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Computer simulations using implicit Lagrangian hydrodynamics in 3D

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Abstract

The method known as Smoothed Particle Hydrodynamics (SPH) is an important tool in modern numerical Astrophysics. It has been extensively used to simulate a large number of systems ranging from planets to clusters of galaxies. Nevertheless current applications of the method are restricted to dynamical situations because of the limitations in the time-step imposed by the Courant condition. Here we describe the main features of a new implicit SPH code which is able to handle with several thousand particles and, therefore, it can be used to simulate slowly evolving systems.

1 Introduction

The SPH is a Lagrangian method of calculation used in the simulation of motion flows. The system is represented by a grid of points where the coordinates move with the fluid. If we have a good resolution the grid will reproduce the behavior of a continuous fluid more accuracy. Each point is associated with a number of local properties, including the mass, so that from now it will identify as a particle. The fluid properties are calculated as the interpolated sum of the properties of particles in their environment.

The advantages of this method are that it allows an implementation in three dimensions more easily than Eulerian methods and, by construction, it exactly conserves mass, linear momentum and angular momentum of the system.

The simplest implementation is through an explicit method and its main disadvantage is that to preserve the model stability, the step of time between iterations can not exceed the *Courant condition*. This restriction forces to use very small time steps, limiting the method to the modeling of dynamic processes of very short duration (such as collisions or mergers).

2 Objectives

The main objective of this work is double. On the one hand, build and implement a multidimensional implicit SPH code incorporating the needed physics to simulate quasi-static [1] pre-explosive phases in compact stellar objects: novae, supernovae and X-ray burst. Moreover applying the SPH code to the study of the ignition conditions of thermonuclear supernovae [3, 4], starting from massive white dwarf, initially in hydrostatic equilibrium and unbalanced by accretion of material.

This pre-explosive phase is barely known and the simulation will be studied based on highly simplified initial conditions. Phase space to explore is very complex, so this type of study will continue calling the attention of the scientific community for many years. Our intention is that the code developed in this work will endure and will be applied in such studies.

Given the huge effort involved in constructing an implicit SPH code, we have intention that it could be used in the study of many astrophysical scenarios. To this end we have chosen a modular design that separates the treatment of basic evolutionary equations (Section 5) from the material properties (equation of state, nuclear reactions, etc.).

The code should be operational with the resources of the GAA (Section 4.2) and available in supercomputers (such as MareNostrum).

3 The state of the art

There have been several attempts to get a functional implicit SPH code. So far the problem has always been the high computational cost of such methods. This is because the properties of the next time step depend on the values of the unknown variables in this time and therefore all must be calculated simultaneously. The consequence is that the whole system of equations must be solved together by inverting a huge sparse matrix (in three dimensions the array size is $(n*8)^2$, where n is the number of particles).

In his thesis, [5] proposes an implicit method based on iterative solvers of Krylov and on Newton-Rapshon corrections. His code has been developed from a previous explicit SPH one: SPHINX of Los Alamos National Laboratory. The Knapp code was developed in 2000 and used a maximum of 6 000 particles, an amount entirely inadequate to describe complex astrophysical scenarios.

Our goal is to work with an amount between 10 000 and 100 000 particles in three dimensions, depending on the complexity of the physics of the problem.

Moreover we include in our implicit SPH code basic physics of the explicit SPH codes available from our group. This has not been done yet, because this basic physics influences on the calculation time, turning it very hard to compute.

[1] Characterized by an evolution time greater than the time that a sound signal takes across the system.

4 Code ISFAA

Based on this previous work, we developed an implicit SPH code where, using the experience in the explicit SPH code of GAA and providing new ideas we have improved the capacity of calculation of the code.

The progress made until today has resulted in a SPH code which meets non-functional requirements proposed and is able to pass a series of basic tests. These tests control the correctness of the code in key functional areas (Section 6).

The current code contains the basic equations of SPH and improvements of the code described by Knapp:

- *Multidimensional Code*: we have done a general solution to the code so it is easy to change the number of dimensions to be addressed in the physical model.
- *Artificial Viscosity* [6, 1]: astrophysical processes that are required to be simulated need this improvement to avoid usual problems such as particle interpenetration.
- *Gravity*: as we work with models where gravity is an essential force our equations need to contemplate this phenomenon.
- *Equation of state (EOS)*: in contrast to Knapp, which uses an ideal gas EOS, we have implemented an EOS that takes into account contributions from the electrons, ions and radiation fitting to the conditions studied.
- *Treatment of the temperature*: needed for EOS and heat diffusion.
- *Centered scheme*: we have modified and implemented the scheme of calculation so that the equations are calculated by leaps centered steps. In terms of numerical accuracy, values of the particle properties are correct until second order.
- *Management of the matrix according to Morton method (Z-order)*: the main problem of solving the system of equations is the dispersion of the matrix to invert. This order ensures the proximity of the particles reducing the dispersion and the computation time.
- *Sparse matrix storage according to the CSR format (compressed by rows)*: you can reduce the amount of memory reserved because only the nonzero cells in the array are stored. The memory savings produced by this property is very important because the rate of filling of the matrix in astrophysical models that treat is about 2%.
- *Resolution of sparse matrices using parallel computing libraries*: the resolution of the system of equations is computationally the most expensive part of the calculation (more than 95% of the time of calculation time). After making a detailed study of parallel computation packages available, we decided to use the PARDISO 4.0 library of the University of Basel [7, 8].

4.1 Functional requirements

The planned physical model is very developed. The requirements not implemented yet and which will improve the behavior of the model approaching it to a more realistic scenario are the following: 1) heat diffusion, and 2) network of nuclear reactions.

4.2 Non-functional requirements

The developed code implements the following requirements: modularity, maintainability, extensibility, scalability, robustness, documentation, efficiency, performance and code correction.

Regarding the software, we can say that the code has been developed in Fortran95 and runs on systems GNU/Linux.

To make the calculations we are using a shared memory and parallel computer machine, purchased by the GAA in November 2009, to support this work. To make this acquisition we made a study of professional processors looking for the best ratio: power versus cost calculation. This study concluded that the best option would be to assemble a workstation "by pieces": it consists of 16 cores (2 Intel Xeon processors at 3.2 Ghz W5580 8-core (4 real cores + 4 virtual cores)) and 48GB of RAM DDR3-1333Mhz.

5 Physical model

Each particle of the model is associated with a group of basic evolutionary equations, derived from the Lagrangian fluid equations [6]:

Continuity equation:

$$\frac{d\rho_i}{dt} = \sum_{j=1}^{N} m_j \left(\mathbf{v}_i - \mathbf{v}_j\right) \nabla_i \tilde{\mathbf{W}}_{ij}. \tag{1}$$

Moment equation:

$$\frac{d\mathbf{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \mathbf{\Pi}_{ij}\right) \nabla_\mathbf{i} \tilde{\mathbf{W}}_{ij} - g\left(\mathbf{r}_i\right). \tag{2}$$

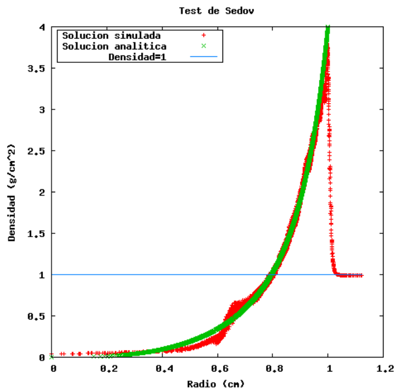
Energy equation:

$$\frac{du_i}{dt} = \sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{\mathbf{\Pi}_{ij}}{2}\right) \left(\mathbf{v}_i - \mathbf{v}_j\right) \nabla_i \tilde{\mathbf{W}}_{ij}, \tag{3}$$

being $\nabla_i \tilde{\boldsymbol{W}}_{ij}$ the gradient of the interpolating function; m_i mass; v_i speed; ρ_i density; P_i pressure; u_i internal energy; $\mathbf{\Pi}_{ij}$ artificial viscosity; $g\left(\mathbf{r}_i\right)$ gravity.

6 Tests cases

To check the validity of the code we have done some tests whose solution is known:



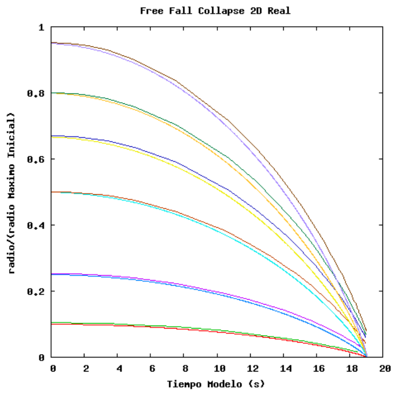


Figure 1: *Left*: Sedov test, density profile with across time $t = 2.16 \times 10^{-2}$ s. *Right*: Collapse of a cylinder of infinite height. It represents the simulated evolution with ISFAA and the theoretical trajectory, beginning with different initial radii.

6.1 Sedov test

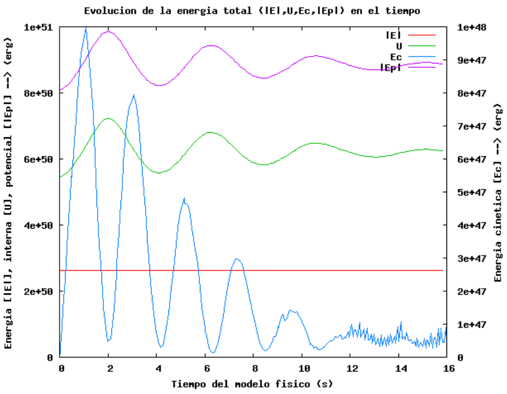
The test [9] examines the ability of the artificial viscosity to represent shock waves. We have a two-dimensional rectangular grid, balanced and equally spaced particles. There is a central disturbance, increasing the density a factor 10^4 by a Gaussian function. The system propagates the density wave to the outside. An analytically description of the change in density between the pre-shock and the post-shock zone could be done and the result is that is a factor of four, as befits a strong shock wave in an ideal gas (see Fig. 1, left).

6.2 Freefall test

The test examines the correction of gravity force in the code. We have a circular grid in two dimensions, balanced and equally spaced particles. (It would be equivalent to a cylindrical three-dimensional distribution of infinite height). The system is allowed to evolve without pressure or artificial viscosity, so it will be a free fall toward the center of mass, which should match with the analytical result [2] (see Fig. 1, right).

6.3 Stability of a white dwarf

We have a white dwarf star in three dimensions, built with a realistic EOS and a mass of 1.2 solar masses, simulated and relaxed with an explicit SPH. The system is allowed to evolve, from a very small step of time and zero speed until the dynamics of the system is relaxed, using steps of time larger than the *Courant time* and getting the stability (see Fig. 2, left).



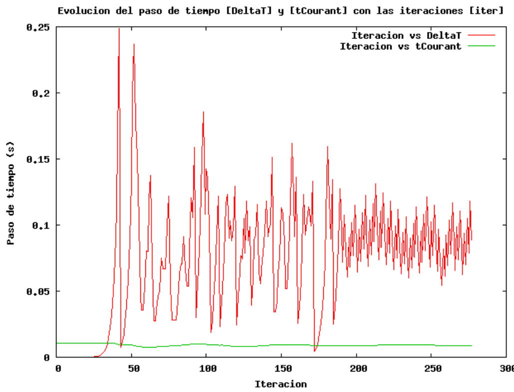


Figure 2: *Left*: Evolution of internal, gravitational and kinetics energy of a 1.15 $M_\odot$ white dwarf. The total energy (E) remains constant. *Right*: The time step vs. the Courant time.

7 Future work

Below we show the temporary planning to completation of the work: 1) add the remainder of the planned physics and calculations for the study of the previous stages to the ignition of supernovas, 2) documentation and reading thesis, and 3) applying the method to other scenarios.

Acknowledgments

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