Methods in Speeding Up PIC-MCC Codes Applied to RF Plasma Discharges

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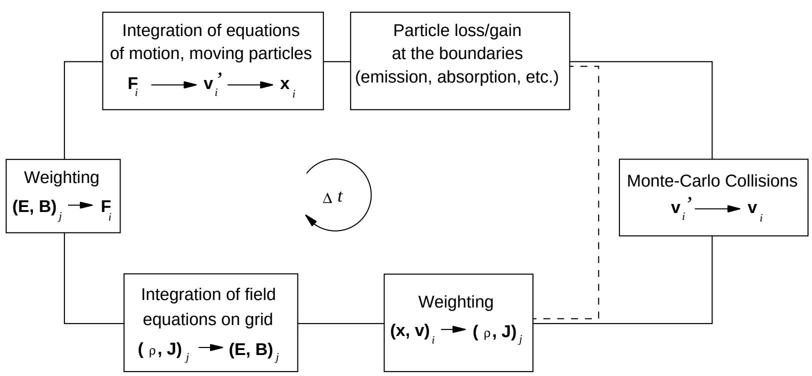
1 Introduction

Our paper presents old and new and combinations of attempts being made to make particle-in-cell, Monte-Carlo collisions, PIC-MCC, codes run faster. The particular application is to RF discharges as used in plasma processing, attempting to reach equilibrium sooner, on single processor machines. We report on speed Gains between 6 and 30 times on argon and oxygen RF discharges, with some runs under one hour, on a 233MHz workstation. It is desirable to keep the first-principle, self-consistent approach in PIC-MCC and to incorporate speed-up mechanisms into PIC-MCC. Below is a flow chart of the PIC-MCC code for bounded models[VS95].



2 PIC-MCC Speedup Methods.

Our base method for comparison is **explicit** coding, with no speed-up applied. Our first speed-up method is **implicit**, with $\Delta t_{implicit} \gg \Delta t_{base}$, yet maintaining stability and accuracy, due to attenuating fields at high frequencies. Our next speed-up is **subcycling** of the electrons, moving the ions every kth electron step ($\Delta t_i = k\Delta t_e$), where k may be 10 to 100. Our next speed-up is use of much **lighter ions**, made in two steps. The first part is with the lighter ions, running to equilibrium. Then we switch back to the heavier (real) masses, M_{real}. Use of **variable weights, initial density profiles** are also discussed.

100 mT Ar	**Runs**		
Model	Base	Implicit	Implicit, Subcycled
Total time(s)	7.1e4	1.75e4	1.1e4
GAIN	**1**	**4.1**	**6.5**
$v_{te}\Delta t_e/\Delta x$	0.43	0.69	0.69
$v_{imax}\Delta t_i/\Delta x$	0.013	0.021	0.42
$\nu_e \Delta t_e$	0.041	0.32	0.32
$\nu_i \Delta t_i$	0.0024	0.019	0.38
$\lambda_{De}/\Delta x$	2.7	0.53	0.53
$\omega_{pe}\Delta t_e$	0.16	1.3	1.3

Table 1: Argon, 100 mT, explicit, implicit, implicit plus subcycled electrons. Run time went from 20 hours to 3.1 hours.

3 Global Cautions

Many of the above accelerations stretch the limits on time steps. We list six global cautions in the Tables below that usually must be obeyed in order to obtain stability and accuracy, and to minimize self-heating. Most are discussed in simulation texts[BL85,BC85]. The stability criterion for conventional explicit PIC requires resolving the electron plasma frequency and the electron Debye length. Implicit schemes allow us to relax the constraints to resolving the RF frequency and the sheath width, but are more complex and require more operations. An additional accuracy condition is for $v_s\Delta t_s/\Delta x < 1$, where v_s is the characteristic velocity and Δt_s is the time step of a particle of species s. This ensures that particles will not travel more than one cell per time step and will sample the electric fields properly. Since the collision handler only assumes one collision per particle per time step, care must be taken to choose a Δt such that the probability of having a particle collide more than once per Δt is low. We can satisfy this condition if $\nu_s \Delta t_s \ll 1$, where ν_s is the maximum collision frequency and Δt_s is the time step of a particle of species s[VS95].

4 Simulations

4.1 100 mT Argon Discharge

We did a base run of a 100 mT Argon discharge for about 1000 RF cycles. A second run of 1000 RF cycles, using an implicit mover with $\Delta t_{implicit} = 8\Delta t_{base}$ reduced the running time by a factor of 4 (Gain = 4). The Gain was not 8 because the implicit mover was roughly twice as costly as the explicit mover. Also, the time spent by the collision handler is not significantly reduced because although the number of calls to the collision handler per RF cycle decreases due to the larger timestep, a larger timestep also leads to an increased number of collisions per timestep. Next we subcycled the electrons in the implicit run with $k = 20$ (the ions are pushed every $20\Delta t_e$). When run for 1000 RF cycles, the Gain in time was 1.6 over the implicit only case, and the total

10 mT Ar	Runs		
Model	Base	Light ions	Light ions, implicit
Total time(s)	5e4	1.2e4	2.7e3
GAIN	**1**	**4.1**	**19**
$v_{te}\Delta t_e/\Delta x$	0.13	0.13	1.0
$v_{imax}\Delta t_i/\Delta x$	6.7e-3	0.12	0.96
$\nu_e\Delta t_e$	4.1e-3	4.1e-2	0.32
$\nu_i\Delta t_i$	2.4e-4	2.4e-3	0.019
$\lambda_{De}/\Delta x$	1.0	1.0	1.0
$\omega_{pe}\Delta t_e$	0.16	0.16	1.3

Table 2: Argon 10 mT base, light ion, light ions plus implicit runs. Current drive of 0.6 A for the base case, with drive of 1.2 A for the light ions. Run time went fom 13.9 hours to 45 minutes.

Gain over the base case was 6.5. In an electro-positive argon discharge where there are roughly an equal number of electrons and ions, the maximum Gain due to subcycling is limited to 2. Our Gain of 1.6 from subcycling is less than 2 since subcycling does not reduce the time spent by the collision handler or the field solve.

4.2 10 mT Argon Discharge

A base run to equilibrium for our 10 mT Argon discharge took roughly 1000 RF cycles. When we applied the light ion speed-up described above, we were able to reach equilibrium in fewer RF cycles, resulting in a Gain of 4.1. A further Gain was made by using the implicit mover ($\Delta t_{implicit} = 8\Delta t_{base}$) with the light ions . The total Gain in time from this combined speed-up was 19.

4.3 100 mT Oxygen Discharge

We did a base run of a 100 mT Oxygen discharge for about 1000 RF cycles. In an electro-negative oxygen discharge, the number of ions is much larger than the number of electrons so that the Gain due to subcycling can be far greater than 2. When we subcycled the electrons by a factor of 80, the Gain in time was 20. Next we did a run using both subcycling and variable weights for the ions. We weighted the ion macroparticles 10 times more than the electron macroparticles. This reduced the number of computer particles in the simulation and increased the total Gain in time to 30.

4.4 Improved Initial Density Profiles

We typically start our simulations with uniform ion and electron density profiles which then evolve to their equilibrium states. The time to reach equilibrium can be improved by starting off with non-uniform initial density profiles that are close to their expected final equilibrium values. These profiles may be calculated

100 mT O_2 Runs

Model	Base	Subcycling	Subcycling, Weighting
Total time(s)	3e5	1.5e4	1e4
GAIN	**1**	**20**	**30**
$v_{te}\Delta t_e/\Delta x$	0.22	0.22	0.22
$v_{imax}\Delta t_i/\Delta x$	6.2e-3	0.5	0.5
$\nu_e \Delta t_e$	0.071	0.071	0.071
$\nu_i \Delta t_i$	8.9e-4	0.071	0.071
$\lambda_{De}/\Delta x$	5.0	5.0	5.0
$\omega_{pe}\Delta t_e$	0.043	0.043	0.043

Table 3: Oxygen, 100 mT, explicit, subcycling, subcycling and variable weights. Run time went from 3.5 days to 2.8 hours.

analytically or deduced from previous runs. For example, using parabolic profiles rather than uniform profiles in the 100 mT argon runs led to a further Gain in time of 4.

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[VS95] V. Vahedi, M. Surendra, Monte-Carlo Collision Model for Particle-in-Cell Method: Application to Argon and Oxygen Discharges, *Computer Physics Communications* **87**, 179-98 1995.

[BL95] C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation*, McGraw-Hill, 1985.

[BC85] J. U. Brackbill and B. I. Cohen, *Multiple Time Scales*, Academic Press, 1985.

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