A Particle-Particle Particle-Mesh Computation without Self Force

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Outline

- Overview
- Numerical Heating-Need to improved sub-grid interpolation and time integrators
- Resolving sub-grid forces through PPPM
- Removing self-force associated with traditional method
- Future work

Equations

Maxwell's Dynamical Equations:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

Subject to the initial value constraints:

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{D} = \rho$$

With the definitions for anisotropic macroscopic media:

$$\mathbf{D} = \boldsymbol{\varepsilon}\mathbf{E} \qquad \mathbf{J} = \boldsymbol{\sigma}\mathbf{E}$$

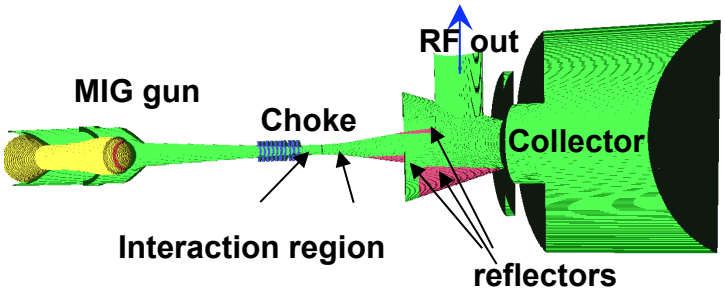
$$\mathbf{B} = \boldsymbol{\mu}\mathbf{H}$$

Relativistic Lorentz Force Law for relativistic velocity *u*=*v*γ:

$$\frac{d\mathbf{u}}{dt} = \frac{q}{m}\left[\mathbf{E} + \frac{\mathbf{u}\times\mathbf{B}}{\gamma}\right]$$

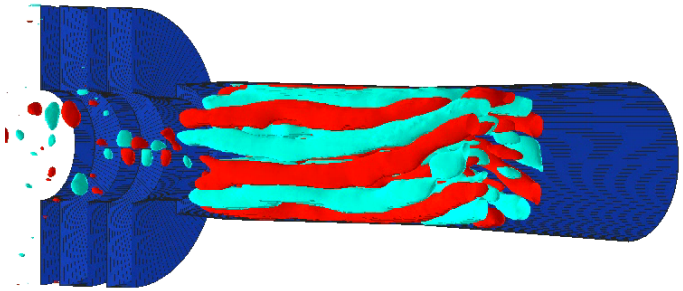
Plasma Physics Integration

Volume Chemistry:
Ionization
Elastic
Excitation
Charge exchange
De/Attachment
Photo Ionization
Recombination
Super Elastic
Penning ionization
Rot-Vib excited states



Surface Physics:
Bremsstrahlung
Thermal heating
Impurity diffusion

Conformal Boundary, Adaptive Bulk Plasma Code



Surface Chemistry:
Electron emission
Adsorption
Desorption
Secondary particle emission

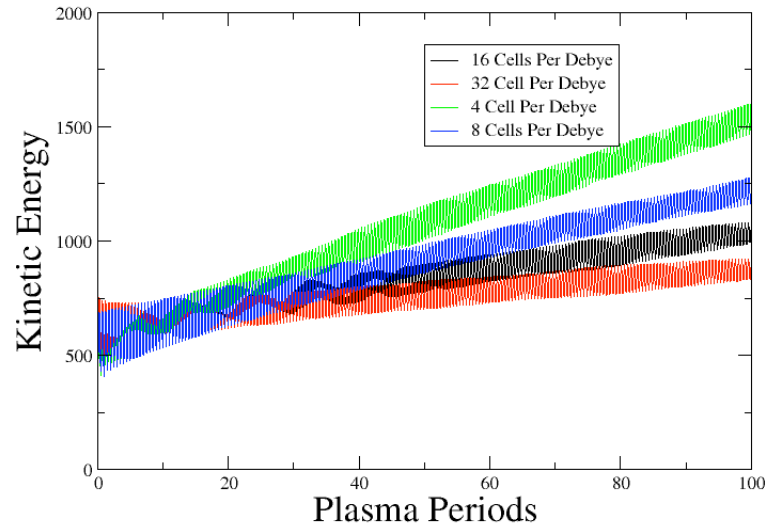
Physics on three time scales
- During a RF pulse (ns)
- Between RF pulse (or long pulse) (ms)
- System thermalization time (s)

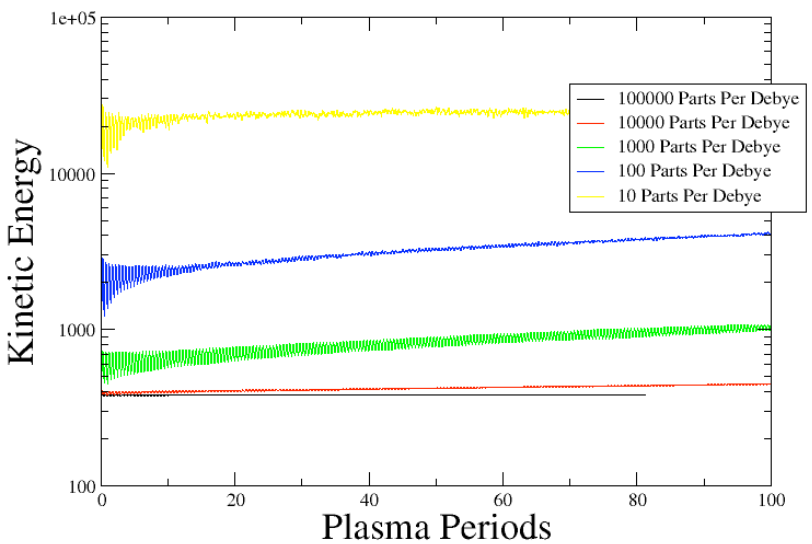
Problems Associated with PIC Simulations

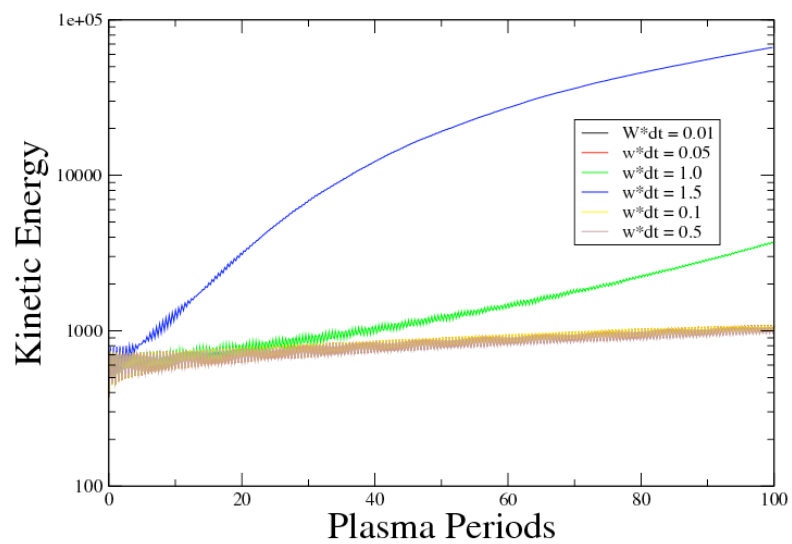
- **Particle-in-Cell (PIC) has been used for many years to accurately simulate plasmas.**
  - **Core technology within ICEPIC**
- **Nominally this technique is second order in space and time if:**
  - **One resolves the Debye length of the system thus resulting in smooth fields over the grids**
  - **One resolves the time signal with respect to the plasma frequency**
  - **One resolves the statistics of the plasma by having enough particles within a cell**
- **If not, plasma gains energy (heating) and produces inaccurate results**

Heating Rates

- **Convergence plots**
  - **Upper right – Convergence as function of grid resolution**
  - **Lower left – Convergence as a function of particle count**
  - **Lower right – Convergence as a function of time step**

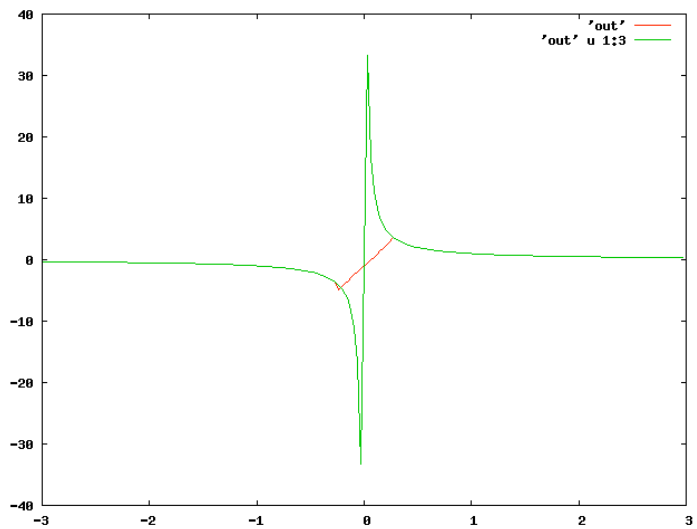






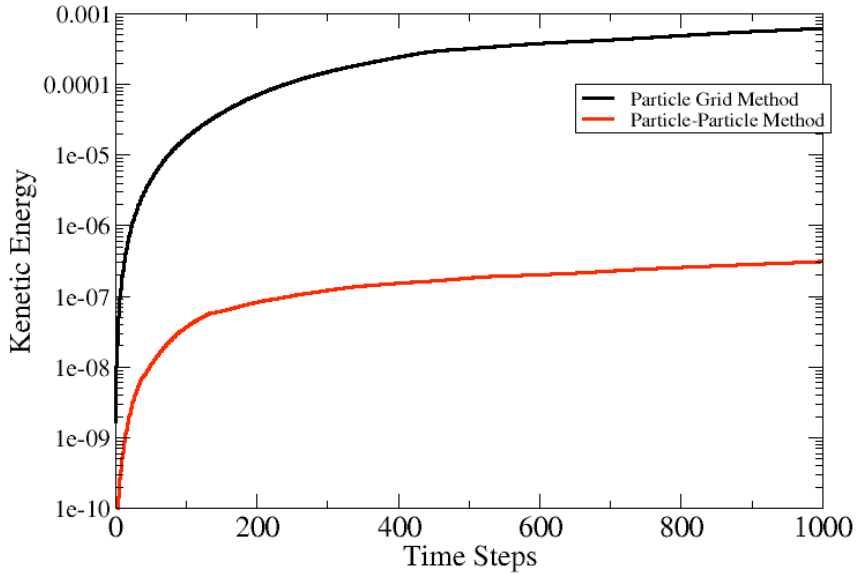
Under-Resolved Spatial Resolution

- The fields are represented on a grid within a simulation
  - Particles are forced by fields on that grid
- Particles feel realistic forces from particles outside their local grid cell
- Local interactions are under predicted.
  - Left – green curve represents physical force on two particles, red is PIC force.
- Resolve by providing a correction to forces locally



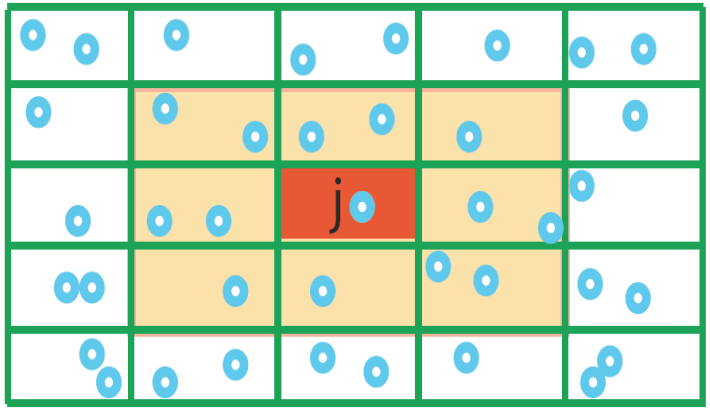
Particle-Particle vs Particle-Grid Heating Rates

- As can be seen computing all particle-particle interactions heats less than going through a grid
- 256x256 grid, 4K particles, Neumann boundaries around the full domain
- Boundary integral method for particle-particle boundary conditions



Particle-Particle-Particle-Mesh PPPM

- Suppose one needs to compute the force on particles in cell j.
  - One has the fields on the grid highlighted in green
  - Standard PIC just interpolates from the green mesh to the particles
- PPPM subtracts the fields on the grid locally due to particles within the yellow domain
- Local forces are then re-added using Green's function (1/r law)



Advantages/Problems with PPPM

- The work to solve this problem is still order N where N is the number of particles
- Accurately resolves local Coulomb collisions
- Particles don't "See" the grid and have associated grid heating – No Debye length issues.
- If the subtraction of local effects does not exactly cancel out what the grid "thinks" the force should be particles can push themselves – self force.
- With large, discontinuous forces integrators are much more critical – More integration errors
- Added complexity
- Hard to extend to electromagnetics

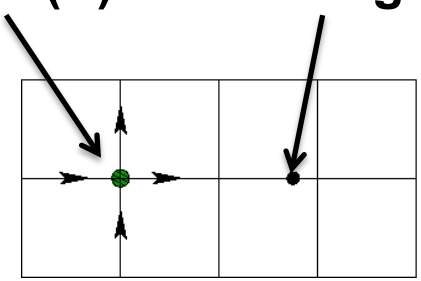
Scheme for PPPM

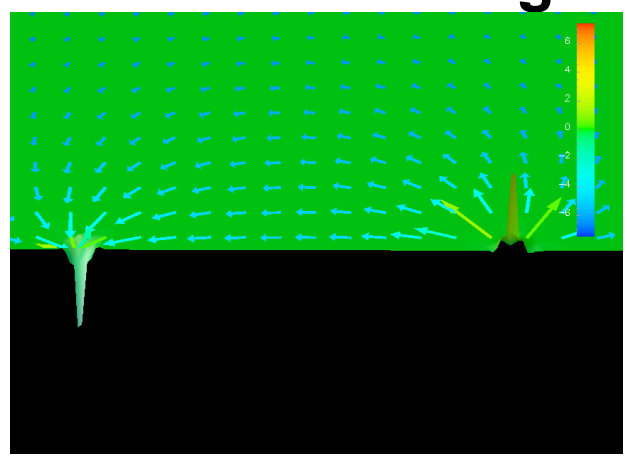
- Steps in electrostatic PIC/PPPM
  - Map charge to grid, typically linear weighting
  - Solve Poisson's equation
  - Subtract local particles forces from grid
  - Interpolate force from grid to particle
  - Add in local particle-particle forces
- No self force assuming:
  - Charge mapping and interpolation are symmetric
  - Subtraction removes all the local contribution to the force

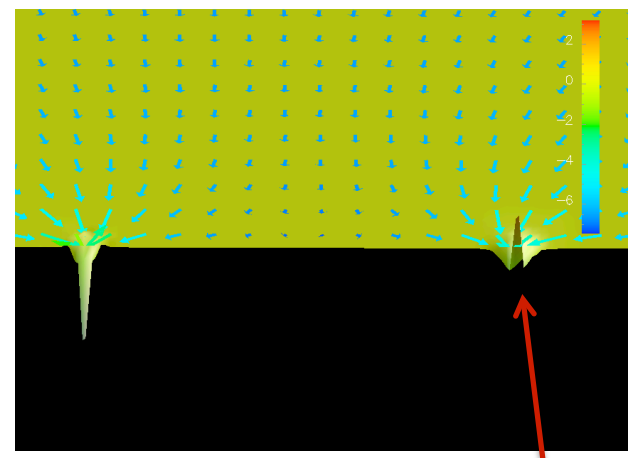
Traditional PPPM

- **Traditional PPPM**
  - **Standard linear weighting of charge to the grid**
  - **2nd or 4th order Poisson solve**
  - **Green's function for removing force**

Div(E) from charge







$$\nabla \cdot E = \frac{8(dx+\zeta)^2}{\pi(dx+2\zeta)(3dx+2\zeta)(5dx^2+8dx\zeta+4\zeta^2)}$$

Charge removed from field

<u>Large residual field</u>

Better Particle Weighting Field

- **Compute electrostatic field on Yee edges using Green's function**

$$E_G\left(i, j+\frac{1}{2}\right) = q(y-y_0)\Big/4\pi\epsilon(r^2+\delta)$$

- **Make irrotational**

$$\sum_{\text{For all Cells}} E_G\left(i+\frac{1}{2}, j\right) + E_G\left(i+1, j+\frac{1}{2}\right) - E_G\left(i+\frac{1}{2}, j+1\right) - E_G\left(i, j+\frac{1}{2}\right) = 0$$

- **Take the discrete divergence, assign to charge**

$$\rho(i,j) = \frac{E_G\left(i-\frac{1}{2}, j\right) - E_G\left(i+\frac{1}{2}, j\right) + E_G\left(i, j-\frac{1}{2}\right) - E_G\left(i, j+\frac{1}{2}\right)}{dx}$$

- **Solve Poisson's equation**

$$\nabla^2\phi_h(i,j) = \rho(i,j)\big/\epsilon$$

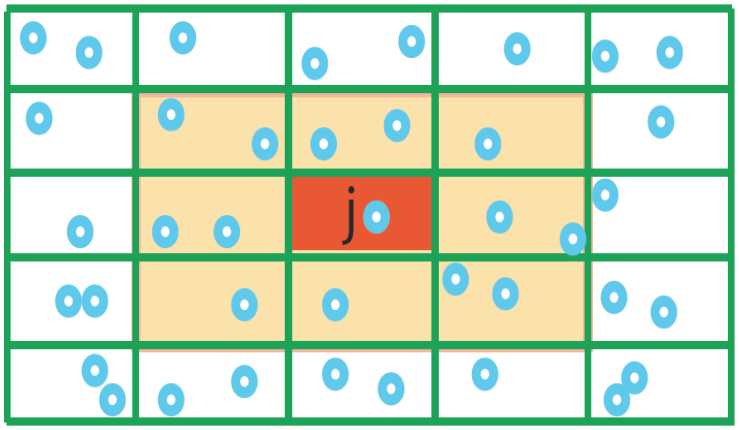
- **Compute discrete E field**

$$E_h\left(i+\frac{1}{2}, j\right) = \frac{\phi_h(i+1,j) - \phi_h(i,j)}{dx}$$

- **This produces an E_h identical to E_G therefore local forces can be subtracted**

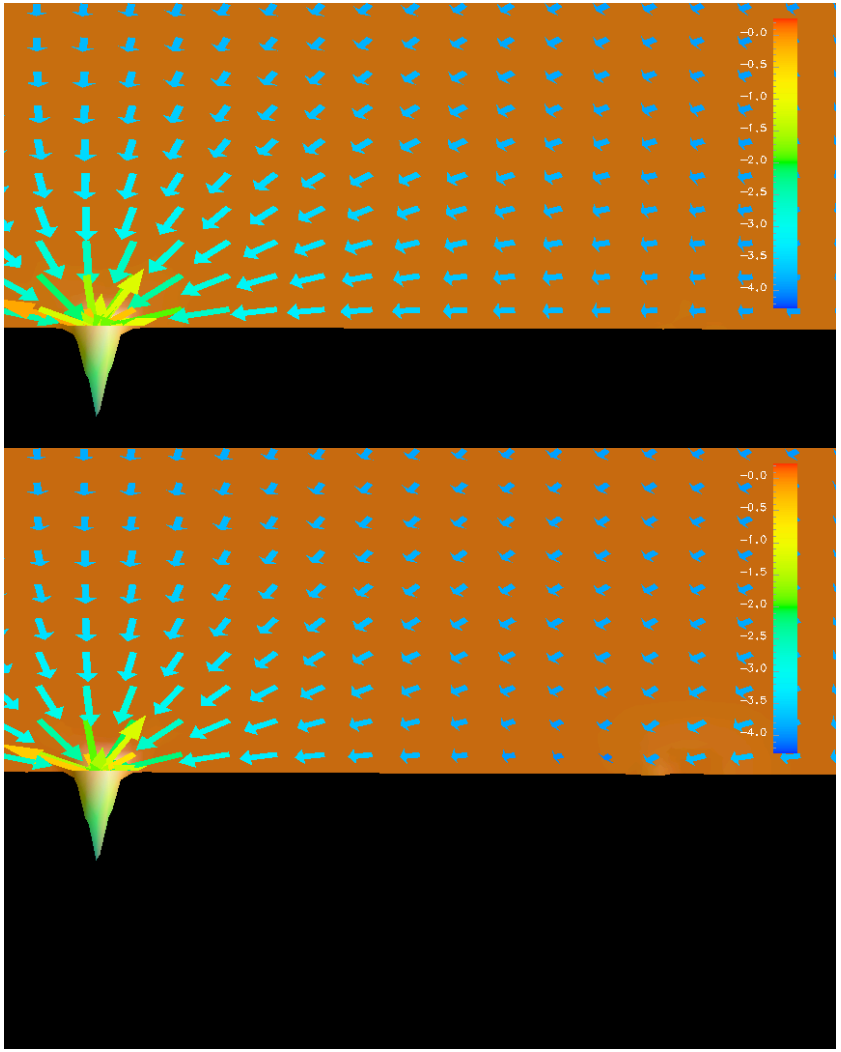
Implementation of Better Weighting

- Two steps are computationally intractable
  - The weighting extends beyond a local range
  - Making fields irrotational is expensive
- Solution
  - Have a finite cutoff radius
    - One cell in picture to right
  - Fields on green edges
  - Densities at nodes touching yellow region
  - Projection to non-rotational space is a onetime matrix inversion and fast multiplication



Electric Field and Divergence as Function of Weighting Radius

100



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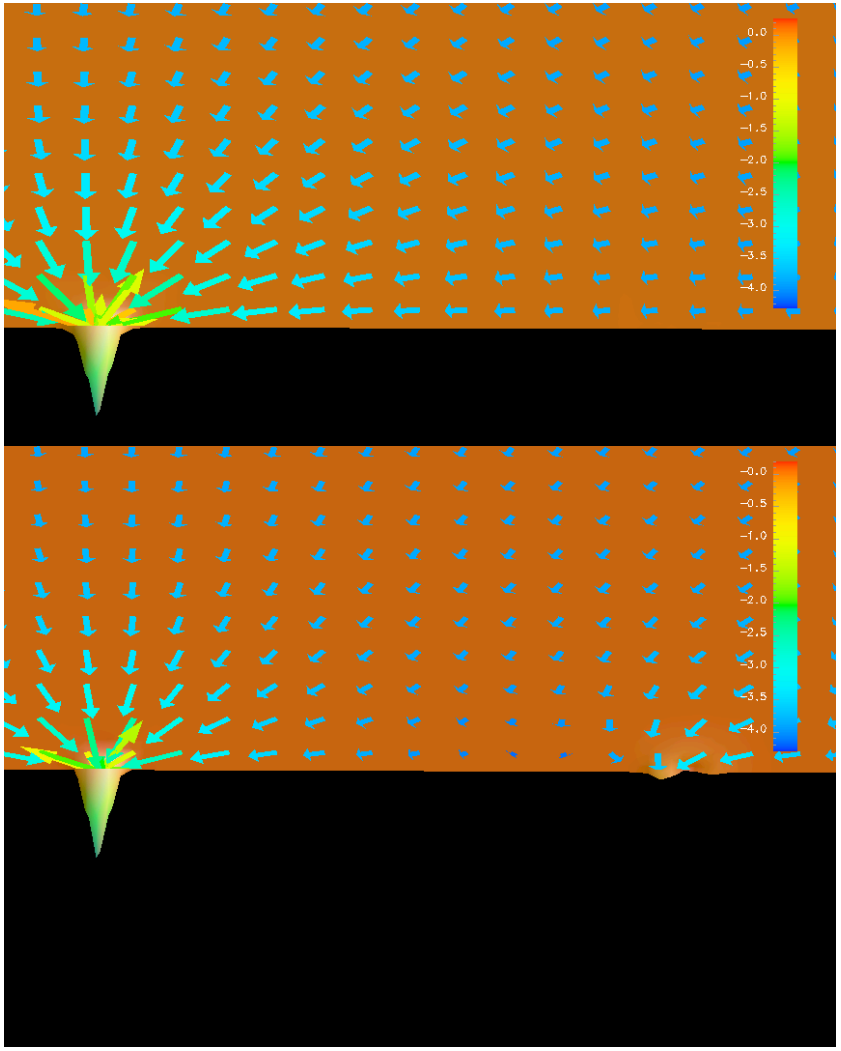

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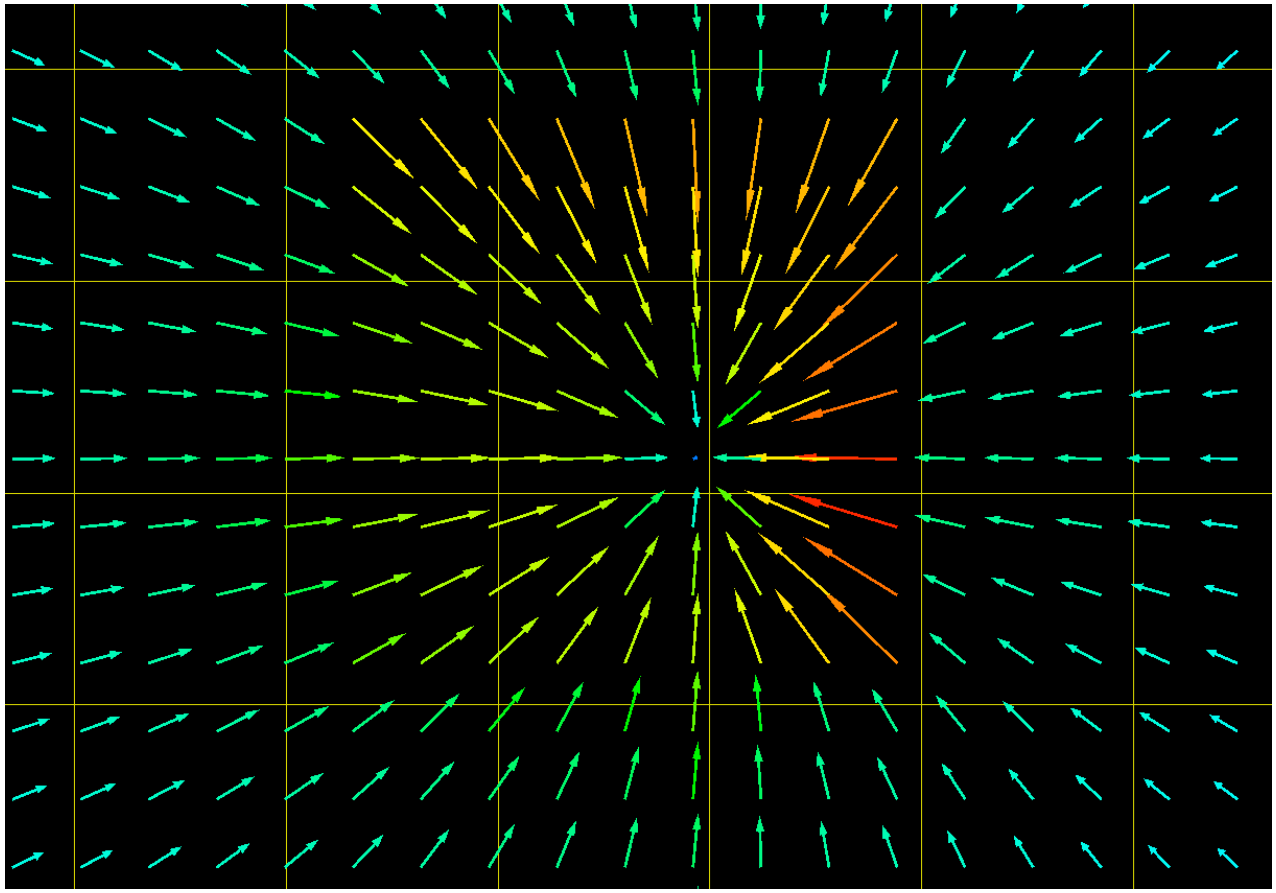
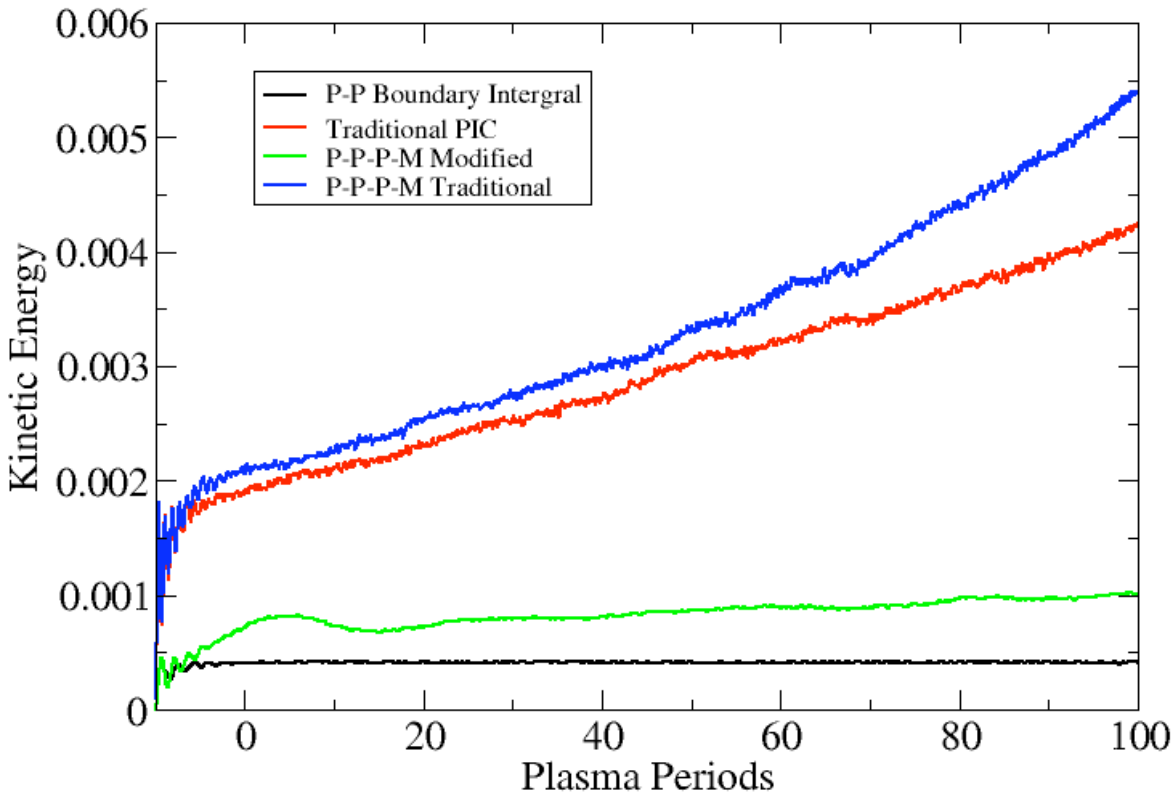
Sub-Grid Resolution

- **Plot shows the potential grid and the sub-grid resolution provided by the PPPM**



Heating Results

- Kinetic Energy for four method with
  - 1000 parts
  - 128x128 grid
  - dt=0.05Wp



Electromagnetic PPPM

- Extending the algorithm to solve electromagnetics
  - Break standard current weighting scheme into two parts
    - Rotational part and electrostatic part
  - Replace electrostatic part with modified charge weighting, and compute current $J = \partial\rho / \partial t$
  - Local subtraction should still cancel out electrostatic fields
  - Electromagnetic fields still transmitted through the grid

Summary

- The grid causes false heating of the particles
- Performing the particle-particle calculations reduces the amount of heating
- PPPM is designed to resolve this issue, however, suffers from a self force
- Modified charge weighting removes the self force
- If weighting scheme is made compact through truncation much of the self force is removed