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**ON THE USE OF PARTICLE-IN-CELL METHODS
FOR THE STUDY OF MAGNETICALLY-CONFINED
FUSION PLASMAS**

**Richard J. Procassini
Massively Parallel Computing Initiative
Lawrence Livermore National Laboratory
Livermore, CA 94550**

and

**Electronics Research Laboratory
University of California
Berkeley, CA 94720**

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Richard J. Procassini

Massively Parallel Computing Initiative

Lawrence Livermore National Laboratory

Livermore, CA 94550

and

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University of California

Berkeley, CA 94720

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Abstract

The applicability of electrostatic particle-in-cell (PIC) methods for the simulation of magnetically-confined fusion plasmas is investigated. The aspects of the PIC methodology which allow one to accurately model the representative charge separations found in hot fusion plasmas with far fewer simulation particles are discussed. The number of simulation particles required to resolve the collective effects of interest (such as the ambipolar potential) above the statistical fluctuations is also analyzed.

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1 Introduction

Particle simulations of magnetically-confined fusion plasmas usually employ on the order of $10^4 - 10^6$ simulation particles to represent high density plasmas with $n_e \simeq n_i \geq 10^{14} \text{cm}^{-3}$, occupying volumes of many cubic centimeters to cubic meters. Hence, while the charge to mass ratio may be the same in the laboratory and computer experiments, each of the simulation particles, or *superparticles*, has a mass and charge that are several orders of magnitude larger than the physical mass and charge of an electron or ion. The larger charge associated with a superparticle, and the smaller number of superparticles that are used to simulate the warm fusion plasma, lead to an increased level of statistical fluctuations of the electrostatic potential. These fluctuations in density about a mean value vary $\sim 1/\sqrt{N_V}$, where N_V is the number of superparticles in the volume V under consideration. The particle-in-cell (PIC) techniques which allow one to model a warm fusion plasma accurately with a limited number of simulation particles, and the criteria that must be met to ensure that the level of the statistical fluctuations is smaller than the desired collective effects are the subjects of this paper. Some of the important advances in the area of particle simulation of thermal plasmas are reviewed in Section 1. In Section 2 we discuss the methods by which a limited number of simulation particles gives rise to the proper charge separation associated with thermal level potential variations. The requirements on the number of simulation particles per wavelength for resolution of the potential structure above the statistical fluctuations are presented in Section 3.

2 Particle Simulation Models Of Fusion Plasmas

Different types of particle simulation methods are applicable to the study of fusion plasmas. The Particle-Particle (PP) method [1], which is based upon the action at a distance formulation of the force law, uses the interparticle spacing to calculate the Coulomb force on one point-sized particle due to all others. While this method is simple to program, and is capable of simulating both collisionless and highly collisional plasmas, it is computationally expensive, requiring $\mathcal{O}(N_p)$ operations per time step, where N_p is the number of particle in the system. In addition, simulation of bounded plasma systems with the PP method is not straightforward.

One of the earliest warm plasmas models to use the PP simulation method was the 1962 one-dimensional model of Dawson [2], which treats the electrons as zero-width charge sheets embedded in a fixed neutralizing background. Dawson's model accurately reproduced the thermalizing properties and stochastic behavior of periodic, thermal plasmas with densities as low as 5 superparticles per Debye length. Time-averaging was employed to reduce the level of statistical fluctuations that are associated with such a small number of "point" particles.

In contrast to the PP method, Particle-Mesh (PM) methods advance the trajectory of the particles using field quantities that are defined on a collection of discrete grid points which span the system. The charge density and current contribution of each particle is weighted to the neighboring grid points according to the shape factor $S_{pg}(x - X_j)$, where x is the particle location and X_j is the location of the j -th grid point. The charge density and current density at each grid point are used to calculate the electric and magnetic field at the grid points. The Lorentz force associated with these fields is interpolated to the particle location via the shape factor $S_{gp}(x - X_j)$. In general, S_{pg} and S_{gp} may use different order interpolating schemes [3]. PM methods that employed various interpolating schemes were developed in the mid to late 1960's, most notably the zero-order Nearest Grid Point (NGP) [4], and the first-order Cloud-In-Cell (CIC) [5] and Particle-In-Cell (PIC) [6] models.

The use of a grid and shape factors (usually in the form of interpolating splines) results in a particle which has finite extent and is tenuous in nature. These properties of the particles lead to a plasma that more closely resembles a continuum fluid, or fluid elements, than the collection of point particles used in the PP method, while retaining some the kinetic nature of point particles. For a given number of particles, PM methods have a lower integrated levels of statistical fluctuations than does the PP method [7, 8]. Therefore, PM methods (such as CIC/PIC) allow one to obtain reasonable accuracy with orders of magnitude fewer particles per Debye length than occur in the physical system that is being modeled *without* resorting to special methods that reduce the statistical noise. On the other hand, PM methods are only capable of resolving forces which are smoothly varying over distances that are longer than a grid spacing Δx . Since some part of Coulomb forces act over a distance that is much shorter than Δx , it is not possible to simulate the short-range Coulomb collisional forces via PM methods, without explicitly modeling the physics

of these short-range collisional processes. Fortunately, for many warm plasmas of interest, large-impact-parameter ($b \simeq \lambda_{De} > \Delta x$), small-angle Coulomb collisions dominate the short-range, large-scattering-angle collisions by a factor of $\ln(N_D)$, where N_D is the number of particles in a cube of length equal to the Debye length λ_D .

3 Charge Separation And Electrostatic Potentials In A Particle-In-Cell Code

The fractional charge separation $(n_i - n_e)/n_e$ which is required to create a potential variation $e\Delta\phi$ (which is some fraction f of the electron thermal energy $k_B T_e$) over a scale length λ may be readily estimated from Poisson's equation

$$\nabla^2 \phi = -4\pi e (n_i - n_e) \quad (1)$$

where ϕ is the electrostatic potential, n_i and n_e are the ion and electron densities and $e = |q_e| = q_i$ is the charge of the ion (i. e. $Z = 1$). For a one-dimensional potential variation along $\hat{x}$, (1) may be rewritten as

$$\frac{d^2 \phi}{dx^2} = -4\pi e (n_i - n_e)$$

which may be approximated by

$$\frac{\Delta \phi}{\lambda^2} \simeq -4\pi e (n_i - n_e). \quad (2)$$

Multiplying both sides of (2) by $\lambda^2 e / k_B T_e$ gives

$$\begin{aligned} \frac{e\Delta\phi}{k_B T_e} &\simeq \lambda^2 \left(\frac{4\pi e^2 n_e}{k_B T_e} \right) \left(\frac{n_i - n_e}{n_e} \right) \\ &\simeq \left(\frac{\lambda}{\lambda_{De}} \right)^2 \left(\frac{n_i - n_e}{n_e} \right) \end{aligned} \quad (3)$$

where λ_{De} is the electron Debye length. Setting $e\Delta\phi/k_B T_e = f$ and rearranging gives

$$\left(\frac{n_i - n_e}{n_e} \right) \simeq f \left(\frac{\lambda_{De}}{\lambda} \right)^2. \quad (4)$$

For typical fusion plasma parameters of $n_e \simeq n_i \simeq 10^{14} \text{ cm}^{-3}$ and $k_B T_e \simeq 20 \text{ keV}$, the electron Debye length is $\lambda_{De} \simeq 10^{-2} \text{ cm}$. For these potential variations with a scale

length $\lambda \simeq 10\text{cm}$ (a reasonable value for present magnetically-confined fusion plasmas), the resultant fractional charge separation is approximately

$$\left(\frac{n_e - n_i}{n_e}\right) \simeq f \times 10^{-6}. \quad (5)$$

The fraction f of the electron thermal energy that is converted to an electrostatic potential is $\simeq 1/N_D$, which is usually much less than one, hence $f \ll 1$. Even for $f \simeq 1$, the expected charge imbalance is very small. Therefore, long-wavelength potential variations are associated with very small fractional charge separations and the plasma is termed *quasineutral*. Since many interesting phenomena in fusion plasma physics are quasineutral with long characteristic wavelengths, equation (5) implies that a simulation of such a plasma must resolve fractional density imbalances over the wavelength of interest to better than 1 part in 10^6 .

On first reading, the fractional charge separation given by (5) may appear to imply using more than 10^6 point particles per wavelength. On this basis, one might argue that the PP method is not practical for the simulation of a fusion plasma which spans several wavelengths. On the other hand, the finite extent of the particles in PM methods allows one to resolve charge separations, which are determined by the location of the centers of the particles, to within the accuracy of the computer. Figure A.1 shows a first-order-weighted CIC/PIC finite-size particle in a gridded system at two successive time steps. At time step n (solid particle shape), the particle i is closer to grid point j than it is to $j+1$, hence the particle's contribution to the charge density at grid point j ($\rho_{i,j}$) is larger than that to grid point $j+1$ ($\rho_{i,j+1}$). The particle is advanced to the right in the time step Δt by the incremental displacement δ . Therefore, at time step $n+1$, the particle contribution to the charge density at grid point j is reduced relative to that at time step n , and vice versa for the charge density at grid point $j+1$. The resolution of the displacement δ is limited only by the accuracy of the computer. Therefore, very small charge imbalances are possible with PM methods, even for a small number of particles per grid cell.

It should be pointed out that the number of superparticles that are required for the simulation of warm plasmas, such as a fusion-grade plasma, is much larger than that required to simulate a cold plasma or a beam. For the latter cases, one only needs a sufficient number of particles to reasonably fill in the configuration "axis" of the (x, v) phase space. However, simulation of a thermal plasma requires enough particles to fill in the phase space region

Figure 1: Location of a finite-size, first-order weighted CIC/PIC particle in a gridded system at two successive time steps. The particle is advanced at a velocity v_i to the right during the time step Δt for an incremental displacement δ .

from $v_{\min}$ to $v_{\max}$, over the entire length of the system, such that the “grainy” simulation phase space closely resembles the nearly continuous physical phase space.

4 Statistical Fluctuations And Electrostatic Potentials In A Particle-In-Cell Code

The goal of particle simulations is to obtain a reasonably accurate description of the physical system that is being modeled, with a finite number of superparticles. Since the number of superparticles used in any simulation of a fusion plasma is many orders of magnitude smaller than the actual number of particles in the physical plasma, the statistical fluctuation level of the simulation plasma is expected to be greater than that for the physical plasma. One must ensure that these fluctuations are not larger than the electrostatic potential which is the result of collective effects in the plasma.

How many superparticles per Debye length are required to resolve small changes in the

potential structure above the statistical fluctuations? The answer may be obtained from the general dispersion relation for an electrostatic wave in an unmagnetized, collisionless plasma. The dispersion relation can be derived from the fluid equations for each species and Poisson's equation (1). Neglecting sources of particles and momentum, the fluid equations become

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (n_s \mathbf{u}_s) = 0 \quad (6)$$

$$m_s n_s \left[\frac{\partial \mathbf{u}_s}{\partial t} + (\mathbf{u}_s \cdot \nabla) \mathbf{u}_s \right] = -\nabla p_s + q_s n_s \mathbf{E} \quad (7)$$

$$p_s = C \rho_s^{\gamma_s}, \quad \nabla p_s = \gamma k_B T_s \nabla n_s. \quad (8)$$

Equations (6), (7) and (8) are the particle continuity equation, momentum balance equation and equation-of-state for species s respectively, with C a constant coefficient. Assuming small-amplitude, plane-wave ($\mathcal{F}(\mathbf{r}, t) = \mathcal{F}_0 \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t)$) perturbations, linearizing about an equilibrium ($\mathbf{u}_{0s} = 0$, $\partial n_{0s}/\partial t = 0$ and $\nabla n_{0s} = 0$) and substituting (8) into (7) produces

$$-i\omega n_{1s} + i\mathbf{k} \cdot (n_{0s} \mathbf{u}_{1s}) = 0 \quad (9)$$

$$-i\omega m_s n_{0s} \mathbf{u}_{1s} = -\gamma k_B T_s i\mathbf{k} n_{1s} - i\mathbf{k} q_s n_{0s} \phi_1 \quad (10)$$

$$k^2 \phi_1 = 4\pi e (n_{1i} - n_{1e}) \quad (11)$$

where (9) is the continuity equation and (10) is the momentum equation for species s , and (11) is Poisson's equation. It is assumed that $|q_e| = q_i = e$. Solving (9) and (10) for the perturbed density gives

$$n_{1s} = \frac{n_{0s} k^2 e \phi_1}{m_s \omega^2 - \gamma k_B T_s k^2} \quad (12)$$

which are inserted into (11) to obtain

$$k^2 \phi_1 = 4\pi n_0 e^2 k^2 \phi_1 \left[\frac{1}{m_i \omega^2 - \gamma k_B T_i k^2} - \frac{1}{m_e \omega^2 - \gamma k_B T_e k^2} \right]$$

which, after cancelling terms and rearranging, becomes

$$1 = \left(\frac{\omega_{pe}}{\omega} \right)^2 \left[\frac{m_e}{m_i - \frac{\gamma k_B T_i k^2}{\omega^2}} - \frac{m_e}{m_e - \frac{\gamma k_B T_e k^2}{\omega^2}} \right]. \quad (13)$$

The definition of the electron plasma frequency $\omega_{pe}^2 \equiv 4\pi e^2 n_0 / m_e$ has been used in deriving (13), where $n_{0e} \equiv n_{0i} = n_0$ is the unperturbed density. Using the definition of the Debye

length $\lambda_D \equiv v_{th}/\omega_F = \sqrt{k_B T/m}/\omega_p$, assuming that the plasma is isothermal ($k_B T_e = k_B T_i = k_B T$) and rearranging gives

$$1 = \left(\frac{\omega_{pe}}{\omega} \right)^2 \left[\frac{1}{\frac{m_i}{m_e} - \frac{\gamma \lambda_D^2 k^2 \omega_{pe}^2}{\omega^2}} - \frac{1}{1 - \frac{\gamma \lambda_D^2 k^2 \omega_{pe}^2}{\omega^2}} \right]. \quad (14)$$

Since quasineutral effects are of interest, examine (14) in the low-frequency ($\omega \ll \omega_{pe}$), long-wavelength ($k\lambda_D < 1$) limit, where

$$\left(\frac{k\lambda_D \omega_{pe}}{\omega} \right)^2 \gg \frac{m_i}{m_e}$$

and

$$\left(\frac{k\lambda_D \omega_{pe}}{\omega} \right)^2 \gg 1.$$

In the quasineutral limit, the dispersion relation reduces to

$$\begin{aligned} 1 &\simeq \frac{1}{\gamma} \left(\frac{\omega_{pe}}{\omega} \right)^2 \left[- \left(\frac{\omega}{k\lambda_D \omega_{pe}} \right)^2 + \left(\frac{\omega}{k\lambda_D \omega_{pe}} \right)^2 \right] \\ &\simeq \frac{1}{\gamma} \left[- \left(\frac{1}{k\lambda_D} \right)^2 + \left(\frac{1}{k\lambda_D} \right)^2 \right]. \end{aligned} \quad (15)$$

Equation (15) indicates that the Laplacian of the perturbed potential $\nabla^2 \phi_1$ is balanced by the difference of the nearly equal species densities n_{1e} and n_{1i} , and that each of the density terms is of order $(1/k\lambda_D)^2 \gg 1$ times greater than the Laplacian term.

The level of the statistical fluctuations may be quantified by the error associated with the process of counting particles to produce the densities n_{1e} and n_{1i} . For a one-dimensional perturbation, the standard deviation about the mean perturbed density ($n_1 = N_\lambda/\lambda$) of either species is defined as

$$\sigma_{n_1} \equiv \frac{n_1}{\sqrt{N_\lambda}} = \left(\frac{N_\lambda}{\lambda} \right) \frac{1}{\sqrt{N_\lambda}} = \frac{1}{\lambda} \sqrt{N_\lambda} \quad (16)$$

where λ is the wavelength of the density perturbations and N_λ is the number of particles per wavelength. Since the perturbed densities are proportional to $(k\lambda_D)^{-2}$ from (15), the statistical fluctuations in the perturbed density and potential scale as

$$\sigma_{n_1} \sim \frac{1}{\sqrt{N_\lambda}} \left(\frac{1}{k\lambda_D} \right)^2. \quad (17)$$

It is desirable to have the signal to noise (statistical fluctuations) ratio be as large as possible, i. e. $\sigma_{n_1} \ll 1$, such that

$$N_\lambda \gg \left(\frac{1}{k\lambda_D} \right)^4. \quad (18)$$

For long-wavelength perturbations ($1/k\lambda_D > 1$), equation (18) appears to be a rather severe requirement on the number of particles per wavelength that are required to obtain accurate results with reasonable statistical fluctuations. Note that this derivation assumes that the particles are effectively *point* sized. The finite extent of the particles used in CIC/PIC simulations leads to a lower integrated level of fluctuations than that encountered in simulations which use the PP method, since wavelengths shorter than the size of a particle are attenuated by the finite extent of the particle. For this reason, equation (18) may be taken as an *upper limit* on the number of particles required per wavelength in a CIC/PIC simulation.

Equation (18) also determines the required number of particles per Debye length, since $k = 2\pi/\lambda$. Fusions plasmas have approximately 10^8 particles per Debye cube in three dimensions ($N_D \equiv n_{3D}\lambda_D^3 \simeq 10^8 \gg 1$). By reducing the system from three dimensions in configuration space down to one, the number of particles per Debye length is $N_D \simeq (n_{3D}\lambda_D^3)^{1/3} \simeq 500$, and the relation $N_D \gg 1$ still holds.

Simulations of long-wavelength phenomena using the PP method requires both $N_\lambda \gg 1$ and $N_D \gg 1$. For a PM method simulation using CIC/PIC techniques, the *grid* (and resulting finite-sized particles) eliminate perturbations with wavelengths that are shorter than $2\Delta x$. In this case, the parameter $\Delta x/\lambda_D$ becomes important. If $\Delta x/\lambda_D \ll 1$, the number of particles required to simulate phenomena with wavelengths on the order of a few grid spacings is much less than N_D , but the $N_D \gg 1$ constraint is still valid. If $\Delta x/\lambda_D \sim 1$, then only $\sim N_D$ particles are needed to simulate the shortest wavelength phenomena. As $\Delta x/\lambda_D$ is increased above 1, the Debye length is no longer resolved, and N_λ replaces N_D as the important linear density. When $\Delta x/\lambda_D \gg 1$, wavelengths on the order of the Debye length are unresolvable, allowing one to reduce the number of particles per Debye length to $N_D \sim 1$. In the large grid cell limit, the required number of particles per wavelength given by (18) is replaced by

$$N_\lambda \gg \left(\frac{1}{k\Delta x} \right)^4. \quad (19)$$

In each of these limits, the constraint $N_A \gg 1$ still holds.

Since implicit formulations of the CIC/PIC method allow one to run at large values of $\omega_{pe}\Delta t$ and $\Delta x/\lambda_{De}$ without incurring numerical instabilities, the total number of particles that are required to simulate long-wavelength or quasineutral phenomena (at the expense of damping out the high-frequency response) is significantly reduced relative to the number required by explicit schemes, which have numerical instability limits on the size of the time step and grid spacing. For this reason, implicit schemes are more attractive than explicit schemes for the simulation of large-scale, quasineutral fusion plasmas.

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