This leads to the opportunity of design systems with such intelligent functions as simultaneous utilization of memory, learning and high-level decision making. Development of adequate models for real industrial processes is usually a complicated task due to the large uncertainties, caused by lack of direct measurements and necessity of inferential approach, high level of non-linearity and different types of disturbances. Building of models accurate enough in a broad range of operational conditions may be successful, if different intelligent modeling techniques are used.

The model-based robust approach for improving the quality of the process can be successfully applied to different industrial processes. Since during industrial production processes there are always errors in process parameters, these errors will affect the quality performance characteristics and will cause variations in their levels. In order to improve the quality, these variations should be minimized through proper choice of process parameters. For each of the quality performance characteristics, on the base of regression, kriging, neural networks or other models, two other models are estimated - for their mean values and their variances. The quality improvement is performed using some overall criterion or simply by the performance characteristic variance minimization, while keeping the mean values close to their target values.

Electron beam melting and refining (EBMR) technology is an advanced vacuum technology for processing of refractory materials in order to meet the ever increasing demands of industry such as aerospace and chemical industry, electronics and nuclear power industry, and medicine for reactive high strength and/or ultra-pure materials suitable for use at high temperatures and aggressive mediums. The simulation of the process can be applied to numerous tasks, connected with investigation of the geometry of the molten pool and the optimization of the form of the crystallization front. The importance of the knowledge of the shape of the crystallization front is directly connected with the quality of the ingot, as a flat crystallization front permits forming of dendrite structures, parallel to the ingot axis as well as the uniform impurity displacement toward the ingot top surface. The enlargement of the depth of the molten pool (with the increase of the beam power and the casting velocity) may lead to regimes at which the molten metal pool and the crystallization process will be controlled mainly by pouring metal heat content. However, the increase of the beam power and the casting velocity lead also to an increase of the evaporation losses through the top surface of the ingot, which is more appropriate for the process electron beam evaporation.

The present study highlights modeling of the process electron beam melting of Ta. The obtained simulated results are verified by comparing with real experimental data. The obtained experimental and simulated results are used for the estimation of regression models (Response surface approach), describing the dependencies of the geometry characteristics of the molten pool, the final concentrations of the impurities or the material losses from the process parameter values and the material losses at EBMR of Ta, depending on process parameters: electron beam power, the casting velocity and the height of the interface ingot-crucible, calculated using the estimated regression models. Other modeling approaches are considered too (kriging and network models). The model-based approach for robust engineering design (in the case of errors of process parameter errors) is implemented in order to make optimization of the quality characteristics and to achieve an efficient and reliable production process.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

# MODELING AND APPLICATION CHALLENGES IN THE CONTAINER TERMINAL OPERATIONS

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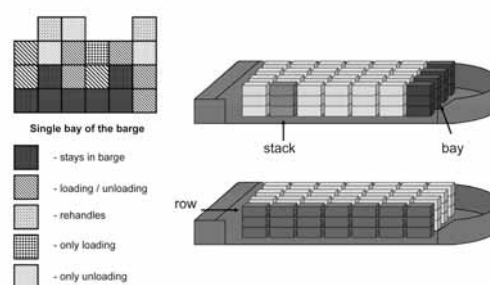
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**Introduction.** Basically there is always a compromise between our desire to create more complex model and computational time necessary to solve that problem. As modeling always implies some simplification of the original system there is also a problem of applicability i.e. implementation of the model and its solution to the real life problems. This paper points out some of these problems within the scope of container terminal modeling. There is great number of scientific papers and publications that analyze these different problems and some of them are modeling the same system (part of the reality) with a different level of approximations. In this paper attempt was made to compare different approaches to the problem on different container terminal processes and to highlight some application problems. A container terminal represents a complex system with highly dynamic interactions between the various handling, transportation and storage units, and incomplete knowledge about future events. There are many decision problems related to logistics planning and control issues of and they can be assigned to three different levels: terminal design, operative planning, and real-time control [1].

**Variety of problems.** Many papers are focused on optimization of only specific process and not the whole container terminal as a system. Main logistic processes inside container terminal are: berth allocation, stowage planning, quay crane assignment, quay crane scheduling, yard crane scheduling, storage and stacking police, rail operations, truck operations and internal transports.

**Modelling challenges.** In scientific literature there are present different models for the same processes. One major example for this is container quay crane scheduling. Despite there are different models and solutions for the same problem, which in this case, mainly arise from the definition of the task to be performed. Tasks are defined by container group, bay and bay area. In the Figure 2 is presented difference between bay and bay area. These models are developed simultaneously over a relatively long period, but only recently in [2] there is proposed a comprehensive method for evaluation of this models and presented significant analysis of this problem.

Exact methodology can't be determined for all problems, so there is a need for creation of some general guidelines for narrow research areas. This is the case with container quay cranes in inland terminals due to a several reasons. Differences are caused by smaller flow of containers in this type of the system, so existing concept of bay areas, bays and container groups is not applicable since each container commonly have different destination - Figure 1



**Figure 1:** Bay inside barge/ship [3]

For the real life systems of this type, this problem was solved optimally. The results showed significant possibilities for time savings. In this paper are presented some problems concerning modelling challenges for container terminals. Since there is an emerging need for an analysis of improvement in all aspects of container transport due to the global increase in the volume of containerised goods.

- [1] K.H. Kim, H.O. Günther. *Container Terminals and Cargo Systems*. Springer-Verlag Berlin Heidelberg 2007.
- [2] F. Meisel, C. Bierwirth. A unified approach for the evaluation of quay crane scheduling models and algorithms. *Computers and operational research* 38, 2011, 683-693.
- [3] E. Pap, V. Bojanić, G. Bojanić and M. Georgijević. Optimization of Container Quay Cranes Operations. 9th IEEE International Symposium on Intelligent Systems and Informatics SISY 2011. September 8-10, 2011, Subotica, Serbia.

# MODELLING THERMO-CHEMICAL HYDROGEN GENERATION IN A SOLAR PLANT

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**Introduction.** Within the framework of Hydrosol II project, a pilot plant was set up at Plataforma Solar de Almería with the aim of obtaining a continuous production of hydrogen from water using as energy source the Sun. The pilot plant is based in a two-step redox cycle system. At the first cycle (hydrolysis), a reduced metal oxide absorbs the oxygen of water producing hydrogen. At the second cycle (regeneration), the oxide is reduced again and releases the absorbed oxygen at the water splitting. Since, these two reactions work at different temperatures, two reactors are required to produce continuous hydrogen flow rate.

For the development of advanced control systems for the plant the Hydrosol II project pilot plant, a dynamic mathematical model was developed. The object-oriented modeling technology implemented in the Dymola tool and the Modelica language were used for developing the model.

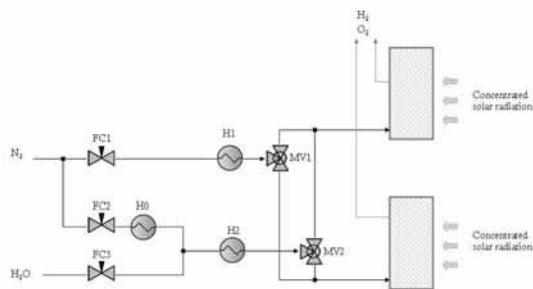
**Mathematical Model.** To develop the model, the system has been divided in two main subsystems: the heliostat field and the process plant, these models are detailed in the article. In particular, the modeling of the kinetic reaction dynamics, which implementation is based on the ThermoFluid library [3], will be explained

**Process Plant Chemical Dynamics.** The model presented in this section is a simplification of the scheme at the figure. The reaction scheme has been reduced to two single reactions [1]:

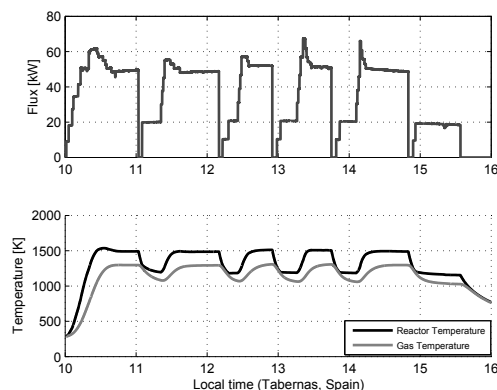


The reaction rate models in the reactors are based in the Arrhenius-type-temperature formulation, obtaining a chemical system similar to the Oregonator system presented in [2], in which mass and energy dynamics are added for the exchange of mass and energy with the environment.

**Simulation results and Ongoing work.** The article will present preliminary results with the interpretation respect to real behaviour of the plant.



(a) Hydrosol II plant diagram



(b) Simulation results with the process plant model

- [1] Christos C. Agrafiotis, Chrysoula Pagkoura, Souzana Lorentzou, Margaritis Kostoglou, and Athanasios G. Konstandopoulos. Hydrogen production in solar reactors. *Catalysis Today*, 127(1-4):265 – 277, 2007.
- [2] M. Tiller. *Introduction to physical modeling with Modelica*, volume 615. Springer, 2001.
- [3] H Tummescheit. *Design and Implementation of Object-Oriented Model Libraries using Modelica*. PhD thesis, Department of Automatic Control, Lund Institute of Technology, Sweden, August 2002.

# MODELLING CHARACTERISTICS OF SHORT TIME SERIES DATA FROM HIGH THROUGHPUT EXPERIMENTS

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**Introduction** Modern biology is interested in better understanding mechanisms within cells. Products of cells like metabolites, peptides, proteins or mRNA are measured and compared under different conditions, like healthy cells vs. infected cells. Recently, there is also a stronger focus on time series data to analyse the behaviour of the cell products over time. Such experiments usually yield regulation or expression values – the abundance or absence of a cell product compared to the initial measurement or a control experiment – for a large number of cell products, but with only a few replicates at a few time points. One of the main problems in the analysis of such data for deriving models of the behaviour of the cell products is the high variance of the data due to noisy measurements and differences in the metabolism of the individual biological organisms. In order to detect cell products with common behaviour over time, simple models need to be fitted to the data taking into account that apart from the noisy measurements there might also be a phase shift as well as variations of the speed of the biological process.

## Problem Formalisation

Time point	$s_1$			...	$s_T$		
Cell product	Replicate 1	...	Replicate R	...	Replicate 1	...	Replicate R
$i_1$	$x_{1,1}^{(1)}$	...	$x_{1,1}^{(R)}$	...	$x_{1,T}^{(1)}$	...	$x_{1,T}^{(R)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$i_N$	$x_{N,1}^{(1)}$	...	$x_{N,1}^{(R)}$	...	$x_{N,T}^{(1)}$	...	$x_{N,T}^{(R)}$

The above table shows the principle structure of the data in the form of expression values. We consider  $N$  cell products (genes, proteins, peptides or metabolites) measured at time points  $s_1, \dots, s_T$  with  $R$  replicates. We assume that behaviour of the measured values of a single cell product  $n$  can be described by some parametric function  $f_n(t; c_n)$ .  $c_n$  denotes a parameter vector that determines the function. For reasons of simplicity, we usually choose a low degree polynomial for  $f_n(t; c_n)$ . We assume that for each replicate there might be a time shift and a different speed for the process. Therefore, we would expect  $x_{n,t}^{(r)} \approx f_n(a_r t + b_r; c_n)$  where  $a_r$  is for the correction of the different speeds of the metabolisms and  $b_r$  for the compensation of the time shift. In order to determine the parameters  $a_r$  and  $b_r$  and the parameter vectors  $c_n$ , we minimise the error function  $E = \sum_{r=1}^R \sum_{n=1}^N \sum_{t=1}^T \delta \left( f_n(a_r s_t + b_r; c_n) - x_{n,t}^{(r)} \right)$  where  $\delta$  is a suitable error measure. The classical least squares approach would use  $\delta(e) = e^2$ . But robust regression (see for instance [1]) provides alternatives that can better cope with outliers.

**Parameter Estimation** The nonlinear minimisation problem posed by the above error function to estimate the parameters is carried out in the following way:

- The parameter sets  $c_n$  and  $(a_r, b_r)$  are adapted alternately.
- For the initialisation we choose  $a_r = 1$  and  $b_r = 0$ .
- The parameter vectors  $c_n$  can be updated independently. If the functions  $f_n$  are polynomials, the  $c_n$  can be calculated in the usual way (least squares regression or robust regression, respectively).
- The  $(a_r, b_r)$  can also be updated independently. However, here a strategy for nonlinear optimisation must be applied, but each time only for a problem with two variables.

The results of this regression problem are then used to detect outliers, to identify cell products with similar behaviour and to match them to signalling networks and pathways.

**Practical Aspects** The algorithm has been implemented in R, offering least squares regression and robust regression based on Huber's loss function and Tukey's biweight. For the estimation of the shift and scale parameters  $a_r$  and  $b_r$ , not all cell products should be used, but only those where it is known that an observable effect is expected, i.e. those ones that are known to be involved in the process stimulated in the experiment. Otherwise, cell products with random fluctuations that are not involved in the process of interest could cause difficulties for the estimation. Then the parameter vectors  $c_n$  of the functions  $f_n(t; c_n)$  for the cell products that have not been considered can be estimated assuming the shift and scale parameters  $a_r$  and  $b_r$  to be fixed. The advantage of robust regression is that it yields weights, so that low weights are an indicator for cell products that might not be involved in the process of interest, since they do not show a coherent behaviour.

[1] P.J. Huber. *Robust Statistics*. Wiley, New York, 2004.

# MORESPACE: DEVELOPMENT OF A DATA INDEPENDENT MODEL STRUCTURE

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**Summary:** The Institute for Analysis and Scientific Computing was intended to create a model to simulate the lecture room reservation at the Vienna University of Technology (TU Vienna). This model called MoreSpace is intended to find and test strategies to increase the efficiency of the lecture room booking by enhancing the utilization of lecture rooms on one hand and the utilization of the capacity on the other hand. The first version of the MoreSpace model was realized in the simulation language Enterprise Dynamics (ED). The part that calculates the time students need to change lecture rooms was implemented in the object oriented programming language JAVA. The topic of this paper is the reimplementing of the MoreSpace model in the object oriented programming language JAVA. It sounds easy to re-implement an already existent simulation model by using another programming language. But in this case it is far more than a simple re-implementation. The aim of the project is to create a more generalised tool that can be used for optimization of facility management in general. The same tool should be able to be used at any university, e.g. the Technical University of Vienna but also in other companies as well. The fact that every company and university has different input data to handle is increasing the complexity of the new system. The achieved results of the software should also be stored in a database. This should be made possible by using only one general data structure which is implemented once and used for all future applications. The data structure has the ability to store different input data in one general scheme. This fact guarantees a flexible but tough basement on which the implemented modules are based.

**Essential components of MoreSpace:** MoreSpace consists of two essential components: the scenario and the experiment. The scenario includes all input data which initializes the database. So whenever some input data changes, the whole scenario changes and the database is initialized again with the new input data. To grant the consistency of the stored data, data used by different scenarios will not be overwritten. A scenario contains several user defined experiments, at least one default one. The experiment is used to work with the input data. The user creates an experiment, selects the input data, defines ranges and co-domains and runs the experiment. The results are stored in the database. The setting of the experiment is done using a dynamic graphical user interface that allows a dynamic setting of user – defined parameters. Every result stored in the database and created by an experiment is reproducible by showing the defined parameters and settings. The results of the experiments in one scenario are also comparable because the input data is provided by the scenario. The focus of this new development of this workflow is on the fact, that the data import, the build – up of the graphical user interface, the creation of the parameters and the initialization of MoreSpace are done by opening a new scenario dynamically. This means that the system is setup up by itself without changing a single line of java code. The system operates the same behavior as the principles of the Model-View-Controller (MVC) as explained in [1] concepts. Model objects are the parts of the application that implement the logic for the application's data domain. Views are the components that display the application's User Interface (UI). The User Interface (UI) is created by the model data. Controllers are the components that handle user interaction, work with the model

**Setup the system:** The implementation of a dynamic application like MoreSpace, with a general data structure legal for different input data requires a dynamic interface between data base and user interface. The core of the program, including the data structure, the implementation of the JAVA classes and the JAVA interfaces for the importer of the different data, written in JavaScript are implemented by the programmer. After the programmers work is done, the dynamic custom process of the tool, comprised the import of different data to the uniform data structure is done by an analyst. The analyst does not need to know anything about object oriented programming languages like JAVA, he/she only needs to supply the correct data for the interfaces . This is done by a script called importer, written in JavaScript using and invokes the defined classes written in JAVA. After depositing the JavaScript importer in the directory structure of MoreSpace, launching MoreSpace imports the new data and the User Interface for the new requirements is setup by the tool dynamically.

This project is supported by “ZIT – Die Technologieagentur der Stadt Wien GmbH”.

[1] Miller F., Vandome A., McBrewster J.: *Model-View-Controller*. VDM Publishing House Ltd., 2010

# MOTION PLANNING OF FORMATIONS OF MOBILE ROBOTS USING RAPIDLY EXPLORING RANDOM TREES AND MODEL PREDICTIVE CONTROL

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**Abstract.** In the paper, a novel method for planning and navigation for formations of mobile robots is proposed. The method relies on Model predictive control (MPC) approach, which is used to plan optimal trajectories over a given time horizon. However, the optimization step in the MPC is time consuming, which disallows to use the method on robots equipped with slow computer. We propose a system for fast trajectory initialization using the Rapidly Exploring Random Trees (RRT) method. The RRT quickly finds a feasible (but non-optimal) solution, which is then passed to the MPC solver. The proposed system has been experimentally verified in simulation and the results show, that it significantly speeds up the planning of the formation movements.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**



## NUMERICAL MODELING OF CROWN FOREST FIRE INITIATION

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**Abstract.** The theoretical investigation of the problems of forest fire initiation was carried out in this paper. Mathematical model of forest fire was based on an analysis of experimental data and using concept and methods from reactive media mechanics. The research was based on numerical solution of three dimensional Reynolds equations. The boundary-value problem is solved numerically using the method of splitting according to physical processes. A discrete analog for the system of equations was obtained by means of the control volume method. The developed numerical model of forest fire initiation and spreading would make it possible to obtain a detailed picture of the variation in the velocity, temperature and chemical species concentration fields with time.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

## ON SOME DISCRETE EQUATIONS IN A HALF-SPACE

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**Introduction.** We consider discrete operator generated by Calderon-Zygmund kernel  $K(x)$ , with is defined for functions of discrete variable  $u_h(\tilde{x})$ ,  $\tilde{x} \in \mathbf{Z}_h^m$ , where  $\mathbf{Z}_h^m$  is integer lattice (modulo  $h$ ) in  $\mathbf{R}^m$ , and corresponding equation

$$au_h(\tilde{x}) + \sum_{\tilde{y} \in \mathbf{Z}_{h,+}^m} K(\tilde{x} - \tilde{y})u_h(\tilde{y})h^m = v_h(\tilde{x}), \quad \tilde{x} \in \mathbf{Z}_{h,+}^m, \quad (1)$$

in the discrete half-space  $\mathbf{Z}_{h,+}^m = \{\tilde{x} \in \mathbf{Z}_h^m : \tilde{x}_m > 0\}$ ,  $u_h, v_h \in L_2(\mathbf{Z}_{h,+}^m) \equiv l_h^2$ .

By definition we let  $K(0) = 0$ , and the symbol of operator

$$u_h(\tilde{x}) \mapsto au(\tilde{x}) + \sum_{\tilde{y} \in \mathbf{Z}_h^m} K(\tilde{x} - \tilde{y})u_h(\tilde{y})h^m, \quad \tilde{x} \in \mathbf{Z}_h^m,$$

is periodic function

$$\sigma_h(\xi) = a + \sum_{\tilde{x} \in \mathbf{Z}_h^m} e^{-i\xi\tilde{x}} K(\tilde{x})h^m \quad (2)$$

with basic cube period  $[-\pi h^{-1}; \pi h^{-1}]^m$ .

The sum in (2) is defined as a limit of partial sums for cubes  $Q_N$

$$\lim_{N \rightarrow \infty} \sum_{\tilde{x} \in Q_N} e^{i\xi\tilde{x}} K(\tilde{x})h^m,$$

$$Q_N = \left\{ \tilde{x} \in \mathbf{Z}_h^m : |\tilde{x}| \leq N, |\tilde{x}| = \max_{1 \leq k \leq m} |\tilde{x}_k| \right\}.$$

Remind the symbol of classical Calderon-Zygmund operator [1] is defined by Fourier transform of the kernel  $K(x)$  in principal value sense

$$\sigma(\xi) = \lim_{\substack{N \rightarrow \infty \\ \varepsilon \rightarrow 0}} \int_{\varepsilon < |x| < N} K(x)e^{i\xi x} dx.$$

It's shown earlier [2] the images of  $\sigma(\xi)$  and  $\sigma_h(\xi)$  are the same, and this fact permits to study such equations in a half-space.

**Basic Conclusion.** The continual analogue of the equation (1) is the equation

$$au(x) + \int_{\mathbf{R}_+^m} K(x-y)u(y)dy = v(x), \quad x \in \mathbf{R}_+^m, \quad (3)$$

in the space  $L_2(\mathbf{R}_+^m)$ .

The topological index for such problem is defined roughly speaking by the variation of argument for the function  $\sigma(\cdot, \xi_m)$ , when  $\xi_m$  is varying from  $-\infty$  to  $+\infty$ . It doesn't depend on  $\xi' (m \geq 3)$ . The same holds for the discrete equation (1) also, and its solvability is determined by the variation of argument of  $\sigma(\cdot, \xi_m)$  under varying  $\xi_m$  on the segment  $[-\pi h^{-1}, \pi h^{-1}]$ . Key point is to obtain the following limit relation

$$\lim_{h \rightarrow 0} \int_{-\pi h^{-1}}^{\pi h^{-1}} d \arg \sigma_h(\cdot, t) = \int_{-\infty}^{+\infty} d \arg \sigma(\cdot, t). \quad (4)$$

The validity of (4) leads immediately to conclusion on solvability (or non-solvability) both the equation (1) and (3). One can assert that (4) holds at least for continuous symbol  $\sigma(\xi)$  on sphere  $S^{m-1}$  and transmission condition  $\sigma(0; +1) = \sigma(0; -1)$ .

[1] Mikhlín S. G., Prössdorf S.: *Singular Integral Operators*. Akademie-Verlag, Berlin, 1986.

[2] Vasilyev V. B.: *Elliptic Equations and Boundary Value Problems in Non-Smooth Domains*. Operator Theory: Advances and Applications, 213 (2011), 105–121.

# ON STABILITY ANALYSIS OF SWITCHED CIRCULANT SYSTEMS

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**Introduction.** There has been a particular attention for circulant systems during the past years. Indeed, these systems exhibit particular mathematical structures that can be found in some engineering applications.

On the other hand there has been a growing interest in the stability analysis of switched and hybrid systems. See e.g., [3] and the references therein.

In this paper we consider a particular class of switched systems, that is a switched linear system where each subsystem is a circulant system. We study then the stability analysis of switched circulant systems. To our knowledge, the only work that addresses the stability of switched circulant systems is the work of [2].

The work in this paper is different from the one in [2] since we derive some necessary and sufficient conditions for the stability of switched circulant systems, particularly by using the matrix pencil calculation. Moreover, in this paper, we also give necessary and sufficient conditions for the stabilizability of switched circulant systems when one of the subsystem is not stable.

**Definitions and Preliminaries.** Definition 1. [1] A  $n \times n$  matrix  $A$  is said to be circulant if it is specified by one vector  $v = [a_1 a_2 \dots a_n]^T$ , which is rotated one element to the right for the next row vectors, as follows:

$$A = \text{circ}\{a_1, a_2, \dots, a_n\} = \begin{bmatrix} a_1 & a_2 & a_3 & \dots & a_n \\ a_n & a_1 & a_2 & \dots & a_{n-1} \\ a_{n-1} & a_n & a_1 & \dots & a_{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_2 & a_3 & a_4 & \dots & a_1 \end{bmatrix} \quad (1)$$

Definition 2. The linear system  $\dot{x}(t) = Ax(t)$ ,  $x(t_0) = x_0$  is said to be a circulant system if  $A = \text{circ}\{a_1, a_2, \dots, a_n\}$ , where  $x(t) = [x_1 x_2 \dots x_n]^T \in \mathbb{R}^n$  is the vector of state variables.

Definition 3. The linear system  $\dot{x}(t) = A_\sigma x(t) = A_i x(t)$ ,  $t \in \mathbb{R}^+$ ,  $i \in \mathcal{S}$  is called switched circulant system if the switching signal  $\sigma$  takes value on the index set  $\mathcal{S}$  and  $\{A_i : i \in \mathcal{S}\}$  is a parametrized compact family of  $x \times n$  circulant matrices.

**Stability Analysis.** One tool to study the stability of a switched system is to find a common quadratic Lyapunov function (CQLF). The conditions for the existence of a CQLF is given as linear matrix inequalities (LMIs). Finding a common quadratic Lyapunov function is not straightforward. Some results dealing with the existence of a CQLF use the notion of matrix pencil. The matrix pencil is defined as follows. Given two matrices  $A_1$  and  $A_2$ , the matrix pencil  $\gamma_\alpha(A_1, A_2)$  is defined as the one-parameter family of matrices  $\gamma_\alpha(A_1, A_2) = \alpha A_1 + (1 - \alpha)A_2$ ,  $\alpha \in [0, 1]$ . The matrix pencil  $\gamma_\alpha(A_1, A_2)$  is said to be Hurwitz if its eigenvalues are in the open left half plane for all  $0 \leq \alpha \leq 1$ .

Theorem 1. Let  $A_1, A_2$  be two Hurwitz circulant matrices in  $\mathbb{R}^{2 \times 2}$ . Then there always exists a CQLF for the switched systems with  $A_1, A_2$  as the 2 subsystems.

Theorem 2. Let  $A_1, A_2$  be two Hurwitz matrices in  $\mathbb{R}^{3 \times 3}$ . Then there always exists a CQLF for the switched circulant system.

If we consider now a particular class of switch circulant systems, where not all the subsystem matrices  $A_i, i \in \mathcal{S}$  are Hurwitz. In that case we study the stabilizability of such class of switched systems.

Theorem 3. Consider a switched circulant system that contains two circulant subsystems,  $\dot{x}(t) = A_i x(t), i = 1, 2$ . If matrices  $A_1$  and  $A_2$  are both unstable, then the switched circulant system is not quadratically stabilizable.

## References.

- [1] Davis, P.J.: Circulant Matrices, New York: John Wiley and Sons, 1994.
- [2] Li, J.H.: Zhao, S.Z., Zhao, J., and Li, Y.P. Stability analysis for circulant systems and switched circulant systems, Proc. of the 43rd IEEE Conference on Decision and Control, 2004, pp. 2805-2809.
- [3] Liberzon, D.: Switching in Systems and Control, Boston: Birkhauser, 2003.

# PARALLEL SIMULATION OF MATHEMATICAL MODELS BY PIPELINE INSTRUCTIONS

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**Introduction.** The power of simulation is that a uniform model execution technique can be used to solve a large variety of systems. A precision of the system modeling with a hybrid approach using both closed-form methods and simulation on the parallel computer systems. Realize simulation difficult mathematical model yourself requires power calculating.

**Preface.** By the simulation good many times repeat in definite period is this demand need has yet expressive. Fulfill mentioned demand be possible by using parallel calculations, this allow today computers. Necessary be suggested mathematical models some that effectively ran on them. Dominating oneself the condition decomposition mathematical model in shape, who be in useful to distributed calculations.

**Mathematical Models and Distributed computing.** In analytical designing of a mathematical models the criterion for control is functional of phase coordinates of the subject  $x_i$  and necessary controls  $u_j$ . Analytical design we are based on differential equations of the type [1]:

$$\dot{x}_i + f_i(x_1, \dots, x_n, t) = \sum_{j=1}^n \varphi_{ij}(x_1, \dots, x_n, t) u_j, \quad (i = 1, 2, \dots, n), \quad (1)$$

defining the functional, where  $f_i$  is the function describing the object,  $\varphi_{ij}$  is the object characteristics..

**Pipelined instruction processing.** The most straightforward method uses a *single pipeline* for all expect floating point (FP) instructions. This variant is often designed as the *master instruction pipeline*, which were the forerunners of pipelined instruction processing, such IBM 801, RISC I, RISC II, MIPS, did not support FP instructions at all. Early RISC pipelines were often built from two or three stages. However, the standard solution has 4-5 pipelines stages. An FP coprocessor (i286, i386) or a pipelined unit (i486, Pentium) has often been added to this master pipeline [2]. A decoded instruction will be sent either to the master pipeline or to the FP pipeline depending on the instruction type. *Both pipelines* operate in parallel, but the FP pipeline has to be synchronized, with the master pipeline. The third approach assumes multiple dedicated pipelines and using *recording* to preserve sequential consistency of writing back the results into a register file or memory, next figure.

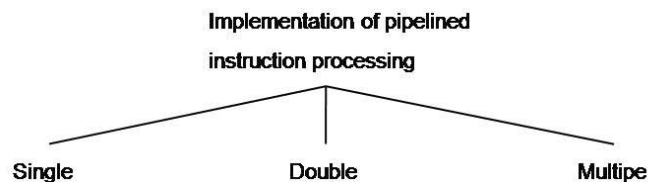


Figure 1 Main approach to implementation of pipeline instruction.

**Parallel Simulation of Mathematical Models.** The operation multiplying uses architecture of the multicore processor. In the first time step the multiplying mathematical model executes  $A_{11} * x_1$  in F stage, in the second time step the multiplying mathematical model executes  $A_{11} * x_1$  in D<sub>1</sub> stage and  $A_{12} * x_2$  in F stage, in the third time step the multiplying mathematical model executes  $A_{11} * x_1$  in D<sub>2</sub> stage and  $A_{12} * x_2$  in D<sub>1</sub> stage and  $A_{13} * x_3$  in F stage, etc..

**Submission.** The original mathematical model is implemented by programming language and is suitable to be simulated in case it does not take a long time. Efficient calculation  $T_p(t)$  is directed from serial processing  $T_s(t)$ . If the time simulation spent on mathematical model is longer then it is necessary to calculate a mathematical model by means of distributed calculation. From numeric results erase effective of results parallel calculation  $T_p(t)$  opposite series calculation  $T_s(t)$ . The  $S(t)$  speedup factor demonstrates the short simulation time in our applications.

- [1] Krasovskij, A., A.: *Sistemy avtomaticheskogo upravlenja poletom i ich analiticheskogo konstruirovanie*. Nauka, Moskva 1980, pp. 589.
- [2] Sima, D., Fountain, T., Kacsuk, P.: *Advanced Computer Architecture a Design Space Approach*. Addison-Wesley, Harlow, England, 1997.
- [3] Zeigler, B., P., Praehofer, H., Kim, T., G.: *Theory of Modeling an Simulation*. Second Edition, Academic Press, San Diego, USA, 2000.

## PEPTIDE POTENTIAL ENERGY SURFACES AND FOLDING

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**Abstract.** The report outlines the utility of a 3D->1D transformation of peptide conformation, which leads to a linearized notation of protein secondary/tertiary structures that may be used for objective description of protein folding. Method is intended to be descriptive and not predictive. It is established from first principles that the idealized 2D-EPSI-PHI map must have nine minima. It is obvious to ask whether all nine conformations are actually occurring in proteins. The objective is to repeat a previous analysis of 258 proteins determined using program ECEPP2, with improved ECEPP2 + polarization. An analysis is performed on 258 proteins with known X-ray structure. Proteins contain 56 495 amino-acids (AAs) with well-defined PHI/EPSI angles. Minima are identified with aid of ECEPP2 minima of Ac-Ala-NHMe with PHI/EPSI +/-40 degrees tolerance. ECEPP2 is improved with inclusion of interacting induced-dipole polarization model, SIMPLEX-MS-3 geometry optimization and calculation of dipole moment from point distribution of net charges. The analysis of 258 proteins determined using ECEPP2 is repeated with the improved ECEPP2 + polarization.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

# POSE TRACKING USING INERTIAL SENSORS AND RECEIVED SIGNAL-STRENGTH INDEX

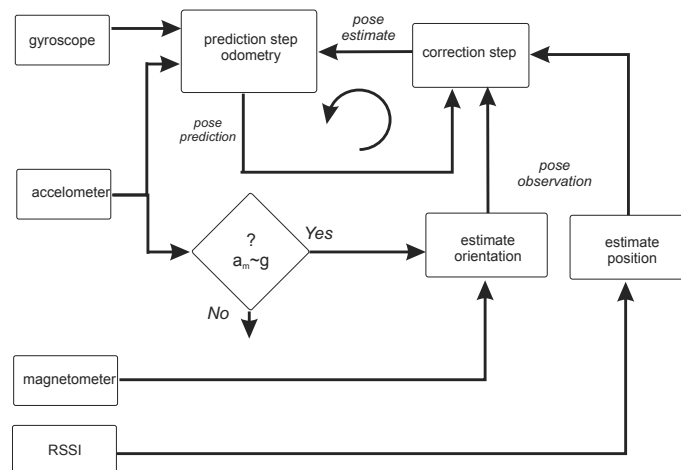
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Inertial navigation systems have received considerable attention in recent years. There have been a number of successful reports such as strapdown inertial navigation systems [1], use of inertial sensors and camera for SLAM [2], positioning using RSSI values [3] and many others.

Indoor localization usually cannot rely on global positioning system (GPS), therefore a combination of alternative localization algorithms based on inertial navigation system (INS) and received signal-strength index (RSSI) fingerprinting is proposed in this paper. To estimate position and orientation a dead reckoning of tri-axis gyroscope and accelerometer sensors are applied. To suppress the growth of position and orientation error due to dead reckoning a tri-axis magnetometer and RSSI measurements are used. These measurements are fused in the extended Kalman filter (EKF) to achieve final pose estimate. To develop and test the pose estimation algorithm a simulator is developed where all sensors are modelled and EKF structure is included. Obtained final pose estimation algorithm is then applied to a low-cost hardware prototype unit.

The orientation estimate is obtained from the direction vectors from the accelerometer and the magnetometer. From these two vectors the orientation of the unit in the world coordinates is estimated and used in the correction step of EKF. Position is estimated from RSSI measurement and fingerprinting on linear regression. Prediction step and correction step for orientation is performed with 1ms time step while the correction step for position is performed with 1s time step. Obtained localization algorithm is validated on real measurements. The indoor environment



EKF based pose tracking system.

is scanned using a mobile robot to obtain map and database for RSSI fingerprinting which is correlated with the environment map. Then the estimated pose using the proposed algorithm is compared to the pose obtained by the already existing robot localization system. The obtained simulation results confirm suitability of the presented localization approach where classic EKF structure is used to integrate information from inertial and absolute information sensors such as magnetometer and RSSI. The results obtained from real sensors are less accurate for estimating position. Accelerometer does not give reliable information, due to high level of noise, insensitivity to low accelerations, virtual acceleration due to unprecise gravity acceleration. Also accuracy and frequency of RSSI measurements should be improved using better RSSI modules. Additionally nonlinear models for estimating position from RSSI models and inclusion of the environment model to consider reflections and weaknesses due to the walls and the like need to be investigated.

- [1] Foxlin E.: *Pedestrian Tracking with Shoe-Mounted Inertial Sensors*. Computer Graphics and Applications 25(6) (2005), 36–46.
- [2] Servant F., Houlier P. and Marchand E.: *Improving monocular plane-based SLAM with inertial measures*. In: International Conference on Intelligent Robots and Systems - IROS 2010, Taipei, 2010, 1986, 3810–3815.
- [3] Mazuelas S., Bahillo A., Lorenzo R.M., Fernandez P., Lago F.A., Garcia E., Blas J. and Abril E.J.: *Robust Indoor Positioning Provided by Real-Time RSSI Values in Unmodified WLAN Networks*. IEEE Journal of selected topics in signal processing, 3(5) (2009), 821–831.

## QUALITATIVE ANALYSIS OF A CHOLERA-BACTERIOPHAGE MODEL

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**Abstract.** Cholera still remains as a severe global threat and is currently spreading in Africa and other parts of the world. The role of lytic bacteriophage as an intervention of cholera outbreaks is investigated using a mathematical model. Dynamics of cholera is discussed on basis of the basic reproduction number. Conditions of Hopf bifurcation are also derived for a positive net growth rate of *Vibrio Cholerae*. Stability analysis and numerical simulations suggest that bacteriophage may contribute to lessening the severity of cholera epidemics by reducing the number of *Vibrio cholerae* in the environment. Hence with the presence of phage virus, cholera is self-limiting in nature. By using phage as a biological control agent in endemic areas, one may also influence the temporal dynamics of cholera epidemics while reducing the excessive use of chemicals. We also performed stochastic analysis which suggests that the model system is globally asymptotically stable in probability when the strengths of white noise are less than some specific quantities.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

## RUNGE-KUTTA BASED PARALLEL COMPUTATIONS

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An important part of contemporary characteristic problems in science and technology is based on simulating and analysing complex systems such as economical models, weather forecast models or technology process control.

Solving most of those problems leads to complex set of linear and non-linear differential and partial differential equations with time changing parameters and large sets of algebraic and transcendental equations. For solving such problems with great emphasis on high accuracy or high speed we need high-performance computer platforms.

The processor's clock frequency is slowly reaching its physical limits. The increase of performance is now possible only by including multiple parallel computing units. This approach is supported by form of some problems. It appears that contemporary sequential methods of solving some problems is not natural.

Even though the idea of parallel computing and parallel connection of high amount of microprocessors is attractive, it is not easy to reach big increase in performance compared to single processor approach. The potential of parallel data processing has already been studied. It was found, that even a small percentage of sequential steps may lead to high reduction of performance of the entire system. This is the consequence of the fact, that most algorithms were not developed for heavy parallel systems.

This paper concentrates on large systems of parallel microprocessors. The idea of this approach comes from analogue methods of computations. Analogue methods are basically parallel methods and their analysing shows that independent parallel cooperation of multiple processors may be implemented by applying differential calculus. Using analogue methods, independent parallel cooperation of microprocessors is going to be effective if each microprocessor is going to be numerically integrating.

The algorithms of parallel cooperation of microprocessors can be derived from one step of numerical solutions. This parallel cooperation of independent microprocessors may be completed using arbitrary chosen numerical integration formula including Euler's method, 2nd, 3rd and 4th order Runge-Kutta method, Adams-Bashforth method etc. As we will present, the system of parallel microprocessors which uses Euler's integration method is going to be relatively fast, but the precision of output is going to be low. Higher precision result can be obtained by applying 2nd Runge-Kutta method to each microprocessor. The accuracy can be increased by increasing the order using 3rd and 4th order Runge-Kutta integration method.

The principal objective of the paper is to provide an idea of Runge-Kutta based parallel computations and the idea of a mathematical background for the practical research in the field of numerical solutions of systems of differential equations. This particularly concerns the problem of transforming a system of differential equations into a new system with polynomials on the right-hand sides. Other results of the paper might also be used by teachers in differential equation courses to find methods of solving in special cases due to the compact form of expressing the problems.



## SIMULATION APPROACH OF CONTAINER TERMINAL MODELLING

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In this paper we have presented an approach that combines the advantages of simulation models and an optimization method related to total cost calculation of an optimal throughput. We have shown that our method is able to generate competitive optimal throughput of CT should be the planning objective since it gives more economical solutions. Computational experiments were conducted to evaluate the performance of the developed models using real data collected from the Korean CTs.

Simulation modelling techniques are being applied to a wide range of container terminal (CT) planning processes and operational analysis of container handling systems. Simulation model (SM) and analysis with ARENA have been developed to CT performance evaluation of Korean CTs. It is shown to provide better results in predicting the actual terminal operations system of the Korean CT. The organization of this paper is as follows. Section 2 provides a literature overview. Section 3 presents a brief description of CT modelling procedure and evaluation of SMs. Also, this section gives model validation and simulation results for selected Korean CT. In Section 4 we show cost analysis of optimal CT throughput with case study of KBCT (Korean Busan CT). Finally, Section 5 concludes the paper.

In Section 2, it is attempted to collect all the papers which are within the criteria of the collection across journals of all including ARENA softer (e.g. Guldogan [1], Wanke [2], among other). Computer algorithms are described in most of the papers to give examples how the SMs are built from sequence of operational procedures which have been conducted to the determination of the CT performance in different environment within various points of view and in heterogeneous cases.

The objective of Section 3 is to develop SMs to analyze the CT performance. This analysis includes the integration of container berth and container yard (CY) simulation planning within CT. Combined planning approaches for different decision levels are expressed here. Implementation of the presented procedure leads to the creation of a simulation algorithm that captures CT performance well. Further, we have carried out the extensive numerical work for the high/low values of the Korean CTs model characteristics. Our numerical experiments are based on different parameters of various Korean CTs. The results obtained using SM with corresponding values of real parameters has also been used for CT performance evaluation. In case of KBCT, current occupancy ratio is estimated to be 50%. However, this is not an appropriate result. As well as CTs consist of four and more berths, the occupancy ratio would increase up to 65% within permissible ship's waiting ratio. The validation of the SM was done by generating CT appropriate capacity and performance from the model at a certain berth throughput level and making comparisons with actual statistics of real CTs parameters.

The Section 4 has tried to analyze the problems originating from ship's waiting and backlogged cargo by means of KBCT. In case that there is any difficult item in analyzing this CT, we have tried to adopt the cases common to many other terminals. The important criteria of this analysis, i.e. the criteria of optimal throughput of a CT, are based on the outputs derived from the SM developed in the Section 3 and results explained in subsection 3.1. The cost increase caused by ship waiting and backlog brings heavy burden not only on the shipping companies and customers, but also on the society. In the case of KBCT, its optimal throughput has been calculated to be from 485,361 to 565,753 TEU as a result of the SM [3].

A simulation approach is explained here, combines the advantages of SMs and an optimization based on relationship between improvement of service facilities and ship's waiting costs. Our contribution is twofold: SMs development and analysis of the integration of container berth and yard simulation planning within CT, and an iterative combination of SM and a method for estimating the optimal throughput per berth or terminal, as well as determining the handling capacity of CY. As a result of our research, it has been found out that KBCT optimal throughput and maximum profit are realized when the waiting ratio of ships is from 3% to 5%.

- [1] Guldogan, E.U: *Simulation-based analysis for hierarchical storage assignment policies in a container terminal*. Simulation, 87(6), 2010, 523–537.
- [2] Wanke, F.P: *Ship-berth link simulation: impact on total demurrage costs*. International Journal of Shipping and Transport Logistics, 3(3), 2011, 261–294.
- [3] Park, N-K., Seo, C-G., Choi, H-R., Dragović, B., Chen, T., Radmilović, Z., Lee, Y-C., Lim, S-Y., Cho, K-S., Lee, J-Y: *Port logistics systems*, TongMyong University, Busan, Korea, in Korean, 2006.

# SIMULATION OF THREE-DIMENSIONAL MOTION OF SMALL AUTONOMOUS UNDERWATER VEHICLE

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**Introduction.** Autonomous Underwater Vehicles (AUV) are torpedo shaped apparatus operating with no physical link with the surface. Carrying a set of relevant sensors they are powerful tool for underwater data gathering. A proposed motion control system is applied to the track-keeping control of an training AUV called “Sea Anemone”, designed and built for the Polish Navy.

**Equations of motion.** The nonlinear dynamical equations of motion of the AUV are given as follows:

$$\mathbf{M}\dot{\mathbf{v}} + \mathbf{C}(\mathbf{v})\mathbf{v} + \mathbf{D}(\mathbf{v})\mathbf{v} + \mathbf{g}(\boldsymbol{\eta}) = \boldsymbol{\tau} \quad (1)$$

where:  $\mathbf{M}$  – inertia matrix,  $\mathbf{C}(\mathbf{v})$  – Coriolis and centripetal terms matrix,  $\mathbf{D}(\mathbf{v})$  – hydrodynamic damping and lift matrix,  $\mathbf{g}(\boldsymbol{\eta})$  – gravitational forces and moments vector,  $\mathbf{v}$  – linear and angular velocity vector in the body-fixed frame,  $\boldsymbol{\eta}$  – position and orientation vector in the inertial frame,  $\boldsymbol{\tau}$  – control inputs (forces and moments) vector.

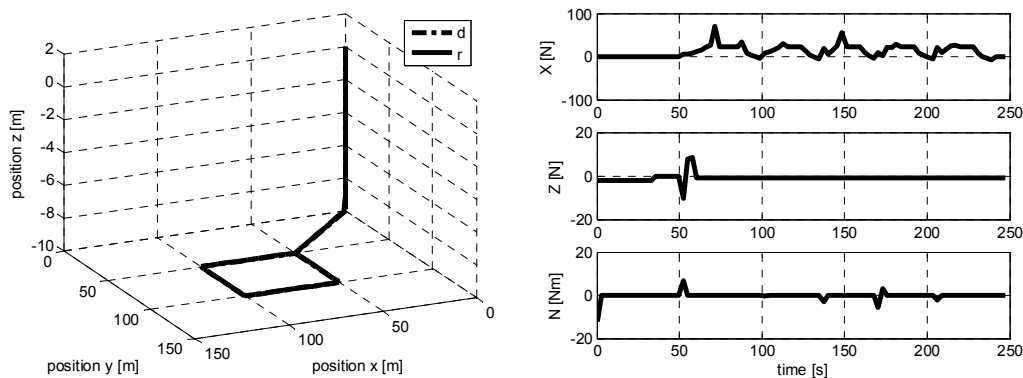
**Adaptive control law.** There are parametric uncertainties in the model (1), and certain parameters are generally unknown. Hence, parameter estimation was necessary in case of using of the model reference adaptive control to track-keeping. A control algorithm with the parameter adaptation law was implemented in an autopilot, consisting of three controllers, responsible for movement along longitudinal and transversal axes, and about a normal axis. The algorithm was worked out basis on a simplified AUV model:

$$\mathbf{M}_d \dot{\mathbf{v}} + \mathbf{D}_d(\mathbf{v})\mathbf{v} = \boldsymbol{\tau} \quad (2)$$

where all kinematics and dynamics cross-coupling terms are neglected. Here  $\mathbf{M}_d$  and  $\mathbf{D}_d(\mathbf{v})$  are diagonal matrices with the diagonal elements of the inertia and damping matrices, consequently. Uncertainties in model (2) are compensated in the designed control system.

**Simulation study.** To validate a performance of the proposed adaptive control law some numerical simulations in the MATLAB/Simulink environment have been conducted by using a nonlinear model (1) of the training underwater vehicle .

Selected results of track-keeping control: desired (d) and realized (r) trajectories in the underwater space (left plot) and command inputs (right plot) are presented below.



**Conclusions.** Simulation results show that the proposed autopilot with adaptive control law implemented assures a good tracking performance. An additional advantage of proposed approach is its usefulness to practical applications due numerical simplicity of the control algorithm.

Research is continuing in a field of tuning of the autopilot’s parameters in relation to the vehicle’s dynamics and testing ability of the applied adaptive control law to compensation of environmental disturbances.

- [1] Fossen T.I.: *Marine Control Systems*. Marine Cybernetics AS, 2002.
- [2] Lantos, B., and Muton, L.: *Nonlinear Control of Vehicles and Robots*. Springer, London, 2011
- [3] Spong, M.W., and Vidyasagar, M.: *Robot Dynamics and Control*. Wiley, Chichester, 1989.

## SIMULATION, STABILITY AND BLOW-UP OF A NON-LINEAR HEAT PROCESS

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**Introduction.** We consider a one-dimensional heat process with exponential internal heat source described by a second order, non-linear, parabolic partial differential equation. The model can describe various physical processes from electric space charge problem, diffusion-reaction processes, some nuclear process or explosion. It has also appeared in the theory of forming Nebulae (interstellar gas and dust). Due to the exponential heat source, stability of the process is an essential question. We investigate under which conditions (i.e. boundary conditions, parameters etc.) the process remains stable and provide the stability region for different boundary conditions. An other important question concerns what happens if the source gain exceeds the stability limit. Then, inevitably, a blow-up happens, that is, given sufficient time, the temperature will grow unbounded. If this happens, then it is of prime importance to estimate the time within blow-up happens. Although the non-linear partial differential equations has no solution in closed form, we provide a reasonable estimate for the blow-up time. Computer simulations verified that the analytic expression provides a good estimate.

**Stability.** We consider the following second order, parabolic non-linear partial differential equation (PDE) in dimensionless form with Robin boundary conditions [1]:

$$\frac{\partial T(\tau, z)}{\partial \tau} = \frac{\partial^2 T(\tau, z)}{\partial z^2} + B e^{T(\tau, z)} \quad \text{in } (0,1) \times (0, \infty)$$

$$\left\{ \begin{array}{l} \frac{\partial T(\tau, 0)}{\partial z} = 0 \\ \frac{\partial T(\tau, 1)}{\partial z} = -\alpha_1^* (T(\tau, 1) - T_a(\tau)) \end{array} \right. \quad \text{in } (0, \infty)$$

where  $T(\tau, z)$  denotes temperature distribution,  $\tau$  is time,  $z$  denotes space coordinate  $z \in [0, 1]$ ,  $B$  denotes the source gain,  $\alpha_1^*$  is the dimensionless heat transfer coefficient and  $T_a$  is the ambient temperature. Since heat generation depends exponentially on the temperature itself, there exist a critical value of  $B$ , beyond which no steady-state solution exists. We define the critical gain  $B_c$  as the largest gain possible still having a stable transient. To investigate the stability of the process it suffices to study the steady-state solution [3]. The critical value of  $B_c$  can then be found for different boundary conditions. In case of Dirichlet B.C.'s an analytic expression has been developed for the critical value of  $B_c$ . For symmetric geometry the method of envelopes has also been developed. In case of Robin b.c.'s, we can define a set of functions which determines the critical value of  $B_c$ . Contrary to general believe, increasing the heat transfer coefficient ( $\alpha_1^* \rightarrow \infty$ ) may not guarantee stability! It is also interesting to note that for a particular boundary condition and value of  $B$ , there exists two different steady-state solutions of which only one is physically realizable.

**Blow-Up.** An other important question concerns "blow-up". This happens if the actual value of  $B$  is higher than the stability limit ( $B > B_c$ ). This problem arises in investigating explosions. If it happens it means that the transient solution becomes unbounded (grows to infinity) for higher-than-critical source gain [2]. If a blow-up happens, then it is important to know when it is going to happen. Unfortunately the PDE has no closed-form analytic solution. However, based on reasonable assumptions we could develop the following formulae to estimate the blow-up time. This is an important result for it provides a closed-analytic expression to estimate the time until a blow-up happens! To simulate the transient process we used Crank-Nicolson finite difference scheme. Care, however, has to be taken regarding the question of how the exponential term can be best approximated. We applied quasi-linearization proposed by R.Bellman which provides fast convergence. We shall detail the numerical method and present typical transients for stable- and unstable parameter value of  $B$ . The results of numerical simulations of unstable processes ( $B > B_c$ ) supports the validity and feasibility of approximate formulae to estimate the blow-up time. We also give examples of the temperature profile during blow-up (explosion).

[1] Carslaw H.S. and Jaeger J.C.: *Conduction of Heat in Solids*, Clarendon Press, Oxford, 2nd edition, 2001.

[2] Samarskii A.A., Galaktionov V.A., Kurdyumov S.P., and Mikhailov A.P.: *Blow-up in Problems for Quasilinear Parabolic Equations*. Walter de Gruyter, Berlin, 1995.

[3] Vajta M.: Stability of a 2<sup>nd</sup> Order Nonlinear PDE with Asymmetric Boundary Conditions, *12<sup>th</sup> Mediterranean Conference on Control and Automation*, CD-ROM, June 6-9, 2004, Kusadasi, Turkey, pp.1248-1252.

## THE CHOICE OF MODEL OF EXTERNAL LOAD IN PROBLEM OF SYNTHESIS OF ADEQUATE MATHEMATICAL DESCRIPTION

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**Abstract.** The problem of mathematical simulation of motion of dynamic systems characteristics and their adequacy to real experimental data which correspond to these characteristics is considered in this paper. The specified problem is still poorly investigated and hardly adapted to formalization. The requirements to the adequate mathematical simulation of dynamic system are considered for the case when mathematical description of coupled systems is represented by linear system of the ordinary differential equations. Two approaches exist to problem of construction of adequate mathematical description. One of these is the following: mathematical model of process is given a priori with inexact parameters and then the models of external loads were determined for which the results of simulation coincide with experiment. The methods of obtaining of the steady models are suggested. The examples of the adequate descriptions of dynamic systems are given.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

# USING SYMBOLIC TECHNOLOGY TO DERIVE INVERSE KINEMATIC SOLUTIONS FOR ACTUATOR CONTROL DEVELOPMENT

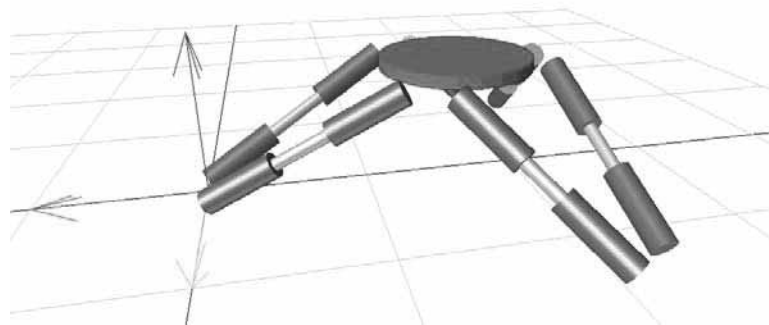
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**Introduction.** In multibody mechanics, the motion analysis for a platform (the kinematics problem) can be classified into two cases: the forward kinematics and the inverse kinematics problems. For the forward kinematics problem, the trajectory of a point on a mechanism (for example, the end effector of a robot arm or the center of a platform support by a parallel link manipulator) is computed as a function of the joint motions. In the inverse kinematics case, the problem is reversed: the goal is to compute the joint motions necessary to achieve a prescribed end effector trajectory.

In general, given the mechanism geometry, it is quite straightforward to solve the forward kinematics problem both numerically and symbolically. In contrast, solving for the inverse kinematic problem typically involves solving a nonlinear system or equation with trigonometric functions. Issues such as singularity, multiple solutions (as in the case of “elbow up” and “elbow down” configurations for a robot arm), and no solution (as in the case in which the specified trajectory goes beyond the workspace of the mechanism) can often come up, further complicating the solution process. The complexity in the inverse kinematics problem is compounded even more for parallel link manipulators.

Because of the complexity involved, the inverse kinematics problem is often solved numerically through iterations, and is computationally expensive. With a numeric approach, however, information about the motion of the mechanism is often lost. In this paper, we will describe how to obtain a symbolic solution to the inverse kinematics problem for two real problems using tools available in MapleSim™. The first, a 2 degrees-of-freedom (DOF) tracking radar gimbal is used to show the principal steps in a relatively simple mechanism. These principles are then demonstrated with a much more complex mechanism: a Stewart-Gough hydraulic platform.



Screenshot of Stewart-Gough platform in MapleSim

Furthermore, we will show how having access to the symbolic Jacobian of the constraint equations allows us to inspect and exploit the underlying matrix structure, which leads to a simplified solution process for obtaining the symbolic solution.

An advantage of having a symbolic solution to the inverse kinematics problem is the possibility of code-generating the symbolic solution so that it can be embedded in real-time hardware-in-the-loop (HIL) applications. This approach can be contrasted with a purely numerical approach where the iterative solution process makes it difficult to use in real-time applications.

- [1] Solving Inverse Kinematic Problems: Tracking-Radar Motion Control. (Online), November 15, 2011.  
[http://www.maplesoft.com/products/maplesim/demo/inverse\\_kinematic\\_gimbal.aspx](http://www.maplesoft.com/products/maplesim/demo/inverse_kinematic_gimbal.aspx).



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**Poster Presentation**





# A COMPARISON OF SYSTEM DYNAMICS AND AGENT-BASED MODELING ON A MODEL OF HEALTH CARE UTILIZATION

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**Introduction.** The choice of an appropriate method for modeling the utilization of health care services is affected by the availability of data and its level of detail. Therefore the question arises whether or not and if so, how the results differ for different methods.

**System Dynamics and Agent-based Modeling.** System dynamics (SD) and agent-based modeling (ABM) are two entirely different approaches to model a system. SD is a top-down modeling method, which means that the system is described from a global perspective, requiring knowledge of the global relations and causalities (see e.g. [2]). ABM on the contrary is a bottom-up approach, where the single acting entities of the system, i.e. the agents, and their behavior are modeled. The global behavior of the system then results from the agents' interactions during simulation. Regarding the simulation of human systems, which are based on individual preferences and decisions, ABM provides a natural description. But it requires individual disaggregated data and soft factors concerning the human psychology for parametrization. Furthermore, depending on the complexity of the system, the simulation can be extremely computation intensive [1]. SD simulation needs less computational power and also the data requirements are often easier to meet. However, it can be a very difficult task to understand and to quantify the causalities needed for the implementation. For comparison a demonstration model of health care utilization is implemented as both an SD and an ABM model with the same parametrization.

**A Model of Health Care Utilization.** The system consists of patients, who can be healthy or sick, and medical providers. To keep the model as simple as possible, only two degrees of severity of the same disease and two corresponding treatments are considered. The patients try to maximize their life quality, which depends on their health state and consequently on the received treatment. The goal of the medical providers is to obtain an optimal mix of achieved income and effectiveness.

Both methods are implemented in AnyLogic, a multi-method simulation modeling tool by XJ Technologies. The agent-based model consists of the agents 'patient' and 'medical provider'. The patient is ruled by two statecharts, one specifying his current health state, the other one depicting his satisfaction with his attending physician, i.e. the medical provider he consults in case of illness. If he is not satisfied, he can change provider in order to achieve a higher life quality. The agent medical provider is able to diagnose the degree of severity (with a certain error rate), to decide on the therapy and to treat a patient. He aims to optimize his performance with respect to his income, the utilization ratio of his working hours, and the effectiveness of his treatments. To attain this goal, he adjusts the criterion, on which his treatment decision is based. In the SD implementation three state variables represent the patients according to their current health state. The medical providers influence the healing rates by prescribing the right therapy. With the help of averaged illness durations and prevalences, a link between the goal of the patients and the resulting behavior of the providers is established. Aggregated income, effective treatments and the influence of the patients then control treatment decisions.

**Results.** First simulation experiments have shown similar behavior of both models with the default parametrization. Also the adaptations of the system to small parameter variations resemble each other. But reactions on drastic changes, like for example a sudden undersupply of medical providers, differ strongly regarding the quantitative outcome, even though the overall trends are the same. Further analyzes and alterations of the models are needed to determine if those differences are inherent in the chosen approach.

**Conclusion.** Both techniques provide the means to describe the dynamics of health care utilization in the specified system. ABM offers the more intuitive approach plus the possibility to easily add or change factors on an individual level, like including effects of distance or social networks on the provider choice (see e.g. [3]). For the implementation of the SD model, the main system components and global feedback mechanisms have to be identified. On the one hand, this requirement helps to gain a better insight into the system on a global level. On the other hand, dynamics due to individual actions or heterogeneities are difficult to describe and to capture.

- [1] E. Bonabeau. *Agent-based modeling: methods and techniques for simulating human systems*. In *Proc. of the National Academy of Sciences of the United States of America*, volume 99 (3), pages 7280–7287, 2002.
- [2] J.W. Forrester. *Industrial dynamics*. M.I.T. Press, Cambridge, Mass., 1961.
- [3] G. Romstorfer, S. Parragh, G. Schneckenreither, M. Landsiedl, P. Einzinger, and M. Scheuringer. *Integration of GIS Data in Health Care Utilization*. In *Tagungsband Abstracts und Fullpapers*. ASIM 2011, 21. Symposium Simulationstechnik, Winterthur, Schweiz, ZHAW School of Engineering, September 2011.

## A CONCEPT TO ENHANCE THE FEEDBACK CAPABILITIES OF MODEL PIPELINES

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Because of the constant growth of the air traffic sector in Germany [1], the Federal Ministry of Education and Research (FMER) commissioned the “efficient airport 2030” cluster of excellence project, to uncover available optimization potential. The goal is to analyze the processes of an airport not supervised by the air traffic control, to discover new insights concerning the streamlining of procedures and expansion of services for the time horizons 2015 and 2030. Therefore, several partners from universities, research organizations and industry have come together to focus their expertise in the fields of logistics, aircraft construction, air traffic management, system development and simulation.

One more specific goal is to analyze the benefits and drawbacks of new technologies developed to face the rapid growth of air activities. In order to do so, the University of Hamburg, the Hamburg University of Technology and the German Aerospace Centre (DLR) are making a collaborative effort to create simulation models of the processes of interest building the chain of events a passenger has to go through to travel from his doorstep to his seat on the airplane. This chain can roughly be partitioned into the following stages: generation of passengers, possible itineraries from their home to the airport itself, passenger movement and luggage handling inside the airport terminal, and finally aircraft movements on the apron. To facilitate the use of already acquired systems knowledge, the project description stipulates that the overall simulation is broken up into individual packages, handled separately by each project partner. Consequently, the implementation of a distributed simulation solution to couple the different models is needed. Considering that the processes are already arranged in a serial fashion, it is noticeable that each model basically only needs the output of the previous model to be able to create a valid input for the next model. Accordingly, Wittmann et al. are suggesting to take advantage of the unidirectional flow of information [2]. Based upon the original idea of pipes for Unix/Linux operating systems, i.e. to use the output of one command as input for the next command, Wittmann et al. proposed to use a model pipeline to couple several models to form a more complex simulation. This pipelining concept is based on the forward oriented dataflow in a model pipeline. Each model gets its data from its predecessor in the line, executes its calculations, and the created output serves as input for the succeeding model in the chain.

One drawback of this basic principle is that feedbacks between models are not taken into account. Yet, in certain scenarios it is indeed a necessity for a model to be able to communicate with a previously executed counterpart, even though the general process structure is forward-oriented. In such cases, Himstedt and Wittmann showed how a feedback functionality can be added, if the computing steps of the overall simulation have a coarse granularity (e.g. a time interval resolution of 1 hour to simulate a day in 24 steps) [3]. To handle feedback situations, the complete simulation chain has to be executed several times, until a complete run has been performed. Because in each rerun, the input is expanded with the outcome of the previous run, the potential impact of a feedback event gets integrated into the rerun. These reruns act as restarting points, which avoids a complex checkpoint management and conserves the black-box character of each model. However, if a single day is subdivided into 24 simulation steps, 24 reruns are required to be able to handle all potential feedback events, even if there are far less actual feedback events produced.

In line with this drawback of the iteratively driven simulation principle [3], this contribution presents a concept to automate the processes involved in the back feeding in model pipelines. The model pipeline prototype is currently handling feedbacks by relying on user specified input. The idea is to improve create a managing entity and allow it to discretely analyze the output of each run, but only in regard of feedback requests, so as to keep the advantages of a generic distributed simulation environment. The rerun of the simulation may then be started automatically, following the instructions of several attributes from the scanned output, in consequence eliminating redundant reruns.

- [1] I.A.T.A., *Strong January Traffic Growth - Oil is the Emerging Worry*, Monthly Traffic Results, 28.02.2011. [http://www.iata.org/pressroom/facts\\_figures/traffic\\_results/Pages/2011-02-28-01.aspx](http://www.iata.org/pressroom/facts_figures/traffic_results/Pages/2011-02-28-01.aspx).
- [2] J. Wittmann, K. Himstedt, D.P.F. Möller, *Ein Pipeliningkonzept zur Modellierung der Passagier und Gepäckbearbeitung am Flughafen*, Simulationstechnik/Simulation Techniques 20. Symposium in Cottbus, Aachen, 2009, S. 404-414.
- [3] K. Himstedt and J. Wittmann, *Modellkopplung und Szenarioanalyse am Beispiel des Projektes ‚Effizienter Flughafen 2030‘*, Simulation in Umwelt- und Geowissenschaften, Aachen, 2010, S. 91-104.

# A CROSS-SCALE MODEL OF TUMOR GROWTH: DO WE NEED TO MODEL MOLECULAR INTERACTIONS IN SEPARATE ARTIFICIAL COMPARTMENTS WITHIN A CELL?<sup>1</sup>

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The glioblastoma (GB) is a common and highly aggressive primary brain tumor with a (still) very poor prognosis for patients. In silico multiscale modeling of tumor growth is a promising area of research that will potentially aid the improvement of existing and the development of new therapeutic strategies in the future.

Here, we modified an existing cross-scale model [1] of avascular tumor growth for GB that establishes a link between the molecular and cellular scale by coupling a gene-protein interaction network with an agent based model. In the original model tumor cells that are further subdivided in 4 artificial compartments are placed on a 2D grid in which each grid point can govern one cell. Each cell is equipped with a network of 14 interacting genes and proteins within each compartment that is represented by a system of 14 nonlinear ordinary differential equations describing the respective concentration changes. Glucose supplied from the environment acts as an input to the system. Depending on the concentrations the cells' phenotypes will be determined as either proliferating, migrating, or quiescent in each time step.

The drawback of this approach is the huge computational effort it implies: Within each artificial compartment the molecular network needs to be updated separately at each time step. To reduce this computational burden we modified the model by renouncing the artificial division of cells on the molecular level.

Originally chemotaxis was modeled through the different concentrations of the protein phospholipase C- $\gamma$  (PLC $\gamma$ ) within the four artificial compartments of a cell. However, in a model that does not use an artificial subdivision of the cells this is not feasible. Since glucose is already included in the model as a nutrient and there is evidence that it also attracts tumor cells we use it as an alternative to decide on the direction of movement.

Now, it is possible to chose between different configurations for the neighborhood from which a cell takes up glucose (using the average of the concentrations on the grid points in the respective neighborhood) and for the neighborhood in which a cell is allowed to move.

In the **compartment based (CB) simulation** cells contain artificial compartments, receive glucose from their von Neumann neighbors, and decide on their direction of movement

setting name	glucose intake source	possible chemotaxis directions
<b>4/4</b>	4 <i>von Neumann</i> neighbors	4 <i>von Neumann</i> neighbors
<b>8/8</b>	8 <i>Moore</i> neighbors	8 <i>Moore</i> neighbors
<b>4/8</b>	4 <i>von Neumann</i> neighbors	8 <i>Moore</i> neighbors

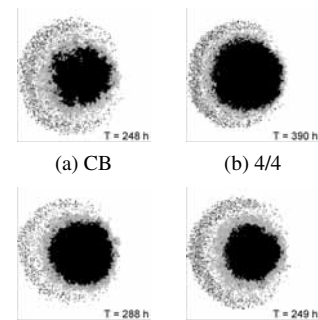
based on the highest PLC $\gamma$  concentrations of all 4 artificial compartments. For the modified model we simulated the settings described in the table.

Results are evaluated by means of images of the spatio-temporal development of the simulated tumors on a cellular scale and quantified according to cell numbers and number of time steps for a simulation to finish.

First, each simulation ran once and generated images showing the spatio-temporal tumor development. The figure allows a comparison between the tumors resulting from the four (CB, 4/4, 8/8 and 4/8) different settings. It shows the tumors in the last time step of each simulation. They exhibit a core of quiescent cells (black) surrounded by a ring of proliferating cells (light grey) and a layer mixed of proliferating and migrating (dark grey) cells. The figure shows that the tumors have a similar shape, but that simulations 4/4 and 8/8 grow more slowly as compared to the CB or 4/8 simulation.

To account for the random character of the model all simulations are also run ten times with different random seeds. On the one hand the so generated data also demonstrated that the tumors in settings 8/8 and, in particular, 4/4 are expanding slower. On the other hand the data show how the computing time is halved in the modified model (computing time for 10 simulation runs could be reduced from 1892 s to 903 s).

Investigating the results one can clearly see that it is possible to simplify the original model and all the same obtain comparable results. With less than half of the computing time the modified 4/8 model is therefore highly favorable.



Tumors are shown when the first cell reaches the boundary

[1] C. Athale, Y. Mansury, and T. S. Deisboeck. Simulating the impacts of a molecular 'decision-process' on cellular phenotype and multicellular patterns in brain tumors. *J. Theor. Biol.*, 233(4):469–481, 2005.

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# A DIFFERENT KIND OF MODELLING: CELLULAR AUTOMATA

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**Introduction.** In a simple case, a cellular automaton consists of a line of cells, each with value 0 or 1. These values are updated in discrete time steps, according to a definite, fixed rule. Denoting the value of a cell at position  $i$  by  $a_i$ , a simple rule gives its new value as  $\tilde{a}_i = \phi(a_{i-1}, a_i, a_{i+1})$ . In general, the cells in a cellular automaton may have any finite number  $k$  of possible values. The rules for updating these cells may depend on values up to any finite distance  $r$  away. In addition, the representation of cellular automaton cells may be arranged not on a line, but on a regular lattice. Cellular automata have a number of basic defining characteristics, see the table below.

Characteristic	Signification
Discrete in space	They consist of a discrete grid of spatial cells.
Discrete in time	The value of each cell is updated in discrete time steps.
Discrete states	Each cell has a finite number of possible values.
Homogeneous	All cells are identical.
Synchronous updating	All cell values are updated in synchrony, each depending on the previous values of neighbouring cells.
Deterministic rule	Each cell value is updated according to a fixed, deterministic rule.
Spatially local rule	The rule at each cell depends only on the values of a local neighbourhood of cells around it.
Temporally local rule	The rule for the new value of a cell depends only on values for a fixed number of preceding steps.

Table: Basic defining characteristics of cellular automata

**Mathematical Definitions.** First, there are some terms, which are important for defining a cellular automaton. The grid  $L$  is a set which is a subset of  $\mathbb{N}$ . The set of the states  $Z$  is the set of all possible states of the cells. In general  $Z$  is a ring with a definite number of real numbers. These possible states are represented by numbers. The value of the cell at position  $i$  and time step  $t$  is denoted by  $a_i^{(t)}$ , with  $a_i^{(t)} \in Z$ . The metric  $d_L$  on  $L$  is defined as  $d_L : L \times L \rightarrow \mathbb{R}$  and  $d_L(x, y) = |x - y|$  for all  $x, y \in L$ . The distance of two cells  $j, k \in L$  is  $d_L(j, k)$ . The neighbourhood with radius (distance)  $r$  of a cell  $j \in L$  is defined as  $E_j^r = \{k \in L : d_L(k, j) \leq r\}$ . An updating rule is any function  $\phi$ , with  $\phi : Z^{2r+1} \rightarrow Z$  and  $\phi$  depends on  $2r + 1$  cells with  $r \in \mathbb{N}$  definite,

$$\phi = \phi \left( a_{i-r}^{(t-1)}, a_{i-r+1}^{(t-1)}, \dots, a_i^{(t-1)}, \dots, a_{i+r-1}^{(t-1)}, a_{i+r}^{(t-1)} \right).$$

With these terms one can define a one-dimensional cellular automaton. A *one-dimensional cellular automaton* consists of a grid of cells. Denote the values of the cells at the beginning with  $a_i^{(0)}$  and  $r$  is a definite constant. The updating of the cells occurs with a definite updating rule  $\phi$ . The updating happens as follows:

$$a_i^{(t)} = \phi \left( a_{i-r}^{(t-1)}, a_{i-r+1}^{(t-1)}, \dots, a_i^{(t-1)}, \dots, a_{i+r-1}^{(t-1)}, a_{i+r}^{(t-1)} \right) \quad \forall t \in \mathbb{N}.$$

**Application Scenarios of Cellular Automata.** There are different application scenarios of cellular automata. There will be mentioned three examples. The first example is the connection of cellular automata and differential equations. There are two different types to create a predator-prey model. On the one hand there is a continuous model, which consists of differential equations (Lotka-Volterra equations), on the other hand there is a discrete model built with a cellular automaton (WATOR). As second example a special type of cellular automata is presented, Lattice Gas Cellular Automata (LGCA). LGCA are a special type of cellular automata, where the updating rule is split into two parts. The third example is that cellular automata have a connection to fractals. Consider a concrete example for a one-dimensional cellular automaton. The values of the cells are elements of  $Z = \mathbb{Z}_2$ . The value of the cell for the next time step is calculated by  $a_i^{(t)} = a_{i-1}^{(t-1)} + a_{i+1}^{(t-1)}$ . The neighbourhood is  $E_j^1 = \{k : |k - j| \leq 1\}$ . At the beginning only one cell has the value 1. The fractal dimension  $D$  of the evolution of this cellular automaton is  $D = \frac{\log 3}{\log 2}$ .

[1] S. Wolfram, *Theory and Applications of Cellular Automata*. World Scientific Publishing Co. Pte. Ltd, 1986.

[2] J. L. Casti, *Reality Rules - Picturing the World in Mathematics: I*. Wiley, New York, 1992.

[3] D. Wolf-Gladrow, *Lattice-Gas Cellular Automata and Lattice Boltzmann Models*. Springer, 2000.

# ARTIFICIAL BOUNDARY CONDITIONS FOR 2D NONLINEAR SCHROEDINGER EQUATION DESCRIBING BOSE-EINSTEIN CONDENSATE

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**Abstract.** In this report we provide the comparison of two types of artificial boundary conditions for 2D nonlinear Schroedinger equation. One of them was developed by us and other was proposed in literature. As it is well-known, the artificial boundary conditions are very important for computer simulation of many problems: laser pulse and beam propagation in nonlinear medium; modelling of BEC; problems of quantum mechanics.

The efficiency of two types of artificial boundary conditions is compared numerically considering the 2D BEC flow interaction with external potential. For this problem we developed conservative finite-difference scheme taking into account the artificial boundary conditions. To realize the conservatism principle we developed new iterative process for the solution of corresponding set of nonlinear difference equations.

**ABSTRACT GENERATED VIA CONFTOOL DATABASE**

# AUTOMATA BASED NANOROBOT FOR MOLECULAR COMMUNICATION IN MEDICAL SCENARIOS

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**Abstract.** In this paper, we aimed to discuss about distributed cooperative routing methods for a team of medical nanorobots in human body and model it as a complex problem. We use the nanonetwork as a communicational structure for optimal routing and movement to a target cancer tissue in a capillary. For this aim, we designed a bacteria based nanorobot that use a probabilistic finite state automaton for its communication tasks and proposed a new multiscale architecture for an in vivo complex nanonetwork.

We try to minimize the needed time for detecting and manipulating cancer cells, with offer a global scenario and mathematically analysis it. As the network nodes are moving in blood vessels, the network structure is inspired from capillary biological communication.

The main innovative aspect of this work is presenting a cooperative routing model in molecular communication area.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

# CHARACTERISATION OF TCR MOTIONS IN REACTION TO IMMUNOGENIC AND NON-IMMUNOGENIC PEPTIDES: A PCA APPROACH

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**Introduction.** The adaptive immune system differentiates between antigens which elicit an immune response and antigens which do not - they are usually referred to as immunogenic and non-immunogenic peptides respectively. These peptides are bound to major histocompatibility complex (MHC) molecules located on the cell surface which present the peptides (p) to T-cell receptors (TCR) of T-cells (TC). If the peptide is considered immunogenic a signalling cascade is triggered.

There are many theories concerning antigen recognition and the induction of this cascade [1]. The purpose of this study is to find indications that the TCR undergoes subtle conformational changes if bound to an immunogenic peptide/MHC complex.

**Method.** To find evidence in order to support this hypothesis molecular dynamics (MD) simulations are a promising approach. MD simulations enable us to analyze atomic motions in detail and have proven to be a powerful tool to study biomolecules [2]. A common approach to extract motions of biological significance is to compute the correlated so-called collective motions. A well known method to extract this information is the principle component analysis (PCA) [3].

We analysed 58 MD simulations of TCRpMHC complexes performed by B. Knapp. Although the considered peptides only differ by one amino acid, this single mutation changes its immunogenicity severely. In order to reduce the amount of data we only considered the C-alpha atoms of amino acids. Furthermore, we removed the overall motions such as rotation and translation to obtain only internal motions. This is achieved by superimposing a reference structure onto the trajectory. As reference structure we chose the crystal structure of the protein data bank (PDB) accession code 1mi5 and superimposed it onto all 58 trajectories.

In the next step we concatenated the trajectories of all 58 simulations which consist of immunogenic as well as non-immunogenic complexes and applied a PCA to this concatenated trajectory. A PCA requires the computation of the covariance matrix of the atomic fluctuation and subsequently its eigenvectors and eigenvalues. The eigenvectors corresponding to the biggest eigenvalues represent the direction of the strongest correlated motions. This procedure was performed using Gromacs 4 which was already employed to realize the MD simulations.

The major hypothesis of this study is that there is a collective motion responsible for signal transduction. By merging all 58 trajectories into one long trajectory and computing its correlated motions, we will be able to find at least one eigenvector which represents the designated motion. By projecting the trajectories onto this eigenvector we should be able to differentiate immunogenic and non-immunogenic TCRpMHC complexes.

The length of the projection is of special interest, since it gives insight how well the eigenvector covers the direction of the molecule's movement and most importantly leads to a considerable data reduction.

**Results and Prospects.** We obtained a considerable amount of 2d-plots each of which represents the projections of the simulations onto two different eigenvectors. To date, the analysis of the data obtained is still in progress and only preliminary results are available. However, on the basis of clustering we are confident to find the collective motions which discriminate best between immunogenic and nonimmunogenic complexes.

Data of another 114 MD simulations of TCRpMHCs is available and will be processed once evidence supporting our hypothesis is found.

- [1] Choudhuri K, van der Merwe PA. *Molecular mechanisms involved in T cell receptor triggering*. Semin Immunol 2007 Aug;19(4):255-61.
- [2] Hansson T, Oostenbrink C, Van Gunsteren WF. *Molecular dynamics simulations*. Curr Opin Struct Biol 2002 Apr;12(2):190-6.
- [3] Berendsen HJ, Hayward S. *Collective protein dynamics in relation to function*. Curr Opin Struct Biol 2000 Apr;10(2):165-9.

## COMPARISON OF INFORMATION CRITERIA FOR MHC HELICAL SEGMENT FITTING

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T-cells and B-cells are major players in the adaptive immune defense of the human body. T-cells have several receptors on their surface. One of them is the so called T-cell receptors (TCR) which can recognize immunogenic and non-immunogenic peptides presented by major histocompatibility complexes (MHC) [1]. The TCR can elicit an adaptive immune response by binding the major histocompatibility complex presenting an immunogenic peptide. It has been frequently hypothesized in the literature that conformational changes of the helical segments, which assemble the MHC binding groove, influence TCR signalling: Miller et al. could show that the TCR/MHC interaction is highly sensitive to single mutations in the MHC helices. Not only the MHC peptide-binding groove, but also the TCR, especially the complementarity Determining Regions (CDR) may change its spatial dynamics due to an immunogenic reaction.

To analyse these conformational changes of the helical segments, we fitted least-squares curves in parametric form to every alpha-helical segment of the MHC of all published crystal structures. These structures are available from the Protein Databank (PDB) and were extracted according to the IMGT database (accessed August 2011). In order to make these coordinate files comparable to each other, we employed a Principal Component Analysis (PCA) via the Statistics Toolbox of Matlab (Version 7.11.0.584) and thereby obtained the coordinates of the complexes in a local coordinate system. Furthermore, we fitted least-squares curves to the alpha-helical segments of four molecular dynamics simulations of previous projects, performed with Gromacs 4 [2].

We intended to find a model for MHCs which characterizes the helical segments in an optimal way, but with a minimum number of model parameters. For this purpose we applied several Information Criteria, which define a certain trade-off between these purposes. Information Criteria have their main applications in applied statistics and econometrics; however, we introduced such a method to immunological problems in structural bioinformatics. We investigated the following criteria to analyse which one is the best to take over in the field of bioinformatics: the "Akaike Information Criterion", the "Bayesian Information Criterion" or the "Hannan-Quinn Information Criterion". Finding an optimal model for MHCs, the value of an Information Criterion is computed for each provided model. These equations are based on the formulation with the minimum variance of the residues and therefore models with minimal values are considered as best. For small sample sizes there is the opportunity to add second order correction term to the particular Information Criterion obtaining a corrected version. On this basis it is necessary to decide which criterion is most applicable for our modelling problem.

We evaluated the Information Criteria with polynomials of degree 1 to 7 and splines with 1 to 2 nodes based on polynomials of degree 1 to 7 for the vector components of our parametric form approach. By a comprehensive literature research and comparison of the results for our modelling problem of the different Information Criteria, we found that the "corrected Akaike Information Criterion" (cAIC) [3] is most appropriate for finding curves representing the helical segments of MHCs in a distinguishing way

$$cAIC = n \log \frac{SSE}{n} + 2k + \frac{2k(k+1)}{n-k-1}.$$

The number of model parameters is described by  $k$ ;  $n$  is the number of data points (in our case the coordinates of the helical segments of the crystal structures);  $SSE$  represents the Sum of Squared Error. The first term of the equation relates to the negative maximum likelihood of the regression model and the second term represents the penalty of each of the Information Criteria. The third term is the added second order correction term to the particular Information Criterion obtaining a corrected version.

This study about finding an appropriate Information Criterion is an important prerequisite for further investigations on the spatial dynamics of different TCRpMHC complexes.

In further studies we will be able to find models for MHC class I and MHC class II for both, the stationary and dynamical case. By calculating parameters from these curves, we will be able to discriminate complexes which cause TC signalling from those which do not.

- [1] Rudolph MG, Stanfield RL, Wilson IA. *How TCRs bind MHCs, peptides, and coreceptors*. Annu Rev Immunol 2006;24:419-66.
- [2] Hess B, Kutzner C, vanderSpoel D, Lindahl E. GROMACS 4: *Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation*. J Chem Theory Comput 2008 Feb 2;4(3):435-47.
- [3] Burnham KP, Anderson DR. *Kullback-Leibler information as a basis for strong inference in ecological studies*. Wildlife Research 2001;28(2):111-9.



# COMSOL-BASED DESIGN STUDIES FOR THE UPCOMING NEUTRON DECAY EXPERIMENT PERC

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**Abstract.** We present a new facility, PERC (Proton and Electron Radiation Channel), for the investigation of neutron beta decay. Neutron decay experiments play an important role in testing the Standard Model of particle physics and searching for new physics beyond it. These experiments are complementary to direct searches in high energy physics.

PERC is designed as a source of neutron decay products, namely electrons and protons. The charged decay products are collected by a strong magnetic field directly from inside a neutron guide. The superconducting magnet system of PERC will consist of three parts on a total length of 11.5 meters. The outer parts are designed as single long solenoids with a length of 8/ 1.5 meters and a magnetic flux density of 1.5/ 0.5 Tesla, respectively. In contrast, the central part consists of a complex system of 8 coils in total. Short tilted coils serve to decouple the neutron beam from its decay products, whereas a solenoid part serves to limit the phase space. Here, the magnetic field varies from 3 to 6 Tesla. PERC is designed to considerably improve the precision of existing neutron decay experiments. Therefore, the magnetic field has to be known with a relative uncertainty of  $10^{-4}$ .

Depending on the decay parameters studied, the analysis of the decay products must be performed with different and specialized detectors. Therefore, an electron energy spectrometer, a proton retardation spectrometer and a magnetic spectrometer are still under development. Besides the electro-/magnetic field calculations, particle tracking simulations are performed in order to understand the behavior of the charged particles in those spectrometers.

In addition, in order to reduce the stray field in the neighborhood of the PERC magnet down to the cardiac pacemaker level, a magnetic field return is under development.

We have designed the magnetic field of the superconducting PERC magnet using COMSOL Multiphysics. The AC/DC module was applied to

- verify the homogeneity constraints of the magnetic field and
- reduce the exterior magnetic field down to cardiac pacemaker level.

Additionally, the Particle Tracing module was used to

- calculate the charged particle beam behavior in PERC and its different post-spectrometers.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

## DECENTRALIZED ACOUSTIC LOCALIZATION

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**Introduction.** This abstract presents a model for decentralized localization of acoustic sources in a hallway employing measurements, i.e. microphones termed sensors [1]. Furthermore, by exploiting the underlying physical structure, the final algorithm is fully decentralized. In this context, the terminology "decentralized" denotes the absence of a fusion center. Thus the computational load is distributed across the sensors.

The investigation belongs to the realm of three commonly disjoint topics merged into a parameter estimation context. The first issue is determined by the physical model of the acoustic field. Secondly, it is embedded into the localization problem by utilizing Bayesian estimation theory. Finally, decentralization brings a consensus algorithm into play.

**State-Space Model.** As compared to the common coarse approximation of acoustic waves by an attenuation factor depending on the distance [2], here we address a different approach. A scalar hyperbolic second-order linear stochastic partial differential equation combined with initial and boundary conditions model the waves. For the localization issue, additional models describe the sources depending on their random position and the random occurrence time. The observations of the sensors are specified by the so-called measurement equation. All equations together form a time-continuous state-space model enabling the usage of a sequential Bayesian maximum a-posteriori estimator for the position estimation.

**Sequential Bayesian Estimation.** Non-linearity due to the sources, non-Gaussian noise and non-Gaussian random states require the use of a Monte-Carlo method termed particle filter [3]. The state-space model is transformed into a discrete representation by a numerical method. A central fusion center is now able to estimate the positions of the sources up to an estimation error. That is, the estimated source positions lie on lattice points defined by the numerical method. Here the finite difference method is chosen.

**Decentralization of the Model.** In the decentralized case, the discrete state-space model is decomposed into  $M$  sub-state space models belonging to the  $M$  sensors. Here the sparsity of the transition matrix is exploited and thus there are only a few coupling terms between the sub-models. These terms cause the transmission between neighbouring sensors. Additionally, in the case of a Sample-Importance-Resample particle filter, the decentralized re-sample step of the particle filter causes an exchange of weights. This can be avoided by using other estimators, but would constrain the probability density functions of the states and noise.

**Consensus.** Every sensor knows only the probability density function of the source positions of its own sub-area. This area corresponds to its sub-state space model. To get the positions with the highest probability across all sensors an argument-maximi consensus algorithm is utilized. This algorithm ensures a global consensus after a number of time steps proportional to the diameter of the sensor graph.

**Summary.** Important properties include the in-cooperation of wave phenomena like echoes and the distribution of the computational load across sensors. On the other hand, there is a significant exchange of messages between neighbouring sensors. Furthermore, there is no approximation compared to the central case. In a real-world application an approximation error would arise due to the necessary source coding of the transmitted messages. Beyond the localization of the position, the occurrence time and the whole wave field is estimated.

- [1] F. Xaver, G. Matz, P. Gerstoft, and C. Mecklenbräuer, "Localization of acoustic sources using a decentralized particle filter," *EURASIP JWCN*, 2011.
- [2] O. Hlinka, O. Slučiak, F. Hlawatsch, P. M. Djurić, and M. Rupp, "Likelihood consensus and its application to distributed particle filtering." Available online: arXiv:1108.6214v2 [stat.AP], Dec. 2012.
- [3] C. Yardim, P. Gerstoft, and W. S. Hodgkiss, "Tracking of geoacoustic parameters using Kalman and particle filters," *The Journal of the Acoustical Society of America*, vol. 125, p. 746, 2009.

# MMT – A SYSTEM OFFERING E-LEARNING OF MODELLING AND SIMULATION IN A DIFFERENT WAY

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**Introduction** The MMT system (MMT stands for Mathematics, Modelling and Tools) was developed as an environment to support e-learning in many ways. The MMT server consists of a huge amount of examples in mathematics as well as modelling and simulation which is constantly increasing.

On the one hand the MMT is used in lectures for students of electrical engineering and geodesy and geomatics engineering by showing examples in Linear Algebra and Analysis. Additionally to the demonstration in the lectures the students get accounts for the MMT to have access to the corresponding examples. This way they are able to train their knowledge and understanding of the current subject by experimenting on the MMT server and comparing the results given by MMT with their own ones.

In lectures about modelling and simulation, the MMT environment is used not only to show results of different modelling approaches but also to give insight to the models itself by showing the underlying source codes. These can be downloaded and modified on the student's own computer, so beginners in modelling can take proved and validated models as a starting point and alter them to gain their own model without having to build a whole complicated model on their own. The examples shown in those lectures are further used in exams via another e-learning platform, e.g. TUWEL, the Moodle-based e-learning system of the Vienna University of Technology.

As mentioned above, the amount of examples on the MMT server is constantly increasing. Apart from models particularly developed for certain educational needs by programmers of the MMath-EL Group, models created by students during projects, bachelor or diploma theses are reviewed, validated and further adjusted and linked to the MMT system.

**Recent Developments** Recently the MMT environment has successfully been updated to enable examples accessing several MATLAB functions as well as Simulink models. Thus it is possible to install models of more or less any complexity at the MMT interface. The various m-files just need to be called from a certain MATLAB function to begin with.

Simulink models are called by a MATLAB function consisting only of the extraction of the input values of the MMT server and the execution of the Simulink model. By having enabled examples using Simulink models, teaching modelling and simulation can now focus also on the method of Physical Modelling.

**Summary and Outlook** Currently in the course of a collaboration of the Vienna University of Technology and the University of Ljubljana complex models of linear and non-linear tank systems and petrinets are included into the MMT system. In this way the different modelling approaches of both universities can be accessed by students in Ljubljana as well as in Vienna, what will additionally extend their modelling skills.

Recently the focus of new MMT models was laid on discrete modelling for the usage of the MMT system in lectures for students of business informatics. Contrary to most of the other examples implemented on the MMT server which are dynamic systems described by ordinary differential equations, discrete models are described by systems of difference equations.

Further goals are the inclusion of other programming languages like Java and Octave into the MMT environment. This will enlarge the possibilities of teaching modelling and simulation via MMT by a significant amount.

- [1] Andreas Körner, Irene Hafner, Martin Bicher, Stefanie Winkler, Felix Breiteneker, *MMT - A Web Environment for Education in Mathematical Modelling and Simulation*. ASIM 21. Symposium Simulationstechnik - Grundlagen, Methoden und Anwendungen in Modellbildung und Simulation, Winterthur, 2011.
- [2] Stefanie Winkler, Andreas Körner, Irene Hafner, *MMT – A web-based e-learning System for Mathematics, Modeling and Simulation using MATLAB*. In: 7th EUROSIM Congress on Modelling and Simulation, Prag, 2010, paper 231.
- [3] Andreas Körner, Günther Zauner, Günther Schneckenreither, *Ein e-learning System für MMT – Mathematik, Modellbildung und Tools, Systemerweiterung und Einbindung von graphischer Modellbildung*. 20th Symposium Simulation Techniques, Cottbus, 2009, 87-94.

# MODELING OF THE CARDIOVASCULAR SYSTEM TAKING INTO ACCOUNT BLOOD PRESSURE REGULATORY MECHANISMS

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**Introduction.** In the work at issue a compartment model of the cardiovascular system was developed. It is based on the PHYSBE-model by John McLeod. I added an extra compartment representing the kidneys. Besides, two different regulatory mechanisms were built in: the one provided by the kidneys and the baroreceptorreflex.

The programming language Matlab Simulink was used to develop these models.

**Basic Model.** Due to the modifications of the PHYSBE-model the whole blood volume and its distribution among the different parts of the cardiovascular system was estimated anew, based on data taken from literature. As a consequence, I had to reconsider the system parameters - namely the compliance and the resistance of the blood vessels. In this process the emphasis was on creating a realistic pressure profile in the "Aorta"-compartment and a good accordance of the simulated heart volume with measured data. The former serves in the further course of the work as correcting variable for the regulatory mechanisms.

**Baroreceptorreflex.** One of the studied regulatory mechanisms was the baroreceptorreflex. This control device is named after pressure receptors which are placed in the central sections of the cardiovascular system. It deals with changes in blood pressure on a short term basis. The baroreflex uses two correcting variables: the alteration of the heart frequency and of the peripheral resistance. Möller and Popovic [3] propose an approach for a mathematical description of the pressure feedback. Due to the differences between the model used in the work at issue and the one applied by Möller and Popovic it was necessary to make some modifications. The pressure-dependent functions representing the changes of the heartfrequency and the peripheral resistance were altered to meet the guidelines set by Arthur Guyton [1]. Guyton indicates that the baroreflex can absorb  $\frac{7}{8}$  of deviations from the normal pressure.

**Kidney-Fluid Mechanism.** The kidneys regulate the blood pressure by increasing and reducing the amount of urine. Among the bodily regulatory mechanisms it is the only one with infinite duration. By using the so-called "renal function curve" the kidney-fluid mechanism is incorporated into the model. The "renal function curve" describes the connection between the mean arterial pressure and the amount of urine excreted through the kidneys. The incorporation of the curve mentioned above was effected through the following exponential function:

$$U := \exp(aP) + b,$$

with the parameters  $a = \frac{1}{91}$  and  $b = -1.95$ .

**Alternative Model Approach.** In the course of work I recognised important drawbacks in the arrangement and the construction of the compartments. To avoid the resulting difficulties a different model structure was contemplated. In this new model vessels were lumped together in compartments according to their lumen. Therefore, I suggested a division into the following compartments: "Right Heart", "Pulmonal Arteries", "Pul.Capillaries", "Pul.Veins", "Left Heart", "Aorta", "Arteries", "Arterioles", "Kidney", "Capillaries", "Small Veins", "Large Veins" and "Vena Cava". With the estimation of the basic parameters I outlined an approach for further research.

**Conclusion.** The pressure control mechanisms taken into account worked well in my simulation. However, the pressure reduction through the baroreflex was not entirely satisfying. During simulation this mechanism was able to absorb  $\frac{2}{3}$  of a pressure increase in contrast to the predicted  $\frac{7}{8}$ .

Besides, the normalization of the blood pressure through the kidney-fluid mechanism takes a lot of time which created difficulties in the simulation run. This challenge was met by the introduction of a scaling constant to speed up the process.

The presented alternative model can be used as a basis for further work on this issue.

- [1] A. C. Guyton. Blood pressure control - special role of the kidneys and body fluids. *Science*, 252:1813–1816, 1991.
- [2] J. McLeod. Physbe - a physiological benchmark experiment. *Simulation*, 7:324–329, 1966.
- [3] Dieter Möller, Dobrivoje Popović, and Georg Thiele. *Modeling, simulation and parameterestimation of the human cardiovascular system*, volume 4 of *Advances in Control Systems and Signal Processing*. Vieweg, 1983.

# MOLECULAR DYNAMICS - THE APPROPRIATE COMBINATION OF CLASSICAL NEWTONIAN AND QUANTUM MECHANICS IN SIMULATING MANY-BODY SYSTEMS

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**Introduction.** A lot of problems in the field of medicine or bio- and nanotechnology deal with many-body systems. Because of the size of the interacting bodies, called particles, a handling at a molecular and atomic level is required, which leads to quantum mechanics. An analytic or numerical solution of the resulting Schrödinger equation is only possible in a few simple special cases - even a system consisting of three bodies cannot be clearly solved. Therefore several approximations and simplifications have to be made when the number of particles increases. The approach to solve many-body systems makes use of the laws of classical Newtonian mechanics and the actually required quantum mechanics.

**Modelling Approach.** The simulation of such systems is based on particle models. In these models the physical system consists of discrete particles and their interactions, therefore very small as well as very big particles can be handled. One particle carries some physical properties, like mass, velocity, position, energy or charge, and the evolution of the system is given by these properties and the interaction of the particles.

Many particle models are based on classical Newtonian mechanics. Newton's second law leads to a system of ordinary differential equations of second order. The acceleration of a particle depends on the force acting on it, and this force depends on the interactions of the particles.

In atomic models one actually needs to make use of the laws of quantum mechanics and solve Schrödinger's equation, representing the equation of motion. Its solution doesn't provide unique trajectories, meaning determined positions and other physical properties. All statements about this system result from the state function, also called wave function,  $\psi$ , given as the solution of the Schrödinger equation

$$i\hbar \frac{\partial \psi(\mathbf{R}, \mathbf{r}, t)}{\partial t} = \hat{H} \psi(\mathbf{R}, \mathbf{r}, t)$$

with  $\mathbf{R}$  representing the positions of the nuclei and  $\mathbf{r}$  the positions of the electrons.

Under the assumption that the Hamilton operator isn't explicitly time dependent a separation approach leads to the stationary Schrödinger equation

$$\hat{H} \psi(\mathbf{R}, \mathbf{r}) = E \psi(\mathbf{R}, \mathbf{r})$$

which is an eigenvalue problem for the Hamilton operator  $\hat{H}$  with the energy eigenvalue  $E$ .

**Simulation Approach.** Within the simulation of many-body systems some simplifications have to be made. The Born-Oppenheimer approximation makes use of the big difference regarding the mass of the atomic nuclei and the electrons. This allows a separation of the equations of motion of the nuclei and the electrons. Also to be mentioned is the Hartree-Fock approach to calculate the potential caused by the electrons.

A simplification concerning the potential is the use of the cut-off radius. For one particle only the interactions with particles in a certain radius are considered. Particles out of this area are treated as if they weren't there, because the distance is too wide and therefore the interaction negligible compared to the interactions with closer particles. For the Lennard-Jones potential  $U(r_{ij})$  with  $r_{ij}$  the distance between two particles, the approximation leads to

$$U(r_{ij}) \approx \begin{cases} 4 \cdot \varepsilon \left( \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right) & r_{ij} \leq r_{cut}, \\ 0 & r_{ij} > r_{cut}. \end{cases}$$

where  $\varepsilon$  is the parameter defining the depth and  $\sigma$  the parameter determining the zero-crossing of the potential.

With regard to the boundary conditions it depends on what system is simulated. In case of a closed box one could work with reflecting boundary conditions. In periodic systems it is common to use periodic boundary conditions. The approach is based on the assumption that a particle leaving the simulation domain on one side reenters on the opposite side. Therefore particles located on opposite sides close to the borders interact with each other.

[1] M. Griebel, S. Knapek, G. Zumbusch, *Numerical Simulation in Molecular Dynamics*. Texts in Computational Science and Engineering 5, (Eds.: T.J. Barth, M. Griebel, D.E. Keyes, R.M. Nieminen, D. Roose, T. Schlick) Springer, Berlin/Heidelberg, 2007.

[2] W. Demtröder, *Experimentalphysik 3. Atome, Moleküle und Festkörper*, Springer, Berlin/Heidelberg, 2005.

## MTA IN MATHEMATICS AND SIMULATION

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**Introduction.** In modelling and simulation there are many different programming languages used. The MMath-EL group especially one part of the working group of simulation focuses on e-learning. The courses of this working group are based on the computer languages Maple and Matlab. These courses simplify the access to simulation tools for the students and additionally teach them mathematical basics in an easy way. Some of the students are not used to code so it is important to introduce the students slowly to these programming languages. This contribution focuses on the e-learning system Maple T.A..

**Maple T.A.** Maple T.A. stands for Maple Testing Assessment and is based on Maple. There is a separate syntax for the Maple T.A. for creating examples but it is also possible to use the common Maple commands. Therefore one can create every kind of plot or algorithm which can be implemented in Maple. Additionally the user interface offers different kind of questions, for *instance multiple choice, question with input window or graphical output*. On the other hand the system supports the creating of testing assignments and the administration of users and their test results.

Another advantage of this system is the possibility to create a kind of example which can be practiced several times without getting exactly the same question. Due to this the students who sit aside at the test are not able to copy the results from their neighbour.

### Motivation

- **Refresher Course** The students of Vienna University of Technology graduated from different schools, for example polytechnic, ordinary highschool oder highschools with other key aspects. So they all have different mathematical levels. The MMath-EL group offers a refresher course for mathematics for every student of Vienna University of Technology. With attending this course it is no longer important which school the student graduated. This course takes one to two weeks. There are lectures and tutorials to every mathematical topic which should be taught at school.  
The refresher course for mathematic is supported by the e-learning system Maple T.A.. So the students have the chance to hear the lectures, participate the tutorials and exercise at home.
- **Mathematic Course** The MMath-EL group organises all parts of the lecture mathematics for the students of electrical engineering. These courses consist of a lecture and a tutorial supported by the e-learning system Maple T.A.. There the students can exercise the examples fitting to the lecture and the tutorial. Also two of three tests on this system have to be passed.  
The students have to deal with the demanded syntax for this system because this course is mandatory. For some students it is the first contact with coding. The advantage of using Maple T.A. is that the students have to learn some syntax which is necessary and basically for every kind of programming and further for modelling and simulation.
- **Modelling and Simulation Course** The students of electrical engineering have to deal with the Maple T.A. system and its syntax for the first three semesters. Due to this fact it is not amazing that the MMath-EL group offers also easy modelling examples in this system. The students can use their aquired knowledge of coding from the mathematics course and advance it.  
The examples help the students of electrical engineering to understand small and easy models. The model discription contains a picture of the block diagram belonging to the example. The students have to calculate for answering the question therefore they have to think about the block diagram and its meaning.

- [1] A. Körner, S. Winkler, V. Urbonaite *E-Learning Einsatz im Auffrischkurs Mathematik an der TU Wien*. eLearning Baltics 2011, 2011, Proc. 4th International eLBa Science Conference, 145-154.
- [2] A. Körner, A. Zimmermann, F. Breiteneker *Blended-Learning mit Maple T.A. in der Lehre für Mathematik und Modellbildung*. ASIM 2009, 2009, Extended Abstracts 20th Symposium Simulation Techniques, 62-64.

# OBJECT-ORIENTED MODELLING OF MACHINE TOOLS FOR ENERGY EFFICIENCY ANALYSIS IN PRODUCTION

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**Introduction.** The research project INFO [1] (sponsored by the Austrian Research Promotion Agency (FFG)) pursues the primary goal to increase energy efficiency in production plants by considering various disciplines of energy technology, production technology and building design in a holistic approach [2]. Qualified and customized predictions and recommendations about the efficiency of different energy saving measures can be made using comprehensive simulation models of the real production plant including all relevant micro- and macro-structures and therefore identify potential savings in manufacturing plants.

One important part of this project investigates the micro-structures of production plants (individual processes and machines) by making extensive energy analysis to point out optimization potential based on simulation models. This also allows gaining knowledge for merging the individual levels in the modelling approach to an ultimately complete simulation. Some of these aspects are studied in more detail by creating a multi-domain model of a turning lathe as an example of a machine tool.

**Modelling Method.** A new high-level object-oriented modelling approach provides the necessary flexibility regarding modularity and reusability. The structured nature of this modelling method allows for simple stepwise development and easy expandability of a multi-domain model including electrical, mechanical and thermal aspects of the machine tool. Simulation results are validated against real measurement data obtained from the actual turning lathe, of which the model is created and which is provided by the Institute for Production Engineering and Laser Technology from the Vienna University of Technology.

Although simulators for object-oriented component-based modelling of physical systems have evolved considerably in the last years (e.g. Dymola, MATLAB/Simscape™, MapleSim), there are still numerical issues when it comes to simulating complex multi-domain systems. Bottom-up modelling of this component-based approach is therefore combined with stepwise top-down modelling in several stages with gradually increasing level of detail for identifying numerical boundaries of the simulation arising from higher level of modelling detail as well as the degree of modelling effort necessary for investigating certain aspects.

**Modelling Stages.** The top-down modelling process is divided into three stages. The first stage consists of the basic mechanical and electrical model including an asynchronous motor for the main drive and servomotors for automatic feed, both represented by linear equation models with parameters extracted from available data sheets. The overall model also includes mechanical loads and a simple calculation model of the cutting forces using common formulas and parameters [3]. However, a simple motor control implementation limits possible simulation scenarios in this stage.

The second stage also takes into account accurate motor control parts, power electronics and waste heat calculations in the drive motors and other components, therefore including thermal aspects in the model. In addition, some adjustments have to be made due to numerical boundaries in order to assure sufficient performance of the simulation and quality of the numerical solution.

The simulation model in the last stage will furthermore include remaining electrical loads, generated heat in the cutting process and additional mechanical details.

**Conclusion.** Object-oriented modelling offers practical ways for structured multi-domain modelling of machine tools leading to modular, easily refinable and modifiable simulation models. However, this approach leads to comparatively complex models with a larger amount of equations, which can profoundly affect the performance during simulation.

Future work will focus on refining the models as part of the next stages in the top-down modelling process as well as parameterization of the remaining components. For model validation it is planned to compare the simulation results of various scenarios against measurement data obtained from the turning lathe.

[1] <http://www.projekt-info.org>

[2] Dorn Ch. and Bleicher F.: *Interdisziplinäre Forschung zur Energieoptimierung in Fertigungsbetrieben*. Junior Science Conference 2010.

[3] Degner W., Lutze H. and Smejkal E.: *Spanende Formung, Theorie - Berechnung - Richtwerte*. Hanser Verlag, 2009.

# PARAMETER ESTIMATIONS OF A MULTI-INPUT AND MULTI-OUTPUT P-CANONICAL DYNAMIC SYSTEM USING THE LEAST SQUARE METHOD

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**Abstract.** This article introduces an algorithm for the parameter estimation of a type of P-canonical multi-input and multi-output (MIMO) model via the least square method. In this article, a LS methodology, its simulation algorithm and the results are presented.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**



## RANDOM GENERATION OF MATHEMATICAL EXAMPLES IN MAPLE T.A.

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**Introduction.** Maple T.A. is an online testing, evaluation and grading software powered by Maple. The Vienna University of Technology uses it to help students preparing to start an intensive education in maths, to refresh basic mathematical skills from high school and improve success in advanced university mathematics. Although this system has its own commands and it is possible to call 80% of Maple functions from Maple T.A. . The common Maple functions are limited in sense of random generation and evaluation of mathematical examples. For this reason at Vienna University of Technology an appended Maple "Random" library was created, which increased example creation opportunities and diversity.

**Random generation of examples in Maple T.A.** A construction of algorithmic variables is the way to randomize the questions in Maple T.A. These algorithmic variables can use the built-in algorithmic generator in Maple T.A. or can use any of Maple's randomization routines. Various functions inside Maple T.A. can be used to create just simple random variables like integers or real numbers. There are also a wide variety of routines and packages in Maple that can be used as straight functions or combinations of functions to create more complex algorithmic variables in this system. But the more complex the objects are, the more complicated Maple T.A. code and creation of question gets. Such Maple random-routines require longer execution time and that leads to some technical problems in case of a large number of students working on the same question at the same time. On the Vienna University of Technology an additional Maple randomization library was developed, which made this process less difficult and less time-consuming.

The following functions are implemented in "Random" library:

- `Random[FromSet](Set, Count)`  
A given number of random elements (with or without replacement; sorted or not) are selected from a set. The data types of the set elements are not restricted.
- `Random[FromInts]([Min1, Max1], [Min2, Max2], . . . , Count)`  
For given interval boundaries (minimum and maximum) the function returns a sequence of either a specified number or all integers between these boundaries.
- `Random [FromRats]([Min, Max, MinDenom, MaxDenom], Count)`  
The function is similar to `FromInts`. In this case the return values are rational numbers, that are restricted by some additional parameters for the denominators.
- `Random[Vec](Set, Dim, zerocount = k)`  
For a given dimension this function returns a random vector with user-defined entries. Number of zeros in the vector can be given.
- `Random[Mat](Set, rows = m, cols = n, zerocount = k, shape = s)`  
The `Mat`-function generates random matrices. It is possible to define the matrix dimension as well as a required shape and number of zero entries.
- `Random[MatInts](Set, rows = m, cols = n, zerocount = k, rank = r, shape = s)`  
Just like the vector function, `MatInts` creates matrices only with integer entries. The rank of the matrix can be also given.
- `Random[MatIntsDef](Max, Pos, Neg, Zero)`  
This function delivers a random symmetric matrix with integer entries and specified numbers of positive (pos), negative (neg) and eigenvalues equal zero (zero). The dimension of the matrix is defined by:  $\text{dim} = \text{pos} + \text{neg} + \text{zero}$ , and the rank equals  $\text{pos} + \text{neg}$ .

- [1] F. Judex, F. Breitenecker, G. Schneckeneither, G. Zauner *Cas-based e-learning for the improvement of refresher courses in mathematics*. Vienna, Argesim Report No. 35, February 11-13 2009, pages 2106x962111.
- [2] A. Körner, S. Winkler, V. Urbonaite *E-Learning Einsatz im Auffrischkurs Mathematik an der TU Wien*. eLearning Baltics 2011, 2011, Proc. 4th International eLBA Science Conference, 145-154.
- [3] A. Körner, A. Zimmermann, F. Breitenecker *Blended-Learning mit Maple T.A. in der Lehre für Mathematik und Modellbildung*. ASIM 2009, 2009, Extended Abstracts 20th Symposium Simulation Techniques, 62-64. eLearning Baltics 2011, 2011, Proc. 4th International eLBA Science Conference, 145-154.
- [4] A. Zimmermann, V. Urbonaite, A. Körner *Advanced randomization and grading in the E-learning system Maple T.A.*. EUROSIM 2010, 2010, 7th Congress on Modelling and Simulation.

# SIMPLIFIED SIMULATION MODEL FOR RADIO CHANNEL SIMULATIONS FOR TYRE PRESSURE MONITORING SYSTEMS

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**Introduction** Tyre pressure monitoring by means of small sensor units embedded in vehicular tyres, is currently seen as a key technology to enhance vehicular comfort and safety standards and enables fuel consumption reduction by maintaining optimum tyre inflation. The transition from traditional bulky, battery powered TPMS to intelligent, energy-efficient, tyre-embedded, low power systems supplied by radio frequency harvesting, requires deeper understanding of the underlying communication channel.

**Problem Description** A typical vehicle contains a centralised onboard unit (OU) and four wheel units (WUs) which exchange data with the OU. For communications with the centralised onboard unit, WUs use radio frequency (RF) transmissions in the ultra high frequency (UHF) domain, especially at 866MHz. The transmission is based on phase shift keying (PSK) and the maximum data rate is below 640kbit/s. Because of the physical proximity between OU, WUs and the metal structures of the vehicle, a combined channel model should be derived which describes propagation effects of the pure RF channel as well as influences of the moving antennas. The OU is equipped with a monopole antenna mounted on the bottom plate of the car. The WUs use shortened dipole antennas for their communication. The model should capture different mounting positions of the WU inside the tyre, as well as all effects caused by moving the vehicle on a potentially rough road surface.

**Channel Model** This problem is best described using a flat fading channel model [1, p. 119], which is justified due to the relatively low data rate and the short distance between OU and WUs [2]. In the downlink channel from WUs to the OU, the received signal  $r_0(t)$ , which is a function of time  $t$ , is described as:

$$r_0(t) = \sum_{i=1}^4 \left[ h_i(\varphi(t), \Theta(t)) + \tilde{h}_i(t) \right] s_i(t) + n(t). \quad (1)$$

It is the sum of four products of the individual OU–WU channels and the corresponding WU transmit signals  $s_i(t)$ , plus a receiver noise term  $n(t)$ , that is assumed to be white and gaussian. The channel coefficient is decomposed into two parts: the deterministic channel component  $h_i(\varphi(t), \Theta(t))$  which captures the variation of the channel caused by changes of the rotational angle  $\varphi$  and the steering angle  $\Theta$ , and the stochastic part  $\tilde{h}_i(t)$  that introduces the channel variations caused by wheel and vehicle vibrations and the roughness of the road surface. The  $2\pi$  periodicity in  $\varphi$  allows for a decomposition of the channel component  $h_i(\varphi, \Theta)$  in a Fourier series, which is not only very helpful to calculate the maximum Doppler shift introduced by tyre rotation [2], but also enables efficient parameter reduction of the channel coefficient.

**Simulation Model** For simulations, we focus on the deterministic channel component  $h_i(\varphi, \Theta)$ . For this work electromagnetic field simulations in Ansoft’s full 3D finite element method (FEM) simulator HFSS (High Frequency Structure Simulator) were performed. While other numerical techniques like Methods of Moments (MoM, also called boundary element method) are in principle better suited to antenna placement problems than FEM, HFSS has the benefit to enable inclusion of lossy, anisotropic, and even nonlinear dielectrics in the simulation model. Unlike [3], where a similar problem is treated in the commercial MoM solver FEKO, this work focuses on the modelling of the areas in proximity to the antennas which have severe impact on antenna efficiency, directivity and input impedance. Based on [4] the complex and very diverse rubber layer structure of a vehicular tyre was first completely modeled in HFSS, including the two layer steel belt common in tyres for cars. It was discovered, that the geometric model had to be simplified to lower the memory demands. Finally, the author used a single rubber layer with effective dielectric permittivity of  $\epsilon_r = 5.5$ , which was found to best capture the near-field detuning effects of the dipole antenna, when compared to measurements of this dipole on a piece of tyre sidewall rubber.

**Simulation Results** Over the rotational angle  $\varphi$  the channel magnitude exhibits strong fluctuation between  $-37\text{dB}$  and  $-77\text{dB}$  for a specific WU antenna mounting, but the changes due to the steering angle  $\Theta$  are relatively small. Similar results were obtained experimentally documented in [5].

- [1] A. F. Molisch, *Wireless communications*, 1st ed. John Wiley & Sons, LTD, 2005.
- [2] G. Lasser and C. F. Mecklenbräuker, “Channel model for tyre pressure monitoring systems (TPMS),” in *Proc. EuCAP’2010 The 4th European Conference on Antennas and Propagation*, Barcelona, Spain, Apr. 2010.
- [3] H. J. Song, H. P. Hsu, R. Wiese, and T. Talty, “Modeling signal strength range of TPMS in automobiles,” *Antennas and Propagation Society International Symposium, 2004. IEEE*, vol. 3, pp. 3167 – 3170, Jun. 2004.
- [4] J. Grosinger, L. W. Mayer, C. F. Mecklenbräuker, and A. L. Scholtz, “Determining the dielectric properties of a car tire for an advanced tire monitoring system,” *Vehicular Technology Conference. VTC 2009-Fall. IEEE 70th*, Sep. 2009.
- [5] G. Lasser and C. F. Mecklenbräuker, “Dual-band channel measurements for an advanced tyre monitoring system,” *Vehicular Technology Conference. VTC 2010-Spring. IEEE 71th*, pp. 1–5, May 2010.

# SIMULATION OF VENTILATION EFFECTS ON INDOOR RADON IN A DETACHED HOUSE

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**Abstract.** Computational fluid dynamics (CFD) is widely used in indoor air quality, air flow pattern, indoor pollutant distribution and thermal comfort as a cost effective and powerful tool.

The intention of this article is to use CFD as a standalone tool to simulate indoor radon distribution and ventilation effects on a one family detached house in Stockholm. A mechanical balanced ventilation system was used to provide the indoor ventilation rate, a continuous radon monitor (CRM) and alpha track detectors were also used to measure the indoor radon levels.

Results of measurements, numerical and analytical study indicated that ventilation rate and infiltration through door or window has significant effects on indoor radon content. As shown in this case study the radon content has reduced whiles the ventilation rates increasing.

**ABSTRACT GENERATED VIA CONF TOOL DATABASE**

# SIMULATIONS OF LONGITUDINAL DYNAMICS IN HYBRID VEHICLES FOR LOAD SPECTRUM PREDICTION

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**Introduction.** Since the automotive industry has just begun to explore the variety of combinations of two different power sources in one car, experience regarding changed loads must be improved. Considering the additional degrees of freedom, ranging from power train topology up to the strategies of realising drivers inputs (i.e. throttle and brake), simulations have become a major instrument in the development process. Depending on the focus of analysis, different methods and tools for simulation are used in the automotive industry. In this paper, representative customer driving cycles are simulated with a model of a complete hybrid car, focusing on the loads of the power train, especially the hybrid components. In general there are two different approaches for realising the simulation, whereas both of them require input in form of a desired vehicle speed. The commonly called backward-simulation calculates the acceleration via the speed profile, the resistances, the longitudinal force on the tire and further, the torque and angle speed at different components of the drive train. This simulation method does not respect dynamic influences (like tire slip) and especially in hybrid cars there is the difficulty of estimating the hybrid strategy made by the controlling unit from the backwards direction. [2] The other approach is the commonly called forward-simulation, which is discussed in this abstract.

**Load spectra.** A load spectrum is classically defined as compressed information about the load (such as force) in time domain on a mechanical part. The methods of compressing the information depends on the mechanism of fatigue. A famous example is the rainflow counting method. [3] For the development of hybrid cars the idea of a load spectrum has been extended to electrical components and overall states of the power train.

**The modelling.** The model of a hybrid power train for the prediction of load spectra with means of forwards-simulation is split into 3 parts:

**The driver:** The driver tries to follow a defined speed. This speed profile might be the output of a measurement-drive with an existing vehicle in a strictly defined cycle representing customer use. This allows the comparison of two (or more) vehicles and/or strategies. The profile has to be defined as speed over distance, so that different speeds, resulting from the driver's inaccuracy in following the profile, won't result in different total distances. For hybrid vehicles, the state of standing still may also be important if. That is why it is reasonable to additionally define stopping distances, within which the driver stops the vehicle for a certain time and then switches back to distance-based speed-lookup. For longitudinal analysis the two main inputs from the driver are the throttle and the brake. At the current status of this project, those two are implemented as PI-controllers, which do not yet represent the true behaviour of human driver. One issue is switching between the two pedals, if the actual speed is oscillating around the desired speed. This results in changes in the control unit and does not represent a human driver. A way to avoid this problem is to additionally define where to brake and where to accelerate in the speed profile.

**The physical model:** The mechanical model used for simulating is basically a rotating system ranging from the combustion engine to the wheel (for longitudinal analysis it's basically the same), where the rotation is transformed into a translation. Torque, defined by the control unit, can be introduced into the system by 3 components: The combustion engine, the electric motor and the brakes. Of course transmissions in the power train have to be respected. If the control unit opens a decoupler, the train splits up into two independent parts. Every part of the power train (especially gears) transforms torque into heat by friction. The electrical model consists of the electrical machine, the inverter, the battery and other electrical aggregates.

**The control unit:** The control unit executes the driver's input by throttle and brake by sending torque requests to the three components described above and sending gear requests to the shift gearbox. This operating strategy can be very complex, since driving and vehicle situations can vary widely and is part of the development philosophy of the automotive industry. The implementation of this strategy has to be reduced to main influences and parameters for realizing a proper simulation of the cycles.

- [1] A. Huber. *Ermittlung von prozessabhängigen Lastkollektiven eines hydrostatischen Fahrtriebsstrangs am Beispiel eines Teleskopladlers*. Karlsruher Schriftenreihe Fahrzeugsystemtechnik, 2010, 16 - 27.
- [2] B.Bertsche, G. Lechner. *Zuverlässigkeit im Fahrzeug- und Maschinenbau: Ermittlung von Bauteil- und Systemzuverlässigkeit*. Springer Verlag, 2004, 292 - 313
- [3] M. Stiegeler. *Entwurf einer vorausschauenden Betriebsstrategie für parallele hybride Antriebsstränge*. Universität Ulm, 2008, 13 - 16.

# THERMODYNAMICAL COUPLING OF A MACHINE TOOL WITH ITS ENVIRONMENT

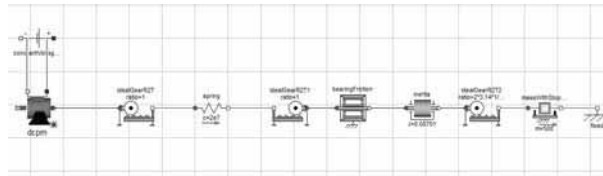
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**Introduction** Energy optimization is a very hot topic at the moment. For this reason, the research project INFO<sup>1</sup>, which is supported by the FFG, the Austrian Research Promotion Agency, tries to make a comprehensive simulation of a production plant, including all aspects, like machines, processes, the building envelope and so on, to be able to make qualified predictions about the impact of certain energy-saving measures. In this context, the issue of coupling different model-parts is very interesting. This work shall present a way to couple a simple machine tool with the environment surrounding it. A linear guiding device is chosen to represent the machine tool and for the environment, the surrounding room is discretised into compartments. The chosen modelling ansatz for both partial models is physical modelling, a block-based, acausal and object-oriented approach to model physical systems.

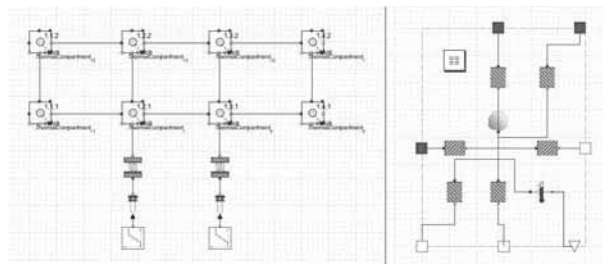
**Machine tool** The linear guiding device is a very simple part of the machine tool. It consists of a permanent magnet DC motor that is connected to a thread bar via a gear belt. The thread bar moves a cart, where the sliding mass is attached. A model of this setup using components of the modelica standard library is depicted in the figure below. The dissipative elements of the system, that are considered in the model are the electric motor, the bearing



Linear guiding device with drive motor model in Dymola

friction and the friction between the thread bar and the cart. The heat emission of these components is calculated in the respective blocks and can then be used as a heating source for the environment model.

**Environment** For the model of the environment the room is discretised into compartments. Each compartment has its own thermal mass, which depends on its volume, and for the heat transfer into adjacent compartments only thermal conductance is considered. The thermal properties of the air, namely the density, specific heat capacity and thermal conductivity, are assumed to be constant, because the rise of temperature in the compartments is expected to be small and therefore an impact of temperature-dependent parameters on the simulation results can be neglected. Additionally the walls of the room are assumed to be perfectly isolated, so there is no heat exchange between the compartments and the adjacent walls and therefor no energy is lost in the system. The figure below depicts the room model and one of its compartments, the parameters for the compartment are the dimensions into the three axes, the rest of the parameters, like volume or thermal capacity are calculated in the parameterblock seen in the top left corner. The components are again taken from the modelica standard library. One advantage of this



Room model and one compartment modelled in MapleSim

modelling approach, using compartments, is, that the model can easily be refined, if a higher resolution should be necessary.

- [1] Modelica Corporation, *Modelica - A Unified Object-Oriented Language for Physical Systems Modeling – Language Specification Version 3.2*, March 24, 2010  
<https://www.modelica.org/documents/ModelicaSpec32.pdf>

<sup>1</sup><http://www.projekt-info.org>

# TRACING HERD IMMUNITY AFTER VACCINATIONS IN SIS-MODELS USING CELLULAR AUTOMATA

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**Introduction.** The aim of our work was to examine the effect of herd immunity in a model for pneumococcal infections. By herd immunity we understand the effect that after the introduction of a vaccination the portion of infected individuals decreases more strongly than just by the portion of vaccinated individuals.

This work was undertaken as an extension to the work of the cooperation between HVB (Hauptverband der österreichischen Sozialversicherungsträger) and Vienna UT (see e.g. [3]) where the decrease of the infection rate under the above conditions was modelled using differential equations and an agent-based approach. We were considering a similar model using a cellular automaton (CA). Making use of this simplified model, we had the advantages of easier implementation as well as lower computational complexity.

**Implementation and Choice of Parameters.** We implemented an FHP-lattice-gas CA in MATLAB (see [1] and [2]). As we represented the hexagonal structure using a matrix, part of the symmetry was lost and we thus had to distinguish between *even* and *odd* rows of the matrix. We described the state of the CA at any point in time with an  $n \times n \times 6$ -matrix. During each time step the FHP-I-transition algorithm (see [2]) was applied.

The model had to be chosen in such a way that it could be used to describe the infection with *Streptococcus pneumoniae*. For this purpose we used the SIS-model: Each particle of the CA represents a person which is either susceptible, infected or vaccinated. After recovery infected individuals return to a susceptible state. By means of the infection probability, immunisation rate and random matrices, we used the number of infected particles in a cell at each time step to calculate the number of infected particles in the subsequent time step. Each time step was presumed to represent a day and the length of infections to be normally distributed with mean 12 days.

Due to the lack of data for infection probabilities, in the initial step we set the rate of vaccination to be zero and chose the infection probability such that the initially assumed proportion of infected individuals within the overall population remained approximately stable over time. We computed the portion of infected individuals (0.1646) by averaging the rates of infections for *Streptococcus pneumoniae* for the different age groups and the population data for Austria as of 2007 (according to Statistik Austria, <http://www.statistik.at/>).

At the next step we introduced a vaccination rate of 0.1. This means that 10% of the population are vaccinated. As we only simulated the CA over the duration of 1 to 2 years, we did not consider the expiration of the protection provided by the vaccination or the influence of restoring immunity by re-vaccination. In order to circumvent effect caused by the great fluctuations in the number of infected individuals in the beginning, we ran the CA for 200 time steps without any vaccinations taking place and took the values thereby obtained as the starting point for the actual simulation incorporating vaccinations.

**Results.** For a  $300 \times 300 \times 6$ -CA which is (statistically) occupied with half of particles possible (which correspond to individuals), an average duration of infection of 12 days and a running time of 500 days, we varied the parameters  $r$  (infection rate) and  $v$  (proportion of vaccinated individuals within the overall population) and averaged over 10 runs each: We used five different values for the infection rate  $r$ :  $r = 0.0385, 0.039, 0.0395, 0.04$  and  $0.0405$ . For all these values we achieved approximately the same portion of infected individuals within the population. Once herd immunity occurred, the effects of different infection rates were different, though. For lower infection rates, the portion of infected individuals decreased more strongly given equal vaccination rates. For the vaccination rate  $v$  we used the four realistic values  $v = 0.05, 0.1, 0.15$  and  $0.2$ , as well as the value  $v = 0.9$  which would correspond to an almost complete immunisation of the population. Unsurprisingly, this value induced the extinction of the infection. We learned that for a relatively low vaccination rate of 5% the portion of infected individuals decreases by approximately 30%. For  $v = 0.2$  that decrease amounted to even about 90%. However, the effect of the herd immunity was proportionately diminished for larger vaccination rates.

- [1] H. Hötzendorfer, N. Popper, F. Breitenecker. *Temporal and Spatial Evolution of a SIR-type Epidemic - AR-GESIM Comparison C17*. Simulation News Europe, 2004, 41/42: C17.
- [2] D. A. Wolf-Gladrow. *Lattice-Gas Cellular Automata and Lattice Boltzmann Models - An Introduction*. Springer, Lecture Notes in Mathematics, Vol. 1725, 2000.
- [3] G. Zauner, N. Popper, F. Breitenecker. *Evaluation of Different Modeling Techniques for Simulation of Epidemics*. Proceedings of the 7th Congress on Modelling and Simulation, (Eds.: M. Snorek, M. Cepek, Z. Buk, J. Drchal) 2010, 2: 791 - 796.

# USING OPEN SOURCE GEO-DATA IN AGENT-BASED MODELS OF HEALTH CARE UTILIZATION

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**Introduction.** The individual choice of a medical service provider depends on a variety of properties. Among them are the type of service required, coverage of health insurance, quality of the facility, accumulation of multiple treatment options and the distance to the patients domicile. The latter is an apparent yet fundamental property, which – in a nation/system wide dynamic simulation of these decision processes – confronts us with different problems. We discuss the integration of geographic information into an agent-based model for simulating the dynamic distribution of patient-provider relations based on real health care and geographic data. Our work is connected to a research cooperation of Vienna University of Technology and the Main Association of Austrian Social Security Institutions.

**Geographic Data.** The basis of processing geographic information is a common coordinate reference system (CRS) and tools like program libraries and database systems which are capable of performing geographic transformations, calculations or queries. Open-source projects like *PostGIS*, *OpenStreetMap* (OSM) and *QuantumGIS* have proven to be the best choice for our purposes. Not only do they provide a free of cost high quality state of the art tool-chain for organising and processing geographic data but they also allow us to use a huge database of cartographic data (OSM) and to combine data from different sources (e.g. *Statistics Austria*) and of different type (e.g. raster data) into a single database.

The most difficult part of obtaining and preprocessing geographic information does clearly not concern cartographic data and tools. The challenge lies in bringing health care data into a geographic context. Especially health care data is very sensitive in terms of protection of privacy and thus must be anonymised, clustered or even blurred. The very direct consequence of anonymised data is that we can no longer identify single individuals and their history of visited providers (i.e. their decisions). This fact is unavoidable but does clearly not render any dynamic simulation based on anonymised data useless in the first place [1].

A greater challenge are incomplete data sets, an inconsistent naming system or the complete lack of information which would enable geographic allocation. The reason for these drawbacks are the great number of different institutions involved in the processes of initial data acquisition and the lack of an immanent necessity to collect geographic information. Furthermore we have to use reverse techniques to regenerate a reasonable distribution of the locations of the patients domiciles. This can be achieved by randomly distributing the domiciles based on the actual population density and the geographic information included in the health care data.

**Techniques.** For integrating geographic information into an agent-based model several steps are necessary:

- Import of all required data into a single database. This involves decompression and extraction of data from different sources and formats, alignment of nomenclature and transformation to a common CRS.
- Basic geographic information (concerning providers and patients) is given in terms of addresses, postcodes or assignments within a political structuring. Based thereon geographic locations (coordinates) must be assigned to all agents of these groups by searching cartographic data (OSM) or by the technique mentioned at the end of the last section. Latter is based on raster data on population count which must be combined with a political structuring. As a consequence we have to solve a large number of *point-in-polygon* problems [2] in order to distribute the patients in the resulting polygon grid (intersections of raster cells and political districts).
- In order to speed up simulations, computationally intensive operations like finding the shortest route between two locations or deciding whether a location lies within a certain area must be precalculated.
- For integrating the resulting database into a dynamic simulation we have to use software libraries or modelling frameworks which are capable of accessing database systems, provide basic geographic processing tools and allow appropriate (even interactive) graphic display of results.

Steps one to three can be combined in an automated preprocessing tool, which allows to quickly react on the highly dynamic geographic data which is available from OSM. For implementing a test model we rely on *AnyLogic*, *GeoTools* and self-written Java classes.

[1] Urach C., Breitenecker F., Miksch F., Popper N., Wilbacher I., Zauner G.: *Distance Dependence on the Willingness of Patients to Participate in Ambulatory Heart Rehabilitation Programs*. SMDM Society for medical Decision Making Europe 2010 - Public Health Decision Making, Target Conferences Ltd., 2010.

[2] Haines E.: *Point in Polygon Strategies*. Graphics Gems IV, (Ed.: Paul Heckbert), Academic Press, 1994, 24-46.

## VALIDATION OF OPTIMAL STRATEGY FOR PORTFOLIO MANAGEMENT USING TECHNICAL ANALYSIS

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At present most of traders use in the portfolio management certain strategy (set of rules). This strategy might be one of the existing popular trading algorithms or developed by trader. Although in case of the utilization of well-known strategy, parameters of rules can vary significantly. In such a way, two essential parts of the trading strategy design are the approximate estimation of the trading strategy efficiency and the validation of the system relevance. The first is carried out due to the algorithm testing on historical data; the second is the optimization process of indicators parameters. Due to the testing and the optimization process one can get the model of rules strategy to utilize in the investment activity. There are a number of appropriate literatures according to the strategy design. Still there is no methodology to estimate the trading algorithm relevance criteria.

At the stage of the identification of the strategy parameters indicators the problem of the optimal values determination appears. Often the strategy optimization is associated with the objective function fitting. Due to the large set of historical data and a number of rules (indicators) of the trading strategy the high profitable trading system might be developed. The optimization of the trading strategy includes several criteria of the effectiveness. In most cases, values that demonstrate the higher return on account or other objective used to determine the best conditions of the entry/exit position are selected as strategy rules. This approach results in unstable performance of the strategy algorithm with identified parameters values in another analyzed set of data or stocks. Consequently, there is need on criteria of the testing results analysis and valid data selection in the strategy design process.

The parameters that were identified as the most optimal in one range of historical data of the financial instrument price might be not necessarily optimal in another range or the security. In such a way, the estimation of the trading strategy should be conducted with the application of the additional criteria of the algorithm efficiency (stability of the algorithm performance). For the strategy developer there is need on the methodology of the relevance identification of the strategy on the adjusted criterion. One of the major problems of the trading strategy design is the estimation of the trading system robustness. Though there is no specific methodology to identify the robustness of the trading strategy. Today, under the robustness requirement is regarded that the system demonstrates stable performance of the trading strategy algorithm. And the problem of relevant choice of obtained results remains unresolved.

Therefore, it is proposed to take additional step after the optimization – the selection of those set of rules that possess the robustness property. It is suggested that robust trading strategies are characterized by the maintenance of the optimal values in various data samples and considered stocks. So, one of the possible ways to verify the strategy relevance is the analysis of the equity curve. Another step in validation of trading strategies is the relevance of obtained parameters on data out of the testing sample. This is usually used at the stage of the strategy testing. Consequently, it is essential to estimate the trading strategy both in the context of major efficiency statistics in given period of time and analysis the average system performance. The system efficiency should be estimate with taking into consideration the next price value out of the sample that reduces in the false treatment of the efficiency indicators set. For the precision rejection in the effectiveness analysis of the investment result it is assumed to use instead of current value of the strategy return in the end of the testing period the average estimation of the investment result. This robustness criterion analysis is assumed to conduct visually with the application of trading strategy efficiency diagrams. So, the robustness estimation currently checked manually. Further research of the strategy robustness determination is focused on the more formalized strategy analysis and the computer-aided robustness criterion evaluation.

In this paper the analysis of the optimization results validation is supposed to solve in the context of stable performance of the strategy algorithm, resulted in the maintenance of the efficiency statistics and obtained rules parameters, equity curve and the interposition of the optimal values areas in different time ranges or list of financial instruments.

- [1] R. Pardo. *Evaluation and Optimization of Trading Strategies*. Wiley John & Sons Incorporated, New York, 2008.
- [2] J. Katz, D. McCormick, D.L. McCormick, J.Owen. *Encyclopedia of Trading Strategies*. McGraw-Hill, New York, 2000.
- [3] F. Hampel, E. Ronchetti, P. Rousseuw, W. Stahel. *Robust Statistics. The approach based on influence functions*. World, Moscow, 1984.



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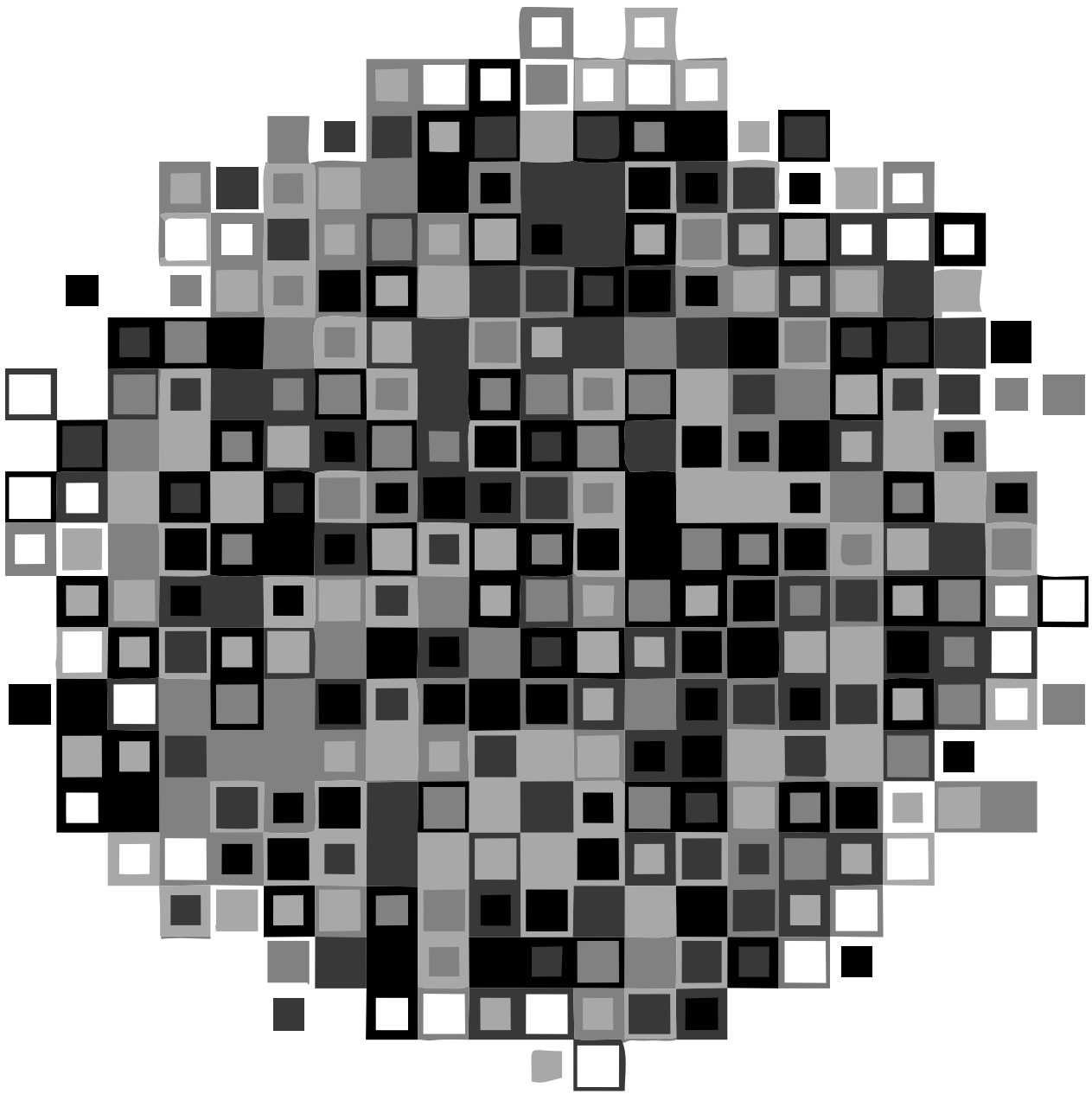


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