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PARALLEL ASPECTS OF MODELLING VERSUS IMPLEMENTATION IN HYBRID SIMULATION APPROACHES

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Abstract. The keyword parallelization is usually applied when speed is of essence. That normally means dividing the problem in such a way that parallel application of similar calculations allows for a quicker arrival at the result („*divide and conquer*"). In this case, the keyword „parallel aspects" is, however, used to make a fundamental statement about the permutability of modelling and implementation while developing a mathematical model in general as well as about the specific implications this has for hybrid models that use different parallel or serial approaches to calculate a real system.
A mathematical model is developed in different stages. A model is first broadly designed, then placed in mathematical phrasing and then suitably implemented. This paper will show that these processes are not, as is usually assumed, utterly independent of each other, but must be considered interdependent. The way each is executed strongly influences the others.
This point will be illustrated at hand of an example of the effects the stages of modelling have on the choice of relevant sets of parameters. These do not only change in terms of numerical stability, but also reflect the structural differences of varying models of one and the same system. These considerations are of course particularly relevant regarding hybrid models. In our case, two or more models of the same real system are calculated in parallel or serially. Several cases must be considered: In the case of model approaches with similar structures, the parametrization follows the same sets of parameters. In a different case, the "permutation" of modelling and implementation described above renders different sets of parameters necessary. Using different model approaches that demand different parametrization leads to problems in validating and verifying the models. On the other hand, however, it also opens up new possibilities for the structural representation of real systems.
Classical controls have to adjust the actual value to a given target value. The same task is given for whole structures in complex real systems. We are dealing with an actual system and a target system. One has to allow for a process change within a simulation. In order to make this possible, the transitions between the different system states must be sufficiently described and clearly implemented. The paper will conclude with some thoughts on the practical applicability of these processes of representation or identification.

1 Introduction

The development of modelling approaches that allow the calculation of simulations occurs via different stages. Classically, the problem is analysed, a model is designed, then phrased mathematically, implemented and finally identified. These stages are usually treated separately, isolated from the other stages and often – especially in larger scale modelling projects – they are worked on by different persons. While this is a sensible procedure with a view to a professional application of projects, it has led to the problem that these stages are now understood as in principle independent from each other.

While working on the *Argesim Comparisons* – a series of sample exercises on analysing modelling questions [2] that are regularly published in the journal SNE (Simulation News Europe) –, the following question arose: Where does the aspect of modelling end and implementation begin? Take the following example: Discretisation of a differential equation means (leaving apart the modelling of the differential equation itself) that an existing exact model is replaced by a less exact but calculable "replacement model". However, this step is in principle absolutely equivalent to the previous step of making assumptions in the process of modeling in order to be able to arrive at the differential equation itself in the first place.

While we can make exact statements on admissibility, area of validity and exactness of the result that is to be calculated thanks to brilliantly developed mathematical theories, this leads to a *difference of the two stages* in their application, but *not in principle*. More precisely, the fact that numerics has established itself as an independent discipline while modelling has not makes the two stages different in how they can be practically solved but not in the problem they pose.

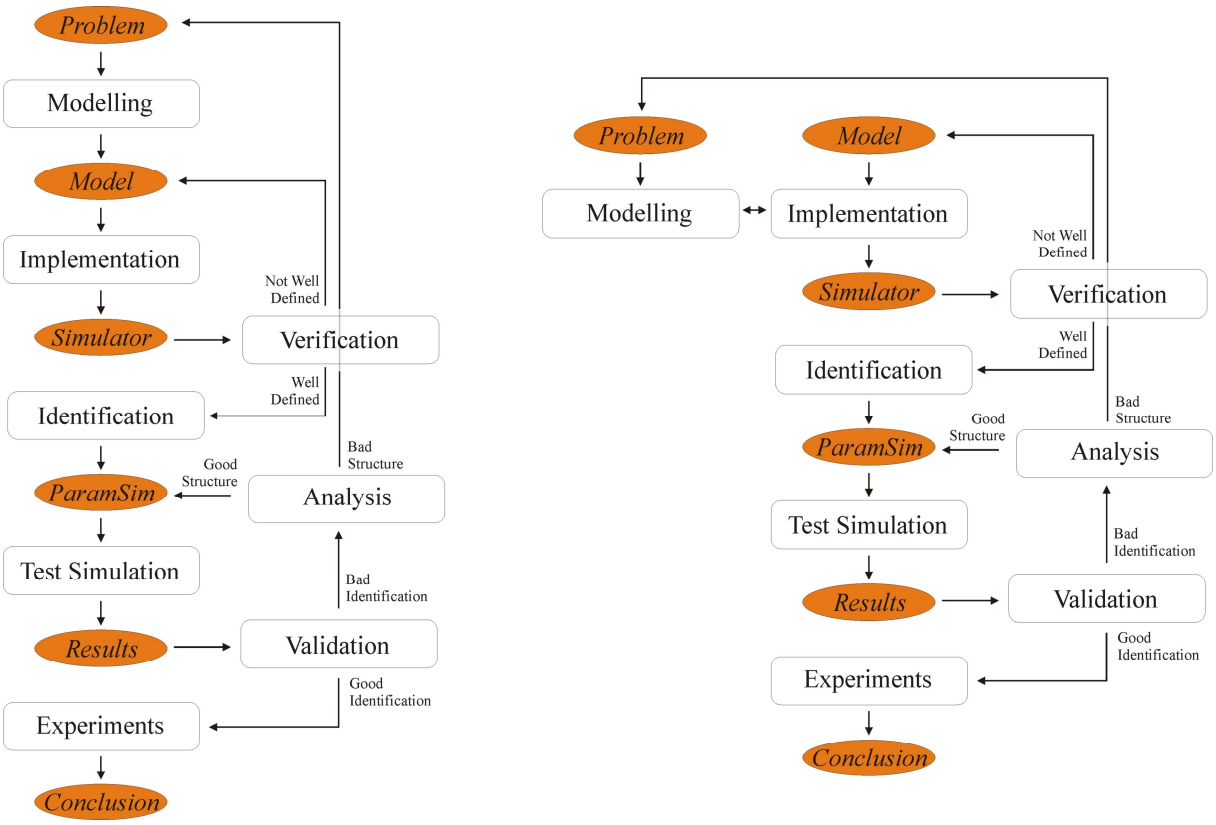

Figure 1. Depiction of the simulation cycle with the simplification of uniting the definition of a formal model and mathematical phrasing into a single step

This principle is the same in both cases. Complexity is reduced in favour of usability of the resulting model. The important aspect of this thought is that the step of discretisation of a differential equation has a lasting effect on the behaviour and structure of the system model just as the assumptions made in the modelling process do. Specifically, each approach demands different parametrizations, which may differ drastically and thus strongly influence modelling and identification. This will be demonstrated in chapter 2 at hand of an epidemic model. The problem of using such different approaches simultaneously in hybrid models (and the interface problems arising thereof) will be sketched out in chapter 3.

The relevance of this research question becomes apparent when looking at problems of model reduction as used e.g., in the calculation of technical systems. We refer as an example to the thesis submitted by W.M. Weidinger [10] from our own research group. In his case, the calculation of a given new type of aeroplane demanded a reduction of the entire system's degree of freedom – i.e., an alteration of the system structure itself – in order to make the model calculable, as purely numerical limitations did not suffice. Further GPU *(Graphics Processing Unit)* models are currently being developed that quite consciously relinquish exactness or partly even the ability to predict the degree of result exactness in favour of faster calculability. They follow the approach of using a "convergent" series of results in order to limit the result range step by step. The aim is to iteratively reach a suitable model by adjusting the model structure and to arrive at an appropriate solution only *via this iteration.*

2 Parameter Identification in Different Models of Epidemic Dynamics of SIR Type

As described above, the choice of model influences the parametrization not only in terms of numerical stability or in potentially leading to problems in the eradication of state events that may arise (see, e.g., Argesim Comparison C12 [6]). Its influence extends also to the quantifiability of parameters, *viz.* the connection between model structure and such quantifiability.

2.1 ODE v. LGCA Model Description

W. O. Kermack and A. G. McKendrick proposed in 1926 a simple SIR model for epidemic spread based upon a system of non-linear ordinary equations. Taking into account different simplifications, the following system arises:

$$\begin{aligned}\frac{\partial S(t)}{\partial t} &= -r \cdot S(t) \cdot I(t) \\ \frac{\partial I(t)}{\partial t} &= r \cdot S(t) \cdot I(t) - a \cdot I(t) \\ \frac{\partial R(t)}{\partial t} &= a \cdot I(t)\end{aligned} \tag{1}$$

Here *r* is the infection rate, a the recovery rate, *S(t)* the number of susceptible individuals, *I(t)* the number of infected individuals and *R(t)* the number of recovered individuals, at time *t* respectively. This classical ODE model does not reflect any spatial distribution.

The spread and recovery of an infection can be interpreted as a diffusion process among particles (= peoples). Therefore, a lattice gas cellular automaton (LGCA) can be considered as describing the epidemic. LGCA are two-dimensional cellular automata with particles moving from cell to cell during each time-step of the automata. We have to distinguish between the HPP (Hardy, de Pazzis, Pomeau - 1973) and the FHP (Frisch, Hasslacher, Pomeau - 1986) model. The FHP model consists of a hexagonal structure containing a maximum of six particles per cell again being defined by its lattice-vectors connecting the cell to its six nearest neighbours. The models can be compared and by showing (under certain assumptions) the equivalence of the models both in quality and quantity different properties of the systems can be described. For a detailed description of the model and the presumptions we refer to [7], for proof of equivalence to [5].

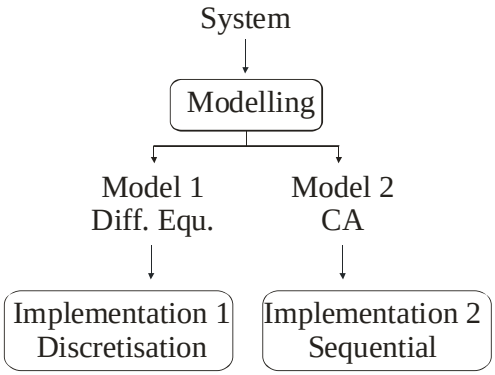

Figure 2. Two Different Models Representing the Epidemic Dynamics

2.2 Parameter Sets

Simulation with the ODE model can be compared with the results of the LGCA model. For this comparison, adequate parameters and spatial distributions have to be chosen. As we chose parameters for the ODE system (Table 1) we can simply use parameters for population sizes in the LGCA model and infection and recovery rates can also at first sight be transformed to the LGCA in a simple way.

$S(t=0) = S_0$	16000
$I(t=0) = I_0$	100
$R(t=0) = R_0$	0
Infection rate *r*	$0.6 \cdot 10^4$
Recovery rate *a*	0.2

Table 1 initial values and parameters for comparison of ODE and LGCA model

A FHP LGCA with a domain size of 100×100 (and therefore 10^4 hexagons), with infection rate of $r = 0.6$ and periodic boundary conditions to remodel the system was implemented (as initial configuration, uniformly distributed individuals of type *S* and *I* were chosen).

However, the results show the problems of parameter identification, as the presented results (figure 3a and 3b) are of similar qualitative nature but differ quantitatively for the different approaches. One reason for this is the fact that infected individuals form spatial groupings in the LGCA and thus slow down the speed of the epidemic. This can be described as a structural difference as we have homogeneous behaviour on the one hand and inhomogeneous behaviour on the other, where infection occurs within one cell of the automaton, rendering the infection probability much lower as no more than a few individuals can “meet” in one cell. When we introduce total

random motion in a HPP-LGCA, the speed of the epidemic slows down even more since nearly no mixture of individuals takes place.

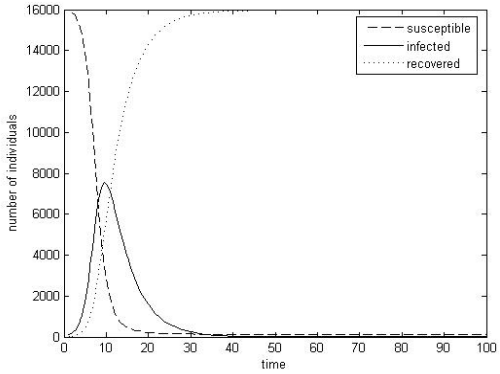

Figure 3a Simulation results for ODE model

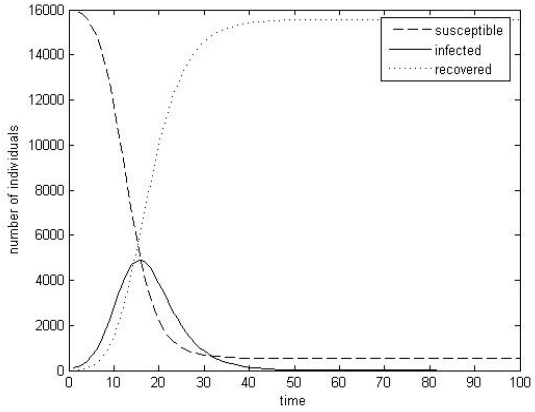

Figure 3b Simulation results for FHP LGCA model

This structural problem can be solved ostensibly. For lattice Boltzmann cellular automata it can be shown that the averaging states converge under certain circumstances to solution of the continuous Boltzmann equation. For the investigated LGCAs, a kind of "convergence" can be shown experimentally. The idea is to prevent clustering in the LCGA and observe again the average states, ensuring perfectly uniform distributions for all three groups of populations (*S(t), I(t), R(t)*) by randomly rearranging all individuals in every time step of the automaton.

However, the "interdependence" of model structure and parametrization cannot be entirely resolved. On the one hand, it soon becomes evident that population size and raster size are directly interdependent and have a direct impact on the quantitative results of the model. On the other hand, one can see that the infection and recovery rates directly react to the resultant concentration. These relationships are obviously manageable in this model, which was consciously chosen for its simplicity. However, the example nevertheless demonstrates that model structure and parametrizability are (or can be) inextricably connected. More complex problems as arise in relevant areas for modelling approaches result in the difficulties described above, as they – if at all recognized – can no longer be suitably - i.e. exactly in the quantitatively same way - parametrized. This is particularly problematic when the two model types are to be used within one and the same simulation.

3 Hybrid Models and Parameter Interfaces

These points are of course particularly pertinent to hybrid models. In hybrid models, two or more models – or model parts – of the same real system are calculated in parallel or serially. This can be necessary or expedient for two reasons. Firstly, complete models are with this method better able to represent different properties of one system – the more appropriate of the methods available can be used. In the example cited in chapter 2, that would be the ability to better mathematically analyse the ODEs with classical models (existence, uniqueness, etc.) on the one hand and the ability to better represent inhomogeneous aspects or the population dynamics using LGCA models on the other.

The second reason for applying hybrid models is the expedience or necessity of modelling different system parts with different models. It must be noted that this problem does not – in contrast to many hybrid models – result

from the existence of, e.g., state events, like, for example, in the „Constrained Pendulum“ (Argesim Comparison C7) but is rather based on a strategy to model different model parts through different models with different properties. While this brings heightened flexibility in adapting the model to system structures on the one hand and existent data sources on the other, one has to pay a price of consistency loss and problems of validation and verification.

3.1 A Hybrid Influenza Model

The research group developed a model on the spread of influenza [4] in real populations based on the epidemic model described above. While classical approaches are based on differential equations, the approach used in the development of this model was based on individuals – in this case leading to a hybrid model consisting of cellular automata and agent-based models. The framework of the model was given by daily routine (working hours, „leisure time“, time at home / family time) and a partition of the population (babies, preschoolers, primary school children, secondary school children, adults, seniors) based on demographic data such as age structure, family size, size of workplaces, schools and childcare facilities. From this framework, it is easy to see that a representation in such detail is not (and in particular not identifiably) possible using classical methods.

The primary structure is an agent-based model. Individuals are represented as agents, who can have different properties, such as infection status, affiliation to neighbourhoods, workplaces, schools, etc., as well as information on age, etc. The agent-based model connects the different partial models with each other.

Those workplaces, schools and neighbourhoods (leisure time environments) are implemented as lattice-gas cellular automata (LGCA) of type FHP-I (see [11] for further information). Within them, the agents move and are at risk of infection through contact with infected agents with respective probabilities. In households, the number of agents is very small and contact can be taken as given. Therefore, households are modelled by simple probabilistic routines. Within the CA the agents loose all their properties except for their unique ID-key. This key becomes the content of particle within the LGCA. If any infections/deaths happen during the runtime of the CA the change is written directly into the affected agent’s column of the look-up table.

This procedure is repeated for all workplaces/schools/childcare facilities. After these are finished the leisure-time neighbourhoods are processed in the same way. This implementation has several advantages. First of all it is necessary to program only one routine for cellular automata. The same routine is used for every unit of the model, the dimensions are simply adjusted to the number of agents within and to the desired density of the CA-population. Thus it would be possible to assign different densities (space per individual) to different “places of work” (e.g. workplaces and schools). Secondly, all agents who are not inside the currently processed automata are not exposed to the model's time. This means that at the end of the day all agents did spend the same amount of time within cellular automata even though they were merely “parked” for most of the time.

Of course this model largely uses simplifications. For example, the routes taken from one unit to another are not modelled. Also, different working times of agents are neglected, as are certain “hot spots” for the spread of diseases such as hospitals. The implementation of the neighbourhoods is also a simplification. All agents are put into their neighbourhood every day with the same other agents. However, this can be interpreted as a pool of personal contacts (ranging from friends via neighbours to doctors and lawyers).

3.2 Interface Problems

The problem of the interface is quite simple in the case of this model. The agents lose all properties when entering the cellular automata, but keep their ID – hence their properties are saved and can be recalled at any time. As ABs and CAs are structurally so similar, there arise no difficulties such as having to translate individual properties into population parameters. Put simply, the parametrization of one part-model is a real subset of the set of parameters of another part-model. This is different in the model described in chapter 2. Hybrid approaches are difficult in that case, as such translations would be necessary. This step would be possible, but it would greatly reduce the ability for consistent validation, which must include a system's parameters and structure.

To sum up, it can be stated that as long as the sets of parameters remain „similar“, i.e., the same parameters can be identified with values that are quantified in the same way, the resultant problems can be limited. In particular, the validation of the model remains easily achievable and a further barrier in the simulation cycle is removed. When, however, the sets of parameters differ strongly in structure and quantifiability – e.g., when, as was described, modelling and implementation are „interchanged“ – this greatly complicates plausible realisation in a hybrid model, as seen above. In such a case, it would be expedient to use the different modelling approaches as reference models, meaning to use two approaches to modelling one system in order to reach further insights by qualitative comparison. This procedure avoids the problem of an exact identical quantitative identification of the models, which is necessary for validation. Conversely, it would be helpful to keep in mind the resultant parametrization when choosing different approaches for hybrid models (and by implication also the structure of the part-models), as was done in the modelling example used in chapter 3.

3.3 Newer Possibilities for Structural Representation of Real Systems

In these cases, one must weigh up the advantages provided by such hybrid models. Particularly the difference of the modelling approaches brings with it the advantages of a hybrid approach, as seen in chapter 2. Despite all considerations concerning validation, one must not forget that actual use usually applies to systems that are already difficult to identify. Thus, hybrid approaches as described here (i.e., not contingent on state events or numerics, but based on system structure) are usually not used in mechanical or physical applications, but in the fields of health economics or sociology. In these fields, validation must always be seen in relation to the entire problem of available data.

4 Modelling Actual and Target Structures

A particular advantage is the possibility to represent a system change via different model approaches. Classical controls have to adjust the actual value to a given target value. The same task is given for whole structures in complex real systems. We are dealing with an actual system and a target system. One has to allow for a process change within a simulation. This means that the change does not only affect parameters or the dimensions of the parameter range, as described in classical models, but that the entire structure of a system is changed so fundamentally that the existing modelling approaches cannot represent both structure states. In order to make this possible, the transitions between the different system states must be sufficiently described and clearly implemented. In future, one will have to decide whether one is dealing with two or more well-defined structures, meaning that these structures are already clear at the time of modelling, or whether one is dealing with a target structure that is not clearly defined and is to be reached via optimising the actual structure. In the latter case, one has to clarify in a first step how the stages or changes in the structural behaviour may be defined. To give an example from practice, we briefly refer to a model for a cost refunding system of an Austrian social insurance agency that is currently in development. This system has to depict both the current structures and the target structures in its processes. This property of future models can and ought to support and make possible the introduction of dynamic modelling and simulations in new areas of application.

5 Model Credibility

In the applications named above, a model's credibility turns on the clear depiction of model structure, the assumptions that have led to this structure and the identified parameters. Classic validation and verifiability are merely single components. Especially when models give out counter-intuitive results, a well-chosen hybrid model may despite all difficulties described here be the key to success. One must, however, carefully evaluate such a choice, as tried and tested criteria for assessing the quality of models and simulation must not be cast off lightly. New approaches for ensuring quality in the realm of hybrid model types are still in their beginnings. An example are the first attempts to consistently classify modelling approaches in order to improve model evaluation [8].

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