Description of Gridless Electrostatic Spectral Particle-in-Cell Code from the UPIC Framework

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I. Introduction

This document presents the mathematical foundation of the gridless periodic Particle-in-Cell electrostatic code in the UCLA Particle-in-Cell Framework. The electrostatic code uses only the Coulomb force of interaction between particles. This is the most fundamental of plasma models and is useful when inductive electric and magnetic fields are not important. The solutions presented are an exact Fourier series. The only approximations made in solving them are truncating the Fourier series and using a finite time step.

II. Electrostatic Plasma Model

The simplest model is the electrostatic model, where the force of interaction is determined by solving only the Poisson equation in Maxwell's equation. The main interaction loop is as follows:

1. Calculate charge density in real space from the particles:

$$\rho(\boldsymbol{x}) = \sum_i q_i S(\boldsymbol{x} - \boldsymbol{x}_i)$$

2. Solve Poisson's equation:

$$\nabla \cdot \boldsymbol{E} = 4\pi\rho$$

3. Advance particle co-ordinates using Newton's Law:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = q_i \int \boldsymbol{E}(\boldsymbol{x}) S(\boldsymbol{x}_i - \boldsymbol{x})\, d\boldsymbol{x} \qquad\qquad \frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$$

The function S(**x**) is the particle shape function. For point particles, this would be a delta function, but in computer modeling extended shapes are commonly used. The codes described here are spectral and solve the electric field using Fourier transforms. For the electrostatic case and periodic boundary conditions, a procedure for a gridless system is as follows:

1. Fourier Transform the charge density:

$$\rho(\boldsymbol{k},t) = \frac{1}{V}\int \sum_i q_i S(\boldsymbol{x} - \boldsymbol{x}_i(t))\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} d\boldsymbol{x} = \sum_i q_i S(\boldsymbol{k})\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i(t)}$$

2. Solve Poisson's equation in Fourier space:

$$\boldsymbol{E}(\boldsymbol{k}) = \frac{-i\boldsymbol{k}}{k^2} 4\pi\rho(\boldsymbol{k})$$

Note that this equation implies that $\rho(\mathbf{k}=0) = 0$. This means that strictly periodic systems are charge neutral.

3. Fourier Transform the Smoothed Electric Field to real space:

$$\boldsymbol{E}_S(\boldsymbol{x}_i) = V \sum_{\boldsymbol{k}=-\infty}^{\infty} \boldsymbol{E}(\boldsymbol{k}) S(\boldsymbol{k})\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}i}$$

For delta function particles shapes, $S(\mathbf{k}) = 1/V$. When solving these equations on the computer, we generally use discrete time co-ordinates and truncate the infinite Fourier series. In discretizing time, the explicit leap-frog integration scheme is commonly used, because it is second order accurate. In this scheme, the particle co-ordinates are known at staggered times. These are the only approximations to an exact solution.

The discrete equations of motion are as follows:

$$\boldsymbol{v}_i(t + \triangle t/2) = \boldsymbol{v}_i(t - \triangle t/2) + \frac{q_i}{m_i}\boldsymbol{E}_S(\boldsymbol{x}_i(t)) \triangle t$$

$$\boldsymbol{x}_i(t + \triangle t) = \boldsymbol{x}_i(t) + \boldsymbol{v}_i(t + \triangle t/2) \triangle t$$

III. Energy and Momentum Flux

For the electromagnetic model, the energy flux is well known to be given by the Poynting vector **S**:

$$\nabla \bullet \boldsymbol{S} + \frac{\partial}{\partial t}\left[\frac{\boldsymbol{E} \bullet \boldsymbol{E}}{8\pi} + \frac{\boldsymbol{B} \bullet \boldsymbol{B}}{8\pi}\right] = -\boldsymbol{j} \bullet \boldsymbol{E}$$

where

$$\boldsymbol{S} = \frac{c}{4\pi}\boldsymbol{E} \times \boldsymbol{B}$$

This equation describes the conservation of energy: the time rate of change of electromagnetic field energy plus the outflow of the energy is equal to the negative of the work done on the particles. This equation is not unique and other energy flux equations can also be derived: only differences in energy and flux are significant. It is less well known that analogous energy flux equations can be derived for the electrostatic and Darwin models.

For the electrostatic model, an energy flux equation is given by:

$$\nabla \bullet \boldsymbol{S} + \frac{\partial}{\partial t}\left[\frac{\boldsymbol{E}_L \bullet \boldsymbol{E}_L}{8\pi}\right] = -\boldsymbol{j} \bullet \boldsymbol{E}_L$$

where

$$\boldsymbol{S} = \left[\boldsymbol{j} - \frac{1}{4\pi}\nabla\frac{\partial\phi}{\partial t}\right]\phi$$

and

$$\boldsymbol{E}_L = -\nabla\phi$$

This equation can be easily shown by making use of the equation of continuity and the identity:

$$\nabla \bullet (f\boldsymbol{V}) = \boldsymbol{V} \bullet \nabla f + f(\nabla \bullet \boldsymbol{V})$$

An alternate form of this equation can be derived by using the result,

$$\nabla \bullet \left[\frac{\phi\nabla\phi}{8\pi}\right] = \frac{\boldsymbol{E}_L \bullet \boldsymbol{E}_L}{8\pi} - \frac{1}{2}\rho\phi$$

to obtain:

$$\nabla \bullet \boldsymbol{S}' + \frac{\partial}{\partial t}\left[\frac{1}{2}\rho\phi\right] = -\boldsymbol{j} \bullet \boldsymbol{E}_L$$

where the alternative energy flux vector is

$$\boldsymbol{S}' = \boldsymbol{j}\phi + \frac{1}{8\pi}\left[\frac{\partial\phi}{\partial t}\nabla\phi - \phi\nabla\frac{\partial\phi}{\partial t}\right]$$

The electrostatic energy in the form $\rho\phi/2$ is useful for isolated systems.

In addition to the energy flux, the momentum flux equation is also useful. For the electromagnetic case, the equation is well known:

$$\nabla \cdot \overleftrightarrow{\mathbf{T}} - \frac{1}{c^2}\frac{\partial \boldsymbol{S}}{\partial t} = \rho \boldsymbol{E} + \boldsymbol{j} \times \boldsymbol{B}/c$$

where

$$\overleftrightarrow{\mathbf{T}} = \frac{1}{4\pi}\Big[\boldsymbol{EE} + \boldsymbol{BB} - \frac{1}{2}(\boldsymbol{E} \cdot \boldsymbol{E} + \boldsymbol{B} \cdot \boldsymbol{B})\,\overleftrightarrow{\mathbf{I}}\,\Big]$$

is the Maxwell Stress Tensor. The quantity $\mathbf{S}/c^2$ is the momentum in the electromagnetic field.

In the electrostatic case, there is no momentum in the longitudinal field and the magnetic field vanishes, so the momentum flux equation reduces to:

$$\nabla \cdot \overleftrightarrow{\mathbf{T}} = \rho \boldsymbol{E}$$

where

$$\overleftrightarrow{\mathbf{T}} = \frac{1}{4\pi}\Big[\boldsymbol{EE} - \frac{1}{2}(\boldsymbol{E} \cdot \boldsymbol{E})\,\overleftrightarrow{\mathbf{I}}\,\Big]$$

These energy and momentum flux equations are not unique, and alternative forms are possible and useful.

IV. Units

These codes use dimensionless grid units, which means that distance is normalized to some distance δ. Generally, this distance δ is the smallest distance which needs to be resolved in the code, such as a Debye length. Time is normalized to some frequency ω_0. Generally this frequency is the highest frequency that needs to be resolved in the code, such as the plasma frequency. Charge is normalized to the absolute value of the charge of an electron e. Mass is normalized to the mass of an electron m_e. Other variables are normalized from some combination of these.

In summary, dimensionless position, time, velocity, charge, and mass are given by:

$$\widetilde{x} = x/\delta \qquad \widetilde{t} = \omega_0 t \qquad \widetilde{\boldsymbol{v}} = \boldsymbol{v}/\delta\omega_0 \qquad \widetilde{q} = q/e \qquad \widetilde{m_e} = m/m_e$$

Dimensionless charge and current densities are given by:

$$\widetilde{\rho} = \rho\delta^3/e \qquad \widetilde{j} = j\delta^3/e\delta\omega_0$$

Dimensionless electric field and potential are given by:

$$\widetilde{\boldsymbol{E}} = e\boldsymbol{E}/m_e\omega_0^2\delta \qquad \widetilde{\phi} = e\phi/m_e\omega_0^2\delta^2$$

Dimensionless energy is given by:

$$\widetilde{W} = W/m_e\omega_0^2\delta^2$$

The dimensionless particle equations of motion are:

$$\widetilde{m_i}\frac{d\widetilde{\boldsymbol{v}_i}}{d\widetilde{t}} = \widetilde{q_i}\left[\widetilde{\boldsymbol{E}} + \widetilde{\boldsymbol{v}_i} \times \widetilde{\boldsymbol{B}}\right] \qquad\qquad \frac{d\widetilde{\boldsymbol{x}_i}}{d\widetilde{t}} = \widetilde{\boldsymbol{v}_i}$$

The dimensionless Poisson equations is:

$$\widetilde{\nabla} \cdot \widetilde{\boldsymbol{E}} = A_f\widetilde{\rho}$$

where

$$A_f = \frac{4\pi e^2}{m_e\omega_0^2\delta^3}$$

defines the relation between the sources and the fields. Whatever time and space scales are chosen, these equations have the same form. Only the constant A_f changes.

In these codes, the normalization length is chosen to be a virtual grid spacing,

$$\delta = L_x/N_x = L_y/N_y = L_z/N_z$$

and the normalization frequency to be the plasma frequency ω_{pe}. In that case, one can show that:

$$A_f = \frac{1}{n_o \delta^3} = \frac{N_x N_y N_z}{N_p}$$

where Np is the number of particles. The grid spacing is then related to some other dimensionless physical parameter, typically the Debye length. Thus:

$$\lambda_{De} / \delta = \frac{v_{the}}{\delta \omega_{pe}} = \tilde{v}_{the}$$

where the dimensionless thermal velocity is an input to the code. Note that if the grid space is equal to Debye length, then A_f is identical to the plasma parameter g which appears as an small expansion parameter in plasma theory.

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