A Code-Verification Plan for Collisional Plasma Dynamics

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Outline

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- Particle-in-Cell Method
- Existing Work
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- Summary

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 $\mathbf{u}_{\text{MS}}$
- 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

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

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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- Particle-in-Cell Method
  - Overview
  - Equations of Motion for Charged Particles
  - Collision Term
  - Maxwell's Equations
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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:

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

- 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
- $\mathbf{F}_p = \dfrac{q}{m}(\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ 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):

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

- 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
- $\mathbf{F}_p = \dfrac{q}{m}(\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ 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:

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

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

Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle (electrostatic):

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

- 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
- $\mathbf{F}_p = \frac{q}{m}(\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \cancelto{\mathbf{0}}{\mathbf{B}(\mathbf{x}_p, t)})$ 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 5D 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 $\nabla \cdot \mathbf{E} = \dfrac{\rho}{\epsilon_0}$

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

Satisfied due to charge conservation

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

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

- Charge conservation $\dfrac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$
- Charge density $\rho(\mathbf{x}, t) = q\displaystyle\int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t)\, d\mathbf{v}$
- Electric current density $\mathbf{J}(\mathbf{x}, t) = q\displaystyle\int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t)\mathbf{v}\, d\mathbf{v}$
- 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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  - Manufactured Solutions
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Collisionless, Electrostatic Plasma Dynamics

Collisionless electrostatic plasma dynamics:

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

- 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

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

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

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

Dependencies require

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

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 ($n = 0$)

$$F_0(\mathbf{v}) = \int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{\pi}[f_{\mathbf{v}}(\tilde{\mathbf{v}})f_{\mathbf{v}}(\tilde{\mathbf{v}}') - f_{\mathbf{v}}(\mathbf{v})f_{\mathbf{v}}(\mathbf{v}')]\sin\chi d\chi\, d\epsilon\, d\mathbf{v}' \qquad (\hat{u} = u/\bar{v},\ \hat{v} = v/\bar{v},\ \hat{w} = w/\bar{v})$$

$$\begin{aligned}
&= \frac{e^{-(\hat{u}^2+\hat{v}^2+\hat{w}^2)}}{720720\sqrt{\pi}\bar{v}^3}[360(\hat{u}^{12}+\hat{v}^{12}+\hat{w}^{12}) - 700(\hat{u}^{10}\hat{v}^2+\hat{u}^{10}\hat{w}^2+\hat{v}^{10}\hat{w}^2+\hat{u}^2\hat{v}^{10}+\hat{u}^2\hat{w}^{10}+\hat{v}^2\hat{w}^{10})\\
&+ 2969(\hat{u}^8\hat{v}^4+\hat{u}^4\hat{v}^8+\hat{u}^8\hat{w}^4+\hat{v}^8\hat{w}^4+\hat{u}^4\hat{w}^8+\hat{v}^4\hat{w}^8) + 1362(\hat{u}^8\hat{v}^2\hat{w}^2+\hat{u}^2\hat{v}^8\hat{w}^2+\hat{u}^2\hat{v}^2\hat{w}^8)\\
&+ 8058(\hat{u}^6\hat{v}^6+\hat{u}^6\hat{w}^6+\hat{v}^6\hat{w}^6) - 4426(\hat{u}^6\hat{v}^4\hat{w}^2+\hat{u}^4\hat{v}^6\hat{w}^2+\hat{u}^6\hat{v}^2\hat{w}^4+\hat{u}^2\hat{v}^6\hat{w}^4+\hat{u}^4\hat{v}^2\hat{w}^6+\hat{u}^2\hat{v}^4\hat{w}^6)\\
&+ 9234\hat{u}^4\hat{v}^4\hat{w}^4\\
&- 988(\hat{u}^{10}+\hat{v}^{10}+\hat{w}^{10}) + 34814(\hat{u}^8\hat{v}^2+\hat{u}^2\hat{v}^8+\hat{u}^8\hat{w}^2+\hat{v}^8\hat{w}^2+\hat{u}^2\hat{w}^8+\hat{v}^2\hat{w}^8)\\
&- 4732(\hat{u}^6\hat{v}^4+\hat{u}^4\hat{v}^6+\hat{u}^6\hat{w}^4+\hat{v}^6\hat{w}^4+\hat{u}^4\hat{w}^6+\hat{v}^4\hat{w}^6) - 76960(\hat{u}^6\hat{v}^2\hat{w}^2+\hat{u}^2\hat{v}^6\hat{w}^2+\hat{u}^2\hat{v}^2\hat{w}^6)\\
&+ 52728(\hat{u}^4\hat{v}^4\hat{w}^2+\hat{u}^4\hat{v}^2\hat{w}^4+\hat{u}^2\hat{v}^4\hat{w}^4)\\
&+ 3718(\hat{u}^8+\hat{v}^8+\hat{w}^8) - 103532(\hat{u}^6\hat{v}^2+\hat{u}^2\hat{v}^6+\hat{u}^6\hat{w}^2+\hat{v}^6\hat{w}^2+\hat{u}^2\hat{w}^6+\hat{v}^2\hat{w}^6)\\
&+ 79794(\hat{u}^4\hat{v}^4+\hat{u}^4\hat{w}^4+\hat{v}^4\hat{w}^4) + 391248(\hat{u}^4\hat{v}^2\hat{w}^2+\hat{u}^2\hat{v}^4\hat{w}^2+\hat{u}^2\hat{v}^2\hat{w}^4)\\
&+ 58344(\hat{u}^6+\hat{v}^6+\hat{w}^6) + 386100(\hat{u}^4\hat{v}^2+\hat{u}^2\hat{v}^4+\hat{u}^4\hat{w}^2+\hat{v}^4\hat{w}^2+\hat{u}^2\hat{w}^4+\hat{v}^2\hat{w}^4) - 19459440\hat{u}^2\hat{v}^2\hat{w}^2\\
&+ 65208(\hat{u}^4+\hat{v}^4+\hat{w}^4) - 401544(\hat{u}^2\hat{v}^2+\hat{u}^2\hat{w}^2+\hat{v}^2\hat{w}^2) + 329472(\hat{u}^2+\hat{v}^2+\hat{w}^2) + 277992]
\end{aligned}$$

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

$$F_1(\mathbf{v}) = \int_{-\infty}^{\infty}\int_0^{2\pi}\int_0^{\pi}[f_{\mathbf{v}}(\tilde{\mathbf{v}})f_{\mathbf{v}}(\tilde{\mathbf{v}}') - f_{\mathbf{v}}(\mathbf{v})f_{\mathbf{v}}(\mathbf{v}')]g^2\sin\chi d\chi\, d\epsilon\, d\mathbf{v}' \qquad (\hat{u} = u/\bar{v},\ \hat{v} = v/\bar{v},\ \hat{w} = w/\bar{v})$$

$$\begin{aligned}
&= \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}) \\
&+ 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}) \\
&+ 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) \\
&- 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) \\
&- 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) \\
&+ 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}) \\
&+ 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) \\
&- 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) \\
&+ 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) \\
&- 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) \\
&+ 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) \\
&+ 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) \\
&+ 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) \\
&+ 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) \\
&+ 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 \\
&+ 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 **E** and **B** on mesh over all time:

$$\varepsilon_{E_x} = \max_t \max_{\mathbf{x}} \left| E_x^h(\mathbf{x},t) - E_{M_x}(\mathbf{x},t) \right|,$$
$$\varepsilon_{E_y} = \max_t \max_{\mathbf{x}} \left| E_y^h(\mathbf{x},t) - E_{M_y}(\mathbf{x},t) \right|,$$
$$\varepsilon_{E_z} = \max_t \max_{\mathbf{x}} \left| E_z^h(\mathbf{x},t) - E_{M_z}(\mathbf{x},t) \right|,$$

$$\varepsilon_{B_x} = \max_t \max_{\mathbf{x}} \left| B_x^h(\mathbf{x},t) - B_{M_x}(\mathbf{x},t) \right|,$$
$$\varepsilon_{B_y} = \max_t \max_{\mathbf{x}} \left| B_y^h(\mathbf{x},t) - B_{M_y}(\mathbf{x},t) \right|,$$
$$\varepsilon_{B_z} = \max_t \max_{\mathbf{x}} \left| B_z^h(\mathbf{x},t) - B_{M_z}(\mathbf{x},t) \right|$$

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? `bafreno@sandia.gov` `brianfreno.github.io`

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