Verification and Convergence Properties of Particle-in-Cell Codes

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Particle-in-cell methods have been widely throughout plasma physics over 50 years. However, there is confusion about the mathematical model used for particle-in-cell (PIC) codes and whether PIC converges or not. Our hypothesis is Klimontovich equation with finite-size particle is the model described by PIC codes. We perform numerical study to compare PIC codes and gridless codes to solve these issues.

I. INTRODUCTION

Plasma is charged particles, the forth state of matter besides solid, liquid, and gas. Techniques of investigating behavior of plasma have been carried out through experiments and mathematical models. Motions of plasma particles can be complex and are invisible by eyes. Therefore, physicists have created different types of models to simulate the behavior of plasma particles.[1]

Of the many mathematical models scientists created for plasma simulation, there are three main types—fluid model, kinetic model, and molecular dynamic model. The fluid model describes plasma as fluids and it is created based on continuity equation. One might think plasma does not behave like fluid since plasma does not have as much collision as fluid; however, 80% of the experiments can be explained by fluid model.[2] The kinetic model uses Valsov equation to describe motions of plasma particles. Kinetic model solves the defect of fluid model not being sensitive to deviation of Maxwellian speed distribution. The molecular dynamic model is also known as Klimontovich models. The Klimontovich equation (Eq.1) is constructed based on Maxwell equations, charge and current density, and Newtons second law.

$$\frac{\partial \boldsymbol{F}(\boldsymbol{x},\boldsymbol{v},t)}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{F} + \frac{q}{m}(\boldsymbol{E}+\frac{\boldsymbol{v}}{c}\times\boldsymbol{B})\cdot\nabla_{\boldsymbol{v}}\boldsymbol{F} = 0 \quad (1)$$

If we would have to rank the accuracy among these three models, the Klimontovich model will be the most accurate model, since it considers interactions between each particle, following by kinetic model and then fluid model.

II. PARTICLE-IN-CELL (PIC) METHOD

The Particle-in-Cell method is used to study motions of plasma particles. There are three main kinds of codes that UCLA plasma simulation group uses—electrostatic, electromagnetic, and Darwin code. Electrostatic code describes Coulomb force of interaction between particles. Electromagnetic code includes all the electric and magnetic fields described by Maxwells equation. Darwin code includes induced electric and magnetic field but excludes radiation.[4] We set initial condition such as positions and velocities of plasma particles. We then use the charge density and Poisson equation to obtain forces acting on each particle. Grids are used to enhance the efficiency of simulation. We interpolate each particle onto the grid and calculate electric field on the grid point. We then integrate equations of motion of particles and calculate forces acting on them. Last, we re-interpolate those particles to their new positions and repeat this process. PIC method has been used over fifty years in plasma research.

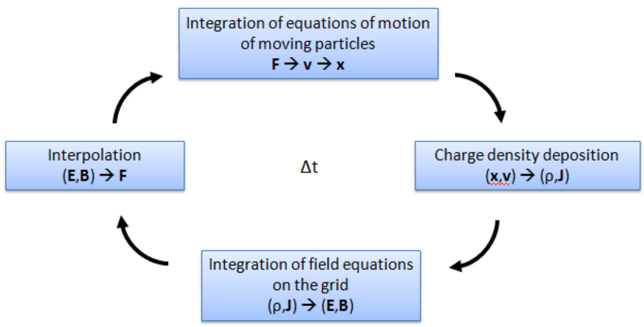
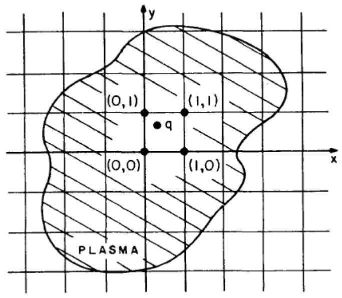
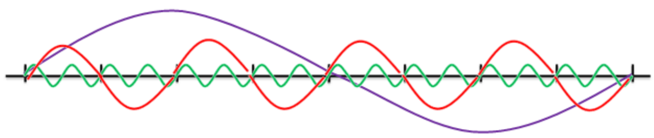


FIG. 1: Flow chart of PIC method

My project is to study the convergence and the mathematical model used for PIC codes by comparing that to gridless codes. Due to the existence of grids in PIC codes, two factors that can lead to inaccuracy arise—interpolation and aliasing. Since we have to use interpolation functions to obtain positions of particles on the grid, different orders of interpolation function used affect the accuracies of the result—using a higher order interpolation function or making the particle size bigger, we are able to obtain more accurate result. The information of particles is resolvable only on the grid points. If we only use few Fourier modes for the simulation, we will lose information on certain grid points. On the other hand, we do not wish to use too many Fourier modes since we are not able to obtain information that is not on the grid points. Therefore, the ultimate way is to use as many Fourier modes as possible but have all the points resolvable. Therefore, there exist a maximum number of Fourier modes (half of the grid points) in PIC code.



(a) 2-D interpolation of a particle onto grid points



(b) Fourier modes
Purple: missing information on grid points (too few modes)
Green: information cannot be obtained within a grid (too many modes)
Red: obtain maximum information
Max mode allow(k_{max})=$\frac{1}{2}$×Number of grids(N_x)

FIG. 2: Two factors of resulting inaccuracy in PIC code

III. STUDY OF CONVERGENCE

I use 1-demensional spectral electrostatic model to obtain exact solution of Klimontovich equation for finite size particle. Spectral codes are periodic; therefore, we can obtain general information by looking into a small area. Since the gridless code does not have a restriction of the maximum number of modes, we will get convergence on our results with a large enough number of modes. The experiment I studied was plasma particles in thermal equilibrium without external beams. The condition of the experiment I studied using PIC code is listed in Table 1.

TABLE I: Condition

Number of grid points (N_x)	512
Total number of particles	18432
dt	0.1

There are 512 grid points and the maximum number of modes allowed in the PIC code is half of the grid points. Therefore, we have 216 modes allowed in PIC codes under this condition. I varied number of modes of the gridless code to see at what number of modes will it allow for complete convergence. The raw data showed the field energy has complete convergence at mode 640.

For particle size (a) = grid size (Δ), the gridless code shows the electric field energy does not converge at mode

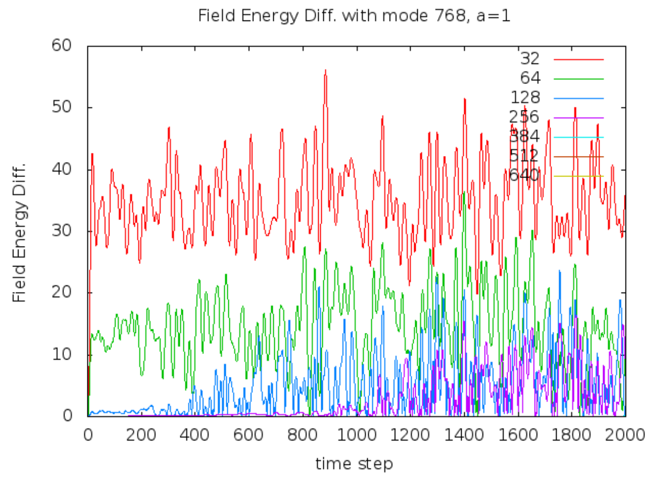
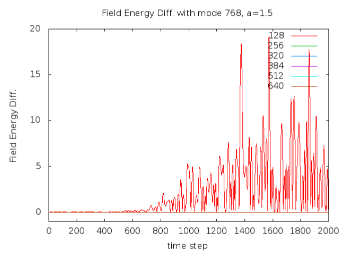
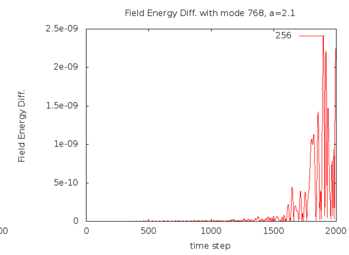


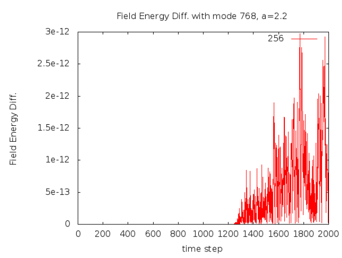
FIG. 3: a (particle size) = 1Δ (grid size)
Field energy difference of varying number of modes with mode 768 vs. time step



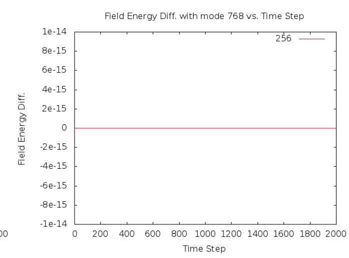
(a) a = 1.5Δ



(b) a = 2.1Δ



(c) a = 2.2Δ



(d) a = 2.25Δ

FIG. 4: Field energy difference compared to mode 768 with varying a

256. I varied the size of the particles and found in order to get complete convergence for mode 256, we have to use a = 2.25Δ. This is an importance result since we had been using a = Δ for PIC code simulations.

The next step is to see how long will the result stay convergent. Figure 5. shows the experiment ran a = 2.25Δ for 10000 timesteps and selectric field energy stays convergent well except for as it goes to 9000 time steps. I also change dt of the experimentwith smaller dt, we will get more accurate result.

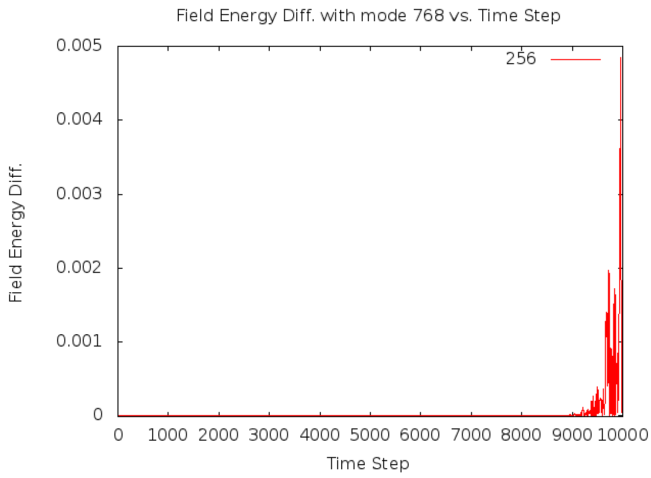


FIG. 5: Field energy difference of varying number of modes with mode 768 vs. 10000 time step (a = 2.25Δ)

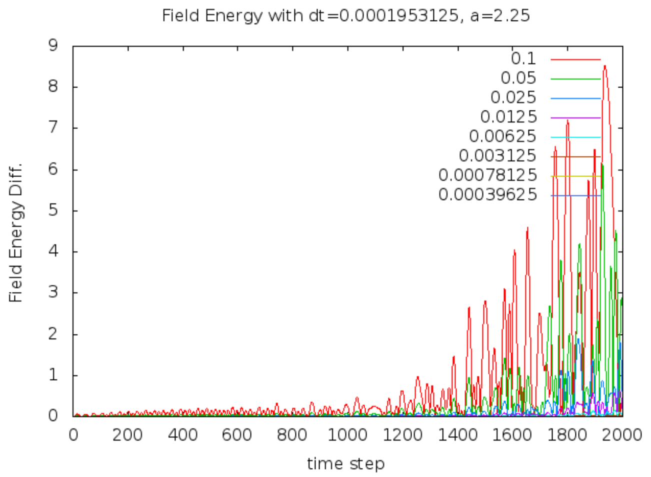


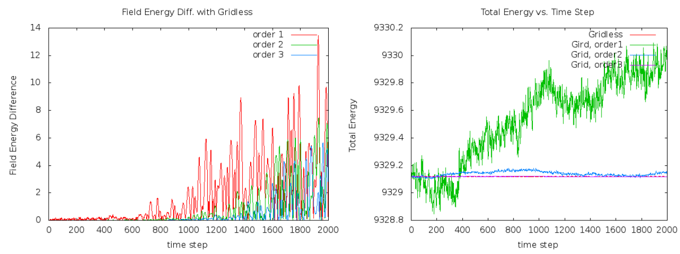
FIG. 6: Change of dt (a = 2.25Δ)

Figure 7 shows PIC codes converge better to the gridless code with higher order of interpolation function.

The last test to verify is the spectrum. Due to the compensation of accuracy by making particle size bigger to avoid aliasing, it will result in dispersion relation. The theoretical equation for dispersion relation is described in Eq. 2.

$$\omega^2 = \omega_{pe}^2 + 3k^2 v_{thermal}^2 \tag{2}$$

Since we use finite size particle, the shape function we use to describe particle size is in Gaussian shape $S(k_i) = e^{(k_i a_i)^2/2}/L_i$ where k is the number of Fourier modes, a is the particle size, and L is the size of the system size. This shape function filter is used to suppress aliasing and the effective particle



(a) Field Energy vs. Time Step (b) Total Energy vs. Time Step

FIG. 7: a = 2.25Δ, dt = 0.0125

shape is given by $S_{eff}(\mathbf{k}) = V \cdot \prod_i W(k_i) S(k_i)$. Then $\omega_{pe}^2 \Rightarrow \omega_{pe}^2 (V \cdot S_{eff}(k_i))$.

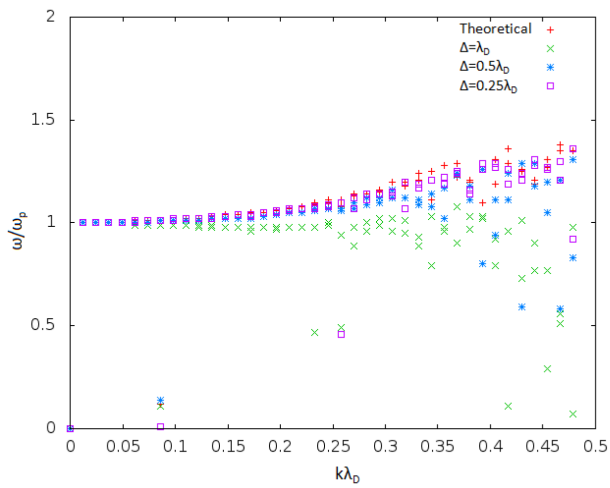


FIG. 8: Spectrum of varying Δ with Debye length (λ_D)

We can see from Fig. 8 that the results converge better to the theoretical value when $\Delta < \frac{1}{2}\lambda_D$. λ_D is Debye length. Combine this result with result earlier that a=2.25Δ, we can conclude that we will obtain results with better convergence if we make the a $\simeq \lambda_D$.

IV. CONCLUSION AND FUTURE WORK

For 1-dimesional electrostatic code with 256 maximum number of modes, we will get most convergent result as we make a=2.25Δ and $\Delta < \frac{1}{2}\lambda_D$. These are important results since we usually use PIC code with a=Δ and $\Delta = \lambda_D$. By performing numerical experiment, we see the results of spectrum PIC code are well-converged with the gridless code. Therefore, we can conclude that the mathematical model behind the PIC code is Klimontovich model. We also verified the results converge more as we approach higher order of interpolation functions or make dt smaller. In the future, we can test if the statement will still hold true on electromagnetic and Darwin codes. We can also rerun some of the previous experiments and compare the difference of the results by using these parameters.

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