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

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Changing the World's Energy Future

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Motivation

- Fusion energy has gained significant interest and funding.
  - Several companies are targeting 2030 for energy generation.
  - Increased urgency for resolving engineering challenges.
- Designing plasma facing components (PFCs) is particularly challenging.
  - PFCs exist in uniquely extreme environments.
  - High ion, neutron, and heat fluxes.
  - Experimental data is rare and expensive.

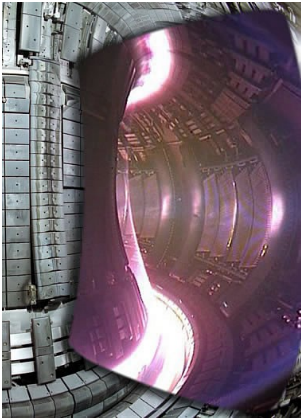


Figure 1: Photo: CCFE, JET

Computational Modeling for Fusion Engineering

- PFCs exist in multiphysics environments.
  - Plasma material interactions are complex.
  - Multiphysics simulation frameworks are required[2].
- Several fluid plasma modeling programs exist.
  - Fluid models make assumptions about particle velocity distributions.
  - These assumptions are not valid in the fusion plasma edge.
  - Higher fidelity plasma models should be used.

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

FENIX Framework

- FENIX - Fusion ENergy Integrated multiphys-X.
  - Open Source.
  - Built upon the MOOSE framework.
- Kinetic plasma capabilities within FENIX.
  - Finite Element based particle-in-cell (PIC) for modeling the edge plasma.
  - Computational particles represent multiple physical particles.
  - Built on MOOSE's Ray Tracing module[2].

[2] Harbour, L. *MOOSE Ray Tracing Module, https://mooseframework.inl.gov/modules/ray_tracing*.

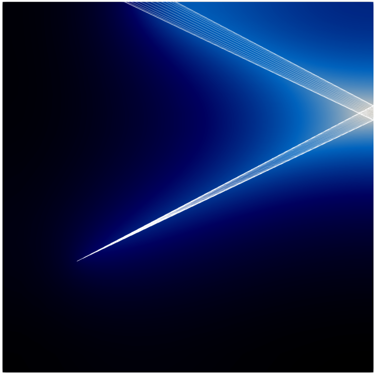
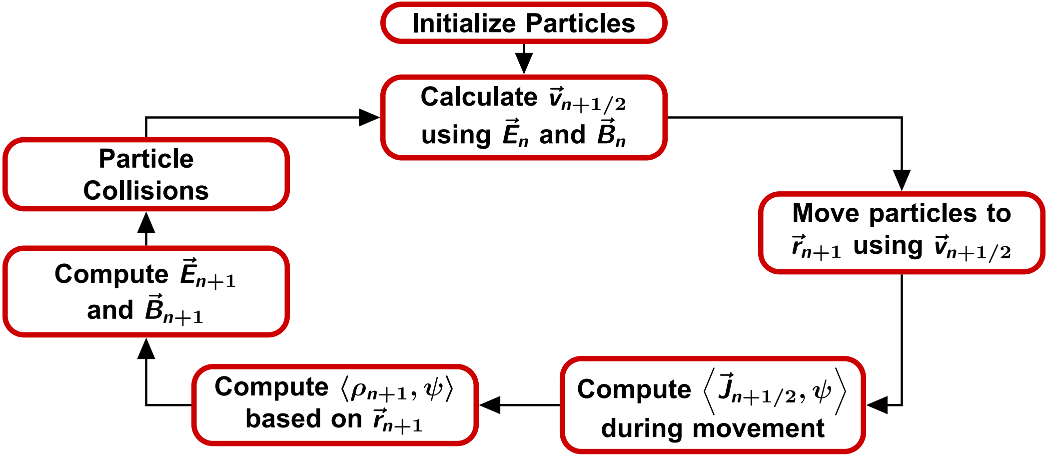


Figure 2: Example Cone Ray Study



$\vec{J}$: Current Density
ρ : Charge Density

ψ : Test Function

$\vec{E}$: Electric Field
$\vec{B}$: Magnetic Field

$\vec{v}$: Velocity
$\vec{r}$: Position

Verification

- Verification:
  - Rigorously demonstrating a model has been implemented correctly.
- Rigorous demonstration of FENIX's PIC capabilities is important.
  - 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.
  - There is not yet a standard verification suite for PIC.[3].

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

Particle Description

- FENIX treats computational particles as point particles.

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

- f : Particle distribution function.
- N : Computational particle count.
- ω_i : Computational particle weight.
- 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.

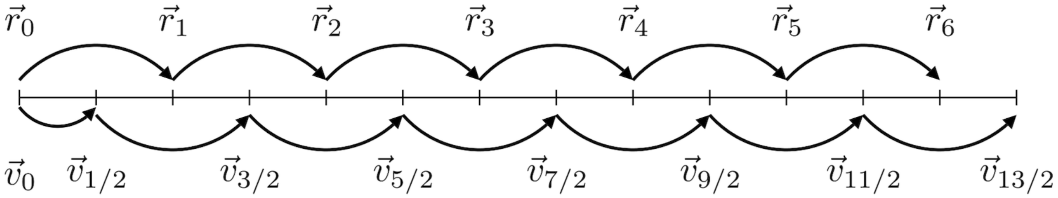
$$\frac{d\,\vec{r}}{dt} = \vec{v}$$

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

- $\vec{E}$ and $\vec{B}$ represent the electric and magnetic fields respectively.
- Established methods for solving these equations numerically are utilized:
  - Leapfrog Method[4]
  - Boris Method[5]

[4] Birdsall, C. K. et al. *Plasma physics via computer simulation*.
[5] Boris, J. P. et al. *Proc. Fourth Conf. Num. Sim. Plasmas*. 1970.

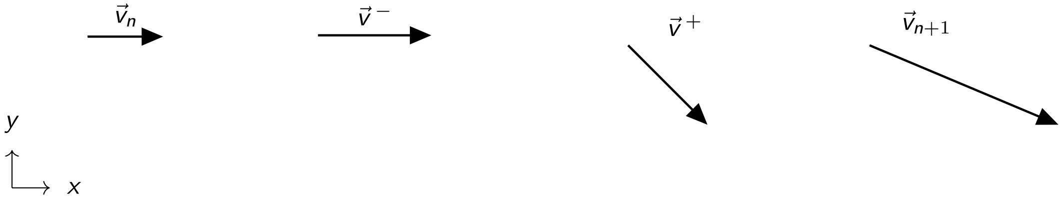
Particle Stepping: Leapfrog Method



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

Particle Stepping: Boris Algorithm

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



1: Initial Velocity at step n

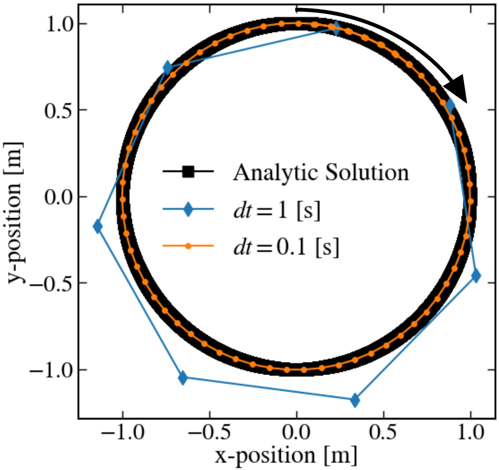
2: Accelerate with $\vec{E}$ through $\Delta t/2$

3: Rotate with $\vec{B}$ through Δt

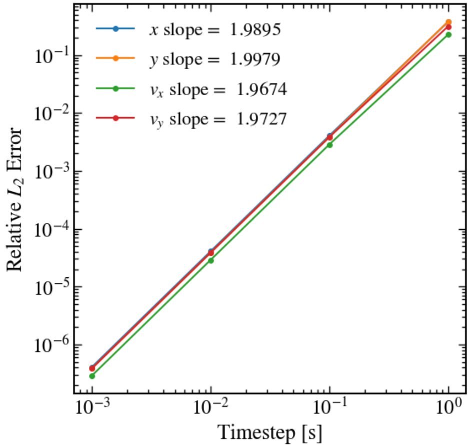
4: Accelerate with $\vec{E}$ through $\Delta t/2$

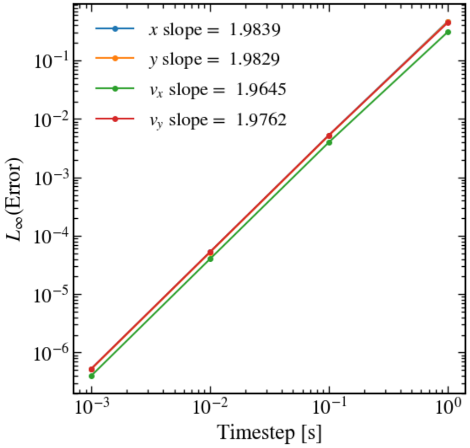
Cyclotron Motion

- Boris Method Verification Problem.
- A single particle in the magnetic field given by $\vec{B} = \hat{z}$ [T]
- Particle Properties:
  - $q = 1$ [C]
  - $m = 1$ [kg]
  - $\omega = 1$ [1/m]
  - $v_\perp = 1$ [m/s]
- $v_\perp$ is the magnitude of the velocity perpendicular to the magnetic field.



Cyclotron Motion Errors





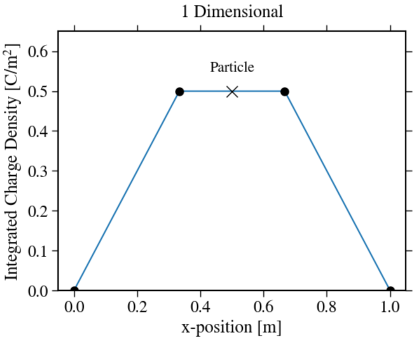
Charge Density Calculation from Particles

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

- The electrostatic 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



Electrostatic Verification Problem

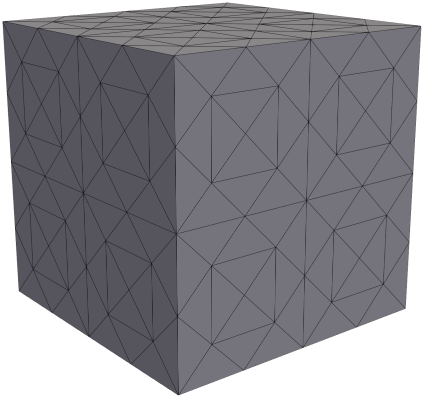
- Represent a uniform charge density profile with computational particles.

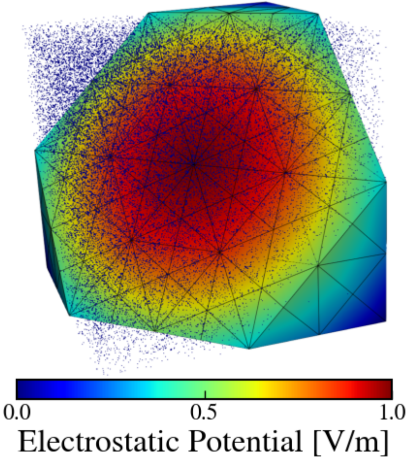
$$\frac{\rho}{\varepsilon_0} = 6 \left[\frac{\mathrm{V}}{\mathrm{m}^2}\right]$$

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

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

Electrostatic Verification Problem





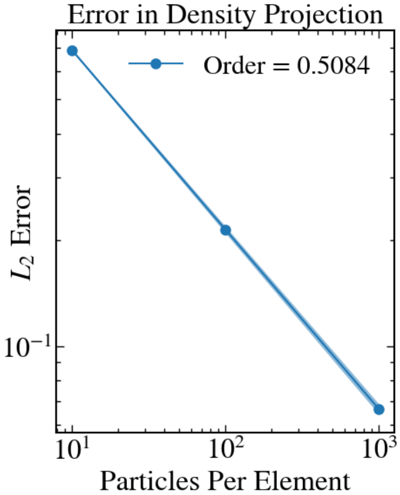
Charge Density

- Weights are assigned based on:
  - Target number density n.
  - Element volume V_E.
  - Particles per element N.

$$\omega = \frac{nV_E}{N}$$

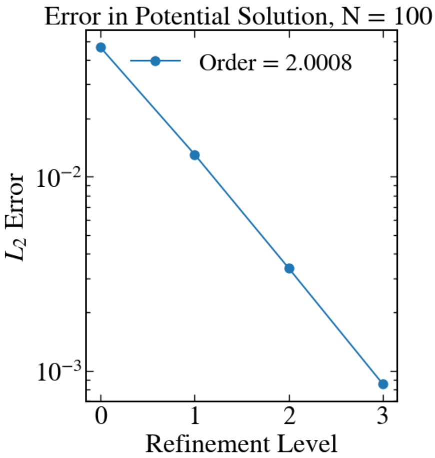
- Particle positions are randomly sampled.
  - Error in the projection of the density follows a sample variance.

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



Electrostatic Potential

- In this example first order finite element basis functions are used.
  - These basis functions have second order convergence.
- Particle source terms should not effect the spatial convergence rate.
- A fixed number of particles per element was used $N = 100$



Current Density

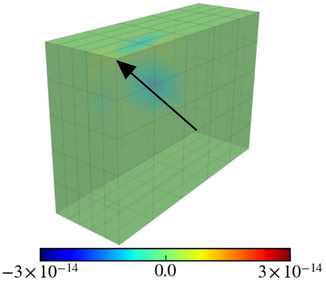
$$\left\langle \vec{J}_{n+1/2}(\vec{r}, t), \vec{\psi}(\vec{r}) \right\rangle = \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \sum_{i=1}^{N} q_i \, \omega_i \vec{v}_i(t) \cdot \vec{\psi}(\vec{r}_i(t)) dt$$

- Time averaging the current density ensures charge conservation[6,7].
    - Conservation is required to ensure Maxwell's equations are well posed.

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

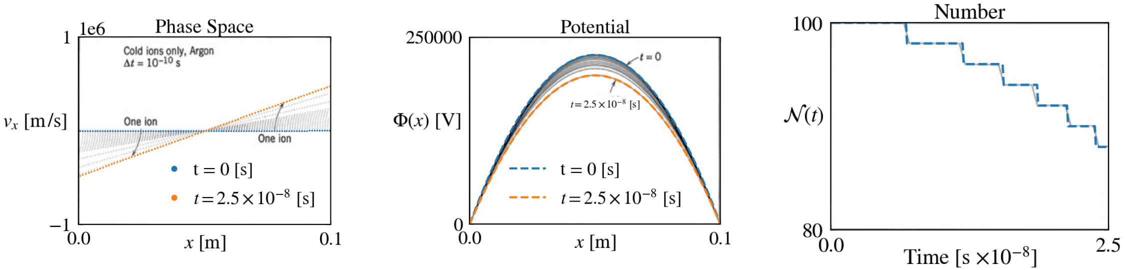
$$\langle \rho_1 - \rho_0, \psi \rangle = \Delta t \left\langle \vec{J}_{n+1/2}, \nabla \psi \right\rangle$$

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



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

Ion Motion Benchmark



- Collisionless single particle simulation demonstration from Lieberman[8].
- Available as a training example in the FENIX documentation.

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

Future Work

- Currently work is underway to verify coupled plasma physics via several textbook phenomena:
  - Landau Damping (Electrostatic)
  - Two-stream instability (Electrostatic)
  - Dory–Guest–Harris instability (Magnetostatic)
- Replication of an analytic solution applicable to both fluid and kinetic simulations[9].
- Direct Simulation Monte Carlo collisions will be implemented.
- Computing heat fluxes from particle fluxes.
- Coupling with other MOOSE modules/applications.
  - Electromagnetics Module.

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

Concluding Remarks

- 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.