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# Method to increase the simulation speed of particle-in-cell (PIC) code

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**Abstract**

An algorithm for time reduction is implemented to an existing particle-in-cell (PIC) code to simulate plasma systems. The algorithm not only guarantees higher simulation speed than the original one but also conserves position, charge density, and energy of the system. Position and charge density are conserved by grouping particles in one cell and energy is conserved by dividing velocity space to several groups. Particle number is reduced by grouping particles that have similar magnitudes and directions of velocity to conserve the total system energy. The speed is improved from two to five times by reducing the simulation particle-numbers in the system. As the particle number is reduced, the stability of code is also improved. © 2001 Elsevier Science B.V. All rights reserved.

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## 1. Introduction

A particle-in-cell (PIC) method [1] is one of the most promising techniques used in a variety of plasma simulation [2–6]. In addition, it is more accurate model compared with fluid codes that use predefined distribution function. The PIC method is based upon super-particles, wherein each super-particle represents a set of many real particles. PIC codes are usually expensive time-wise, and hence require considerably large computation time to achieve a steady state in a typical simulation. In the case of plasma discharge evolution, the number of charged particles eventually increases by a several orders of magnitude. This consequently leads to poor speed of the simulation code. The speed of such code can be significantly improved by reducing the number of particles to a certain extent, without the loss of generality of the physical problem. The reduction of particle number in the simulation may lead to adverse effects, for example, violation of charge and energy conservation laws. The stability critically relies upon the conservation of such quantities. Nevertheless, the instantaneous reduction in the number of particle may cause trivial or unpredictable results. A number reduction method must be dealt with an utmost care.

In the past, to overcome the problems of kinetic simulation particle splitting and sifting method was applied to one-dimensional system [7,8]. Usually, the particle simulation suffers from too many particles in

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the total system and too small particles in the cathode fall region. In this method, the authors [7,8] separated the particle species in the bulk and cathode fall region. Large-weighted particles are used in the bulk and small-weighted particles are used in the cathode fall region. Thus, particle number in the cathode fall region is increased enough such that spurious fluctuations are removed and particle numbers in the bulk region are reduced to obtain speed gain. The particle species are changed at the boundary of bulk and cathode fall region. The boundary was determined by the particle energies. Also, in Refs. [7,8], different time steps are used for different species.

In this report, we present an alternative particle number reduction scheme as applicable to a PIC code that preserves not only the conservation laws but reduces the time of simulation. In contrast to the previous work [7,8], we initially use one species. If the particle number reach a certain criteria, we make another large-weighted particle species by dividing the phase space. By this method, we reduce the particle number without discriminating the bulk and cathode fall region. We also extended this method to two-dimensional system. In the next section, we describe the number reduction method. Simulation results of the new method are presented in Section 3, and a comparison with the original method is also presented therein. Section 4 contains summary and conclusions.

## 2. Number reduction method

A particle number reduction method has been employed to speed up simulation [9] in which particle numbers are reduced in the simulation by combining several particles to one particle that has higher charge. We apply this method to one- and two-dimensional PIC codes namely XPDP1 [10] and XPDP2 [11] to obtain a speed gain. While implementing the technique, it is important to ensure that the conservation laws are satisfied. We achieve the charge conservation law by merging particles in the same cell or closest cells. The momentum and energy conservation laws may not be satisfied simultaneously because the degrees of freedom decrease with the reduction of particle number. The errors that may occur in the merging process increase and generate the numerical instability of the simulation code.

In order to conserve the charge of the system, particle merging is performed within one cell. Then the phase space of particles in each cell is divided into several small segments by the magnitude and the direction of velocity. The particles are ordered from lower to higher energy ones in the phase space. We merge particles, that have closest energies in the same segment of phase space, into smaller number of particles, and simultaneously maintain momentum and energy as close as possible to the original ones. The speed and the stability of the code are enhanced by this method.

### 2.1. One-dimensional number reduction method

The one-dimensional PIC code (XPDP1) follows one position coordinate ($x$) and three-dimensional direction velocities. The phase space of one-dimensional system is divided into two by $x$-direction velocity only

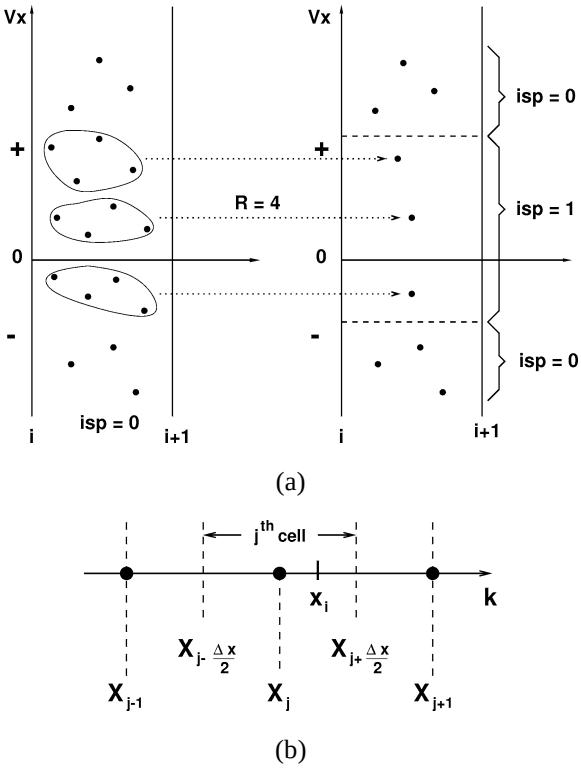


Fig. 1. The reduction method in one dimension. (a) $R$ is the reduction rate, and isp means the species-group number, (b) charge assignment of PIC method.

as shown in Fig. 1(a). The concerned velocity direction is only $x$-direction because applied voltage is along the direction. If the two particles that have the same but reverse-direction velocity are merged, energy cannot be conserved. Therefore our scheme divides velocity system into two domains to prevent such situations. To conserve the momentum, particles are sorted from the minimum to maximum velocity. The merging process begins from the minimum energy particles. This procedure is applied to each divided phase space domain ($+x$- and $-x$-direction velocities in one dimension). We preserve concerned direction velocity momentum and energy by the method. The time for sorting and merging is small enough compared with the whole simulation time. As the reduction rate, $R$ (the number ratio of merging particle to new super-particle) increases, the speed of simulation also increases.

It is possible to merge several particles to one particle in one dimension because the charge conservation law requires only one new spatial degree of freedom. If several particles are merged to one particle, there are five degrees of freedom, position, charge, and three velocities of the new particle. The new charge is then determined by the total charge of merging particle. The charge density in the PIC code is determined by [1]

$$q_j = q_c\left[\frac{\Delta x - (x_i - X_j)}{\Delta x}\right] = q_c\frac{X_{j+1} - x_i}{\Delta x}, \tag{1}$$

$$q_{j+1} = q_c\frac{x_i - X_j}{\Delta x}, \tag{2}$$

where $q_j$ and $q_{j+1}$ are charge densities at the $j$th and $(j+1)$th grid point, $q_c$ is total charge in the $j$th cell, $x_i$ is $i$th particle's position, and $X_j$ is grid point [Fig. 1(b)]. The total charge $q_c$ in the cell is determined by the particle number before merging. Therefore the only degree of freedom in the above equations is particle position ($x_i$). The position of new particle can be estimated by the above equations, or by averaging the positions of particles that will be merged because the averaged position does not disturb the original charges on the grids.

The new $x$-direction velocity is obtained as follows. Firstly, we sort the particles in a cell. The particles that have velocities in opposite directions ($+v_x$ and $-v_x$) are ordered separately in the process. The velocity of new particle is generated by averaging $R$ particle velocities from lower energy particles to higher energy particles,

$$v_{\text{new}} = \frac{\sum_i^R v_i}{R}, \tag{3}$$

where the summation corresponds to old (to be merged) particles. We divide new species from the original species to separate the remains. If we merge more than two particles, then some particles are left over. We refer to them as residual particles. The new merged-particles and residual particles are treated as different species in our scheme. It means that we have several electron species which have different masses and charges. But the change of mass and charge does not affect substantially because particles follow the equations that depend on the same $q/m$ value [1]. The example of merging four particles ($R = 4$) is shown in Fig. 1(a). The residual particles have higher energies than the merged particles. The new $x$-direction velocity ($v_x$) is obtained from the average of merging particle velocities. The $y$- and $z$-direction velocities are assigned to the particles by obtaining the total magnitude of $y$- and $z$-direction velocities and slopes in the $y$–$z$ phase space with random number generation. This means that $y$- and $z$-direction energies do not change in this process. The loss of total energy can be reduced by the method because $+x$- and $-x$-direction velocities are combined separately and merged-particle velocities are close to each other.

### 2.2. Two-dimensional number reduction method

Two-dimensional PIC code (XPDP2) follows two position coordinates $(x, y)$ and three components of velocities. The concept of reducing the number of particles in two dimension is same as that in one dimension case. Two groups ($+v_x$ and $-v_x$) of velocities are enough to conserve momentum and energy in one dimension, but grouping of phase space becomes complex in two-dimensional system because two components of velocity ($v_x$ and $v_y$) are concerned. The particles that will be merged in two dimension have to be arranged such that each velocity component of the particles have close magnitude and direction to conserve velocities and energy. As shown in Fig. 2(a), we divide the $v_x$–$v_y$ phase space into several domains by angle between particle velocity and $v_x$ direction to satisfy above condition. The magnitude of domain angle

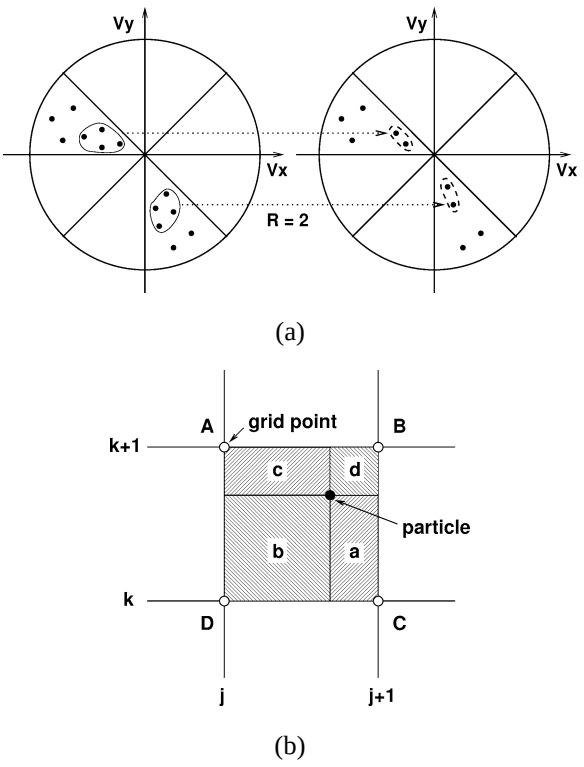


Fig. 2. The reduction method in two dimension. (a) $R$ is reduction rate, (b) charge assignment of PIC method.

determines the uniformity of the velocities of particles in each domain. As the angle between domains becomes smaller, the directions of particle velocities become more uniform. If the angle is too small, uniformity of velocities becomes better but the number of residual particle becomes larger. After grouping the particles into several directions, particles in each group are sorted out separately by the magnitude of velocity ($\sqrt{v_x^2 + v_y^2}$) in the $v_x$–$v_y$ phase space. Each component of new velocities is then obtained by averaging the velocities of the particles that will be combined, as in one dimension. The phase space ordering is adapted in the same cell of coordinate space to conserve charge density in the cell. Each direction ($x$ and $y$) momentum as well as energy can be conserved by the method.

To conserve the charge density, we need at least two new particles because number of spatial degree of freedom increases in two-dimensional system. It is sufficient to specify position of a new particle in one-dimensional system. However at least four new variables are required in two-dimensional system to conserve charge density of the system. The reason is as follows. Electric fields and potential are calculated at the grid points in PIC codes. When we solve the Poisson equation, the potential is obtained from the charge density source which is already evaluated at each grid. If we consider the procedure of specifying the grid point charge density in PIC code as shown in Fig. 2(b), four grid points (A, B, C, D) are involved in each cell [1]. If there is only one particle in the cell, the charge densities at each grid points are assigned by the area weighting divided by the particle position as shown in Fig. 2(b). Furthermore charge densities $Q$(A), $Q$(B), $Q$(C), and $Q$(D) are determined by the weighting of area a, b, c, and d. Total charge densities of each grid-point are obtained by the sum of charge densities at each grid point by particles in the cell. The charge densities of each grid point have to be conserved to obey charge conservation law. If we assume that there are $N$-particles to be combined and converted to new super-particles, we need at least two new super-particles to conserve the four grid-point charge densities [$Q$(A), $Q$(B), $Q$(C), and $Q$(D)] because there are four degrees of freedom in one cell. Therefore we need to merge several particles to at least two super-particles in two dimension. The example of merging four particles to two super-particles is shown in Fig. 2(a).

## 3. Simulation results

Figs. 3, 4, and 5 are the comparison of simulations with and without the method of particle reduction. Fig. 3 represents one-dimensional simulation results. The system of Figs. 3(a)–3(d) consists of two electrodes and a dielectric barriers on the cathode. The system of Figs. 3(e)–3(f) consists of two dielectric barriers on each electrode. The gap size between anode and cathode is 10 mm and the width of each dielectric barrier is 1 mm. They are one-dimensional dielectric barrier systems or one-dimensional AC Plasma Display Panel (PDP) systems [4,12–14]. Typical PDP simulations have been done by fluid simulation. PIC simulation retains kinetic effects as electron and ion energy distribution (EEDF and IEDF) which provide important information to understand the discharge phenom-

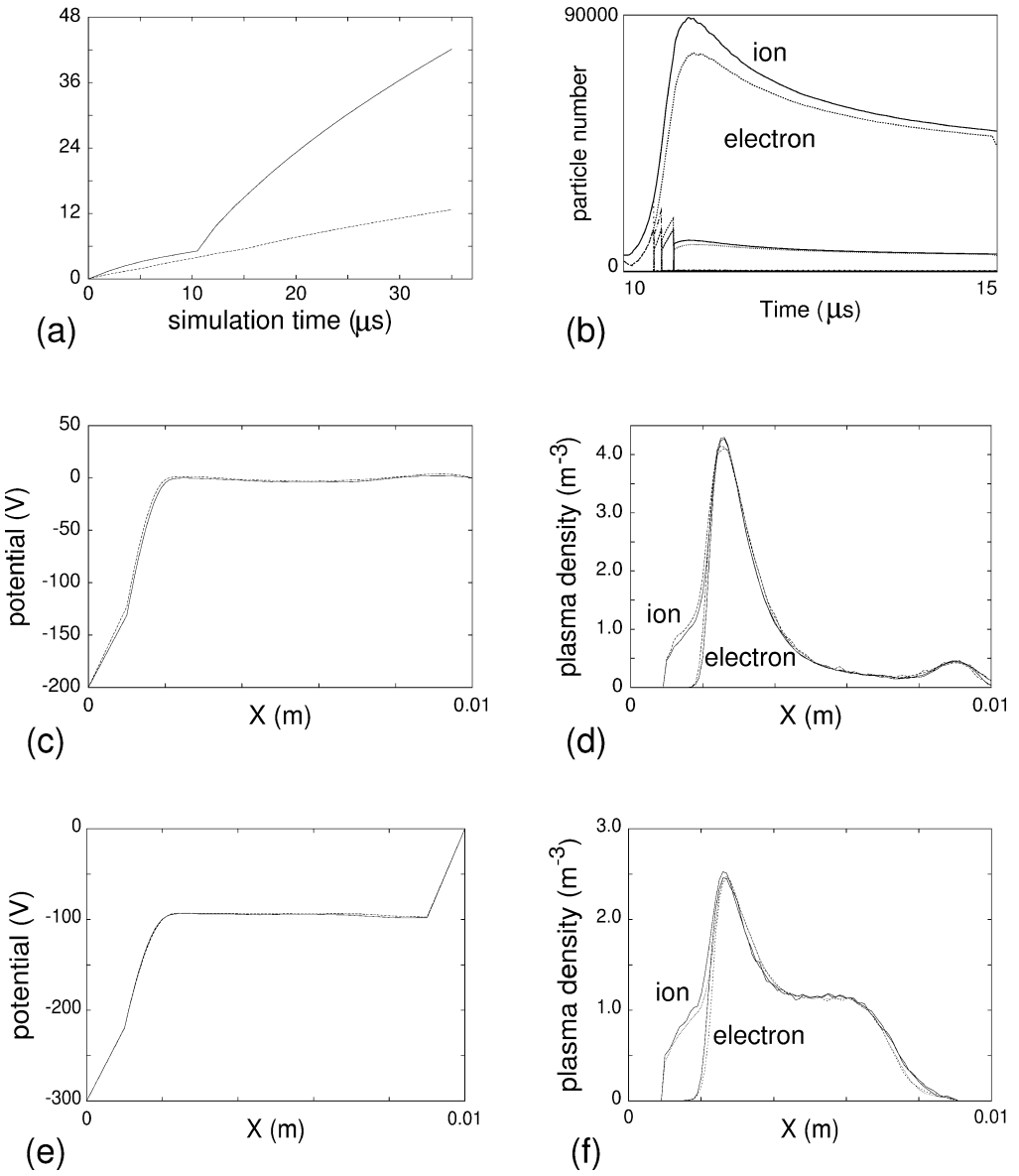


Fig. 3. Simulation results in one dimension. (a) Speed comparison between original (real line) and new (dotted line) methods, (b) total particle numbers, the upper lines are the original and the lower ones are the modified codes for the comparison of (c) potential profiles, (d) density profiles ($\times 10^{16}$) of one dielectric system, and of (e) potential profiles, (f) density profiles ($\times 10^{16}$) of two dielectric system between the original and the modified codes after several conversions.

enon. Such studies are not possible with fluid simulation [4,14]. The discharge extinguishes after the peak density of plasma. At this time the potential due to the charges on the dielectric surface reduces the applied potential. The applied voltage, to begin with, is –200 V (–300 V for two dielectric barrier) and 0 V on each electrode. The pressure of the systems is 5 Torr. The applied voltages are sustained till 5 μs and set to 0 V during the next 5 μs, which makes one period. The polarity is changed during the next pulse period to uti-

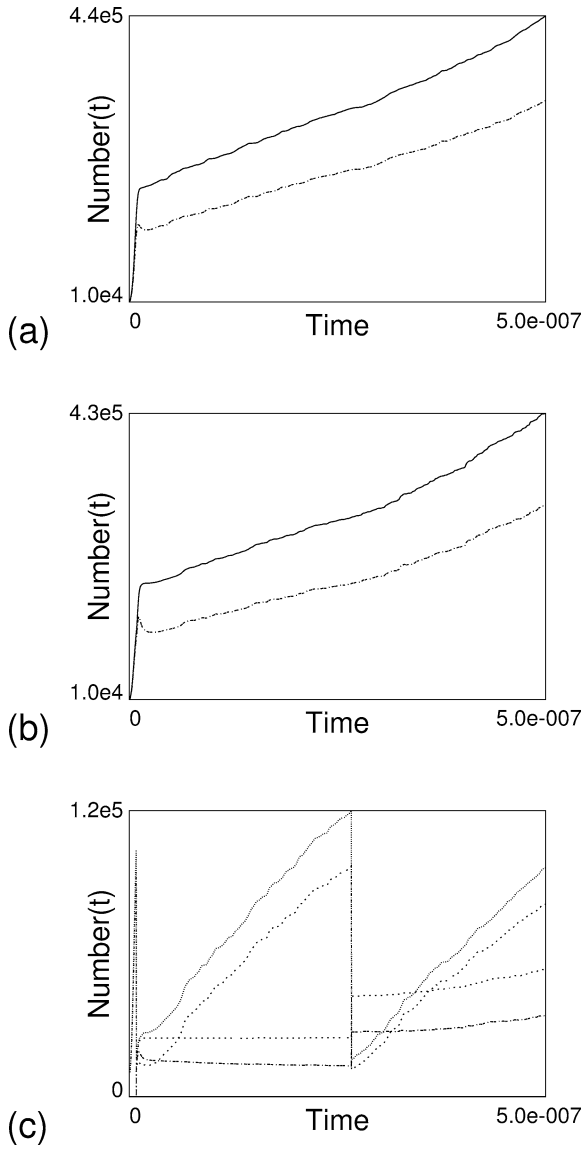


Fig. 4. Simulation results in two dimension. Total simulation particle numbers in the (a) original code and (b) the modified code with weighting. (c) Simulation particle numbers in the modified code.

lize surface charge of previous period as in the PDP system.

The boundary condition at the interface between the dielectric surface and the plasma is followed,

$$(\epsilon_0 \mathbf{E}_0 - \epsilon_1 \mathbf{E}_1) \cdot \mathbf{n}_s = \sigma, \tag{4}$$

where $\mathbf{E}_0$ and $\mathbf{E}_1$ are the electric field in the plasma and at the dielectric surface, respectively, $\mathbf{n}_s$ is the unit vector perpendicular to the dielectric surface. $\sigma$ is the time integration of charge densities entering the dielectric surface. The initial density for each electron and ion species is $1 * 10^{15}/\mathrm{m}^3$. The time step ($dt$) of the system is $1 * 10^{-11}$ s. The number of total initial particles is 10 000 for each species. The converting ratio ($R$) is taken as 2 in the one-dimension. Unlike fluid code, we can calculate the self-consistent distribution function of electron and ions by PIC method without assuming any predefined distribution functions. The distribution function shows the ion energies impinging into the dielectric surface that is known to be important to estimate the secondary electron emission coefficient of the materials [15].

The speeds of the original and the new methods are compared in Fig. 3(a). The time for simulation has no difference until 10 μs because the number of particles is small and the number reduction is not being executed. The slopes of simulation time differ after this time. The simulation by the new method is three times faster than the original one at 35 μs for the first system (one dielectric barrier system). The speed gain in the modified code for the second system (two dielectric barrier system) is 5.2 times the original one until 20 μs. The comparison of particle number between 10 and 15 μs is presented in Fig. 3(b). The upper two lines correspond to plasma particle-numbers in the original code simulation and lower ones show plasma particle-numbers in the modified code simulation. The three peaks in Fig. 3(b) indicate that the reduction occur three times. This means that the particles have $R^3$ times higher charge and mass than the original particles. The number of species is increased to four (isp = 0, 1, 2, 4) for each electron and ion. The dotted lines just above time axis represent residual particle numbers that are not merged at the reduction process, and are very few in number in the one-dimensional simulation. The next figures represent physical quantities such as potential and electron density in the system. Figs. 3(c) and 3(d) are potential and density profiles of the first system and Figs. 3(e) and 3(f) are those of the second system. The plasma profiles do not change even after several conversion and coincide well with unmodified simulation results.

Two-dimensional simulation results are shown in Fig. 4. The system is a typical parallel plate system with anode and cathode. The applied voltage is 400

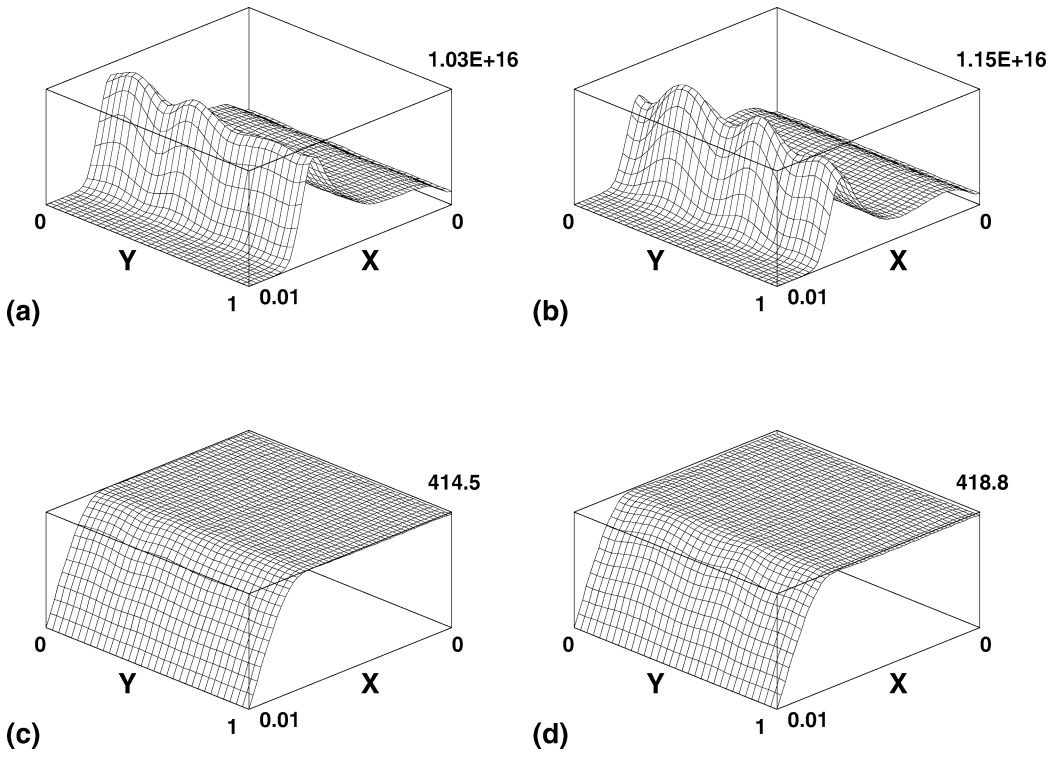


Fig. 5. Simulation results in two dimension. Electron density profiles of the (a) original code and (b) the modified code. Potential profiles of the (c) original code and (d) the modified code.

and 0 V on each electrode, the gap distance between electrodes is 10 mm, and neutral gas pressure is 2 Torr. As the residual particles (not merged at the reduction process) are more populated in two-dimensional system than one-dimensional one (lowest dotted lines of Fig. 3(b) and highest two lines of Fig. 4(c)), the speed gain in two-dimensional system is smaller than that in one dimension. When the number of particles reaches a specified value, the reduction occur and the particle numbers are reduced. The difference between Figs. 3(b) and 4(c) is that the residual particle number is very few in one dimension, but larger than the merged-particles in two dimension after one reduction, which reflects the speed gain. At the second reduction, the residual particles are reduced by the reduction method, but the merged-particles are not combined together because the population is lower than residual particles and specified conversion value. When the reduction process occurs, the species number increases in one dimension because reduction processes are adapted to merged-particles. But the species number does not change at the second reduction in two dimension because the upper grade particle numbers are not enough to experience conversion process. These differences originate from the reduction method that uses fine grid in two dimension to group particle directions [Fig. 2(a)].

As we merge from the lower energy particles, the new species (merged particles) have lower energy than pre-existing species (particles before merging). The number of new species particles (two flat lines in Fig. 4(c)) does not change much because these particles correspond to the bulk plasma and does not make significant contribution to the ionization process. On the contrary, pre-existing lower grade species have sufficient energy to ionize the neutral gas and the number of species increases with time. The maximum electron density increases by 12% as compared with the

usual PIC method [Figs. 5(a) and 5(b)]. However, the total particle number decreases by only 3% [Figs. 4(a) and 4(b)]. The averaged potential is nearly the same (1% difference in the peak value) [Figs. 5(c) and 5(d)]. These results show that the merging process does not affect to the physical quantities and the software is working stably and with sufficient accuracy. As we compare the real simulation particle numbers in the two simulations, the number of new method is maintained below $1/3$ of the original PIC simulation. This reflects the speed gain of the new method.

## 4. Summary and discussion

We have presented a method based on particle-reduction technique to speed up a PIC code. Not only by reducing the particles numbers but also by maintaining the physical quantities, we obtained the accurate results with an improved speed. The conservation of charge, velocities, and energies was accomplished by the method. The velocity phase space was divided and ordered to merge particles without losing the original quantities. The number of new particles was different in different dimensions to maintain the degrees of freedom. The simulation speed of this scheme was several times faster than that of the original PIC method in one- and two-dimensional systems. The speed gain would have been more if the simulation time were longer than our examples. The stability of the code is also improved because the physical profiles did not change even after several conversions of particle numbers. This method can be adaptable to three-dimensional system and other PIC codes to reduce the simulation time and to improve the accuracy.

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