Parallel closures: Analytical and numerical accomplishments and plans

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Analytical accomplishments for parallel closures

- Higher-order moment model derived and tested.
  - Reproduces Braginskii in collisional limit and provides corrections.
  - Converges through moderately collisionless limit hence appropriate for $\Psi$ - Center applications.

- Complete Chapman-Enskog-like model derived.
  - Converges in collisional through extremely collisionless limits
  - Expand-and-fit algorithm developed.

- Time-dependent derivation for linear closures completed.
  - Uses full moment form of collision operator.
  - Imparts time-dependent effects needed in $\Psi$ - Center applications.
5-moment fluid model for plasmas:

**What are closures?**

\[
\frac{\partial f_a}{\partial t} + \mathbf{v} \cdot \frac{\partial f_a}{\partial \mathbf{x}} + \frac{e_a}{m_a} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_a}{\partial \mathbf{v}} = \sum_b C(f_a, f_b)
\]

- Density, velocity, energy moments (1+3+1)

\[
\frac{\partial n_a}{\partial t} + \nabla \cdot (n_a \mathbf{u}_a) = \int d\mathbf{v} 1C = 0
\]

\[
m_a n_a \frac{d\mathbf{u}_a}{dt} - n_a e_a (\mathbf{E} + \mathbf{u}_a \times \mathbf{B}) + \nabla p_a + \nabla \cdot \mathbf{\pi}_a = \int d\mathbf{v} m\mathbf{v} C
\]

\[
\frac{3}{2} n_a \frac{dT_a}{dt} + n_a T_a \nabla \cdot \mathbf{u}_a + \nabla \cdot \mathbf{q}_a + \mathbf{\pi}_a : \nabla \mathbf{u}_a = \int d\mathbf{v} \frac{1}{2} m\mathbf{v}^2 C
\]
Moment expansion

\[ f_a = f_a^{(0)} \sum_{l_k} P_{a}^{l_k} \cdot M_{a}^{l_k} = f_a^{(0)} \sum_{l_k} L_k^{(l+1/2)} (s_a^2) P^l \cdot M^{l_k} \]

\[ = f_a^{(0)} [L_0^{(1/2)} M^{00} + L_1^{(1/2)} M_{a}^{01} + L_2^{(1/2)} M_{a}^{02} + \cdots \]

\[ + \mathbf{v} \cdot (L_0^{(3/2)} M_{a}^{10} + L_1^{(3/2)} M_{a}^{11} + \cdots ) \]

\[ + (\mathbf{vv} - \frac{1}{3} v^2 l) : (L_0^{(5/2)} M_{a}^{20} + L_1^{(5/2)} M_{a}^{21} + \cdots ) + \cdots ] \]

= Maxwellian x (orthogonal velocity polynomials)

\[ f_a^{(0)} = \frac{n_a}{\pi^{3/2} v_T^3} e^{-s_a^2}, \quad s_a = \frac{\mathbf{v}}{v_T a}, \quad v_T a = \sqrt{\frac{2T_a}{m_a}} \]

- \( M^{00}: n, \quad M^{01}: T(p), \quad M^{10}: V, \quad M^{11}: q, \quad M^{20}: \pi, \quad M^{21}: \)

- Irreducible harmonic and Sonine polynomials
Coulomb Collision operator

Rosenbluth potentials

\[ C(f_a, f_b) = \frac{\gamma_{ab}}{2m_a} \nabla \cdot [\nabla \cdot (f_a \nabla \nabla G_b) - 2(1 + \frac{m_a}{m_b}) f_a \nabla H_b] \]

\[ H_b(v) = \int d^3v' f_b(v') \frac{1}{|v - v'|}, \quad \nabla H_b = -4\pi f_b \]

\[ G_b(v) = \int d\mathbf{v}' f_b(\mathbf{v}') |\mathbf{v} - \mathbf{v}'|, \quad \nabla^2 G_b = 2H_b \]

- Integro-differential op. -> Differential op.

\[ G^{lk}(v) = P^l(\hat{v}) \cdot M^{lk}[g_E(v)\text{erf}(v) + g_e(v)\text{erf}'(v)] \]
\[ H^{lk}(v) = P^l(\hat{v}) \cdot M^{lk}[h_E(v)\text{erf}(v) + h_e(v)\text{erf}'(v)] \]

= speed polynomials x (error functions)
Collision operators in the moment expansion

\[ C(f_a, f_b) = C\left(\sum_{lk} f_a^{(0)} P_{a}^{lk} \cdot M_{a}^{lk}, f_b^{(0)}\right) + C\left(\sum_{lk} f_a^{(0)}, f_b^{(0)} P_{b}^{lk} \cdot M_{b}^{lk}\right) \]

\[ = f_a^{(0)} P^{l}(\hat{\mathbf{v}}) \cdot \sum_{lk} \left[ M_{a}^{lk} \nu_{ab}^{(lk,0)}(\mathbf{v}) + M_{b}^{lk} \nu_{ab}^{(0,lk)}(\mathbf{v}) \right] \]

Collisional moments:
Linear combination of fluid moments

\[ \int d\mathbf{v} P^{l} L_{p}^{(l+1/2)} C(f_a, f_b) = \sum_{k} (A_{ab}^{lpk} M_{a}^{lk} + B_{ab}^{lpk} M_{b}^{lk}) \]
General moment equations

\[
\frac{\partial f_a}{\partial t} + \mathbf{v} \cdot \frac{\partial f_a}{\partial \mathbf{x}} + \frac{e_a}{m_a} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_a}{\partial \mathbf{v}} = \sum_b C(f_a, f_b)
\]

\[
\begin{pmatrix}
D^0 & D^0+ & 0 & 0 \\
D^{1-} & D^1 & D^{1+} & 0 \\
0 & D^{2-} & D^2 & D^{2+} \\
0 & 0 & D^{3-} & D^3
\end{pmatrix}
\begin{pmatrix}
M_a^0 \\
M_a^1 \\
M_a^2 \\
M_a^3
\end{pmatrix}
= \sum_b \begin{pmatrix}
A_{ab}^0 M_a^0 \\
A_{ab}^1 M_a^1 \\
A_{ab}^2 M_a^2 \\
A_{ab}^3 M_a^3
\end{pmatrix}
+ \begin{pmatrix}
B_{ab}^0 M_b^0 \\
B_{ab}^1 M_b^1 \\
B_{ab}^2 M_b^2 \\
B_{ab}^3 M_b^3
\end{pmatrix}
\]

\[
D^l = \partial_t + \Xi^l (\partial_t \ln T) + \Omega_a \hat{b} \times \mathbf{t}
\]

\[
D^{l\pm} = v_T \Psi^{l\pm} \nabla + v_T \Phi^{l\pm} (\nabla \ln T) + v_T^{-1} \frac{e_a}{m_a} \Theta^{l\pm} \mathbf{E}
\]
Moment equations for parallel closures

- Drift kinetic equation
  - Magnetized plasma (strong magnetic field)
  - Fast short-scale gyrating motions averaged out
- Parallel components of general moment equation
General parallel closures

\[ \Psi \partial_L \vec{M} = C \vec{M} + \vec{G} \]

\[ \partial_z \vec{M} = \Psi^{-1} C \vec{M} + \Psi^{-1} \vec{G} \]

\[ \Psi^{-1} C \vec{W}_I = k_I \vec{W}_I \]

\[ W = (\vec{W}_1, \vec{W}_2, \ldots, \vec{W}_N) \]

\[ \vec{m} = W^{-1} \vec{M}, \quad \vec{g} = W^{-1} \Psi^{-1} \vec{G} \]

\[ \partial_z \vec{m} = W^{-1} \Psi^{-1} C W \vec{m} + \vec{g} \]

\[ \frac{d}{dz} m_I = k_I m_I + g_I \]

\[ m_I(z) = e^{k_I(z-z_0)} m_I(z_0) + \int_{z_0}^z e^{k_I(z-z')} g_I(z') dz' \]

\[ m_I^\pm(z) = \int_{\pm\infty}^z g_I(z') e^{k_I^\pm(z-z')} dz' \]

\[ q_\parallel(z) = \sum_j W_{q,j} m_j(z) = \int_{-\infty}^z K_-(z-z') \frac{dT}{dz'} + \int_{+\infty}^z K_+(z-z') \frac{dT}{dz'} \]

- **Truncate:**
  - \( N \times N \) matrix
- **Diagonalize:**
  - Decoupled ODEs
- Initial (boundary) conditions
- Confined field lines
- Inverse transform
Convergence of the general closures

- Closure calculations should not be sensitive to the truncation
- For a given collisionality \( L_{\text{mfp}} / L_T \), there exist \( l \) and \( k \) such that the closure calculations do not change by increase of \( l \) and/or \( k \)
- The longer \( L_{\text{mfp}} \) requires the larger \( l \) and \( k \)
- Kernel functions are calculated from the 1600 (\( L=40, k=40 \)) parallel moment approximation (\( L_{\text{mfp}} / L_T = 20 \))
Convergence test $T = T_0 - T_1 \sin(L/L_T)$

Heat flux
Parallel heat flux for $T = T_0 - T_1 \sin(L/L_{mfp})$
Parallel heat flux for a monotonically varying temperature: \( T(L) = T_0 - T_1 \tanh(L/L_T) \)
Temperature along field lines in SSPX
Analytical accomplishments for parallel closures

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Numerical accomplishments for parallel closures

• Heat flow implemented for higher-order moment model.
  • Improved implementation of boundary conditions and convergence test.
  • Preliminary results for SSPX electron heat confinement show reduction in parallel transport compared to Braginskii prediction.

• Parallelization of closure calculation decoupled from fluid.
  • Arbitrary number of nodes strictly calculate closure (CEMM).
  • Strong scaling shown to 4096 processors (CEMM).

• Expand-and-fit algorithm implemented.
  • Accelerates closure calculation for confined field lines.
  • Further development may be needed for unconfined field lines.
Previous closure implementation had all processors doing both fluid and closure calculations.

NIMROD nodes 1 - 1000

1. Exchange local variables so processors can integrate anywhere in global domain.
2. Calculate closures.
3. Advance fluid equations.
Calculate fluid and closure problems on separate groups of processors.

1) pass fluid variables

fluid nodes
~100's -1000

receiving closure nodes
same # as fluid
Calculate fluid and closure problems on separate groups of processors.

1) pass fluid variables 1 to 1

fluid nodes
~100's -1000

receiving closure nodes
same # as fluid

2) advance fluid equations with latest closures.

3) compute drives and exchange

slave closure nodes
~1000's-10,000
Calculate fluid and closure problems on separate groups of processors.

1) pass fluid variables 1 to 1

fluid nodes ~100's - 1000

2) advance fluid equations with latest closures.

3) compute drives and exchange

4) calculate closures

receiving closure nodes same # as fluid

slave closure nodes ~1000's - 10,000
Calculate fluid and closure problems on separate groups of processors.

1) pass fluid variables 1 to 1
2) advance fluid equations with latest closures.
3) compute drives and exchange
4) calculate closures
5) return closures

fluid nodes
~100's -1000

receiving closure nodes
same # as fluid

slave closure nodes
~1000's -10,000
Expand-and-fit algorithm implemented.

- Harmonic expansion permits analytic calculation of closure:
  \[ T = T_0 + \sum_i \left( T_{ci} \cos(k_i L) + T_{si} \sin(k_i L) \right) \]

Poincare surface of section from NIMROD SSPX simulation

Even when field lines are stochastic, T perturbations well-approximated by finite set of sinusoidal functions.
Expand-and-fit algorithm implemented.

- Harmonic expansion permits analytic calculation of closure:
  \[ T = T_0 + \sum_i \left( T_{ci} \cos(k_i L) + T_{si} \sin(k_i L) \right) \]
Short integration provides spectral content.
Fit approximately valid over longer distances.
Unconfined field lines that suddenly move to boundary more difficult to treat.
Plans for parallel closures (analytical)

• Derive parallel electron and ion stress in higher-order moment model including precise conservation laws.

• Derive complete form for collisional closures with comparison to Braginskii.

• Derive small-mass-ratio form for collision operator in moment expansion with arbitrary flow speeds.

• Develop nonlinear time-dependent CEL closures.
Plans for parallel closures (numerical).

- Complete steady-state heat transport studies for SSPX including integral parallel heat flow closure.
- Implement general parallel electron stress and test numerical stability using fluid form as si operator.
- Extend expand-and-fit algorithm to handle field lines terminating on material boundaries.
- Perform time-dependent simulations of SSPX during enhanced confinement stage.
- **Improve efficiency of closure calculations.**