Kinetic Plasma Simulation in the MOOSE Framework: Verification of Electrostatic Particle In Cell Capabilities

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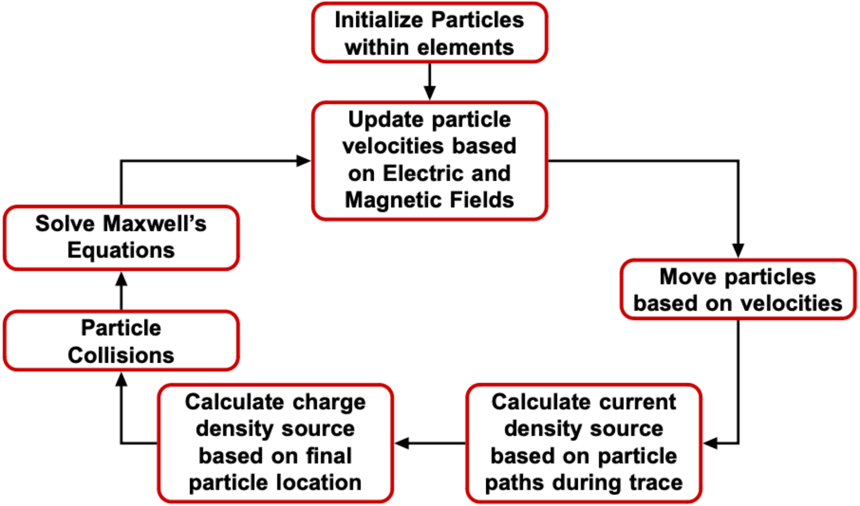
Motivation

- In recent years, Fusion energy has gained significant interest and funding.
  - Several fusion energy companies are targeting 2030 as the goal for energy generation.
- However, the design plasma facing components (PFCs) is particularly challenging.
  - PFCs exist in a highly coupled multiphysics environment.
  - Experimental data is rare and expensive.
- In order to meet this challenge scalable multiphysics frameworks are required[1].
  - To address this need kinetic plasma modeling capabilities are being developed as a part of the Fusion ENergy Integrated multiphys-X (FENIX) framework.
  - FENIX benefits from all of the flexiblity and scalability of the MOOSE framework.

[1] Carter, T. et al. 2020.

Particle-In-Cell

- Individual computational particles that represent multiple physical particles are tracked.
    - In FENIX this is build on MOOSE's Ray Tracing module.
- Maxwell's equations are solved based on computational particle positions and path.
    - Typically, finite difference solvers with uniform grids are used.
- FENIX is built on top of the MOOSE framework, this enables
    - Finite element based simulations.
    - 1D,2D, or 3D simulations.
    - Non-uniform domain discritizations.
    - Massive parallelization.
    - Rhobust software quality assurance and testing.
    - Coupling with other physics modules.


Initialize Particles within elements
Update particle velocities based on Electric and Magnetic Fields
Move particles based on velocities
Calculate current density source based on particle paths during trace
Calculate charge density source based on final particle location
Particle Collisions
Solve Maxwell's Equations

Verification Motivation

- Rigorous verification denomstrates the proper implemenation of FENIX's PIC capabilities.
    - Gives researchers a higher degree of confidence when exploring new devices/regimes.
    - Enables an easier road for licensing of designs based on FENIX calculations.
- PIC is heavily utilized by the Low Temperature Plasma (LTP) community.
    - Verification studies are not prioritized and are rarely published in the LTP community[2].

[2]Alves, L. L. et al. *Plasma Sources Science and Technology*. 2023.

Particle Description

- FENIX treats computational particles as point particles.

$$f(\vec{r}, \vec{v}, t) = \sum_{i=1}^{N} \omega_i q_i \delta\left(\vec{r} - \vec{r}_i(t)\right) \delta\left(\vec{v} - \vec{v}_i(t)\right) \quad (1)$$

- f : Particle distribution function.
- N : Computational particle count.
- ω_i : Computational particle weight.
- q_i : Computational particle charge.
- δ : Dirac Delta Function.
- $\vec{r}$: Particle position.
- $\vec{v}$: Particle velocity
- t : Simulation time

Single Particle Motion

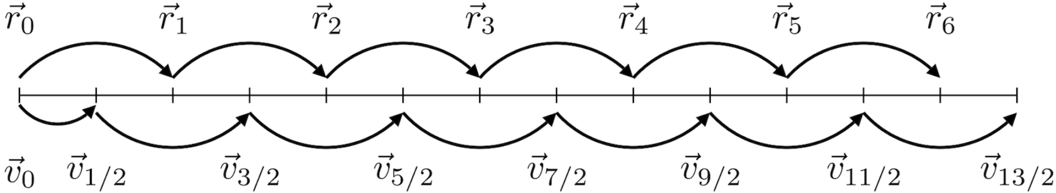
The equations of motion are solved for each computational particle, individually.

$$\frac{d\vec{r}}{dt} = \vec{v} \tag{2}$$

$$\frac{d\vec{v}}{dt} = \frac{q}{m}\left(\vec{E} + \vec{v} \times \vec{B}\right) \tag{3}$$

$\vec{E}$ and $\vec{B}$ represent the electric and magnetic fields repsectively.

Leapfrog Particle Stepping



Boris Stepping

Particles are stepped through electromagnetic fields using the boris algorithm[3].

$$\vec{v}^{-} = \vec{v}_n + \frac{q}{m}\vec{E}_n\frac{\Delta t}{2} \tag{4}$$

$$\vec{v}^{+} = \vec{v}^{-} + \vec{v}^{\,\prime} \times \vec{s} \tag{5}$$

$$\vec{v}^{\,\prime} = \vec{v}^{-} + \vec{v}^{-} \times \vec{l} \tag{6}$$

$$\vec{l} = \frac{q}{m}\vec{B}_n\Delta t \tag{7}$$

$$\vec{s} = \frac{2\vec{l}}{1 + \vec{l}\cdot\vec{l}} \tag{8}$$

$$\frac{\vec{v}^{+} - \vec{v}^{-}}{\Delta t} = \frac{q}{m}\left(\vec{v}^{+} + \vec{v}^{-}\right) \times \vec{B}_n \tag{9}$$

$$\vec{v}_{n+1} = \vec{v}^{+} + \frac{q}{m}\vec{E}_n\frac{\Delta t}{2} \tag{10}$$

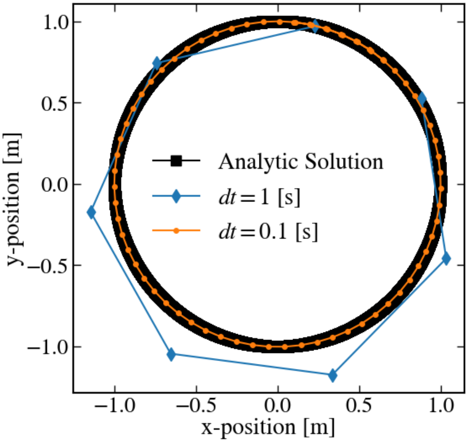
$\vec{E}$ and $\vec{B}$ represent the electric and magnetic fields respecitvely, and n is denotes the number of the current timestep.

[3] Boris, J. P. et al. *Proc. Fourth Conf. Num. Sim. Plasmas.* 1970.

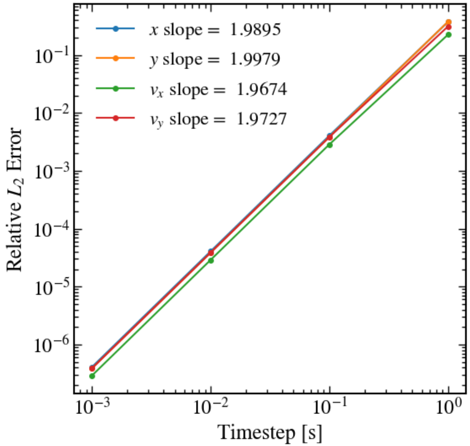
Cyclotron Motion

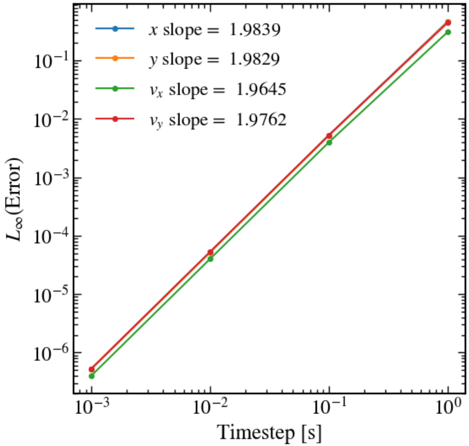
- A single particle in the magnetic field given by $\vec{B} = 1\hat{z}$
- Particle Properties:
  - $q = 1$ [C]
  - $m = 1$ [kg]
  - $\omega = 1 \left[\frac{1}{\mathrm{m}}\right]$
  - $v_\perp = 1 \left[\frac{\mathrm{m}}{\mathrm{s}}\right]$

$v_\perp$ is the magnitude of the velocity perpendicular to the magnetic field.



Cyclotron Motion Errors





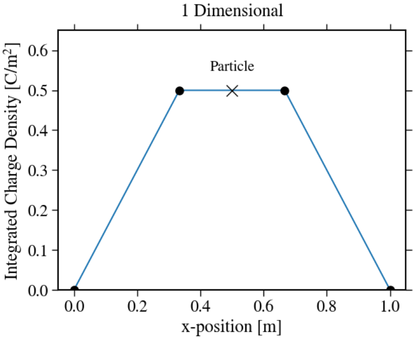
Charge Density Calculation

$$\langle \rho(\vec{r}), \phi_i(\vec{r}) \rangle = \sum_{j=1}^{N_i} q_j \omega_j \psi\,(\vec{r} - \vec{r}_j) \tag{11}$$

- Solving for the electric field requires solving Poisson's equation.

$$\nabla^2 \phi = \frac{\rho}{\varepsilon_0} \tag{12}$$

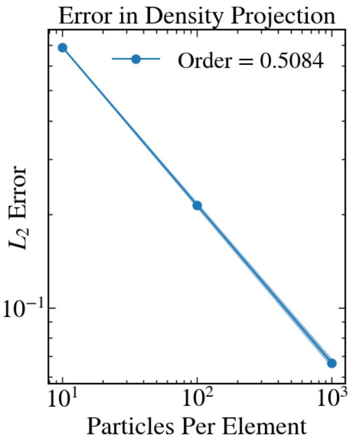
- This requies evaluating the inner product of the computational charge distribution and the basis functions, ψ



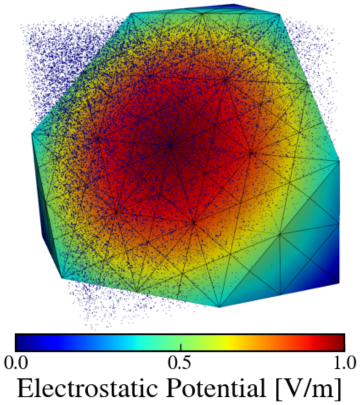
Particle Initialization

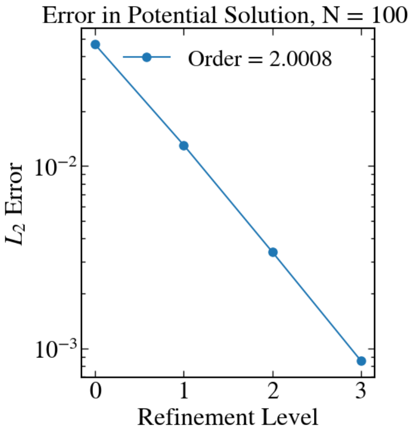
- A widely used initial condition for particles is a uniform distribution throughout the domain.
  - In FENIX each elements volume is uniformly sampled.
- Initial particle position is a randomly sample quantity so the error in the projection of the particle density onto the mesh follows a standard sample variance.

$$S^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \overline{x})^2 \qquad (13)$$



Electrostatic Potential





Current Density

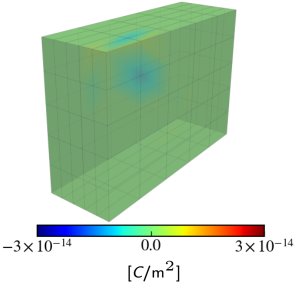
$$\left\langle \vec{J}_{n+1/2}\left(\vec{r},t\right), \vec{\psi}(\vec{r}) \right\rangle = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \sum_{i=1}^{N} q_i \omega_i \vec{v}_i(t)\cdot\vec{\psi}(\vec{r}_i(t))dt \quad (14)$$

- Current density is often a parameter of interest and is required to solve the full set of Maxwell's equations

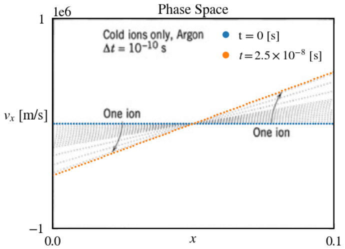
$$\frac{\partial\rho}{\partial t} = -\boldsymbol{\nabla}\cdot\vec{J} \quad (15)$$

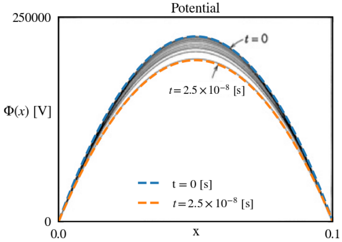
$$\langle\rho_1-\rho_0,\psi\rangle = \Delta t\left\langle \vec{J}_{n+1/2}, \boldsymbol{\nabla}\psi\right\rangle \quad (16)$$

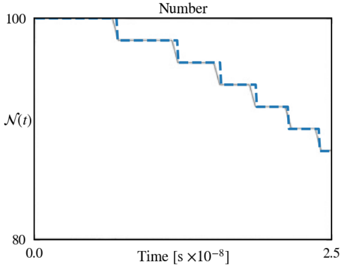
$<\rho_1-\rho_0,\psi> - \Delta t <\vec{J}_{1/2},\nabla\psi>$



Lieberman Benchmark







A simple collisionless single particle simulation demonstration from Lieberman[4] was replicated and documented as a training example.

[4] Lieberman, M. A. et al. *Principles of plasma discharges and materials processing*.

Future Work

- Currently work is underway to demonstrate some canonical kinetic plasma instabilities:
  - Landau Damping
  - Two-stream instability
  - Dory–Guest–Harris
- Replication of an analytic solution applicable to both fluid and kinetic simulations[5].
- Particle-Particle collisions will be implemented.
- Computing heatfluxes from particle fluxes.
- Coupling with other MOOSE applications.

[5] Lafleur, T. *Plasma Sources Science and Technology*. 2022.

Summary

- The fundamental capabilities for PIC have been verified.
- FENIX will enable FEM PIC simulations within the MOOSE frameowork.
- FENIX can perform simulations in 1D, 2D, and 3D.
- FENIX will be one of the only openly available massively parallel kinetic plasma simulation tools.
- Rhobust verification enables FENIX to be able to utilized as an engineering tool.