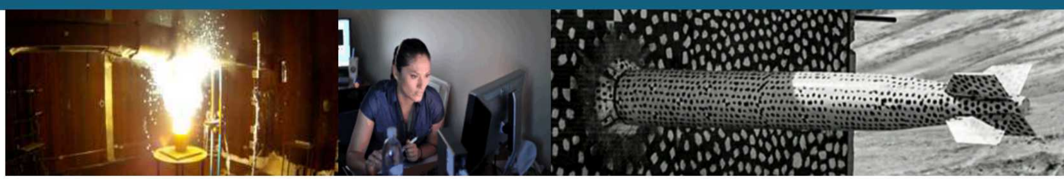
SAND2019-10287C

# Hybrid fluid-kinetic models for high-energy-density plasmas



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# Motivation

Sandia's applications are primarily focused on high energy density regimes where plasmas interact with material structures.

Collisional process in the high-energy density (HED) regime are dependent on both charged and neutral interactions.

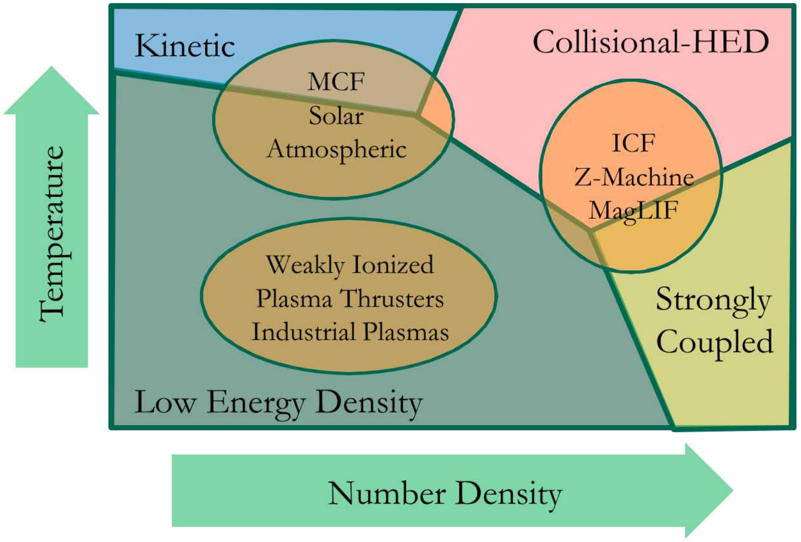
- Understanding energy deposition and heating processes requires high-fidelity representations of kinetic plasma effects.

Existing strategies attempt to resolve physics using particle-based sampling schemes.

- Highly collisional systems (e.g. dense plasmas or background neutral gas) lead to slow collisional evaluations.

**Goal**: Use a fluid to accelerate a particle scheme in regimes dominated by collisional transport.

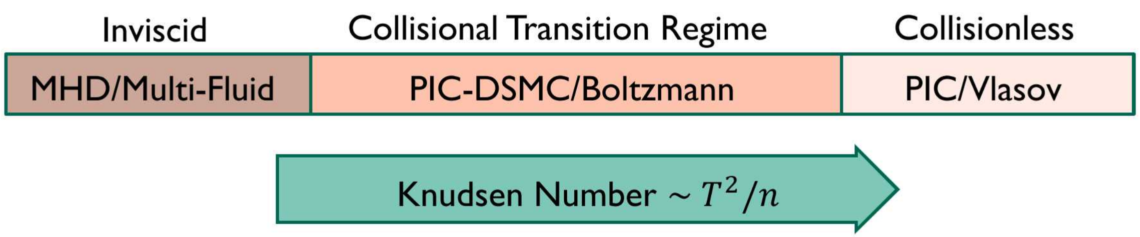
Plasma Regimes vs Applications



# Collisional Processes in Plasmas

Collisional transport in plasmas is strongly dependent on temperature, density, and background material properties (e.g. neutral gas).

- There are three main regimes for model development in plasma physics:




The rule of thumb is:

- Fluid models: Fast and accurate, but misses important physics.
- Kinetic (particle) models: Slow and noisy, but include missing physics.

Magnetization plays a large role in collisional transport, as the magnetic field reduces collisional mean free paths in directions orthogonal to the field. Hall Parameter $H$ is the ratio of collisional time scales to cyclotron time scales

- Fluid approach: Braginskii closures – limited to highly collisional regime with moderate magnetic fields ($H \leq 1$)
- Kinetic approach: Gyrokinetic models – valid for strongly magnetized systems ($H \gg 1$)

# Kinetic Plasmas – Boltzmann Model

Kinetic models for plasmas attempt to represent the full phase space form for the particle distribution.

- The full Boltzmann model evolves a phase space distribution $f_\alpha$ for a species $\alpha$ through advective, electromagnetic, and collisional effects.

$$\mathcal{L}[f_\alpha] = \partial_t f_\alpha + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{v}\, f_\alpha) + \nabla_{\boldsymbol{v}} \cdot \left( \frac{q_\alpha}{m_\alpha} (\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})\, f_\alpha \right) = (\partial_t f_\alpha)_{col}$$

The electromagnetics are represented by Maxwell's equations.

$$\partial_t \boldsymbol{E} - c^2 \nabla \times \boldsymbol{B} = -\frac{1}{\epsilon_0} \sum_\alpha q_\alpha \int \boldsymbol{v}\, f_\alpha\, d^3 v$$

$$\partial_t \boldsymbol{B} + \nabla \times \boldsymbol{E} = 0$$

6D model → Extremely large scale simulation if discretized on 6D mesh.

- **Particle-in-cell (PIC)**: Sample the distribution in velocity space and evolve samples in time.

# Kinetics via Particle-In-Cell (PIC)

PIC approximates 6D Vlasov/Boltzmann by sampling velocity space
- Highly magnetized/dense plasmas require 100's or 1000's of particles per cell.
- Each particle update uses the simplified equations of motion:

$$\mathcal{L}[f_\alpha] = \partial_t f_\alpha + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{v}\, f_\alpha) + \nabla_{\boldsymbol{v}} \cdot \left( \frac{q_\alpha}{m_\alpha} (\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})\, f_\alpha \right) \rightarrow \begin{cases} \partial_t \boldsymbol{x}_p^\alpha = \boldsymbol{v}_p^\alpha \\ \partial_t \boldsymbol{v}_p^\alpha = \dfrac{q_\alpha}{m_\alpha} \left( \boldsymbol{E} + \boldsymbol{v}_p^\alpha \times \boldsymbol{B} \right) \end{cases}$$

Maxwell's Equations are solved on a mesh:
- Issue of projecting particle data onto unstructured mesh, and mesh data onto particles.
- Divergence errors in magnetic fields cause issues with PIC.

Direct-Simulation Monte-Carlo (DSMC) collides particles to model thermalization
- High-density regimes require many stochastic collisions.
- Collisions can generate new particles (problem size grows over time).

Our discretization uses a Dirac-delta distribution shaping function in both physical and velocity space for each sample.
- Leads to noise and Debye heating.
- Moments of particles are very noisy (needs 1000s of particles per cell)

# Reducing Kinetic to Fluid Representation

Fluid models are derived by taking moments of the Boltzmann model and making assumptions about how to close the system.

- Limiting the phase space distribution to a Maxwell-Boltzmann distribution leads to a complete set of five moments:

$$\langle g(\boldsymbol{v})\rangle_\alpha = m_\alpha \int_{-\infty}^{\infty} g(\boldsymbol{v})\, d^3v \rightarrow \begin{cases} \rho_\alpha = \langle f_\alpha(v)\rangle_\alpha & \text{Mass Density} \\ \boldsymbol{p}_\alpha = \langle \boldsymbol{v} f_\alpha(v)\rangle_\alpha & \text{Momentum Density} \\ \epsilon_\alpha = \frac{1}{2}\langle \boldsymbol{v}^2 f_\alpha(v)\rangle_\alpha & \text{Total Isotropic Energy Density} \end{cases}$$

- Moments of the Boltzmann model give the Euler fluid equations:

$$\langle \mathcal{L}[f_\alpha]\rangle_\alpha = \langle C_\alpha\rangle_\alpha \qquad \text{Continuity Equation}$$

$$\langle \boldsymbol{v}\mathcal{L}[f_\alpha]\rangle_\alpha = \langle \boldsymbol{v} C_\alpha\rangle_\alpha \qquad \text{Momentum Equation}$$

$$\frac{1}{2}\langle \boldsymbol{v}^2\mathcal{L}[f_\alpha]\rangle_\alpha = \frac{1}{2}\langle \boldsymbol{v}^2 C_\alpha\rangle_\alpha \qquad \text{Energy Equation}$$

System is closed assuming the distribution $f_\alpha$ remains in local thermal equilibrium.

- Deviations from equilibrium treated using viscous closure (Navier-Stokes, Braginskii, etc.)

# Euler Fluid: Moments of Boltzmann Model

Fluids are linked to kinetics through the anisotropic pressure $\boldsymbol{\Pi}$ and heat flux $\boldsymbol{q}$, electromagnetics, and collisions:

- Continuity Equation: $\partial_t \rho + \nabla \cdot \boldsymbol{p} = 0$
- Momentum Equation: $\partial_t \boldsymbol{p} + \nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{p} + P\boldsymbol{I} + \boldsymbol{\Pi}) = qn(\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B}) + \boldsymbol{R}$
- Energy Equation: $\partial_t \epsilon + \nabla \cdot (\boldsymbol{u}(\epsilon + P) + \boldsymbol{u} \cdot \boldsymbol{\Pi} + \boldsymbol{q}) = qn\boldsymbol{u} \cdot \boldsymbol{E} + \boldsymbol{u} \cdot \boldsymbol{R} + Q$

Model is discretized using a discontinuous Galerkin (DG) representation:

- Strong Form: $\partial_t u + \nabla \cdot \boldsymbol{f} = s, \quad u \in \{\rho, \boldsymbol{p}, \epsilon\}$

Discontinuous Basis: $\phi_i^K$ in element $K \in \Omega$

- Weak Form: $\int_{\mathrm{K}} \phi_i^K \partial_t u \, dV + \oint_{\partial \mathrm{K}} \phi_i^K \hat{\boldsymbol{n}} \cdot \boldsymbol{f} \, dS - \int_{\mathrm{K}} \boldsymbol{f} \cdot \nabla \phi_i^K dV = \int_{\mathrm{K}} \phi_i^K s \, dV$

Scheme is chosen due to its nice computational properties:

- Arbitrary order of accuracy.
- Can be embedded easily into fast/scalable implicit-explicit time integration schemes.
- Supports various stabilization methods.

Discretization relies on consistency condition on the normal flux on the surface of each cell to be globally conservative.

# Exact Sequence Discretization for EM

A compatible finite element discretization is used to enforce the divergence constraints for the electric and magnetic fields.

- Fluids are represented by an **HGrad** (node) basis $\rho \in V_{\nabla}$.
- The electric field is represented by an **HCurl** (edge) vector basis **E** $\in \boldsymbol{V}_{\nabla\times}$.
- The magnetic field is represented by an **HDiv** (face) vector basis **B** $\in \boldsymbol{V}_{\nabla\cdot}$.

Formulation supports the discrete preservation of the De Rham Complex.

- In this case, the discretization supports the divergence involutions for Gauss' laws:

$$\partial_t \boldsymbol{B} + \nabla \times \boldsymbol{E} = 0 \qquad \text{Strongly Enforces:} \quad \partial_t(\nabla \cdot \boldsymbol{B}) = 0$$

$$\partial_t \boldsymbol{E} - c^2 \nabla \times \boldsymbol{B} = -\frac{1}{\epsilon_0}\boldsymbol{j} \qquad \text{Weakly Enforces:} \quad \partial_t(\epsilon_0 \nabla \cdot \boldsymbol{E} - \rho_c) = 0$$

This has been shown to work for continuous discretizations [1] and PIC, currently working to extend its validity to discontinuous fluid discretizations.

[1] S. T. Miller, et al. *IMEX and exact sequence discretization of the multi-fluid plasma model*. JCP 2019

# Hybrid Kinetic Modeling by Species

Low temperature, high density species are represented by a fluid.

- Closures (collisional coupling) are either inviscid, Navier-Stokes, or Braginskii.

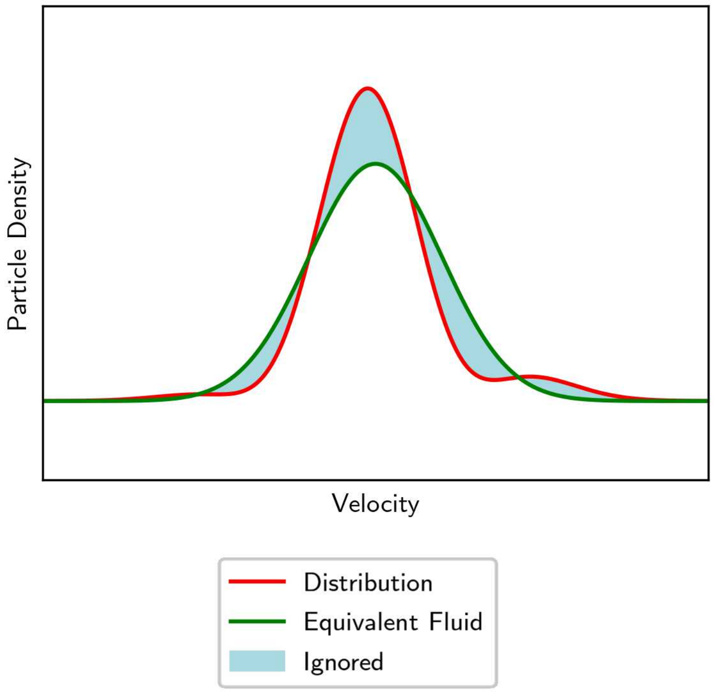
High temperature, low density species are represented using PIC.

- Direct-simulation Monte-Carlo (DSMC) is used to represent collisions if required.

The main challenge with this approach is that there is a limited application regime where this is accurate.

- Fluid will generate incorrect wave speeds for collisional/electrostatic/acoustic processes.
- Currents associated with the fluid can have a dramatic influence on electromagnetics when the fluid is outside its validity regime.

**Inherent problem**: Fluids potentially ignore much of the distribution.



# Hybrid Kinetic Modeling by Component

$\delta f$ models mix fluid and kinetic representations to reduce computational cost associated with the kinetic representation for dense plasma regimes.

The model is based on assuming the phase space distribution $f$ is represented by a Maxwell-Boltzmann distribution $f_m$ and a deviation $\delta f = f - f_m$ such that

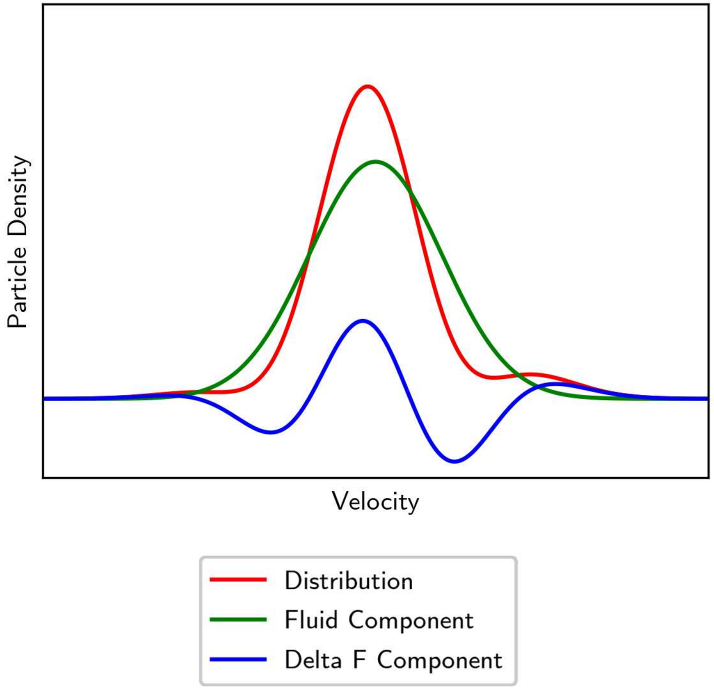
$$\mathcal{L}[f] = C \rightarrow \mathcal{L}[\delta f] = -\mathcal{L}[f_m] + C = S$$

- $\mathcal{L}[\delta f]$ is modeled with a kinetic representation.
- $\mathcal{L}[f_m]$ is modeled with a fluid representation.

To keep this scheme consistent, we have to couple the kinetic model to the fluid evolution.

- For PIC this means generating deviatoric particles.

The $\delta f$ component feeds the missing kinetic component back into the model.



# Kinetic Representation for $\delta f$ Model

The Maxwell-Boltzmann distribution is defined by the number density $n$, flow velocity $\boldsymbol{u}$, and standard deviation $\sigma = T/m$ as

$$f_m = n\left(\frac{1}{2\,\pi\,\sigma^2}\right)^{\frac{3}{2}} \exp\left(-\frac{1}{2}\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{\sigma^2}\right)$$

Which means that the chain rule can be used to define the kinetic source using the fluid mass density $\rho$, momentum $\boldsymbol{p}$, and energy $\epsilon$

$$S = -\partial_\rho f_m(\partial_t\rho + \boldsymbol{v}\cdot\nabla\rho) - \nabla_p f_m\cdot(\partial_t\boldsymbol{p} + \boldsymbol{v}\cdot\nabla\boldsymbol{p})$$
$$-\partial_\epsilon f_m(\partial_t\epsilon + \boldsymbol{v}\cdot\nabla\epsilon) - \boldsymbol{a}\cdot\nabla_v f_m + C$$

- $\partial_t\rho$, $\partial_t\boldsymbol{p}$, $\partial_t\epsilon$, $\nabla\rho$, $\nabla\boldsymbol{p}$, and $\nabla\epsilon$: taken from the fluid representation.
- $\partial_\rho f_m$, $\nabla_p f_m$, $\partial_\epsilon f_m$, and $\nabla_v f_m$: have analytic solutions.

**Challenges**:

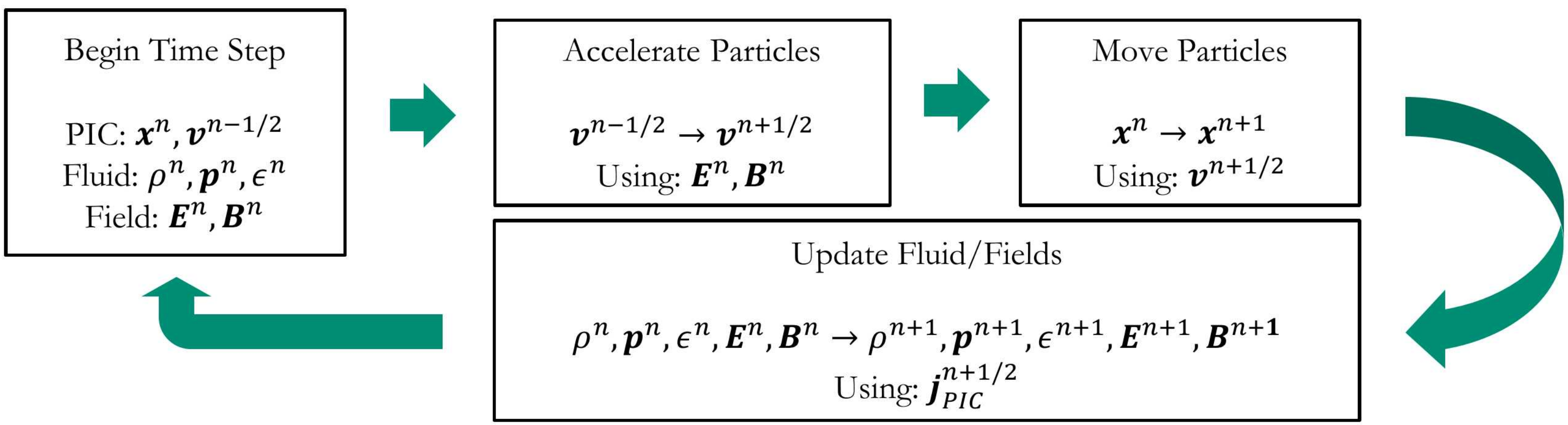
- How do we generate particles to represent this source?
- How many particles do we need to add?
- What is the impact of negative weight particles on electromagnetics?

# Time Integration

Time integration for hybrid models is challenging and not well understood.

- PIC: Simplectic time integrators or L-stable implicit integrators.
- Fluid: Dissipative (SSP) Runge-Kutta (RK) explicit integrators and SSPRK-IMEX
- Maxwell: Linear equation set - supports everything.

To retain stability in the fluid solve, the initial implementation merges a leap-frog integrator with a 3rd order SSP-RK method:



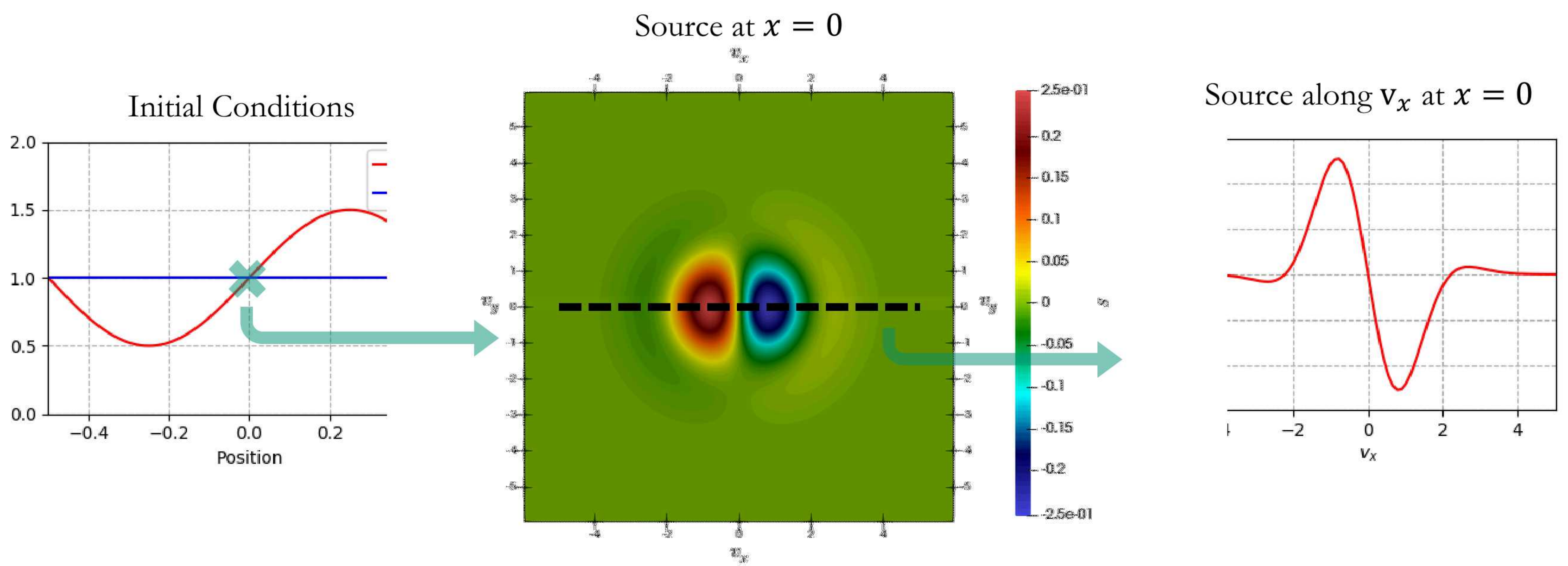

**Challenges**:

- Can we get greater than first order time convergence?
- How does dissipation in field integrator affect particles?

# Full PIC vs Hybrid (Neutral)

The simplest test for the $\delta f$ particle source is a direct comparison with Full PIC for a continuous solution where the gradients are well defined for the fluid.

- Constant pressure with sine wave in density → temperature gradient.




This is a static solution for a inviscid fluid, however, the kinetic solution evolves to where the density is constant.

# Hybrid Closure - Good Agreement With PIC

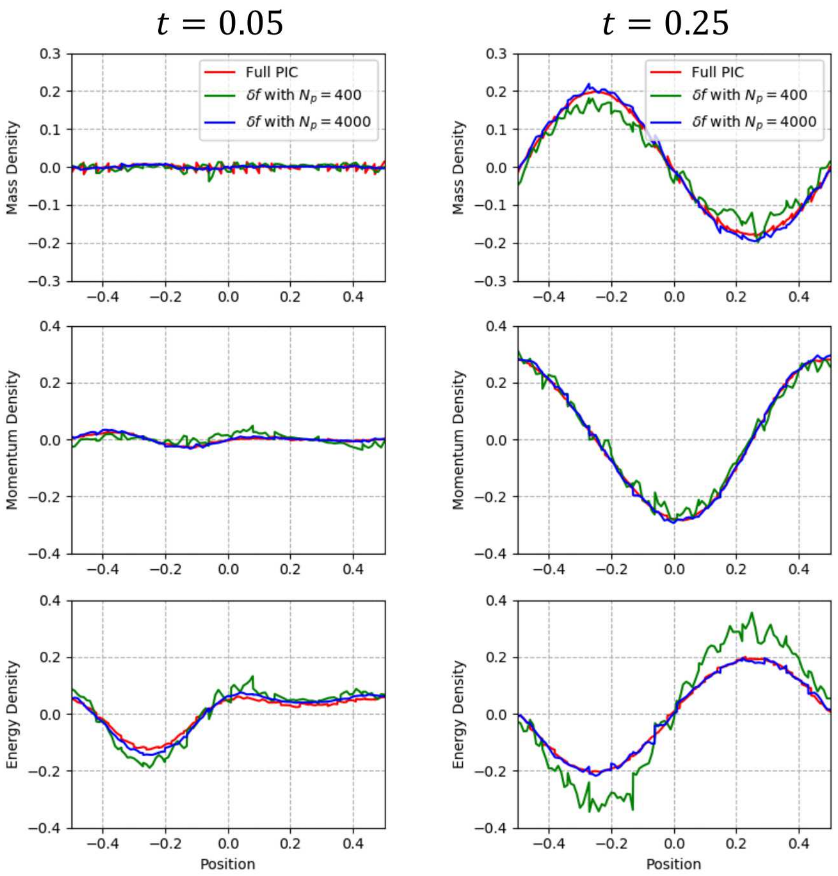
Tested against number of particles added to a cell per time step ($N_p$).

- Full PIC simulation initialized with $100k$ particles per cell.
- $\delta f$ particles are placed every $\Delta t = 0.01$.

Good agreement seen between full PIC simulation and high particle count $\delta f$ simulation.

Lower particle count $\delta f$ simulation is seen to predict the wrong mass and energy, and is very noisy.

Results can be cleaned up with a better particle placement strategy.



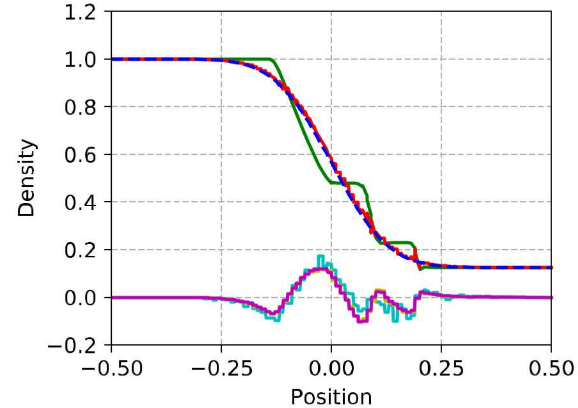
# Dynamic Fluids Also Show Good Agreement

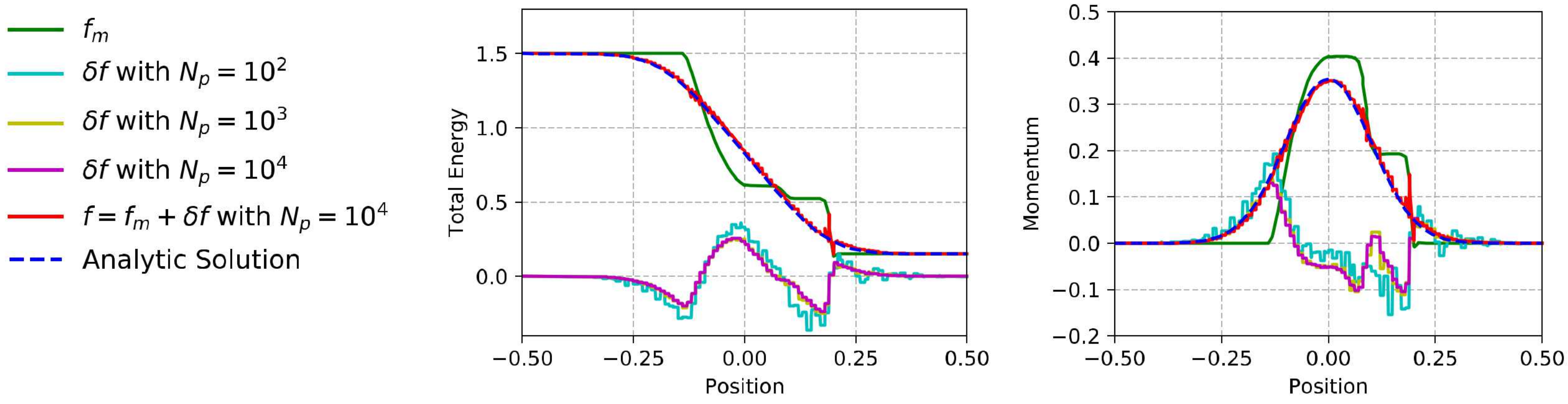
A shock tube simulation is more challenging as the fluid evolves and must remain consistent with the analytic solution.

- Example adds at most 1000 particles to each of 200 cells at 120 equally spaced times ending at 0.1.
- Particles are only added if their weight is sufficient.

The main challenge with shock physics is resolving the steep gradients that feed into the particle source.

**Sod Shock Tube:** Good agreement in smooth areas. Poor agreement at shock interfaces.



# Full PIC vs Hybrid (Electromagnetic)

Electromagnetic simulation uses same initialization as neutral wave, however now with imposed magnetic component.

- Single positron species.
- Speed of sound set to $v_s = 0.1c$.
- Density is chosen to have 20 Debye lengths in the domain to reduce Debye heating.
- Magnetic coupling length scales are chosen to be similar to Debye length: $\omega_p = 2\omega_c$.

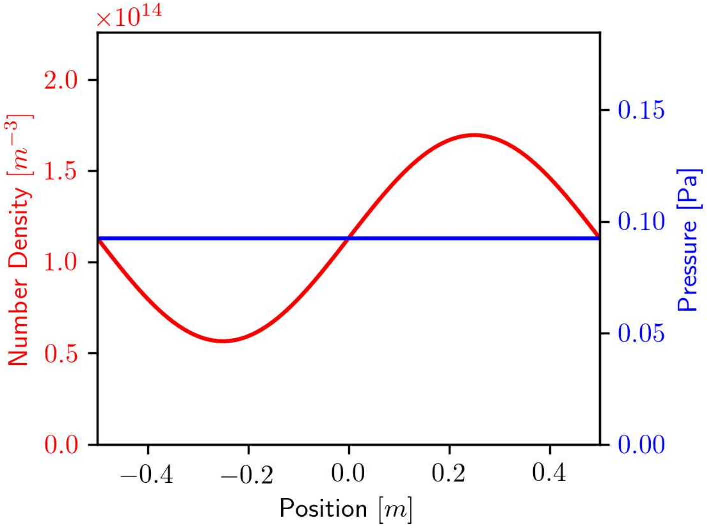
PIC initialized with 40 million particles.

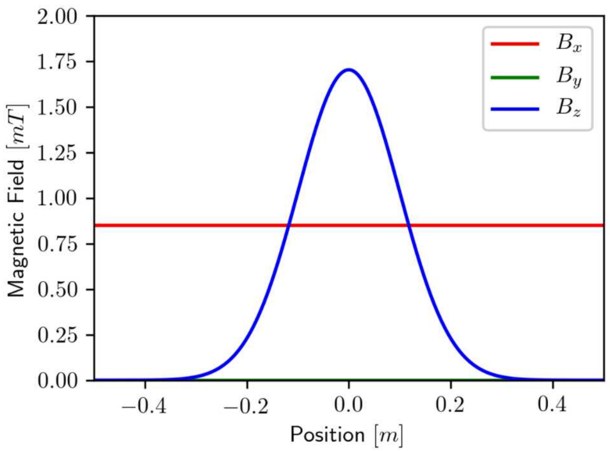
- Overkill, but needed to reduce noise in moments.

Delta F initialized with 0 particles, but particles are added over time.

- As few as 5 particles per time step per cell give accurate electromagnetic response.

**Goal**: Problem is designed to see full electromagnetic and electrostatic response of the Delta F model in comparison to pure fluid and PIC.



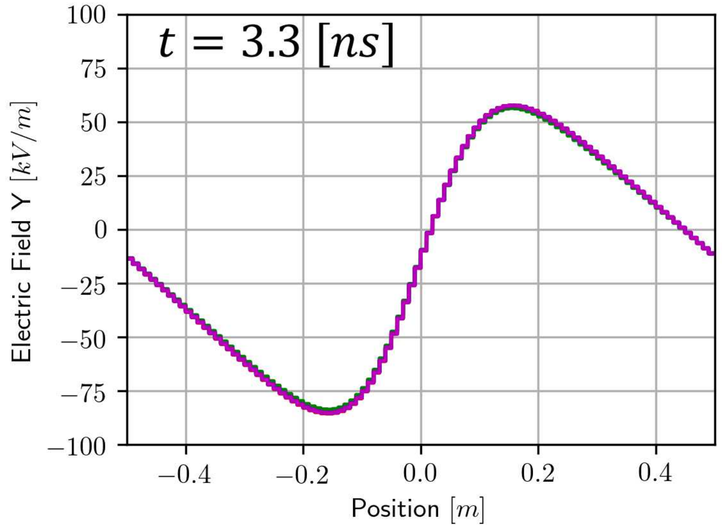
# Electromagnetic Hybrid Shows Good Agreement

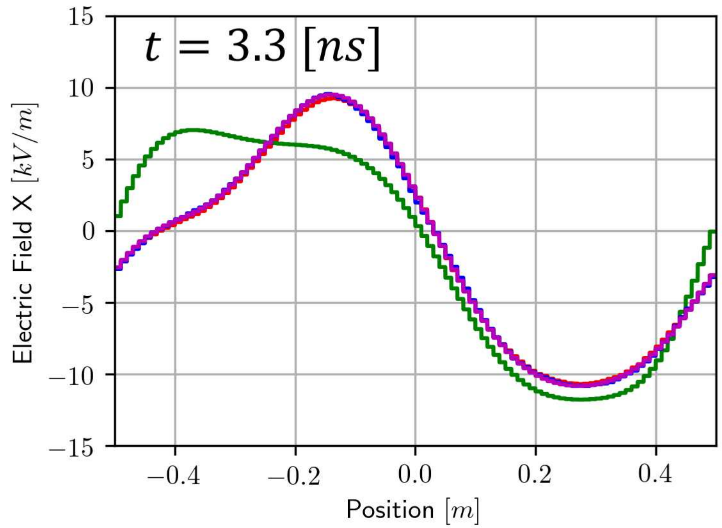
Electromagnetic response, $E_y$, shows little difference between pure fluid, PIC, and the hybrid closure.

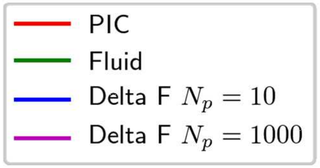
Electrostatic response $E_x$ deviates between fluid and PIC due to the thermal response of the inviscid fluid.

- The hybrid closure scheme brings these effects back into the model to give a consistent electric response.
- Two particle counts per time step are shown, results show minor deviations between them associated with noise.

**Result**: The choice of using a species separated hybrid, or hybrid closure scheme is strongly tied to the physical behavior of interest.



# Electromagnetic Hybrid Moments Show Impact of Delta F

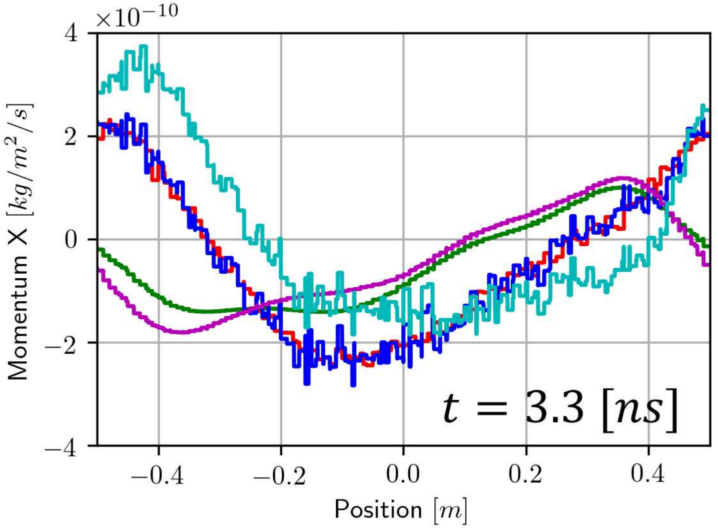
The impact of the closure is more easily seen when viewing the moments.

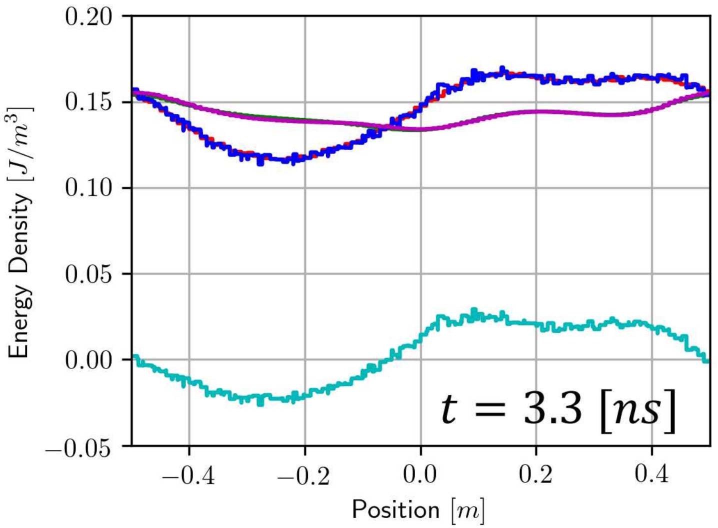
- Example: Delta F has 10 particles added per cell per time step.

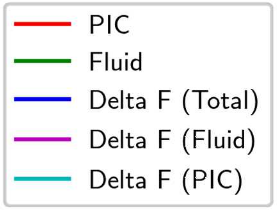
Momentum along the acoustic direction is seen to deviate from the particle response by a large factor.

- The hybrid closure acts to represent the missing current, however magnitude of PIC moments can exceed fluid components.
- Due to field effects, the fluid component of Delta F does not agree with the fluid-only simulation.

**Result**: To reduce particle counts we must couple the PIC moments back into the fluid.



## Summary

Neutral $\delta f$ compares well to full kinetic solution for:

- Static, well-resolved fluid.
- Shock based fluid evolution.

Electromagnetic $\delta f$ compares well to full kinetic solution over pure fluid solution.

Choice of sampling scheme for particle source is important.

Stable evolution of discontinuous Galerkin fluid using exact sequence discretized electromagnetics was shown.

- Noise from PIC did not affect fluid stability for smooth problems.

# The Next Steps

The main pieces missing include feedback and collisions:

$$\partial_t \rho + \nabla \cdot \boldsymbol{p} = 0$$

$$\partial_t \boldsymbol{p} + \nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{p} + P\boldsymbol{I} + \boldsymbol{\Pi}) = \frac{q}{m}(\rho \boldsymbol{E} + \boldsymbol{p} \times \boldsymbol{B}) + \boldsymbol{R}$$

$$\partial_t \epsilon + \nabla \cdot (\boldsymbol{u}(\epsilon + P) + \boldsymbol{u} \cdot \boldsymbol{\Pi} + \boldsymbol{q}) = \frac{q}{m}\boldsymbol{p} \cdot \boldsymbol{E} + \boldsymbol{u} \cdot \boldsymbol{R} + Q$$

$$S = -\partial_\rho f_m(\partial_t \rho + \boldsymbol{v} \cdot \nabla \rho) - \nabla_p f_m \cdot (\partial_t \boldsymbol{p} + \boldsymbol{v} \cdot \nabla \boldsymbol{p})$$

$$-\partial_\epsilon f_m(\partial_t \epsilon + \boldsymbol{v} \cdot \nabla \epsilon) - \boldsymbol{a} \cdot \nabla_v f_m + C$$

Optimization of the algorithm is needed:

- Particle merge algorithm to reduce the number of particles in a simulation.
- Automated/adaptive control of how many particles are added per cell.

Additionally, we are looking into IMEX time integration to step over plasma frequency, cyclotron frequency, and fluid time scales.