Implementing moment equations for parallel closures in NIMROD

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Motivation

- Implementing general moment equations in NIMROD (Integrating over velocity variables).
- Calculating exact parallel moment equation avoiding integrals along the field lines.
- In a large Knudsen number, trying to capture some kinetic effects about parallel dynamics for magnetized plasmas.
- Trying to incorporate time-dependent and non-linear effects in integral closures.

General parallel moment equation

- Landau (Fokker-Planck) kinetic equation

$$\frac{\partial f_a}{\partial t} + \mathbf{v} \cdot \nabla f_a + \frac{q_a}{m_a}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_a}{\partial \mathbf{v}} = \sum_b C(f_a, f_b)$$

- Take gyro-average and linearize

$$v_\parallel \frac{\partial \overline{f_a^{\mathrm{N}}}}{\partial \ell} = \overline{C_{\mathrm{L}}(f_a^{\mathrm{N}})} - v_\parallel \frac{\partial \overline{f_a^{\mathrm{M}}}}{\partial \ell} + \overline{C_{\mathrm{L}}(f_a^{\mathrm{M}})}$$

- Moment expansion

$$\overline{f_a^{\mathrm{N}}} = \hat{f}_a^{\mathrm{m}} \sum_{lk \neq \mathsf{M}} \hat{P}_a^{lk} n_a^{lk}$$

with $\hat{f}_a^{\mathrm{m}} = \frac{1}{\pi^{3/2} v_{Ta}^3} \exp(-s_a^2)$ and $\mathbf{s}_a = \frac{\mathbf{v}}{v_{Ta}}$

$$\hat{P}_a^{lk} = \frac{1}{\sqrt{\bar{\sigma}_l \lambda_k^l}} s_a^l P_l(\xi) L_k^{(l+1/2)}(s_a^2)$$

where $\xi = v_\parallel / v$,P_l is a Legendre polynomial.

General parallel moment equation

$$v_\parallel \frac{\partial \overline{f^{\mathrm{N}}}}{\partial \ell} = \overline{C_{\mathrm{L}}(f^{\mathrm{N}})} - v_\parallel \frac{\partial \overline{f^{\mathrm{M}}}}{\partial \ell} + \overline{C_{\mathrm{L}}(f^{\mathrm{M}})}$$

- Multiply $\hat{P}^{jp}$and integrate over velocity space

$$v_T \sum_{lk \neq \mathrm{M}} \overline{\Psi}^{jp,lk} \frac{\partial n^{lk}}{\partial \ell} = \frac{1}{\tau} \sum_{lk \neq \mathrm{M}} c^{jp,lk} n^{lk} + \frac{1}{\tau} g^{jp}$$

$$\begin{aligned}
\overline{\Psi}^{jp,lk} &= \int d\mathbf{v} \hat{P}^{jp} s_\parallel \hat{f}^{\mathrm{m}} \hat{P}^{lk} \\
c^{jp,lk} &= \tau \int d\mathbf{v} \hat{P}^{jp} C_{\mathrm{L}}(\hat{f}^{\mathrm{m}} \hat{P}^{lk}) \\
g^{jp} &= \int d\mathbf{v} \hat{P}^{jp} [\tau \overline{C_{\mathrm{L}}(f^{\mathrm{M}})} - v_T \tau \frac{\partial \overline{f}^{\mathrm{M}}}{\partial \ell}]
\end{aligned}$$

Integral closures for arbitrary collisionality

- Truncate the system to $N = LK$ moments with $j, l = 0, 1, ..., L-1$ and

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

$$\sum_{B=1}^{N} \Psi_{AB} \frac{\partial n_B}{\partial \eta} = \sum_{B=1}^{N} C_{AB} n_B + g_A$$

- $d\eta = d\ell/\lambda_c$,normalized arclength along a magnetic field line by the collision length.

$$n_A(\eta) = \sum_B \int_{-\infty}^{\infty} K_{AB}(\eta - \eta') g_B(\eta') d\eta'$$

- Fitted kernel functions for arbitrary collisionality are available for electron and ion. [Ji *et al*, PoP 23,032124 (2016)],[Ji *et al*, PoP 24,022127 (2017)]

Closures for sinusoidal drives

- Parallel closures are related to the general moments by

$$
\begin{aligned}
h_{\|} &= -\frac{\sqrt{5}}{2} v_T T n^{11} \\
R_{\|} &= \frac{m_{\mathrm{e}} v_{T,\mathrm{e}}}{\tau_{\mathrm{ei}}} \left[-n_{\mathrm{e}} \frac{V_{\mathrm{ei},\|}}{v_{T,\mathrm{e}}} + \frac{1}{\sqrt{2}} \sum_{k=1} a_{\mathrm{ei}}^{10k} n^{1k} \right] \\
\pi_{\|} &= \frac{2}{\sqrt{3}} T n^{20}
\end{aligned}
$$

- For sinusoidal drives, $T = T_0 + T_1 \sin\varphi$, $V_{||} = V_0 + V_1 \sin\varphi$, $V_{\mathrm{ei},||} = V_{\mathrm{ei}} \cos\varphi$, where $\varphi = 2\pi\ell/\lambda + \varphi_0$.

$$
\begin{aligned}
h_{\|}(\ell) &= -\frac{1}{2} n T_1 v_T \hat{h}_h \cos\varphi + n T_0 V_{\mathrm{ei}} \hat{h}_R \cos\varphi - n T_0 V_1 \hat{h}_\pi \sin\varphi \\
R_{\|}(\ell) &= -n T_1 \frac{2\pi}{\lambda} \hat{R}_h \cos\varphi - \frac{m n V_{\mathrm{ei}}}{\tau_{\mathrm{ei}}} \hat{R}_R \cos\varphi - n m V_1 \frac{2\pi v_T}{\lambda} \hat{R}_\pi \sin\varphi \\
\pi_{\|}(\ell) &= -n T_1 \hat{\pi}_h \sin\varphi + 2 n T_0 \frac{V_{\mathrm{ei}}}{v_T} \hat{\pi}_R \sin\varphi - n T_0 \frac{V_1}{v_T} \hat{\pi}_\pi \cos\varphi
\end{aligned}
$$

- Calculated closures are compared with theoretical values.

NIMROD Fluid equations and closures

- Fluid closures are calculated by moment equations.

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

- Collisional momentum exchange

$$
\begin{aligned}
\eta J_{||} &\rightarrow \frac{R_{||}}{n_\mathrm{e} e} \\
\frac{R_{||}}{n_\mathrm{e} e} &= \frac{m_\mathrm{e} v_{T,\mathrm{e}}}{n_\mathrm{e} e \tau_\mathrm{ei}} \left[-n_\mathrm{e} \hat{V}_{\mathrm{ei},||} + \frac{1}{\sqrt{2}} \sum_{k=1} a_\mathrm{ei}^{10k} n^{1k} \right]
\end{aligned}
$$

Algorithm

- By using whole $N = LK$ moments in a single vector, we can use the matrix form of Ψ.

$$\left(1 + \Delta t f_\psi \left[\psi\right] \partial_\parallel + \Delta t f_c \left[c\right]\right) \left[\Delta n\right]_{\text{pass}} = \Delta t(\left[c\right] \left[n\right]^k + \left[\psi\right] \partial_\parallel \left[n\right]^k + \left[g\right])$$

Tested in a single time shot by taking off mass matrix term

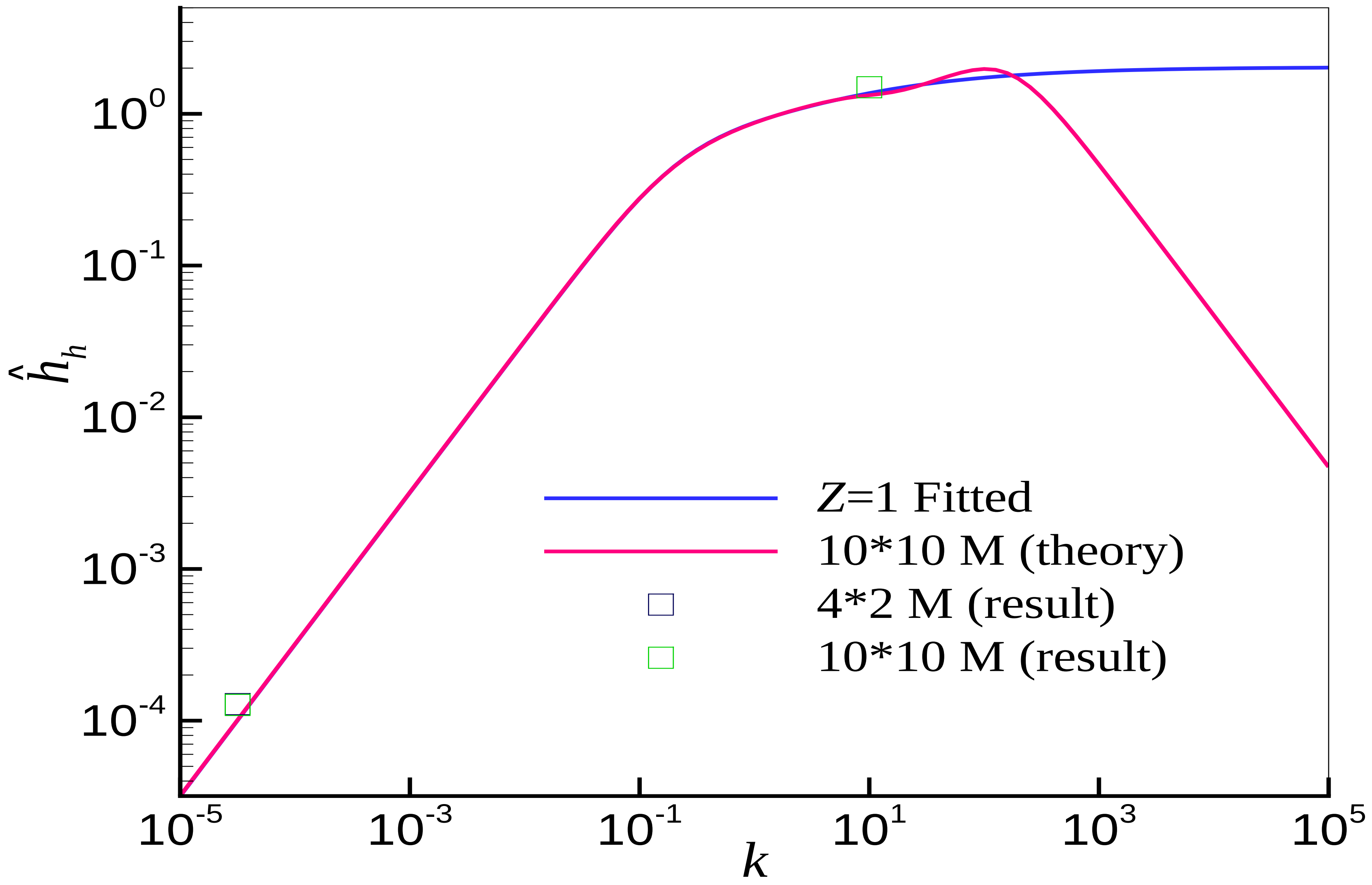
- Alternatively, an algorithm for separated vectors of odd and even l moments is possible(ongoing).

$$\begin{aligned}
\partial_t \left[n\right]^{\text{even}} &= \left[c\right] \left[n\right]^{\text{even}} + \left[\psi\right] \left[n\right]^{\text{odd}} + \left[g(n, T, \nabla \mathbf{V})\right] \\
\partial_t \left[n\right]^{\text{odd}} &= \left[c\right] \left[n\right]^{\text{odd}} + \left[\psi\right] \left[n\right]^{\text{even}} + \left[g(n, T, \mathbf{V}_{\text{ei}})\right]
\end{aligned}$$

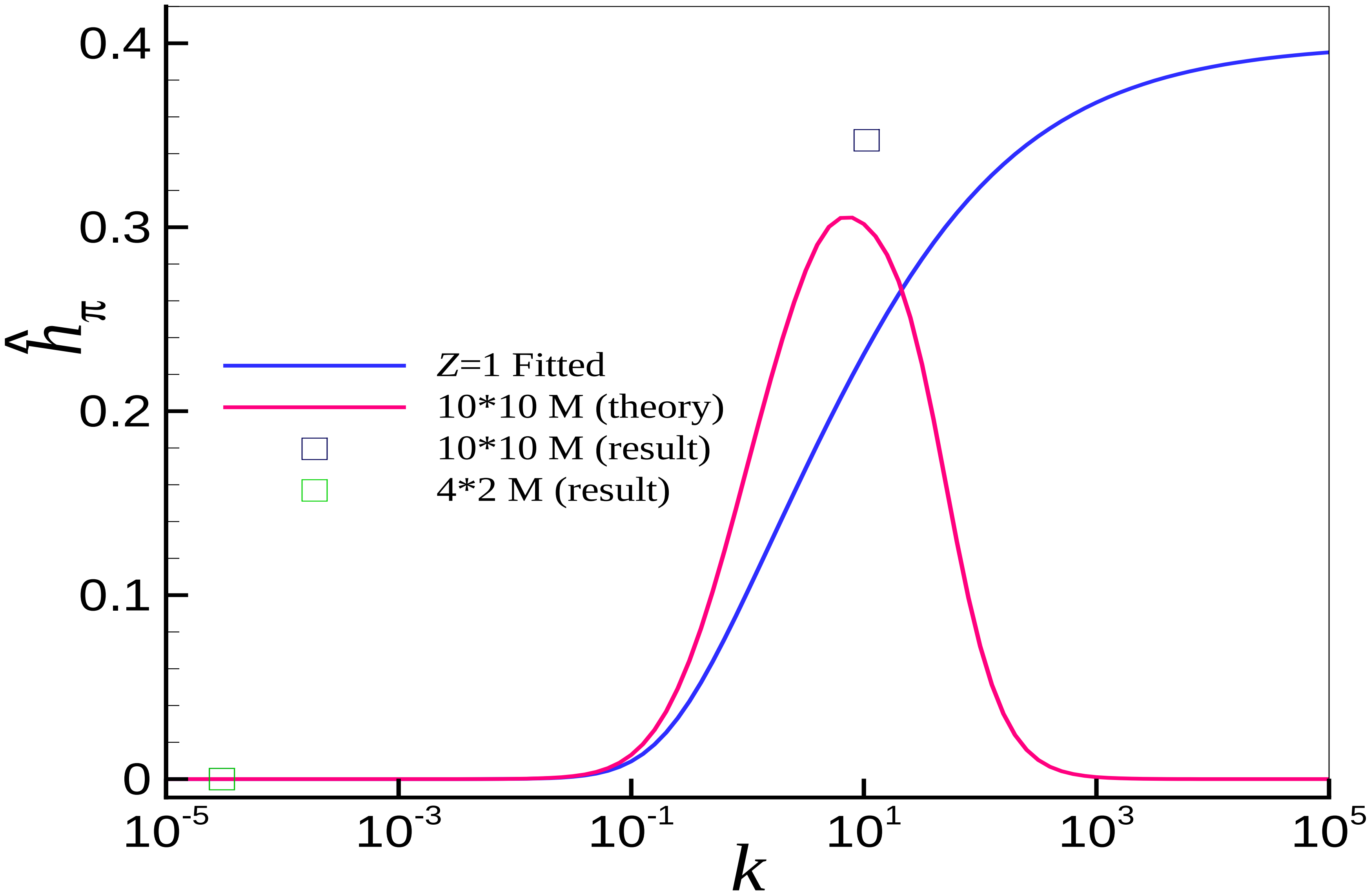
Predictor-corrector time advance $t^k \rightarrow t^{k+1}$

$$\left(1 + \Delta t f_{[n]} \left[c\right]\right) \left[\Delta n\right]_{\text{pass}} = \Delta t(\left[c\right] \left[n\right]^k + \left[\psi\right] \left[n\right]^{k+1/2} + \left[g\right])$$

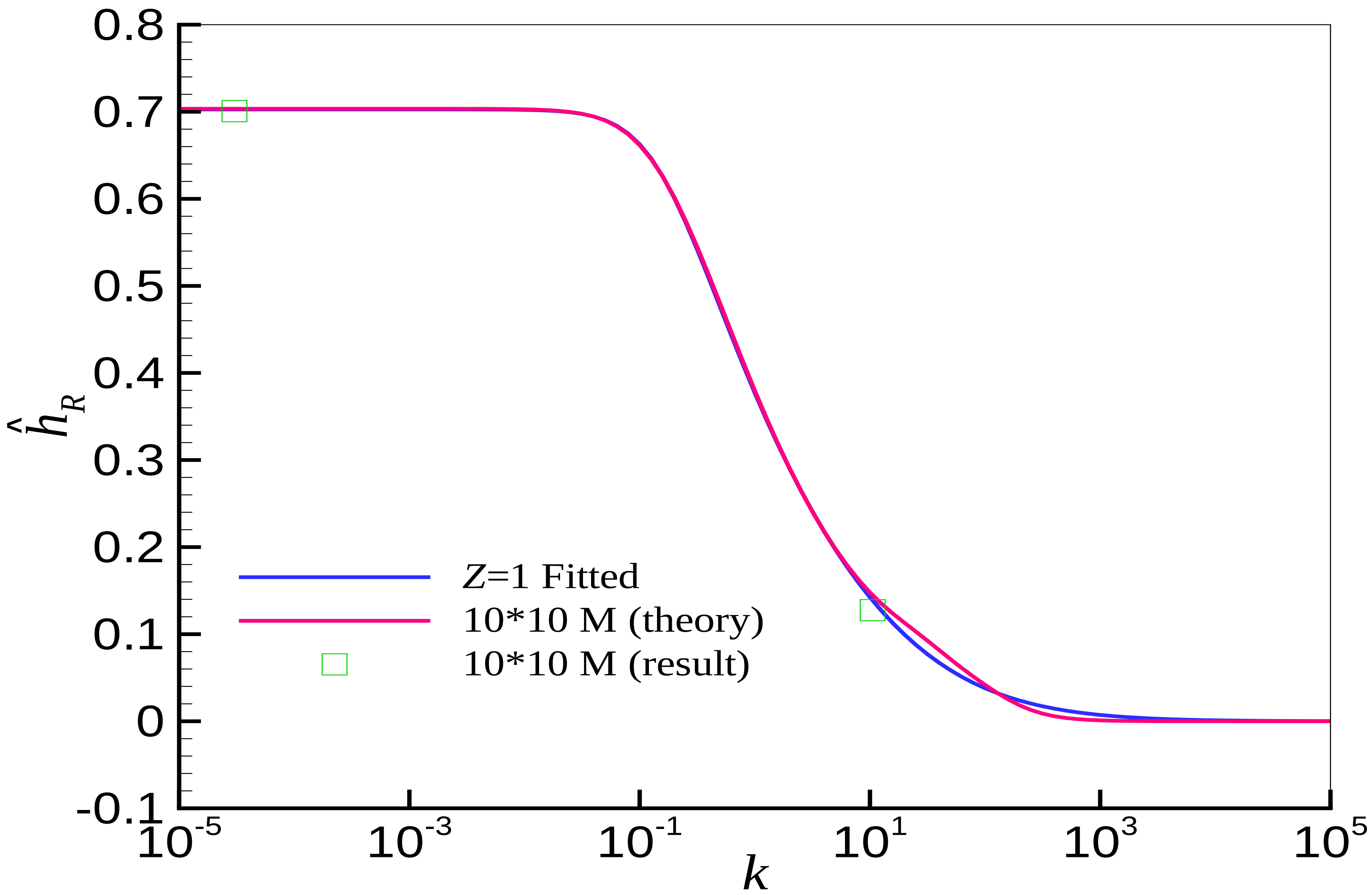
Electron $\hat{h}_h$ closure



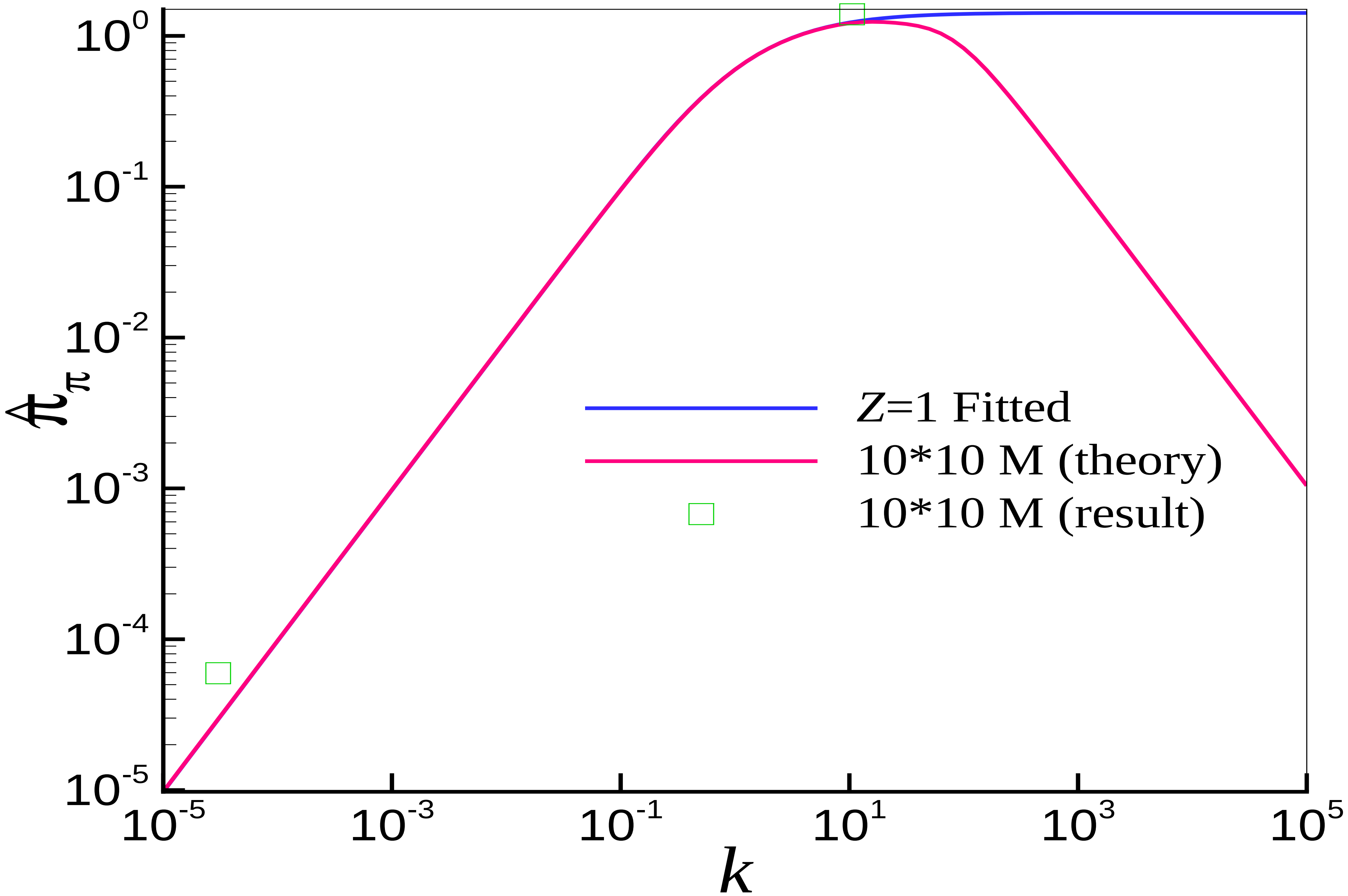
Electron $\hat{h}_\pi$ closure



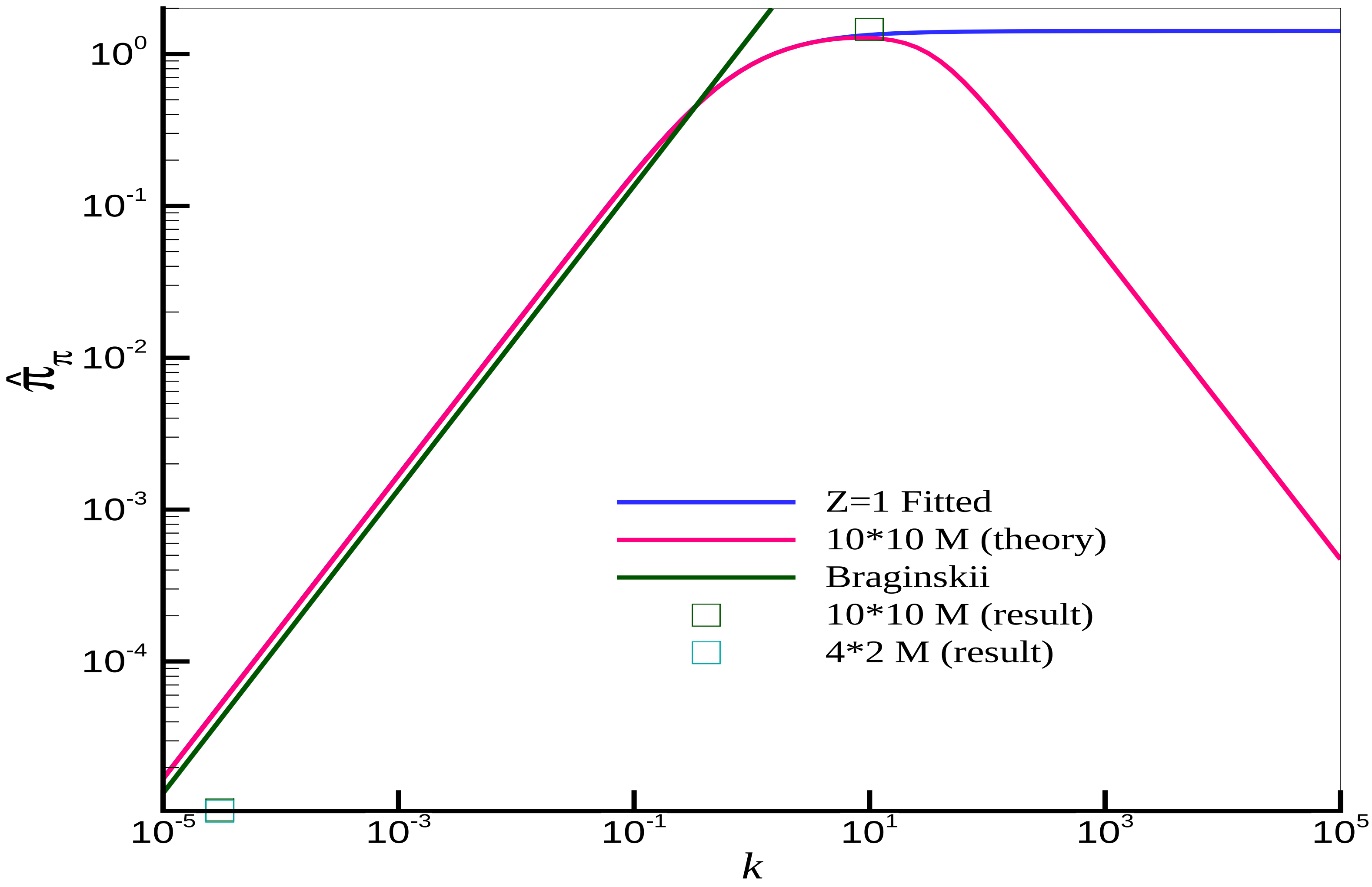
Electron $\hat{h}_R$ closure



Electron $\hat{\pi}_\pi$ closure



Ion $\hat{\pi}_\pi$ closure ($T_\mathrm{i} = T_\mathrm{e}$)



Future plan

$$\partial_t \bar{N}_{\parallel}^{lp} + \sum_k \Big[\bar{\Xi}_{pk}^{l} (\partial_t \ln T) \bar{N}_{\parallel}^{lk} + v_T (\bar{\Psi}_{pk}^{l+} \partial_{\parallel}^{l+} + \bar{\Phi}_{pk}^{l+} \partial_{\parallel} \ln T + \frac{q}{2T} \bar{\Theta}_{pk}^{l+} E_{\parallel}) \bar{N}_{\parallel}^{l+1,k}$$

$$+ v_T (\bar{\Psi}_{pk}^{l-} \partial_{\parallel}^{l-} + \bar{\Phi}_{pk}^{l-} \partial_{\parallel} \ln T + \frac{q}{2T} \bar{\Theta}_{pk}^{l-} E_{\parallel}) \bar{N}_{\parallel}^{l-1,k} \Big] = \sum C^{lpk} \bar{N}_{\parallel}^{lk} + C^{(2)} + G^{lp}$$

$$\partial_{\parallel}^{l+} = \partial_{\parallel} - \frac{l+2}{2} (\partial_{\parallel} \ln B)$$

$$\partial_{\parallel}^{l-} = \partial_{\parallel} + \frac{l-1}{2} (\partial_{\parallel} \ln B)$$

- Adding temperature gradient coupling (blue terms).
- Adding magnetic field gradient coupling (green terms).
- Verification in equilibrium states [Held, E. D., *et al.* "Verification of continuum drift kinetic equation solvers in NIMROD." Physics of Plasmas 22.3 (2015)]
    - High aspect ratio equilibrium
    - High beta DIII-D like equilibrium