Parallel Algorithm for Supercomputing Simulation of Dust-Gaseous Gravitating Systems Using Particle-In-Cell and SPH Methods

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Abstract.

We present a supercomputer numerical model for simulating 3D dynamics of dust-gas gravitating circumstellar disk. The model combines SPH method for solving gas dynamical equations, particle-in-cell (PIC) method for solving Vlasov equation, and convolution FFT-based grid method for solving Poisson equation. The approach is based on 3D domain decomposition, sorting of particles with regard to grid cell, and transferring necessary amount of particles between subdomains. The algorithm is aimed to be run on supercomputers with distributed memory and on hybrid supercomputers.

1. Introduction

One of the important problems of modern computational astrophysics is to develop supercomputing models for simulation of planets formation in circumstellar dust-gas disks. A lot of observational data regarding formation of exoplanets appeared in the last two decades [1]. This data requires theoretical interpretations and explanations with the help of numerical experiments, conducted with high resolution and for large timescale to track fragmentation of disk into clumps and their subsequent migration.

In this regard meshless method of smoothed particle hydrodynamics [2] (SPH) has some advantages over grid methods: it allows to treat rapid changes in density on a very small space scale. On the other hand a traditional implementation of gravitational solver used in conjunction with SPH makes use of tree-code algorithms [3], and it is more complicated and less scalable in comparison with grid-based Poisson solvers.

In this paper we describe numerical model and developed parallel algorithm which combines particle-in-cell method for simulating collisionless dust component, SPH method for simulating 3D dynamics of two-phase dust-gas mixture, and grid FFT-based method for calculating gravitational potential. This numerical model was previously used for simulating thin 2D gas disk [4], while present work is focused on its 3D version.

2. Numerical model

In the developed software we use two approaches for simulating dynamics of dust. First one is based on the solving Vlasov equation using particle-in-cell method, while the second approach
employs gas-dynamics equations solved with SPH with pressure term equal to zero. Depending on the particular numerical experiment we can use either PIC method or SPH.

2.1. Gravitating Dust Component

Vlasov equation (known also as Boltzmann collisionless equation) consists of distribution function \( f = f(t, r, u) \), which is dependent on time \( t \), space coordinate \( r \) and velocity \( u \), with the initial distribution \( f^0(r, u) \):

\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial r} - \nabla \Phi(t, r) \frac{\partial f}{\partial u} = 0, \quad f(0, r, u) = f^0(r, u)
\]

Dynamics of dust is governed by self-consistent gravitational force with potential \( \Phi = \Phi(t, r) \) with boundary conditions imposed on isolated system:

\[
\Delta \Phi(t, r) = 4\pi G \rho(t, r), \quad \Phi(t, r)|_{r\to\infty} = 0,
\]

where \( G \) – gravitational constant.

Density \( \rho = \rho(t, r) \) is calculated by distribution function \( f \):

\[
\rho(t, r) = \int f(t, r, u) du.
\]

Solving Vlasov equation is made on a uniform Cartesian grid with a standard implementation of particle-in-cell method [5, 6].

Gravitational potential is calculated with convolution method [5]. Instead of solving Dirichlet problem for Poisson equation in infinite domain:

\[
\Delta \Phi(x) = \rho(x), \quad \Phi(x)|_{x\to\infty} = 0,
\]

we then calculate the Poisson integral:

\[
\Phi(x_0) = -\int \frac{\rho(x)dx}{|x_0-x|}.
\]

Such approach allows to use fast Fourier transform and accomplish the calculations in \( O(M^3 \log M) \) operations (where \( M \) is a number of grid nodes in one dimension).

2.2. SPH method for simulating dynamics of dust-gas mixture

We consider three dimensional two-phase dust-gas mixture where dust and gas interact with each other by friction force and by gravitational force:

\[
\frac{\partial \rho_g}{\partial t} + \nabla (\rho_g v) = 0, \quad \frac{\partial v}{\partial t} + (v \cdot \nabla) v = -\nabla P - \frac{K(v-u)}{\rho_g} - \frac{\Phi}{\rho_g},
\]

\[
\frac{\partial \rho_d}{\partial t} + \nabla (\rho_d u) = 0, \quad \frac{\partial u}{\partial t} + (u \cdot \nabla) u = -\frac{K(v-u)}{\rho_d} - \frac{\Phi}{\rho_d},
\]

where \( \rho_g \) and \( \rho_d \) – density of gas and dust, \( v \) and \( u \) – velocities of gas and dust, \( P \) – pressure, \( K(v-u) \) – friction force between dust and gas:

\[
K = \frac{\rho_d}{t_{stop}}.
\]
Equation (4) means that dynamics of dust is modeled as a continuous medium with pressure term set to zero.

For solving this equation we use SPH implementation of [7] in Cartesian grid with the following smoothing kernel $W_{ab}(q)$ for particles $a$ and $b$:

$$W_{ab}(q) = \frac{1}{\pi h^3} \begin{cases} 
1 - \frac{3}{2}q^2 + \frac{3}{4}q^3, & \text{if } 0 \leq q \leq 1, \\
\frac{1}{4}(2-q)^3, & \text{if } 1 < q \leq 2, \\
0, & \text{otherwise}
\end{cases}$$

where $q = \frac{\bar{r}_a - \bar{r}_b}{h}$, and $h$ is a smoothing radius.

Method of calculating friction force is available in details in paper [8].

Testing of the method implementation is done using three dimensional shock tube problem in a rectangular domain with periodic boundary conditions, where shock wave propagates along $x$ axis. Such condition allows to compare solution of 3D problem with solution of 1D problem.

We use an equation for internal energy of gas $e$:

$$\rho_g \left( \frac{\partial e}{\partial t} + v \nabla e \right) = -p \nabla v,$$

which is tied with the pressure using the following equation of state, where $\gamma$ is an adiabatic exponent:

$$p = \rho_g e(\gamma - 1).$$

Computational domain is set up to the rectangle $[0, 1] \times [0, 0.1] \times [0, 0.1]$, and is divided in 2 parts by plane $x = 0.5$. Initial parameters in left and right parts are set to:

$$[\rho_l, p_l, v_l, e_l] = [1, 1, 0, 2.5],$$
$$[\rho_r, p_r, v_r, e_r] = [1, 0.8, 0, 2],$$
$$\gamma_l = \gamma_r = 7/5.$$

Relation between mass of dust and mass of gas is set to $\varepsilon = 1$.

Periodical boundary conditions are set for $y$ and $z$, providing propagating of shock along $x$ axis.

$$v|_{y=0} = v|_{y=0.1}, \quad v|_{z=0} = v|_{z=0.1},$$
$$u|_{y=0} = u|_{y=0.1}, \quad u|_{z=0} = u|_{z=0.1},$$
$$\rho_g|_{y=0} = \rho_g|_{y=0.1}, \quad \rho_g|_{z=0} = \rho_g|_{z=0.1},$$
$$\rho_d|_{y=0} = \rho_d|_{y=0.1}, \quad \rho_d|_{z=0} = \rho_d|_{z=0.1}.$$

We used constant smoothing radius $h = 0.01$, and time step $\tau = 0.001$, satisfying Courant condition $CFL = 0.1$.

Figure 1 demonstrates results of the obtained numerical solution at time $t = 0.1$ for coefficient of friction force $K = 500$. For this test we used sequential (non-parallel) version of the program with moderate number of particles $N = 2 \times 300 \times 32 \times 32$. It can be seen that solution is able to reproduce main features of reference solution, but for better precision it is required to use significantly more particles.
Figure 1. Solution of 3D problem of shock tube for time $t = 0.1$ and $t_{stop} = 0.002$, $K = 500$, $\varepsilon = 1$. Projection on $x$ axis is shown. Upper pictures show gas functions, lower pictures show dust functions. Density is shown on the left, velocity is shown on the right. Red dots mark solution obtained with SPH method; black line marks reference solution. Number of particles is $N = 2 \times 300 \times 32 \times 32$, $h = 0.01$ and $\tau = 0.001$.

3. Parallel Algorithm

The developed parallel algorithm is essentially the same for both SPH and PIC particles, mainly dealing with calculating new positions of particles and transferring them among subdomains. Parallel implementation of 3D FFT-based gravitational solver uses a standard method of data transposing [9, 10].

Initial 3D computational domain is divided into $K$ subdomains of the same size $S_1, S_2, ..., S_K$ by $x$ axis. Group of processors $G_k$ is assigned to each subdomain $S_k$. Number of processors in group $G_k$ is equal to $P_k$, $P_k \geq 1$. Total number of processors is $P = \sum P_k$.

For each subdomain we assign a grid, which is used for calculating gravitational potential and for calculating friction force between gas and dust phases. Number of nodes (cells) in each grid is chosen in such a way that all grid functions can be stored in RAM of one computational device and keep enough memory for particles (coordinates, velocities and gasdynamical functions). Typically it is equal to $0.5 \div 2$ million of nodes ($128^3$). Number of processors in group $G_k$ is chosen to provide approximately the same amount of particles on the same processor and it may change during a numerical experiment in case if more particles will be accumulated in some particular subdomains.

The general scheme of the algorithm for 3D PIC method was suggested earlier in [11]. Its main features adopted for solving both SPH and PIC are the following.

- We use sorting of the particles (both SPH and PIC) with regard to the cell of the grid. This sorting is done on each time step and it allows to search efficiently for all neighbour particles.
- To optimize searching for neighbour in one cell (in case if number of SPH particles is big) the construction of K-d trees can be used inside each cell.
The main computational efforts are concentrated in the calculating gas-dynamical functions in SPH method. Calculating gravitational potential is the least time-consuming part of the algorithm.

The amount of computations required for processing one PIC or SPH particle (calculating its coordinates and gas parameters) is much higher than transferring this particle from RAM of one processor to another. It means that it is reasonable to have a moderate number of communications (transferring of particles) between subdomains for each step.

In order to satisfy Courant condition for a single timestep SPH particle can move between nearest cells only. Because of this fact the number of particles which needed to be transferred between subdomains doesn’t exceed 0.1 - 1% of the total number of SPH-particles.

Processing of SPH particles requires that neighbour particles are located on the same processor. This suggests to use so-called "ghost" zones or overlapping zones between subdomain: when the information about particles located near the boundaries of subdomains is distributed on both subdomains.

The results of preliminary proof-of-concept numerical experiments with number of SPH particles $N_{SPH} = 10^8$, and PIC particles $N_{PIC} = 10^8$ on $2048 \times 256 \times 256$ grid nodes, and using 128 CPU-cores of Intel Xeon X5570 (at Lomonosov Supercomputer Center), showed the calculation of a single timestep is about 20 seconds, with less than half of computations spent on communications.

4. Conclusions
We developed parallel algorithm for numerical model which combines SPH method for solving 3D gas-dynamics equations, PIC method for solving Vlasov equation and grid FFT-based method for calculating gravitational potential. It is based on domain decomposition and dynamic load balancing of particles and group of processors re-assigned to the subdomains depending on the particular density distribution.

First tests have shown that algorithm is promising for conducting numerical experiments with a big number of SPH and PIC particles on supercomputers with distributed memory. It could be employed for the simulation of non-stationary astrophysics problems, which require series of computations with tens of thousands of time steps.

Acknowledgements. Nikolay Snytnikov is supported by budget project 0315-2019-0009 for ICMMG SB RAS. Numerical experiments have been conducted using Siberian Supercomputer Center (Novosibirsk) and Lomonosov supercomputer in MSU.

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