ENABLING TOOLS AND TECHNIQUES FOR THE OPTIMIZATION OF THE HERACLES SIMULATION PROGRAM

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Abstract

Simulations conducted on high-performance, massively parallel mainframes have become a central tool in the study of astrophysical plasmas. HERACLES is a radiation hydrodynamics program used in particular to investigate turbulences in interstellar molecular clouds. In the framework of the COAST engineering project conducted at Saclay, a special effort has been undertaken to provide enabling tools and techniques for the HERACLES program, including the development of a multiple-grid approach to overcome spatial resolution limitations, optimization and parallelization methods, data handling facilities and visualization tools. COAST (for Computational Astrophysics) is a CEA/DAPNIA project dedicated to high performance computing in astrophysics. The originality of the project is the collaborative work of astrophysicists and software engineers with the aim to develop common tools and techniques for different independent astrophysical simulation programs. In particular, the techniques of multiple-grid and interlocked meshes are being developed in the finite volumes HERACLES program; these developments rely on parallelized algorithms for which optimization is pursued. The SD*vision* graphical interface, implemented in the framework of IDL object programming, is also presented, as the visualization tool for analysis of the computation results.

Keywords: Simulation, Data handling, Astrophysics, Visualization.

Presenting Author's biography

Valérie Gautard. Doctor in Applied Mathematics, Valérie Gautard launched her career on shape optimization in aeronautics at Aerospatiale and ONERA, before joining in 1999 the DAPNIA 'Laboratory of research into the fundamental laws of the universe' at CEA/Saclay as a research engineer. She was involved in the LHC/ATLAS experiment at CERN, as a developer of the muon detector software. She is now member of the COAST project (Computational Astrophysics), committed to the development of numerical methods in finite volumes astrophysical simulation codes. Furthermore, she is a teacher in computing at the University of Marne-la-Vallée for Master degree students.

1 The COAST project: a general approach of astrophysical simulation software

The COAST (for Computational Astrophysics) project [1,2,3] started in 2005 in CEA/DAPNIA at Saclay is an extensive program of simulations of astrophysical plasmas; astrophysicists and software engineers collaborate to rationalize and optimize the development of simulation programs by creating a core of common specific modules and using common software tools for data handling, post-treatment, visualization, numerical methods, parallelization and optimization. Physics studies involving various scales are performed, including cosmological structures formation, dynamics of the interstellar medium, stellar evolution and formation of proto-planetary disks. At this time, four simulation codes are developed, corresponding to each astrophysical domain. HERACLES [4] is one these programs.

2 The HERACLES program

2.1 Physics goal

The HERACLES program is mostly used for studying turbulences in the interstellar gas [5], which is of great importance to understand the formation of structures such as molecular clouds and is therefore determinant in the star formation process. HERACLES is also used for the study of inertial fusion plasmas [6].

Current studies focus on the thermal fragmentation of turbulent flows of interstellar hydrogen [7]. Molecular clouds form through the condensation of a warm and diffuse state into a cold and dense one. The thermal condensation of interstellar hydrogen gas involves four different spatial scales, each related to different physical mechanisms, from few 10 light-years to about 10^{-3} light-years, to be treated simultaneously. This dynamic range of 10^4 requires the introduction of multiple resolution techniques in the code, such as block meshes, multiple-grid and interlocked meshes methods.

2.2 Software status

HERACLES is a 1-D, 2-D and 3-D code in Cartesian, cylindrical or spherical coordinates in finite volumes using currently a fixed regular grid. It solves the equations of radiative transfer coupled to hydrodynamics. The fluid evolution is determined by the classical conservation equations (mass, momentum, energy) with source terms characterizing the momentum and energy exchanges between the fluid and the external radiation. The transfer equations are solved by a second order Godunov type method and integrated implicitly using iterative solvers such as Gauss-Seidel or GMRES.

HERACLES is written in Fortran 90 and parallelized with the MPI library [8], using up to 2048 processors in parallel on supercomputers like the massively parallel mainframes of CEA Computing Center in France or MareNostrum in Barcelona.

3 Numerical methods developments

3.1 Mesh status

All the HERACLES results up to now have been produced on fixed regular grids. The domain, the number of cells and the coordinate system are defined by the user. The domain decomposition is by default regular but can be adapted easily. The software is running on multiple-processor machines. Once the number of CPUs is known, the number of processors dedicated to each direction can be determined. Taking the Cartesian coordinate system example and introducing respectively

(i) Nx, Ny, Nz the number of cells in the x, y and z direction for the global domain

(ii) Ncpux, Ncpuy, Ncpuz the number of cells in the x, y and z direction for each cpu.

Ncpux, Ncpuy and Ncpuz are calculated to satisfy the equations (1):

$$Nx/Ncpux = Ny/Ncpuy = Nz/Ncpuz \qquad (1)$$

The physic quantities, such as the density, the velocity, the momentum, the pressure, the temperature and the energy are defined in each cell. Communications between cells are managed in the center and the corners of the cells. Finally, the boundary conditions are tackled.

The current fixed grid implementation implies limitation in domain shape and numerical resolution. The issue of the complex domain geometries can be addressed using a block meshes approach. Concerning the numerical resolution, 1200^3 cells are currently implemented while the physics would benefit from much higher resolution, typically about 10000^3 cells. To overcome this limitation, the COAST team is implementing the techniques of interlocked meshes and multiple-grid, as previously implemented in the JUPITER program [9] for studies of proto-planetary disks.

3.2 Current developments

3.2.1 Block meshes method

In order to better fit complex geometries, while optimizing the total number of cells, a block meshes method is currently implemented. As illustrated in Fig.1, basic fixed regular grids are positioned side by side in order to encompass the region of physical interest. The main drawback of this technique lies in the treatment of the communications between blocks, which adds a layer of difficulty in the parallelization process.

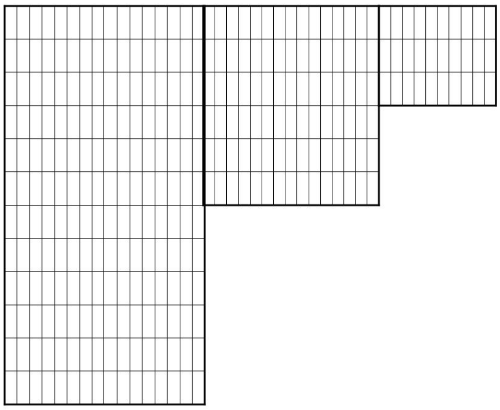

Fig.1 An example of multiple blocks mesh.

3.2.2 Multiple-grid method

To obtain more precision on special regions in the mesh, a multiple-grid method is being implemented, which consists of using refined meshes in the regions of higher gradients, as shown in Fig.2. A first, basic approach is to predefine several fine embedded meshes in the interesting regions and iterate on these meshes during the calculations. A dynamic way to perform the calculations will then be implemented, based on the experience of the manual method.

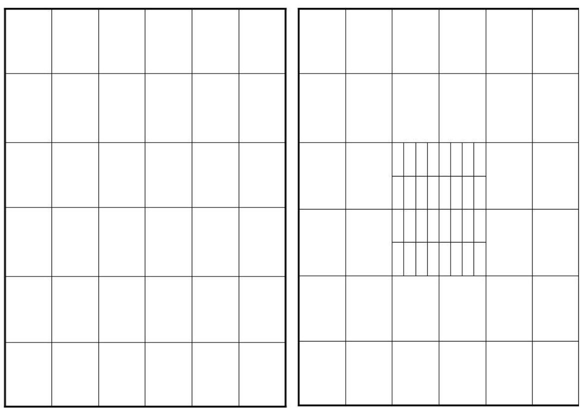

Fig.2 Two levels multiple grid meshes example; calculations, initially based on the left grid, are refined in the central region as shown on the right.

3.2.3 Interlocked meshes method

With the fixed grid version of HERACLES, radiation calculations are performed with an implicit scheme, which is very costly in time. For these calculations, interlocked meshes method consisting of embedded coarse-grained grids (Fig.3) used to make up-and-down iterations is under development. Comparisons will be made with previous version of the program to evaluate the improvement in computing time for a given precision.

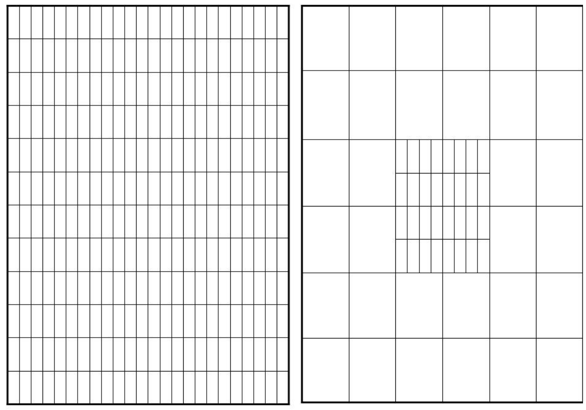

Fig.3 Two levels interlocked meshes example; calculations, initially based on the left high-resolution grid, are pursued on the grid shown on the right, where the resolution is degraded in peripheral regions.

3.2.4 MPI parallelization

The use of the MPI library for parallelization adds a layer of complexity in the implementation of multiples meshes methods in HERACLES. For efficiency reasons, the MPI optimization must be pursued; this implies to group the meshes in bundles, each bundle dedicated to one processor. This decomposition must be done automatically depending on the number of processors and the number of grids used by the modeling. Boundary conditions are managed at the same time on the MPI cutting and on the multiple grids of the mesh.

4 Data Handling

A unique format, HDF5 [10], the Hierarchical Data Format developed by the NCSA (National Center for Supercomputing Applications), has been chosen for storing data produced by the different codes of the COAST project. This choice allows the rationalization of the post-treatment and visualization tools. The HDF5 libraries are optimized for efficient parallel input and output. Post-processing and visualization benefit from fast and simplified navigation capabilities within the hierarchical structures. HDF5 is the latest version of HDF able to store the huge amount of data produced by the massively parallel simulations of the COAST project.

5 Visualization

The visualization plays a very important role in the development of simulations codes. It enables the control of the impacts of the codes' development lifecycle. Fundamental aspects including domain decomposition, initial conditions, message passing and parallelization, treatment of boundary limits, can be controlled and evaluated qualitatively through visualization. Once in production phase, visualization is also used one in the validation, analysis and interpretation of the results. A complete graphical interface named SD*vision* [11,12] has been developed in order to participate in the development of the simulation codes and visualize the large astrophysical simulation datasets produced in the context of the COAST program. It is used in particular to enable the development and use of the HERACLES code.

5.1 The SD*vision* graphical interface

The interface is implemented as a graphical widget providing interactive and immersive 3-dimensional navigation capabilities. The baseline technology is the object-oriented programming offered by IDL's Objects Graphics [13]. It benefits from hardware acceleration through its interface to the OpenGL libraries. An example of the widget displayed in its running state is shown in Fig.4.

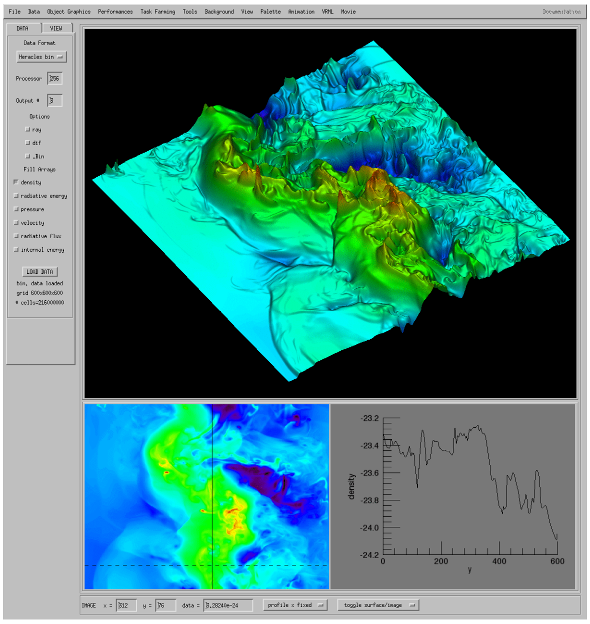

Fig.4 The SD*vision* widget used to visualize results from a 600x600x600 simulation of the turbulences in the interstellar medium obtained with HERACLES. In this example, a surface of the density distribution on a slice is displayed with a colored texture, together with an image and a profile plot.

5.2 Visualization of 3D scalar fields

The SD*vision* interface can be used to visualize interactively the scalar three-dimensional fields distributed over regular Cartesian grids produced by HERACLES. The visualization of such data fields is proposed in three different, complementary ways.

The first approach is the volume projection obtained by casting rays through the data grid. Using an optimized class of the IDL object library, such visual representation provides at a glance a complete, global view of the volume under scrutiny. Several compositing functions are available to account for the contribution of each individual voxel of the data set. An example of volume visualization obtained by maximum intensity projection is shown in Fig.5 for a large, 1.728 billion cells, HERACLES simulation. Another technique is the alpha-blending method used to favor sub-samples of the data volume by finely tuning the color and transparency tables. An example of such a visual representation is shown in Fig.6.

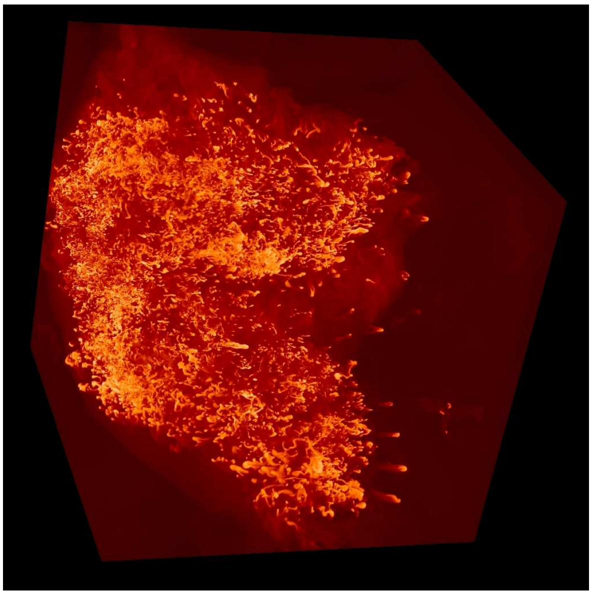

Fig.5 Visualization of the density field obtained in a high-resolution 1200^3 HERACLES simulation of turbulences in the interstellar medium. The rendering of the volume is obtained with the SD*vision* graphical tool using a ray-tracing algorithm.

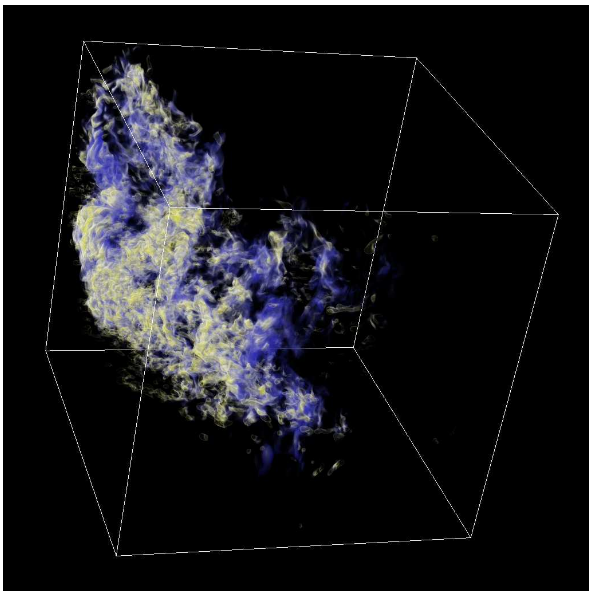

Fig.6 Visualization of the density field in a 600x600x600 HERACLES simulation obtained by volume projection using the alpha-blending technique.

The second approach is the isosurface representation. An isosurface is a 3D contour surface obtained using a method based on the marching cube algorithm [14]. In this purely three-dimensional approach, multiple isosurfaces of multiple variables can be generated by interactively setting the contour value on histograms of the corresponding data. The represented objects are Gouraud-shaded polygons that benefit from lighting by selected sources of illuminations. An example of multiple isosurfaces is shown in Fig.7

Finally, in a third approach, slices of the data volume can be visualized as RGB images to which the current 3D transformation is applied. Such a representation is displayed in Fig.8.

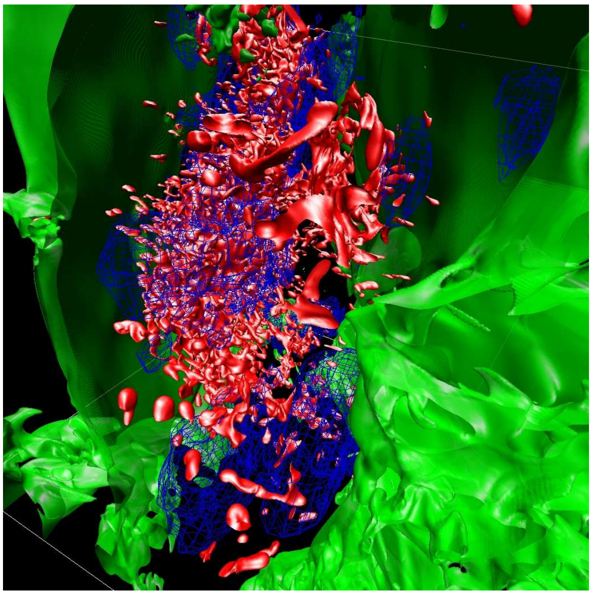

Fig.7 Visualization of isosurfaces of scalar fields in a 600x600x600 HERACLES simulation. In this closeup view, the Gouraud-shaded red polygons correspond to an isosurface of high density while the green, slightly transparent one is associated to a low density value. The blue wire-frame polygon is an isosurface of the pressure field. The scene is illuminated by three sources : ambient, frontal, and top directional.

5.3 Visualization of 3D vector fields

Vector fields can be visualized either by hedgehog-type display or by streamlines display. Streamlines are computed using an optimized IDL procedure that traces the path of a massless particle through the vector field. The seeds of the streamlines are distributed on 2D or 3D rectangular grids, or set by interactive picking in the scene. An example of a collection of streamlines seeded in this way can be seen in Fig.8

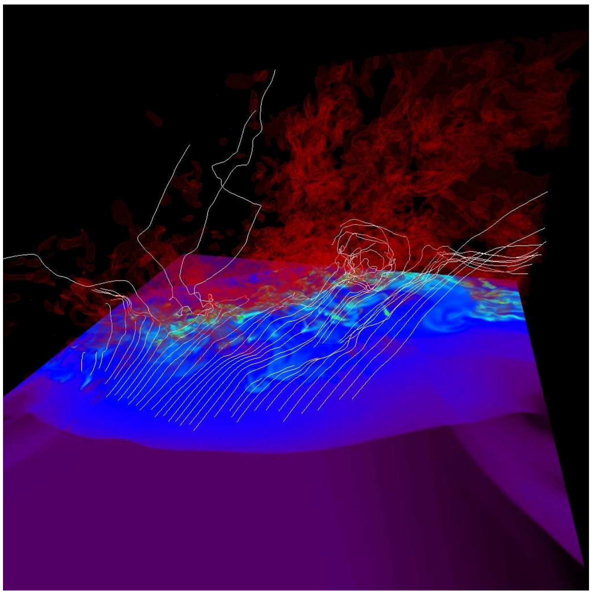

Fig.8 Visualization of multiple objects of a 600x600x600 HERACLES simulation. The planar object is an RGB image of the density field transformed in the current 3D model. The red haze is a quasi-transparent isosurface associated to a high value of the hydrodynamical density. The velocity field is visualized as streamlines that are seeded by interactively clicking on the image.

5.4 Current developments

Developments in the SD*vision* interface are focused on the handling of complex data structures, such as multiple embedded grids or AMR (Adaptive Mesh Refinement) octree mesh. Visualization of multiple grid will benefit to the forthcoming HERACLES meshing scheme, and preliminary results have been obtained in the context of the JUPITER code. This code is used to study the formation of protoplanetary systems using a multiple grid technique similar to the one developed in HERACLES. Visualization of multiple image objects each corresponding to a given grid level is achieved.

6 Conclusions and perspectives

From the physics point of view, the HERACLES program is now entering another phase of development with the introduction of the MHD (magnetohydrodynamics) equations treatment. This work is part of the MAGNET collaboration [15], a French collaboration dedicated to the study of MHD in the context of astrophysics and geophysics.

The multiple-grid methods are first implemented in a non-MHD version of the code; the comparison of the results with a regular grid version is on the way and the program must be validated before taking into account the complete set of new MHD equations. Furthermore, an application designed to interactively control and monitor the initialization and execution of the HERACLES program will be developed in the IDL framework. Such tool is a major added value for the distribution of the code in the different collaborations, as well as the use of appropriate versioning tool.

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