Advanced parallel closures using general moment equations for NIMROD simulations

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Motivation

- Obtain closures from general moment equations without velocity variable grid points

- Avoid integrals along field lines in NIMROD.

- In a low-collisionality regime, capturing kinetic effects by using fluid models in NIMROD.

- Incorporate time-dependent and non-linear effects in closures for large variations of magnetic and temperature fields along field lines.
Obtaining general parallel moment equations

- Take gyro-average and linearize
  \[v \parallel \frac{\partial f_a^N}{\partial \ell} = C_L(f_a^N) - v \parallel \frac{\partial f_a^M}{\partial \ell} + C_L(f_a^M)\]

- Moment expansion
  \[f_a^N = \hat{f}_m \sum_{lk \neq M} \hat{P}_a^{lk} N_{a\parallel}^{lk}\]
  \[\hat{P}_a^{lk} = \frac{1}{\sqrt{\bar{\sigma}_l \lambda_k^l}} s_a^l P_l(\xi) L_k^{(l+1/2)}(s_a^2)\]
  where \(\xi = v \parallel / v\), \(P_l\) is a Legendre polynomial.

- \(\hat{f}_m = \frac{1}{\pi^{3/2}v_T^3} \exp(-s_a^2)\) and \(s_a = \frac{v}{v_T a}\).

- Multiply \(\hat{P}^{jp}\) and integrate over velocity space
  \[v_T \sum_{lk \neq M} \left[ \Phi_B^{jp,lk} \frac{\partial \ln B}{\partial \ell} N_{\parallel}^{lk} + \Psi^{jp,lk} \frac{\partial N_{\parallel}^{lk}}{\partial \ell} + \Phi^{jp,lk} \frac{\partial \ln T}{\partial \ell} N_{\parallel}^{lk} \right] = \frac{1}{\tau} \sum_{lk \neq M} c^{jp,lk} N_{\parallel}^{lk} + g^{jp}\]
Neoclassical transport in general parallel moments

- Parallel moment equations

\[
\frac{\partial N_{jp}}{\partial t} + v_T \sum_{lk\neq M} \left[ \Psi_B^{jp,lk} \frac{\partial \ln B}{\partial \ell} N_{lk} + \Psi_{jp,lk} \frac{\partial N_{lk}}{\partial \ell} + \Phi_{jp,lk} \frac{\partial \ln T}{\partial \ell} N_{lk} \right] + \frac{q}{2T} E_{\parallel} \Theta_{jp,lk} N_{jp} = \frac{1}{\tau} \sum_{lk\neq M} c_{jp,lk} N_{lk} + g_{jp}
\]

- \( \frac{\partial \ln B}{\partial \ell} N_{lk} \) plays a crucial role for neoclassical transport on the flux surface

\[
\frac{\partial N_{jp}}{\partial t} + v_T \sum_{lk\neq M} \left[ \Psi_B^{jp,lk} \frac{\partial \ln B}{\partial \ell} N_{lk} + \Psi_{jp,lk} \frac{\partial N_{lk}}{\partial \ell} \right] = \frac{1}{\tau} \sum_{lk\neq M} c_{jp,lk} N_{lk} + g_{jp}
\]

- To obtain parallel general moments, we need to truncate the set of equations
Truncation of the parallel moment equation

- Truncate the system to \( \iota = LK \) moments with \( l = 0, 1, ..., L - 1 \) and

\[
k = \begin{cases} 
2, 3, ..., K + 1, & l = 0 \\
1, 2, ..., K, & l = 1 \\
0, 1, ..., K - 1, & l > 1
\end{cases}
\]

- The unknown \([N]\) has \( \iota = LK \) components, and begins from \( N[1] \rightarrow N^{02} \) to \( N[\iota] \rightarrow N^{(L-1)(K-1)} \)

- (e.g.) \((L, K) = (3, 3)\)

\[
\begin{bmatrix}
N^{02} \\
N^{03} \\
N^{04} \\
N^{11} \\
\vdots \\
N^{22}
\end{bmatrix} \Rightarrow \begin{bmatrix}
N[1] \\
N[2] \\
N[3] \\
N[4] \\
\vdots \\
N[9]
\end{bmatrix}
\]
In matrix form,

\[
\frac{\partial}{\partial t} [N] + v_T \Psi \partial_{\parallel} [N] + v_T \Psi_B (\partial_{\parallel} \ln B) [N] = \frac{C}{\tau} [N] + [g]
\]

- \([N]\): unknown (initialized as 0)
- \([g]\): thermodynamic drives (rhs)
- \(\Psi, \Psi_B, C\): constant matrices

\[
(1 + \Delta t f_\Psi v_T [\Psi] \partial_{\parallel} + \Delta t v_T f_B [\Psi_B] (\partial_{\parallel} \ln B) - f_C \frac{\Delta t}{\tau} [C]) [\Delta N] \\
= \Delta t \left( \frac{1}{\tau} [C] [N]^k - v_T [\Psi] \partial_{\parallel} [N]^k - v_T [\Psi_B] (\partial_{\parallel} \ln B) [N]^k + [g] \right)
\]

- \(\partial_{\parallel} \rightarrow \alpha_i (\mathbf{b} \cdot \nabla) \alpha_j\)
- Use centering parameters \(f_\Psi, f_C, f_B\) for the implicit scheme
\( \Psi \) and \( \Psi_B \) matrix

- \( v_T \sum_{l_k \neq M} \Psi_{p_k}^l \partial_{N_{l+1,k}}^l + \Psi_{p_k}^l \partial_{N_{l-1,k}}^l \)
- \( \Psi_{p_k}^{l+} = \frac{l+1}{\sqrt{(2l+1)(2l+3)}} \left[ \sqrt{l + p + \frac{3}{2} \delta_{p,k} - \sqrt{p} \delta_{p-1,k}} \right] \)
- \( \Psi_{p_k}^{l-} = \frac{l}{\sqrt{(2l-1)(2l+1)}} \left[ \sqrt{l + p + \frac{1}{2} \delta_{p,k} - \sqrt{p + 1} \delta_{p,k-1}} \right] \)
- \( \Psi_{B,p_k}^{l+} = -\frac{j+2}{2} \Psi_{p_k}^{l+}, \Psi_{B,p_k}^{l-} = \frac{j-1}{2} \Psi_{p_k}^{l-} \)

\[
\begin{pmatrix}
\overline{\Psi}_0^{0+} & \overline{\Psi}_2^{0+} & \overline{\Psi}_3^{0+} \\
\overline{\Psi}_1^{21} & \overline{\Psi}_2^{22} & \overline{\Psi}_3^{23} \\
\overline{\Psi}_1^{12} & \overline{\Psi}_2^{12} & \overline{\Psi}_3^{13} \\
\overline{\Psi}_1^{10} & \overline{\Psi}_2^{11} & \overline{\Psi}_3^{11} \\
\end{pmatrix}
\]

- For the numL=3, numK=3 case
Code verification with ion integral closures

- Time independent, homogeneous magnetic field problem in matrix form,

\[
(1 - \frac{\Delta t}{\tau} C + \Delta t v_T \Psi \partial_{\parallel}) \Delta [N] = [g] \Delta t
\]

- For sinusoidal drives, \( T = T_0 + T_1 \sin \varphi \), \( V_{\parallel} = V_0 + V_1 \sin \varphi \), where \( \varphi = 2\pi \ell / \lambda + \varphi_0 \).

\[
\begin{align*}
\hat{h}(\ell) &= -\frac{1}{2} n T_1 v_T \hat{h} \cos \varphi - n T_0 V_1 \hat{\pi} \sin \varphi \\
\hat{\pi}(\ell) &= -n T_1 \hat{\pi} \sin \varphi - n T_0 \frac{V_1}{v_T} \hat{\pi} \cos \varphi
\end{align*}
\]

\[1\text{[Ji et al, PoP 23,032124 (2016)], [Ji et al, PoP 24,022127 (2017)]\]
• Parallel closures are related to the general moments by

\[
\begin{align*}
    h_\parallel &= -\frac{\sqrt{5}}{2} v_T T n^{11} \\
    R_\parallel &= \frac{m_e v_{T,e}}{\tau_{ei}} \left[ -n_e \frac{V_{ei,\parallel}}{v_{T,e}} + \frac{1}{\sqrt{2}} \sum_{k=1}^\infty a_{ei}^{10k} n_1^{1k} \right] \\
    \pi_\parallel &= \frac{2}{\sqrt{3}} T n^{20}
\end{align*}
\]

• For sinusoidal drives, \( T = T_0 + T_1 \sin \varphi \), \( V_\parallel = V_0 + V_1 \sin \varphi \), \( V_{ei,\parallel} = V_{ei} \cos \varphi \), where \( \varphi = 2\pi \ell/\lambda + \varphi_0 \).

\[
\begin{align*}
    h_\parallel(\ell) &= -\frac{1}{2} nT_1 v_T \hat{h}_h \cos \varphi + nT_0 V_{ei} \hat{h}_R \cos \varphi - nT_0 V_1 \hat{h}_\pi \sin \varphi \\
    R_\parallel(\ell) &= -nT_1 \frac{2\pi}{\lambda} \hat{R}_h \cos \varphi - \frac{mnV_{ei}}{\tau_{ei}} \hat{R}_R \cos \varphi - nmV_1 \frac{2\pi v_T}{\lambda} \hat{R}_\pi \sin \varphi \\
    \pi_\parallel(\ell) &= -nT_1 \hat{\pi}_h \sin \varphi + 2nT_0 \frac{V_{ei}}{v_T} \hat{\pi}_R \sin \varphi - nT_0 \frac{V_1}{v_T} \hat{\pi}_\pi \cos \varphi
\end{align*}
\]
Ion $\hat{h}_h$, $\hat{\pi}_\pi$ closures ($T_i = T_e$)

Figure 1: Ion $\hat{h}_h$ closure (left) Ion $\hat{\pi}_\pi$ closure (right)

- x axis: Knudsen number (mean free path)
- error $\sim 0.1\%$
Ion $\hat{h}_\pi$, $\hat{\pi}_h$ closures ($T_i = T_e$)

Figure 2: Ion $\hat{h}_\pi$ closure (left) Ion $\hat{\pi}_h$ closure (right)

- $\hat{h}_\pi$ closure: heat flux responding to the parallel rate of strain tensor
Electron $\hat{h}_h$, $\hat{\pi}_\pi$ closures ($Z = 1$)

Figure 3: Electron $\hat{h}_h$ closure (left) Electron $\hat{\pi}_\pi$ closure (right)
Electron $\hat{h}_\pi, \hat{R}_\pi$ closures ($Z = 1$)

Figure 4: Electron $\hat{h}_\pi$ closure (left) Electron $\hat{R}_\pi$ closure (right)

- $\hat{R}_\pi$ closure: Collisional momentum exchange responding to the parallel rate of strain tensor
Electron $\hat{h}_R$, $\hat{R}_R$ closures ($Z = 1$)

Figure 5: Electron $\hat{h}_R$ closure (left) Electron $\hat{R}_R$ closure (right)
Computational complexities

- $mx=16, my=16$

- $poly\_degree=1$

- Using 16 processors during one step

- About 30 minutes

- Maximum number of moments in NIMROD (current state): 400 moments $= 20 \times 20$

- Restriction on NERSC for 1 GB matrix allocations

- New block allocation method is required
NIMROD fluid equations and closures

- Fluid closures are calculated by moment equations.

\[
\begin{align*}
\rho D_t V &= J \times B - \nabla p - \nabla \cdot \pi \\
\frac{n}{\gamma - 1} D_t T &= -p \nabla \cdot V - \pi : \nabla V - \nabla \cdot h + Q \\
E &= -V \times B + \frac{1}{ne} J \times B + \frac{m_e}{ne^2} \left[ \frac{\partial J}{\partial t} + \nabla \cdot (JV + VJ) - \frac{e}{m_e} (\nabla p) \right] \\
&\quad - \frac{1}{ne} \nabla \cdot \pi + \eta J
\end{align*}
\]

- Collisional momentum exchange

\[
\begin{align*}
\eta J|| &\rightarrow \frac{R||}{ne e} \\
\frac{R||}{ne e} &= \frac{m_e v_{T,e}}{ne e \tau_{ei}} \left[ -n_e \hat{V}_{e,||} + \frac{1}{\sqrt{2}} \sum_{k=1} a_{ei}^{10k} n^{1k} \right]
\end{align*}
\]
Time-dependent neoclassical transport: initial conditions

Figure 6: 32×48 spatial grid following flux surfaces for aspect-ratio-ten tokamak. An annulus poloidal mesh can be used to avoid numerical issues on boundaries (left). The equilibrium profile along major radius $R$ (right). [Held, E. D., et al. "Verification of continuum drift kinetic equation solvers in NIMROD." Physics of Plasmas 22.3 (2015)]

- Starting from equilibrium temperature profile on the high aspect ratio tokamak
- Applying parallel moments for each time-step
Time-dependent neoclassical transport: ongoing results

Figure 7: Time-slicing profiles of the heat flux ($h_\parallel$) along the radial direction for electron (left) and ion (right)

- Plan to solve the numerical instability issue by using the proper boundary value
Figure 8: Spatial grid for the high-beta, DIII-D like equilibrium (left). The equilibrium profile along major radius $R$ (right)

- Obtaining closures for high-beta DIII-D type equilibrium
- Comparing the bootstrap current research with the CEL approach result
- Equilibrium ion and electron velocities would be surface-averaged to obtain $\langle J_\parallel B \rangle$
- Adding temperature gradient coupling
Conclusion

- Parallel moment equations are implemented in NIMROD.

\[
\frac{\partial N_{jp}^{||}}{\partial t} + v_T \sum_{lk \neq M} \left[ \Psi_B^{jp,lk} \frac{\partial \ln B}{\partial \ell} N^{lk} + \Psi^{jp,lk} \frac{\partial N^{lk}^{||}}{\partial \ell} \right] = \frac{1}{\tau} \sum_{lk \neq M} c^{jp,lk} N^{lk}_{||} + g^{jp}
\]

- For the time independent and homogenous magnetic field problem, the code thoroughly reproduces analytic results.

- To solve the time dependent and nonlinear problem, the code requires proper boundary conditions for numerical stability issues.