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

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Pacific Basin Nuclear Conference 2024

Supported by the Idaho National Laboratory, Laboratory Directed Research & Development (LDRD) Program

Motivation

- In recent years, Fusion energy has gained significant interest and funding.
    - Several companies are targeting 2030 for energy generation.
- However, designing plasma facing components (PFCs) is particularly challenging.
    - PFCs exist in uniquely extreme environments.
    - Experimental data is rare and expensive.

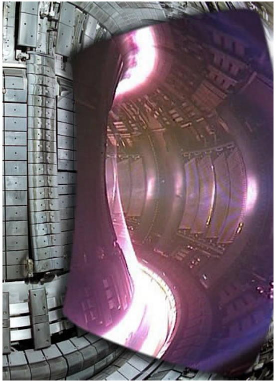


Figure 1: Interior of the Joint European Torus. Photo: CCFE, JET

Modeling Needs

- To facilitate the design of PFCs multiphysics simulation frameworks are required[2].
- Plasma material interactions in fusion devices are complex and multiphysics effects are significant.
- Typically fluid plasma models make assumptions about the velocity distributions which can be invalid in the fusion pasma edge.
    - As a result higher fidelity plasma models should be used.

[2] Carter, T. et al. *Powering the future: Fusion & plasmas*. 2020.

FENIX

- To address modeling needs the Fusion ENergy Integrated multiphys-X (FENIX) framework is being developed.
  - FENIX is built on top of the MOOSE framework.
- FENIX utilizes a Finite Element based Particle-In-Cell (PIC) method for modeling the edge plasma.
  - Individual computational particles that represent multiple physical particles are tracked.
  - In FENIX this is built on MOOSE's Ray Tracing module.

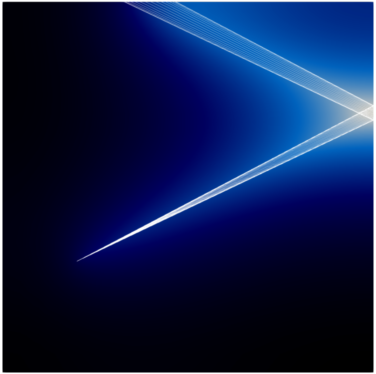
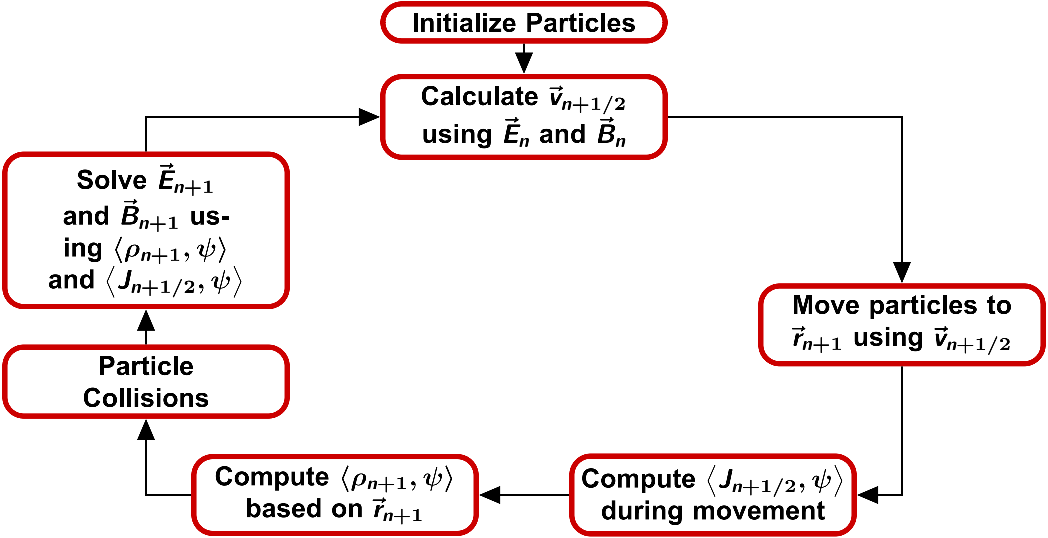


Figure 2: Example Cone Ray Study


Initialize Particles
Calculate $\vec{v}_{n+1/2}$ using $\vec{E}_n$ and $\vec{B}_n$
Move particles to $\vec{r}_{n+1}$ using $\vec{v}_{n+1/2}$
Compute $\langle J_{n+1/2}, \psi \rangle$ during movement
Compute $\langle \rho_{n+1}, \psi \rangle$ based on $\vec{r}_{n+1}$
Particle Collisions
Solve $\vec{E}_{n+1}$ and $\vec{B}_{n+1}$ using $\langle \rho_{n+1}, \psi \rangle$ and $\langle J_{n+1/2}, \psi \rangle$

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[3].

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

Particle Description

- FENIX treats computational particles as point particles.

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

- 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

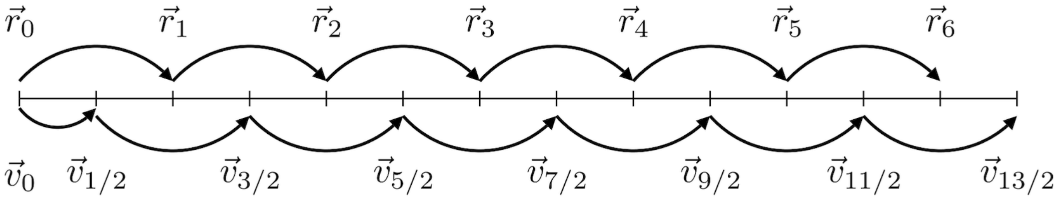
The equations of motion are solved for each computational particle, individually.

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

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

- $\vec{E}$ and $\vec{B}$ represent the electric and magnetic fields repsectively.
- The standard methods for doing this numerically are the Leapfrog method and the Boris method.

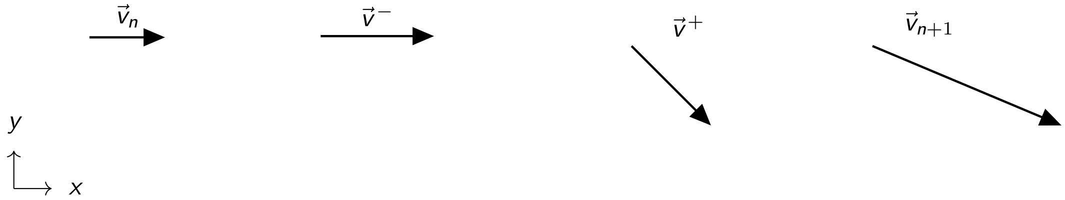
Leapfrog Particle Stepping



$$\vec{r}_{n+1} = \vec{r}_n + \vec{v}_{n+1/2}\Delta t$$

Boris Stepping

$\vec{E} = E_0 \hat{x}$ $\vec{B} = B_0 \hat{z}$



1: Initial Velocity at step n

2: Accelerate with $\vec{E}$ through $\Delta t/2$

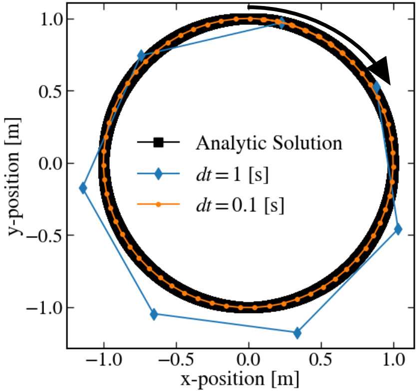
3: Rotate with $\vec{B}$ through Δt

4: Accelerate with $\vec{E}$ through $\Delta t/2$

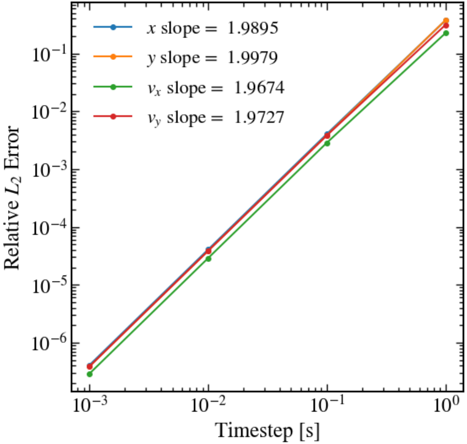
Cyclotron Motion

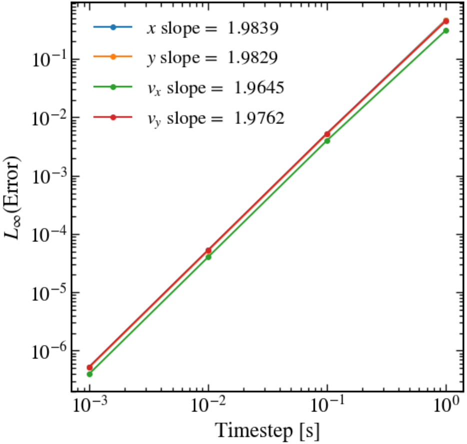
- A single particle in the magnetic field given by $\vec{B} = \hat{z}$ [T]
- Particle Properties:
  - $q = 1$ [C]
  - $m = 1$ [kg]
  - $\omega = 1 \left[\frac{1}{\mathrm{m}}\right]$
  - $v_\perp = 1 \left[\frac{\mathrm{m}}{\mathrm{s}}\right]$

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



Cyclotron Motion Errors





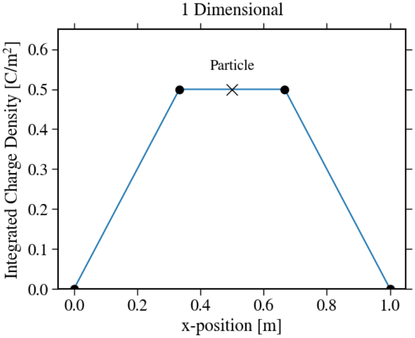
Charge Density Calculation

$$\langle \rho_n, \psi \rangle = \sum_{j=1}^{N_i} q_j \omega_j \psi \left(\vec{r} - \vec{r}_j(t_n) \right) \quad (1)$$

- When using electrostatics the electric field can be calculated via Poisson's equation.

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

- The variational formulation requies evaluating the inner product of the computational charge distribution and the basis functions, ψ



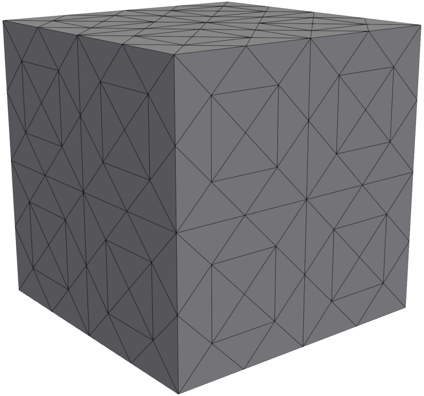
Verification Problem

- Represent a uniform charge density profile with computational partilces.

$$\frac{\rho}{\varepsilon_0} = 6\left[\frac{\mathrm{V}}{\mathrm{m}^2}\right]$$

- Solve for an electric potential consistent with the charge density profile.

$$\phi(x, y, z) = x(1 - x) + y(1 - y) + z(1 - z) \;\; [\mathrm{V}]$$



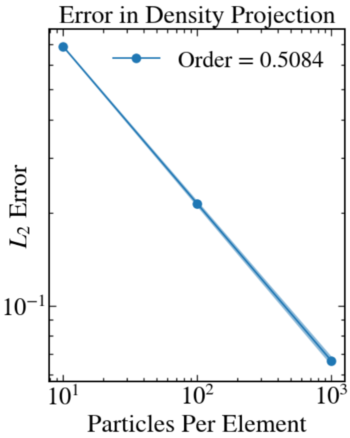
Charge Density

- Weights are assigned based on target number density ρ_n element volume V_E and particles per element, N.

$$\omega = \frac{\rho_n V_E}{N}$$

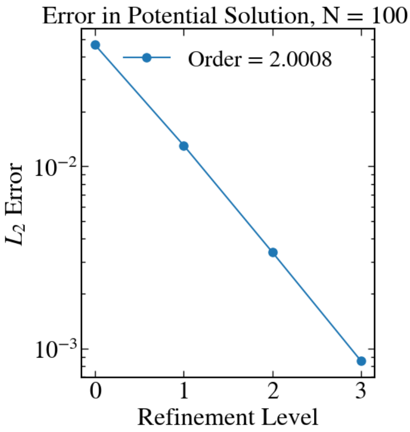
- Position are randomly sampled so the error in the projection of the density onto the mesh follows a sample variance.

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



Electrostatic Potential

- In this example first order finite element basis functions are used.
  - These basis functions have second order convergence.
  - Using particles as the source terms should not effect the spatial convergence rate of the system.



Current Density

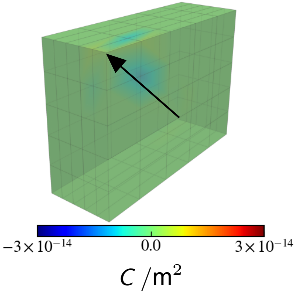
$$\left\langle \vec{J}_{n+1/2}\left(\vec{r},t\right), \vec{\psi}(\vec{r})\right\rangle = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \sum_{i=1}^{N} q_i \omega_i \vec{v}_i(t)\cdot\vec{\psi}(\vec{r}_i(t))dt$$

- Time averaging the current density ensures charge conservation[4,5].
    - Conservation is required to ensure Maxwell's equations are well posed.

$$\frac{\partial\rho}{\partial t} = -\boldsymbol{\nabla}\cdot\vec{J}$$

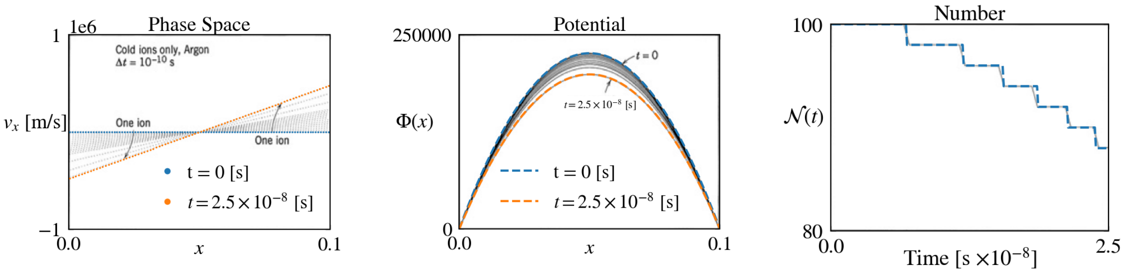
$$\langle \rho_1 - \rho_0, \psi\rangle = \Delta t\left\langle \vec{J}_{n+1/2}, \boldsymbol{\nabla}\psi\right\rangle$$

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



[4]Eastwood, J. W. *Computer Physics Communications*. 1991.
[5]Pinto, M. C. et al. *Comptes Rendus Mecanique*. 2014.

Lieberman Benchmark



A simple collisionless single particle simulation demonstration from Lieberman[6] was replicated and documented as a training example.

[6] 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[7].
- Direct Simulaiton Monte Carlo collisions will be implemented.
- Computing heatfluxes from particle fluxes.
- Coupling with other MOOSE applications.

[7] 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.
- Rhobust verification enables FENIX to be able to utilized as an engineering tool.
- Once DSMC has been implemented FENIX will be capable of modeling the conditions in fusion plasma edges.