Time advance schemes for continuum drift kinetics and extended MHD*

J. Andrew Spencer, Eric D. Held, Jeong-Young Ji
Department of Physics
UtahStateUniversity

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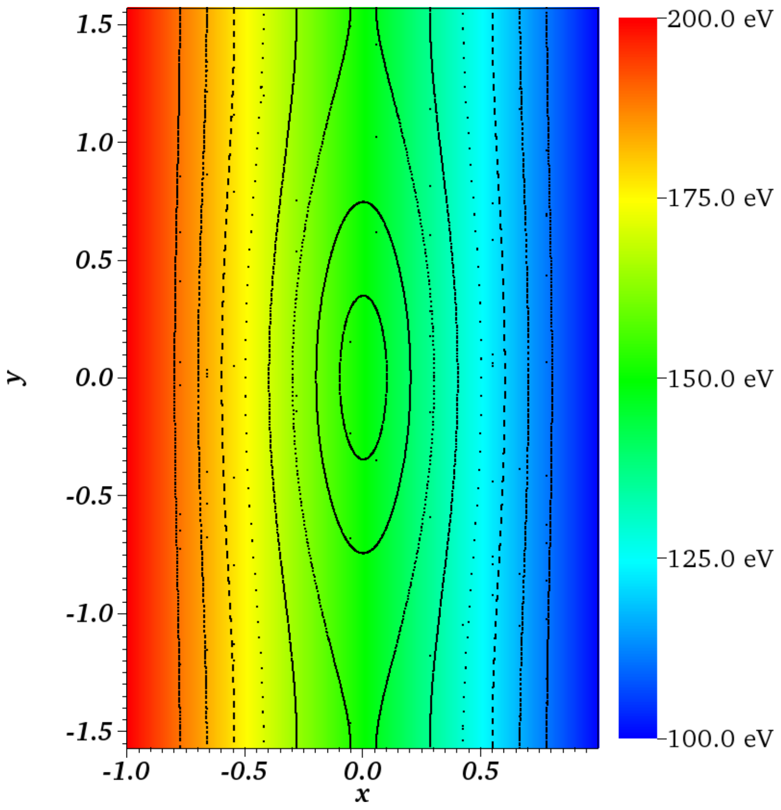
A simple model of a magnetic island

Research Objective: Understand challenges of solving the fluid + CEL drift kinetic system

- Strong nonlinear coupling between fluid quantities and kinetic distortion
- Scaling velocity by thermal speed
- Implicit advance for large stable time steps
- Introduce new fluid equations incrementally
- Start with a simplified coupling:
  - Thermal transport with kinetic parallel heat flux
  - Slab island geometry
  - Periodic in vertical direction

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



Initial linear T profile flattens across island as t evolves

CEL drift kinetic equation

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

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

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

where

$$\begin{aligned}
\mathbf{v}_{\mathrm{gc}} &= v_T s\xi\mathbf{b} + \frac{\mathbf{E}\times\mathbf{B}}{B^2} + \frac{Ts^2}{qB}\left(1+\xi^2\right)\mathbf{b}\times\nabla\ln B + \frac{2Ts^2}{qB^2}\left[\xi^2\left(\mathbf{I}-\mathbf{bb}\right) + \frac{1}{2}\left(1-\xi^2\right)\mathbf{bb}\right]\cdot\nabla\times\mathbf{B} + \frac{mv_T s\xi}{qB^2}\mathbf{b}\times\frac{\partial\mathbf{B}}{\partial t} \\
\dot{s} &= -\frac{s}{2}\frac{d\ln T}{dt} + \frac{s\left(1-\xi^2\right)}{2}\frac{\partial\ln B}{\partial t} + \frac{q\mathbf{v}_{\mathrm{gc}}\cdot\mathbf{E}}{2sT} \\
\dot{\xi} &= \frac{1-\xi^2}{2\xi}\left\{-\xi^2\frac{\partial\ln B}{\partial t} + \left(\mathbf{v}_{\parallel} + \mathbf{v}_{\mathrm{c}}^*\right)\cdot\left(\frac{q\mathbf{E}}{Ts^2} - \nabla\ln B\right) + \xi^2\frac{\mathbf{E}\times\mathbf{B}}{B^2}\cdot\nabla\ln B\right. \\
&\quad \left. -\frac{\xi^2}{B^2}\left[\mathbf{bb}\cdot(\nabla\times\mathbf{B})\right]\cdot\mathbf{E} - 2\frac{Ts^2\xi^2}{q}\mathbf{b}\cdot\nabla\left[\frac{\mathbf{b}\cdot(\nabla\times\mathbf{B})}{B^2}\right] + \frac{mv_T s\xi}{qB}\nabla\cdot\left(\mathbf{b}\times\frac{\partial\mathbf{b}}{\partial t}\right)\right\} \\
\mathbf{v}_c^* &= \frac{2Ts^2\xi^2}{qB^2}\left(\mathbf{I}-\mathbf{bb}\right)\cdot\nabla\times\mathbf{B} + \frac{mv_T s\xi}{qB^2}\mathbf{b}\times\frac{\partial\mathbf{B}}{\partial t}
\end{aligned}$$

*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).

Continuum kinetics in NIMROD used to study thermal transport

- Temperature equation $\frac{3}{2}n\frac{\partial T}{\partial t} = \kappa_{\perp}\nabla\cdot[(\mathbf{I}-\mathbf{bb})\cdot\nabla T] - \nabla\cdot\mathbf{q}_{\parallel}$

- Two options for closures (fluid or kinetic):
  1) Fourier conduction $\mathbf{q}_{\mathrm{i}\parallel} = -\kappa_{\parallel}(\mathbf{b}\cdot\nabla T)\,\mathbf{b}$
  2) Kinetic heat flux $\mathbf{q}_{\mathrm{e}\parallel} = \pi m_{\mathrm{e}} v_{T\mathrm{e}}^{6}\int_0^{\infty} ds\int_{-1}^{1} d\xi\, s^5\xi F_{\mathrm{e}}\mathbf{b}$

     Chapman-Enskog-Like (CEL) DKE

$$\frac{\partial F_{\mathrm{e}}}{\partial t} + \mathbf{v}_{\parallel}\cdot\nabla F_{\mathrm{e}} - \frac{1-\xi^2}{2\xi}\mathbf{v}_{\parallel}\cdot\nabla\ln B\frac{\partial F_{\mathrm{e}}}{\partial\xi} - \frac{s}{2}\left(\mathbf{v}_{\parallel}\cdot\nabla + \frac{\partial}{\partial t}\right)\ln T_{\mathrm{e}}\frac{\partial F_{\mathrm{e}}}{\partial s}$$
$$= C_{\mathrm{ee}}\left(f_{\mathrm{e}}^{\mathrm{M}}, F_{\mathrm{e}}\right) + C_{\mathrm{ee}}\left(F_{\mathrm{e}}, f_{\mathrm{e}}^{\mathrm{M}}\right) + \left(\frac{3}{2}-s^2\right)\mathbf{v}_{\parallel}\cdot\nabla\ln T_{\mathrm{e}} f_{\mathrm{e}}^{\mathrm{M}} + \frac{2}{3nT_{\mathrm{e}}}\left(s^2-\frac{3}{2}\right)\left(\nabla\cdot\mathbf{q}_{\mathrm{e}\parallel}\right)f_{\mathrm{e}}^{\mathrm{M}}$$

(red terms have electron temperature dependence)

Semi-implicit time advances

Problem: Tight nonlinear coupling of fluid and kinetic distortion

- Staggered advance

$$\begin{tikzcd} T_\mathrm{e}\left(t^k\right) \arrow[rr, bend left] & F_\mathrm{e}\left(t^{k+\frac{1}{2}}\right) \arrow[rr, bend right] & T_\mathrm{e}\left(t^{k+1}\right) & F_\mathrm{e}\left(t^{k+\frac{3}{2}}\right) \end{tikzcd}$$

- Simultaneous advance (***Picard iterations*** or ***Newton iterations***)

$$T_\mathrm{e}\left(t^k\right), F_\mathrm{e}\left(t^k\right) \longrightarrow T_\mathrm{e}\left(t^{k+1}\right), F_\mathrm{e}\left(t^{k+1}\right)$$

- NIMROD staggers flow and remaining quantities (How should F be centered in time?)

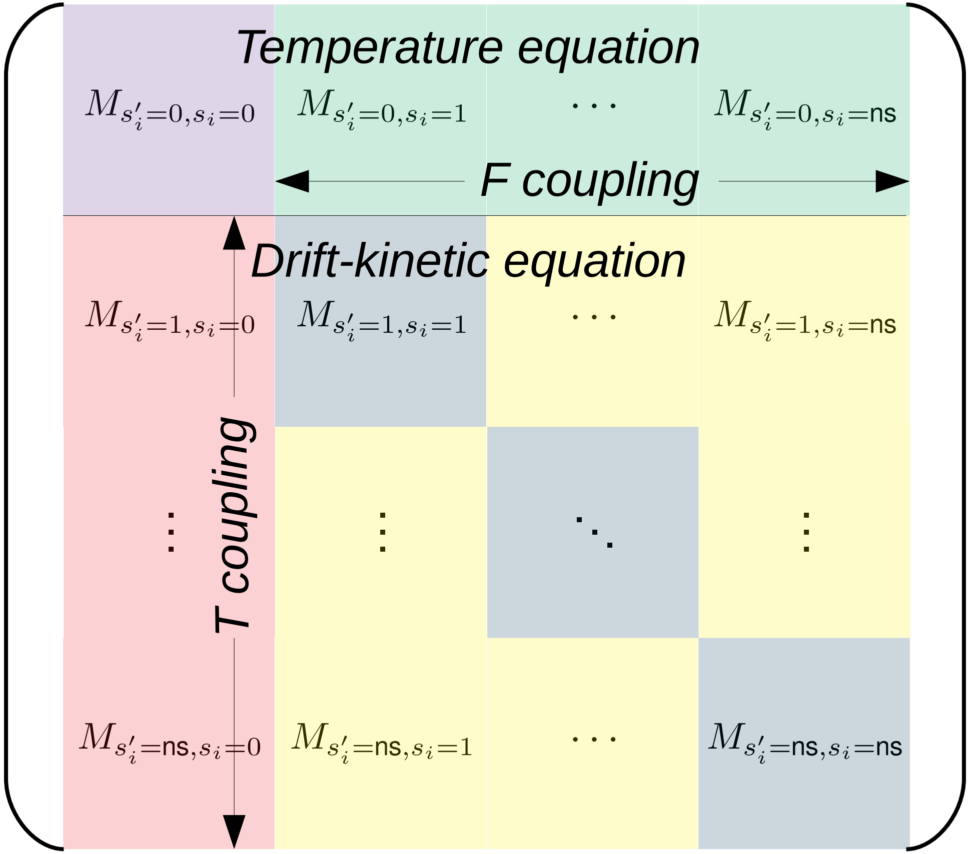
$$\begin{tikzcd} \left[\mathbf{u}, F_\mathrm{i}\right]\left(t^k\right) \arrow[rr, bend left] & \left[n_\mathrm{i}, \mathbf{B}, T_\mathrm{i}\right]\left(t^{k+\frac{1}{2}}\right) \arrow[rr, bend right] & \left[\mathbf{u}, F_\mathrm{i}\right]\left(t^{k+1}\right) & \left[n_\mathrm{i}, \mathbf{B}, T_\mathrm{i}\right]\left(t^{k+\frac{3}{2}}\right) \end{tikzcd}$$

J.R.Jepson, et al., *Phys. Plasmas* **28**, 082503 (2021)

$$\begin{tikzcd} \mathbf{u}\left(t^k\right) \arrow[rr, bend left] & \left[n, \mathbf{B}, T_\mathrm{e}, T_\mathrm{i}, F_\mathrm{e}\right]\left(t^{k+\frac{1}{2}}\right) \arrow[rr, bend right] & \mathbf{u}\left(t^{k+1}\right) & \left[n, \mathbf{B}, T_\mathrm{e}, T_\mathrm{i}, F_\mathrm{e}\right]\left(t^{k+\frac{3}{2}}\right) \end{tikzcd}$$

Centers F_e with Ohm's law

The linear operator's toroidal-blocks can be written in the following matrix form

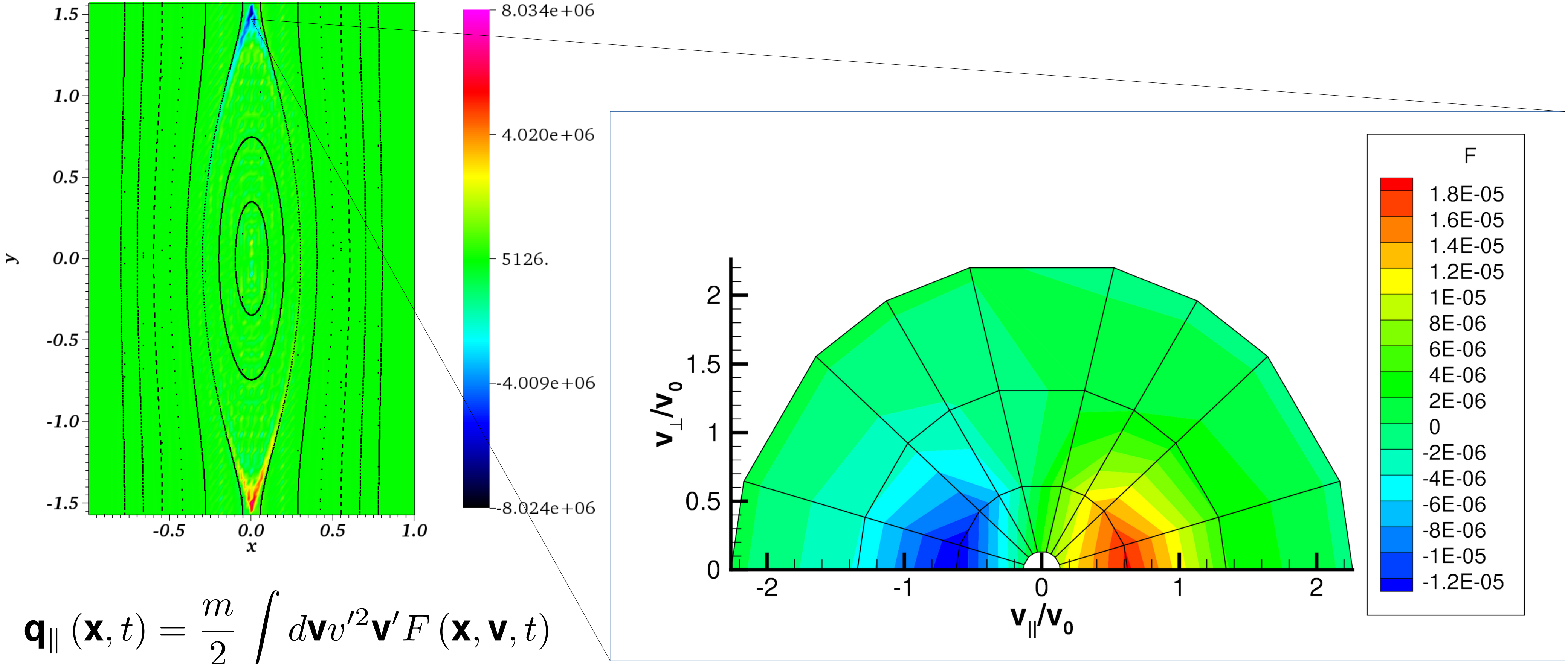


A few preconditioning strategies implemented:

1) Full preconditioner includes all terms
2) Block Jacobi inverts & s-blocks excluding:
   - ✗ off-diagonal collision operator terms
   - ✗ thermodynamic drives
   - ✗ s-derivative
   - ✗ heat-flux in temperature equation
3) New block preconditioner uses , & s-blocks is similar, but includes:
   - ✓ heat-flux in temperature equation

s-blocks are tailored to pitch-angle scattering operator and low-collisionality

Heat flux moment of distribution function



$$\mathbf{q}_{||}(\mathbf{x},t) = \frac{m}{2}\int d\mathbf{v} v'^2 \mathbf{v}' F(\mathbf{x},\mathbf{v},t)$$

Rosenbluth potentials coupling arrays

Normalize speed $s \equiv v/v_{\mathsf{T}a}$ and use collocation method

$$F_{a,l'}\left(v_{\mathsf{T}a}s\right) = \sum_{k=1}^{N_s} F_{a,l',k} L_k\left(s\right) \mathsf{e}^{-s^2}$$

$$\int_0^\infty ds L_j\left(s\right) L_k\left(s\right) \mathsf{e}^{-s^2} = \delta_{jk}$$

$$F_{a,l'}\left(v_{\mathsf{T}a}s\right) = \sum_{k=1}^{N_s} \sum_j w_j L_{k'}\left(s_j\right) F_{a,l'}\left(v_{\mathsf{T}a}s_j\right) L_k\left(s\right) \mathsf{e}^{-s^2}$$

$$\int_{-1}^{1} d\xi H_b\left(v_{\mathsf{T}a}s_i,\xi\right) Q_l\left(\xi\right) = v_{\mathsf{T}a}^2 s_i^2 \sum_{l'} \sum_j \mathsf{H}_{a,b,l,i,l',j} F_{b,l'}\left(v_{\mathsf{T}b}s_j\right)$$

$$\int_{-1}^{1} d\xi \frac{\partial H_b}{\partial v}\left(v_{\mathsf{T}a}s_i,\xi\right) Q_l\left(\xi\right) = v_{\mathsf{T}a} s_i \sum_{l'} \sum_j \mathsf{H}'_{a,b,l,i,l',j} F_{b,l'}\left(v_{\mathsf{T}b}s_j\right)$$

$$\int_{-1}^{1} d\xi \frac{\partial^2 G_b}{\partial v^2}\left(v_{\mathsf{T}a}s_i,\xi\right) Q_l\left(\xi\right) = v_{\mathsf{T}a}^2 s_i^2 \sum_{l'} \sum_j \mathsf{G}''_{a,b,l,i,l',j} F_{b,l'}\left(v_{\mathsf{T}b}s_j\right)$$

where

$$\mathsf{H}_{a,b,l,i,l',j} = \int_0^\infty d\bar{v} \sum_k w_j L_k\left(s_j\right) L_k\left(v_{Ta}s_i\bar{v}/v_{\mathsf{T}b}\right) \mathsf{e}^{-\left(v_{Ta}s_i\bar{v}\right)^2/v_{\mathsf{T}b}^2} \mathsf{K}_{ll'}\left(\bar{v}\right)$$

$$\mathsf{H}'_{a,b,l,i,l',j} = \int_0^\infty d\bar{v} \sum_k w_j L_k\left(s_j\right) L_k\left(v_{Ta}s_i\bar{v}/v_{\mathsf{T}b}\right) \mathsf{e}^{-\left(v_{Ta}s_i\bar{v}\right)^2/v_{\mathsf{T}b}^2} \left[\mathsf{Kp}_{ll'}\left(\bar{v}\right) - \frac{1}{2}\mathsf{K}_{ll'}\left(\bar{v}\right)\right]$$

$$\mathsf{G}''_{a,b,l,i,l',j} = \int_0^\infty d\bar{v} \sum_k w_j L_k\left(s_j\right) L_k\left(v_{Ta}s_i\bar{v}/v_{\mathsf{T}b}\right) \mathsf{e}^{-\left(v_{Ta}s_i\bar{v}\right)^2/v_{\mathsf{T}b}^2} \mathsf{Epp}_{ll'}\left(\bar{v}\right)$$

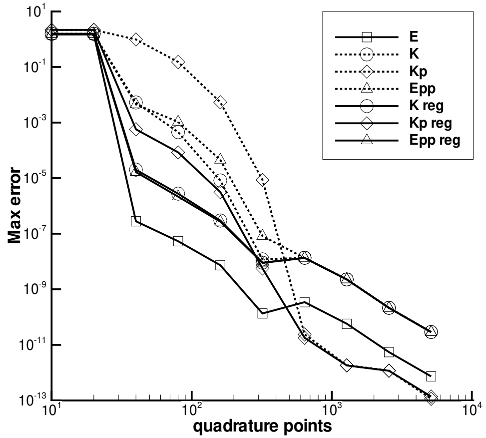
Several convergence tests of kernels and coupling arrays shown in
J.A.Spencer, et al., *J. Comput. Phys.*, **450** (2022) 110862

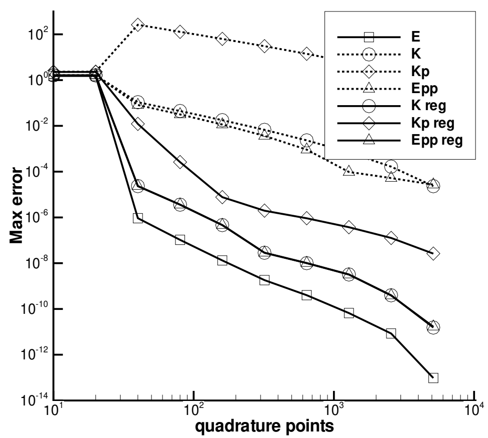
Convergence of kernels near singularity

GLL basis, $p_\xi = 3$, $\bar{v} = 0.99$ GLL basis, $p_\xi = 3$, $\bar{v} = 0.9999$

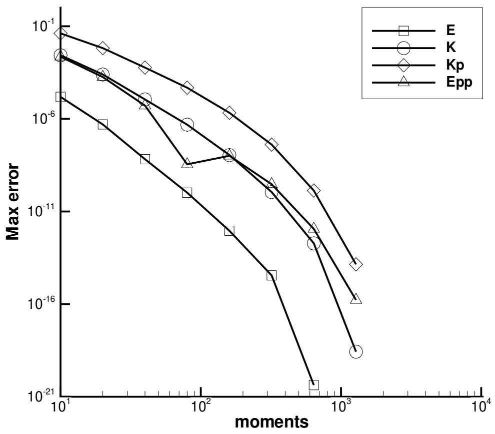
Max error = $\max_{l,l'} \left\{ \left| \mathsf{K}_{ll'}^{N_\xi}(\bar{v}) - \mathsf{K}_{ll'}^{10,240}(\bar{v}) \right| \right\}$

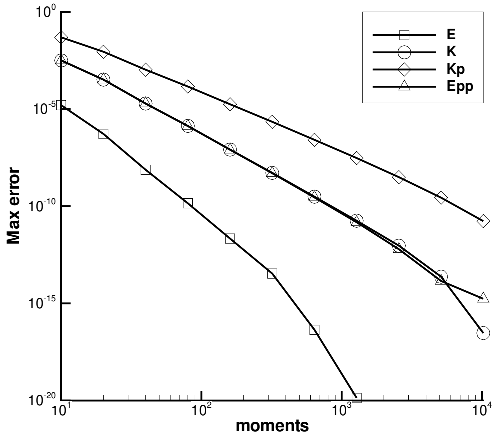
Regularization improves accuracy of closed form near singularity





Moment expansion performs better even near singularity





Collisional moments* test

$$B_{ab}^{lpk} = \frac{1}{\bar{\sigma}_l}\int d\boldsymbol{v} s_a^l P_a^l(\xi) L_p^{(l+1/2)}(s_a^2)\, C\left(f_a^M, s_b^l P_b^l(\xi) L_k^{(l+1/2)}(s_b^2) f_b^M\right)$$

$$\epsilon_{ab} \equiv \mathrm{max}_{l,p,k}\left|\mathrm{B}_{ab}^{lpk} - \mathrm{B}_{ab}^{*lpk}\right| \text{ for all } l,p,k \le 4$$

$$N_{\bar{v}1} = N_{\bar{v}2} = 256,\ N_{\bar{v}3} = 32,\ p_\xi = 10,\ N = 400$$

$N_s = 48$

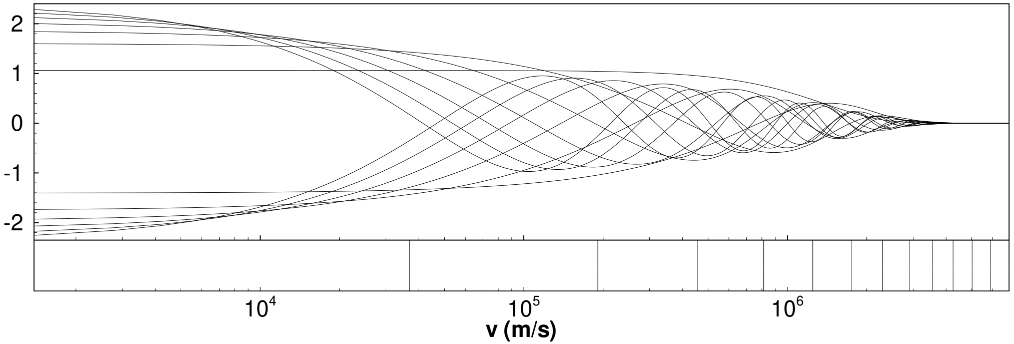
$\boxed{\epsilon_{\mathrm{ee}} = \epsilon_{\mathrm{ii}} \approx 4.8 \times 10^{-13}}$

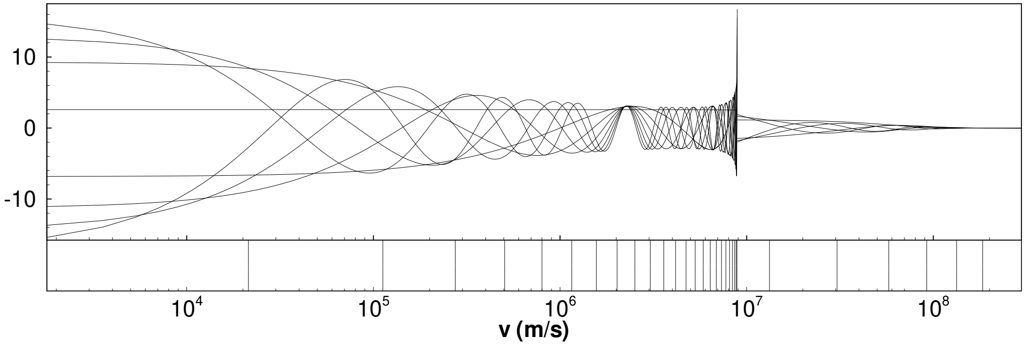
$N_s = 13$

$\boxed{\epsilon_{\mathrm{ie}} \approx 1.3 \times 10^{-14}}$

$N_{s1} = 24,\ N_{s2} = 6,\ s_{\mathrm{mid}} = 0.15$

$\boxed{\epsilon_{\mathrm{ei}} \approx 3.1 \times 10^{-15}}$



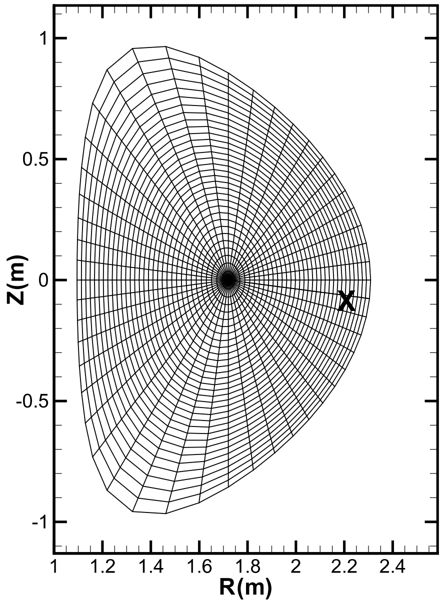


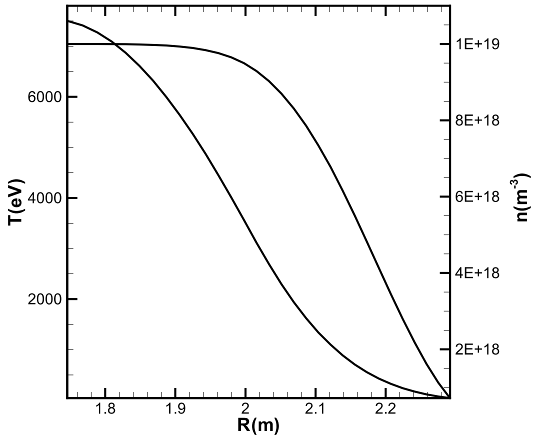
*Ji and Held, *Phys. Plasmas* **13**, 102103 (2006), J. Ji, et al, *Phys. Plasmas* **23**, 032124 (2016).

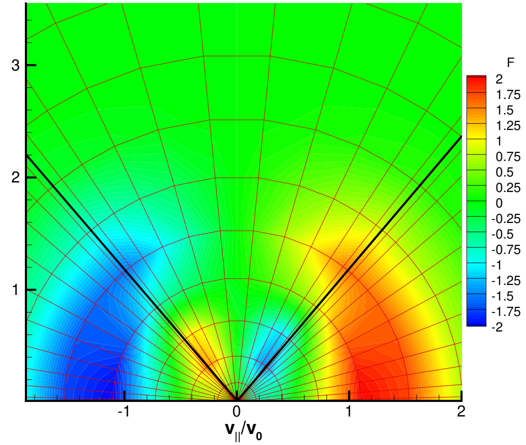
FE pitch-angle basis improves bootstrap current

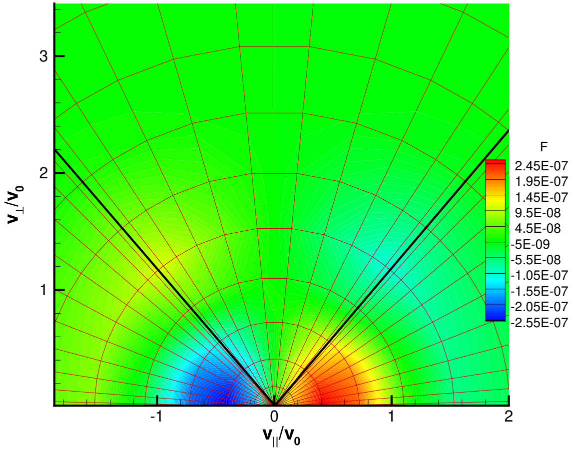
$$\mathbf{v}_{\|}\cdot\left[\nabla F-\frac{1-\xi^2}{2\xi}\nabla\ln B\frac{\partial F}{\partial\xi}\right]-C\left(F\right)=-\mathbf{v}_D\cdot\left(\nabla\ln n_0-\left(\frac{3}{2}-s^2\right)\nabla\ln T_0\right)f_0$$

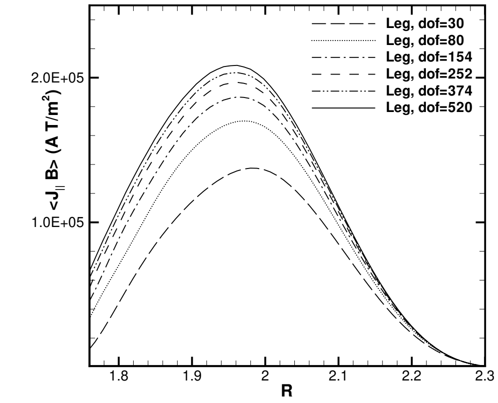
$$\langle J_{\|}B\rangle=\sum_b q_b\left\langle B\int d\mathbf{v}v_{\|}F_b\right\rangle$$

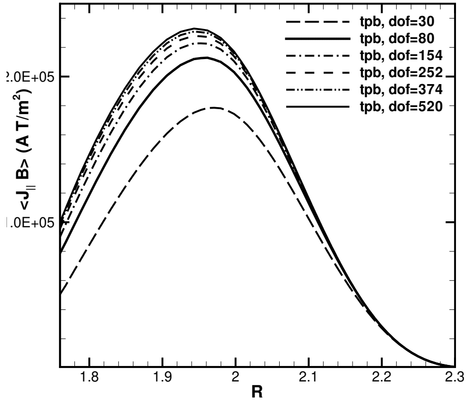


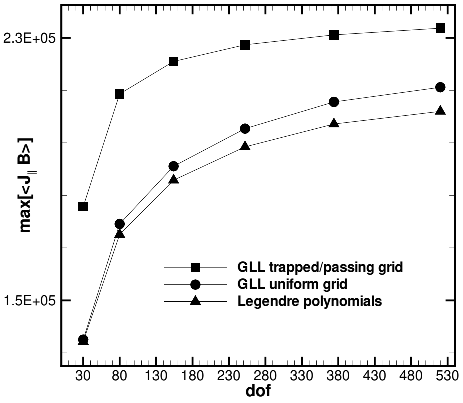


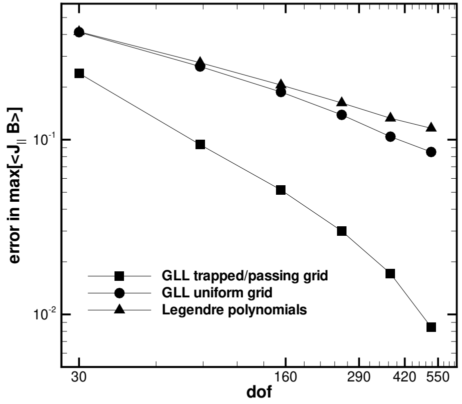












Working to implement thermal transport problem in NIMROD with i-e energy exchange

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

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

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

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

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

$$\frac{\partial F_{\mathrm{e}}}{\partial t} + \mathbf{v}_{\|}\cdot\nabla F_{\mathrm{e}} - \frac{1-\xi^2}{2\xi}\mathbf{v}_{\|}\cdot\nabla\ln B\frac{\partial F_{\mathrm{e}}}{\partial\xi} - \frac{s}{2}\left(\mathbf{v}_{\|}\cdot\nabla + \frac{\partial}{\partial t}\right)\ln T_{\mathrm{e}}\frac{\partial F_{\mathrm{e}}}{\partial s} =$$

$$C_{\mathrm{ee}}\left(f_{\mathrm{e}}^{\mathrm{M}}, F_{\mathrm{e}}\right) + C_{\mathrm{ee}}\left(F_{\mathrm{e}}, f_{\mathrm{e}}^{\mathrm{M}}\right) + C_{\mathrm{ei}}\left(f_{\mathrm{e}}^{\mathrm{M}}, f_{\mathrm{i}}\right) + C_{\mathrm{ei}}\left(F_{\mathrm{e}}, f_{\mathrm{i}}^{\mathrm{M}}\right) + \left(\frac{3}{2} - s^2\right)\mathbf{v}_{\|}\cdot\nabla\ln T_{\mathrm{e}} f_{\mathrm{e}}^{\mathrm{M}} + \frac{2}{3nT_{\mathrm{e}}}\left(s^2 - \frac{3}{2}\right)\left(\nabla\cdot\mathbf{q}_{\mathrm{e}\|} - Q_{\mathrm{ei}}\right) f_{\mathrm{e}}^{\mathrm{M}}$$

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

Time-centering scheme for above model

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

Goal for future time-centering scheme

$$\begin{tikzcd}
\mathbf{u}(t^k) \arrow[rr, bend left] & {[n, \mathbf{B}, T_{\mathrm{e}}, T_{\mathrm{i}}, F_{\mathrm{e}}]\left(t^{k+\frac{1}{2}}\right)} \arrow[rr, bend right] & \mathbf{u}(t^{k+1}) & {[n, \mathbf{B}, T_{\mathrm{e}}, T_{\mathrm{i}}, F_{\mathrm{e}}]\left(t^{k+\frac{3}{2}}\right)}
\end{tikzcd}$$

Summary

Improved NIMROD's axisymmetric Coulomb collision field operator

Parallelism over speed collocation points improves memory usage

Tests in 2022 JCP paper:

- "Poison solve", H, tested with method of manufactured solutions
- Low order collisional moments
- L_{32} Sauter coefficient calculation
- Bootstrap current using different pitch-angle bases adds to the story in 2015 PoP paper*

Implementation of kinetic closures with nonlinear implicit simultaneous advance of ion and electron temperatures and electron distribution function with more fluid quantities on the way

*E. D. Held, S. E. Kruger, J.-Y. Ji, E. A. Belli, and B. C. Lyons, Physics of Plasmas, 22, 032511 (2015).