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Supercomputer simulation of plasma electron dynamics in a magnetic trap with inverse magnetic mirrors and multipole magnetic walls*

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Abstract. The problem of simulation of plasma electron dynamics in the magnetic trap with inverse magnetic mirrors and multipole magnetic walls is considered. The model is built on the basis of Particle-In-Cell method. The complexity of processes under study and the necessary in a high precision of results required the development of a highly-scalable computational algorithm. Such an algorithm must be capable of computing billions of particle trajectories in a reasonable time. In order to achieve uniform and complete workload of the computational nodes of a supercomputer, the mixed Eulerian–Lagrangian decomposition is used. A dynamic time step is taken into account. This approach results in a high scalability and a significant decrease in the computational time.

1. Introduction

Powerful neutral beams for controlled fusion installations are obtained in the best way by neutralizing the negative ion beams in a target plasma trap. In the Budker Institute of Nuclear Physics SB RAS for solving this problem, a linear axially symmetric trap with inverse magnetic mirrors was proposed [1]. A target plasma trap 130 cm long with 10 cm aperture was created for carrying out experimental research. The objective of this project is to minimize plasma losses in the trap. The main source of plasma losses is wide aperture holes in the end faces of the trap. These holes contain inverse magnetic mirrors. One more source of plasma losses is the exit of plasma particles to the trap vacuum chamber through the cylindrical multipole magnetic walls of the trap.

A full-scale investigation of physical processes in plasma may be performed only by means of an integrated approach, i.e., the approach combining experimental research and numerical simulation. The simulation techniques involved must describe the physical processes correctly. In order to avoid simplifications and to obtain a qualitatively correct physical pattern it is necessary to develop a mathematical model as complete as possible.

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It is generally accepted that a good basical model is a system of equations that consists of the Boltzmann equation for the distribution functions for electrons and ions [2]:

$$\frac{\partial f_\alpha}{\partial t} + \vec{v}\frac{\partial f_\alpha}{\partial \vec{r}} + \vec{F}_\alpha \frac{\partial f_\alpha}{\partial \vec{p}} = \mathrm{St}\{f_\alpha\}, \quad \vec{F}_\alpha = q_\alpha(\vec{E} + \frac{1}{c}[\vec{v}, (\vec{H} + \vec{H}_0)]), \qquad (1)$$

and Maxwell's equations for the self-consistent electromagnetic field:

$$\mathrm{rot}\,\vec{H} = \frac{4\pi}{c}\vec{j} + \frac{1}{c}\frac{\partial \vec{E}}{\partial t} = \frac{4\pi}{c}\sum_\alpha q_\alpha \int f_\alpha \vec{v}\, d\vec{v} + \frac{1}{c}\frac{\partial \vec{E}}{\partial t}, \qquad (2)$$

$$\mathrm{rot}\,\vec{E} = -\frac{1}{c}\frac{\partial \vec{H}}{\partial t}, \qquad (3)$$

$$\mathrm{div}\,\vec{E} = 4\pi\rho = 4\pi\sum_\alpha q_\alpha \int f_\alpha\, d\vec{v}, \qquad (4)$$

$$\mathrm{div}\,\vec{H} = 0. \qquad (5)$$

Here the subscript α stands for the sort of particles (either electrons or ions); $f_\alpha(\vec{r}, \vec{v}, t)$ is the distribution function for the particles of the sort α; q_α is the particle charge; $\vec{j}$ is the current density, ρ is the charge density; $\vec{E}$ is the electric field; $\vec{H}$ is the magnetic field; $\vec{H}_0$ is the trap magnetic field; $\mathrm{St}\{f_\alpha\}$ is the collision term that describes the following physical processes:

- hydrogen atom ionization,
- ionization and dissociation of H^2 molecule,
- dissociation excitation and dissociation recombination of H^{2+},
- dissociation recombination of D^{2+},
- charge exchange between protons and hydrogens atoms.

The PIC method is the multi-purpose and most widely used method for solving these equations [3]. This method can be briefly described in the following way. Plasma is represented by a sufficient large number of model particles, that are moving according to the classical mechanics laws. The motion of particles is determined by the self-consistent electromagnetic field. Each model particle represents the motion of a large number of real particles. Thus, a model particle has also a number of attributes of real particles such as mass, charge, impulse, kinetic energy, etc. In order to obtain a correct description of processes within the whole trap it is necessary to use up to 10^9–10^{13} model particles and 10^6–10^9 grid nodes in the 2D case. The PIC method is an essentially parallel method since the trajectories of particles may be evaluated independently. Nevertheless, the development of a scalable

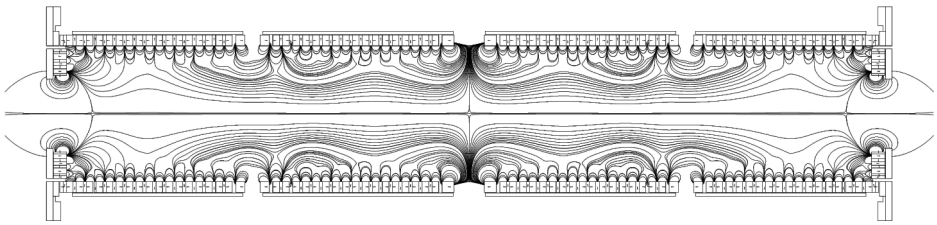

Figure 1. The geometry of the target plasma trap and contours of the magnetic field

parallel implementation of the PIC method is a complex task depending on peculiarities of the physical processes under study [4].

One of such peculiarities is the complex pattern of the magnetic field within the trap. Figure 1 shows the geometry of the ringed magnets with iron screens. The magnetic field pattern forms the target plasma trap. The magnetic field of the trap in some regions varies from 50 Gs to 7 kGs.

Such a considerable difference (two orders of magnitude) in the value of the magnetic field greatly affects the Larmor radius. It results in a decrease of a time step at the stage of the particle trajectory computation. In this paper, the problem of an adaptive time step for particles in various parts of the trap is also considered.

2. Solving the main equations

In an axially symmetric trap with a ring magnetic field, the azimuthal field component is absent as well as the stationary azimuthal electric field. Thus, in such a trap the wall-normal plasma drift is impossible. Due to this reason the 2D statement of the problem in the cylindrical R–Z coordinates is optimal. All the three components of particle velocities and impulses are taken into account.

2.1. Solving the Boltzmann equations. The Boltzmann equation solution is reduced by means of the splitting technique to solving the Vlasov equation

$$\frac{\partial f_\alpha}{\partial t} + \vec{v}\frac{\partial f_\alpha}{\partial \vec{r}} + \vec{F}_\alpha \frac{\partial f_\alpha}{\partial \vec{p}} = 0,$$

and to the correction of particle trajectories to provide $\mathrm{St}\{f_\alpha\} = 0$ considering ionization and dissipation processes by means of Monte Carlo methods [5].

Solving the Vlasov equation is performed in the Lagrangian coordinates. The characteristic equations for the Vlasov equation, yield the equations of motion for model particles:

$$\frac{\partial \vec{p}}{\partial t} = q_\alpha\Big(\vec{E} + \frac{1}{c}[\vec{v}, (\vec{H} + \vec{H}_0)]\Big), \qquad \frac{\partial \vec{r}}{\partial t} = \vec{v}.$$

Here $\vec{H}$ includes the self-consistent magnetic field for particles and the external field created by the trap. In order to avoid the numerical errors at the symmetry axis, in the present paper, the Boris correction scheme is used [6]. The scheme involves solving the equations of motion for a particle in the Cartesian coordinates and further local conversion of the result to cylindrical coordinates. In this case, the following scheme could be used for the particle trajectory evaluation:

$$\frac{\vec{p}_i^{\,m+1/2} - \vec{p}_i^{\,m-1/2}}{\tau} = q_\alpha\left(\vec{E}_i^m + \frac{1}{c}\left[\frac{\vec{v}_i^{\,m+1/2} + \vec{v}_i^{\,m-1/2}}{2}, \vec{H}_i^m\right]\right). \qquad (6)$$

Here τ is the time step; superscript shows the moment of time to which the value corresponds. The subscript i shows the number of the model particle under consideration.

2.2. Solving the Maxwell's equations. Maxwell's equations are solved in the Eulerian coordinates. The necessary current and charge densities are evaluated with the velocities and coordinates of model particles:

$$\rho(\vec{r}, t) = \sum_j q_j R(\vec{r}, \vec{r}_j(t)), \qquad \vec{j}(\vec{r}, t) = \sum_j q_j \vec{v}_j(t) R(\vec{r}, \vec{r}_j(t)).$$

Here q_j is the charge of a particle with number j; the function $R(\vec{r}, \vec{r}_j(t))$ (the kernel function) gives the form and size of the particle as well as the charge distribution within the particle. In the case under consideration, the charge and current densities are evaluated by means of the formulas similar to those in [7]. The formulas from [7] were modified to satisfy a finite difference analog of equation (4) in the cylindrical coordinate system. This enables significantly to speed up computations. The electric and magnetic fields are evaluated by means of the scheme proposed by Langdon and Lasinsky [8]. According to this scheme, the fields are defined from the finite difference analog of Faradey and Ampere laws:

$$\frac{\vec{H}_i^{\,m+1/2} - \vec{H}_i^{\,m-1/2}}{\tau} = -c\,\mathrm{rot}_h\,\vec{E}^m, \qquad (7)$$

$$\frac{\vec{E}_i^{\,m+1} - \vec{E}_i^{\,m}}{\tau} = -4\pi\vec{j}^{\,m+1/2} + c\,\mathrm{rot}_h\,\vec{H}^{m+1/2}. \qquad (8)$$

In such a way, solving the problem consists of the three stages. At the first (Lagrangian) stage, particle velocities and coordinates are evaluated according to scheme (6). At the same time, components of the current density $\vec{j}^{\,m+1/2}$ and the charge density ρ_{m+1} are defined. At the second

stage, particle trajectories are corrected, particles are added and removed with allowance for ionization and dissipation. These processes are treated with Monte Carlo methods. The particles that have escaped the trap are also removed. At the third (Eulerian) stage, Maxwell's equations are solved according to scheme (7)–(8). Thus, the values $\vec{H}^{m+1/2}$ and $\vec{E}^{m+1}$ are determined in the grid nodes. The values of electric and magnetic fields at the position of each particle are evaluated by means of the bilinear interpolation.

2.3. Adaptive mass alteration. Particles can appear and disappear (due to ionization and recombination) and, also, escape from the trap at each time step. Thus, it appears necessary to inspect the local density alteration in each cell at each time step. The problem is in that the number of real physical recombining particles could be much lesser than the number of real particles corresponding to one model particle. In this case, removing one model particle in order to simulate recombination may result in a dramatic non-physical density alteration. In order to avoid such non-physical effects, the PIC method with adaptive mass alteration was proposed [9]. For each sort of particles, a constant $s = \frac{q}{m}$ is introduced, which is the charge to mass ratio. The model particle stores the charge value that is proportional to the density in the cell. New particles are created according to the following algorithm [9]:

- the total mass in the cell is computed,
- the average velocity is computed,
- the new mode particles are added with a necessary velocity distribution (the average velocity of the added super-particles is 0),
- the new mass of a model particle in this cell is computed (the total mass is divided into the new number of super-particles). This mass is assigned to each super-particle in this cell,
- the average velocity is added to the velocities of the new model particles.

Removing the model particles is done in the same way.

3. Parallel implementation of the algorithm

At every time step, the algorithm performs the following actions:

- evaluation of electric and magnetic fields,
- evaluation of the motion of particles,
- evaluation of the new charge and current densities, collision term evaluation,
- particle mass alteration.

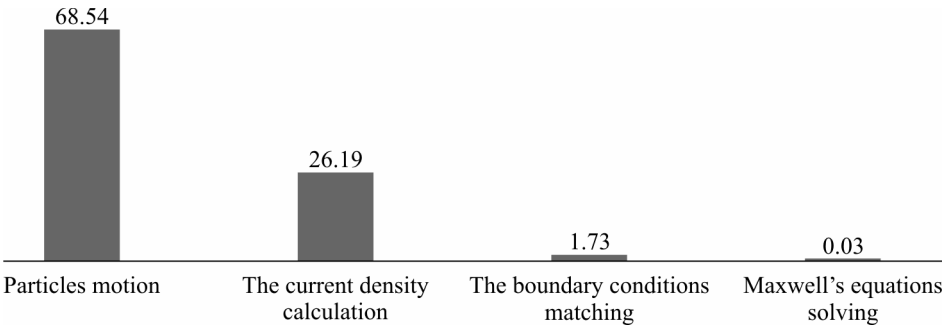

Figure 2. The working time distribution (%) for 128×128 grid with 200 particles per cell

The working time for all these procedures was measured by *gprof* profiler. The results are given in Figure 2.

From Figure 2 one can see that the main time to run the code is spent on the operations with particles, namely, on the calculation of the particle motion and the current density for each particle. Consequently, there are a few schemes for parallelization: the uniform particle distribution by processors, the Euler domain decomposition and distribution of particles among processors depending on their position, distribution of particles depending on each time step for a single processor. The advantage of the Euler–Lagrange domain decomposition for a constant time step is shown in [4] (Figure 3).

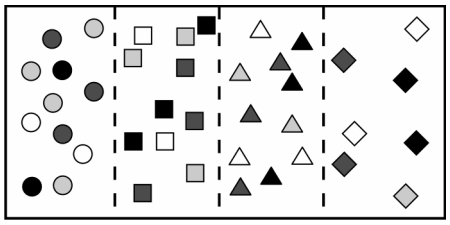

Figure 3. The Euler–Lagrange domain decomposition

The solution domain is divided into a few sectors along the axis Y. The particles of each subdomain are distributed among the processors of each type, uniformly and independent of the coordinate. Different symbols denoting particles such as a circle, a square, a triangle, a diamond refer to particles of a different processor type. Here 16 processors were used.

4. Numerical experiment

The calculation of the trajectories of model particles has been carried out using the following physical and model parameters: the plasma temperature is 5 eV, the domain size is 61×12 cm^2, the electron (ion) density $2 \cdot 10^{13}$ cm^{-3}, the grid has 4096×128 nodes, the total number of model particles is 5,242,880,000. The calculations were performed on the supercomputer "Lomonosov" using up to 8192 processor cores. The average time

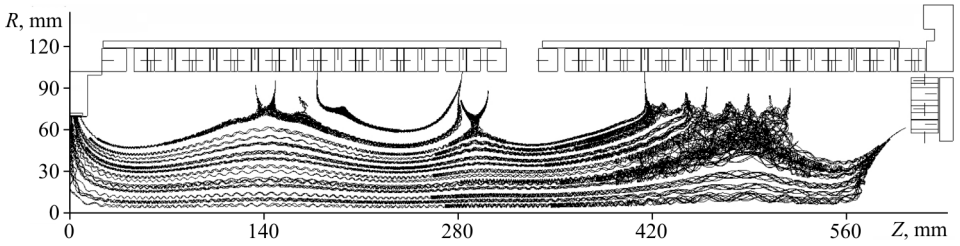

Figure 4. The electron motion trajectories of the plasma target electrons under the influence of the magnetic field

of one step calculation is 0.326 s, the average time for running the code is 24 hours. There are shown trajectories of some plasma electrons in Figure 4. Here the influence of ionization and dissipation was not taken into account.

From Figure 4, it can be seen that inverse magnetic plugs on the ends keep plasma in the trap sufficiently well. At the same time, there is a loss of plasma on the trap walls and the inverse plug boundaries. In the future, for the combined description of the plasma loss, the influence of the electron dispersion will be taken into account in the future.

5. Conclusion

In this paper, it has been shown that the use of modern supercomputers permits us to successfully solve a physical problem. The developed parallel algorithm is well scalable, i.e., very good up to tens of thousands processor cores and takes into account a capacity balance on the processors. In spite of the fact that even in a two-dimensional case a vast computational burden is necessary to calculate trajectories of the billions of model particles, we succeeded to estimate the plasma loss on the trap walls and inverse plug boundaries. In the computational experiment, a reduced model of the experimental trap, with the side ratio 1 : 5 was considered. In the future, we are planning to consider a real size of the trap in our calculations by increasing the number of processor cores up to 100 000 and by using graphical accelerators.

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References

[1] Dimov G.I., Emelev I.S., et al. Multicusp trap with circular geometry for confinement of low-temperature plasma // Transactions of fusion science and technology. — 2011. — Vol. 59, No. 1T FUSTE8 (2). — P. 1–324.

[2] Vlasov A.A. Many-Particle Theory and its Application to Plasma. — Gordon and Breach, 1961.

[3] Berezin Y.A., Vshivkov V.A. Particle Method in Rareed Plasma Dynamics. — Novosibirsk: Nauka, 1980 (In Russian).

[4] Berendeev E.A., Efimova A.A. Implementation of the effective parallel computations to model big problems of the plasma physics using the particle-in-cell method // Proc. Intern. Conf. "Parallel Computational Technologies (PCT) 2012", Novosibirsk. — 2012. — P. 380–385 (In Russian).

[5] Birdsall C.K. Particle-in-cell charged-particle simulation plus Monte Carlo collisions with neutral atoms, PIC-MCC // IEEE Trans. Plasma Sci. — 1991. — Vol. 19, No. 2. — P. 65–83.

[6] Boris J.P. Relativistic plasma simulation - optimization of a hybrid code // Fourth Conference on Numerical Simulation of Plasmas, Washington. — 1970. — P. 3–67.

[7] Villasenor J., Buneman O. Rigorous charge conservation for local electromagnetic field solver // Computer Phys. Comm. — 1992. — Vol. 69. — P. 306–316.

[8] Langdon A.B, Lasinski B.F. Electromagnetic and relativistic plasma simulation models // Meth. Comput. Phys. — 1976. — Vol. 16. — P. 327–366.

[9] Snytnikov A.V., Vshivkov V.A., Goedheer W.J. Adaptive mass alteration to model ion-ion recombination ia a Particle-in-Cell simulation of silane radio-frequency discharges // Computer Phys. Comm. — 2010. — Vol. 181. — P. 1743–1749.

[10] Andrianov A.N., Efimkin K.N. Approach for implementation parallel PIC method. — 2009. — (Preprint / Keldysh Institute of Applied Mathematics; 9).