

A CODE-VERIFICATION PLAN FOR COLLISIONAL PLASMA DYNAMICS

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ASME Verification, Validation, and Uncertainty Quantification Symposium
April 9–10, 2025

Outline

- Introduction
- Particle-in-Cell Method
- Existing Work
- Proposed Approach
- Summary

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 - Plasma Dynamics
 - Verification and Validation
 - Code Verification
 - Code-Verification Goal
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Plasma Dynamics

- Plasma dynamics important for many scientific and engineering applications
 - Fusion energy research – stable conditions for nuclear fusion
 - Space physics – interactions between solar wind and planetary magnetospheres
 - Accelerator physics – particle beam dynamics for research, medicine, industry
 - Semiconductor manufacturing – plasma-assisted processes for circuits
- Plasma dynamics commonly modeled by particle-in-cell (PIC) method
 - Maxwell's equations to compute electromagnetic fields on grid
 - Equations of motion due to Lorentz force for large number of charged particles
 - Fields interpolated to particles, particle properties distributed to grid

Verification and Validation

Credibility of computational physics codes requires verification and validation

- **Validation** assesses how well models represent physical phenomena
 - Compare computational results with experimental results
 - Assess suitability of models, model error, and bounds of validity
- **Verification** assesses accuracy of numerical solutions against expectations
 - *Solution verification* estimates numerical error for particular solution
 - *Code verification* assesses correctness of numerical-method implementation

Discretization Error

Code verification assesses correctness of numerical-method implementation

- Continuous equations are numerically discretized

$$\mathbf{r}(\mathbf{u}) = \mathbf{0} \quad \rightarrow \quad \mathbf{r}_h(\mathbf{u}_h) = \mathbf{0}$$

- Discretization error is introduced in solution

$$\mathbf{e} = \mathbf{u}_h - \mathbf{u}$$

- Discretization error should decrease as discretization is refined

$$\lim_{h \rightarrow 0} \mathbf{e} = \mathbf{0}$$

- More rigorously, should decrease at an expected rate

$$\|\mathbf{e}\| \approx Ch^p$$

- Measuring error requires exact solution – usually unavailable

Manufactured Solutions

Manufactured solutions are popular alternative

- Manufacture an arbitrary solution \mathbf{u}_{MS}
- Insert manufactured solution into continuous equations to get residual term

$$\mathbf{r}(\mathbf{u}_{\text{MS}}) \neq \mathbf{0}$$

- Add residual term to discretized equations

$$\mathbf{r}_h(\mathbf{u}_h) = \mathbf{r}(\mathbf{u}_{\text{MS}})$$

to coerce solution to manufactured solution

$$\mathbf{u}_h \rightarrow \mathbf{u}_{\text{MS}}$$

Code-Verification Goal

- Existing code-verification work
 - Plasma dynamics without collisions: distribution modeled by Vlasov equation
 - Electrostatics (negligible magnetic field influence): Poisson equation
 - 1D-1V, 2D-2V
- Our code-verification goal
 - Plasma dynamics with collisions: distribution modeled by Boltzmann equation
 - Electromagnetics: Maxwell's equations
 - 3D-3V

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 - Overview
 - Equations of Motion for Charged Particles
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Overview

- Place weighted computational particles randomly in phase space (according to distribution function)
- Interpolate particle charge onto spatial mesh nodes
- Solve Maxwell's equations on spatial mesh for electromagnetic fields
- Interpolate fields onto particles
- For each particle, integrate equations of motion

Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle:

$$\frac{dw_p}{dt} = \frac{(\delta f / \delta t)_{\text{coll}}}{f(\mathbf{x}_p(0), \mathbf{v}_p(0), 0)}, \quad \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad \frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_p}{m}$$

- w_p is computational particle weight, $(\delta f / \delta t)_{\text{coll}}$ is numerical collision term
- $f(\mathbf{x}_p, \mathbf{v}_p, t)$ is particle distribution function
- $\mathbf{F}_p = \frac{q}{m}(\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ is Lorentz force
- \mathbf{E} and \mathbf{B} are electric and magnetic fields
- m and q are species mass and charge

Increasing N_p , distribution function evolution approaches Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

- $(\partial f / \partial t)_{\text{coll}}$ is analytical collision term

Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle (**collisionless**):

$$\frac{dw_p}{dt} = \frac{\cancel{(\delta f / \delta t)}_{\text{coll}}^0}{f(\mathbf{x}_p(0), \mathbf{v}_p(0), 0)}, \quad \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad \frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_p}{m}$$

- w_p is computational particle weight, $(\delta f / \delta t)_{\text{coll}}$ is numerical collision term
- $f(\mathbf{x}_p, \mathbf{v}_p, t)$ is particle distribution function
- $\mathbf{F}_p = \frac{q}{m}(\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ is Lorentz force
- \mathbf{E} and \mathbf{B} are electric and magnetic fields
- m and q are species mass and charge

Increasing N_p , distribution function evolution approaches ~~Boltzmann~~ ^{Vlasov} equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \cancel{\left(\frac{\partial f}{\partial t}\right)_{\text{coll}}}^0$$

- $(\partial f / \partial t)_{\text{coll}}$ is analytical collision term

Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle (**electrostatic**):

$$\frac{dw_p}{dt} = \frac{(\delta f / \delta t)_{\text{coll}}}{f(\mathbf{x}_p(0), \mathbf{v}_p(0), 0)}, \quad \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad \frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_p}{m}$$

- w_p is computational particle weight, $(\delta f / \delta t)_{\text{coll}}$ is numerical collision term
- $f(\mathbf{x}_p, \mathbf{v}_p, t)$ is particle distribution function
- $\mathbf{F}_p = \frac{q}{m} (\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ is Lorentz force
- \mathbf{E} and \mathbf{B} are electric and magnetic fields
- m and q are species mass and charge

Increasing N_p , distribution function evolution approaches Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

- $(\partial f / \partial t)_{\text{coll}}$ is analytical collision term

Collision Term

Analytical collision term for binary elastic collisions is 6D integral

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int_{-\infty}^{\infty} \int_{\Omega} [f(\mathbf{x}, \tilde{\mathbf{v}}, t) f(\mathbf{x}, \tilde{\mathbf{v}}', t) - f(\mathbf{x}, \mathbf{v}, t) f(\mathbf{x}, \mathbf{v}', t)] g \sigma(g, \Omega) d\Omega d\mathbf{v}'$$

- \mathbf{v} and \mathbf{v}' are pre-collision velocities of two particles
- $\tilde{\mathbf{v}}$ and $\tilde{\mathbf{v}}'$ are post-collision velocities of two particles
- $g = |\mathbf{v}' - \mathbf{v}| = |\tilde{\mathbf{v}}' - \tilde{\mathbf{v}}|$ is relative speed
- σ is differential scattering cross section of collision
- Ω is solid angle defining direction of post-collision particle scattering

Odd power of g complicates analytical evaluation of integral

Maxwell's Equations

Gauss's law $\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$

Gauss's law for magnetism $\nabla \cdot \mathbf{B} = 0$

Faraday's law of induction $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$

Ampère's circuital law $\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$

- Charge conservation $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$
- Charge density $\rho(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$
- Electric current density $\mathbf{J}(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v}$
- ϵ_0 and μ_0 are permittivity and permeability of free space

Maxwell's Equations (Electromagnetic Case)

Gauss's law	$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$	} Satisfied due to charge conservation
Gauss's law for magnetism	$\nabla \cdot \mathbf{B} = 0$	

Faraday's law of induction	$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$
Ampère's circuital law	$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$

- Charge conservation $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$
- Charge density $\rho(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$
- Electric current density $\mathbf{J}(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v}$
- ϵ_0 and μ_0 are permittivity and permeability of free space

Maxwell's Equations (Electrostatic Case)

Gauss's law

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

$$\mathbf{E} = -\nabla\phi \rightarrow \Delta\phi = -\frac{\rho}{\epsilon_0}$$

Gauss's law for magnetism

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

Faraday's law of induction

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

Ampère's circuital law

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$$

- Charge conservation $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$
- Charge density $\rho(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$
- Electric current density $\mathbf{J}(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v}$
- ϵ_0 and μ_0 are permittivity and permeability of free space

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Collisionless, Electrostatic Plasma Dynamics

Collisionless electrostatic plasma dynamics:

$$\frac{dw_p}{dt} = 0, \quad \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad \frac{d\mathbf{v}_p}{dt} = \frac{q}{m} \mathbf{E}_p, \quad \Delta\phi = -\frac{\rho}{\epsilon_0}$$

- Riva et al., *Physics of Plasmas* (2017)
 - 1D, electrons
 - Maximum error in \mathbf{E} computed over all \mathbf{x}_p and t
 - Multiple approaches with varying expense to measure error in f
 - Results convincingly converge at expected rates
- Tranquilli et al., *Journal of Computational Physics* (2022)
 - 2D, positively and negatively charged particles
 - L^2 norm of error in ρ , \mathbf{E} , and ϕ
 - Argues against the need to measure error in f

Manufactured Solutions

Manufacture

- Particle distribution function $f_M(\mathbf{x}, \mathbf{v}, t) = f_{\mathbf{x}}(\mathbf{x}, t) f_{\mathbf{v}}(\mathbf{v})$
- Electromagnetic field $\mathbf{E}_M(\mathbf{x}, t)$

Compute source terms based on Vlasov and Poisson equations

$$S_f(\mathbf{x}, \mathbf{v}, t) = \frac{\partial f_M}{\partial t} + \mathbf{v} \cdot \nabla f_M + \frac{q}{m} \mathbf{E}_M \cdot \frac{\partial f_M}{\partial \mathbf{v}}, \quad S_{\mathbf{E}}(\mathbf{x}, t) = \nabla \cdot \mathbf{E}_M - \frac{\rho}{\epsilon_0}$$

Modify weight evolution equation to be

$$\frac{d}{dt} w_p(t) = \frac{\frac{d}{dt} f_M(\mathbf{x}_p(t), \mathbf{v}_p(t), 0)}{f_0(\mathbf{x}_p(0), \mathbf{v}_p(0))} = \frac{S_f(\mathbf{x}_p(t), \mathbf{v}_p(t), t)}{f_0(\mathbf{x}_p(0), \mathbf{v}_p(0))},$$

where

$$w_p(0) = \frac{f_M(\mathbf{x}_p(0), \mathbf{v}_p(0), 0)}{f_0(\mathbf{x}_p(0), \mathbf{v}_p(0))}$$

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Particle Distribution Function

Assume f_M takes the form of 3D analog of previous work:

$$f_M(\mathbf{x}, \mathbf{v}, t) = f_{\mathbf{x}}(\mathbf{x}, t) f_{\mathbf{v}}(\mathbf{v}),$$

where

$$f_{\mathbf{v}}(\mathbf{v}) = f_v(u) f_v(v) f_v(w), \quad f_v(u) = \frac{2}{\sqrt{\pi}} \frac{u^2}{\bar{v}^3} e^{-u^2/\bar{v}^2}$$

Dependencies require

$$\int_{-\infty}^{\infty} f_v(u) du = 1, \quad \int_V f_{\mathbf{x}}(\mathbf{x}, t) d\mathbf{x} = \bar{n} \cdot V,$$

where \bar{n} is average number density and V is domain volume

Collisionless Plasma Dynamics

- Follow approach of Riva et al., start with 1D electrostatic plasma dynamics
- After achieving expected convergence rates, generalize to account for
 - Additional dimensions
 - Magnetic field influence
 - Multiple species

Collisional Plasma Dynamics: Weight Evolution

With collisions, weight evolution is

$$\frac{d}{dt}w_p(t) = \frac{(\delta f / \delta t)_{\text{coll}}}{f_0(\mathbf{x}_p(0), \mathbf{v}_p(0))}$$

Method of manufactured solutions modifies collisional weight evolution to be

$$\frac{d}{dt}w_p(t) = \frac{S_f + (\delta f / \delta t)_{\text{coll}}}{f_0(\mathbf{x}_p(0), \mathbf{v}_p(0))},$$

where

$$S_f = \frac{\partial f_M}{\partial t} + \mathbf{v}_p \cdot \nabla f_M + \frac{\mathbf{F}_M}{m} \cdot \frac{\partial f_M}{\partial \mathbf{v}_p} - \left(\frac{\partial f_M}{\partial t} \right)_{\text{coll}}$$

Collisional Plasma Dynamics: Collision Integral

Assume isotropic scattering, same mass for particles, and cross-section form

$$\sigma = \sum_{n=0}^{n_{\max}} \sigma_n g^{2n-1}$$

- Precedent for manufacturing convenient cross sections: Maxwell molecules
- σ_n can be chosen to optimally fit actual cross-section data

Cross-section form yields closed-form expression for collision integral

$$\left(\frac{\partial f_M}{\partial t} \right)_{\text{coll}}(\mathbf{x}, \mathbf{v}, t) = f_{\mathbf{x}}(\mathbf{x}, t) \sum_{n=0}^{n_{\max}} \sigma_n F_n(\mathbf{v}),$$

where, in spherical coordinates with χ and ϵ polar and azimuthal angles,

$$F_n(\mathbf{v}) = \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} [f_{\mathbf{v}}(\tilde{\mathbf{v}}) f_{\mathbf{v}}(\tilde{\mathbf{v}}') - f_{\mathbf{v}}(\mathbf{v}) f_{\mathbf{v}}(\mathbf{v}')] g^{2n} \sin \chi d\chi d\epsilon d\mathbf{v}'$$

Collisional Plasma Dynamics: Collision Integral ($n = 0$)

$$\begin{aligned}
 F_0(\mathbf{v}) &= \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} [f_{\mathbf{v}}(\tilde{\mathbf{v}})f_{\mathbf{v}}(\tilde{\mathbf{v}}') - f_{\mathbf{v}}(\mathbf{v})f_{\mathbf{v}}(\mathbf{v}')] \sin \chi d\chi d\epsilon d\mathbf{v}' & (\hat{u} = u/\bar{v}, \hat{v} = v/\bar{v}, \hat{w} = w/\bar{v}) \\
 &= \frac{e^{-(\hat{u}^2 + \hat{v}^2 + \hat{w}^2)}}{720720\sqrt{\pi}\bar{v}^3} [360(\hat{u}^{12} + \hat{v}^{12} + \hat{w}^{12}) - 700(\hat{u}^{10}\hat{v}^2 + \hat{u}^{10}\hat{w}^2 + \hat{v}^{10}\hat{w}^2 + \hat{u}^2\hat{v}^{10} + \hat{u}^2\hat{w}^{10} + \hat{v}^2\hat{w}^{10}) \\
 &\quad + 2969(\hat{u}^8\hat{v}^4 + \hat{u}^4\hat{v}^8 + \hat{u}^8\hat{w}^4 + \hat{v}^8\hat{w}^4 + \hat{u}^4\hat{w}^8 + \hat{v}^4\hat{w}^8) + 1362(\hat{u}^8\hat{v}^2\hat{w}^2 + \hat{u}^2\hat{v}^8\hat{w}^2 + \hat{u}^2\hat{v}^2\hat{w}^8) \\
 &\quad + 8058(\hat{u}^6\hat{v}^6 + \hat{u}^6\hat{w}^6 + \hat{v}^6\hat{w}^6) - 4426(\hat{u}^6\hat{v}^4\hat{w}^2 + \hat{u}^4\hat{v}^6\hat{w}^2 + \hat{u}^6\hat{v}^2\hat{w}^4 + \hat{u}^2\hat{v}^6\hat{w}^4 + \hat{u}^4\hat{v}^2\hat{w}^6 + \hat{u}^2\hat{v}^4\hat{w}^6) \\
 &\quad + 9234\hat{u}^4\hat{v}^4\hat{w}^4 \\
 &\quad - 988(\hat{u}^{10} + \hat{v}^{10} + \hat{w}^{10}) + 34814(\hat{u}^8\hat{v}^2 + \hat{u}^2\hat{v}^8 + \hat{u}^8\hat{w}^2 + \hat{v}^8\hat{w}^2 + \hat{u}^2\hat{w}^8 + \hat{v}^2\hat{w}^8) \\
 &\quad - 4732(\hat{u}^6\hat{v}^4 + \hat{u}^4\hat{v}^6 + \hat{u}^6\hat{w}^4 + \hat{v}^6\hat{w}^4 + \hat{u}^4\hat{w}^6 + \hat{v}^4\hat{w}^6) - 76960(\hat{u}^6\hat{v}^2\hat{w}^2 + \hat{u}^2\hat{v}^6\hat{w}^2 + \hat{u}^2\hat{v}^2\hat{w}^6) \\
 &\quad + 52728(\hat{u}^4\hat{v}^4\hat{w}^2 + \hat{u}^4\hat{v}^2\hat{w}^4 + \hat{u}^2\hat{v}^4\hat{w}^4) \\
 &\quad + 3718(\hat{u}^8 + \hat{v}^8 + \hat{w}^8) - 103532(\hat{u}^6\hat{v}^2 + \hat{u}^2\hat{v}^6 + \hat{u}^6\hat{w}^2 + \hat{v}^6\hat{w}^2 + \hat{u}^2\hat{w}^6 + \hat{v}^2\hat{w}^6) \\
 &\quad + 79794(\hat{u}^4\hat{v}^4 + \hat{u}^4\hat{w}^4 + \hat{v}^4\hat{w}^4) + 391248(\hat{u}^4\hat{v}^2\hat{w}^2 + \hat{u}^2\hat{v}^4\hat{w}^2 + \hat{u}^2\hat{v}^2\hat{w}^4) \\
 &\quad + 58344(\hat{u}^6 + \hat{v}^6 + \hat{w}^6) + 386100(\hat{u}^4\hat{v}^2 + \hat{u}^2\hat{v}^4 + \hat{u}^4\hat{w}^2 + \hat{v}^4\hat{w}^2 + \hat{u}^2\hat{w}^4 + \hat{v}^2\hat{w}^4) - 19459440\hat{u}^2\hat{v}^2\hat{w}^2 \\
 &\quad + 65208(\hat{u}^4 + \hat{v}^4 + \hat{w}^4) - 401544(\hat{u}^2\hat{v}^2 + \hat{u}^2\hat{w}^2 + \hat{v}^2\hat{w}^2) + 329472(\hat{u}^2 + \hat{v}^2 + \hat{w}^2) + 277992]
 \end{aligned}$$

Collisional Plasma Dynamics: Collision Integral ($n = 1$)

$$\begin{aligned}
 F_1(\mathbf{v}) &= \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} [f_{\mathbf{v}}(\tilde{\mathbf{v}})f_{\mathbf{v}}(\tilde{\mathbf{v}}') - f_{\mathbf{v}}(\mathbf{v})f_{\mathbf{v}}(\mathbf{v}')] g^2 \sin \chi d\chi d\epsilon d\mathbf{v}' & (\hat{u} = u/\bar{v}, \hat{v} = v/\bar{v}, \hat{w} = w/\bar{v}) \\
 &= \frac{e^{-(\hat{u}^2 + \hat{v}^2 + \hat{w}^2)}}{1441440\sqrt{\pi}\bar{v}} [720(\hat{u}^{14} + \hat{v}^{14} + \hat{w}^{14}) - 680(\hat{u}^2\hat{v}^{12} + \hat{u}^{12}\hat{v}^2 + \hat{u}^{12}\hat{w}^2 + \hat{v}^{12}\hat{w}^2 + \hat{u}^2\hat{w}^{12} + \hat{v}^2\hat{w}^{12}) \\
 &\quad + 4538(\hat{u}^{10}\hat{v}^4 + \hat{u}^4\hat{v}^{10} + \hat{u}^{10}\hat{w}^4 + \hat{v}^{10}\hat{w}^4 + \hat{u}^4\hat{w}^{10} + \hat{v}^4\hat{w}^{10}) - 76(\hat{u}^{10}\hat{v}^2\hat{w}^2 + \hat{u}^2\hat{v}^{10}\hat{w}^2 + \hat{u}^2\hat{v}^2\hat{w}^{10}) \\
 &\quad + 22054(\hat{u}^8\hat{v}^6 + \hat{u}^6\hat{v}^8 + \hat{u}^8\hat{w}^6 + \hat{v}^8\hat{w}^6 + \hat{u}^6\hat{w}^8 + \hat{v}^6\hat{w}^8) \\
 &\quad - 190(\hat{u}^8\hat{v}^4\hat{w}^2 + \hat{u}^4\hat{v}^8\hat{w}^2 + \hat{u}^8\hat{v}^2\hat{w}^4 + \hat{u}^2\hat{v}^8\hat{w}^4 + \hat{u}^4\hat{v}^2\hat{w}^8 + \hat{u}^2\hat{v}^4\hat{w}^8) \\
 &\quad - 1588(\hat{u}^6\hat{v}^6\hat{w}^2 + \hat{u}^6\hat{v}^2\hat{w}^6 + \hat{u}^2\hat{v}^6\hat{w}^6) + 764(\hat{u}^6\hat{v}^4\hat{w}^4 + \hat{u}^4\hat{v}^6\hat{w}^4 + \hat{u}^4\hat{v}^4\hat{w}^6) \\
 &\quad + 1504(\hat{u}^{12} + \hat{v}^{12} + \hat{w}^{12}) + 77664(\hat{u}^{10}\hat{v}^2 + \hat{u}^2\hat{v}^{10} + \hat{u}^{10}\hat{w}^2 + \hat{v}^{10}\hat{w}^2 + \hat{u}^2\hat{w}^{10} + \hat{v}^2\hat{w}^{10}) \\
 &\quad + 23847(\hat{u}^8\hat{v}^4 + \hat{u}^4\hat{v}^8 + \hat{u}^8\hat{w}^4 + \hat{v}^8\hat{w}^4 + \hat{u}^4\hat{w}^8 + \hat{v}^4\hat{w}^8) - 55266(\hat{u}^8\hat{v}^2\hat{w}^2 + \hat{u}^2\hat{v}^8\hat{w}^2 + \hat{u}^2\hat{v}^2\hat{w}^8) \\
 &\quad - 104626(\hat{u}^6\hat{v}^6 + \hat{u}^6\hat{w}^6 + \hat{v}^6\hat{w}^6) + 70506(\hat{u}^6\hat{v}^4\hat{w}^2 + \hat{u}^4\hat{v}^6\hat{w}^2 + \hat{u}^6\hat{v}^2\hat{w}^4 + \hat{u}^2\hat{v}^6\hat{w}^4 + \hat{u}^4\hat{v}^2\hat{w}^6 + \hat{u}^2\hat{v}^4\hat{w}^6) \\
 &\quad + 45270(\hat{u}^4\hat{v}^4\hat{w}^4 + \hat{u}^6\hat{v}^4\hat{w}^4 + \hat{u}^4\hat{v}^6\hat{w}^4 + \hat{u}^4\hat{v}^4\hat{w}^6) \\
 &\quad - 18096(\hat{u}^{10} + \hat{v}^{10} + \hat{w}^{10}) - 184574(\hat{u}^8\hat{v}^2 + \hat{u}^2\hat{v}^8 + \hat{u}^8\hat{w}^2 + \hat{v}^8\hat{w}^2 + \hat{u}^2\hat{w}^8 + \hat{v}^2\hat{w}^8) \\
 &\quad + 347568(\hat{u}^6\hat{v}^4 + \hat{u}^4\hat{v}^6 + \hat{u}^6\hat{w}^4 + \hat{v}^6\hat{w}^4 + \hat{u}^4\hat{w}^6 + \hat{v}^4\hat{w}^6) + 1942096(\hat{u}^6\hat{v}^2\hat{w}^2 + \hat{u}^2\hat{v}^6\hat{w}^2 + \hat{u}^2\hat{v}^2\hat{w}^6) \\
 &\quad + 409500(\hat{u}^4\hat{v}^4\hat{w}^2 + \hat{u}^4\hat{v}^2\hat{w}^4 + \hat{u}^2\hat{v}^4\hat{w}^4) \\
 &\quad + 257114(\hat{u}^8 + \hat{v}^8 + \hat{w}^8) + 800228(\hat{u}^6\hat{v}^2 + \hat{u}^2\hat{v}^6 + \hat{u}^6\hat{w}^2 + \hat{v}^6\hat{w}^2 + \hat{u}^2\hat{w}^6 + \hat{v}^2\hat{w}^6) \\
 &\quad + 1512654(\hat{u}^4\hat{v}^4 + \hat{u}^4\hat{w}^4 + \hat{v}^4\hat{w}^4) - 43229472(\hat{u}^4\hat{v}^2\hat{w}^2 + \hat{u}^2\hat{v}^4\hat{w}^2 + \hat{u}^2\hat{v}^2\hat{w}^4) \\
 &\quad + 751608(\hat{u}^6 + \hat{v}^6 + \hat{w}^6) + 3289572(\hat{u}^4\hat{v}^2 + \hat{u}^2\hat{v}^4 + \hat{u}^4\hat{w}^2 + \hat{v}^4\hat{w}^2 + \hat{u}^2\hat{w}^4 + \hat{v}^2\hat{w}^4) - 190640736\hat{u}^2\hat{v}^2\hat{w}^2 \\
 &\quad + 1403688(\hat{u}^4 + \hat{v}^4 + \hat{w}^4) - 3181464(\hat{u}^2\hat{v}^2 + \hat{u}^2\hat{w}^2 + \hat{v}^2\hat{w}^2) + 4839120(\hat{u}^2 + \hat{v}^2 + \hat{w}^2) + 4169880]
 \end{aligned}$$

Error Metrics: Electromagnetic Field

Measure maximum error in \mathbf{E} and \mathbf{B} on mesh over all time:

$$\varepsilon_{E_x} = \max_t \max_{\mathbf{x}} |E_x^h(\mathbf{x}, t) - E_{M_x}(\mathbf{x}, t)|,$$

$$\varepsilon_{E_y} = \max_t \max_{\mathbf{x}} |E_y^h(\mathbf{x}, t) - E_{M_y}(\mathbf{x}, t)|,$$

$$\varepsilon_{E_z} = \max_t \max_{\mathbf{x}} |E_z^h(\mathbf{x}, t) - E_{M_z}(\mathbf{x}, t)|,$$

$$\varepsilon_{B_x} = \max_t \max_{\mathbf{x}} |B_x^h(\mathbf{x}, t) - B_{M_x}(\mathbf{x}, t)|,$$

$$\varepsilon_{B_y} = \max_t \max_{\mathbf{x}} |B_y^h(\mathbf{x}, t) - B_{M_y}(\mathbf{x}, t)|,$$

$$\varepsilon_{B_z} = \max_t \max_{\mathbf{x}} |B_z^h(\mathbf{x}, t) - B_{M_z}(\mathbf{x}, t)|$$

Error Metrics: Particle Distribution Function

Measure difference between manufactured and empirical f on boundaries:

$$\begin{aligned}\varepsilon_{f_x} &= \max_t \max_x \left| \int_{-\infty}^x \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{\mathbf{x}}(x', y, z, t) dy dz dx' - \sum_{p=1}^{N_p} \hat{w}_p \theta(x - x_p) \right|, \\ \varepsilon_{f_y} &= \max_t \max_y \left| \int_{-\infty}^y \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{\mathbf{x}}(x, y', z, t) dx dz dy' - \sum_{p=1}^{N_p} \hat{w}_p \theta(y - y_p) \right|, \\ \varepsilon_{f_z} &= \max_t \max_z \left| \int_{-\infty}^z \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{\mathbf{x}}(x, y, z', t) dx dy dz' - \sum_{p=1}^{N_p} \hat{w}_p \theta(z - z_p) \right|, \\ \varepsilon_{f_u} &= \max_t \max_u \left| \left(\int_{-\infty}^u f_v(u') du' \right) \left(\int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}, t) d\mathbf{x} \right) - \sum_{p=1}^{N_p} \hat{w}_p \theta(u - u_p) \right|, \\ \varepsilon_{f_v} &= \max_t \max_v \left| \left(\int_{-\infty}^v f_v(v') dv' \right) \left(\int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}, t) d\mathbf{x} \right) - \sum_{p=1}^{N_p} \hat{w}_p \theta(v - v_p) \right|, \\ \varepsilon_{f_w} &= \max_t \max_w \left| \left(\int_{-\infty}^w f_v(w') dw' \right) \left(\int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}, t) d\mathbf{x} \right) - \sum_{p=1}^{N_p} \hat{w}_p \theta(w - w_p) \right|\end{aligned}$$

Extension of approach from Riva et al. – most tractable option for multiple dimensions

Error Metrics: Discretization Error

- Discretization error depends on
 - Time step Δt
 - Mesh size Δx
 - Number of computational particles N_p
 - Problem dimension
- Convergence rates are less straightforward

Outline

- Introduction
- Particle-in-Cell Method
- Existing Work
- Proposed Approach
- **Summary**
 - Closing Remarks

Closing Remarks

- Presented a code-verification plan for 3D-3V collisional plasma dynamics
- Collisionless contributions follow established approaches
- Collisional approach achieved by analytically evaluating integral
- Manufacture differential scattering cross section of collision
- Expected convergence rates are not straightforward

Questions?

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