PROGRESS ON CODE VERIFICATION FOR COLLISIONAL PLASMA DYNAMICS

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Outline

- Introduction
- Particle-in-Cell Method
- Existing Work for Collisionless Plasma Dynamics
- Approach for Collisional Plasma Dynamics
- Numerical Examples
- Summary



Introduction • 000000 Outline

- Introduction
 - Collisional Plasma Dynamics
 - Verification and Validation
 - Code Verification
 - Code-Verification Goal
- Particle-in-Cell Method
- Existing Work for Collisionless Plasma Dynamics
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Collisional Plasma Dynamics

- Important for many scientific and engineering applications
 - Hypersonic and reentry air plasmas affecting heat loads and radiation
 - Environmental and biomedical plasmas for ozone, sterilization, and cleaning
 - Electric propulsion plasmas in Hall-effect thrusters and ion engines
 - Semiconductor and thin-film plasmas for etching and deposition
- Modeled via particle-in-cell (PIC) with collision algorithm (MCC/DSMC)
 - Solve Maxwell's equations to compute electromagnetic fields on grid
 - Solve particle equations of motion due to Lorentz force and collisions
 - Interpolate EM fields to particles, distribute particle properties to grid
 - Model particle collisions with direct simulation Monte Carlo (DSMC)



Introduction

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Verification and Validation

Introduction

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

Introduction

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

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

• More rigorously, should decrease at an expected rate

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

Measuring error requires exact solution – usually unavailable



Manufactured Solutions

Introduction

Manufactured solutions are popular alternative

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

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

• Add residual term to discretized equations

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

to coerce solution to manufactured solution

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



Code-Verification Goal

Introduction

- 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 due to
 - Lorentz force from electromagnetic fields
 - Collisions between particles



Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle:

$$\frac{dw_p}{dt} = 0,$$
 $\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p,$ $\frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_p}{m} + \mathbf{a}_{\text{coll}}$

- w_p is computational particle weight
- $\mathbf{F}_p = \frac{q}{m} (\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ is Lorentz force
- E and B are electric and magnetic fields
- m and q are species mass and charge
- **a**_{coll} is acceleration due to collision

Increasing N_p , distribution function evolution approaches Boltzmann equation:

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

• $f(\mathbf{x}_p, \mathbf{v}_p, t)$ is particle distribution function, $(\partial f/\partial t)_{\text{coll}}$ is collision term

Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle (collisionless):

$$\frac{dw_p}{dt} = 0, \qquad \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \qquad \frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_p}{m} + \mathbf{a}_{\text{coll}} \mathbf{v}_0^0$$

- w_p is computational particle weight
- $\mathbf{F}_p = \frac{q}{m} (\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ is Lorentz force
- E and B are electric and magnetic fields
- m and q are species mass and charge
- **a**_{coll} is acceleration due to collision

Vlasov Increasing N_p , distribution function evolution approaches Boltzmann equation:

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

• $f(\mathbf{x}_p, \mathbf{v}_p, t)$ is particle distribution function, $(\partial f/\partial t)_{\text{coll}}$ is collision term

Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle (electrostatic):

$$\frac{dw_p}{dt} = 0,$$
 $\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p,$ $\frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_p}{m} + \mathbf{a}_{\text{coll}}$

- w_n is computational particle weight
- $\mathbf{F}_p = \frac{q}{m} (\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \mathbf{B}(\mathbf{x}_p, t))$ is Lorentz force
- E and B are electric and magnetic fields
- m and q are species mass and charge
- **a**_{coll} is acceleration due to collision

Increasing N_p , distribution function evolution approaches Boltzmann equation:

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

• $f(\mathbf{x}_p, \mathbf{v}_p, t)$ is particle distribution function, $(\partial f/\partial t)_{\text{coll}}$ is collision term

Maxwell's Equations

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

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

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

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

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

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
$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \qquad \rightarrow \qquad \boxed{\Delta \phi = -\frac{\rho}{\epsilon_0}}$$
Gauss's law for magnetism
$$\nabla \cdot \mathbf{B} = 0 \qquad \uparrow$$

Faraday's law of induction
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}_0}{\partial t}$$
 \rightarrow $\mathbf{E} = -\nabla \phi$
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



Existing Work

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- Existing Work for Collisionless Plasma Dynamics
 - Collisionless, Electrostatic Plasma Dynamics
 - Manufactured Solutions
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Collisionless, Electrostatic Plasma Dynamics

Collisionless electrostatic plasma dynamics:

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

- Riva et al., Physics of Plasmas (2017)
 - 1D, electrons
 - Maximum error in **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, electrons and ions
 - L^2 norm of error in ρ , **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

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

- Particles move without regard to manufactured distribution function
- \mathbf{x}_p and \mathbf{v}_p , when weighted by w_p , approach f_M
- Risk of negative weights



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Manufactured 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

$$f_{\mathbf{x}}(\mathbf{x},t) = N \prod_{i=1}^{3} f_{x_i}(x_i,t), \qquad f_{\mathbf{v}}(\mathbf{v}) = \prod_{i=1}^{3} f_{v_i}(v_i), \qquad f_{v_i}(v_i) = \frac{2}{\sqrt{\pi}} \frac{v_i^2}{\bar{v}^3} e^{-v_i^2/\bar{v}^2},$$

and

$$\int_0^{L_{x_i}} f_{x_i}(x_i, t) dx_i = 1, \qquad \int_{-\infty}^{\infty} f_v(v_i) dv_i = 1, \qquad \int_V f_{\mathbf{x}}(\mathbf{x}, t) d\mathbf{x} = N$$

- \bullet N is the number of physical particles in the volume
- $V = \prod_{i=1}^{3} L_{x_i}$ is the volume

Collisionless Plasma Dynamics

- $\bullet\,$ 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 without Lorentz Force

Apply method of manufactured solutions to equations of motion:

$$\dot{\mathbf{x}}_p = \mathbf{v}_p + \dot{\mathbf{x}}_M - \mathbf{v}_M, \qquad \dot{\mathbf{v}}_p = \left(\frac{\Delta \mathbf{v}_p}{\Delta t}\right)_{\text{coll}} + \dot{\mathbf{y}}_M - \left(\frac{\Delta \mathbf{v}_M}{\Delta t}\right)_{\text{coll}}$$

- Avoids negative weights
- \mathbf{x}_M and \mathbf{v}_M obtained from uniform random samples $F_{\mathbf{x}_p}, F_{\mathbf{v}_p} \in [0, 1]$
- Inversely query cumulative distribution functions $F_{\mathbf{x}}(\mathbf{x}_p, t)$ and $F_{\mathbf{v}}(\mathbf{v}_p)$
- Obtain \mathbf{x}_M and \mathbf{v}_M for each computational particle at each time step
- In general, $\dot{\mathbf{x}}_M \neq \mathbf{v}_M$
- $\dot{\mathbf{v}}_M = \mathbf{0}$ since $f_{\mathbf{v}}(\mathbf{v})$ does not depend on time
- $(\Delta \mathbf{v}_M/\Delta t)_{\text{coll}}$ represents analytic expression for the change due to collisions

Example time discretization (forward Euler):

$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \underbrace{\left(\Delta \mathbf{v}_p\right)_{\text{coll}}^n}_{\text{stochastic}} - \underbrace{\left(\Delta \mathbf{v}_M\right)_{\text{coll}}^n}_{\text{deterministic}}, \qquad \mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \mathbf{v}_p^{n+1} \Delta t + \mathbf{x}_M^{n+1} - (\mathbf{x}_M^n + \mathbf{v}_M \Delta t)$$



Source Term for Binary Elastic Collisions (same mass)

Post-collision velocities are obtained from conservation of momentum and energy:

$$\mathbf{v}' = \frac{1}{2}(\mathbf{v}_1 + \mathbf{v} - g\mathbf{n}), \qquad \mathbf{v}_1' = \frac{1}{2}(\mathbf{v}_1 + \mathbf{v} + g\mathbf{n}), \qquad \mathbf{n} = \begin{cases} \cos \epsilon \sin \chi \\ \sin \epsilon \sin \chi \\ \cos \chi \end{cases},$$

where $g = |\mathbf{v} - \mathbf{v}_1| = |\mathbf{v}' - \mathbf{v}_1'|$ is the relative speed

For a given particle, the change in velocity is $\Delta \mathbf{v} = \mathbf{v}' - \mathbf{v} = \frac{1}{2}(\mathbf{v}_1 - \mathbf{v} - g\mathbf{n})$

Compute expected change in velocity for particle across possible collision partners:

$$\langle \Delta \mathbf{v}_M \rangle_{\text{coll}} = \frac{\frac{1}{2} \int_V \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} \frac{P_{\text{coll}}(g)(N_p - 1)(\mathbf{v}_1 - \mathbf{v}_p - g\mathbf{n}) f_M(\mathbf{x}, \mathbf{v}_1, t) p(\chi, \epsilon) d\chi d\epsilon d\mathbf{v}_1 d\mathbf{x}}{\int_V \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} f_M(\mathbf{x}, \mathbf{v}_1, t) p(\chi, \epsilon) d\chi d\epsilon d\mathbf{v}_1 d\mathbf{x}},$$

 $P_{\text{coll}}(g)$ is likelihood of collision happening, $p(\chi, \epsilon)$ is probability density function

 $\langle \Delta \mathbf{v}_M \rangle_{\mathrm{coll}}$ is deterministic, should be computed analytically – complicated by g

Manufactured Anisotropy

Model probability density function as separable: $p(\chi, \epsilon) = p_{\chi}(\chi)p_{\epsilon}(\epsilon)$, where

$$\int_0^{2\pi} \int_0^{\pi} p(\chi, \epsilon) d\chi d\epsilon = 1, \qquad \int_0^{2\pi} p_{\epsilon}(\epsilon) d\epsilon = 1, \qquad \int_0^{\pi} p_{\chi}(\chi) d\chi = 1$$

Azimuthally symmetric scattering: $p_{\epsilon}(\epsilon) = \frac{1}{2\pi}$

In expression for $\langle \Delta \mathbf{v}_M \rangle_{\text{coll}}$,

$$g \int_0^{2\pi} \int_0^{\pi} \mathbf{n} p(\chi, \epsilon) d\chi d\epsilon = \frac{g}{2\pi} \int_0^{2\pi} \int_0^{\pi} \mathbf{n} p_{\chi}(\chi) d\chi d\epsilon = g \left\{ 0, 0, \underbrace{\int_0^{\pi} p_{\chi}(\chi) \cos \chi d\chi}_{=0} \right\}$$

Avoid dependency on g from anisotropy: $\int_0^{\pi} p_{\chi}(\chi) \cos \chi d\chi = 0$

Avoid isotropy: $p_{\chi}(\chi) \neq \frac{\sin \chi}{2}$

For $F_{\nu_{\star}}^{-1}$, use ansatz $p_{\chi}(\chi) = (C_0 + C_1 \cos \chi + C_2 \cos^2 \chi + C_3 \cos^3 \chi) \sin \chi$

 C_2 and C_3 satisfy constraint, C_0 and C_1 minimize $\int_0^{\pi} (p_{\chi}(\chi) - \bar{p}_{\chi}(\chi))^2 d\chi$

Manufactured Cross Section

With
$$\int_0^{\pi} p_{\chi}(\chi) \cos \chi d\chi = 0,$$

$$\langle \Delta \mathbf{v}_M \rangle_{\text{coll}} = \frac{w_p \Delta t (N_p - 1)}{2V} \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{g}) \mathbf{g}(\mathbf{v}_1 - \mathbf{v}_p) f_{\mathbf{v}}(\mathbf{v}_1) d\mathbf{v}_1$$

If
$$\sigma(g) = \sum_{n=0}^{N_{\sigma}-1} \sigma_n g^{2n-1}$$
,

$$\langle \Delta \mathbf{v}_M \rangle_{\text{coll}} = \frac{w_p \Delta t (N_p - 1)}{2V} \sum_{n=0}^{N_\sigma - 1} \sigma_n \mathbf{f}_n(\mathbf{v}_p),$$

where $\mathbf{f}_n(\mathbf{v}_p) = \int_{-\infty}^{\infty} g^{2n}(\mathbf{v}_1 - \mathbf{v}_p) f_{\mathbf{v}}(\mathbf{v}_1) d\mathbf{v}_1$ can be computed exactly:

$$\mathbf{f}_0(\mathbf{v}_p) = -\mathbf{v}_p, \quad \mathbf{f}_1(\mathbf{v}_p) = -\frac{1}{2}(15\bar{v}^2 + 2v_p^2)\mathbf{v}_p, \quad \mathbf{f}_2(\mathbf{v}_p) = -\frac{1}{4}(231\bar{v}^4 + 84\bar{v}^2v_p^2 + 4v_p^4)\mathbf{v}_p$$

Velocity Evolution

$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + \underbrace{\left(\Delta \mathbf{v}_p\right)_{\mathrm{coll}}^n}_{\mathrm{stochastic}} - \underbrace{\left\langle\Delta \mathbf{v}_M\right\rangle_{\mathrm{coll}}^n}_{\mathrm{deterministic}}$$

- $(\Delta \mathbf{v}_p)_{\text{coll}}^n$ is computed from a collision algorithm
- Collision algorithms are stochastic consider random subset of collisions
- ullet Run collision algorithm $N_{
 m avg}$ times, average outcome for each particle

Summary

- Get uniform random samples for each position and velocity component
- Integrate equations of motion
- Each time step, get \mathbf{x}_M and \mathbf{v}_M from inverse of time-varying CDF
- Measure discrete L^p norm of particle position and velocity errors
 - \rightarrow One simulation per refinement



Refinement Ratios

Measure error using discrete L^p norm of particle positions and velocities

- Discretization error depends on Δt , Δx , N_p , N_{avg} , h_{interp}
- Refinement ratios: $r_{\Delta t} = \frac{\Delta t_1}{\Delta t_2}$, $r_{N_p} = \frac{N_{p_2}}{N_{p_1}}$, $r_{N_{\text{avg}}} = \frac{N_{\text{avg}_2}}{N_{\text{avg}_1}}$, $r_{h_{\text{interp}}} = \frac{h_{\text{interp}_1}}{h_{\text{interp}_2}}$
- Time integration error is locally $\mathcal{O}(\Delta t^2)$, globally $\mathcal{O}(\Delta t)$
 - Decrease N_p error at same rate as global time error
 - Decrease N_{coll} error at same rate as local time error
- Error due to N_p is $\mathcal{O}(N_p^{-1/2})$ (central limit theorem) $\rightarrow r_{N_p} = r_{\Delta t}^2$
- Error due to the collisions is $\mathcal{O}(N_{\text{coll}}^{-1/2})$, $N_{\text{coll}} \sim N_{\text{avg}} N_v \Delta t \rightarrow r_{N_{\text{avg}}} = r_{\Delta t}^3$
- Error due to interpolating inverse CDFs is $\mathcal{O}(h_{\text{interp}}^2)$ \rightarrow $r_{h_{\text{interp}}} = r_{\Delta t}$

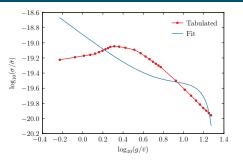


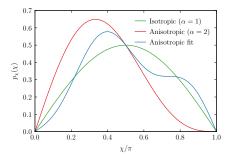
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Manufactured Cross Section and Anisotropy





- Cross section $\sigma(g) = \sum_{n=0}^{\infty} \sigma_n g^{2n-1}, \qquad N_{\sigma} = 3$
 - Log-scale least squares fitting of data from Itikawa J. Phys. Chem. Ref. (2009)
- Anisotropy $F_{p_{\chi}}^{-1}$, $p_{\chi}(\chi) = (C_0 + C_1 \cos \chi + C_2 \cos^2 \chi + C_3 \cos^3 \chi) \sin \chi$
 - $-\bar{p}_{\gamma}(\chi) = \alpha \cos(\chi/2)^{2\alpha-1} \sin(\chi/2), \qquad 1 \le \alpha \le 2,$ (variable soft sphere)
 - Isotropic ($\alpha = 1$), anisotropic ($\alpha > 1$)

Manufactured Distribution Function and Discretizations

• Particle distribution function $f_M(\mathbf{x}, \mathbf{v}, t) = f_{\mathbf{x}}(\mathbf{x}, t) f_{\mathbf{v}}(\mathbf{v})$,

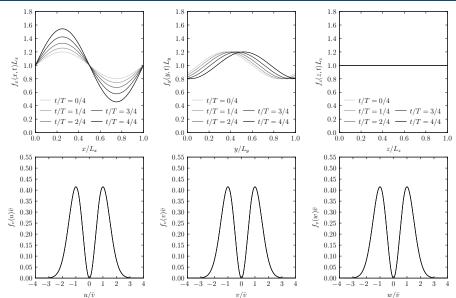
$$f_{\mathbf{x}}(\mathbf{x},t) = N \prod_{i=1}^{3} f_{x_i}(x_i,t), \qquad f_{\mathbf{v}}(\mathbf{v}) = \prod_{i=1}^{3} f_v(v_i)$$

•
$$\bar{v} = 10^6 \text{ m/s}$$
, $L_{x_i} = 3/2 \text{ m}$, $T = L_{x_i}/(10\bar{v})$, periodic BCs

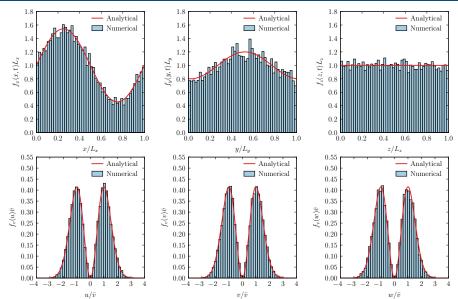
Discretizations

Disc.	N_p	$T/\Delta t$	$N_{ m avg}$	$1/h_{\mathrm{interp}}$
1	50	10	50	1000
2	200	20	400	2000
3	800	40	3200	4000
4	3200	80	25600	8000
5	12800	160	204800	16000

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

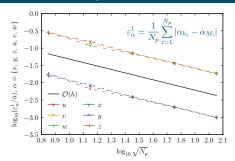


Particle Distribution Function $f_M(\mathbf{x}, \mathbf{v}, T) = f_{\mathbf{x}}(\mathbf{x}, T) f_{\mathbf{v}}(\mathbf{v})$



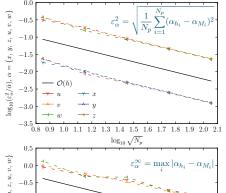


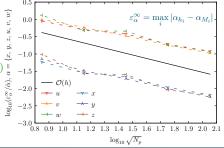
Error Convergence at t = T



- Discrete L^p error norms for particle positions and velocities: $p = 1, 2, \infty$
- Each component converges at expected rate $\mathcal{O}(h)$

$$h \sim \Delta t \sim N_p^{-1/2} \sim N_{\rm avg}^{-1/3}$$





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Closing Remarks

- Presented code-verification progress for 3D-3V collisional plasma dynamics
- Add manufactured source terms to equations of motion, weights unmodified
- Manufacture distribution function, cross section, anisotropy
- Analytically compute manufactured source terms, average collisions
- Achieved expected convergence rates without Lorentz force



References

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- P. Tranquilli and L. Ricketson and L. Chacón
 A deterministic verification strategy for electrostatic particle-in-cell
 algorithms in arbitrary spatial dimensions using the method of
 manufactured solutions
 Journal of Computational Physics (2022)



