

CODE-VERIFICATION TECHNIQUES FOR PARTICLE-IN-CELL SIMULATIONS WITH DIRECT SIMULATION MONTE CARLO COLLISIONS

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Outline

- Introduction
- Governing Equations
- Manufactured Solutions for PIC Simulations with DSMC
- Error Analysis
- Numerical Examples
- Summary

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- Introduction
 - Collisional Plasma Dynamics
 - Code Verification
 - This Work
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Collisional Plasma Dynamics

- Important for many scientific and engineering applications
 - **Hypersonic & reentry air plasmas** affecting heat loads and radiation
 - **Plasma devices** such as lightning arresters and plasma switches
 - **Pulsed power** for simulating Sandia flagship experimental facilities
 - **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 field on grid
 - Solve particle equations of motion due to Lorentz force and collisions
 - Interpolate field onto particles, distribute particle properties onto grid
 - Model particle collisions with direct simulation Monte Carlo (DSMC)

Code Verification

- Code verification assesses correctness of numerical-method implementation
- Most rigorously measures rate at which error decreases with refinement
- Error requires exact solution – usually unavailable
- Manufactured solutions are popular alternative: $\mathbf{r}(\mathbf{u}) = \mathbf{0} \rightarrow \mathbf{r}(\mathbf{u}) = \mathbf{r}(\mathbf{u}^M)$
 - Manufacture an arbitrary solution \mathbf{u}^M
 - Insert manufactured solution into equations to get residual term $\mathbf{r}(\mathbf{u}^M)$
 - Add residual term to equations to make manufactured solution a solution
- For *collisionless* PIC simulations, few instances of code verification exist
- Significant code-verification challenges with *collisional* PIC simulations:
 - Discretization errors from space and time discretization
 - Statistical sampling error from finite number of computational particles
 - Stochasticity from collision modeling – considering random subset of collisions

Existing Work: Collisionless Particle-in-Cell Simulations

- Riva et al., *Physics of Plasmas* (2017), 10.1063/1.4977917
 - Modify particle weights to achieve manufactured distribution function
 - Particles move independently of manufactured distribution function
 - Particle weights modified according to Vlasov equation
 - 1D, electrons
 - Measure electric field error
 - Multiple approaches with varying expense to measure dist. function error
 - Many runs per discretization
- Tranquilli et al., *Journal of Computational Physics* (2022), 10.1016/j.jcp.2021.110751
 - Extend the approach of Riva et al. to 2D, electrons and ions
 - Measure charge density, electric field, and electric potential errors
 - Derive expected convergence rates for statistical sampling errors in fields
 - Argue against the need to measure error in distribution function
 - Single run per discretization

This Work: Collisional Particle-in-Cell Simulations

- Apply method of manufactured solutions to equations of motion
 - Weights are unmodified – no negative weights, collision-algorithm modifications
 - Obtain manufactured particle positions and velocities at each time step
 - Inversely query cumulative manufactured distribution function
- Balance collision-algorithm velocity change with manufactured source term
 - Average outcomes from multiple collision-algorithm runs at each time step
 - Compute analytic expected change in velocity due to collisions
 - Manufacture cross section and anisotropy
- Apply method of manufactured solutions to Poisson equation
 - Manufacture electric scalar potential
- Compute field errors and particle errors
 - Single run per discretization
- Demonstrate approach for collisional and collisionless PIC simulations

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- Governing Equations
 - Particle-in-Cell Method Overview
 - Equations of Motion for Charged Particles
 - Maxwell's Equations
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Particle-in-Cell Method Overview

- Place (weighted) computational particles randomly in phase space (according to distribution function)
- Interpolate particle charge onto spatial mesh
- Solve Maxwell's equations on spatial mesh for electromagnetic field
- Interpolate electromagnetic field onto particles
- For each particle, integrate equations of motion due to
 - Lorentz force from electromagnetic field
 - Collisions between particles

Equations of Motion for Charged Particles (single species, electrostatic)

Equations of motion for each particle p :

$$\dot{w}_p(t) = 0, \quad \dot{\mathbf{x}}_p(t) = \mathbf{v}_p(t), \quad \dot{\mathbf{v}}_p(t) = \frac{\mathbf{F}_p(t)}{m} + \left(\frac{\Delta \mathbf{v}_p(t)}{\Delta t} \right)_{\text{coll}}$$

- w_p , \mathbf{x}_p , and \mathbf{v}_p are computational particle weight, position, and velocity
- $\mathbf{F}_p(t) = q\mathbf{E}_p(t)$ is electrostatic Lorentz force, $\mathbf{E}_p(t) = \mathbf{E}(\mathbf{x}_p(t), t)$
- \mathbf{E} is electric field
- m and q are species mass and charge
- $(\Delta \mathbf{v}_p / \Delta t)_{\text{coll}}$ is instantaneous change in \mathbf{v}_p per Δt due to collision algorithm

Distribution function evolution approximates 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 (electrostatic case – negligible magnetic field)

Gauss's law

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

→

$$\Delta\phi = -\frac{\rho}{\epsilon_0}$$

Gauss's law for magnetism

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

↑

Faraday's law of induction

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}_0}{\partial t}$$

→

$$\mathbf{E} = -\nabla\phi$$

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

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- Manufactured Solutions for PIC Simulations with DSMC
 - Manufactured Particle Distribution Function
 - Manufactured Solutions through the Equations of Motion
 - Manufactured Source Term for Binary Elastic Collisions
 - Manufactured Solutions for the Poisson Equation
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Manufactured Particle Distribution Function

Assume f^M takes the form of 3D analog of previous work:

$$f^M(\mathbf{x}, \mathbf{v}, t) = f_{\mathbf{x}}(\mathbf{x}, t) f_{\mathbf{v}}(\mathbf{v}, t),$$

where

$$f_{\mathbf{v}}(\mathbf{v}, t) = \prod_{i=1}^3 f_{v_i}(v_i, t), \quad f_{v_i}(v_i, t) = \frac{2}{\sqrt{\pi}} \frac{v_i^2}{\hat{v}_i(t)^3} e^{-v_i^2/\hat{v}_i(t)^2}, \quad \int_{-\infty}^{\infty} f_{v_i}(v_i, t) dv_i = 1,$$

and

$$f_{\mathbf{x}}(\mathbf{x}, t) = N \prod_{i=1}^3 f_{x_i}(x_i, t), \quad \int_0^{L_{x_i}} f_{x_i}(x_i, t) dx_i = 1, \quad \int_V f_{\mathbf{x}}(\mathbf{x}, t) d\mathbf{x} = N$$

- N is the number of physical particles in the volume $V = \prod_{i=1}^3 L_{x_i}$
- Separability of $f_{\mathbf{x}}(\mathbf{x}, t)$ imposed for convenience
- $f_{\mathbf{v}}(\mathbf{v}, t)$ is deliberately non-Maxwellian, $\hat{v}_i(t)$ incorporates time variation

Manufactured Solutions through the Equations of Motion

Apply **method of manufactured solutions** to equations of motion:

$$\dot{\mathbf{x}}_p = \mathbf{v}_p + \dot{\mathbf{x}}_p^M - \mathbf{v}_p^M, \quad \dot{\mathbf{v}}_p = \frac{q}{m} \mathbf{E}_p + \left(\frac{\Delta \mathbf{v}_p}{\Delta t} \right)_{\text{coll}} + \dot{\mathbf{v}}_p^M - \frac{q}{m} \mathbf{E}_p^M - \left(\frac{\Delta \mathbf{v}_p^M}{\Delta t} \right)_{\text{coll}}$$

- **Weights unmodified – no negative weights, collision-algorithm modifications**
- At $t = 0$, for component i , take uniform random samples $\xi_{x_{i_p}}, \xi_{v_{i_p}} \in [0, 1]$
- Inversely query cumulative dist. functions to obtain $x_{i_p}^M(t)$ and $v_{i_p}^M(t)$:

$$F_{x_i}(x_{i_p}^M(t), t) = \xi_{x_{i_p}}, \quad F_{v_i}(v_{i_p}^M(t), t) = \xi_{v_{i_p}}$$

- Differentiate to obtain $\dot{x}_{i_p}^M(t)$ and $\dot{v}_{i_p}^M(t)$
- In general, $\dot{\mathbf{x}}_p^M \neq \mathbf{v}_p^M$
- $\mathbf{E}^M = -\nabla \phi^M$ is electric field from manufactured potential ϕ^M
- $(\Delta \mathbf{v}_p^M / \Delta t)_{\text{coll}}$ is manufactured collision term

Manufactured Source Term for Collisions

Velocity equation

$$\dot{\mathbf{v}}_p = \frac{q}{m} (\mathbf{E}_p - \mathbf{E}_p^M) + \frac{(\Delta \mathbf{v}_p)_{\text{coll}} - (\Delta \mathbf{v}_p^M)_{\text{coll}}}{\Delta t} + \dot{\mathbf{v}}_p^M$$

Requires velocity changes due to collisions at each time step:

- $(\Delta \mathbf{v}_p)_{\text{coll}}$ due to **stochastic** collision algorithm
- $(\Delta \mathbf{v}_p^M)_{\text{coll}}$ due to corresponding **deterministic** manufactured source term

At each time step, make collision-algorithm outcome **less stochastic**:

- Run collision algorithm N_{avg} independent times, average velocity change
- Replace $(\Delta \mathbf{v}_p)_{\text{coll}}$ with $\langle \Delta \mathbf{v}_p \rangle_{\text{coll}} = \frac{1}{N_{\text{avg}}} \sum_{k=1}^{N_{\text{avg}}} (\Delta \mathbf{v}_p)_{\text{coll}}^k$
- Derive expected velocity change for each particle: $(\Delta \mathbf{v}_p^M)_{\text{coll}} = \langle \Delta \mathbf{v}_p^M \rangle_{\text{coll}}$

Expected Change in Velocity (binary elastic collisions)

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

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

where $g = |\mathbf{v}_p - \mathbf{v}_q| = |\mathbf{v}'_p - \mathbf{v}'_q|$ is relative speed

The velocity change for particle p is $\Delta\mathbf{v}_p = \mathbf{v}'_p - \mathbf{v}_p = \frac{1}{2}(\mathbf{v}_q - \mathbf{v}_p + g\mathbf{n})$

Compute expected velocity change across possible collision partners:

$$\langle \Delta\mathbf{v}_p^M \rangle_{\text{coll}} = \frac{\frac{N_p^{\text{cell}} - 1}{2} \int_{\Delta V} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} P_{\text{coll}}(g)(\mathbf{v}_q - \mathbf{v}_p + g\mathbf{n}) f^M(\mathbf{x}, \mathbf{v}_q, t) p(\chi, \epsilon) d\chi d\epsilon d\mathbf{v}_q d\mathbf{x}}{\int_{\Delta V} \int_{-\infty}^{\infty} \int_0^{2\pi} \int_0^{\pi} f^M(\mathbf{x}, \mathbf{v}_q, t) p(\chi, \epsilon) d\chi d\epsilon d\mathbf{v}_q d\mathbf{x}}$$

$P_{\text{coll}}(g) = \frac{\sigma(g)gw\Delta t}{\Delta V}$ is collision likelihood, $p(\chi, \epsilon)$ is probability density function, $\sigma(g)$ is cross section

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

→ Manufacture anisotropy and cross section

Manufactured Anisotropy (to avoid dependency on g due to \mathbf{np})

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

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

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

In expression for $\langle \Delta \mathbf{v}_p^M \rangle_{\text{coll}}$,

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

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

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

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

$$\langle \Delta \mathbf{v}_p^M \rangle_{\text{coll}} = \frac{w\Delta t(N_p^{\text{cell}} - 1)}{2\Delta V} \int_{-\infty}^{\infty} \sigma(g) g(\mathbf{v}_q - \mathbf{v}_p) f_{\mathbf{v}}(\mathbf{v}_q, t) d\mathbf{v}_q$$

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

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

where $\mathbf{f}_n = \int_{-\infty}^{\infty} g^{2n}(\mathbf{v}_q - \mathbf{v}_p) f_{\mathbf{v}}(\mathbf{v}_q, t) d\mathbf{v}_q$ can be computed analytically

Numerical and manufactured source terms balanced with manufactured p_χ and σ

Additional Error Metrics for Collisions

- Coding errors are **not detected** if the expected collision error is zero
- A necessary (but insufficient) condition for zero expected collision error is

$$\int_0^{2\pi} \int_0^\pi \mathbf{n} p(\chi, \epsilon) d\chi d\epsilon = \mathbf{0}$$

- Additionally measure convergence of $p_\chi(\chi)$ and $p_\epsilon(\epsilon)$ by recording

$$\chi = \cos^{-1} \frac{g'_z}{g}, \quad \epsilon = \tan^{-1} \frac{g'_y}{g'_x},$$

and measuring difference between analytic and empirical CDFs

- Additional metrics detect problems with
 - Scattering angles
 - Constant scaling of the variance of the collision error

Manufactured Solutions for the Poisson Equation

Manufacture the electric scalar potential $\phi^M(\mathbf{x}, t)$ and solve

$$\Delta\phi = -\frac{\rho}{\epsilon_0} + \Delta\phi^M + \frac{\rho^M}{\epsilon_0},$$

where $\Delta\phi^M$ is evaluated analytically

Evaluate manufactured charge density analytically as well:

$$\rho^M(\mathbf{x}, t) = q \int_{-\infty}^{\infty} f^M(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} = q f_{\mathbf{x}}(\mathbf{x}, t)$$

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Discretization Parameters

- Discretize spatial domain with uniform cells of length Δx_i
- Numerically integrate with time-step size Δt
- Represent physical particles with N_p computational particles
- Run the collision algorithm N_{avg} times, average the outcomes

Refine these quantities together:

$$\Delta x_i \sim \Delta t \sim h,$$

$$N_p \sim h^{-q}, \quad N_{\text{avg}} \sim h^{-r}, \quad N_{\text{cell}} \sim h^{-3}, \quad N_p^{\text{cell}} \sim h^{-(q-3)}$$

Measure discrete L^1 , L^2 , and L^∞ norms, refine so error in L^∞ is at most $\mathcal{O}(h^2)$

- Collisional: $q = 7 \rightarrow N_p \sim h^{-7}, \quad r = 5 \rightarrow N_{\text{avg}} \sim h^{-5}$
- Collisionless: $q = 5 \rightarrow N_p \sim h^{-5}$

Error Sources

Field Quantities

- Trilinear basis functions: $\mathcal{O}(h^2)$ for ϕ , $\mathcal{O}(h^2)$ recovery for $\mathbf{E} = -\nabla\phi$
- Sampling error: $\mathcal{O}(N_p^{-1/2})$ for ϕ , $\mathcal{O}(N_p^{-1/2}h^{-1/2})$ for \mathbf{E} (Tranquilli et al., 2022)
- Particle-position error: $\mathcal{O}(h^{p_x})$ for ϕ and \mathbf{E}

Particles (second-order-accurate velocity-Verlet time integration)

$$\mathbf{v}_p^{n+1/2} = \mathbf{v}_p^n + \frac{1}{2} \left(\Delta t \frac{q}{m} (\mathbf{E}_p - \mathbf{E}_p^M)^n + \langle \Delta \mathbf{v}_p \rangle_{\text{coll}}^n - \langle \Delta \mathbf{v}_p^M \rangle_{\text{coll}}^n + \Delta t (\dot{\mathbf{v}}_p^M)^n \right) + \boldsymbol{\tau}_{\mathbf{v}_p}^n,$$

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \Delta t (\mathbf{v}_p + \dot{\mathbf{x}}_p^M - \mathbf{v}_p^M)^{n+1/2} + \boldsymbol{\tau}_{\mathbf{x}_p}^n,$$

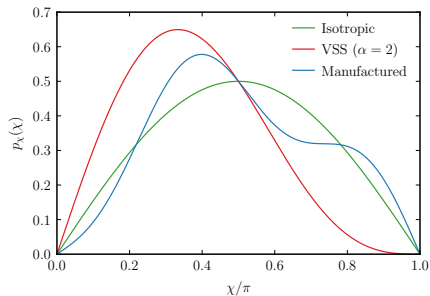
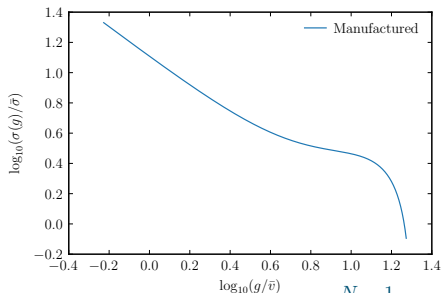
$$\mathbf{v}_p^{n+1} = \mathbf{v}_p^{n+1/2} + \frac{1}{2} \left(\Delta t \frac{q}{m} (\mathbf{E}_p - \mathbf{E}_p^M)^{n+1} + \langle \Delta \mathbf{v}_p \rangle_{\text{coll}}^{n+1/2} - \langle \Delta \mathbf{v}_p^M \rangle_{\text{coll}}^{n+1/2} + \Delta t (\dot{\mathbf{v}}_p^M)^{n+1} \right) + \boldsymbol{\tau}_{\mathbf{v}_p}^{n+1/2}$$

- Per-step collision error: $\mathbf{e}_{\text{coll}_p}^n = \langle \Delta \mathbf{v}_p \rangle_{\text{coll}}^n - \langle \Delta \mathbf{v}_p^M \rangle_{\text{coll}}^n$
- Per-step Lorentz-force acceleration error: $\mathbf{e}_{\text{acc}_p}^n = \Delta t \frac{q}{m} (\mathbf{E}_p - \mathbf{E}_p^M)^n$
- Time-integration truncation errors: $\boldsymbol{\tau}_{\mathbf{v}_p}^n + \boldsymbol{\tau}_{\mathbf{v}_p}^{n+1/2} \sim \mathcal{O}(\Delta t^3)$, $\boldsymbol{\tau}_{\mathbf{x}_p}^n \sim \mathcal{O}(\Delta t^3)$

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Manufactured Cross Section and Anisotropy



- **Cross section** $\sigma(g) = \sum_{n=0}^{N_\sigma-1} \sigma_n g^{2n-1}$
 - $N_\sigma = 3$, $\bar{\sigma} = 1 \text{ \AA}^2$, $\bar{v} = 10^6 \text{ m/s}$

- **Anisotropy** $F_{p_\chi}^{-1}, p_\chi(\chi) = (C_0 + C_1 \cos \chi + C_2 \cos^2 \chi + C_3 \cos^3 \chi) \sin \chi$
 - $\bar{p}_\chi(\chi) = \alpha \cos(\chi/2)^{2\alpha-1} \sin(\chi/2)$, $1 \leq \alpha \leq 2$, (variable soft sphere)
 - **Isotropic** ($\alpha = 1$), **anisotropic** ($\alpha > 1$)

Manufactured Solutions and Discretizations

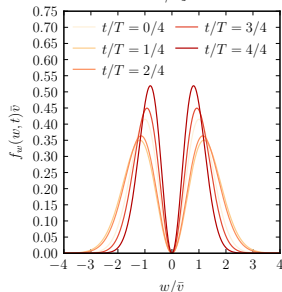
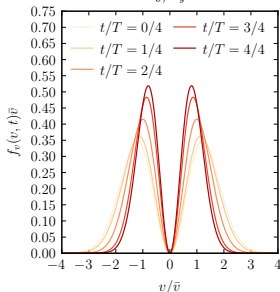
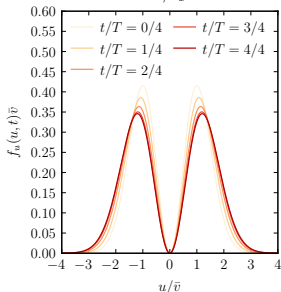
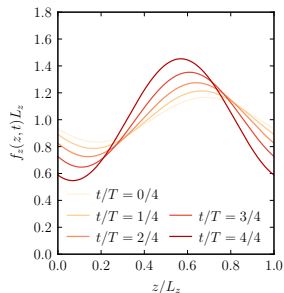
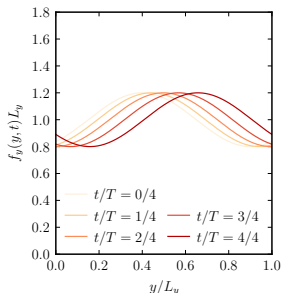
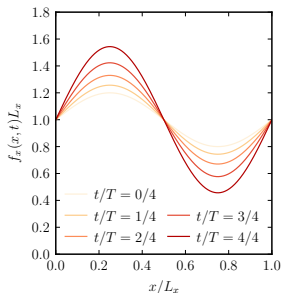
Particle distribution function: $f^M(\mathbf{x}, \mathbf{v}, t) = f_{\mathbf{x}}(\mathbf{x}, t) f_{\mathbf{v}}(\mathbf{v}, t)$,

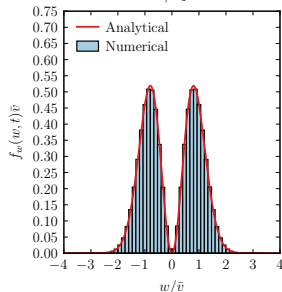
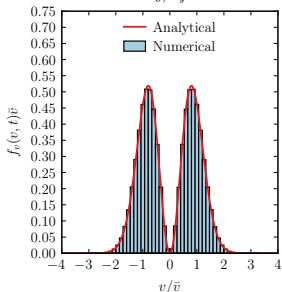
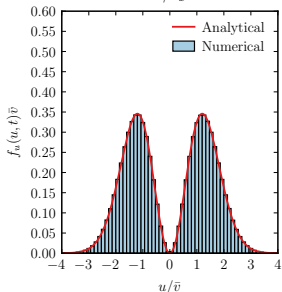
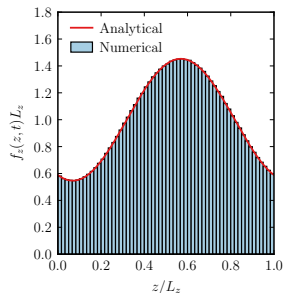
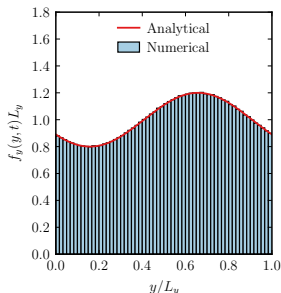
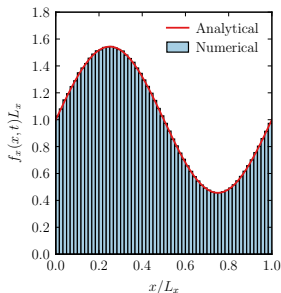
$$f_{\mathbf{x}}(\mathbf{x}, t) = N \prod_{i=1}^3 f_{x_i}(x_i, t), \quad f_{\mathbf{v}}(\mathbf{v}, t) = \prod_{i=1}^3 f_{v_i}(v_i, t),$$

Potential: $\phi^M(\mathbf{x}, t) = \bar{\phi} e^{t/(2T)} \sin\left(2\pi\left[\frac{x}{L_x} - \frac{1}{7}\right]\right) \sin\left(2\pi\left[\frac{y}{L_y} - \frac{1}{5}\right]\right) \sin\left(2\pi\left[\frac{z}{L_z} - \frac{1}{3}\right]\right)$

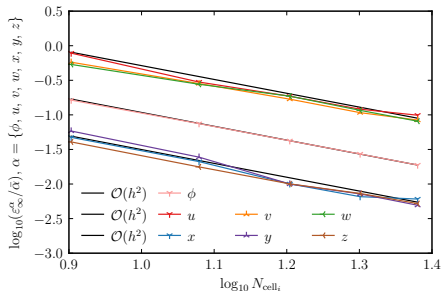
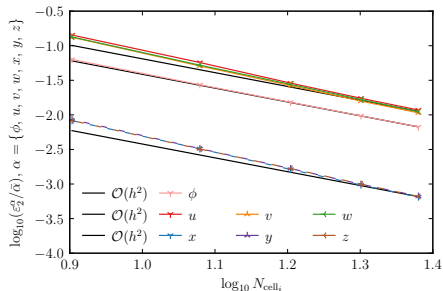
$$\begin{aligned} \bar{v} &= 10^6 \text{ m/s}, & L_{x_i} &= 3/2 \text{ m}, & T &= L_{x_i}/(10\bar{v}), & N &= 10^{20} \text{ particles} \\ q &= e, & m &= 3 \times 10^8 m_e, & \bar{\phi} &= 10^{10} \text{ V}, & & \text{periodic BCs} \end{aligned}$$

Disc.	$T/\Delta t$	N_{cell_i}	N_{cell}	Collisional			Collisionless	
				N_{avg}	N_p	N_p/N_{cell}	N_p	N_p/N_{cell}
1	8	8	512	32	10,240	20.00	10,240	20.00
2	12	12	1,728	243	174,960	101.25	77,760	45.00
3	16	16	4,096	1,024	1,310,720	320.00	327,680	80.00
4	20	20	8,000	3,125	6,250,000	781.25	1,000,000	125.00
5	24	24	13,824	7,776	22,394,880	1620.00	2,488,320	180.00

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

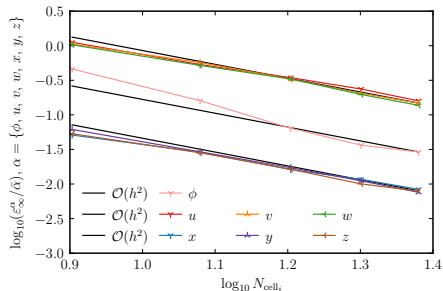
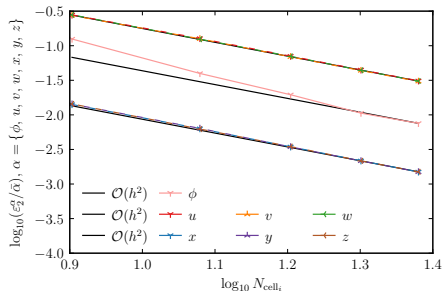
Particle Distribution Function $f_M(\mathbf{x}, \mathbf{v}, t) = f_x(\mathbf{x}, t)f_v(\mathbf{v}, t), t = T$ 

Error Convergence at $t = T$: Collisional, Uncoupled



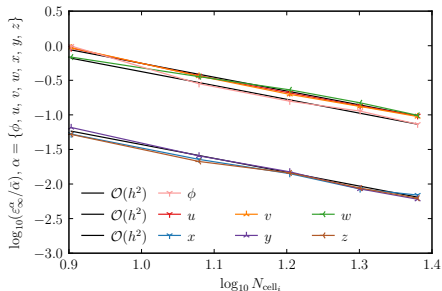
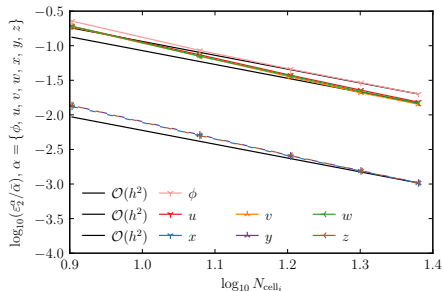
- Particles and field **uncoupled** (single run)
 - Field does not affect particles ($q/m = 0$)
 - Particles do not affect field ($q = 0$)
- Particle error due to **collisions**, **time integration**
 - Velocity and position: $\mathcal{O}(h^2)$ in L^1, L^2, L^∞
- Field error due to **basis functions**
 - Potential: $\mathcal{O}(h^2)$ in L^1, L^2, L^∞

Error Convergence at $t = T$: Collisional, One-Way Coupled



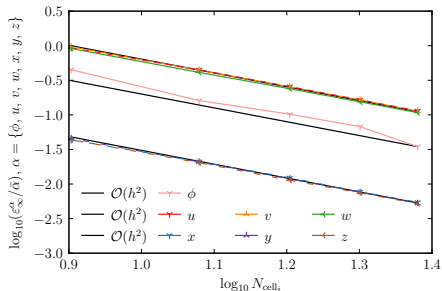
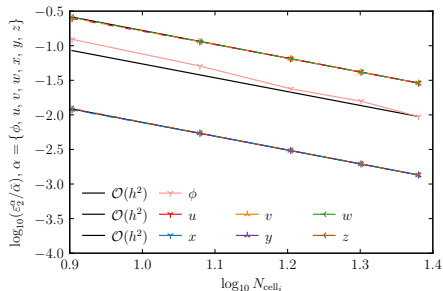
- Particles and field **one-way coupled** (2 separate runs)
 - Field affects particles but is not affected by particles ($q/m \neq 0, q = 0$)
 - Particles affect field but are not affected by field ($q \neq 0, q/m = 0$)
- Particle error due to **collisions**, **time integration**, **field basis function error**
 - Velocity and position: $\mathcal{O}(h^2)$ in L^1, L^2, L^{∞}
- Field error due to **basis functions**, **finite sampling**, **collisions**, **integration**
 - Potential: $\mathcal{O}(h^2)$ in L^1, L^2, L^{∞}

Error Convergence at $t = T$: Collisional, Fully Coupled



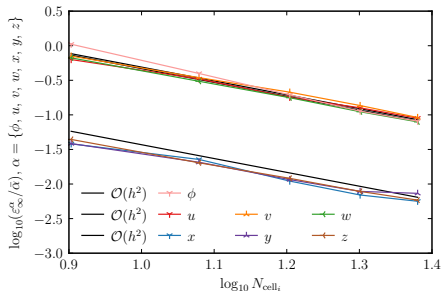
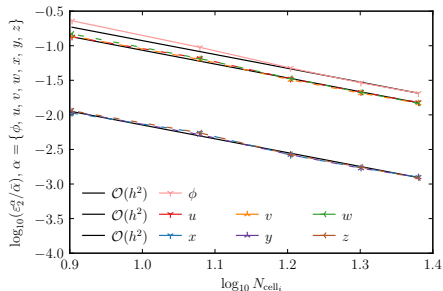
- Particles and field **fully coupled** (single run)
 - Field affects particles ($q/m \neq 0$)
 - Particles affect field ($q \neq 0$)
- Particle error due to **collisions**, **time integration**, **all field errors**
 - Velocity and position: $\mathcal{O}(h^2)$ in L^1, L^2, L^∞
- Field error due to **basis functions**, **finite sampling**, **all particle errors**
 - Potential: $\mathcal{O}(h^2)$ in L^1, L^2, L^∞

Error Convergence at $t = T$: Collisionless, One-Way Coupled



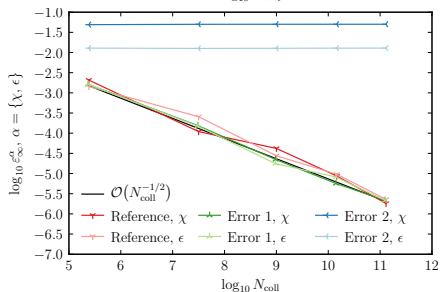
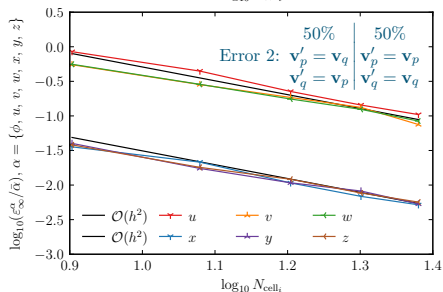
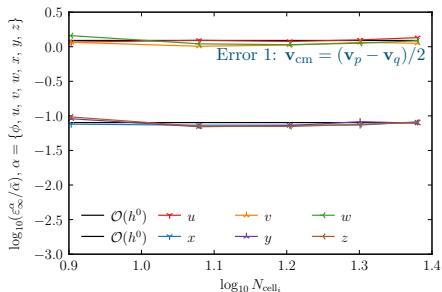
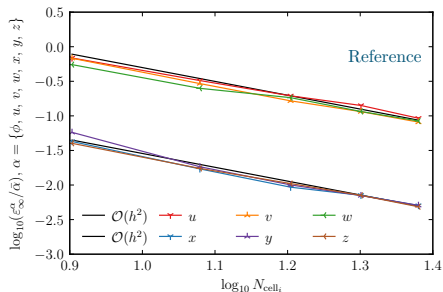
- Particles and field **one-way coupled** (2 separate runs)
 - Field affects particles but is not affected by particles ($q/m \neq 0, q = 0$)
 - Particles affect field but are not affected by field ($q \neq 0, q/m = 0$)
- Particle error due to **time integration**, **field basis function error**
 - Velocity and position: $\mathcal{O}(h^2)$ in L^1, L^2, L^{∞}
- Field error due to **basis functions**, **finite sampling**, **particle time integration**
 - Potential: $\mathcal{O}(h^2)$ in L^1, L^2, L^{∞}

Error Convergence at $t = T$: Collisionless, Fully Coupled



- Particles and field **fully coupled** (single run)
 - Field affects particles ($q/m \neq 0$)
 - Particles affect field ($q \neq 0$)
- Particle error due to **time integration**, **all field errors**
 - Velocity and position: $\mathcal{O}(h^2)$ in L^1, L^2, L^{∞}
- Field error due to **basis functions**, **finite sampling**, **all particle errors**
 - Potential: $\mathcal{O}(h^2)$ in L^1, L^2, L^{∞}

Coding Errors (Collisions Only)



Outline

- Introduction
- Governing Equations
- Manufactured Solutions for PIC Simulations with DSMC
- Error Analysis
- Numerical Examples
- **Summary**
 - Closing Remarks

Closing Remarks

- Presented code-verification approach for collisional PIC simulations
- Added manufactured source terms to equations of motion (weights unmodified)
- Manufactured distribution function, potential, cross section, and anisotropy
- Computed manufactured source terms analytically, averaged collisions
- Achieved expected convergence rates with one simulation per discretization
 - For collisional and collisionless cases with varying degrees of coupling
 - With and without coding errors

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