Implementing methods of PIC simulation by a special purpose computer system for gravitational N-body problems

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Particle In Cell (PIC) simulation using GRAPE-6 (G6), a special-purpose computer for gravitational N-body problems, is demonstrated. The calculation time is decreased by approximately 20 times, as compared to the usual method. There are two problems associated with simulation of plasma by the G6. First, G6 calculates only Coulomb force and three-dimensional (3D) calculations, which means that one-dimensional (1D) and two-dimensional (2D) simulations cannot be performed. Calculation of the electric field is achieved by arranging virtual particles. Virtual particles are arranged on a plane in 1D and along a line in 2D. As a result, in addition to 3D simulations, 1D and 2D simulations can be performed using the G6, and the PIC method can be applied. In addition, the G6 can only be used in free space. The FFT method assumes a cyclic boundary condition. This problem is solved by calculating the electric field outside the simulation space. The obtained external electric field is added to the electric field in the simulation space. By this operation, the error can be suppressed to approximately 1/80, as compared to the case in which this operation is not performed.

Keywords: Plasma, Simulation, Special-purpose computer, Vortex, Boundary condition

1. Introduction

Simulating the physical phenomena of celestial bodies and plasma requires significant calculations. Therefore, a special purpose computer has been developed in order to reduce the cost of hardware required for simulations and short calculation times. A special-purpose computer is typically a massive parallel-processing computer that has numerous custom LSI chips specifically designed to calculate a few expressions. By limiting the versatility of the calculation, the hardware complexity can be drastically reduced. Therefore, a special-purpose computer can contain a greater number of processors on one chip, as compared to a personal purpose computer. The GRAPE-6 (G6) (Hamamatsu Metrix Co., Ltd.) is a special-purpose computer that was designed to perform *N*–body gravitational simulations [1]. The G6 can rapidly calculate the gravitational force between particles using its specialized pipeline processors. The peak performance of a G6 unit reaches 985 GFlops. We have used the G6 for the calculation of the Coulomb interactions, which have the same form as the gravitational force, in order to determine the acceleration in the plasma simulation [2].

However, the calculation of only Coulomb's force cannot be performed by the PIC method of the primary technique of the plasma particle simulations for studying plasma physics. If the simulation of the PIC method can be performed using the G6, the application range of the G6 is expanded, and the possibility exists that a larger-scale plasma simulation can be achieved in the future. We introduce application to the PIC method by solving various problems using the G6 special purpose computer.

2. Calculations using GRAPE-6

A single G6 unit includes 32 custom LSI chips, each containing six pipeline processors for the calculation of gravitational interactions between particles. Since one pipeline processor works logically as eight pipelines, the G6 has a total of 1,536 pipelines per unit. Fast calculations by the G6 result from efficient use of the pipelines in parallel. The G6 is connected to a personal purpose host computer (CPU: Pentium-4) through a communication interface. The G6 calculates only the force due to the gravitation between particles, and the host computer performs the other calculations. The user program runs on the host computer and can only use the G6 by calling library functions. The architecture of the G6 is fairly simple from the user's viewpoint. The G6 is comprised of multiple memory units and pipeline processors. Each LSI chip has its own memory unit, and all of the particle data that must be stored are distributed to these memory units. Thus, the calculation of the force that is exerted on a particle is divided among all LSI chips. In addition, the G6 calculates the forces on different particles in parallel using pipeline processors on the LSI chip. The architecture of the G6 is shown in Fig. 1.

The gravitational force calculated by a pipeline of the G6 is given by

$$\boldsymbol{a}_i = G\sum_j m_j \frac{\boldsymbol{r}_{ij}}{(r_{ij}^2 + S^2)^{3/2}} \quad (1)$$

$$\boldsymbol{r}_{ij} = \boldsymbol{x}_i - \boldsymbol{x}_j \quad (2)$$

where $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ and m_i and m_j are the positions and masses, respectively, of particles i and j, G is the gravitational constant, and S is a softening parameter used to suppress any divergence of the force at $\boldsymbol{r}_{ij} \rightarrow 0$. The Coulomb force between charged particles is expressed by

$$\boldsymbol{F}_i = \frac{-q_i}{4\pi\varepsilon_0}\sum_j q_j \frac{\boldsymbol{r}_{ij}}{(r_{ij}^2 + S^2)^{3/2}} \quad (3)$$

where q_i and q_j are the charges of particles i and j, respectively, and ε_0 is the electric constant. This equation shows that the computation can be accelerated using the G6 for the system including Coulomb interaction, by replacing G, m_i, and m_j in Eq. 1 with $-1/4\pi\varepsilon_0$, q_i, and q_j, respectively. In the case of the simulations presented in the following sections, the host computer integrated the equation of motion and calculates the charging process and external forces. The G6 calculates the interaction between grids. The interparticle force is calculated as the Coulomb force using Eq. 3.

3. Application to the PIC method using the G6

In general, when a calculation is performed using the PIC method, the electric field is requested by performing FFT by the space after the charge is distributed to each grid point. On the other hand, when the G6 is used, the electric field is requested directly by calculating coulomb interaction from the charge density of each grid point [3], [4]. The distribution of the charge on grid points and the electric field on the particle positions is calculated by a personal computer. From the charge distribution on grid points, G6 calculates the force at each grid point, rather than the force on each particle.

However, there is a problem in that the character of the plasma simulation that uses the G6 is solved only by Coulomb force and three-dimensional (3D) calculations. This has the advantage of automatic 3D calculability. However, this means that 1D and 2D simulations cannot be calculated. In order to solve this problem, the electric field was calculated by arranging virtual particles, which are arranged on a plane in 1D (Fig. 2) or along a line in 2D (Fig. 3). In Fig. 2, the plane is constructed from 400 virtual particles for one particle. In Fig. 3, the line is formed from 50 virtual particles for one particle.

As a result, in addition to 3D simulations, 1D and 2D simulations can performed by the G6, and the PIC method can be applied [4].

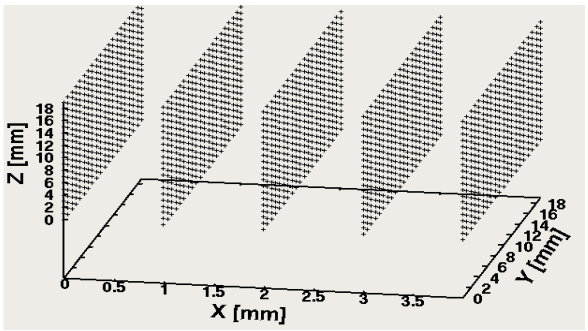

Fig. 2: Arrangement of virtual particles in 1D.

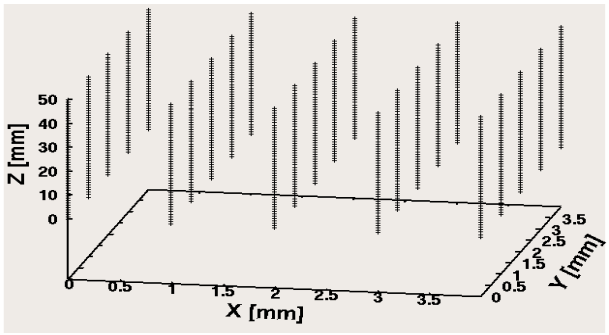

Fig. 3: Arrangement of virtual particles in 2D.

4. Comparison with the FFT method

We proposed a technique by which to obtain results similar to those provided by the usual Fast Fourier Transform (FFT) method in solving the Poisson's equation using the G6. The FFT method has generally been used to solve Poisson's equation in the PIC method. The FFT method assumes a cyclic boundary condition. However, the G6 only performs calculations in free space. Therefore, the potential distribution calculated by the usual PIC code yields a result that is different from that obtained using the G6 [5].

This problem is solved as follows. We calculate the electric field based on the distribution of the charge density in the simulation region, and the electric field outside the simulation region is calculated by the expansion of the electric field calculation region. The boundary condition is a cyclic boundary, and we calculated the influence of the cyclic charge density outside the simulation region by the superposition of the electric field obtained by the charge density outside the simulation region calculated in the first step to the electric field calculated using the inner simulation region. Using this method, the calculation amount decreases because of the interaction between the charge densities inside and outside the simulation region. We superposed the electric field by the charge density near the simulation region and neglected the electric field outside the simulation region.

To confirm the correctness of this method, we compared the electric field calculated by this method using the G6 to that calculated by the normal FFT method

using a PIC. For example, figure 4 shows the electric field component calculated in the X direction at Z=64 mm when the positive charge was distributed uniformly in space. For the cyclic boundary conditions, the charge is effectively distributed uniformly throughout space, so the electric field is constant in the simulated region. As shown in Fig. 4(a), the electric field is not constant for the case in which there is no correction for the effect of the charge outside the simulation region. In the G6 calculation, when the charge is positive, the electric field outside the simulation region is generated by the lack of charge in the region outside the simulation region. Here, the uniform charge density results in the electric field component in the X direction depending largely on X; Y dependence is very weak as well as Z dependence (not shown in Fig.4). For 3D simulation, we must compute the electric field in the X, Y, and Z space. When the original computational space is doubled in each direction and the electric field in the extended space is additively duplicated to the original space, the electric field error was suppressed to approximately 1/80 compared to the case without the extended space.

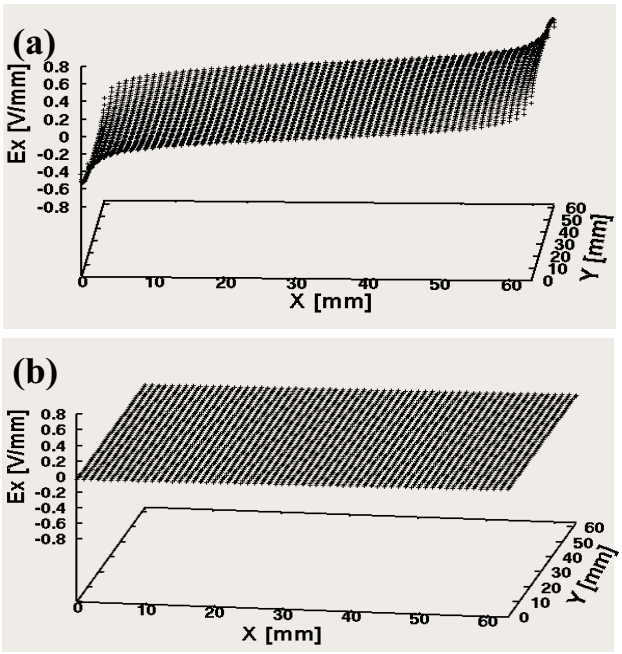

Fig. 4: Electric field component in the X direction for the cyclic boundary calculated using the G6. (a) no correction and (b) correction.

5. An example of a PIC simulation result obtained by the GRAPE-6

Plasma is a medium that easily forms vortices and a variety of vortex structures have recently been observed [6]. It would be useful to simulate the vortex motion of the plasma. In this section, the simulation result of the vortex motion of electron plasma is shown. Electron plasmas with an initial annular z-direction distribution located in a uniform magnetic field were considered. For such an initial distribution, the appearance of certain modes has been experimentally observed. We perform calculation not by the fluid vortex method, but rather using the following equation of motion:

$$\boldsymbol{F} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \qquad (4)$$

The first term of Eq. (4) is calculated using the G6. In general, significant computational time is required when computation is performed using Eq. 4 for the individual particles. However, the PIC method calculated by the G6 can simulate the phenomena of large-scale plasma. In addition, the algorithm of the vortex method is very simple compared with the conventional fluid vortex method, because the motion equation is solved directly instead of by the conventional fluid vortex method. The simulation of electron plasmas with an initial annular distribution is shown Fig. 5(a), and the electrons are distributed in equal intervals. Moreover, 100 particles are distributed on the line at intervals of 0.01 mm within the range from 0 mm to 1 mm in the Z direction of each particle of Fig. 5.

In this simulation, the number of electrons is 120,000, and number of grid points is 20,000. A full 3D simulation is calculated by the G6. The electron density is 10^{13} m^{-3}, and the external magnetic field is 0.048 T. The electrons divide into four vortices in the experiment results (Fig. 5(b)). We were able to obtain simulation results that were similar to the experiment results. Furthermore, the simulation when the thickness of the ring is changed is shown in Fig. 6. Under this condition, the vortex divides into eight clusters. The observed behavior was similar to the Kelvin-Helmholtz instability that occurs on the surface of the sea. In an electron plasma, this instability is called a diocotron instability [7].

6. Evaluation of the calculation time of the G6

In order to evaluate the calculation time of the G6 for the simulations, the calculation time of the G6 was compared with that of a personal computer (Pentium-4 3 GHz). We compared the CPU time of Poisson's solver by the personal computer with that of the counterpart (calculation of force on the grid points) by G6. The results are shown in Figure.7 with the CPU time of FFT in the Poisson's solver by personal computer. When the number of grid points is 10,000 or less, the calculation time of G6 is long. In the G6, when the calculation amount is small, the dead time for the communication time between the host computer and the G6 is dominant. For the same calculation, the G6 is approximately 300 times faster than a personal computer. However, when the FFT method is compared with the G6, the difference in

calculation times depends on the number of grid points. When the number of grid points is approximately 50,000, the calculation time of the G6 is shorter than that of the FFT method. At present, the calculation time of the G6 is approximately 20 times shorter than the calculation times of FFT methods. The difference in calculation time between the G6 and the FFT method is reduced when the number of grid points exceeds 50,000 points. In addition, when the number of grid points exceeds one million, the calculation time of the FFT method exceeds that of the G6, because the scaling of the amount of calculation is log (N) in the FFT and is N^2 in the Coulomb method.

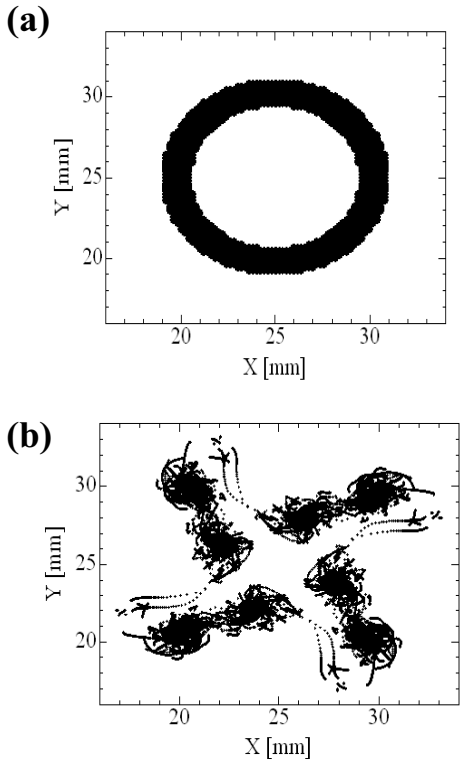

Fig. 5: Vorticity as a function of time for an annular distribution with an initial inner radius of 4.5 mm and an outer radius of 6 mm. (a) t = 0 ns and (b) t = 360 ns.

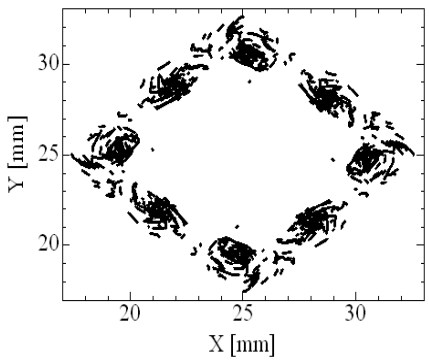

Fig. 6: Vorticity as a function of time for an annular distribution with an initial inner radius of 4.8 mm and an outer radius of 6 mm, t = 220 ns.

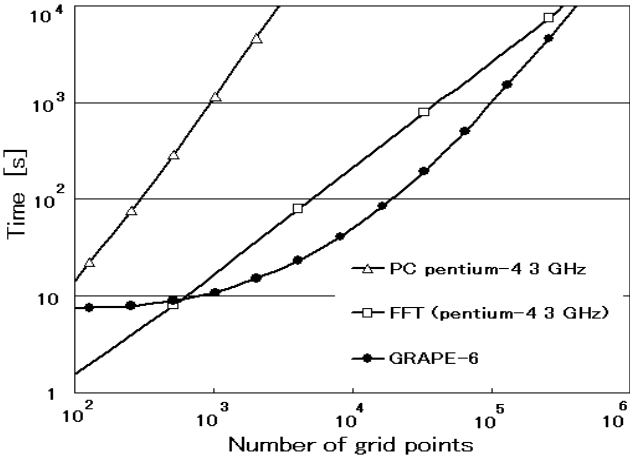

Fig. 7: Comparison of calculation times of the G6 and a personal computer.

7. Conclusion

We enabled the PIC method to be performed using the G6. The inability to perform calculations other than 3D calculations is one problem associated with the G6 special-purpose computer. This problem was solved by arranging the virtual particles as shown in Section 3.

The G6 calculates only the plasma simulation in the free space in the normal method because it calculates only Coulomb force. This is a limitation of G6 simulation. However, the implementation of the proposed method enables the cyclic boundary conditions to be calculated.

Finally, when the number of grid points is less than one million, the calculation time of the G6 is, at maximum, 20 times shorter than that of a personal computer. However, the following problems remain. The calculation amount increases in the case of 1D and 2D simulations for arranging virtual particles. The calculation time of the FFT method is shorter than that of the G6 when the number of grid points exceeds one million. If these problems can be solved, the application range of the G6 can be expanded, and a larger-scale plasma simulation may be achieved in the future.

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