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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  - 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:

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

- 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	$\nabla \cdot \mathbf{E} = \dfrac{\rho}{\epsilon_0}$	$\rightarrow$	$\boxed{\Delta\phi = -\dfrac{\rho}{\epsilon_0}}$
Gauss's law for magnetism	$\nabla \cdot \mathbf{B} = 0$		$\uparrow$
Faraday's law of induction	$\nabla \times \mathbf{E} = -\dfrac{\partial \cancelto{\mathbf{0}}{\mathbf{B}}}{\partial t}$	$\rightarrow$	$\mathbf{E} = -\nabla\phi$
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

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- Governing Equations
- 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

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

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

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

- 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 $v_{i_p}^M(t)$:

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

- 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:

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

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:

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

$P_{\text{coll}}(g) = \frac{\sigma(g) g w \Delta t}{\Delta V}$ 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 $\mathbf{n}p$)

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

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

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 $\langle \Delta \mathbf{v}_p^M \rangle_{\text{coll}}$ 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

$$\chi = \cos^{-1} \frac{g_z'}{g}, \qquad \epsilon = \tan^{-1} \frac{g_y'}{g_x'},$$

  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:

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

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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:

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

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

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

- Collisional: $q = 7 \rightarrow N_p \sim h^{-7}, \qquad r = 5 \rightarrow N_{\text{avg}} \sim h^{-5}$
- 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: $\mathcal{O}\big(N_p^{-1/2}\big)$ for ϕ, $\mathcal{O}\big(N_p^{-1/2}h^{-1/2}\big)$ for $\mathbf{E}$ (Tranquilli et al., 2022)
- Particle-position error: $\mathcal{O}\big(h^{p_\mathbf{x}}\big)$ for ϕ and $\mathbf{E}$

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

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

- 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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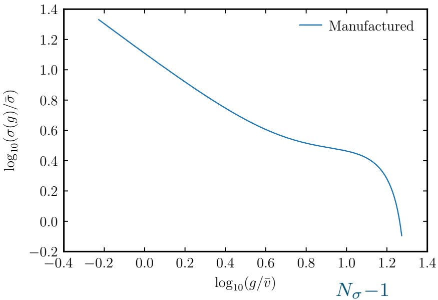
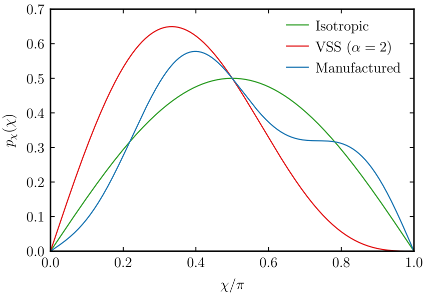
Manufactured Cross Section and Anisotropy





- **Cross section** $\sigma(g) = \sum_{n=0}^{N_\sigma - 1} \sigma_n g^{2n-1}$
  - $N_\sigma = 3, \qquad \bar{\sigma} = 1\ \text{Å}^2, \qquad \bar{v} = 10^6\ \text{m/s}$
- **Anisotropy** $F_{p_\chi}^{-1},\ p_\chi(\chi) = (C_0 + C_1 \cos\chi + C_2 \cos^2\chi + C_3 \cos^3\chi)\sin\chi$
  - $\bar{p}_\chi(\chi) = \alpha\cos(\chi/2)^{2\alpha-1}\sin(\chi/2), \qquad 1 \leq \alpha \leq 2, \qquad$ (variable soft sphere)
  - Isotropic ($\alpha = 1$), anisotropic ($\alpha > 1$)

Manufactured Solutions and Discretizations

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

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

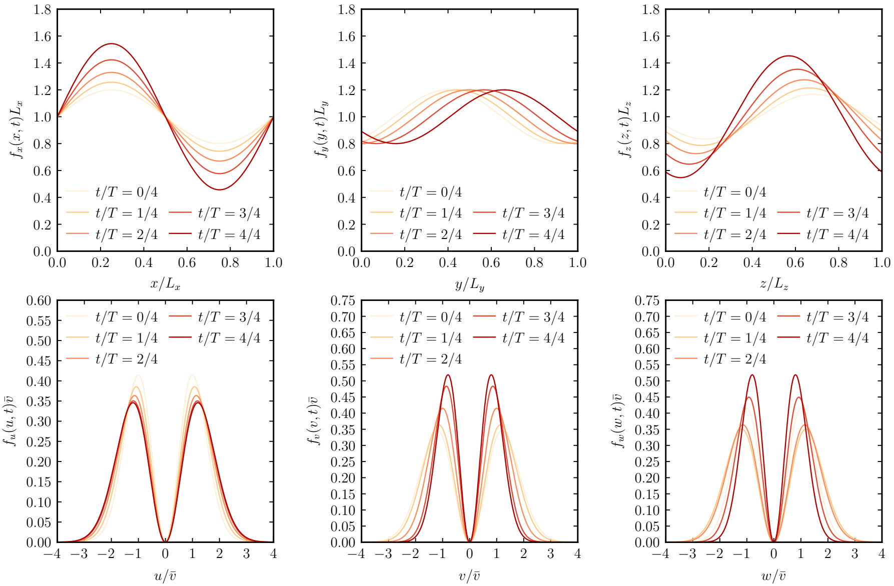
Potential: $\phi^M(\mathbf{x},t) = \bar{\phi} e^{t/(2T)} \sin\left(2\pi\left[\frac{x}{L_x} - \frac{1}{7}\right]\right) \sin\left(2\pi\left[\frac{y}{L_y} - \frac{1}{5}\right]\right) \sin\left(2\pi\left[\frac{z}{L_z} - \frac{1}{3}\right]\right)$

$\bar{v} = 10^6$ m/s, $\quad L_{x_i} = 3/2$ m, $\quad T = L_{x_i}/(10\bar{v})$, $\quad N = 10^{20}$ particles

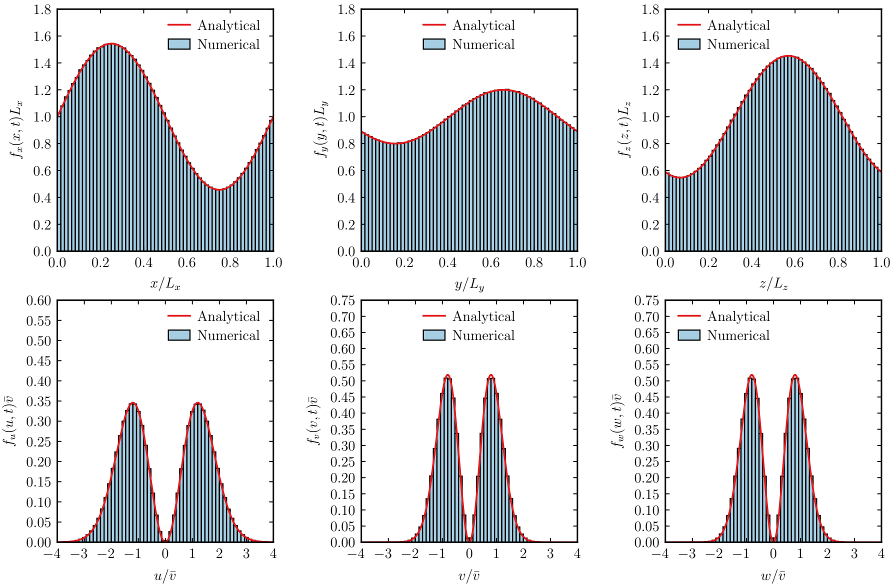
$q = e$, $\quad m = 3 \times 10^8 m_e$, $\quad \bar{\phi} = 10^{10}$ V, $\quad$ periodic BCs

				Collisional			Collisionless	
Disc.	$T/\Delta t$	N_{cell_i}	N_{cell}	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

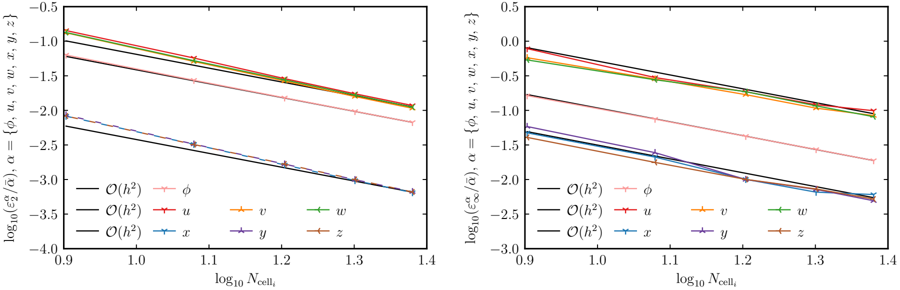
Particle Distribution Function $f_M(\mathbf{x},\mathbf{v},t) = f_{\mathbf{x}}(\mathbf{x},t) f_{\mathbf{v}}(\mathbf{v},t)$



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

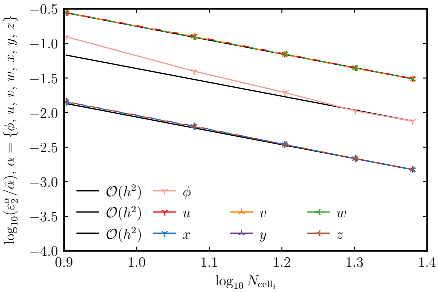


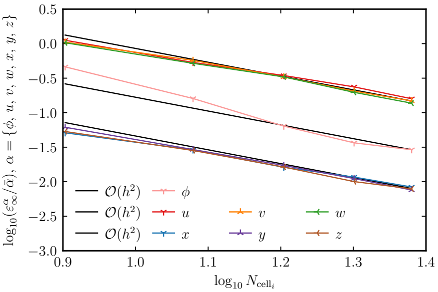
Error Convergence at $t = T$: Collisional, Uncoupled



- 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^∞

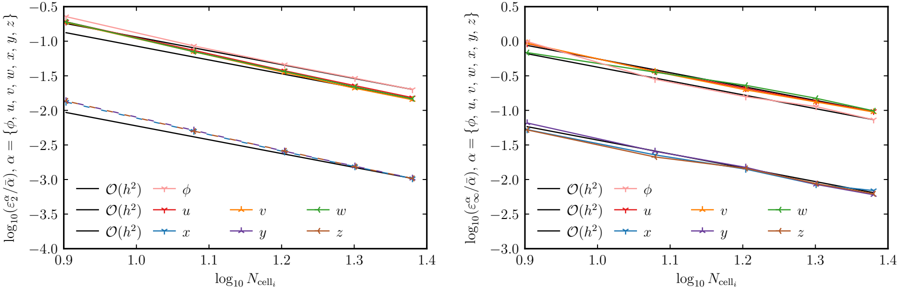
Error Convergence at $t = T$: Collisional, One-Way Coupled





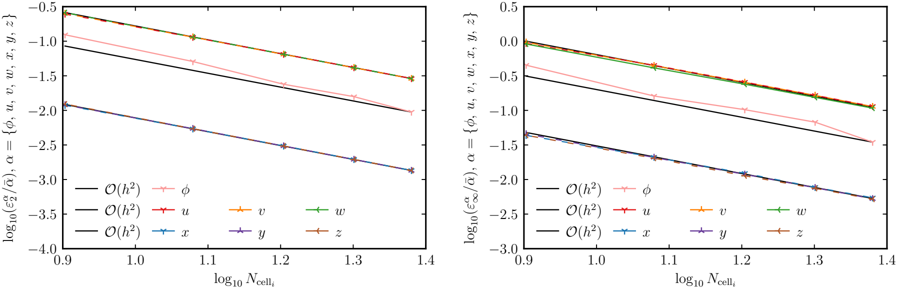
- Particles and field **one-way coupled** (2 separate runs)
  - Field affects particles but is not affected by particles ($q/m \neq 0$, $q = 0$)
  - Particles affect field but are not affected by field ($q \neq 0$, $q/m = 0$)
- Particle error due to collisions, time integration, field basis function 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



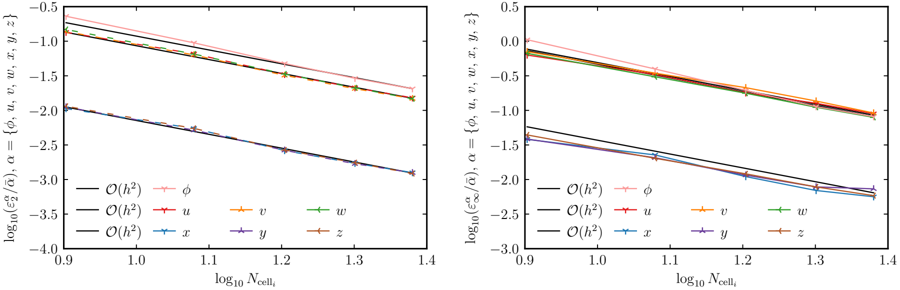
- Particles and field **fully coupled** (single run)
  - Field affects particles ($q/m \neq 0$)
  - Particles affect field ($q \neq 0$)
- Particle error due to collisions, time integration, all field errors
  - Velocity and position: $\mathcal{O}(h^2)$ in L^1, L^2, L^∞
- Field error due to basis functions,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



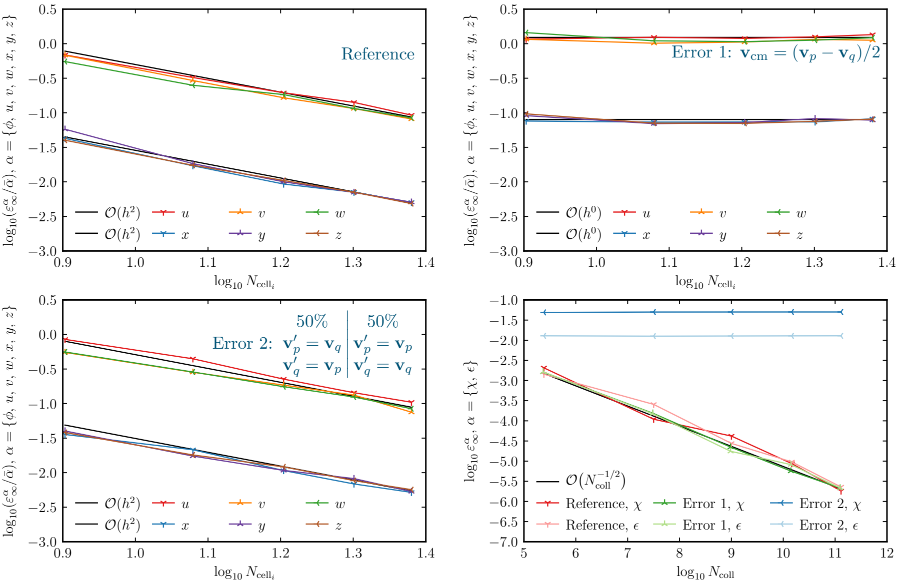
- Particles and field **one-way coupled** (2 separate runs)
  - Field affects particles but is not affected by particles ($q/m \neq 0$, $q = 0$)
  - Particles affect field but are not affected by field ($q \neq 0$, $q/m = 0$)
- Particle error due to time integration, field basis function error
  - Velocity 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

Questions?

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- David Sirajuddin
- Tom Smith

References

- B. Freno, W. McDoniel, C. Moore, N. Matula
  Code-verification techniques for particle-in-cell simulations with DSMC collisions
  `arXiv:2602.15130`

- F. Riva and C. Beadle and P. Ricci
  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)