On the energy conservation electrostatic particle-in-cell/Monte Carlo simulation: Benchmark and application to the radio frequency discharges*

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We benchmark and analyze the error of energy conservation (EC) scheme in particle-in-cell/Monte Carlo (PIC/MC) algorithms by simulating the radio frequency discharge. The plasma heating behaviors and electron distributing functions obtained by one-dimensional (1D) simulation are analyzed. Both explicit and implicit algorithms are checked. The results showed that the EC scheme can eliminated the self-heating with wide grid spacing in both cases with a small reduction of the accuracies. In typical parameters, the EC implicit scheme has higher precision than EC explicit scheme. Some "numerical cooling" behaviors are observed and analyzed. Some other errors are also analyzed. The analysis showed that the EC implicit scheme can be used to qualitative estimation of some discharge problems with much less computational resource cost without much loss of accuracies.

Keywords: particle-in-cell/Monte Carlo simulation, energy conservation, grid heating, discharging simulation

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1. Introduction

Particle-in-cell (PIC) simulation is a key method for tenuous plasma modeling.[1] In PIC simulation, the kinetic effects are considered self-consistently. On the other hand, PIC simulation gets rid of the full modeling in phase space through the particle sampling.[2] With the Monte Carlo (MC) method, it can be used to simulate the discharge problems in detail. As a result, PIC simulation becomes an important technology in dealing with the problems of gas pressure discharge.[3–8]

However, PIC simulation has some shortcomings.[9] One of them is the space–time scale limit. In convenient PIC algorithms, the grid spacing and time steps are constrained by

$$\begin{aligned} \Delta t &< \frac{2}{\omega_{\mathrm{p}}}, \\ \Delta t &< \frac{\Delta x}{c}, \\ \Delta x &< \xi \lambda_{\mathrm{D}}, \end{aligned} \tag{1}$$

where ω_{p} is plasma electron frequency, λ_{D} is plasma Debye length, ξ is a factor having the order of 1 and is determined by the electron velocity distributions. For electrons with a Maxwellian distribution, it is $\xi \sim 3$. These constraints come from the leap-frog algorithms, the Courant–Friedrichs–Lewy limit (CFL) and fine grid instability (FGI) separately.[9,10] In discharge plasma devices, these constraints cause a very large number of grid cells and the time steps, so that the simulation can incur very large computational costs.

In typical low temperature discharging plasmas, the inpractical huge computational costs cause severely difficult problems. It is because both the leap-frog limit and the fine grid instabilities become critical (even the FGI can be neglected in many other cases). When the leap-frog constraint is violated, the simulation diverges immediately. When the FGI constrain is violated, an effect named "self heating" takes place and increases the particle kinetic energy. However, in the gas discharges, the plasma is kept by collision and the collisional cross sections are sensitive to the particle energy. When the self-heating tries to increase the particle energy, more collisional ionizing should occur instead. Hence, the self-heating does not increase the energy of particles largely but increase the densities of plasma. Furthermore, the increasing plasma densities decrease the Debye length and cause more self-heating. This positive feedback intensively disturbs the simulation and often leads to a slow divergence. Therefore, in the discharge PIC/MC simulation, we need to use very small time and space steps. Because of the computational resource costs being proportional to $1/(\Delta x^D \Delta t)$ in D-dimensional simulations, it becomes impractically huge in industrial applications. This difficulty is called the "space–time scale problem". In multi-dimensional simulating, the FGI constraint is more critical.

To overcome the the space–time scale problem, we can apply some variants to the algorithms or the physical model-

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ing. For example, the scaling method resizes the simulation region by adjusting the colliding rates to reduce the computational costs.[11] This method depends on the scale similar law and can be used in very narrow regions. We should mention that there are other tricks to mitigate the grid self-heating (sometimes is called "grid heating"). The method is to apply the high-order weighting scheme to the particle/current and field weighting. This trick can reduce the aliasing error greatly and slow the increase of self-heating.[12] Hence, it has been applied to solve the problems when the simulating time is not extremely long.[13,14] However, the self-heating is slowed down instead of being eliminated. In addition, a very high order weighting scheme will introduce complexity in parallelization.

There are also two kinds of variant algorithms overcoming the space-time limits. One is the implicit PIC method[15,16] and the other is the energy-conservation (EC) algorithm.[1,10] The implicit PIC method eliminates the time step limits by damping the high-frequency oscillations in the time domain, consequently, it will be stable for very long Δt. The damping also decreases the self-heating of the plasma. When the time step is increased by the grid spacing, the self-heating will be decreased and FGI will be eliminated.[17]

The EC scheme introduces the total energy (field energy plus particle kinetic energy) conservation of the plasma. Theoretically, the self heating takes place in some modes and increases the particles kinetic energy. When the total energy is constrained to conserve, the self heating can not increase to diverge, then the EC scheme can eliminate the FGI constraint but does not affect the time step limit.

Both of the two algorithms are used in large-scale or high density plasma simulations. Implicit algorithms are used in capacitive coupled plasma (CCP) discharging,[18] geophysics,[19] and high energy densities physics.[20] Some variants of the EC scheme are used in some electromagnetic PIC simulating softwares.[21,22] The one-order weighting EC scheme has some problems such as stochastic noise. However, high-order weighting can cure them. Recently, some development of EC is introduced to simulate the high-power devices.[23] We should point out that these EC schemes are always approximate energy conservation with finite dt. One kind of accuracy energy conservation PIC algorithms are introduced[24] and promise to work well in the future. However, these algorithms are very complex and difficult in the equation solving and coding, which we will discuss in another paper.

The reduction of computational resources causes the reduction of accuracy. e.g., implicit PIC simulating can cause plasma self-cooling.[25] We can recognize that the implicit PIC method worked by the whole region oscillation damping, and the grid heating source is not cured indeed because the grid heating does not relate to the Langmuir oscillation. Similarly, the EC scheme suppresses the energy increasing from the grid heating. However, some self-force is introduced and the particle distribution in phase space can be disturbed[27] Therefore, it could cause some errors of kinetic behavior.

Therefore, we need detailed benchmarks and error analysis of the application of these methods in discharge simulation. Vahedi[18] studied the implicit methods and compared them with the explicit simulation in CCP, while no benchmarks are performed for the EC algorithms with MC up until now. Hence, a detailed investigation of the accuracy and errors in EC algorithms is needed. In addition, the effective combination of the EC scheme and implicit algorithms has not been reported.

In the present paper, we analyze the simulation results and compare convenient PIC algorithms (referred to as the "momentum conservation scheme" or the "MC sheme") with EC algorithms and obtain the validity and applicability of these algorithms. The benchmark model is a one-dimensional CCP discharging plasma. Because the driving frequency is as low as tens of MHz, electrostatic modeling is used. To model the collision in plasma, the MC procedure is applied. We show that the combined EC-implicit PIC algorithm could be a qualitative method for the discharge simulation. In addition, the errors and their origin are discussed.

2. Numerical algorithms of the PIC and EC scheme

In this paper, we test and analyze a series of PIC algorithms. The base algorithms are the convenient explicit PIC algorithms ("explicit") and the direct implicit PIC algorithms ("implicit"). The detail of these algorithms can be found in our early papers.[17,28] In the early paper, all of the algorithms used the momentum conservation scheme (MC). In the present paper, we patch them with the energy conservation scheme (EC). The major idea of the EC scheme can be found in Ref. [23]. We describe it here very briefly.

The energy conservation scheme is only slightly different from the momentum convenient conservation scheme. Denote the middle point of x_g and x_{g+1} by $x_{g+1/2}$, then the weighting of the charge should be alternated to

$$\rho(x_g) = \sum_{\mathrm{p}} q_{\mathrm{p}} S_m(x_g - x_{\mathrm{p}}). \tag{2}$$

The interpolation of fields should be alternated to

$$F(x_{\mathrm{p}}) = \sum_{g} q E_g S_{m-1}(x_{\mathrm{p}} - x_{g+1/2}), \tag{3}$$

where $S_m(x)$ is the standard PIC interpolation function (see Ref. [12]). The other algorithms are not changed (both for explicit and implicit algorithms). Then there are four PIC schemes.

(i) MC explicit scheme, the scheme is the same as that in Ref. [28]. In fact, this is the standard electrostatic particle-in-cell/Monte Carlo algorithm in literature.

(ii) EC explicit, the scheme applies the patch to the Ref. [28].

(iii) MC implicit, the scheme is the same as that in Ref. [17]. In literature, these algorithms are called the "direct implicit particle-in-cell" method.

(iv) EC implicit, the scheme applies the patch to the Ref. [17].

In consideration of reduction stochastic noise by interpolation, one should set $m = 2$ and a larger m can also be applied. In this paper, we choose $m = 2$ in the EC scheme only. Under this chosen parameter, only the particle weighting (Eq. 2) becomes more complex and the field interpolation is almost the same as the convenient scheme. Then the coding work and the computational cost is minimum.

Theoretically, the simulation running time equals $t = (T_{\text{physical}}/\Delta t)t_{\text{step}}$, where T_{physical} is the physical time of the system and t_{step} is the time for one PIC step simulation. Then increasing Δt will decrease the simulation costs but the increase is limited by leap-frog constraints and MC collision, t_{step} is related to the field solving time t_{f} and the particle pushing/Monte Carlo time t_{ptcls}. For Monte Carlo subroutine accuracy and noise control, the PPC must be set to larger than some limit (say, 100). If we fix the particle number per cell (PPC) according to the Monte Carlo code required, t_{ptcls} will be in direct proportion to the cell number and t_{f} will also be positively correlated to the cell number. Thus increasing the grid spacing will reduce the computational cost. On the other hand, our EC scheme needs a two-order weighting of particles, while implicit algorithms need some more complex pushing codes. Hence, the EC and implicit scheme will run slightly slower than the convenient PIC scheme when the same grid spacing is applied. Anyway, in almost all cases, the grid spacing effects are dominant.

3. Discharge model and the simulation

We simulated a CCP discharge with the above 1D model. In the CCP discharges, the electrode is driven by radio-frequency (RF). The electrons bounce on the sheaths and get slight acceleration. Then the electrons are scattered by gas atoms in the background and the electrons velocities are dephased. In these processes, the energy of the electric field is converted into electron stochastic energy. The energy conversion is called stochastic heating. The stochastic heating transfers energy into the plasma and causes ionization. This mechanism is the dominant physics issue of low gas pressure CCP. This behavior exists widely in many kinds of low pressure discharge problems. Similarly, RF sheath formation and stochastic heating are key mechanisms of these discharges. Therefore, the analysis and benchmark of them in CCP simulation can be used to estimate the effects of the algorithm applying to these discharge problems.

The geometry of the model is 1D symmetric planar for the sake of simplicity. The Ar gas is put between two electrodes with RF voltage source being applied. The frequency of the RF source is 27 MHZ and the voltage amplitude is 200 V. The gap length between electrodes is 4 cm. The MC procedure identical to Ref. [28] is used to describe the electron–atom and ion–atom collisions. The gas pressure is set to 50 mTorr and the secondary electrons are neglected.

The conceptual behavior of the CCP simulation can be described by energy balance. The heating process is the discharging plasma generator. On the other hand, when electrons and ions diffuse to the electrode, they are absorbed. This process is the plasma eliminator. At the beginning of the simulation, the plasma are filled uniformly between the electrodes. Then the bipolar diffusion causes the sheath formation. After the sheath formation, the stochastic heating and the electrode absorbtion compete with each other and evolve the plasma densities. When the two effects reach a balance, the simulation converges to a stable result.

We can recognize that if the grid heating is too large, the simulation will diverge for the positive feedback mentioned in Section 1. However, the absorbing rates are related to the plasma densities. If the grid heating is not very large, the simulation can still converge. Because of the error of the total heating (and the total heating rate profile), the simulation results are essentially wrong. In addition, when the gas pressure is low, the stochastic heating causes the bi-Maxwellian while the colliding and absorbing cause cutting Maxwellian distribution. Hence, even if the simulation converges, the simulation can possibly be wrong without a careful check. On the other hand, the complexity and the sensitivity of CCP discharge causes it to be a good tester of the PIC/MC algorithms.

In our benchmark simulations, the initial plasma densities are set to $2.0 \times 10^{16}/\text{m}^3$ uniformly and are lower than the densities when reaching equilibrium. With the simulation running, the macro particle numbers and the plasma densities will increase slowly (after a short decrease to construct the sheath). If the simulation converge, the macro particle numbers will converge to a fixed value, when all physical parameters are given, and will only fluctuate slightly around it. In the convenient PIC regime, we set the grid number to 800 and could see the simulation converge after about 16000–22000 RF periods. Theoretically, for the electron Maxwell distribution, when the $Dx < 3\lambda_{\text{D}}$, the grid heating effects can be ignored.[9] In this case, the stable plasma density is about 5.2×10^{16}, and the electron Debye length is about 3.3×10^{-5} m. Thus the $\text{d}x \sim 1.4\lambda_{\text{D}}$ and $\omega_{\text{p}}\,\text{d}t \simeq 0.2$. When the grid spacing increases to more than $3\lambda_{\text{D}}$, the macro particle number will keep increasing and diverge finally. Similarly, in the momentum conservation direct implicit PIC simulation, the divergence can also be observed. The phenomena take place while the time step $\text{d}t$ of implicit simulation is small and the grid spacing is

much larger than λ_D. In contrast, the EC scheme causes convergence results after likely RF periods for all the grid spacing but the stable plasma densities are not the same for the different grid spacings. When the grid spacing becomes lower than λ_D and the time step $dt < 0.2/\omega_p$, all of the codes get equal densities as expected.

As the discussion in Section 2, the increasing grid spacing can greatly reduce computational cost. For the convergence periods in different cases are closes, we can benchmark the computational time per RF period (T_{period}) to estimate the simulation cost. Table 1 gives a simple benchmark results on a PC with PPC = 400 in all cases.

Table 1. T_{period} by second with alternative algorithms and grid spacings. We choose a status with the same physical time in the simulation, and $dt = 1.5 \times 10^{-11}$ for all cases. "N/A" means this simulation will not converge.

Grid number	MC explicit	EC explicit	MC implicit	EC implicit
800	32.5	35.2	41.7	57.5
400	15.9	16.7	21.0	26.5
200	N/A	8.0	N/A	12.3
64	N/A	2.3	N/A	3.1

One can recognize that the computational cost can be reduced by one-order in 1D cases with the increase of the grid spacing when the EC scheme is applied: At the benchmark system, MC explicit grid = 800 simulation runs for about 10 days while EC implicit grid = 64 simulation runs for less than one day. If the simulation is 2D modeled or the time step Δt is increased, the cost will be reduced much more (see as Ref. [17]).

Anyway, the macro particle number can affect the stochastic noise and cause error in the results. In most of the simulations, we set the initial macro particle number per cell (PPC) to 400 except the section about the PPC effects. We will discuss the effects of these parameters as follows.

3.1. Effects of grid spacing

We should point out that the grid spacing limit is more critical than the time step limit in discharge simulation. The reason is that the grid number increases as dx^{-D} where $D = 1, 2, 3$ is the simulation's dimensions. Therefore, if we increases dx 10 times, the resource cost decreases 1000 times for 3D simulation. In addition, the CFL can relate the time step to the grid spacing: $v_{max}\Delta t < \Delta x$, where v_{max} is the maximal physical characteristic velocity in the systems. Then the Δt could be increased while the Δx is increased and the computational cost will be reduced more. In fact, if the grid spacing can be increased greatly and the convergence can be kept, we can endure some system errors of the simulation. Here, we will discuss the grid spacing effects of the EC scheme.

We believe that when the grid becomes dense enough, the results from different schemes will become the same. In this case, when grid = 800 ($Dx = 1.4\lambda_D$), the four schemes give very close results and can not be distinguished from each other in the figure. A more dense grid causes little change. Hence, we use the MC explicit results with 800 cells to a benchmark data, i.e., the closer the result is to the MC explicit 800 result, the higher the accuracy is.

3.1.1. Plasma densities

We show the plasma densities and the average electric potential with stable discharge in Figs. 1, 2, and 3. The time step is set to 1.5×10^{-11} s and the grid numbers vary from 800 to 64. Because we are interested in the EC scheme, we show the MC explicit results for the benchmark only.

For all cases, the potential profiles are very similar and the values are close. A difference of the potential is only observable when the grid spacing is too large. The plasma densities seem to be more sensitive to the grid spacing. As we know, the MC explicit PIC simulation will diverge when the grid spacing is larger than $3\lambda_D$.

When the grid spacing increases, the EC scheme will give lower plasma densities. Even when the grid spacing becomes much larger than the Debye length, the profile of plasma densities is still similar and can be fitted with a multiplying factor. In the most extreme cases, when $\Delta x \sim 18\lambda_D$, the plasma densities are equal to about 60% of the $\Delta x = 1.4\lambda_D$ cases by the EC explicit scheme. It seems that the EC implicit scheme obtains more accurate results: When the grid number is equal to 64, the

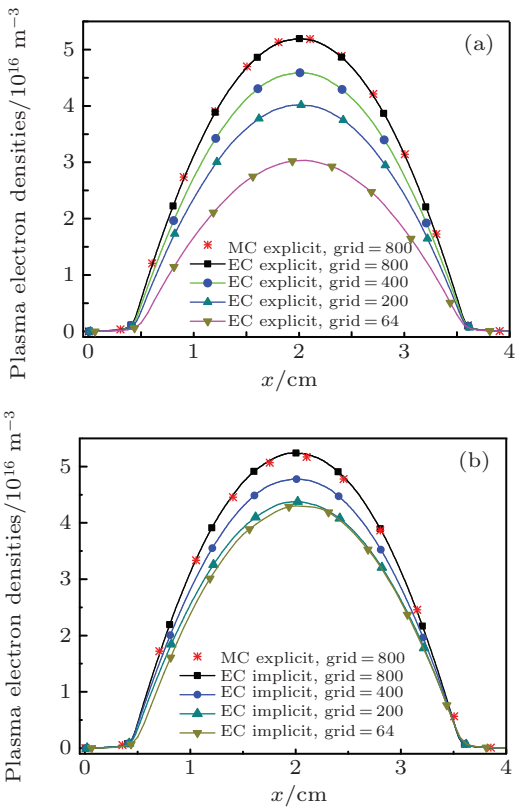


Fig. 1. (color online) Electron densities by EC scheme: (a) explicit, (b) implicit.

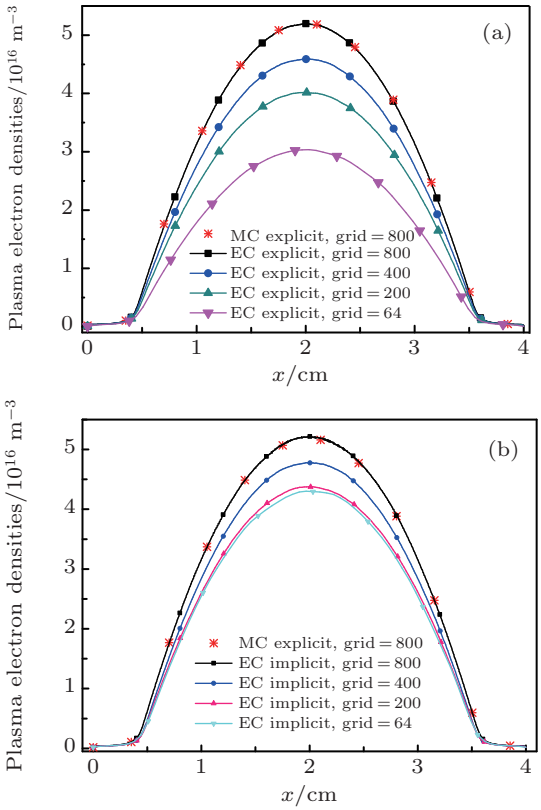


Fig. 2. (color online) Ion densities by EC scheme: (a) explicit, (b) implicit.

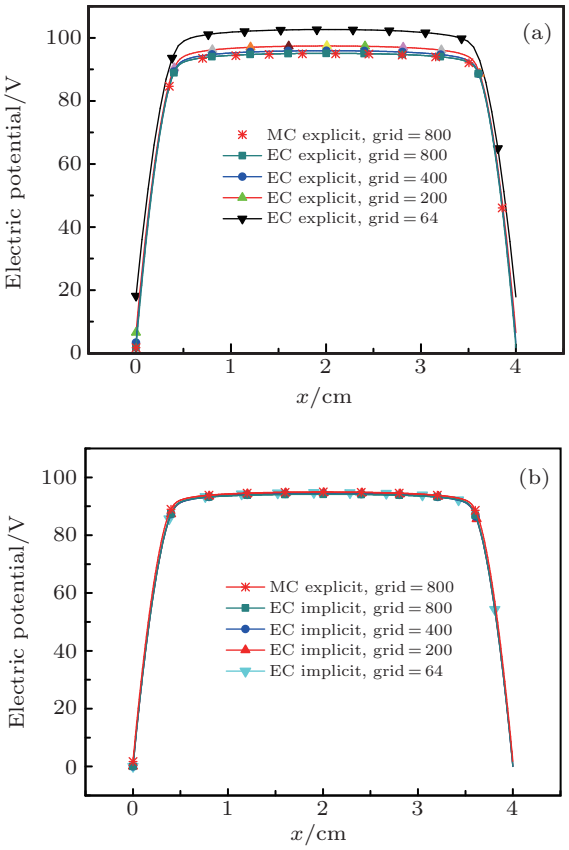


Fig. 3. (color online) Average Phi: (a) explicit, (b) implicit .

result error is less than 20%. Because of the convergence characteristic of the EC PIC algorithm, we think that it can be used to estimate qualitatively the plasma distribution for engineering. If the time step constraint is not very critical, both the EC explicit scheme and EC implicit scheme can be applied to qualitative analysis. However, for the very wide grid, the EC implicit scheme can work better.

3.1.2. Sheath behavior

For the CCP discharge, the sheath behaviors are very important. In fact, many of the interesting processes and the major physical mechanisms are working in the sheathes. For the ratio frequency CCP, the sheathes are oscillating. We show the average $\delta n = n_{\rm i} - n_{\rm e}$ in Fig. 4, where $n_{\rm i}$ and $n_{\rm e}$ are the plasma ion and electron densities, respectively. The profile of the δn can be seen as the sheath boundary. One can find that the sheath thicknesses are all the same. Especially, when grid = 64, the EC implicit scheme can give out correct potential while the EC explicit scheme shows about 5% error in the potential. Because the sheath thickness is determined by the particle diffusion, we conclude that the EC scheme can model the particle diffusion process correctly.

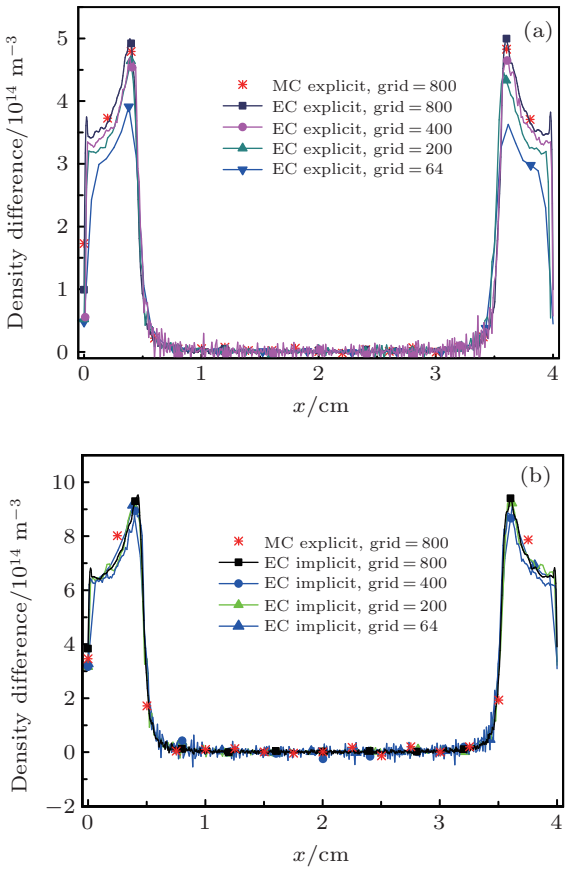


Fig. 4. (color online) The $\delta n = n_{\rm i} - n_{\rm e}$ shows the sheath structure: (a) explicit, (b) implicit.

3.1.3. Heating rates

The electron heating rates with stable discharge are shown in Fig. 5. It can be found that the heating rates of the EC scheme are lower and the peaks are more narrow than that

of the MC scheme, which can be explained by considering the sheath heating mechanism:[3] the electron collides with the moving sheath and is accelerated. This can be considered as an electron being bounced with an oscillating sheath. After being bounced back from the oscillating sheath, it runs towards the bulk plasma and the other electrode. The accelerating behavior depends on the phase matching of the plasma sheath oscillating and the electron oscillating. On the other hand, the EC scheme causes the self force of particles. The self force gives the particle a slight and fast oscillation.[27] Then the EC scheme causes orbit error slightly, the error will accumulate and disturb the acceleration. Hence the phase matching lengths are shorter and the heating rates peaks are more narrow. The implicit algorithms work better than the explicit algorithms: when grid = 64, the heating peak height (comes from scholastic heating) reduces to about 70% in the EC explicit scheme. In contrast, the peak height keeps almost the same value in the EC implicit scheme grid = 64. We think the possible reason is that the implicit algorithms damp the high frequency oscillation which includes the self force disturbance, then the accelerating phase is more accurate. In addition, the higher accuracy of heating rates should be the origin of more precise density and voltage.

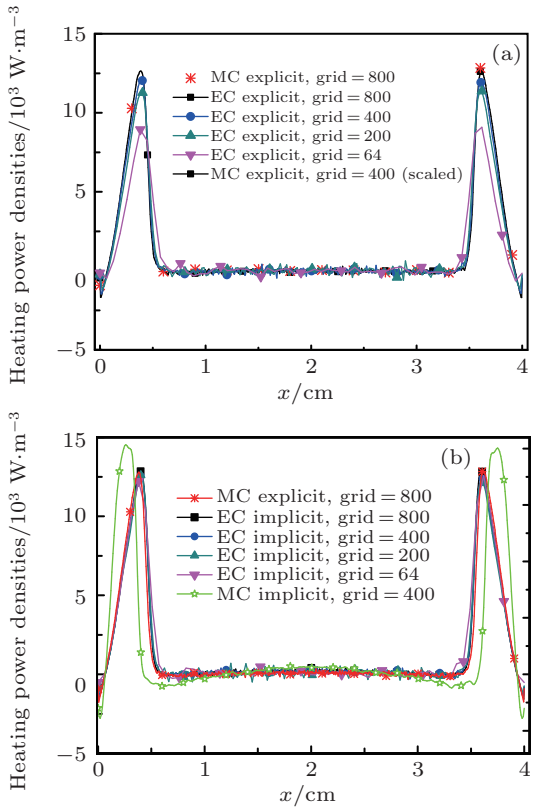


Fig. 5. (color online) Electron heating rates with stable discharge: (a) explicit, (b) implicit. The left axis scale in panel (b) is for the results of the benchmark and the EC scheme. The result with MC implicit (green line) is re-scaled to fit in the figure and can be read with the right axis scale. One can find that the heating rates of the MC implicit grid 400 are much larger than the others and have a peak in the middle.

As a comparison, we show the heating rates of MC implicit scheme with grid = 400 and the same dt. In fact, under these parameters, the MC implicit simulation can give out convergent results but with higher densities. When the grid spacing becomes wilder, the MC implicit scheme diverges like the MC explicit scheme. We can find the reason in the heating rate profile. The scale of this case is shown on the right. We can find the peak heating rates in this case are totally wrong (perhaps because of the incorrect densities). In addition, we find a bulk heating region in the middle of the discharge area. The larger the grid spacing becomes, the stronger the bulk heating becomes. Even if the MC scheme can give out some convergence results, it is qualitatively wrong when $Dx > 3\lambda_{\mathrm{D}}$, which is the major strongpoint of the EC scheme.

3.1.4. Energy distribution

The electron energy distribution is shown in Fig. 6. At 50-mTorr pressure, the energy distribution of electrons has a slight bi-Maxwellian distribution. The results of the EC explicit simulation are more close to single temperature Maxwellian, especially when the grid spacing becomes large. In addition, the electron's average energy in the EC explicit scheme becomes slightly higher (about 5%–10%) than the MC benchmark. These effects come partially from the particle stochastic noise increasing (for the particle number decreasing) and partially from the essentiality of the EC scheme. In theory, the particle self force in the EC scheme causes more "momentum exchangr" between the particle and the grid and can also induce more energy re-distribution among the electrons. Therefore, the results are not unexpected.

The behavior of the EC implicit scheme is slightly more complex. In the EC explicit scheme, the increase in grid spacing causes the electron energy probability function (EEPF) to be thermalized. However, the direct implicit scheme causes some damping and stronger bi-Maxwellian distribution. Accordingly, we can see some lines below the benchmark and some others above. Anyway, for very large grid spacing, the EC implicit will be always better than the EC explicit scheme.

For the analysis, we draw out the result of the MC implicit scheme while the grid spacing is larger than $\xi\lambda_{\mathrm{D}}$. The distribution of electron energy has a very long tail which indicates self-heating. This is in agreement with our judgement: the MC scheme causes qualitatively incorrect results while $\mathrm{d}x > \xi\lambda_{\mathrm{D}}$.

For the convenience of the analysis, we show the $\langle mv_x^2/2\rangle$ in Fig. 7. In 1D simulation, the electron bounce and acceleration are occurring in the x direction and transfer the kinetic energy to the other directions by collision. Thus the equivalence kinetic energy $\langle mv_x^2/2\rangle$ can indicate the bounce and acceleration. One can find the distribution of the equivalence kinetic energy in the x direction is a standard two temperature Maxwellian distribution. When the grid spacing increases, the temperature

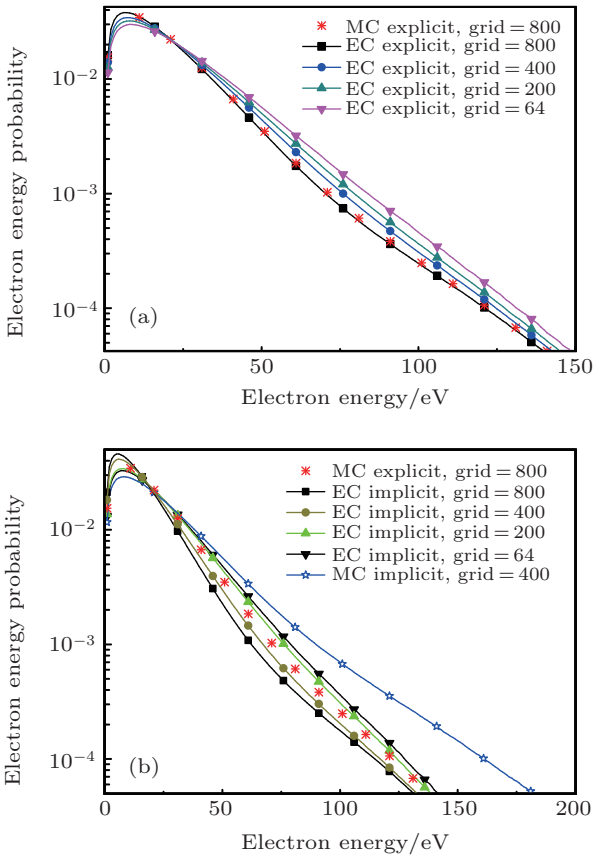


Fig. 6. (color online) The EEPF of the electrons: (a) explicit, (b) implicit. When the grid increases, the electron distribution becomes single temperature Maxwellian. The results of MC implicit grid 400 (green line) is also shown in panel (b). The very long tail shows self (grid)-heating.

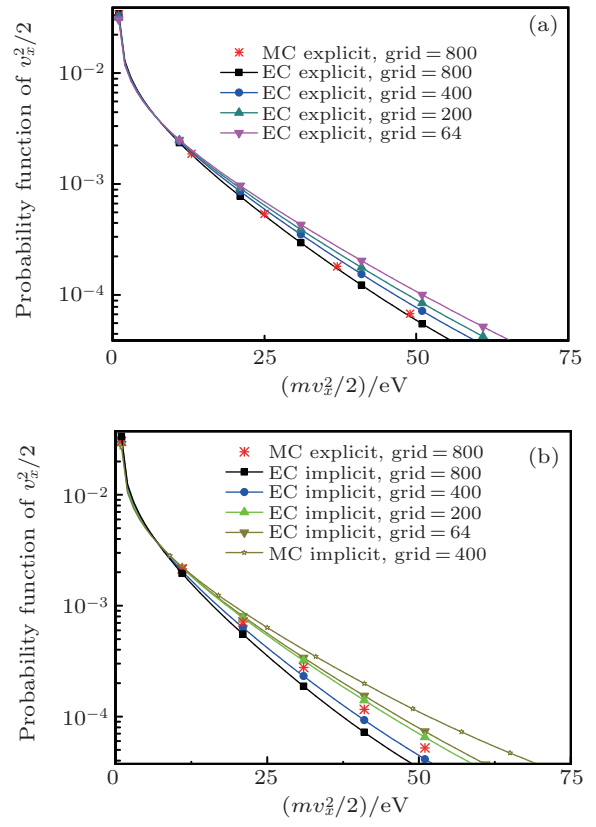


Fig. 7. (color online) The distribution of the electron equivalence kinetic energy in the x direction: (a) explicit, (b) implicit. When the grid increases, the high energy part increases the temperature slightly.

of the high energy part increases slightly in the EC scheme. This increase is caused partially by the decreased particle number and partially by the EC self-force disturbance. The MC implicit results are also shown in the figure. There is a longer tail in it but not as evident as in the energy distribution figure. It agrees with the judgement that the grid heating took place in all directions and was not a resonance effect.

3.2. Effects of time steps

Theoretically, the explicit PIC algorithm will diverge while $\mathrm{d}t > 2./\omega_\mathrm{p}$ and the implicit algorithm can give out stable results. However, because of the grid heating and the Monte Carlo couple of the particles, the results could change. We show that the average electron densities and heating rates with $\mathrm{d}t = 1.5 \times 10^{-11}$ to $\mathrm{d}t = 1.0 \times 10^{-10}$ in Figs. 8 and 9. One can find that the relations between $\mathrm{d}t$ and the average electron densities are slightly complex. The reason can be found in Fig. 9. As we expected, the increase of the $\mathrm{d}t$ causes the decrease of the peaks of the stochastic heating in implicit algorithms, while this increase affects little the peaks in the explicit algorithms. The effects can be explained by the well known "self-cooling" effects of direct implicit PIC algorithms. However, some bulk heating results appear in the large $\mathrm{d}t$ simulations. The bulk heating seems to increase more in implicit algorithms. We are not very clear about its source. We think that it is some pseudo Ohmic heating. That is, when the $\mathrm{d}t$ becomes large, the average acceleration in one step is slightly larger than the real field acceleration for the error of the leap-frog scheme, which enables some pseudo Ohmic heating to occur. In the implicit algorithms, the algorithms decrease the high frequency distorts of fields (decrease the collision damping) then make the situation even worse. In fact, when the $\mathrm{d}t > 2./\omega_\mathrm{p}$, we find that even the implicit algorithms can not give out convergence results. Anyway, the pseudo Ohmic heating is small when the $\mathrm{d}t < 0.5/\omega_\mathrm{p}$ ($< 5\%$ of the scholastic heating) and shows no heating peak in all cases.

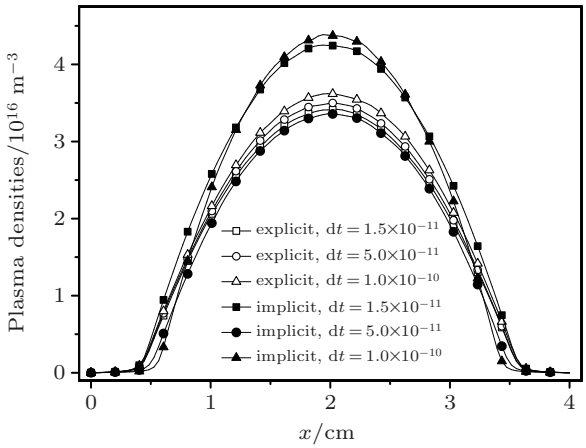


Fig. 8. The average electron densities versus $\mathrm{d}t$. The grid numbers are set to 100.

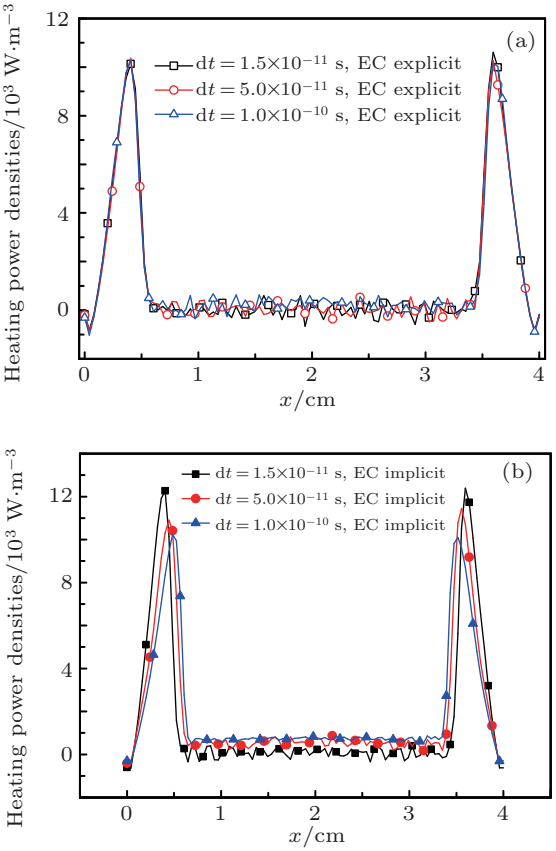


Fig. 9. (color online) The average heating rates versus dt: (a) explicit, (b) implicit. The grid numbers are set to 100.

3.3. Effects of macro particle numbers per cell (PPC)

As Tunner showed,[30] the PIC/MC simulation results can be affected by macro particle per Debye length (N_D) and total macro particle number (N_T). In our problems, the effects can be shown with the results by PPC. This effect comes from stochastic noise and can cause simulation breakdown if N_D is too small. We showed the effects of PPC with the EC implicit and EC explicit schemes while grid numbers are 100 and 200 in Fig. 10, respectively. The results are more complex than the upper effects. The PPC effects can be found easily, and implicit schemes work better than the explicit scheme always. However, in the case of the implicit scheme, the PPC effects can overrun the grid number effects. The reason could be that the grid number effects have been reduced much in the implicit scheme.

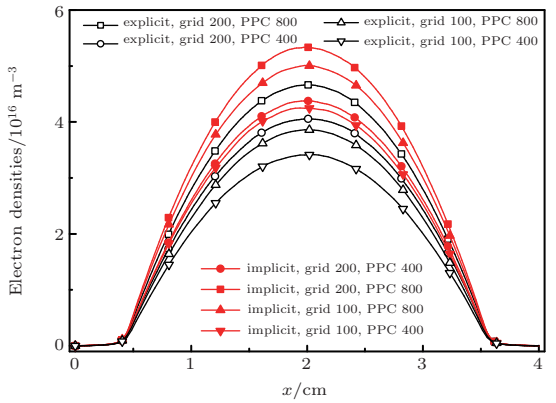


Fig. 10. (color online) The electron densities by PPC = 400 to 800 while grid numbers are 100 and 200, respectively.

4. Discussion

In the above simulations, we have compared the results between the convenient momentum conservation PIC scheme and the energy conservation PIC scheme. The EC scheme has shown that it can control self-heating behavior and can converge with a much wider grid. However, while the grid spacing becomes very wide, numerical cooling-like effects will obviously appear. Fortunately, the important physics is still preserved. In our simulation, Not only are the diffusion behaviors like sheath formation always correct, but also the kinetics effects such as power absorption are conceptually correct. In addition, the combination of the implicit and the EC scheme showed higher accuracy than the conventional explicit EC scheme.

A contrasting result is the MC implicit scheme. Although the implicit scheme introduces numerical damping and counteracts the self heating partially, the self heating causes divergence in many cases. In addition, the heating rates showed that the MC implicit scheme can give out qualitatively incorrect results in some worst cases.

We can conclude that the combination of the EC scheme and the direct implicit algorithm is the optimum numerical scheme for the PIC/MC simulations, especially as very large space and time steps in this scenario can be adopted, so that the computational cost can be significantly reduced. At the same time, the physical properties of the system are preserved well and numerical instability can be avoided, if the space and time steps are not too large. While in the conventional MC scheme, the numerical error may lead to non-physical heating of the plasma, because the energy is not exactly conserved.

However, this scheme also has some shortcomings. Because the momentum is not conserved, the energy distributions of the electrons will be slightly disturbed by the self force when the particles pass the cell boundaries. There is no effective technology to overcome this problem at present. Fortunately, the disturbance is small in most cases. The major properties of the system like the plasma density and temperature are still simulated well.

We also showed that some other non-physical effects of the particles in the EC scheme will occur at very large space and time steps. The results indicate that the error of the stochastic heating rates comes from the small oscillation of the EC scheme. Because the essential oscillation is controlled by the grid spacing, there is no perfect method to get rid of the error. However, our results indicate that the error is only impor-

tant in the sheath heating region and implicit algorithms migrate them a lot. For the gas discharge simulations, we could apply a multi-scale method to overcome the problem. That is, we can use a much finer grid in the sheath region and use a wider grid in the other regions. For the other problem (for example, ECR), more powerful technologies are needed. If the problems are not dominated by the stochastic heating and the orbit resonance, the EC scheme could give more accurate results and could be applied credibly.

The final problem is of pulse discharge. In these kinds of discharge, the heating rates are important, especially their profile. We have shown that the EC implicit scheme can give out a correct stochastic heating rate profile. In addition, we can expect the resonance heating and Ohmic heating can be qualitatively correct in the scheme. When the dt becomes large, a subtle problem shows that some non-physical heating (perhaps pseudo Ohmic heating) appears, but it is not very large. We expect that the shortcomings will not prevent its application in pulse discharge simulation.

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