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The cuFFT code for N-body simulation

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Abstract. The complexity of astrophysical processes lies in the joint consideration of components of various nature. For example, in the collision problem of galaxies, the three-dimensional dynamics of an interstellar gas and a stellar component is considered. The modeling of these components can be based on completely different classes of numerical methods. One possible solution to this problem is to use the Eulerian-Lagrangian approach, in which physical quantities are concentrated at material points, which is typical for the SPH (Smoothed Particle Hydrodynamics) method, and the forces are calculated on an adaptive grid attached to a system of material points. This approach uniformly takes into account both the dynamics of a continuous medium and discrete particles, and also eliminates a number of drawbacks inherent in the original method. The calculation of gravitational interaction is carried out by solving the Poisson equation for the gravitational potential. In this case, all particles are projected onto the computational grid and the potential values in each cell are already calculated on it. The solution of the Poisson equation for the gravitational potential is performed using the fast Fourier transform. The article describes the new cuFFT code Virtual Planetarium for modeling astrophysical objects based on the SPH method, supplemented by the Godunov method for calculating pressure and momentum flows between particles, and the fast Fourier transform method for solving the Poisson equation for the gravitational potential. The paper describes the rationale for the transition to such a computational model, kinetic and hydrodynamic approaches are described in detail. Simulation of the collapse of an isothermal gas cloud is performed. Method to reproduce the evolution of instabilities in form of two density arms is realized.

1. Introduction

Modern theoretical astrophysics has practically exhausted the possibilities of analytical and semi-analytical solutions that can be obtained under the assumptions of spatial symmetry of the processes under consideration. A computational experiment has become main tool of theoretical astrophysics. The complexity of astrophysical processes can be explained by the joint consideration of components of various nature. To describe such a process, it is necessary to solve the equations of hydrodynamics to describe gas motion and to solve kinetic equation for recording the stars motion. Solution methods are based on completely different classes of numerical methods. One of the trends for resolving such problems is the use of Lagrangian-Eulerian methods (Arbitrary Lagrangian-Eulerian - ALE in foreign literature), which are simultaneously suitable both for solving hydrodynamic equations and for describing particles motion. Although it is worth noting that there are studies on the modification of mathematical models to describe various components by a single class of hyperbolic equations [1]. We will
focus on the development of the Lagrangian-Eulerian approach.

In the last decade, several codes have been created in the field of computational astrophysics, successfully and at the same time in various ways, implementing the Lagrangian-Eulerian approach. Among them are AREPO [2], BETHE-HYDRO [3], GIZMO [4] codes. One way or another, all codes are based on representing the solution in the form of a set of material points with physical characteristics placed in them, which is typical for the method of smoothed particles [5] (Smooth Particles Hydrodynamics - SPH in foreign literature). Next, different mechanism is used for the method of interaction with neighboring points. In particular, it is a way to build grids. Let us dwell on the codes description in details.

The AREPO code is based on moving mesh technology which in turn is based on the Voronoi and Delaunay triangulations with Lloyd regularization. This approach allows you to adapt the grid to the solution. The classical Godunov method is used as the main for solving the hydrodynamic equations. This is due to the fact that it is rather difficult to build a higher-order scheme on a moving mesh. To solve the Poisson equation, an approach is used based on writing the equation for the total mechanical energy into the equation for the sum of all types of energy (internal, kinetic and potential). Such an equation for the total energy on the right side has a time derivative of the potential and its gradient, which is calculated using the Poisson integral by particle-grid methods. An individual time step is used for time integration. This approach with all the advantages is quite difficult in terms of computational costs. And the question about of the quality of solution in the areas described by less detailed grid cells remains open. However, the AREPO code is one of the most used in the World at the moment.

The BETHE-HYDRO code is based on the ALE approach combining the advantages of both the Eulerian and Lagrangian approaches. The hydrodynamic equations are formulated in a Lagrangian non-conservative form and are solved on an unstructured grid. The numerical method is based on the operator approach, which allows one to construct consistent schemes for approximating the gradient and divergence operators. To solve the Poisson equation in a one-dimensional formulation, the sweep method (or the Thomas method in foreign literature) is used. In the two-dimensional formulation of the Poisson equation, it is solved using the conjugate gradient method. Then, the potential is corrected to preserve the total energy (the sum of the kinetic, internal and potential energies) of the system. It is worth noting that it is still not possible to save the full energy of the system completely. But the error in the collapse problem is about 10-2 percent that is negligible. Unfortunately, the code was not developed for the three-dimensional case.

In the GIZMO program code, a new meshless approach to solving the equations of gravitational gas dynamics is developed and implemented. The approach is based on a combination of classical grid methods and the SPH method. The method consists in using the equations of gas dynamics in Euler coordinates, which, using the Galerkin variational principle, are multiplied by trial functions. Feature of these functions is the fact they are not tied to the computational grid, but to individual particles, similar in nature to SPH particles. To determine the values at the boundaries of the region, we apply solution of the Riemann problem using the Godunov method.

An analysis of these codes shows that the main computational problem is the construction of grid (or its analogue) to describe the interaction between particles. At the same time, the ideology of the kinetic approach based on the description of the motion of material points is preserved in all methods. In this concept, computational model is developed and described in the paper. To organize the calculations, we will use a uniform cubic grid in which a cloud of particles will be placed. This approach makes it quite simple to organize the Eulerian stage of calculations.

The kinetic computational model and the numerical methods that is used to solve them are described in second section. The third section is devoted to discussion points that is a natural
extension of the models and implementations described in the paper. The fourth section is devoted to the results of computational experiments.

2. The Numerical Model

We write the equations of gravitational hydrodynamics with zero pressure in the form of mass (1) and angular momentum (2) conservation laws in Euler coordinates:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \quad (1)
\]

\[
\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \times \vec{u}) = -\rho \nabla \Phi, \quad (2)
\]

supplemented by the Poisson equation for the gravitational potential (3):

\[
\Delta \Phi = 4\pi G \rho, \quad (3)
\]

where \(\rho\) is the density, \(\vec{u}\) is the velocity vector, \(\Phi\) is the gravitational potential, \(G\) is the gravitational constant.

We will consider the dynamics of an arbitrary number of material points (particle). The mass conservation law of particle is obtained naturally when integrating the equation (1) in a small neighborhood of a point at which other particles do not fall. We write the second Newton’s law for an arbitrary number of particle using equation (2) in the Lagrangian formulation:

\[
\rho \frac{d\vec{u}}{dt} = -\rho \nabla \Phi. \quad (4)
\]

In equation (4), it is necessary to reduce the density function, which is nonzero in a small neighborhood of the point. As a result, we obtain the equations for the particles motion:

\[
\frac{d\vec{u}}{dt} = -\nabla \Phi, \quad \frac{d\vec{x}}{dt} = \vec{u}. \quad (5)
\]

To solve equations (5), we need to calculate the potential gradient. To do this, we introduce a uniform cubic Eulerian grid with a step \(h\) in each direction and project each particle onto the corresponding cell. It means each particle will contribute to the mass of the corresponding cell \((i, j, k)\). Thus, in each cell, we can calculate the density by the equation (6):

\[
\rho_{i,j,k} = \frac{\sum_l M_l}{h^3}, \quad (6)
\]

where \(M_l\) is the mass of the particle falling into the cell \((i, j, k)\). Knowing the density in each cell of the computational domain using the method based on the fast Fourier transform, we can find the gravitational potential. The study and description of the method for solving the Poisson equation is described in [6, 7] in details. Since the function of the gravitational potential is a smooth function, we will use the central differences to find the potential gradient.

To solve equations (5) for a particle in time step, we will use a two-layer scheme with stepping, where velocities are calculated by the equation (7):

\[
u_x^{m+1/2} = u_x^m - \frac{\tau}{2h} (\Phi_{i+1,j,k} - \Phi_{i-1,j,k}),
\]

\[
u_y^{m+1/2} = u_y^m - \frac{\tau}{2h} (\Phi_{i,j+1,k} - \Phi_{i,j-1,k}),
\]
\[ u_{m}^{n+1/2} = u_{m}^{n} - \frac{\tau}{2h} (\Phi_{i,j,k+1} - \Phi_{i,j,k-1}) \]

Coordinates are calculated using formula (8):
\[ \vec{x}^{n+1} = \vec{x}^{n} + \tau \vec{u}^{n+1/2}. \] (8)

Such a scheme corresponds to the Euler-Lagrangian approach used by the team of authors earlier [1, 6, 7]. Choice of appropriate time step is an important condition for numerical scheme stability. To do this, we use the Courant-Friedrichs-Levy condition

3. The Discussion

In this section, we describe discussion points related to the constructed computational model and to the software implementation. These discussion points are not yet included in the code, but can be used when developing the code.

(i) In the introduction, it was said about using only uniform cubic grid. This is done only to simplify the description of the computational model and its use for the needs of the Novosibirsk planetarium. Of course, the use of material points allows us to introduce adaptive meshes (Adaptive Mesh Refinement - AMR in foreign literature) in a fairly simple and natural way, applying the appropriate numerical methods to restore the gravitational potential. In the future, we plan to develop our approach in this direction.

(ii) In the second section, we used the pressureless equation of state, which depends only on the density function. For the projection of particles on an Eulerian grid, it is sufficient to use the masses conservation law to determine the density. However, to describe the ideal gas, it is necessary to use thermodynamic variable – entropy, and projection method similar to the projection of material points velocities onto a cell.

(iii) The simplest projection of material points onto computational grid was also used. To eliminate computational noise, it is necessary to use smoothing kernels similar to SPH and particle-in-cell methods. In the future, if necessary, the question of choosing a core will be considered separately.

(iv) The formulas for recalculating the velocities and coordinates of material points are written in vector form explicitly. That fact explains usage of vector SSE extensions built into Intel and AMD processors of modern personal computers. The developed program code is oriented for such computing devices. Also, most of personal computers are equipped with NVIDIA graphics accelerators, for which special libraries have been created to perform fast Fourier transform calculation that is a part of the CUDA technology. It shall be noted, that the developed code works using cuFFT.

4. The Numerical Simulation

As a model problem, we consider the collapse of an isothermal cloud in dimensionless variables. To do this, we introduce an auxiliary computational grid in a cubic region of domain size. At the initial moment of time, in a sphere of unit radius we uniformly distribute particles of total mass with a model temperature and Keplerian rotation speed. In our model problem, we will study the behavior of gas particles ensemble at various values of velocity dispersion. The problem of studying the fragmentation of rotating cold cloud is especially interesting in the context of the evolution process of elliptical galaxies [8]. Analysis of the simulation results shows (see fig. 1) that instabilities evolve into two density arms form when increasing velocity dispersion up to the same initial density distribution. In the present study, we do not plan to analyze evolution of such instabilities similar to [7]. The ability to reproduce such disturbances by the developed computational model is the main result of computational experiments. In the future, we will consider evolution of instabilities in many bodies system in the context of modeling planetary systems and galaxies [9] in details.
5. Conclusion
The new cuFFT code “Virtual Planetarium” for astrophysical objects simulation was discussed. The program code is based on the Eulerian-Lagrangian combination of the smoothed particle method and Godunov method. The rationale for transition to such a computational model was also discussed. Using the developed code, the simulation of collapse of a rotating gas cloud was performed.

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