Comparisons of Collisional Interactions between Kinetic and Fluid Models

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Abstract

A previous Code Comparison Infrastructure (CCI) study focused on non-collisional plasma expansion problems. Here we build on that work by considering collisional plasma behavior. We seek to understand the physics of collisions and how they are modeled in both Particle-In-Cell (PIC) and multifluid plasma codes with an overarching goal of establishing and demonstrating model consistency. We also seek to identify limitations of the methods and codes to better inform approaches to hybrid modeling which strives to enable dramatic gains in performance without sacrificing modeling fidelity.

Problems and Codes

Codes	0-D Maxwell Mol. Thermalize (w/o drift)	0-D Maxwell Mol. Thermalize (w. drift)	0-D Coulomb Thermalize	1-D Neutral Expanding Slab
Aleph - PIC	x	x	x	x
Drekar - fluid	x		x	x
Empire-PIC	x			x
Empire-fluid	x	x		x

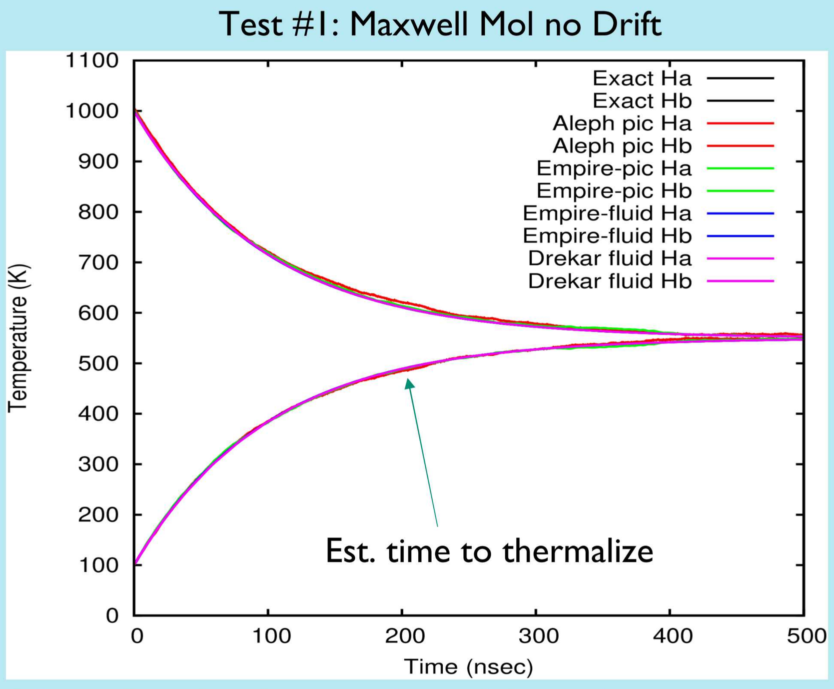
Outcomes of this activity include the following:

- Construct code-to-code comparison tests in CCI
- Understand how to achieve consistency between PIC and fluid operators
- Understand how to achieve consistency in problem specifications across the respective codes
- Understand how to identify the onset of non-Maxwellian evolution from collisions and how it relates to delta-f

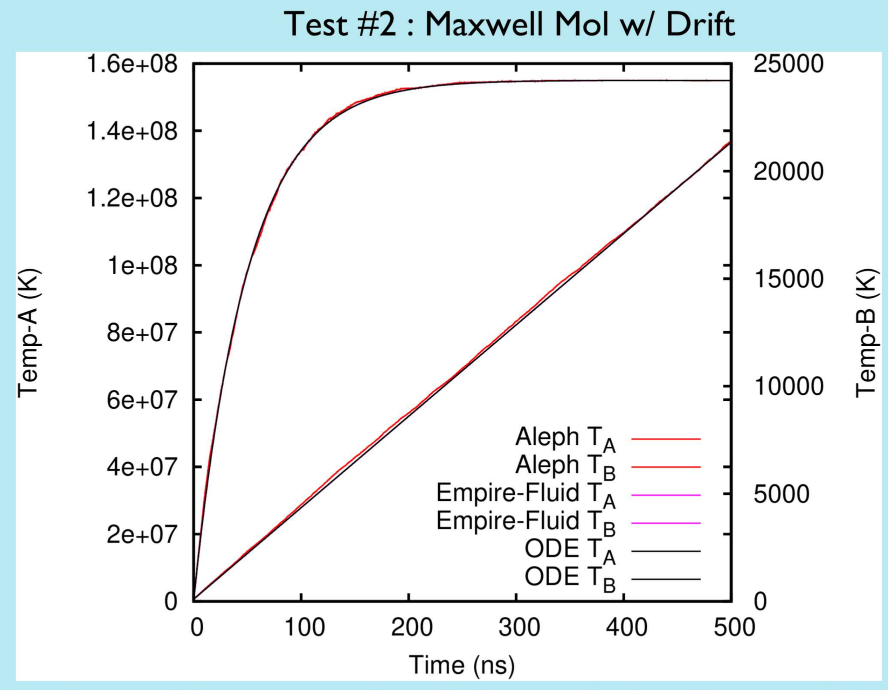
Maxwell Molecule Model Thermalization

Cross-section for PIC: $\sigma = \frac{\sigma_0}{||\mathbf{v}_\alpha - \mathbf{v}_\beta||}$ → Constant fluid collision rate: $\nu = n < \sigma v >$

Test #1: Maxwell Mol no Drift

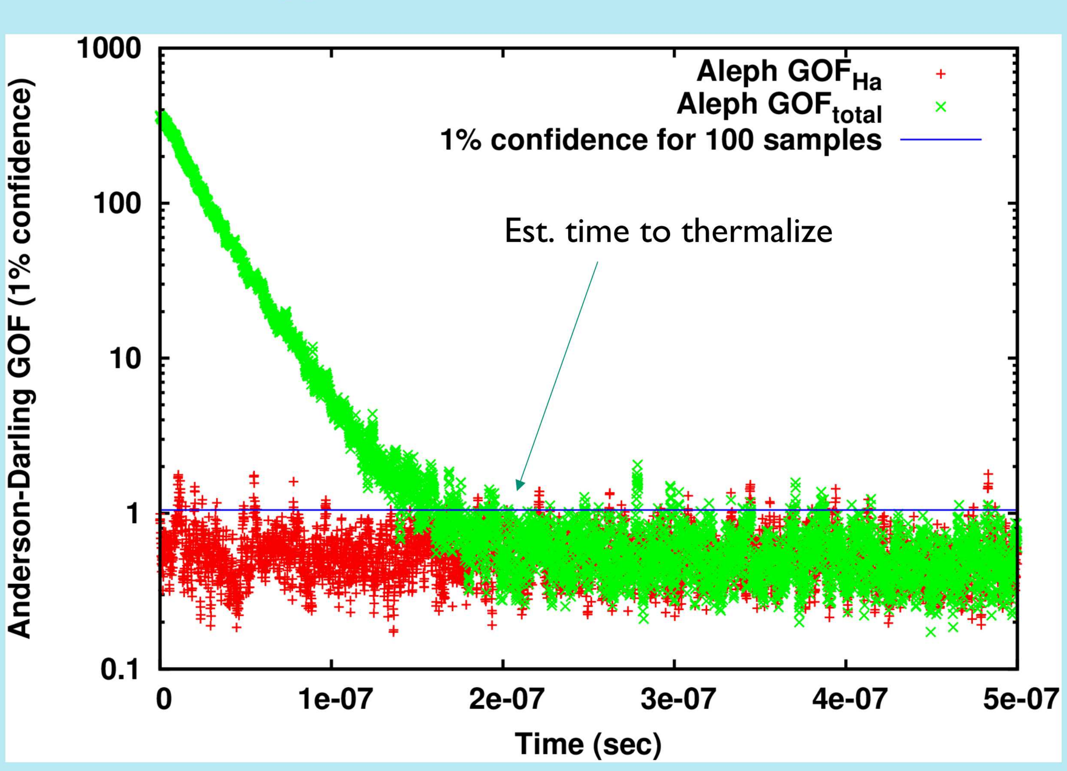


Test #2 : Maxwell Mol w/ Drift



Maxwell molecules permit model consistency across codes along with an exact closed-form solution for non-drifting particles. Additional modeling terms become active with drifted distributions and can be compared against a known solution for a subset of the codes.

CCI allows rigorous comparisons across codes (and models) along with verification against known solutions when applicable.



Maxwellian Expectation

Anderson-Darling Goodness-of-Fit to estimate (with confidence level) how Gaussian a discrete VDF is. This metric can indicate time to thermalize, opportunity to switch between fluid and kinetic models and possibly inform delta-f hybrid approaches.

Points below Blue Line are time steps with 99% confidence of being from a Maxwellian (thermalized) distribution.

Coulombic Thermalization

Fluid Model
Martinez-Gomez

$$\frac{\partial \rho_s}{\partial t} = 0$$
$$\frac{\partial \rho_s \mathbf{u}_s}{\partial t} = \sum_{t \neq s} \alpha_{st}\rho_s\rho_t(\mathbf{u}_t - \mathbf{u}_s)$$
$$\frac{\partial \rho_s \mathcal{E}_s}{\partial t} = \sum_{t \neq s}\left[\alpha_{st}\rho_s\rho_t\mathbf{u}_s\cdot(\mathbf{u}_t-\mathbf{u}_s) + \frac{\alpha_{st}\rho_s\rho_t}{m_s+m_t}\left[3k_B(T_t-T_s)+m_t(\mathbf{u}_t-\mathbf{u}_s)^2\right]\right]$$

$$\alpha_{st} = \frac{Z_s^2 Z_t^2 e^4 \ln\Lambda_{st}}{6\pi\sqrt{2\pi}\epsilon_0^2 m_s m_t m_{st}(k_B T_s/m_s + k_B T_t/m_t)^{3/2}}$$
$$m_{st} = \frac{m_s m_t}{m_s + m_t}$$
$$\ln\Lambda_{st} = 15.9$$

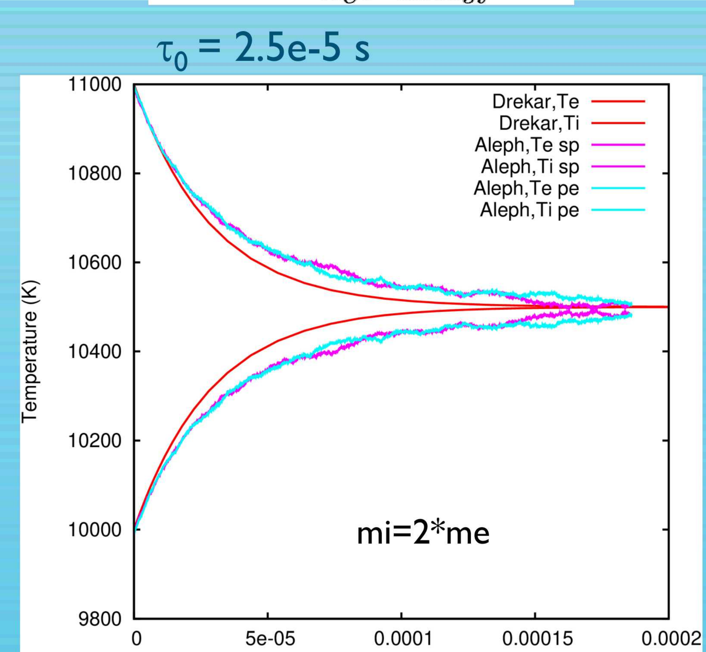
$$\tau_{st} = \frac{6\pi\sqrt{2\pi}\epsilon_0^2 m_s m_t (k_B T_s/m_s + k_B T_t/m_t)^{3/2}}{3(\gamma-1)Z_s^2 Z_t^2 e^4 \ln\Lambda_{st}(n_s+n_t)}$$

τ_{st} = 2.9e-5 s

Kinetic (PIC) Model
Nanbu cumulative small-angle collision operator , DSMC

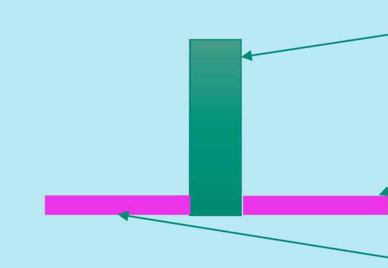
$$\tau_0 = \frac{8\pi\epsilon_0^2\sqrt{2m_e k_B T_e} k_B T_e}{n_e e^4 \ln\Lambda_{st}}$$

τ_0 = 2.5e-5 s

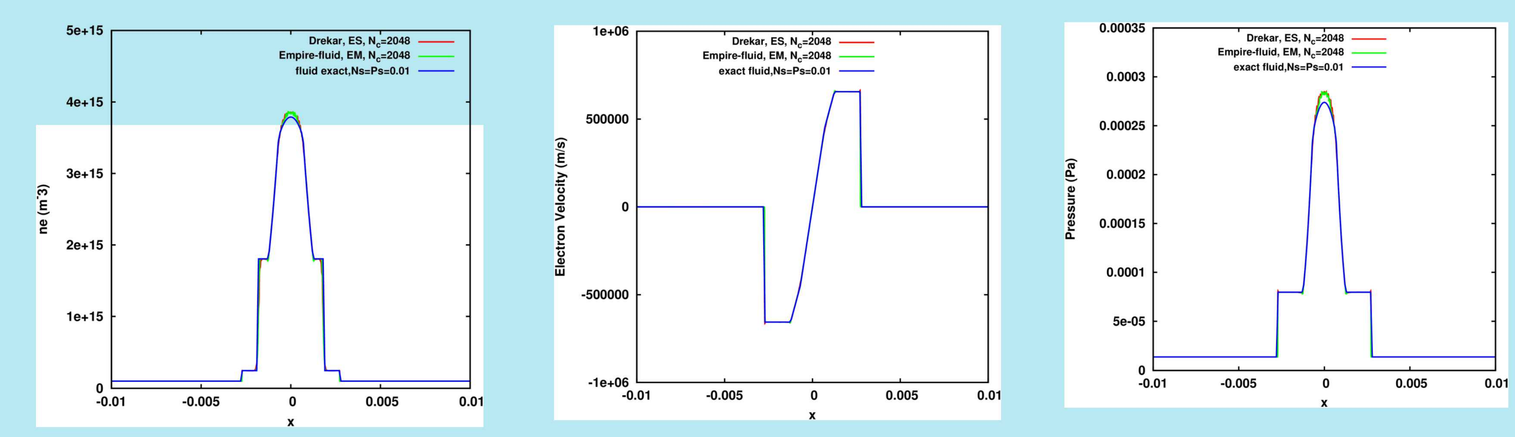


Neutral Expanding Slab Kinetic (VHS)/Fluid Solutions

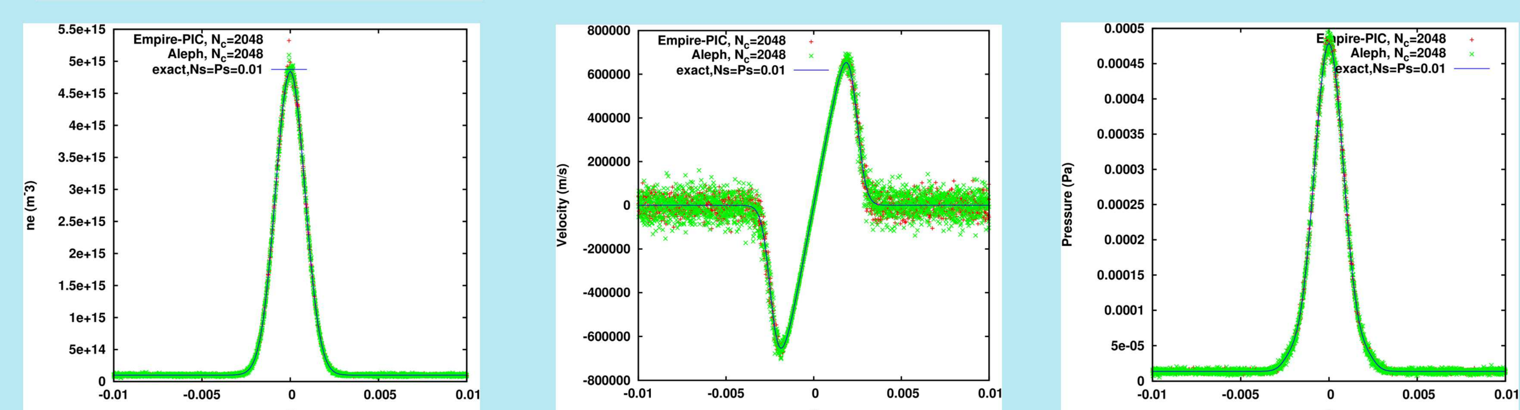
- 1D slab of electrons and ions (Z=1) with same density
- No external Electric field
- Te=Ti
- T0=T1 = 10,000 K
- mi = me
- ne = ni = 1e16
- Time duration = 2 ns
- L = 0.02 m
- Lp = 0.001 m



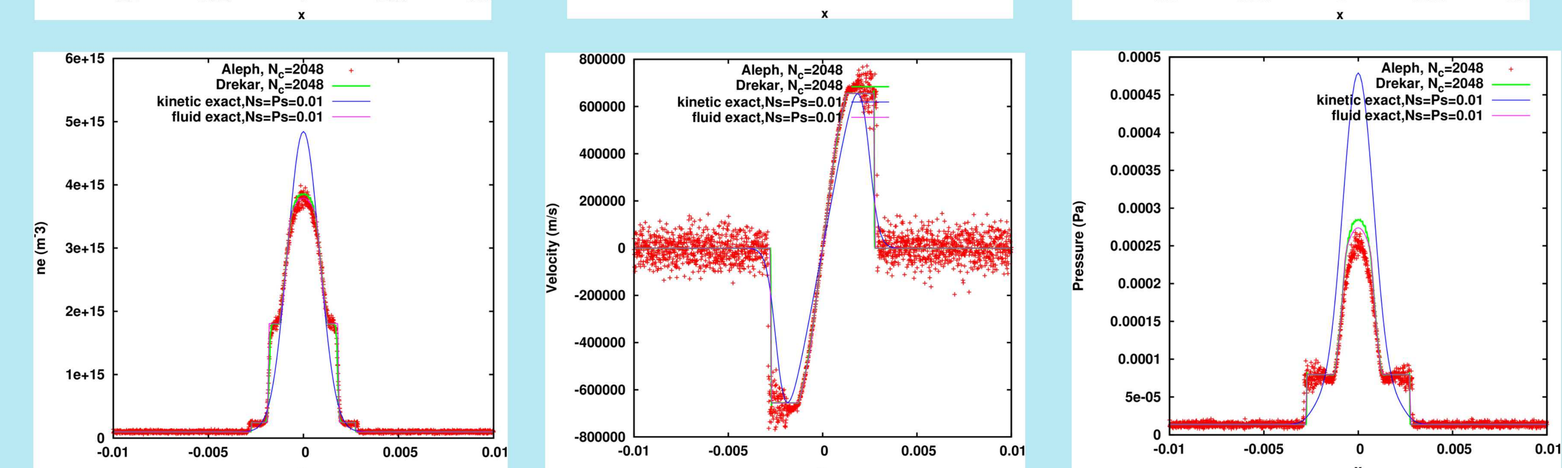
Fluid Solution
Ns=Ps=0.01
$Kn \approx 0$



Kinetic Solution
Ns=Ps=0.01
$Kn \approx$ 1e7



Fluid Solution
Ns=Ps=0.01
$Kn \approx 1$



$Kn = \lambda/L = 1/(L*\sigma*n) \approx$ 1e7
L = initial plasma width
λ = mean free path
$\sigma \approx \pi d^2$
σ = cross sectional area
d = particle diameter

→ Reduce $Kn \approx 1$ by increasing diameter to 1e7

Summary

- **We are integrating four tests into the CCI test suite focused on elastic collisional interactions.**
- **Neutral Expanding Slab** – Tests have demonstrated both kinetic and fluid solutions to the neutral expanding slab problem in a PIC code by adjusting the Knudsen number from the non-collisional regime to the collisional regime.
- **Maxwell Molecule Thermalization** – Tests allows rigorous verification across kinetic and fluid codes for isotropic scattering of neutral species. In the case of zero drift velocity four codes were exercised and show good agreement between codes and exact solution. For the case including drift velocity, two codes reproduce the numerically integrated ODE.
- **Coulomb Collision Thermalization –** Using native Coulomb collision operators, we have shown reasonable agreement of an ion-electron thermalization problem.

Lessons Learned

- Differences due to methods (PIC vs. fluid) and assumptions (dropped terms, regimes) can be subtle and must be identified and understood for quantitative comparison across codes solving "the same problem."
- If capability is not tested it is broken (or soon will be).
- The CCI infrastructure standardizes problem descriptions and enforces comparable solution resolution (mesh size, time step and particle statistics) and is invaluable for benchmarking, preserving and protecting capability.
- Confidence is best built by evidence.
- CCI fosters a culture of iterative understanding and improvement moving toward a shared goal of credible predictive mod/sim.
- Experience gained from design/implementation and testing relatively simple elastic tests is a necessary pre-requisite for including more complex inelastic collisional interactions such as ionizaton/recombination.

Next Steps

- Adopt a parameterized Maxwell molecule model to allow deviations from Maxwellian intra-particle distributions to assess greater non-local thermodynamic equilibration and inform hybrid approaches based on such deviations (e.g. delta-f).
- Augment Drekar with Maxwell molecule model for comparison to existing drift velocity results.
- Investigate possibility of constructing an inelastic collisional interaction test
- Extend 0-dimensional collisions to 1,2,3-D along with fields to benchmark interplay between PIC and explicit collision operators.

References

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