A Newton-Krylov Method for Simultaneous Semi-Implicit Time-advance of Extended MHD with Kinetic Closures*

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Newton-Krylov Simultaneous Time-advance

- Motive:
  Replacing heuristic closures in Eric Howell's NTM simulations with kinetic closures

- Smaller cases:
  - Frozen B-field temperature flattening
  - Thermal Equilibration

$$[\mathbf{u}, F_\mathrm{i}]\left(t^k\right) \quad n, [T_\mathrm{e}, T_\mathrm{i}, \mathbf{B}, F_\mathrm{e}]\left(t^{k+\frac{1}{2}}\right) \quad [\mathbf{u}, F_\mathrm{i}]\left(t^{k+1}\right) \quad n, [T_\mathrm{e}, T_\mathrm{i}, \mathbf{B}, F_\mathrm{e}]\left(t^{k+\frac{3}{2}}\right)$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left[\overbrace{-\mathbf{u} \times \mathbf{B} - \frac{\mathbf{J} \times \mathbf{B}}{n_\mathrm{e} q_\mathrm{e}} + \frac{\nabla \cdot \mathbf{p}_\mathrm{e}}{n_\mathrm{e} q_\mathrm{e}} - \frac{\mathbf{R}_\mathrm{e}}{n_\mathrm{e} q_\mathrm{e}} + \frac{m_\mathrm{e}}{n_\mathrm{e} q_\mathrm{e}^2} \frac{\partial \mathbf{J}}{\partial t}}^{\mathbf{E}} \right]$$

$$\frac{3}{2} n_a \frac{\partial T_a}{\partial t} + \frac{3}{2} n_a \mathbf{V}_a \cdot \nabla T_a + n_a T_a \nabla \cdot \mathbf{V}_a + \nabla \cdot \mathbf{q}_a + \nabla \mathbf{V}_a : \pi_a = Q_a$$

$$\mathbf{J} = \mu_0^{-1} \nabla \times \mathbf{B}$$

$$\mathbf{p}_a = \pi_a + n_a T_a \mathbf{I}$$

$$\pi_{\mathrm{e}\|} = \pi m_\mathrm{e} v_{T\mathrm{e}}^5 \int_0^\infty ds s^4 \int_{-1}^1 d\xi \left(3\xi^2 - 1\right) F_\mathrm{e}$$

$$\mathbf{R}_\mathrm{e} = \eta_\perp \mathbf{J} + \sum_b 2\pi m_\mathrm{e} v_{T\mathrm{e}}^4 \int ds s^3 \int_{-1}^1 d\xi \xi \left[C\left[F_\mathrm{e}, f_b^M\right] + C\left[f_b^M, F_\mathrm{e}\right] \right]$$

$$\mathbf{q}_a = -\kappa_{a\perp} \left(\mathbf{I} - \mathbf{bb}\right) \cdot \nabla T_a - \kappa_{a\times} \mathbf{b} \times \nabla T_a + q_{a\|} \mathbf{b}$$

$$q_{\mathrm{i}\|} = -\kappa_{\mathrm{i}\|} \mathbf{b} \cdot \nabla T_\mathrm{i}$$

$$q_{\mathrm{e}\|} = \pi m_\mathrm{e} v_{T\mathrm{e}}^6 \int_0^\infty ds s^5 \int_{-1}^1 d\xi \xi F_\mathrm{e}$$

$$(s, \xi) \equiv \left(\left|\mathbf{v} - \mathbf{u}\right| / v_T, (\mathbf{v} - \mathbf{u}) \cdot \mathbf{b} / \left|\mathbf{v} - \mathbf{u}\right| \right)$$

CEL drift kinetic equation

Starting from the DKE* project out Maxwellian part, $f = f^{\mathrm{M}} + F$

$$\frac{\partial F}{\partial t} + \mathbf{v}_{\mathrm{gc}} \cdot \nabla F + \dot{s}\frac{\partial F}{\partial s} + \dot{\xi}\frac{\partial F}{\partial \xi} = C - f^{\mathrm{M}}\left[\frac{d\ln n}{dt} + \frac{2\mathbf{s}}{v_T}\cdot\frac{d\mathbf{u}}{dt} + \left(s^2 - \frac{3}{2}\right)\frac{d\ln T}{dt}\right]$$

where

$$s \equiv |\mathbf{v} - \mathbf{u}|/v_T, \xi \equiv (\mathbf{v} - \mathbf{u})\cdot\mathbf{b}/|\mathbf{v} - \mathbf{u}|$$

$$\mathbf{v}_{\mathrm{gc}} = v_T s\xi\mathbf{b} + \frac{\mathbf{E}\times\mathbf{B}}{B^2} + \frac{Ts^2}{qB}\left(1+\xi^2\right)\mathbf{b}\times\nabla\ln B + \frac{2Ts^2}{qB^2}\left[\xi^2\left(\mathbf{I} - \mathbf{bb}\right) + \frac{1}{2}\left(1-\xi^2\right)\mathbf{bb}\right]\cdot\nabla\times\mathbf{B} + \frac{mv_T s\xi}{qB^2}\mathbf{b}\times\frac{\partial\mathbf{B}}{\partial t}$$

$$\dot{s} = -\frac{s}{2}\frac{d\ln T}{dt} + \frac{s\left(1-\xi^2\right)}{2}\frac{\partial\ln B}{\partial t} + \frac{q\mathbf{v}_{\mathrm{gc}}\cdot\mathbf{E}}{2sT}$$

$$\dot{\xi} = \frac{1-\xi^2}{2\xi}\left\{-\xi^2\frac{\partial\ln B}{\partial t} + \left(v_T s\xi\mathbf{b} + \mathbf{v}_{\mathrm{c}}^*\right)\cdot\left(\frac{q\mathbf{E}}{Ts^2} - \nabla\ln B\right) + \xi^2\frac{\mathbf{E}\times\mathbf{B}}{B^2}\cdot\nabla\ln B - \frac{\xi^2}{B^2}\left[\mathbf{bb}\cdot\left(\nabla\times\mathbf{B}\right)\right]\cdot\mathbf{E} - 2\frac{Ts^2\xi^2}{q}\mathbf{b}\cdot\nabla\left[\frac{\mathbf{b}\cdot\left(\nabla\times\mathbf{B}\right)}{B^2}\right] + \frac{mv_T s\xi}{qB}\nabla\cdot\left(\mathbf{b}\times\frac{\partial\mathbf{b}}{\partial t}\right)\right\}$$

$$\mathbf{v}_c^* = \frac{2Ts^2\xi^2}{qB^2}\left(\mathbf{I} - \mathbf{bb}\right)\cdot\nabla\times\mathbf{B} + \frac{mv_T s\xi}{qB^2}\mathbf{b}\times\frac{\partial\mathbf{B}}{\partial t}$$

*R.D. Hazeltine, *Plasma Phys.* **15**, 77 (1973); R.D. Hazeltine and J.D. Meiss, Plasma Confinement (Adisson-Wesley, Redwood City, 1992); J. J. Ramos, *Phys. Plasmas* **17**, 082502 (2010).

Semi-implicit Newton-Krylov method

$$\frac{\partial \boldsymbol{f}}{\partial t} = \boldsymbol{\mathcal{L}}\left(\boldsymbol{f}\right) + \boldsymbol{\mathcal{S}} \quad \xrightarrow{\text{semi-implicit time-discretization}} \quad \frac{\boldsymbol{f}^{k+1} - \boldsymbol{f}^{k}}{\Delta t} = \theta \boldsymbol{\mathcal{L}}\left(\boldsymbol{f}^{k+1}\right) + (1-\theta)\,\boldsymbol{\mathcal{L}}\left(\boldsymbol{f}^{k}\right) + \boldsymbol{\mathcal{S}}$$

$$\underbrace{\boldsymbol{f}^{k+1} - \theta\Delta t\left[\boldsymbol{\mathcal{L}}\left(\boldsymbol{f}^{k+1}\right)\right]}_{\mathbf{A}\left(\boldsymbol{f}^{k+1}\right)} = \underbrace{\underbrace{\Delta t\left[\boldsymbol{\mathcal{L}}\left(\boldsymbol{f}^{k}\right) + \boldsymbol{\mathcal{S}}\right]}_{\mathbf{b}\left(\boldsymbol{f}^{k}\right)} + \underbrace{\left\{\boldsymbol{f}^{k} - \theta\Delta t\left[\boldsymbol{\mathcal{L}}\left(\boldsymbol{f}^{k}\right)\right]\right\}}_{\mathbf{A}\left(\boldsymbol{f}^{k}\right)}}_{\mathbf{b}^{*}\left(\boldsymbol{f}^{k}\right)}$$

Use preconditioned GMRES to solve

$$\mathbf{J}\left(\boldsymbol{f}^{k+1,n}\right) \cdot \left(\boldsymbol{f}^{k+1,n+1} - \boldsymbol{f}^{k+1,n}\right) = \left[\mathbf{b}^{*}\left(\boldsymbol{f}^{k}\right) - \mathbf{A}\left(\boldsymbol{f}^{k+1,n}\right)\right]$$

where

$$J_{ij}\left(\boldsymbol{f}^{k+1,n}\right) = \partial A_i / \partial f_j \left(\boldsymbol{f}^{k+1,n}\right)$$

Iterate until satisfied with residual

Solution Convergence Criteria

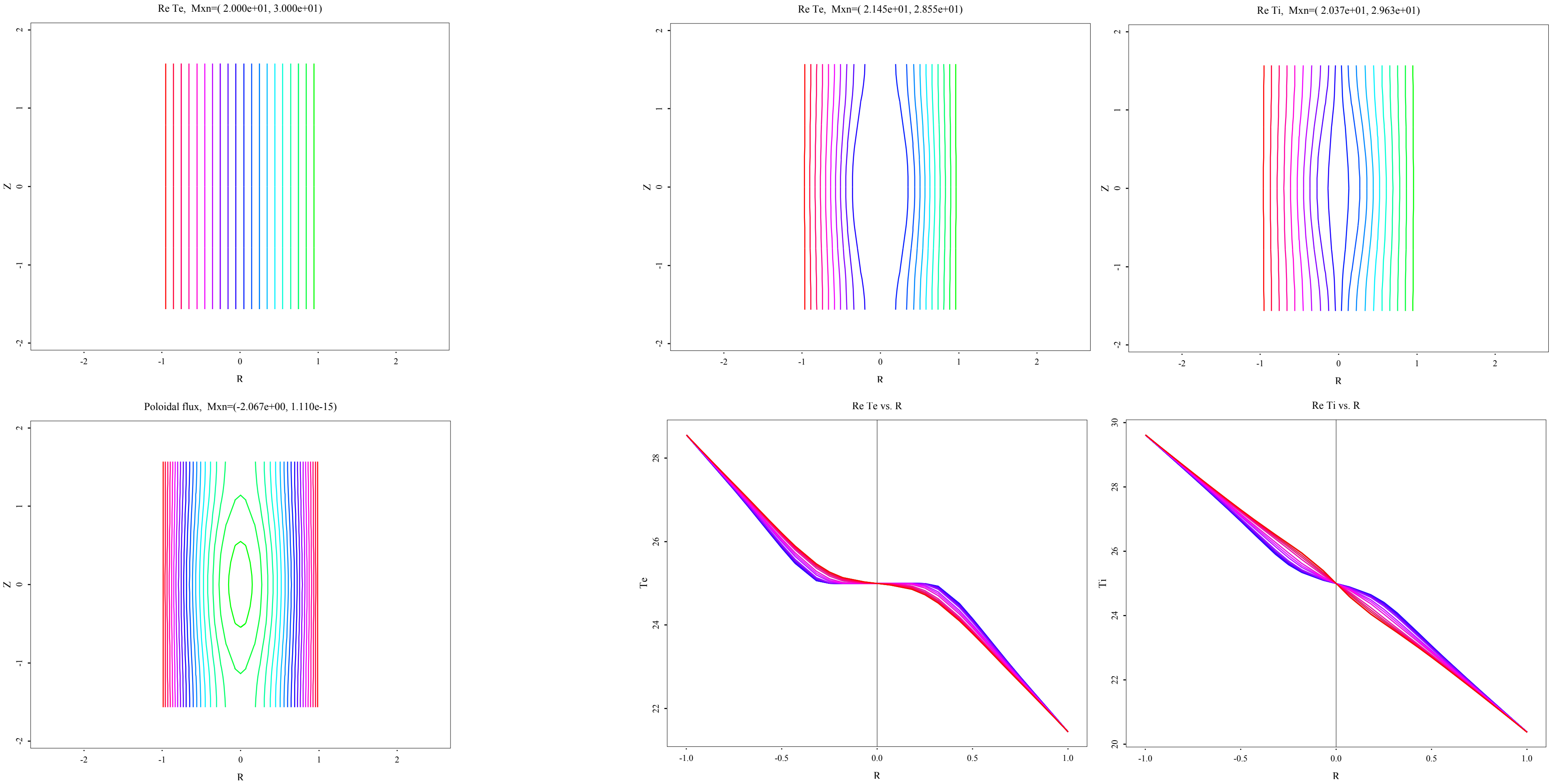
GMRES convergence criteria:

$$\frac{\left|\mathbf{J}\left(\boldsymbol{f}^{k+1,n}\right)\left(\boldsymbol{f}^{k+1,n+1}-\boldsymbol{f}^{k+1,n}\right)-\left[\mathbf{b}^*\left(\boldsymbol{f}^{k}\right)-\mathbf{A}\left(\boldsymbol{f}^{k+1,n}\right)\right]\right|}{\left|\mathbf{b}^*\left(\boldsymbol{f}^{k}\right)-\mathbf{A}\left(\boldsymbol{f}^{k+1,n}\right)\right|}<\text{tol}\,\frac{\left|\mathbf{b}\left(\boldsymbol{f}^{k}\right)\right|}{\left|\mathbf{b}^*\left(\boldsymbol{f}^{k}\right)-\mathbf{A}\left(\boldsymbol{f}^{k+1,n}\right)\right|}$$

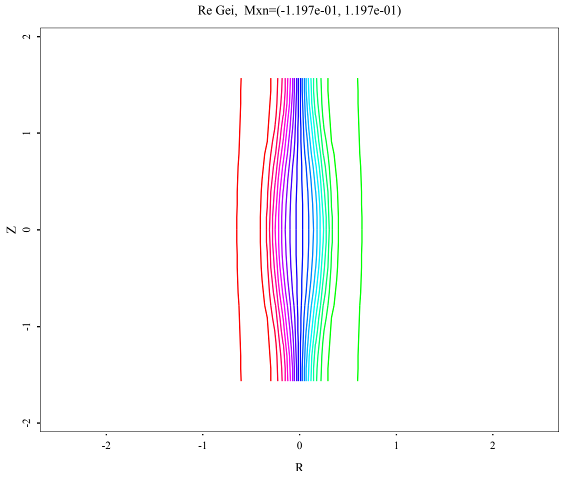
Newton iterations convergence criteria:

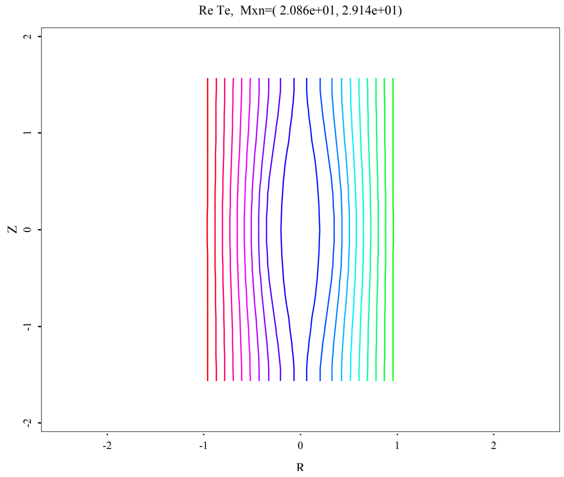
$$\frac{\left|\mathbf{b}^*\left(\boldsymbol{f}^{k}\right)-\mathbf{A}\left(\boldsymbol{f}^{k+1,n+1}\right)\right|}{\left|\mathbf{b}\left(\boldsymbol{f}^{k}\right)\right|}<\text{tol} \qquad \text{or} \qquad \left|\mathbf{b}^*\left(\boldsymbol{f}^{k}\right)-\mathbf{A}\left(\boldsymbol{f}^{k+1,n+1}\right)\right|<\text{tol}$$

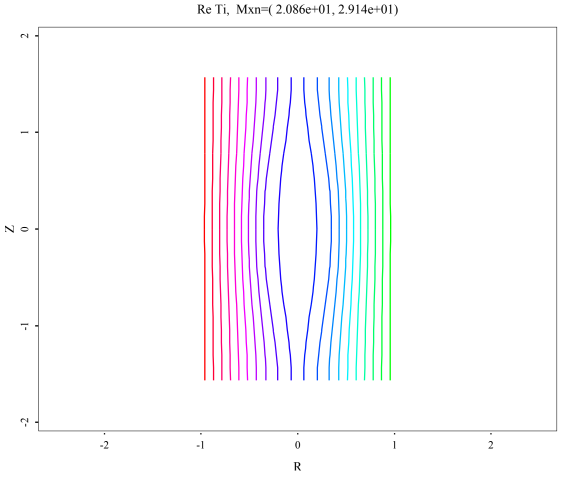
Anisotropic Heat Flow in Frozen Magnetic Island (fluid closures)

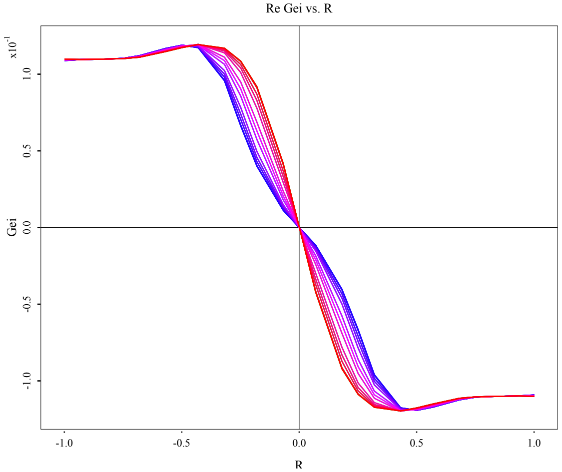


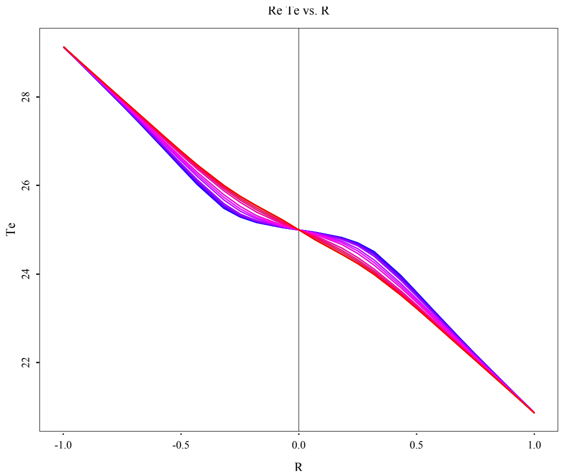
Anisotropic Heat Flow with i-e Energy Exchange in Frozen Magnetic Island (fluid closures)

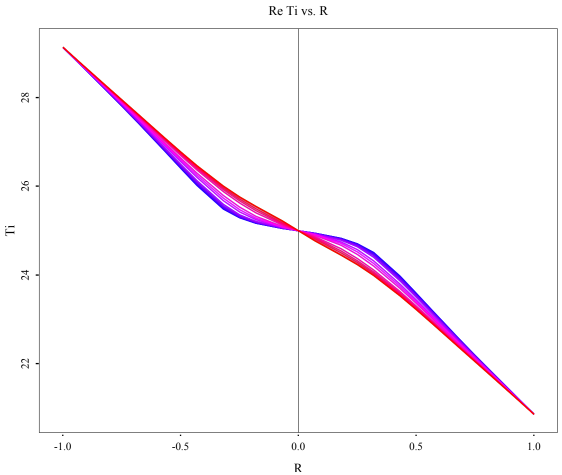










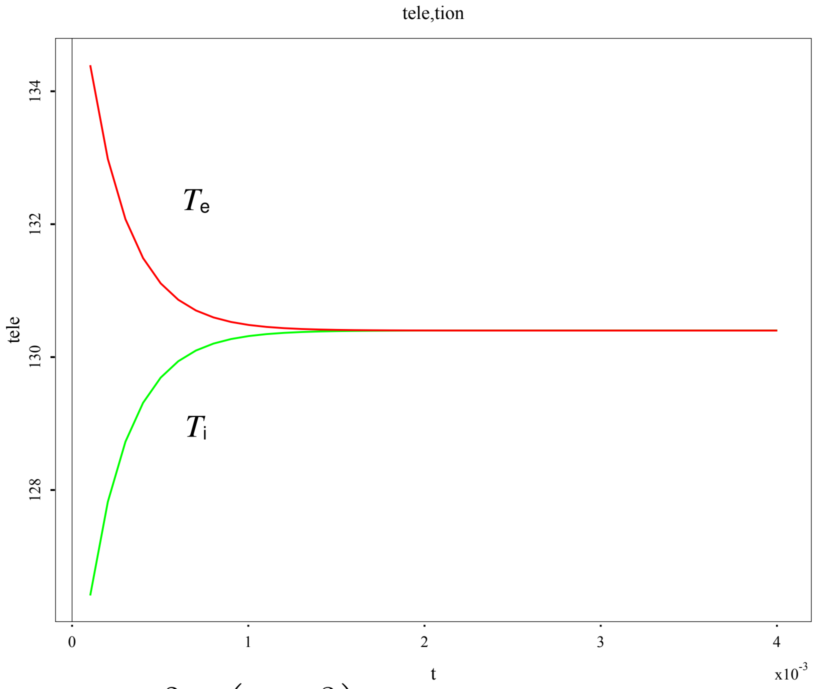


Thermal Equilibration with i-e Energy Exchange

$$\frac{\partial \mathbf{B}}{\partial t} = 0,\ \nabla \to 0,\ \mathbf{u} = \mathbf{J} = 0,\ T_{\mathsf{e}} > T_{\mathsf{i}}$$

Time-centering scheme for above model

$$[T_{\mathsf{e}}, T_{\mathsf{i}}, F_{\mathsf{e}}]\left(t^{k+\frac{1}{2}}\right) \longrightarrow [T_{\mathsf{e}}, T_{\mathsf{i}}, F_{\mathsf{e}}]\left(t^{k+\frac{3}{2}}\right)$$



$$\frac{3}{2} n \frac{\partial T_{\mathsf{e}}}{\partial t} = Q_{\mathsf{ei}} \qquad \frac{3}{2} n \frac{\partial T_{\mathsf{i}}}{\partial t} = -Q_{\mathsf{ei}}$$

$$\frac{\partial F_{\mathsf{e}}}{\partial t} - \frac{s}{2}\frac{\partial}{\partial t}\ln T_{\mathsf{e}} \frac{\partial F_{\mathsf{e}}}{\partial s} = C_{\mathsf{ee}}\left(f_{\mathsf{e}}^{\mathsf{M}}, F_{\mathsf{e}}\right) + C_{\mathsf{ee}}\left(F_{\mathsf{e}}, f_{\mathsf{e}}^{\mathsf{M}}\right) + C_{\mathsf{ei}}\left(f_{\mathsf{e}}^{\mathsf{M}}, f_{\mathsf{i}}\right) + C_{\mathsf{ei}}\left(F_{\mathsf{e}}, f_{\mathsf{i}}^{\mathsf{M}}\right) + \frac{2}{3nT_{\mathsf{e}}}\left(s^2 - \frac{3}{2}\right)\left(-Q_{\mathsf{ei}}\right) f_{\mathsf{e}}^{\mathsf{M}}$$

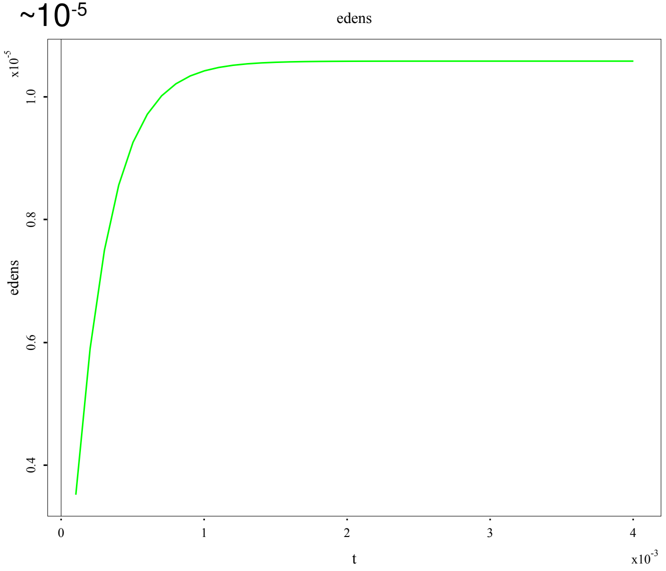
$$Q_{\mathsf{ei}} = \pi m_e v_{T\mathsf{e}}^5 \int_0^\infty ds \int_{-1}^1 d\xi s^4 \left[C_{\mathsf{ei}}\left(f_{\mathsf{e}}^{\mathsf{M}}, f_{\mathsf{i}}\right) + C_{\mathsf{ei}}\left(F_{\mathsf{e}}, f_{\mathsf{i}}^{\mathsf{M}}\right)\right]$$

Using reduced form of electron-ion collision operator and energy exchange from J. J. Ramos, *Phys. Plasmas* **17**, 082502 (2010).

Partition of Maxwellian and Non-Maxwellian Is Well Preserved Numerically

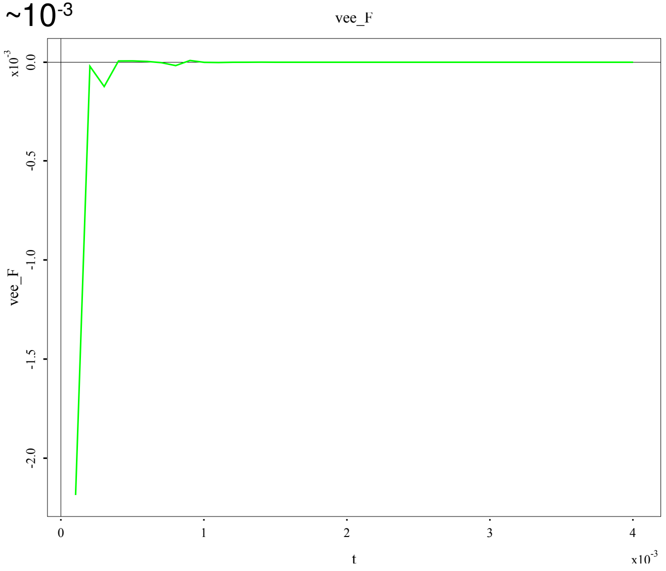
Maxwellian Moments of Non-Maxwellian Distribution Function

~10^{-5}



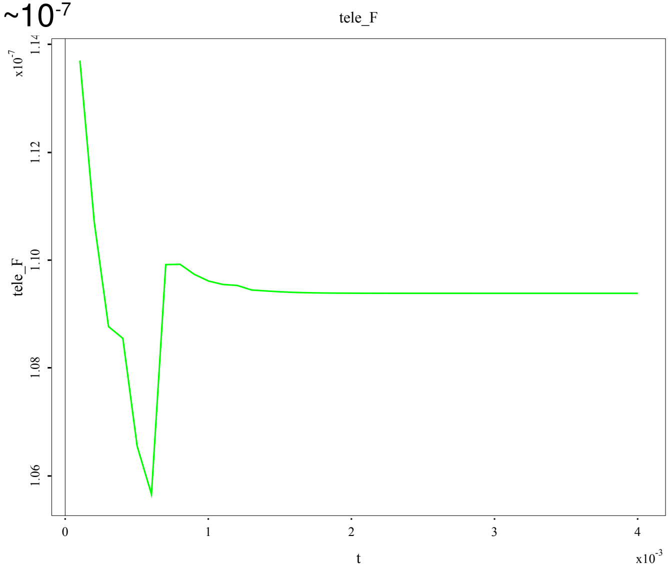
Error Density Moment

~10^{-3}



Error Flow Moment

~10^{-7}



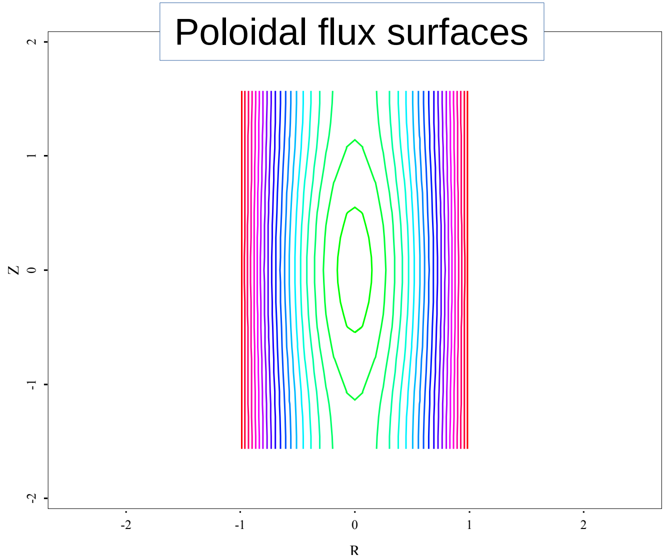
Error Temperature Moment

Implementing Kinetic Closures for Parallel Heat Flow and i-e Energy Exchange

$$\frac{\partial \mathbf{B}}{\partial t} = 0$$

Time-centering scheme for above model

$$[T_e, T_i, F_e]\left(t^{k+\frac{1}{2}}\right) \longrightarrow [T_e, T_i, F_e]\left(t^{k+\frac{3}{2}}\right)$$



$$\frac{3}{2} n \frac{\partial T_e}{\partial t} = \kappa_\perp \nabla \cdot [(\mathbf{I} - \mathbf{bb}) \cdot \nabla T_e] - \nabla \cdot \mathbf{q}_{e\|} + Q_{ei}$$

$$\frac{3}{2} n \frac{\partial T_i}{\partial t} = \kappa_\perp \nabla \cdot [(\mathbf{I} - \mathbf{bb}) \cdot \nabla T_i] - \nabla \cdot \mathbf{q}_{i\|} - Q_{ei}$$

$$\mathbf{q}_{i\|} = -\kappa_\| \left(\mathbf{b} \cdot \nabla T\right) \mathbf{b}$$

$$\mathbf{q}_{e\|} = \pi m_e v_{Te}^6 \int_0^\infty ds \int_{-1}^1 d\xi s^5 \xi F_e \mathbf{b} \qquad Q_{ei} = \pi m_e v_{Te}^5 \int_0^\infty ds \int_{-1}^1 d\xi s^4 \left[C_{ei}\left(f_e^M, f_i\right) + C_{ei}\left(F_e, f_i^M\right)\right]$$

$$\frac{\partial F_e}{\partial t} + v_{Te} s \xi \mathbf{b} \cdot \nabla F_e - \frac{1-\xi^2}{2\xi} v_{Te} s \xi \mathbf{b} \cdot \nabla \ln B \frac{\partial F_e}{\partial \xi} - \frac{s}{2}\left(v_{Te} s \xi \mathbf{b} \cdot \nabla + \frac{\partial}{\partial t}\right) \ln T_e \frac{\partial F_e}{\partial s} =$$

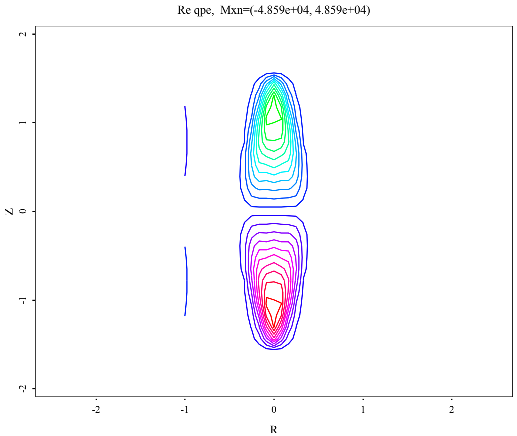
$$C_{ee}\left(f_e^M, F_e\right) + C_{ee}\left(F_e, f_e^M\right) + C_{ei}\left(f_e^M, f_i\right) + C_{ei}\left(F_e, f_i^M\right) + \left(\frac{3}{2} - s^2\right) v_{Te} s \xi \mathbf{b} \cdot \nabla \ln T_e f_e^M + \frac{2}{3nT_e}\left(s^2 - \frac{3}{2}\right)\left(\nabla \cdot \mathbf{q}_{e\|} - Q_{ei}\right) f_e^M$$

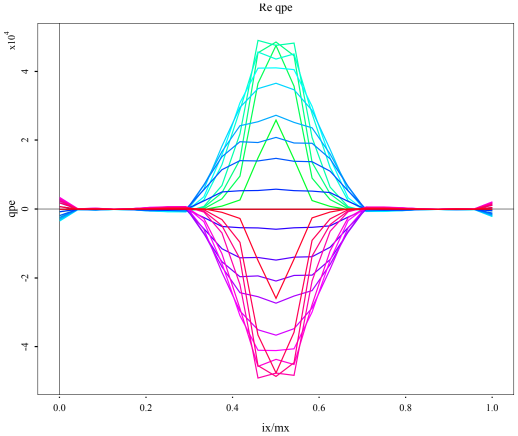
Using reduced form of electron-ion collision operator and energy exchange from J. J. Ramos, *Phys. Plasmas* **17**, 082502 (2010).

Kinetic heat flux and i-e Energy Exchange

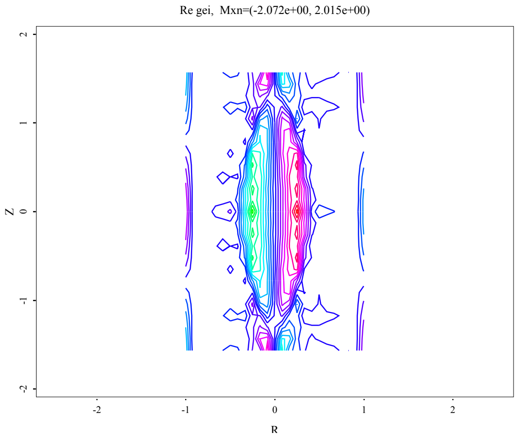
10^{-7} s later with kinetic closures

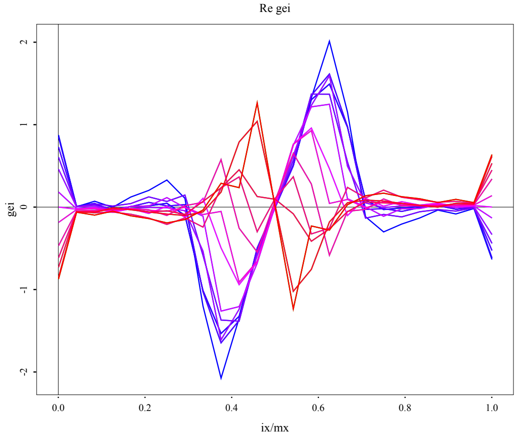
$q_{||e}$ (-4.859x10^4, 4.859x10^4)





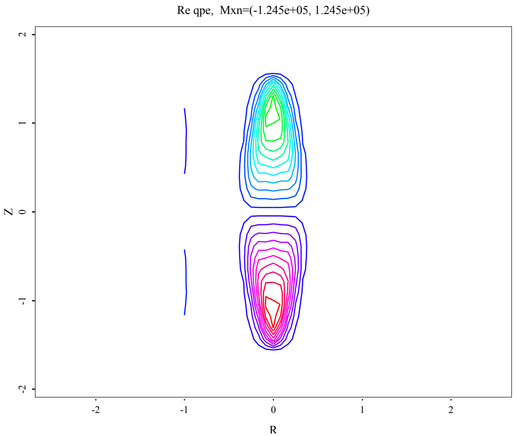
Q_{ei} (-2.072, 2.015)

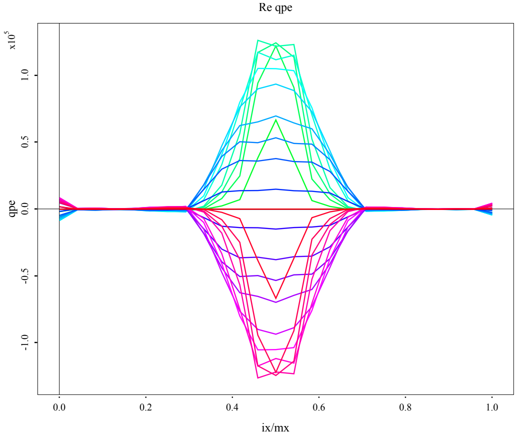




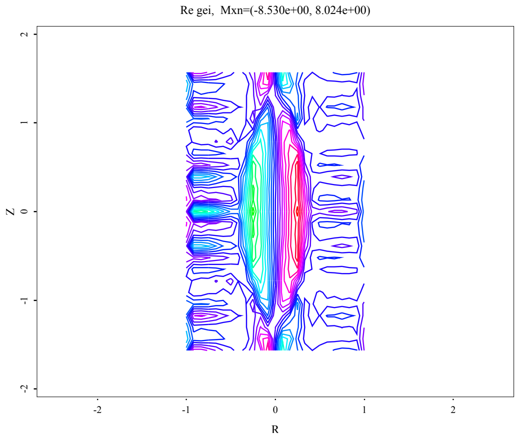
19 x 10^{-7} s later with kinetic closures

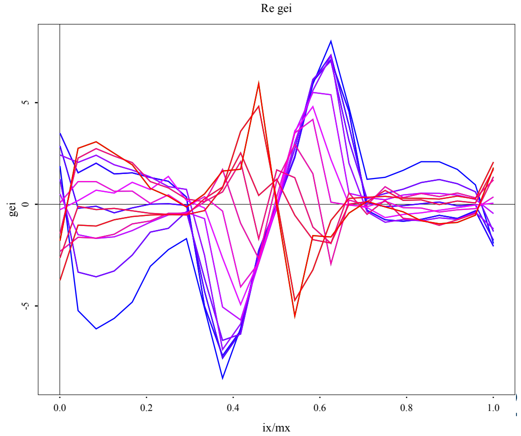
$q_{||e}$ (-1.245x10^5, 1.245x10^5)





Q_{ei} (-8.530, 8.024)





Summary and Future Work

- Thermal Equilibration
  - s-parallelism working
  - Single s-domain working
  - Two s-domains working
  - Convergence tests
  - Will compare with Picard iterations
- Anisotropic thermal diffusion
  - Preconditioning needs work
  - Debug boundary conditions or seaming issue
- Bring in B field
  - Picard iteration with B?
  - Fully implicit NK?
- Tokamak NTM (replace heuristic closures with kinetic closures in Eric Howell's simulations)