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Three-dimensional particle-in-cell simulation of scrape-off-layer plasmas

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Abstract. Three-dimensional particle-in-cell simulation code for the investigation of physics in scrape-off-layer plasmas is developed. The code is parallelized by using High Performance Fortran (HPF) and good performance is attained in the computation at the Plasma Simulator at the National Institute for Fusion Science (NIFS) (NEC SX-7/160M5). The code represents resonable physics related to sheath and presheath formation as well as the formation of the self-consistent potential structure related to blob transport across a magnetic field.

1. Introduction

There is a growing interest in the investigation of three-dimensional (3D) kinetic effects of scrape-off-layer (SOL) plasmas in magnetic fusion devices. In a blob transport in a SOL of tokamak plasmas, the drift motion of charged particles, the sheath near diverter plates and the self-consistent potential structure play important roles [1,2]. The particle-in-cell (PIC) simulation method is one of the candidates for kinetic treatment. Unfortunately, because of the large spatiotemporal scale in SOL plasma, usual PIC simulation cannot treat the whole system of the SOL. However some important physics, such as the self-consistent potential structure formation and transport, can be presented by using a system with reduced space and time scale. In addition, PIC simulation takes an important part in multi-layer SOL simulation in which fluid type simulation and kinetic type simulation may be self-consistently connected. With these situations in mind, we have been developing 3D PIC simulation code for the investigation of dynamic plasma behavior in a SOL. Since a 3D PIC simulation needs a lot of computer resources, it is necessary to use parallel supercomputers efficiently. In this paper we would like to present the parallelization method of 3D PIC code by High Performance Fortran (HPF) [3] and some preliminary results of 3D bounded PIC code including the potential formation in relation to a blob transport.

2. Parallelization of 3D PIC code by HPF

In this section, we would like to briefly describe the parallelization of 3D PIC code by HPF which is a distributed parallel processing language for Fortran.

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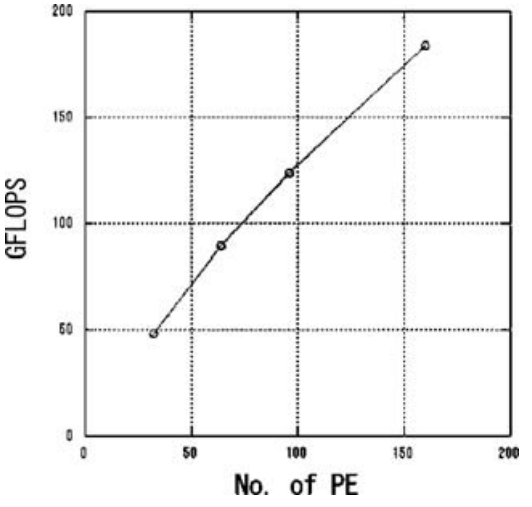


Figure 1. Dependence of the computing performance (GFLOPS) as a function of the total number of PEs.

Programmers can make a parallel program by specifying the distribution of arrays and adding some directives. The Plasma Simulator NEC SX7/160M5 supercomputer system at the National Institute for Fusion Science has five nodes and each node has 32 processor elements (PEs). In order to use this supercomputer efficiently we have to use parallelization in distributed memories among nodes as well as parallelization in shared memory.

Usual PIC code uses much CPU time for the deposition of particle position to grids and particle accelerations, while use of CPU time for solving Maxwell's equation is quite small. Thus, we should efficiently parallelize the parts related to particle information. We prepare two-dimensional arrays for particle velocities and positions and use a block distribution in terms of second index which corresponds to the processor number. The parts related to particles are parallelized in distributed memories with HPF and in shared memory with the automatic parallelization of the sxf90 compiler. On the other hand, the parts of solving Maxwell's equations are parallelized only in shared memory.

Figure 1 shows the FLOPS as a function of number of PEs in the case with $128 \times 128 \times 512$ spatial grids and 1 073 741 824 particles. Computation speed increases in proportion with the number of processor. This indicates that the parallelization is efficiently done.

3. 3D PIC simulation model for SOL plasmas

Configuration of our 3D PIC simulation code was carried out as follows. External magnetic field is pointing into the z direction. Particle absorbing boundaries corresponding to diverter plates are placed at the both ends of the z-axis. A particle absorbing plate corresponding to the first wall is also placed at one end of the x-axis. A particle reflecting plate is placed at the other end of the x-axis. A particle impinging to the absorbing boundaries is removed from the system. In the y direction, a periodic boundary condition is applied. First of all, we present the results with uniform magnetic field and smooth initial particle loading. The employed simulation

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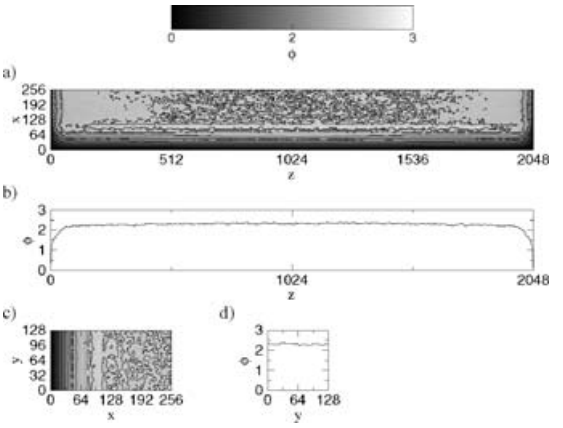


Figure 2. (a) Grayscale plot of potential profile in the x–z plane at $y = L_y/2$, (b) potential profile in the z direction at $x = 3L_x/4$ and $y = L_y/2$, (c) grayscale plot of potential profile in the x–y plane at $z = L_z/2$, and (d) potential profile in the y direction at $x = 3L_x/4$ and $z = L_z/2$ in the case with a uniform magnetic field and no density hump at $t = 500$.

parameters are as follows. The system sizes $L_x \times L_y \times L_z$ are $256 \times 128 \times 2048$ and a $256 \times 128 \times 2048$ spatial grid system is used. The ion to electron mass ratio $m_\mathrm{i}/m_\mathrm{e}$ is fixed at 100 and the ion to electron temperature ratio $T_\mathrm{i}/T_\mathrm{e}$ is 0.25. The ratio of the electron cyclotron to electron plasma frequency is $\omega_\mathrm{ce}/\omega_\mathrm{pe} = 2.5$, and the ratio of the ion cyclotron frequency to electron plasma frequency is $\omega_\mathrm{ci}/\omega_\mathrm{pe} = 0.025$. The time step width is 0.05 where the time is normalized by ω_pe^{-1}. The electrons and ions are initially loaded such as $n(x, y, z) = 0.5n_0(\tanh(x - 128)/32 + 1)$ where n_0 is the plasma density of the high-density region. It is noted that averaged plasma density of the whole system is $n_0/2$. The length is normalized by the Debye length of the high-density region.

Figure 2 shows the potential profiles (a) in the x–z plane at $y = 64$, (b) in the z direction at $y = 64$ and $x = 192$, (c) in the x–y plane at $z = 1024$, and (d) in the y direction at $x = 192$, $z = 1024$ at $t = 500$, where each profile is averaged over twice the length of the plasma period. Here, the potential ϕ is normalized by e/T_e, where e is the electronic charge. The potential profile is almost symmetrical about the $z = 1024$ plane. In the left-hand side, the potential is almost constant from the center of the system to the region at $z \sim 50$ in the z direction. It gradually goes down to $z \sim 5$ and strongly goes down to the boundary. This indicates that an ion sheath is created in the vicinity of the boundary. The potential difference between the center of plasma region and the boundary is about $\phi \sim 2$, which is almost equal to the value of simple estimation $\phi = 0.5 \ln(m_\mathrm{i}/m_\mathrm{e}) \sim 2.3$. The position which the potential starts to decrease is $x \sim 50$. This is almost equal to $x = c_\mathrm{s}t = 50$, where c_s is the ion acoustic speed. There is no significant potential structure in the y direction. These results indicate that the sheath and presheath regions are reasonably created in the 3D PIC simulation.

Finally, we show the results with the density hump placed and with grad-B in the x direction. The magnetic field along the z-axis is given by $B_z(x, y, z) = B_0(512/(768-x))$ and the initial density profile is given by $n(x, y, z) \propto ((\tanh(x-128)/32+1) + 4\exp-((x-192)/32)^2)(4\exp(-((y-64)/32)^2) + 1)$. The averaged density is $n_0/2$, which is the same as the previous case. The other simulation parameters are

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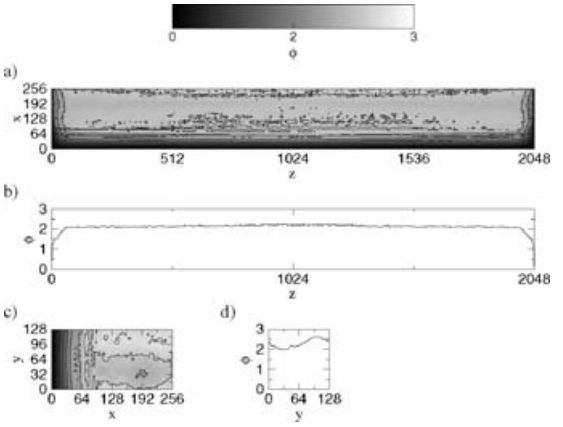


Figure 3. (a) Grayscale plot of the potential profile in the x–z plane at $y = L_y/2$, (b) potential profile in the z direction at $x = 3L_x/4$ and $y = L_y/2$, (c) grayscale plot of the potential profile in the x–y plane at $z = L_z/2$, and (d) potential profile in the y direction at $x = 3L_x/4$ and $z = L_z/2$ in the case with a non-uniform magnetic field and a density hump at $t = 500$.

also the same as in the previous case. Figure 3 shows the potential profiles. The potential profile in the z direction at $y = 64$ and $x = 192$ is almost the same as that of the previous simulation. On the other hand, a potential structure can be clearly observed in the y direction. The potential difference is approximately $\phi \sim 0.5$. The ions move in the positive y direction and electrons move in the negative y direction due to grad-B drift. The positive edge of the density hump with $y \sim 100$, thereby, is positively charged and the negative edge of density hump with $y \sim 30$ is negatively charged. As a result, the potential difference in the y direction is self-consistently created. This self-consistent electric field pointing to the negative y direction plays a role to push the density hump to the negative x direction due to $E \times B$ drift. At later times the density hump moves in the negative x direction at the speed $v \sim 0.1 c_s$.

4. Summary and discussion

We have developed 3D PIC simulation code for the investigation of SOL physics. Simulation code is parallelized by using HPF and automatic parallelization of the sxf90 compiler and is optimized for the SX7/160M5 system at the National Institute for Fusion Science. Several simulation runs were performed and reasonable results were attained. The self-consistent electric field creation which causes the transport of a blob across a magnetic field is demonstrated without significant assumptions. In our 3D simulation, instabilities related to the field aligned plasma flow, such as shear flow instability, can be taken into acount. These instabilities could collapse the blob. These kinds of subjects will be studied in the future.

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