Progress on Code Verification for Collisional Plasma Dynamics

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Outline

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

Collisional Plasma Dynamics

- Important for many scientific and engineering applications
  - **Hypersonic & reentry air plasmas** affecting heat loads and radiation
  - **Environmental & biomedical plasmas** for ozone, sterilization, and cleaning
  - **Electric propulsion plasmas** in Hall-effect thrusters and ion engines
  - **Semiconductor & 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)

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

$$\|\mathbf{e}\| \approx C h^p$$

- Measuring error requires exact solution $\mathbf{u}$ – usually unavailable

Manufactured Solutions

Manufactured solutions are popular alternative

- Manufacture an arbitrary solution $\mathbf{u}_{\mathrm{MS}}$
- 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

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

Code-Verification Goal

- Existing code-verification work
  - Collisionless plasma dynamics
  - Electrostatics (negligible magnetic field influence)
  - 1D-1V, 2D-2V
- Our code-verification goal
  - Collisional plasma dynamics
  - Electromagnetics
  - 3D-3V

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- Introduction
- Particle-in-Cell Method
  - Overview
  - Equations of Motion for Charged Particles
  - 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 due to
  - Lorentz force from electromagnetic fields
  - Collisions between particles

Equations of Motion for Charged Particles (Single Species)

Equations of motion for each particle:

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

- 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
- $\mathbf{E}$ and $\mathbf{B}$ are electric and magnetic fields
- m and q are species mass and charge
- $\mathbf{a}_{\text{coll}}$ 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):

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

- 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
- $\mathbf{E}$ and $\mathbf{B}$ are electric and magnetic fields
- m and q are species mass and charge
- $\mathbf{a}_{\text{coll}}$ is acceleration due to collision

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

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

- $f(\mathbf{x}_p, \mathbf{v}_p, t)$ 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):

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

- w_p is computational particle weight
- $\mathbf{F}_p = \dfrac{q}{m}\left(\mathbf{E}(\mathbf{x}_p, t) + \mathbf{v}_p \times \cancelto{\mathbf{0}}{\mathbf{B}(\mathbf{x}_p, t)}\right)$ is Lorentz force
- $\mathbf{E}$ and $\mathbf{B}$ are electric and magnetic fields
- m and q are species mass and charge
- $\mathbf{a}_{\text{coll}}$ 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

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

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

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 $\rho(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$
- 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	$\nabla \cdot \mathbf{E} = \dfrac{\rho}{\epsilon_0}$	Satisfied due to charge conservation
Gauss's law for magnetism	$\nabla \cdot \mathbf{B} = 0$	
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)

$$\boxed{\text{Gauss's law} \qquad \nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}} \quad \rightarrow \quad \boxed{\Delta\phi = -\frac{\rho}{\epsilon_0}}$$

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

$$\boxed{\text{Faraday's law of induction} \qquad \nabla \times \mathbf{E} = -\frac{\partial \cancel{\mathbf{B}}^{\,\mathbf{0}}}{\partial t}} \quad \rightarrow \quad \mathbf{E} = -\nabla\phi$$

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

- 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

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  - Collisionless, Electrostatic Plasma Dynamics
  - 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, electrons and ions
  - 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

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

- 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

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

and

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

- N is the number of physical particles in the volume
- $V = \prod_{i=1}^{3} L_{x_i}$ is the 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 without Lorentz Force

Apply method of manufactured solutions to equations of motion:

$$\dot{\mathbf{x}}_p = \mathbf{v}_p + \dot{\mathbf{x}}_M - \mathbf{v}_M, \qquad \dot{\mathbf{v}}_p = \left(\frac{\Delta \mathbf{v}_p}{\Delta t}\right)_{\text{coll}} + \cancelto{0}{\dot{\mathbf{v}}_M} - \left(\frac{\Delta \mathbf{v}_M}{\Delta t}\right)_{\text{coll}}$$

- 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):

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

Source Term for Binary Elastic Collisions (same mass)

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

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

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:

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

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

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

Manufactured Anisotropy (to avoid dependency on g due to $\mathbf{n}p$)

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: $p_\epsilon(\epsilon) = \dfrac{1}{2\pi}$

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: $\displaystyle\int_0^{\pi} p_\chi(\chi)\cos\chi d\chi = 0$

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

For $F_{p_\chi}^{-1}$, 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 $\displaystyle\int_0^{\pi}\left(p_\chi(\chi) - \bar{p}_\chi(\chi)\right)^2 d\chi$

Manufactured Cross Section (to evaluate $\langle \Delta \mathbf{v}_M \rangle_{\text{coll}}$ analytically)

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

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

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 analytically:

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

Velocity Evolution

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

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

  $(\Delta \mathbf{v}_p)_{\text{coll}}^n \rightarrow \langle \Delta \mathbf{v}_p \rangle_{\text{coll}}^n$

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 discrete L^p norm of particle position and velocity errors

- Discretization error depends on Δt, $\Delta \mathbf{x}$, N_p, N_{avg}, h_{interp}
- Refinement ratios: $r_{\Delta t} = \dfrac{\Delta t_1}{\Delta t_2}$, $r_{N_p} = \frac{N_{p2}}{N_{p1}}$, $r_{N_{\text{avg}}} = \frac{N_{\text{avg}_2}}{N_{\text{avg}_1}}$, $r_{h_{\text{interp}}} = \frac{h_{\text{interp}_1}}{h_{\text{interp}_2}}$
- 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) $\quad\rightarrow\quad r_{N_p} = r_{\Delta t}^2$
- Error due to the collisions is $\mathcal{O}(N_{\text{coll}}^{-1/2})$, $N_{\text{coll}} \sim N_{\text{avg}} N_p \Delta t \quad\rightarrow\quad r_{N_{\text{avg}}} = r_{\Delta t}^3$
- Error due to interpolating inverse CDFs is $\mathcal{O}(h_{\text{interp}}^2) \quad\rightarrow\quad r_{h_{\text{interp}}} = r_{\Delta t}$

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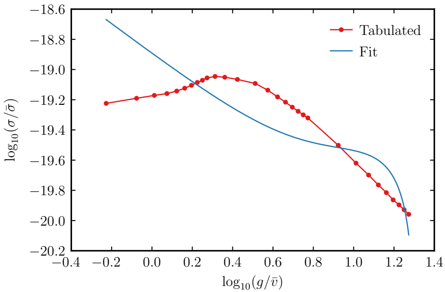
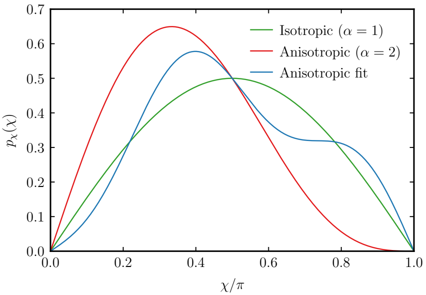
Manufactured Cross Section and Anisotropy





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

Manufactured Distribution Function and Discretizations

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

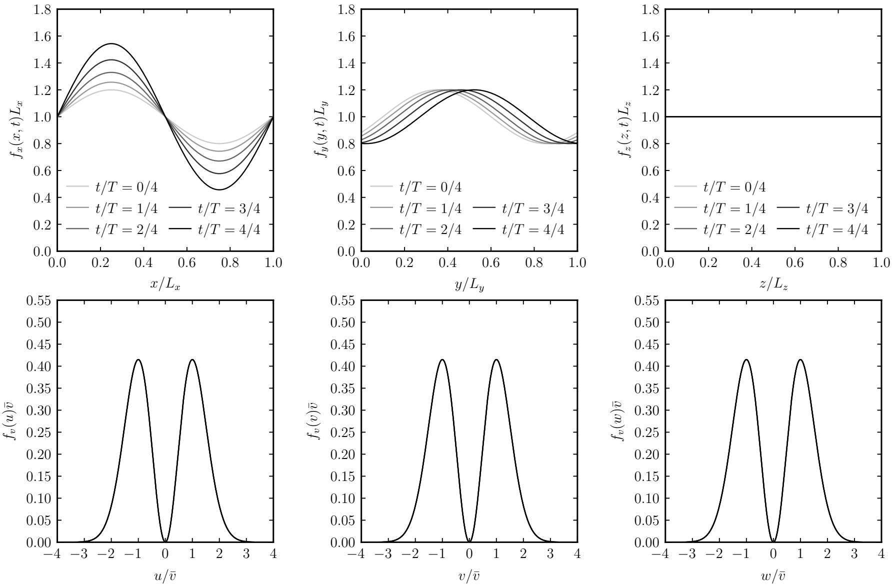
$$f_\mathbf{x}(\mathbf{x},t) = N\prod_{i=1}^{3} f_{x_i}(x_i,t), \qquad f_\mathbf{v}(\mathbf{v}) = \prod_{i=1}^{3} f_v(v_i)$$

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

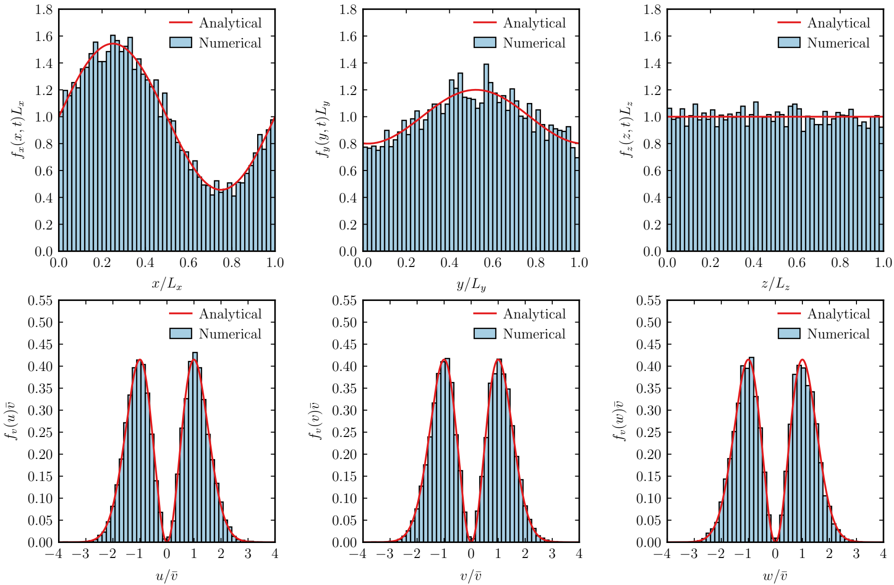
- Discretizations

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

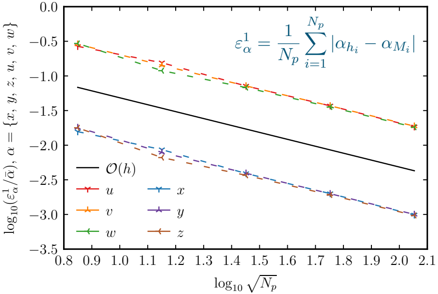
Particle Distribution Function $f_M(\mathbf{x}, \mathbf{v}, t) = f_{\mathbf{x}}(\mathbf{x}, t) f_{\mathbf{v}}(\mathbf{v})$

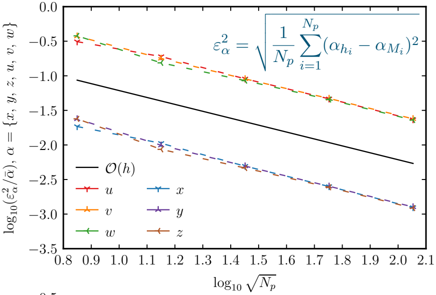


Particle Distribution Function $f_M(\mathbf{x},\mathbf{v},t) = f_\mathbf{x}(\mathbf{x},t) f_\mathbf{v}(\mathbf{v})$ at $t = T$



Error Convergence at $t = T$

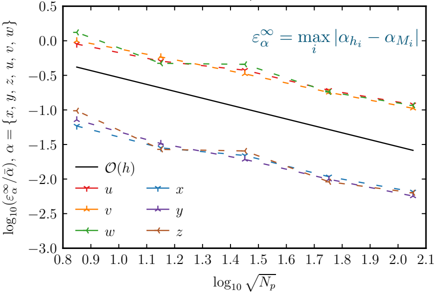




- Discrete L^p error norms for particle positions and velocities: $p = 1,\ 2,\ \infty$

- Each component converges at expected rate $\mathcal{O}(h)$

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



Outline

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

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, and anisotropy
- Analytically compute manufactured source terms, average collisions
- Achieved expected convergence rates without Lorentz force

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References

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  A methodology for the rigorous verification of particle-in-cell simulations
  Physics of Plasmas (2017)

- 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)