High-Performance Computing in Astrophysical Simulations

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Abstract. The author’s approach for simulating of multiscale astrophysical objects with using of supercomputers is described in the paper. Astrophysical objects consists of several components with different nature, and as a result are described with different mathematical models. This fact leads us to need of formulation of mathematical model and numerical method for each component. The two-phase model (gas + particles) was used in case of simulation of protoplanetary disks. The numerical method and details of parallel implementation for that model were disclosed. The mathematical model for galactic objects, describing stellar component and dark matter, based on the first momenta of Boltzmann equation was built. Such approach allows us to use unified numerical method to describe collisionless and gas component of galaxies.

1. Introduction
Observational astrophysics plays an important role in the study of the universe, formation of multiscale objects and different flows. However, observational data often just makes a question about formation of one or another configuration, but it couldn’t give an answer about how any particular galaxy or planetary system was formed. Therefore, the main, and sometimes the only possible way to do that is to use mathematical modeling.

In recent years, with discovering of a big amount of planets, the problem of planet formation has become popular. Todays hypotheses about planet formation are based on the Kant-Laplace theory. It describes the structure of the Solar system very well, but for some of other planetary systems it faltering. For example, many Hot Jupiters (gaseous giant planets with a very short orbit) were found. The question about how much time is needed to form the planet systems is opened too. As expected, it takes a hundreds of millions of years, but in fact the value is ten times less. Besides, it’s not clear how multiple systems forms. Nowadays a couple of theories exist, described in [1], but they should be proved with using of mathematical modeling.

Also, the variety of observed galaxies is of great interest. An ordinary galaxy has up to a ten of collisions for a period of the Hubble time, that leads to formation of complex structures of galaxies. The observed variety of galaxies is directly related to collisions between them [2]. These observations led to the hypothesis that was proved with mathematical modeling [3].
The main problem in modeling of protoplanetary systems and galaxies is that it is necessary to model two different components – collisional (gas and dust in case of galaxies, and gas in case of protoplanetary disks) and collisionless (stellar component and dark matter in galaxies, and the dust component in protoplanetary disks). The gas component is described with system of gravitational gasdynamics equations, but the collisionless component is described with N-body problem, that leads to a couple of difficulties in its joint modeling.

The alternative to N-body problem is model based on the first momenta of the Boltzmann equation [4]. The ability of using such approach for describing of the collisionless component of colliding galaxies was experimentally proved [5]. This model isn’t universal of course. It could be used only if: we are interested in the behaviour of cluster of collisionless component (it is true for the dynamics of stars in galactic scales); the velocity of cluster, as usually, has a directional movement and low dispersion of speed (it is also true for interacting galaxies, moreover, the very dispersion of speed of stellar component is observed in galaxies); there is no heat conduction (it is typical for all astrophysical processes).

The obvious advantage of the model is based on the first momenta of Boltzmann equation is ability of thermodynamically coherent phase transition between stellar and gas components. The mass and momentum conservation laws are satisfied but the entropy decreases in case of the N-body model. For example, in star formation process it is possible to save internal energy of the system while transition from gas component to collisionless component, but the mass and momentum are lost, that leads in fact to increasing of the gas entropy in the medium. But there is no contribution to the internal energy of the gas in case of supernovae feedback while transition from stellar component to gas with using of N-body model. The limitation on the description of small number of bodies, that holds in the case of protoplanetary disks, is the main disadvantage of this model. Nevertheless, such problem could be solved in two dimensional formulation, as opposed to simulation of colliding galaxies. So it need less computational resources and, consequently, is less demanding on the numerical methods in terms of performance.

The complexity and need of high detail of model leads to necessity of using the most powerful of the available supercomputers. Today the most powerful supercomputers are based on hybrid architecture with graphics accelerators and Intel Xeon Phi accelerators. For example, in the july 2015 version of Top500 the two first supercomputers (and four of Top10) are built with using of these technologies. It is quite clear, that first exaflop supercomputer will be built on the basis of hybrid architecture. The using of the unified numerical method for describing of two components will allow us to use such hybrid computational resources [6].

2. Mathematical model
The equations of gravitational gasdynamics are used to describe gaseous component of galaxies and protoplanetary disks. The stellar component of galaxies is described with using of the first momenta of Boltzmann equation, and the dust component of protoplanetary disks is described with N-body model in 2D. The used model was substantiated in introduction, so let us give a formal description of it.

2.1. Equations
The gravitational gasdynamics equations could be written in redefined form.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad \frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla (p) - \rho \nabla (\Phi)$$
$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \vec{u}) = -(\gamma - 1) \rho \varepsilon \nabla \cdot (\vec{u}) \quad \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \vec{u}) = -\nabla \cdot (p \vec{u}) - (\rho \vec{u} \cdot \nabla (\Phi))$$

where $\rho$ – is a density, $\vec{u}$ – velocity, $p$ – pressure, $\varepsilon$ – internal energy, $E$ – full energy, $\Phi$ – gravitational potential, $\gamma$ – adiabatic index. The full energy is connected with internal energy...
by means of equation $\rho E = \rho e + \frac{1}{2} \rho \vec{u}^2$. Internal energy and pressure are connected by equation of state for ideal gas $p = (\gamma - 1) \rho e$.

Expressions for the first momenta of Boltzmann equation with using of diagonal tensor of velocity dispersion could be written in redefined form:

\[
\frac{\partial n}{\partial t} + \nabla \cdot (n \vec{v}) = 0 \\
\frac{\partial n \vec{v}}{\partial t} + \nabla \cdot (n \vec{v} \vec{v}) = -\nabla \left( \pi \xi \xi \right) - n \nabla (\Phi)
\]

\[
\frac{\partial \pi \xi \xi}{\partial t} + \nabla \cdot (\pi \xi \xi \vec{v}) = -2\pi \xi \xi \nabla \cdot (\vec{v}) \\
\frac{\partial \rho W}{\partial t} + \nabla \cdot (\rho W \vec{v}) = -n \nabla \left( \pi \xi \xi \vec{v} \right) - (n \vec{v}, \nabla (\Phi))
\]

where $n$ – density, $\vec{v}$ – velocity, $\pi \xi \xi$ – elements of diagonal tensor of velocity dispersion, $W$ – full mechanical energy. The full energy is connected with a trace of diagonal tensor of velocity dispersion with relation: $\rho W = \frac{1}{2} \pi \xi \xi + \frac{1}{2} \rho \vec{u}^2$.

Equations of particles movement is:

\[
\frac{d^2 x}{dt^2} = \frac{\nabla (\Phi)}{m}
\]

where $m$ – particle mass.

Poisson equation generally written as

\[
\Delta \Phi = 4\pi G (\rho + n + \sigma)
\]

where $\sigma$ – density of particles, defined by an ansamble of particles using kernel.

### 2.2. Numerical method

To solve the equations of gasdynamics and first momenta of the Boltzmann equation, the combination of Fluids-in-Cells method (operator-splitting approach), Godunov method and piecewise-parabolic method on local stencil for achievement of high order of accuracy are used. The special modification of the Roe averaging scheme is used to average the quantity on the borders of cells. To recompute internal energy (or tensor of velocity dispersion in case of Boltzmann equation) in the region with high density and to correct the magnitude of velocity vector on the gas-vacuum border area and in the area rarefied space the redefined system of equations is used.

It is very important to know the movement trajectories of each particle with high accuracy in the case of simulation of planet formation process. The Particle-Mesh method with Clouds-in-Cells approach is used to simulate the dynamics of dust component of protoplanetary disk. According to it, the particles are discrete bodies translated into the same grid as used for gas density. Herewith, the mass of each particle is spreaded by some finite area, called “cloud”, which make a contribution to the distribution of density in gravitational potential and gravitational interaction between gas and particles without loosing of the ability of tracking each particle separately [7].

### 2.3. Parallel implementation

Geometrical decomposition of the computational area is in the heart of the parallel implementation of interacting galaxies model. Unique feature of the mathematical model allows us to formulate unified numerical method and, consequently, parallel algorithm and it’s implementation. The implementation on heterogeneous supercomputer RSC PetaStream equipped with Intel Xeon Phi had achieved 134x acceleration on one Intel Xeon Phi, and 92% of efficiency was shown on 64 Intel Xeon Phi accelerators.
Graphics accelerators with Nvidia CUDA technology were used for parallel implementation of model of protoplanetary disks dynamics. The most expensive stage of simulation is solving of Poisson equation. The Fast Fourier Transform is used to solve the equation and it is implemented on GPU in cuFFT library. The computation of border conditions and potential in harmonic space are ported on GPU to improve performance. In this way the data transferring from host to device and back is minimal. So, almost 10x acceleration was achieved on Nvidia GeForce G210M opposed to one core of Intel Core2Duo. The particles simulation was implemented on GPU too, that had increased performance in 4 times. Simulation of gasdynamics is computed on CPU in the same time as particles dynamics computed on GPU.

3. Numerical experiments
The main focus of the paper is on demonstration of various models for describing of collisionless component. So let us make an experiment of one-dimension impact of density waves with using of different models. Also the late stage of protoplanetary disk evolution and collision of galaxies with different masses will be shown.

3.1. One-dimensional impact of density waves
We use three models to simulate the collision between two waves: models with particles with some initial speed and without collision; pressureless hydrodynamics model; model with first momenta of Boltzmann equation. The last one is equal to gasdynamics model with $\gamma = 3$ in 1D. Density distribution with using of these models is shown on the figure 1. In case of pressureless model the solution is $\delta$-function, that makes it useless for describing of collisionless model. One can see the scattering of waves after collision in case of the third model, that could be used in galaxy collision. This fact was proved in paper [5].

3.2. The late stage of evolution of protoplanetary disk
L
ets look at the process of evolution of protoplanetary disk from the moment when a couple of protoplanets formed. Let us make a gas disk with radius $R = 4$, density $\rho(r) = 3.5 \frac{(R-r)(R+r)}{R^2}$, pressure $p(r) = 0.8 \frac{(R-r)(R+r)}{R^2}$ and angular velocity $\omega = 1$ in the area $[-5, 5] \times [-5, 5]$. The protoplanets are 10 particles that distributed uniformly within a disk with radius $R \in [1.0, 2.5]$ and has masses $m \in [9e - 3, 9e - 2]$ and angular velocity $\omega = 2.5 + \epsilon$, $\epsilon \sim N(1.0, 0.5)$. The result is shown on figure 2. Formation of three gaseous objects with high density, which could be interpreted as possible stars, is shown on it. Also, there is a rarefying space in the left of central star. It was formed as a result of stellar wind that threw matter away to the outer part.
3.3. Simulation of collision of galaxies with different masses

As a model problem, let us compute a central collision of galaxies with mass fraction 1 : 20 with total mass of “big” one $10^{13} M_\odot$. The fraction of halo mass to disk mass is 10 : 1 in both galaxies. Each component is given by the equilibrium configuration. The results (dimensionless density distribution) are in figure 3. The instabilities after the massive galaxy because of ram-pressure mechanism made by the “small” galaxy are shown on the figure 3.

4. Conclusion

The author’s approach for modeling of multiscale astrophysical objects with supercomputers is described in this paper. The two-phase model (gas + particles) was used to simulate the dynamics of protoplanetary disks. Also the numerical method and details of parallel implementation were described for it. The mathematical model based on the first momenta of Boltzmann equation for describing of stellar component and the dark matter of galactic objects is given. Such approach allows us to use unified numerical method to simulate collisionless and gaseous component of galaxies and also get high efficiency of the parallel implementation. The process of collision of two galaxies with different masses and the late stage of evolution of protoplanetary disk were simulated.

Figure 2. Simulation of the late stage of evolution of protoplanetary disk, $t = 9.5$

Figure 3. Simulation of galaxies collision. Dimensionless distribution of gas density (left), stellar component and dark matter (center), total density (right)
Acknowledgments
Acknowledgements This work was partially supported by Russian Foundation for Basic Research (grants 15-31-20150, 15-01-00508, 13-07-00589, and 14-01-31199) and by Grant of the President of Russian Federation for the support of young scientists number MK – 6648.2015.9. This project was partially supported by the Russian Ministry of Education and Science.

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