A multispecies 13-moment model for capturing magnetized collisional transport in plasmas

Sean Miller and Uri Shumlak

University of Washington

Aerospace and Energetics Research Program

Sherwood Theory Conference

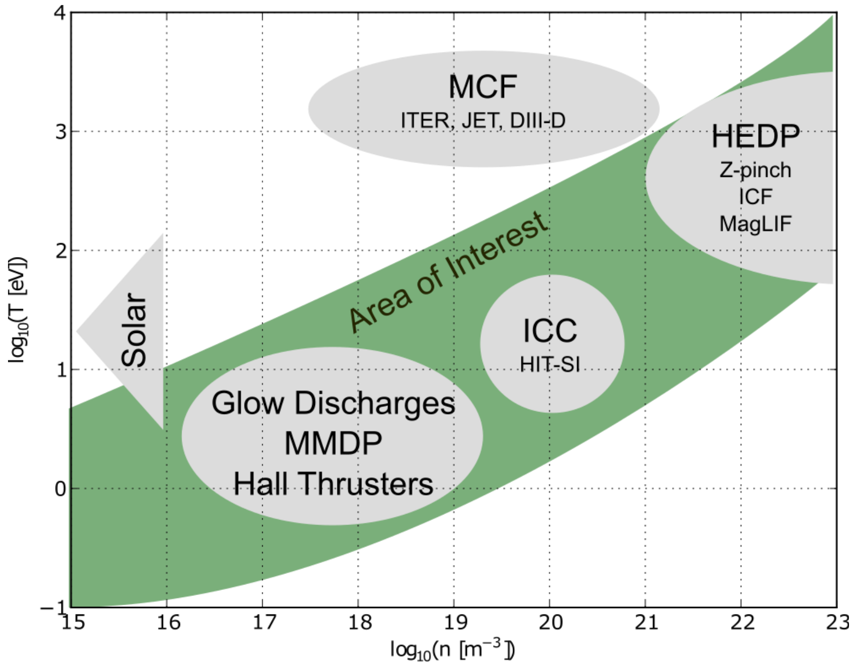
April 4th -6th, 2016

This work is supported by a grant from the United States Air Force Office of Scientific Research

UNIVERSITY of WASHINGTON

Motivation for this research

- **Goal**: Develop computationally efficient methods for capturing multispecies collisional transport in plasmas.
- Multispecies plasma models capture neutral, ion, electron, and electromagnetic dynamics separately with **disparate time scales**.
  - Bulk plasma dynamics are much slower than electron response.
  - Single-fluid plasma models can be inadequate for many applications including tokamak edge plasmas and inertial confinement fusion.
- **Computationally efficient models** beyond single fluid are lacking.
  - Kinetic models are the most general, but are computationally expensive.
- **Approach**: Higher-moment[1] plasma models offer a **cost effective** means to capture **kinetic effects** beyond standard fluid descriptions.



[1] e.g. *Torrilhon (2011)*; *McDonald and Torrilhon (2013)*; *Cai, Fan, and Li (2012)*

Continuum kinetics: Boltzmann-Maxwell model

- The **Boltzmann equation** describes the evolution of this phase space distribution based on interactions with the electromagnetic fields and collisions C_α

$$\partial_t f_\alpha + v_i \partial_{x_i} f_\alpha + \frac{q_\alpha}{m_\alpha}\left(E_i + \epsilon_{ijk} v_j B_k\right)\partial_{v_i} f_\alpha = \sum_\beta C_{\alpha\beta}$$

- **Maxwell's equations** describe the evolution of the electric and magnetic fields

$$\partial_t E_i = c^2 \epsilon_{ijk} \partial_{x_j} B_k - \frac{1}{\epsilon_0}\sum_\alpha q_\alpha \iiint_{-\infty}^{\infty} v_i f_\alpha \, d^3 v \qquad \partial_{x_i} B_i = 0$$

$$\partial_t B_i = -\epsilon_{ijk} \partial_{x_j} E_k \qquad \partial_{x_i} E_i = \frac{1}{\epsilon_0}\sum_\alpha q_\alpha \iiint_{-\infty}^{\infty} f_\alpha \, d^3 v$$

- Model is robust, but is six dimensional.
  - Solving the Boltzmann-Maxwell model requires a massive computational effort.
- The scale of the Boltzmann model can be reduced using moment models.

Deriving moment models

- Moment models are generated by taking **velocity space moments** of the Boltzmann equation thereby converting a six-dimensional equation into a three dimensional set of equations.

$$\iiint_{-\infty}^{\infty} v^n \cdot \left(\partial_t f_\alpha + v_i \partial_{x_i} f_\alpha + \frac{q_\alpha}{m_\alpha}\left(E_i + \epsilon_{ijk} v_j B_k\right)\partial_{v_i} f_\alpha = \sum_\beta C_{\alpha\beta}\right) d^3v$$

- The moments themselves can be written more compactly

$$\langle v^n \cdot f_\alpha \rangle = \iiint_{-\infty}^{\infty} v^n \cdot f_\alpha \, d^3v$$

- In general, taking moments results in an infinite series:

$$v^0 = 1 \quad \Rightarrow \quad \partial_t \langle f_\alpha \rangle + \partial_{x_i} \langle v_i f_\alpha \rangle + \frac{q_\alpha}{m_\alpha} E_i \langle \partial_{v_i} f_\alpha \rangle + \frac{q_\alpha}{m_\alpha} \epsilon_{ijk} B_k \langle v_j \partial_{v_i} f_\alpha \rangle = \sum_\beta \langle C_{\alpha\beta} \rangle$$

$$v^1 = v_i \quad \Rightarrow \quad \partial_t \langle v_i f_\alpha \rangle + \partial_{x_j} \langle v_i v_j f_\alpha \rangle + \frac{q_\alpha}{m_\alpha} E_j \left\langle v_i \partial_{v_j} f_\alpha \right\rangle + \frac{q_\alpha}{m_\alpha} \epsilon_{jkl} B_l \left\langle v_i v_k \partial_{v_j} f_\alpha \right\rangle = \sum_\beta \langle v_i C_{\alpha\beta} \rangle$$

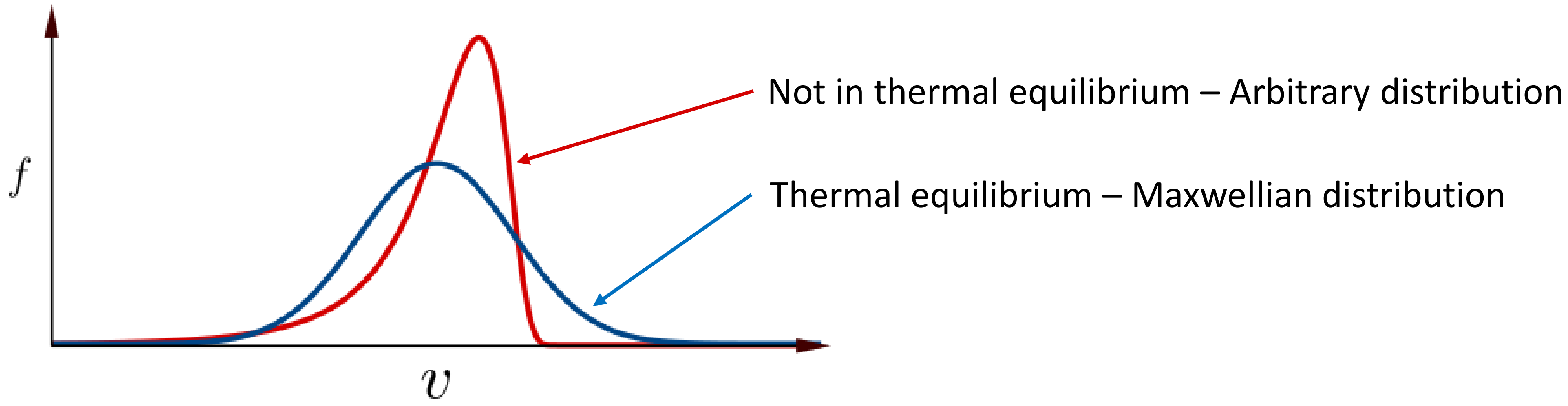
$$v^2 = v_i v_j \quad \Rightarrow \quad \partial_t \langle v_i v_j f_\alpha \rangle + \partial_{x_k} \langle v_i v_j v_k f_\alpha \rangle + \frac{q_\alpha}{m_\alpha} E_k \langle v_i v_j \partial_{v_k} f_\alpha \rangle + \frac{q_\alpha}{m_\alpha} \epsilon_{klm} B_m \langle v_i v_j v_l \partial_{v_k} f_\alpha \rangle = \sum_\beta \langle v_i v_j C_{\alpha\beta} \rangle$$

$$\vdots$$

- **Closure**: Moment models have to be truncated by relating higher moments to lower moments.

Thermal equilibrium as a basis for closure

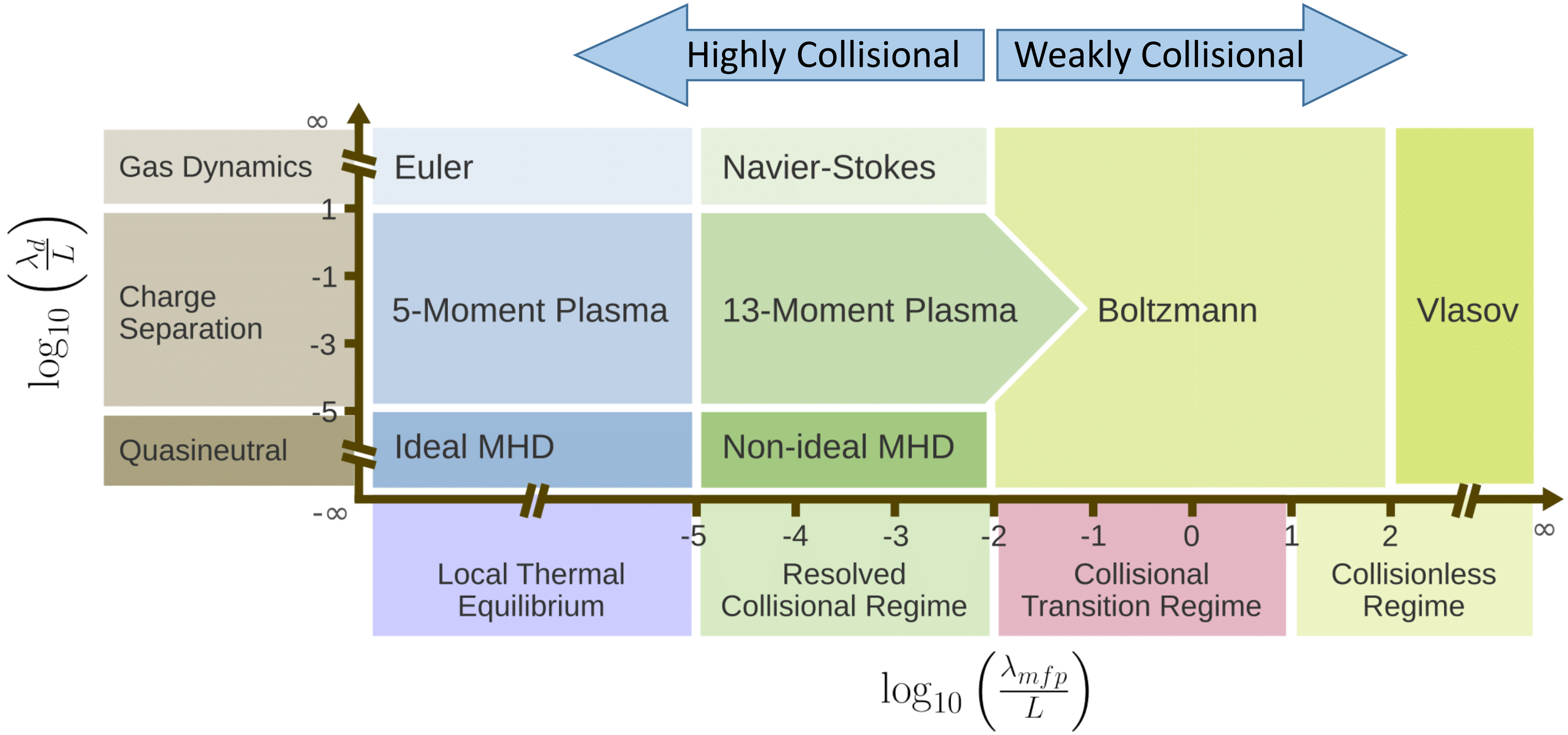
- Boltzmann H-theorem: In the limit of infinite collisions, the velocity distribution reaches an **thermal equilibrium** described by a **Maxwellian**.



- A gas in thermal equilibrium is fully described by 5 moments: **density**, **flow velocity** (mean), and **isotropic pressure** (variance).
  - This implies that if the system is near thermal equilibrium, then only 5 moments need to be modeled.
  - **Important**: The system must be highly collisional to assume a locally thermalized system.
- The H-theorem can be used as a basis for closing higher-moment models.
  - The unknown higher moments can be related to deviations from thermal equilibrium.

Moment models and plasma regimes

- Thermal equilibrium is important for deriving closure schemes, but these closures are limited to a highly collisional plasma regime.
- Higher-moment models attempt to extend this collisional regime by including additional moments.



Multispecies 5-moment plasma model

- Continuity equation

$$\partial_t \rho_\alpha + u_i^\alpha \partial_{x_i} \rho_\alpha = -\rho_\alpha \partial_{x_i} u_i^\alpha$$

- Momentum equation

$$\partial_t u_i^\alpha + u_j^\alpha \partial_{x_j} u_i^\alpha = -\frac{1}{\rho_\alpha} \partial_{x_j} P_{ij}^\alpha + \frac{q_\alpha}{m_\alpha}\left(E_i + \epsilon_{ijk} u_j^\alpha B_k\right) + \frac{1}{\rho_\alpha} \sum_\beta R_i^{\alpha\beta}$$

- Isotropic pressure equation

$$\partial_t P_\alpha + u_i^\alpha \partial_{x_i} P_\alpha = -P_\alpha \partial_{x_i} u_i^\alpha - \frac{2}{3} P_{ij}^\alpha \partial_{x_i} u_j^\alpha - \frac{2}{3} \partial_{x_i} q_i^\alpha + \sum_\beta Q_{\alpha\beta}$$

- The pressure tensor P_{ij}^α and heat flux vector q_i^α can be defined for **weakly magnetized plasmas near thermal equilibrium**

$$P_{ij}^\alpha = P_\alpha \delta_{ij} - \mu\left(\partial_{x_i} u_j^\alpha + \partial_{x_j} u_i^\alpha - \frac{2}{3}\delta_{ij} \partial_{x_k} u_k^\alpha\right)$$

$$q_i^\alpha = -\kappa \partial_{x_i} T_\alpha$$

- To understand the effect of strong magnetization on the 5-moment closure, we extend the moment model to 13-moments.

Extension to 13 moments

- The 13-moment model includes additional effects related to larger deviations from thermal equilibrium.
- The isotropic pressure equation is extended to evolve the full pressure tensor P_{ij}^{α}

$$\partial_t P_{ij}^{\alpha} + u_k^{\alpha} \partial_{x_k} P_{ij}^{\alpha} = -P_{ik}^{\alpha} \partial_{x_k} u_j^{\alpha} - P_{jk}^{\alpha} \partial_{x_k} u_i^{\alpha} - P_{ij}^{\alpha} \partial_{x_k} u_k^{\alpha} - \partial_{x_k} h_{ijk}^{\alpha}$$
$$+ \frac{q_\alpha}{m_\alpha} B_l \left(\epsilon_{ikl} P_{jk}^{\alpha} + \epsilon_{jkl} P_{ik}^{\alpha} \right) + \sum_{\beta} Q_{ij}^{\alpha\beta}$$

- Three additional moments are given by the heat flux equation

$$\partial_t q_i^{\alpha} + u_j^{\alpha} \partial_{x_j} q_i^{\alpha} = -q_j^{\alpha} \partial_{x_j} u_i^{\alpha} - q_i^{\alpha} \partial_{x_j} u_j^{\alpha} - h_{ijk}^{\alpha} \partial_{x_j} u_k^{\alpha} - \frac{1}{2} \partial_{x_j} g_{ij}^{\alpha} + \frac{3}{2} \frac{P_\alpha}{\rho_\alpha} \partial_{x_j} P_{ij}^{\alpha} + \frac{P_{ik}^{\alpha}}{\rho_\alpha} \partial_{x_j} P_{jk}^{\alpha}$$
$$+ \frac{q_\alpha}{m_\alpha} \epsilon_{ijk} q_j^{\alpha} B_k + \sum_{\beta} \left(\frac{1}{2} W_i^{\alpha\beta} - \frac{3}{2} \frac{P_\alpha}{\rho_\alpha} R_i^{\alpha\beta} - \frac{P_{ij}^{\alpha}}{\rho_\alpha} R_j^{\alpha\beta} \right)$$

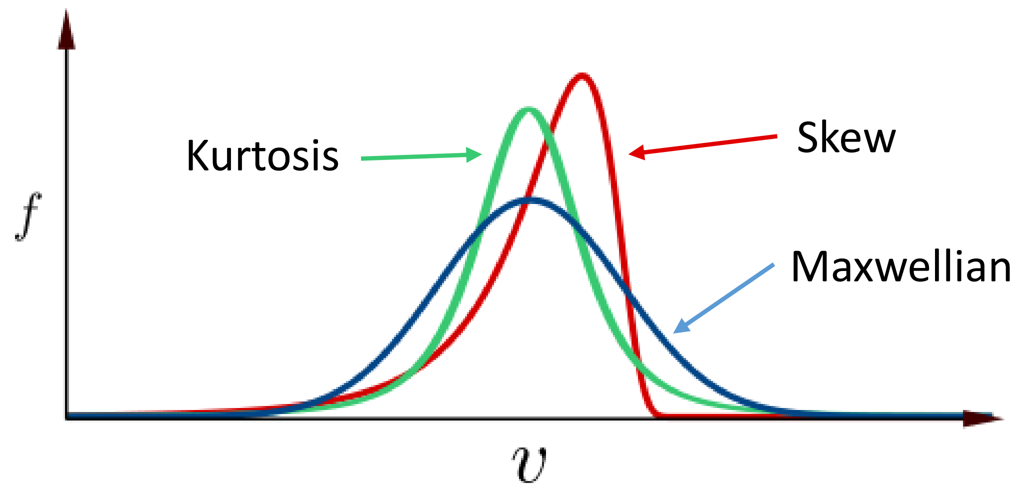
- Unlike the 5-moment model, P_{ij}^{α} and q_i^{α} are now directly evolved.
- The full heat flux tensor h_{ijk}^{α} and higher moment variable g_{ij}^{α} must still be related to the known moments.

Pearson type-IV closure

- Closure is derived for applications in rarefied gas dynamics[1].
- The Pearson type-IV distribution is used in statistics to analyze skew and kurtosis in datasets.

$$f_{P4}(x,v) \propto \underbrace{\left(1+\left(\frac{v-\lambda(x)}{a(x)}\right)^2\right)^{-\gamma(x)}}_{\text{Kurtosis}} \underbrace{e^{-\eta(x)\tan^{-1}\left(\frac{v-\lambda(x)}{a(x)}\right)}}_{\text{Skew}}$$

- Skew is closely tied to the heat flux h^{α}_{ijk}, while kurtosis defines g^{α}_{ij}.



[1] *Torrilhon, CCP (2010)*

Deriving the Pearson type-IV closure

- Given a distribution $f_{P4}(\vec{v}, \phi_0(\vec{x}), \phi_1(\vec{x}), \phi_2(\vec{x}), \ldots)$, its spatial variables $\phi_i(\vec{x})$ are related to the known moments through moment integration.

$$\langle f_{P4} \rangle \to \rho \qquad \langle v_i v_j f_{P4} \rangle \to P_{ij}$$
$$\langle v_i f_{P4} \rangle \to u_i \qquad \langle v_i v^2 f_{P4} \rangle \to q_i$$

$$\Rightarrow \quad \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \vdots \end{bmatrix} = \boldsymbol{A} \cdot \begin{bmatrix} \rho \\ u_i \\ P_{ij} \\ q_i \end{bmatrix}$$

- The relation between the distribution variables and the known moments defines the closure.

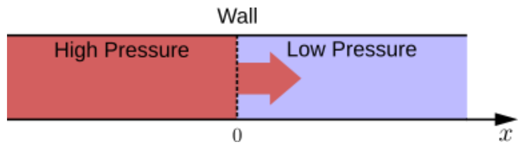
$$\langle v_i v_j v_k f_{P4} \rangle \to h_{ijk}$$
$$\langle v_i v_j v^2 f_{P4} \rangle \to g_{ij}$$

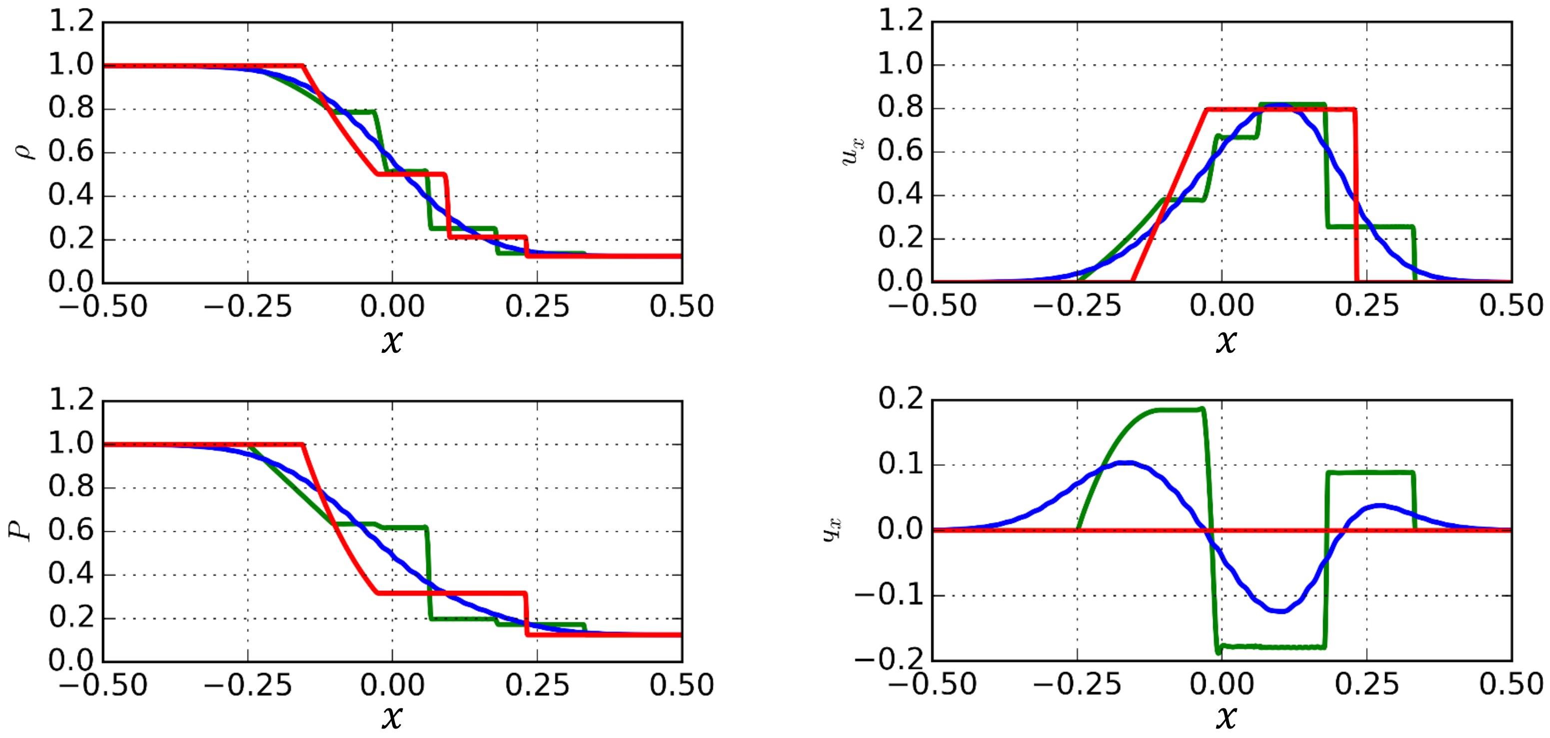
$$\Rightarrow \quad \begin{bmatrix} h_{ijk} \\ g_{ij} \end{bmatrix} = \boldsymbol{B} \cdot \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \vdots \end{bmatrix} = (\boldsymbol{B} \cdot \boldsymbol{A}) \cdot \begin{bmatrix} \rho \\ u_i \\ P_{ij} \\ q_i \end{bmatrix}$$

- Relation between known moments and distribution variables ϕ_i is nonlinear.
- The 6D Pearson type-IV distribution has 14 variables to describe 13 moments.
  - Infinite possible solutions for h_{ijk} and g_{ij}.
  - Additional constraint is chosen to enforce **hyperbolicity** and/or **realizability**.
- While the solution enforces hyperbolicity and/or realizability, the closure is not physically accurate on its own.

Pearson type-IV closure leads to artificial waves

- The neutral species shock tube is used to test closures.
  - Collisionality determines the resulting profile which can vary from discontinuous (highly collisional) to smooth (weakly collisional).
  - The Pearson-IV closure attempts to capture weakly collisional dynamics, but with only 13 waves.





- Collision operators are used to damp the artificial waves.

Including collisions within a species

- Collisions within a species are captured using a BGK collision operator to drive f_α towards a Maxwellian $\tilde{f}_\alpha$ over a time scale $\tau_{\alpha\alpha}$.

$$C_{\alpha\alpha} = -\frac{1}{\tau_{\alpha\alpha}}\left(f_\alpha - \tilde{f}_\alpha\right)$$

- Intraspecies scattering collisions do not affect density, momentum, or isotropic energy, consistent with the 5-moment model

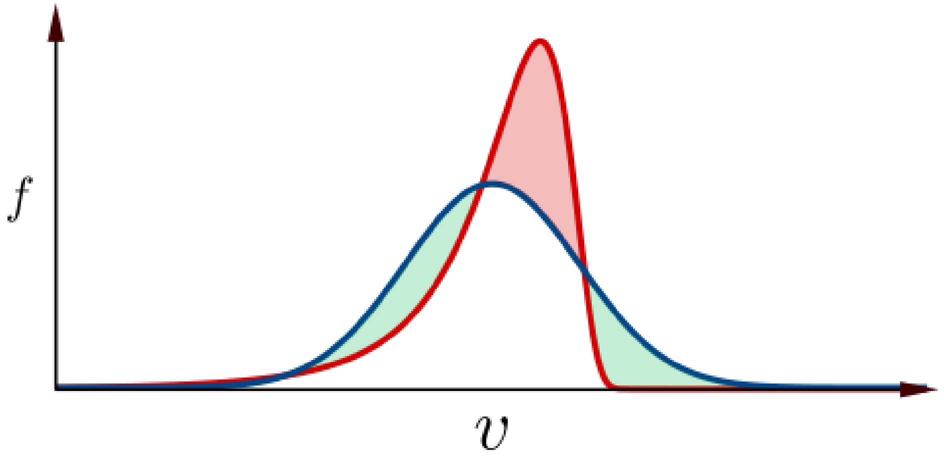
$$\langle C_{\alpha\alpha} \rangle = R_i^{\alpha\alpha} = Q_{ii}^{\alpha\alpha} = 0$$

- Collisions do drive the pressure tensor to isotropy

$$Q_{ij}^{\alpha\alpha} = -\frac{1}{\tau_{\alpha\alpha}}\left(P_{ij}^{\alpha} - P_\alpha \delta_{ij}\right)$$

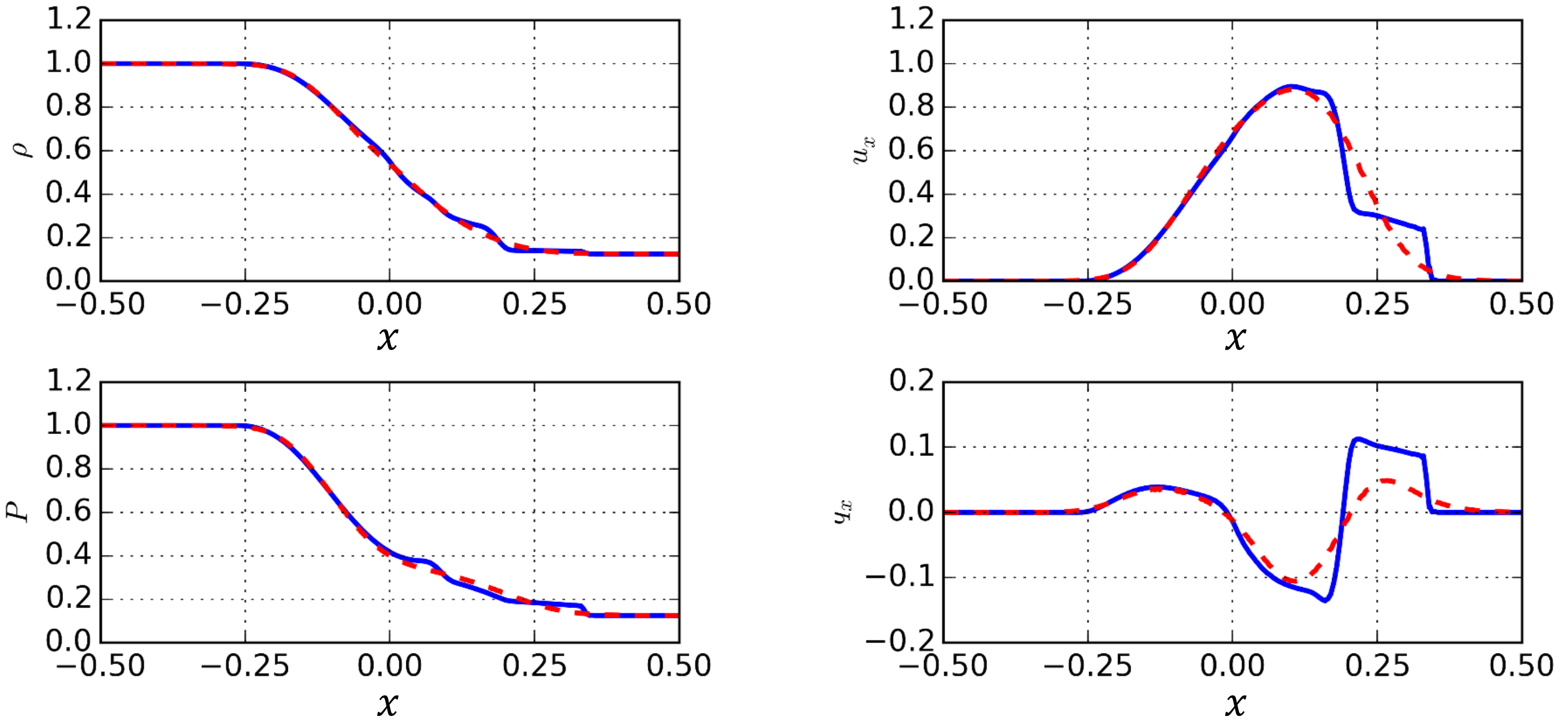
- And the heat flux vector q_i^α is driven to zero

$$W_i^{\alpha\alpha} = -\frac{2}{\tau_{\alpha\alpha}} q_i^\alpha$$



BGK collision operator improves the behavior

- Shock tube is now simulated with moderate collisionality to show the effect of the BGK collision operator.
  - The collisional time scale is dependent on the temperature and density $\tau_{\alpha\alpha} = 0.01\, T_\alpha^{3/2}/n_\alpha$ so the domain has a region of high collisionality area ($x < 0$) and low collisionality ($x > 0$).
  - The Boltzmann model is used to show that a smooth shock is expected.
  - The BGK operator captures the smooth profile in the highly collisional area, but the artificial waves still appear in the weakly collisional area.



- An additional operator is required to treat the weakly collisional regime.

Diffusion eliminates artificial wave structure

- To counter the artificial waves of the Pearson-IV closure, a diffusive stabilization operator is developed based on the BGK collision operator.

$$C_{\alpha\alpha} = \partial_{x_i}\left(D_\alpha \partial_{x_i}\left(f_\alpha - \tilde{f}_\alpha\right)\right)$$

- As with the relaxation form, the diffusion operator does not affect the density, momentum, or isotropic energy.

$$\langle C_{\alpha\alpha}\rangle = R_i^{\alpha\alpha} = Q_{ii}^{\alpha\alpha} = 0$$

- A stabilizing diffusion is added to the anisotropic pressure terms and helps keep the pressure tensor positive definite.

$$Q_{ij}^{\alpha\alpha} = \partial_{x_i}\left(D_\alpha \partial_{x_i}\left(P_{ij}^{\alpha} - P_\alpha \delta_{ij}\right)\right)$$

- And it drives the heat flux vector to zero

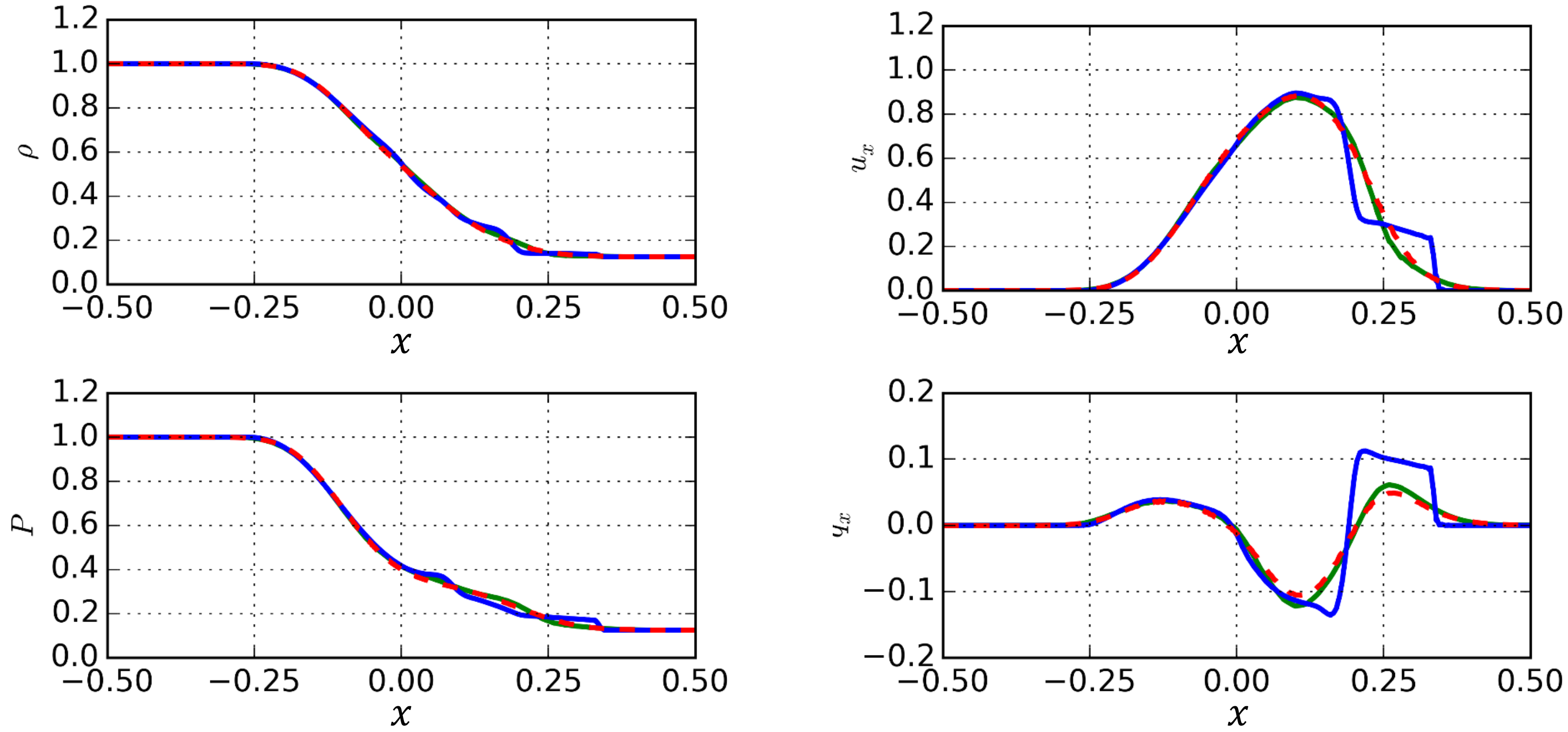
$$W_i^{\alpha\alpha} = \partial_{x_i}\left(2D_\alpha \partial_{x_i} q_i^{\alpha}\right)$$

- The diffusion coefficient is similar to those found using Chapman-Enskog expansion methods

$$D_\alpha \approx \frac{P_\alpha \tau_{\alpha\alpha}}{\rho_\alpha}$$

Diffusion operator is consistent with kinetic model

- The shock tube is again simulated with the Boltzmann model and Pearson-IV model with BGK collisions, but now includes the Pearson-IV model with BGK collisions and diffusion operator.
  - The diffusive operator helps damp out the artificial waves in the weakly collisional area.
  - Adds stability to the model for multidimensional applications and magnetized flow, as well as increase the physical accuracy of the closure.



Including collisions between species

- Scattering collisions do not affect density $\langle C_{\alpha\beta} \rangle = 0$.
- **Momentum exchange** drives velocities together (friction) at a rate related to the interspecies thermalization time scale $\tau_{\alpha\beta}$

$$R_i^{\alpha\beta} = -\frac{\rho_\alpha}{\tau_{\alpha\beta}}\left(u_i^\alpha - u_i^\beta\right) = -\frac{\rho_\alpha}{\tau_{\alpha\beta}} u_i^{\alpha\beta}$$

- **Heat exchange** drives temperatures together

$$Q_{ij}^{\alpha\beta} = -\frac{2\rho_\alpha}{\tau_{\alpha\beta}(m_\alpha + m_\beta)}\left(T_{ij}^{\alpha\beta} - m_\beta u_i^{\alpha\beta} u_j^{\alpha\beta}\right)$$

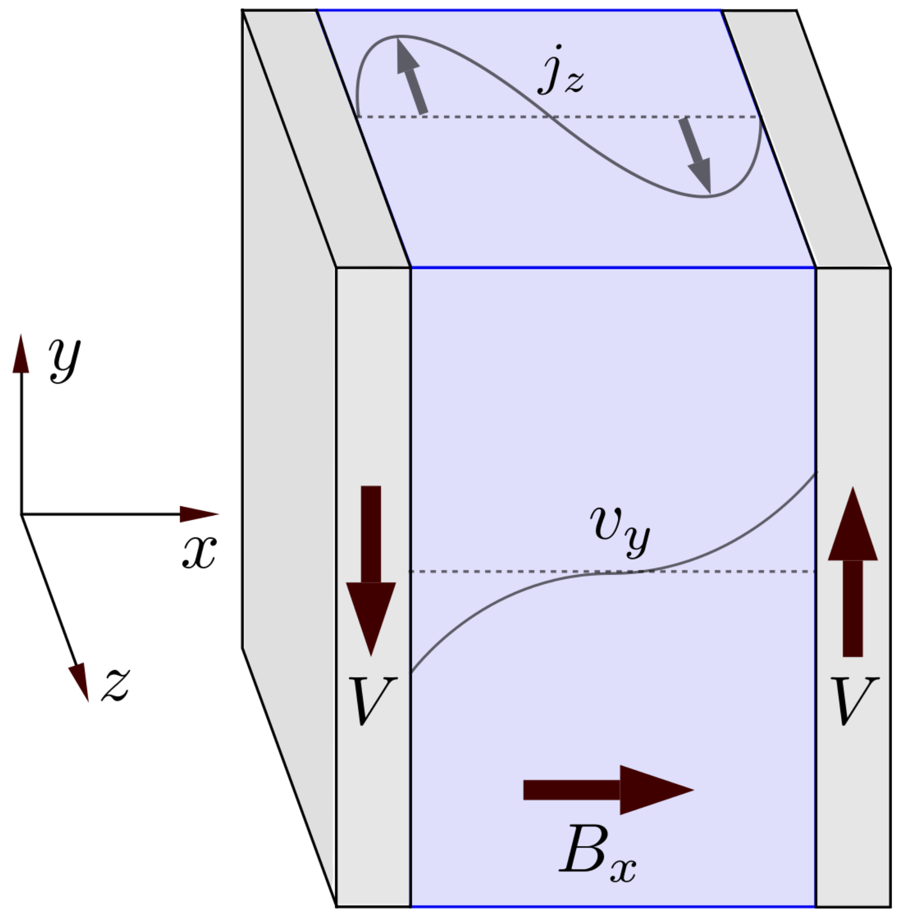
- **Heat flux exchange** drives the flow of temperature together

$$W_i^{\alpha\beta} = -\frac{\rho_\alpha}{\tau_{\alpha\beta}(m_\alpha + m_\beta)}\left(\frac{q_i^\alpha}{n_\alpha} - \frac{q_i^\beta}{n_\beta}\right) + \frac{2\rho_\alpha m_\beta}{\tau_{\alpha\beta}(m_\alpha + m_\beta)}\left(3u_i^{\alpha\beta} T_{\alpha\beta} + 2u_j^{\alpha\beta} T_{ij}^{\alpha\beta} + \frac{3}{2}(m_\alpha - m_\beta) u_{\alpha\beta}^2 u_j^{\alpha\beta}\right)$$

- The 13-moment plasma model is now complete.

Multispecies Hartmann flow benchmark

- Used to benchmark **resistive**, **magnetic**, and **viscous** effects in plasmas.
- Benchmark is an extension of the MHD Hartmann flow based on MHD generators.
- Interplay between frozen-in magnetic field, resistive diffusion, and viscous drag result in complex shear velocity profile.



Solution to multispecies Hartmann flow problem

- For low Mach number applications, the Hartmann flow is the solution to a coupled set of elliptic equations derived from the multispecies 5-moment plasma model.

$$\partial_x^2 u_y^\alpha = -\lambda_\alpha u_z^\alpha + \sum_\beta \gamma_{\alpha\beta} \left(u_y^\alpha - u_y^\beta \right)$$

$$\partial_x^2 u_z^\alpha = \lambda_\alpha u_y^\alpha + \sum_\beta \gamma_{\alpha\beta} \left(u_z^\alpha - u_z^\beta \right)$$

$$\partial_x B_y = \mu_0 \sum_\beta q_\alpha n_\alpha u_z^\alpha$$

$$\partial_x B_z = -\mu_0 \sum_\beta q_\alpha n_\alpha u_y^\alpha$$

- With the coefficients

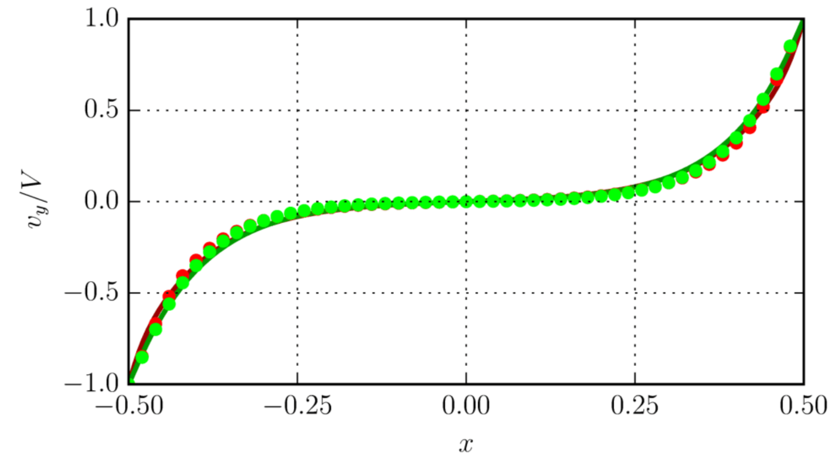
$$\lambda_\alpha = \frac{q_\alpha B_x}{T_\alpha \tau_{\alpha\alpha}}$$

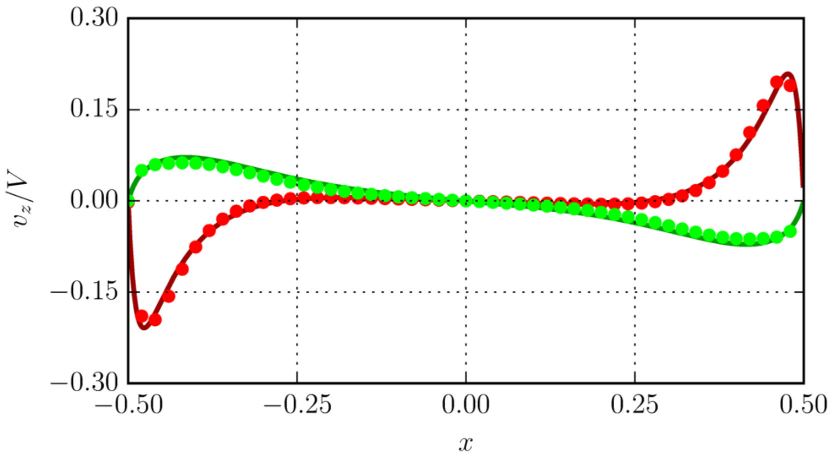
$$\gamma_{\alpha\beta} = \frac{m_\alpha \tau_{\alpha\beta}}{T_\alpha \tau_{\alpha\alpha}}$$

- This equation set is solved numerically.

Multispecies Hartmann flow comparison

- At high collisionality and weak magnetization, the 13-moment model converges to the 5-moment analytical solution.
- Simulations results (dots) and analytical solution (solid line) for a two-fluid application with ions ($m_i = 1$, $q_i = 1$) and electrons ($m_e = 0.01$, $q_e = -1$).
- The 13-moment model accurately captures magnetized collisional plasma effects at **moderate to high collisionalities** and **weak to moderate magnetic field strengths**.





Summary

- Presented a new multispecies 13-moment plasma model for capturing magnetized collisional transport that extends the applicability of fluid theory.
  - Model closure assumes a Pearson type-IV distribution in velocity space.
  - A BGK collision operator is used to treat intraspecies interactions in highly collisional plasmas.
  - A diffusive operator treats intraspecies interactions in rarefied regimes.
  - Interspecies collision operators add resistive and thermal exchange effects.
  - Model was benchmarked against the multispecies Hartmann flow problem and was shown to be valid for moderate to high collisionalities with weak to moderate levels of magnetization.
- Up to this point the model has been developed as a foundation, but research is still underway.
  - Developing a more physically consistent closure.
  - Developing ionization, recombination, and charge exchange operators for low temperature applications.
  - Developing benchmarks for non-equilibrium plasmas.