Comparison of several algorithms of the electric force calculation in particle plasma models

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Abstract. This work is devoted to plasma modelling using the technique of molecular dynamics. The crucial problem of most such models is the efficient calculation of electric force. This is usually solved by using the particle-in-cell (PIC) algorithm. However, PIC is an approximative algorithm as it underestimates the short-range interactions of charged particles. We propose a hybrid algorithm which adds these interactions to PIC. Then we include this algorithm in a set of algorithms which we test against each other in a two-dimensional collisionless magnetized plasma model. Besides our hybrid algorithm, this set includes two variants of pure PIC and the direct application of Coulomb's law. We compare particle forces, particle trajectories, total energy conservation and the speed of the algorithms. We find out that the hybrid algorithm can be a good replacement of direct Coulomb's law application (quite accurate and much faster). It is however probably unnecessary to use it in practical 2D models.

1. Introduction

Computer modelling is a very important approach in plasma physics. This work is focussed on the molecular dynamics, i.e. deterministic particle modelling, which is used for the detailed study of plasma behaviour in cases like plasma-solid interaction. In molecular dynamics, the motion of individual particles is modelled using Newton's second law. The crucial point is the calculation of forces. In self-consistent models, the forces are updated in each step according to the actual particle positions (and velocities if we include magnetic field). This usually takes lots of computation time and many optimizations have to be done to make the model run reasonably fast (say, days instead of years of computation time).

We focus on high-temperature plasma so we have to include the electric and magnetic forces in our model. In low-temperature plasma, we would have to add the collisions with neutral particles.

Apparently the most widely used method for the calculation of electric force is the particle-in-cell (PIC) technique. It is relatively fast, relatively simple and it allows easy application of most types of boundary conditions. The main drawback of particle-in-cell is that it greatly underestimates the short-range interactions between charged particles as it sums their charges in the cells of the grid. The question is how much this inaccuracy affects practical plasma models.

According to [1], it seems that the short-range interactions (alias Coulomb collisions) are quite important in the case of magnetized plasma, as shown in figure 1. However, it has been found that the effect is probably exaggerated in the right picture and the truth lies somewhere in the middle. This is one of the reasons why we study this problem.
2. Our model
Our model is two-dimensional and self-consistent and represents a region in a collisionless magnetized plasma. For the comparison of different electric force calculation algorithms, it is necessary to use the same boundary conditions for all the algorithms. We found periodic boundary conditions to be the only boundary conditions that satisfy this requirement. Hence our model is fully periodic.

We include the magnetic field in the simplest way – as a constant field along the $x$ axis. We use the algorithm referred to as half acceleration, rotation, half acceleration [2].

3. The methods
Here we describe the electric force calculation methods which we have used.

3.1. Particle-in-cell
This technique consists in solving the discretized field equations
\[ \Delta \varphi = -\frac{\rho}{\epsilon_0}, \quad (1) \]
\[ \mathbf{E} = -\nabla \varphi \quad (2) \]
on a grid covering the modelled region. There exist several variants of PIC which differ in the way how the charges of the particles are counted (or weighted) to the cells and, after solving (1) and (2), how the electric field (evaluated at the grid points) is weighted back to the particles (both weightings should be the same) [2]. We use these two variants: PIC with nearest-grid-point (zero order) weighting, which we will refer to as PIC-NGP, and PIC with linear (first order) weighting, so called cloud-in-cell, which we will refer to as PIC-CIC.

3.2. Coulomb’s law
This is the most direct and theoretically the most accurate method of calculating the electric force. In our model, Coulomb’s law does not have the well-known form. In a two-dimensional model, the particles must be regarded as infinite charged rods, so Coulomb’s law takes the form
\[ \mathbf{E} = \frac{\lambda r}{4\epsilon_0 r^2} \quad (3) \]
where $\lambda$ is the linear charge density. Furthermore, our model is periodic so when we calculate the force at particle 1 caused by particle 2, we have to count in all the images of particle 2 in the whole 2D space. So we use a double infinite sum of (3) in our program.

3.3. **Hybrid algorithm**

The aim of our hybrid algorithm is to be more accurate than PIC and faster than Coulomb's law. Here we will give a brief description of the algorithm.

First, PIC-NGP is performed so we have the electric field calculated at the cell centres. Then, for each particle, we subtract the Coulomb forces (3) of the eight neighbouring cells (see figure 2), using the coordinates of the cell centres. Finally, we add Coulomb forces of all the particles inside the grey region in figure 2 (except for the target particle, of course).

![Figure 2. Part of the grid for the explanation of the hybrid algorithm. The blue spot represents the target particle (i.e. the particle for which we calculate the electric field) and the crosses represent cell centres.](image)

4. **Non-physical heating**

Non-physical heating is a common problem in molecular dynamics. It is a result of inaccurate time integration due to the finite time step. This problem arises especially in the Coulomb and hybrid methods. In Coulomb collisions, the particles have large acceleration and large trajectory curvature. In the model, they usually get closer together than they would in reality, so they gain additional energy, producing non-physical heating.

We have devised and tested the following method of reducing the non-physical heating. At the beginning of the program, we estimate the maximal particle velocity, according to Maxwell-Boltzmann distribution and the number of particles. Then, during the model run, we check the velocity of each particle each time it is updated. If the velocity is larger than the precomputed limit, we change it to this limit, preserving the original direction.

5. **Results**

Table 1 summarizes the input parameters we have used.

| Parameter               | Value                |
|-------------------------|----------------------|
| Gas                     | Deuterium            |
| Plasma density          | $1 \times 10^{18}$ m$^{-3}$ |
| Plasma temperature      | $1 \times 10^6$ K    |
| Magnetic field          | 1 T                  |
| Number of particles     | Various              |
| Modelled region size    | 2 cm $\times$ 2 cm   |
| Grid                    | $100 \times 100$ cells |
| Time step               | $1 \times 10^{-12}$ s |

5.1. **Force comparison**

We have made histograms which show the correlation between the electric field calculated by the given method and the electric field calculated by the periodic Coulomb's law (taken as the reference). These histograms were created using 40 000 particles and they are shown in figure 3.
5.2. Particle trajectories
We originally performed the computations with only 2000 particles (1000 ions and 1000 electrons) because of the very slow periodic Coulomb calculations; but there was a huge non-physical heating and other problems. As our hybrid algorithm seems to be a good replacement of the direct Coulomb calculation (see figure 3), we decided to exclude the Coulomb algorithm from testing and repeat the computations with 200,000 particles. The resulting trajectories are shown in figure 4.

5.3. Energy conservation
Because there are no physical energy sources or leaks in our model, the total energy should remain constant. Figure 5 shows the total energy evolution for the tested algorithms. These results come from the same computations as the trajectories in figure 4 (i.e. with 200,000 particles).

5.4. Speed
Our computations have been performed on an ordinary PC (Athlon64 @ 1.8 GHz). The computation times are summarized in table 2.
6. Discussion and conclusions

The proposed hybrid algorithm really does what it is supposed to do – it calculates the forces very close to the results of exact Coulomb's law calculations while it is much faster. On the other side, it suffers from the non-physical heating markedly just like the direct Coulomb's law calculations. The proposed method of reducing the non-physical heating does really reduce the non-physical heating but it obviously cannot do wonders. It also distorts the energy distribution function (however, the non-physical heating distorts it in another way).

The most important result of our contribution can be found in figure 4 – particle trajectories. For given parameters (typical edge plasma), we have found no transitions between magnetic field lines even if we use Coulomb's law for close particle encounters (the hybrid algorithm). Moreover, we have found no such transitions even in the case of 2 000 particles and using the periodic Coulomb's law directly (picture not presented). We performed the computations also for the parameters of low-temperature plasma (though physically impossible without neutral particles) and the results were

Figure 4. Trajectories of 10 almost randomly chosen electrons during the time of $1 \times 10^{-8}$ s. All the pictures show the trajectories of the same electrons for the same initial conditions.
almost the same. So it is probably useless to use such complicated algorithms in practical plasma models, at least in the case of two-dimensional models.

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References
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[2] Birdsall C K and Langdon A B 1991 Plasma physics via computer simulation (Bristol: IOP Publishing Ltd)

Figure 5. Total energy evolution in time for the tested algorithms: PIC-NGP, PIC-CIC, hybrid and hybrid with the non-physical heating reduction. Sampling rate: 10 steps. Please note the logarithmic scale for energy.

Table 2. Comparison of the speed of the algorithms.

| Algorithm            | Computation time per step [ms] |
|----------------------|---------------------------------|
|                      | 2 000 particles | 200 000 particles |
| PIC-NGP              | 12               | 36                |
| PIC-CIC              | 13               | 70                |
| Periodic Coulomb a   | 5 825             | Not tried b       |
| Hybrid               | 16               | 5 749             |

a Periodic Coulomb is considerably (at least 13, maybe 100 times) slower than ordinary Coulomb.
b Our estimate is 58 million ms, i.e. 16 hours.