

PIC Algorithm with Multiple Poisson Equation Solves During One Time Step

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Abstract: In order to reduce the overall computational time of a PIC (particle-in-cell) computer simulation, an attempt was made to utilize larger time step sizes by implementing multiple solutions of Poisson's equation within one time step. The hope was this would make the PIC simulation stable at larger time steps than an explicit technique can use, and using larger time steps would reduce the overall computational time, even though the computational time per time step would increase. A three-dimensional PIC code that tracks electrons and ions throughout a three-dimensional Cartesian computational domain is used to perform this study. The results of altering the number of times Poisson's equation is solved during a single time step are presented. Also, the size of the time that can be used and still maintain a stable solution is surveyed. The results indicate that using multiple Poisson solves during one time step provides some ability to use larger time steps in PIC simulations, but the increase in time step size is not significant and the overall simulation run time is not reduced

1. Introduction

Basically, there are three types of models used in plasma modeling: fluid models, fully kinetic models (or particle-in-cell), and hybrid models. The advantage of the particle-in-cell (PIC) method is its physical fidelity and the detailed results that it produces. The disadvantage of PIC methods, especially the explicit technique, is very long computational time. It is desired to find a technique to reduce these computational times. This was the motivation for this investigation.

In order to decrease the computation time for the PIC method, the implicit PIC technique has been under development for a number of years. Implicit methods in the most general sense fall under one of two categories, the direct implicit method [2] or the implicit moment method [3]. The direct implicit method is a predictor-corrector type of method which requires an iterative solution to be fully implicit. The implicit moment method aims to use fluid assumptions in order to estimate spatial properties, such as the electric field and the magnetic field, at a future time. Though the goal of the implicit and semi-implicit methods is to increase the size of the time step, while keeping the simulation stable, they are generally still restricted by the need for the particle to cross less than one cell in a single time step [4]. This is a restrictive limitation in sheath regions of high density plasmas where the relevant length scale is on the order of the Debye length.

In this paper, using multiple Poisson equation solves within one time step is investigated. The authors have not been able to find this technique documented in the literature and thus have undertaken this work to test this idea. Because we have not been able to find this technique documented in the literature, we will give it a name. We will call this method of PIC solution, the multiple Poisson solves technique. The ultimate goal of testing the multiple Poisson solves technique is to decrease the overall computational time of the PIC simulation by increasing the maximum stable time step size that can be used in the simulation. Of course, the time step has to be large enough to



overcome the extra computational time for solving Poisson's equation several times for each time step.

2. Mathematical Model

2.1. Charged particle kinetics equations

Two important equations for describing the motions of charged particles in an electric field are the Newton-Lorentz equation and Poisson's equation. The Newton-Lorentz equation is

$$m \frac{d\vec{v}}{dt} = \vec{F} = q(\vec{E} + \vec{v} \times \vec{B}), \quad (1)$$

where m is the mass of the particle, \vec{v} is the velocity, t is the time, \vec{F} is the force, q is the particle's charge, \vec{E} is the electric field, and \vec{B} is the magnetic field. While the electric field vector can change both the speed of the particle and its direction of travel, the magnetic field can only change the direction of the particle's travel and is unable to increase or decrease its speed.

The electric field value is determined from the gradient of the electric potential, $\vec{\Phi}$, using

$$\vec{E} = -\nabla \vec{\Phi}. \quad (2)$$

The electric potential is found using Poisson's equation,

$$-\frac{\rho}{\epsilon_0} = \nabla^2 \Phi, \quad (3)$$

where ρ is the charge density and ϵ_0 is the permittivity of free space. The charge density is found using the particle number densities of ions, n_i , and electrons, n_e ,

$$\rho = q(n_i - n_e). \quad (4)$$

The three-dimensional PIC code used in this work includes the solution of Poisson's equation to determine the electric fields throughout the computational domain that are caused by the boundary conditions and the charged particles. Also included is the solution of the Newton-Lorentz equation of motion to obtain the path of all ions and electrons when traveling through these electric fields. While the developed PIC code can handle magnetic fields, no magnetic fields are included in the simulations performed for this paper. Full coupling between the particle motion calculations (equation 1) and the electric field calculation (equations 2, 3, and 4) is maintained. The details of the solving process of equations (1) through (4) can be found in reference [5] and are not given here.

2.2. Explicit Stability Criteria

The explicit PIC algorithm is subject to a number of stability criteria [6] which limit its performance capabilities. These criteria define limits of the numerical parameters used, which include the maximum time step size, maximum grid spacing, and minimum number of computational particles per cell. These limiting values typically depend on characteristics of the plasma such as plasma frequency, Debye length, and electron velocity (electron temperature). The criteria which apply to the explicit PIC technique are:

$$n_{cell} \geq 20, \quad (5)$$

$$v_{p,x} \Delta t \leq \Delta x, v_{p,y} \Delta t \leq \Delta y, v_{p,z} \Delta t \leq \Delta z, \quad (6)$$

$$\omega_{pe} \Delta t \leq 2 \quad (7)$$

and

$$\frac{\lambda_D}{0.3} \leq \min(\Delta x, \Delta y, \Delta z). \quad (8)$$

In equations (5) through (8), n_{cell} is the number of computational particles per cell for one species, $v_{p,x}$, $v_{p,y}$ and $v_{p,z}$ are the particle velocities in each of the three Cartesian directions, Δx , Δy and Δz are the control volume sizes in each of the three Cartesian directions, ω_{pe} is the plasma frequency, and λ_D is the Debye length.

2.3. Multiple Poisson Solves Technique

The idea behind the multiple Poisson solves technique is to prevent unrealistic charge separation during one time step. This technique is classified as semi-implicit because it evaluates the electric fields a number of times during the course of a single time step. In the multiple Poisson solves technique some fraction of the total number of computational particles are moved using the Newton-Lorentz equation, then Poisson's equation is solved using the new positions of the particles, then another fraction of the computational particles are moved using the Newton-Lorentz equation, then Poisson's equation is solved again, and so on. This process is repeated within a given time step until all computational particles have been moved. Figure 1 shows the flow chart for the multiple Poisson solves technique, and, for comparison purposes, the flow chart of the explicit technique. The difference between the two techniques can be seen from this figure. This figure shows that multiple Poisson solves can be done during the movement of the electrons and during the movement of the ions. For the results presented in this work, multiple solves are only done during the electron moves. Multiple solves during the ion moves have been tried and shown to have little effect. The reason is that ions move such a small distance relative to the electrons for a given time step.

An important input parameter used in the multiple Poisson's solve technique is Npps. This stands for the number of particles per solve. This number indicates how many computational particles are moved between Poisson solves. The lower this number the more Poisson solves per time step. The number of Poisson equation solves per time step can be obtained by dividing the total number of computational electrons by Npps.

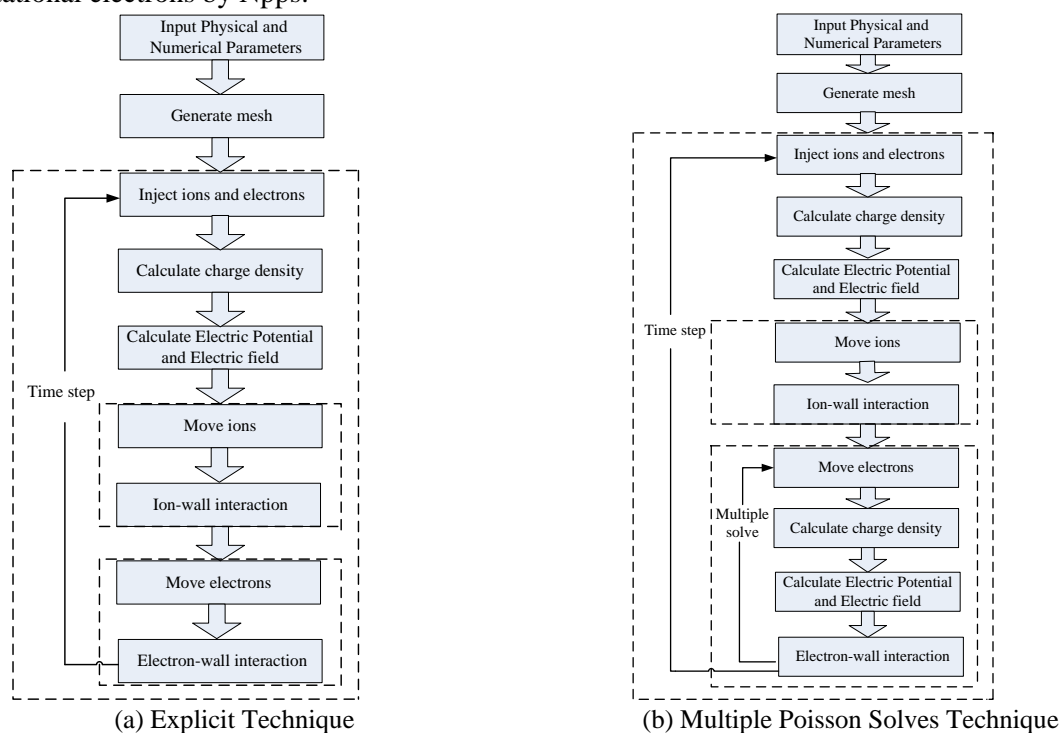


Figure 1. Flow charts of the explicit PIC technique and multiple Poisson solves PIC technique.

3. Results

3.1. Geometry and Physical Conditions

The geometry used to test the multiple Poisson solves technique is a simple cubical box with the wall at $x = 0$ set to 3 volts and the wall at $x = 10\text{mm}$ set to 6 volts. The walls at $y = 0$, $y = 10\text{mm}$, $z = 0$, and $z = 10\text{mm}$ are dielectric walls that are specular reflectors of all particles incident upon them. This particular problem could have been simulated in two dimensions, but the computer program developed to perform this work is a full three-dimensional simulation. Validation results for this newly developed computer program are given in reference [5].

Only electrons and positively charged hydrogen ions are considered in this analysis and these particles are injected uniformly throughout the cubical box at equal rates of 2.5×10^{14} particles/second. Thus the plasma in the box is a low density plasma with no neutral particles and only consists of electrons and positive ions. The initial velocity distribution of the electrons and ions are uniform and the magnitudes of these velocities are 100,000 m/s and 1,000 m/s, respectively. The total number of the particles increases as the time increases, until the number of injected particles is equal to the rate at which particles are lost to the absorbing 3 and 6 volt walls.

The cell size used in all simulations is $0.5 \times 0.5 \times 0.5$ mm; thus 8000 cells are used to cover the cubical computational domain. The weighting of the computation particles is 500 real particles per computational particle. The time step size is varied depending on the particular study being undertaken. The total simulation time to reach steady state is about 1×10^{-5} seconds which is 10,000 time steps when a time step size of 1×10^{-9} seconds is used.

3.2. Stable Multiple Poisson Solves Technique Results

Figure 2 shows electric potential profiles across different planes of the cubical computational domain that intersect the z-axis at different locations. All of the results are basically the same and the figures show that the electric potential in the bulk of the plasma is 6.4 volts. The sheaths that form in the vicinity of the two walls with voltages of 3 volts and 6 volts are clearly visible. The explicit PIC technique and analytical results give a bulk plasma potential of 6.3 volts. Thus the multiple Poisson solves technique increases the plasma potential by 0.1 volts. The results shown in Figure 2 were obtained with the multiple Poisson solves technique using a time step size of 1×10^{-9} seconds, a Npps of 30,000, and a total number of time steps of 10,000. A Npps value of 30,000 for this case means Poisson's equation was solved 27 times per time step when the solution reached its steady state number of particles. There are about 810,000 particles in the cubical box when the particle number reaches steady state. Poisson's equation was solved fewer times per time step as the electrons were building up to their steady state value.

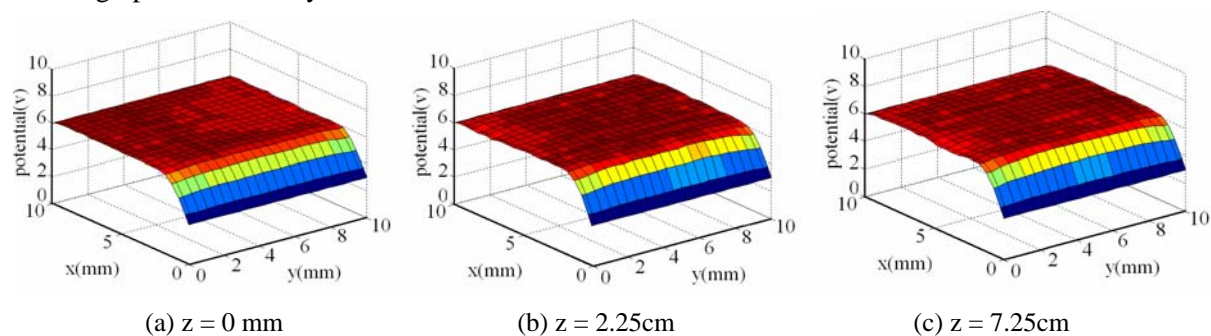


Figure 2. Electric potential profiles at different slices using the multiple Poisson solves technique with a Npps value of 30,000 and a time step size of 1×10^{-9} seconds.

3.3. Effect of Time Step and Npps

Figure 3 gives the time history of the total number of electrons in the computational domain for different computational techniques. Figure 3(a) gives the time history of the number electrons in the computational domain using the explicit technique with a number of different time steps. Figures 3(b) and 3(c) provide total number of electron history plots using the multiple Poisson solves technique with different Npps values and time steps of 2×10^{-9} and 4×10^{-9} seconds. Note that the explicit technique results are also shown on these graphs. It can be seen from these three graphs that the explicit technique results are stable when the time step size is less than or equal to 1×10^{-9} seconds, but it is unstable when time steps greater than or equal to 2×10^{-9} seconds are used. The multiple Poisson solves technique is stable for time steps up to and including 2×10^{-9} seconds when the Npps values are 5,000, 10,000 and 30,000. If Npps is 50,000, 70,000 or 90,000 the multiple Poisson solves technique is unstable at time steps of 2×10^{-9} . For a time step of 4×10^{-9} seconds all techniques are unstable. The flat lines seen in Figure 3(c) do not indicate stability, but are flat because particles are

leaving the chamber rapidly and the effects of the sheaths are being bypassed. These results clearly indicate that the multiple Poisson solves technique enhances stability at slightly larger time steps if the Npps value is chosen correctly. However, these results also indicate that the multiple Poisson solves technique produces slightly different numbers of electrons in the computational domain than the explicit technique.

Figure 4 gives the electric potentials at the z-direction mid-plane, for different time step sizes, using the multiple solves technique. Reasonable electric potential profiles are seen for time steps of 1×10^{-9} and 2×10^{-9} seconds, but greatly enlarged values are seen with a time step of 4×10^{-9} seconds. The reason for this is the simulation results are unstable with a time step of 4×10^{-9} seconds, and this is obvious if one watches a video of the voltage profiles changing as a function of time.

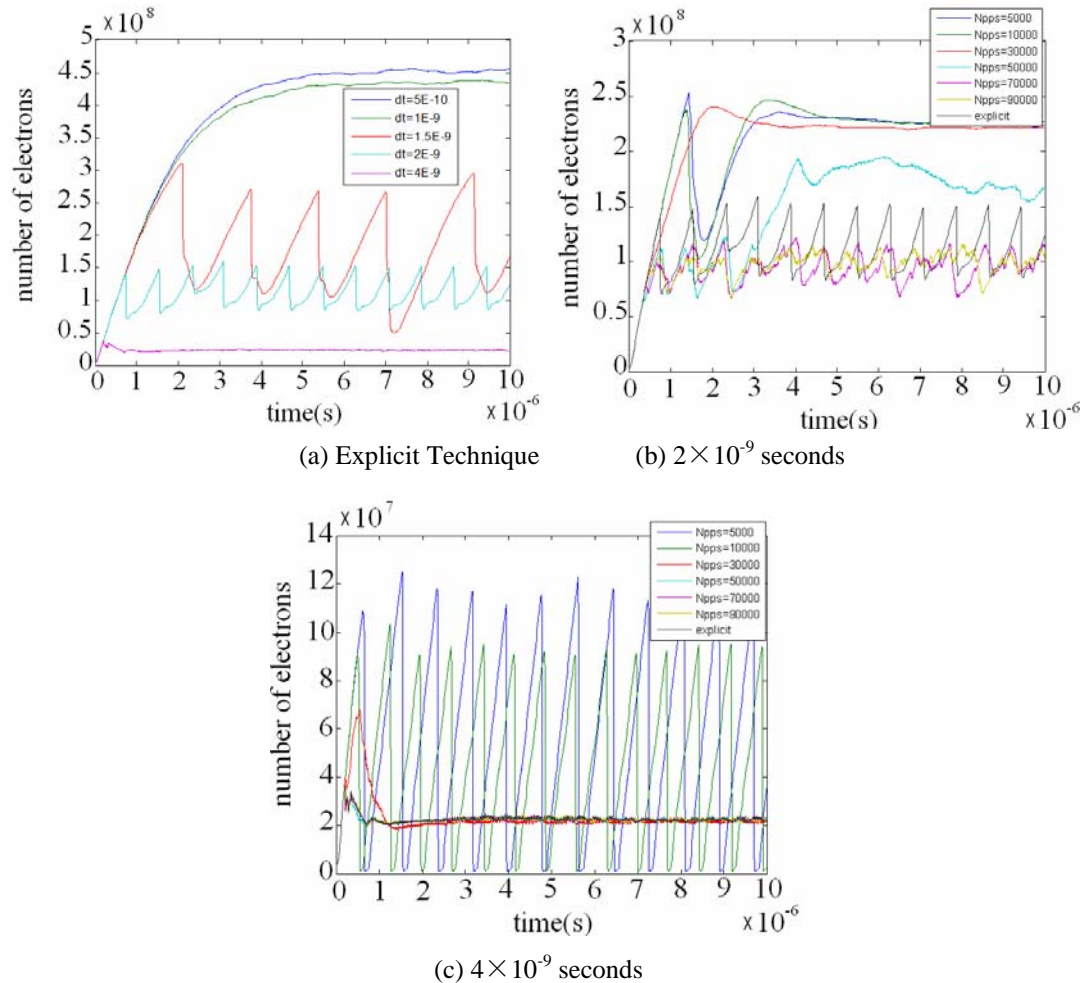


Figure 3. Time history plots of the total number of electrons in the computational domain for (a) the explicit technique using different time step sizes, (b) the multiple Poisson solves technique with a time step size of 2×10^{-9} seconds using different Npps values, and (c) the multiple Poisson solves technique with a time step size of 4×10^{-9} seconds using different Npps values.

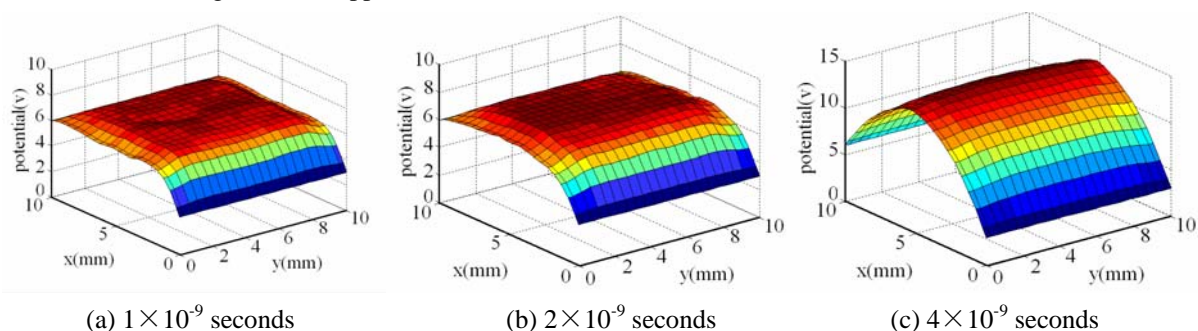


Figure 4. Electrical potential surface plots at the mid-plane of the z-direction using different time steps with the multiple Poisson solves technique.

Figure 5 gives the electron density as a function of the time step size and Npps. The black line is the explicit result and these results converge when the time step size is less than 1×10^{-9} seconds. When the time step size is bigger than 1×10^{-9} seconds, the results with the multiple Poisson solves technique are different than the explicit technique results; however, decreasing the time step size causes the multiple Poisson solves technique results to converge with the explicit technique results.

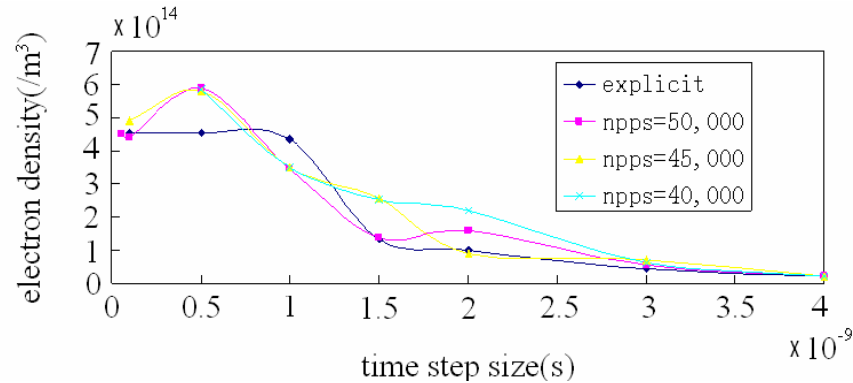


Figure 5. Electron density as a function of the time step size and Npps.

3.4. Computational Times

Table 1 shows the comparison of computational times for different time steps and different values of Npps. The first line in this Table provides times for the explicit technique. The cases were run on a computer equipped with an AMD Phenom II x6 1045 T 2.7 GHz processor. The least computational time with the multiple Poisson solves technique producing a stable result is 3.75 hours using at time step size of 2×10^{-9} seconds and a Npps of 40,000. However, this time is still larger than the time of 1.91 hours obtained with the explicit technique using a time step size of 1×10^{-9} seconds. Thus the goal of decreasing the computation time with the multiple Poisson solves technique has not been obtained.

Table 1. Computational times in hours using different time step sizes and different Npps.

Npps \ Δt	1×10^{-9} s	1.5×10^{-9} s	2×10^{-9} s	3×10^{-9} s
Explicit	1.91	0.80	0.47	0.28*
5,000	120.22	47.40	35.67	5.96*
10,000	59.64	25.76	16.41	3.02*
30,000	19.49	9.59	6.28	1.42*
40,000	19.85	10.04	3.75	0.94*
45,000	18.61	8.18	1.80*	0.79*
50,000	12.59	3.15*	2.56*	0.72*
70,000	5.11*	2.09*	1.04*	0.48*
90,000	3.32*	1.66*	0.93*	0.44*

*unstable results

4. Conclusions

In this work results of the effects of altering the number of times Poisson's equation is solved during one time step are presented. The results include a study of the effect of time step and the number of times the Poisson equation is solved in a single time step via the parameter Npps (number of particles per solve). The results indicate that small increases in the time step size over that which can be used with a purely explicit technique can be obtained; however, overall computational times are not decreased because of the extra time required to perform multiple Poisson solves in a single time step. In addition, the results produced by the multiple Poisson solves technique are slightly different than those produced by the explicit technique, except for the cases where very small time steps are used. This work was able to find no advantages of using the multiple Poisson solves technique over a purely explicit PIC technique.

Acknowledgments

The authors would like to thank the National Aeronautics and Space Administration (NASA), Glenn Research Center, for funding this project under the 2011 Phase-II Small Business Technology Transfer Research (STTR) program. We would also like to thank our technical monitors Dr. Jon Van Noord and George Soulas.

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