Continuum closure plans and efforts*

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CTTS work at USU

Continuum energetic particle physics implemented using δf drift kinetic equation (DKE) with stress tensor coupling in NIMROD's flow evolution equation.

- Resistive Wall Modes
  - Piggyback on Tech-X resistive wall development in NIMROD.
  - Yr 4 Explore kinetic effects on stability with NIMROD, M3D-C1/DK4D: Compare with MARS-K
  - Yr 5 Explore disruptions caused by energetic particles (fishbone modes) interacting with RWMs.

Continuum Chapman-Enskog-like (CEL)-DKEs implemented with tight coupling of collisional friction, anisotropic stress, conductive heat flow and collisional energy exchange closures in NIMROD's fluid model.

- Neoclassical Tearing Modes
  - Ys 1-2 Identify suitable equilibria for NTM/locked mode disruptions on DIII-D for modeling (Tech-X).
  - Yr -1 Implement Ramos-form of CEL-DKE closures in NIMROD (USU).
  - Yr 1 NIMROD DKE closures in fixed magnetic island geometry (USU) by testing anisotropic thermal transport with tight CEL-DKE/temperature coupling.

Various forms for the δf DKE

The drift-kinetic equation may be written using several sets of variables:

1. Hazeltine*

$$\bar{f}\left(U,\mu,\mathbf{x},t\right) \rightarrow \frac{\partial \bar{f}}{\partial t} + \mathbf{v}_{\mathrm{gc}} \cdot \nabla \bar{f} + \frac{dU}{dt}\frac{\partial \bar{f}}{\partial U} + \frac{d\mu}{dt}\frac{\partial \bar{f}}{\partial \mu} = C$$

2. Ramos†

$$\bar{f}\left(v_{\parallel},v_{\perp},\mathbf{x},t\right) \rightarrow \frac{\partial \bar{f}}{\partial t} + \mathbf{v}_{\mathrm{gc}} \cdot \nabla \bar{f} + \frac{dv_{\parallel}}{dt}\frac{\partial \bar{f}}{\partial v_{\parallel}} + \frac{dv_{\perp}}{dt}\frac{\partial \bar{f}}{\partial v_{\perp}} = C$$

3. NIMROD‡

$$\bar{f}\left(s,\xi,\mathbf{x},t\right) \rightarrow \frac{\partial \bar{f}}{\partial t} + \mathbf{v}_{\mathrm{gc}} \cdot \nabla \bar{f} + \frac{ds}{dt}\frac{\partial \bar{f}}{\partial s} + \frac{d\xi}{dt}\frac{\partial \bar{f}}{\partial \xi} = C$$

*Hazeltine and Meiss, Plasma Confinement (Adisson-Wesley, RedwoodCity, 1992)
†Ramos, Phys Plasmas 15, 082106 (2008)
‡Held,*et al*, Phys Plasmas 22, 032511 (2015)

δf DKE in NIMROD for studies of energetic particle effects

The δf DKE implemented in NIMROD uses the coordinates $(\mathbf{x}, t, s, \xi)$, where $s = v/v_0$ and $\xi = v_\parallel / v$

$$
\begin{aligned}
\mathbf{v}_{\rm gc} &= v_0 s\xi\mathbf{b} + \frac{\mathbf{E}\times\mathbf{B}}{B^2} + \frac{T_0 s^2}{qB}\left(1+\xi^2\right)\mathbf{b}\times\nabla\ln B \\
&+ \frac{2T_0 s^2}{qB^2}\left[\xi^2\left(\mathbf{I}-\mathbf{bb}\right) + \frac{1}{2}\left(1-\xi^2\right)\mathbf{bb}\right]\cdot\nabla\times\mathbf{B} + \frac{m v_0 s\xi}{qB^2}\mathbf{b}\times\frac{\partial\mathbf{B}}{\partial t} \\
\dot{s} &= -s\frac{d\ln v_0}{dt} + \frac{s\left(1-\xi^2\right)}{2}\frac{\partial\ln B}{\partial t} + \frac{q}{2T_0 s}\left(\mathbf{v}_\parallel + \mathbf{v}_{\rm c}\right)\cdot\mathbf{E} + \frac{s}{2}\left(1+\xi^2\right)\frac{\mathbf{E}\times\mathbf{B}}{B^2}\cdot\nabla\ln B \\
\dot{\xi} &= \frac{1-\xi^2}{2\xi}\left\{-\xi^2\frac{\partial\ln B}{\partial t} + \left(\mathbf{v}_\parallel + \mathbf{v}_{\rm c}^*\right)\cdot\left(\frac{q\mathbf{E}}{T_0 s^2} - \nabla\ln B\right) + \xi^2\frac{\mathbf{E}\times\mathbf{B}}{B^2}\cdot\nabla\ln B\right\} \\
&- \xi(1-\xi^2)\left\{\frac{\mu_0}{2B^2}\mathbf{J}_\parallel\cdot\mathbf{E} + \frac{T_0 s^2}{q}\mathbf{b}\cdot\nabla\left(\frac{\mu_0 J_\parallel}{B^2}\right)\right\} + (1-\xi^2)\frac{T_0 s}{v_0 qB}\nabla\cdot\left(\mathbf{b}\times\frac{\partial\mathbf{b}}{\partial t}\right)
\end{aligned}
$$

This agrees exactly with Hazeltine's DKE, and includes additional terms in red.
Green term enters from $\dot{\mu}$ and is called the "twist" term by Ramos.

Linearization of δf DKE

Assuming $\mathbf{E}_0 = 0$ and using a speed norm v_0 that is constant in time yields

$$
\begin{aligned}
\delta \mathbf{v}_{gc} =& v_0 s\xi \mathbf{b}_1 + \frac{\mathbf{E}_1 \times \mathbf{B}_0}{B_0^2} + \frac{T_0 s^2}{qB_0^3}(1+\xi^2)\left[(\mathbf{I} - 4\mathbf{b}_0\mathbf{b}_0)\cdot \mathbf{B}_1 \times \nabla B_0 + \mathbf{b}_0 \times \nabla(\mathbf{B}_0 \cdot \mathbf{B}_1)\right] \\
&+ \frac{T_0 s^2}{qB_0^2}\left\{(1-3\xi^2)\delta\left(\mathbf{bb}\right)\cdot \nabla \times \mathbf{B}_0 + \left[2\xi^2(\mathbf{I}-\mathbf{b}_0\mathbf{b}_0) + (1-\xi^2)\mathbf{b}_0\mathbf{b}_0\right]\cdot \nabla \times \mathbf{B}_1\right\} \\
&- \frac{2T_0 s^2}{q}\frac{\mathbf{b}_0 \cdot \mathbf{B}_1}{B_0^3}\left[2\xi^2(\mathbf{I}-\mathbf{b}_0\mathbf{b}_0) + \left(1-\xi^2\right)\mathbf{b}_0\mathbf{b}_0\right]\cdot \nabla \times \mathbf{B}_0 + \frac{m v_0 s\xi}{qB_0^2}\mathbf{b}_0 \times \frac{\partial \mathbf{B}_1}{\partial t} \\
=& v_0 s\xi \mathbf{b}_1 + \frac{\mathbf{E}_1 \times \mathbf{B}_0}{B_0^2} + \frac{T_0 s^2}{qB_0^3}(1+\xi^2)\left[(\mathbf{I} - 4\mathbf{b}_0\mathbf{b}_0)\cdot \mathbf{B}_1 \times \nabla B_0 + \mathbf{b}_0 \times \nabla(\mathbf{B}_0 \cdot \mathbf{B}_1)\right] \\
&+ \frac{2T_0 s^2}{qB_0^2}\left\{\xi^2\left(\mathbf{J}_{\perp 1} - \delta(\mathbf{bb})\cdot \mathbf{J}_0 - \frac{2\mathbf{B}_0\cdot\mathbf{B}_1}{\mathbf{B}_0^2}\mathbf{J}_{\perp 0}\right) + \frac{1-\xi^2}{2}\left(\mathbf{J}_{||1} + \delta(\mathbf{bb})\cdot \mathbf{J}_0 - \frac{2\mathbf{B}_0\cdot\mathbf{B}_1}{\mathbf{B}_0^2}\mathbf{J}_{||0}\right.\right. \\
&+ \frac{m v_0 s\xi}{qB_0^2}\mathbf{b}_0 \times \frac{\partial \mathbf{B}_1}{\partial t}
\end{aligned}
$$

where $\mathbf{b}_1 = (\mathbf{I} - \mathbf{b}_0\mathbf{b}_0)\cdot \mathbf{B}_1/B_0$ and $\delta(\mathbf{bb}) = \mathbf{b}_1\mathbf{b}_0 + \mathbf{b}_0\mathbf{b}_1$.

Linearization of δf DKE (cont.)

Linearizing the acceleration terms yields

$$\delta\dot{s} = -\frac{s\left(1-\xi^2\right)}{2B_0^2}\mathbf{B}_0\cdot\nabla\times\mathbf{E}_1 + \frac{q}{2sT_0}\mathbf{v}_{gc}\cdot\mathbf{E}_1 - s\delta\mathbf{v}_{gc}\cdot\nabla\ln v_0$$

$$= -\frac{s\left(1-\xi^2\right)}{2B_0^2}\mathbf{B}_0\cdot\nabla\times\mathbf{E}_1 + \frac{q}{2T_0 s}\left(\mathbf{v}_\parallel + \mathbf{v}_c\right)_0\cdot\mathbf{E}_1 + \frac{s}{2}\left(1+\xi^2\right)\frac{\mathbf{E}_1\times\mathbf{B}_0}{B_0^2}\cdot\nabla\ln B_0$$

$$-s\delta\mathbf{v}_{gc}\cdot\nabla\ln v_0$$

$$\delta\dot{\xi} = \frac{1-\xi^2}{2\xi}\left\{\frac{\xi^2\mathbf{B}_0}{B_0^2}\cdot\nabla\times\mathbf{E}_1 + \left(\mathbf{v}_\parallel + \mathbf{v}_c^*\right)\cdot\left(\frac{q\mathbf{E}_1}{T_0 s^2} - \nabla\ln B_1\right) - \delta\left(\mathbf{v}_\parallel + \mathbf{v}_c^*\right)\cdot\nabla\ln B_0\right.$$

$$+\xi^2\frac{\mathbf{E}_1\times\mathbf{B}_0}{B_0^2}\cdot\nabla\ln B_0 - \frac{\xi^2\mu_0}{B_0^2}\mathbf{J}_{\parallel 0}\cdot\mathbf{E}_1 - 2\frac{T_0 s^2\xi^2}{q}\left(\mathbf{b}_0\cdot\nabla\delta\left(\frac{\mu_0 J_\parallel}{B^2}\right) + \mathbf{b}_1\cdot\nabla\left(\frac{\mu_0 J_{\parallel 0}}{B_0^2}\right)\right)$$

$$\left.+\frac{2T_0\xi s}{v_0 q B_0}\nabla\cdot\left(\mathbf{b}_0\times\frac{\partial\mathbf{b}_1}{\partial t}\right)\right\}$$

Continuum CEL-DKEs implemented in NIMROD for NTM studies

Qualities of Chapman-Enskog like (CEL) method*:

- Separates fluid and kinetic parts of distribution function
- Fluid equations govern lowest order fluid quantities, n_a, $\mathbf{V}_a$, and T_a
- Kinetic equation governs kinetic distortion, F_a
- n_a, $\mathbf{V}_a$, and T_a provide thermodynamic drives for F_a
- Moments of F_a close fluid equations

Research Objective: Understand challenges

- Strong nonlinear coupling between fluid and F_a
- Scaling velocity by thermal speed
- Implicit advance for large time steps

*S. Chapman and T.G. Cowling, The Mathematical Theory of Non-Uniform Gases (Cambridge University Press, Cambridge, 1939); Z. Chang and J.D. Callen, Phys. Fluids 4, 1167 (1992).

CEL method separates fluid and kinetic physics

Starting from the DKE* project out Maxwellian part, $f = f^{\mathrm{M}} + F$,
and transform to coordinates, $(s, \xi) \equiv (|\mathbf{v} - \mathbf{V}| / v_T, \mathbf{v} \cdot \mathbf{B} / |\mathbf{v}| |\mathbf{B}|)$:

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

where

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

*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).

Challenges highlighted in kinetic thermal transport case studies

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

Calculate parallel heat flux as moment of kinetic distortion

$$\mathbf{q}_\parallel = \frac{m}{2}\int d\mathbf{v} v^2 v_\parallel F = \pi m v_T^6 \int_{-1}^{1} d\xi \int_0^\infty ds \left(s^5 \xi F\right)$$

$$\frac{\partial F}{\partial t} + \mathbf{v}_\parallel \cdot \nabla F - \frac{1-\xi^2}{2\xi}\mathbf{v}_\parallel \cdot \nabla \ln B \frac{\partial F}{\partial \xi} - \frac{s}{2}\left(\mathbf{v}_\parallel \cdot \nabla + \frac{\partial}{\partial t}\right)\ln T \frac{\partial F}{\partial s}$$
$$= C + \left(\frac{5}{2} - s^2\right)\mathbf{v}_\parallel \cdot \nabla \ln T f^{\mathrm{M}} + \frac{2}{3nT}\left(s^2 - \frac{3}{2}\right)\left(\nabla \cdot \mathbf{q}_\parallel - Q\right) f^{\mathrm{M}}$$

(red terms have temperature dependence.)

Possible θ-centered semi-implicit time advances

Problem: tight nonlinear coupling of fluid and kinetic distortion

$$\frac{\partial T}{\partial t} = G(T, F)$$
$$\frac{\partial F}{\partial t} = H(T, F)$$

complex nonlinear combinations of T and F

- Staggered advance

$$T\left(t^k\right) \longrightarrow F\left(t^{k+\frac{1}{2}}\right) \longrightarrow T\left(t^{k+1}\right) \longrightarrow F\left(t^{k+\frac{3}{2}}\right)$$

$$\Delta T - \theta \Delta t G_{\text{lin}}\left(\Delta T, F^{k+\frac{1}{2}}\right) = \Delta t G\left(T^k, F^{k+\frac{1}{2}}\right)$$
$$\Delta F - \theta \Delta t H_{\text{lin}}\left(T^{k+1}, \Delta F\right) = \Delta t H\left(T^{k+1}, F^{k+\frac{1}{2}}\right)$$

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

$$T\left(t^k\right), F\left(t^k\right) \longrightarrow T\left(t^{k+1}\right), F\left(t^{k+1}\right)$$

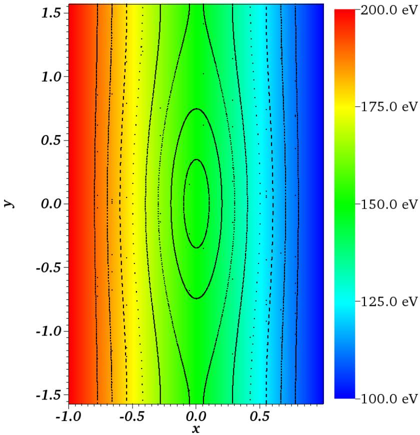
$$\Delta T - \theta \Delta t G\left(T^{k+1}, F^{k+1}\right) = (1-\theta)\, \Delta t G\left(T^k, F^k\right)$$
$$\Delta F - \theta \Delta t H\left(T^{k+1}, F^{k+1}\right) = (1-\theta)\, \Delta t H\left(T^k, F^k\right)$$

GMRES fails to solve

Test case: thermal transport in magnetic island

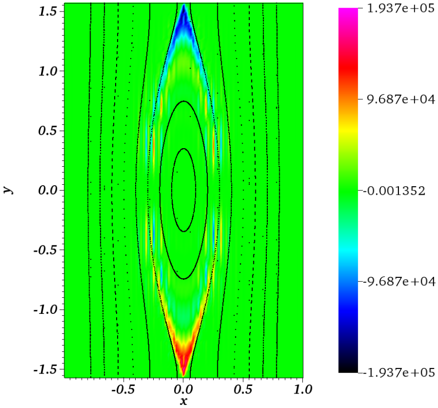
Kinetic parallel thermal transport across magnetic island in slab geometry

- $n = 9.5175 \times 10^{18}\,\mathrm{m}^{-3}$, $\mathbf{V} = 0$
- Ignore electron-ion and ion-electron collisions
- Boundary condition: periodic in Z direction
- Objective: take as large time steps as possible to get to steady state with kinetic parallel heat flux
- 32x32 grid in xy-plane
- 3rd degree polynomials



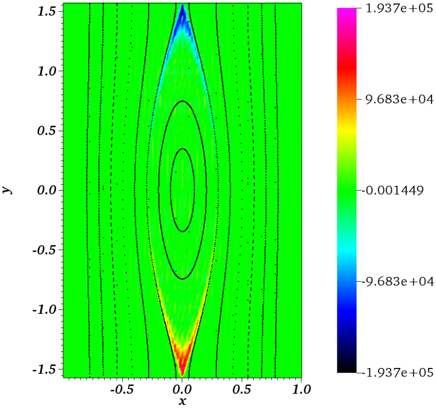
Initial temperature is a linear gradient that flattens across island as T evolves

Standard and mixed finite element steady state parallel heat flux with conductivity $\kappa_\parallel = 1.5 \times 10^7$



Standard fluid steady state

$q_\parallel \; [\mathrm{W/m^2}]$



Mixed finite element steady state

$q_\parallel \; [\mathrm{W/m^2}]$

Picard and Newton methods implemented for simultaneous T and F advance.

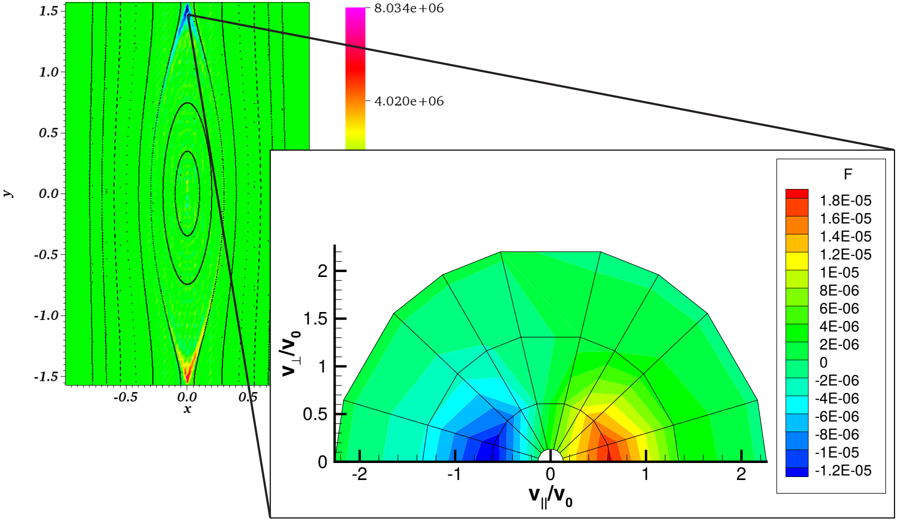
Implicit advance of F:

$$\frac{F^{k+1}-F^k}{\Delta t}+\sqrt{\frac{2T}{m}}s\xi\left(\nabla_\parallel F^{k+1}-\frac{1-\xi^2}{2\xi}\nabla_\parallel \ln B\frac{\partial F^{k+1}}{\partial \xi}\right)-\frac{s}{2T}\left(\sqrt{\frac{2T}{m}}s\xi\nabla_\parallel+\frac{\partial}{\partial t}\right)T\frac{\partial F^{k+1}}{\partial s}$$
$$=C\left(T,F^{k+1}\right)+\left[\left(\frac{5}{2}-s^2\right)\sqrt{\frac{2}{mT}}s\xi\nabla_\parallel T+\frac{2}{3nT}\left(s^2-\frac{3}{2}\right)\left(\nabla\cdot\mathbf{q}_\parallel\left(F^{k+1},T\right)-G\right)\right]f^{\mathrm{M}}\left(T\right)$$

Implicit advance of T:

$$\frac{3}{2}n\frac{T^{k+1}-T^k}{\Delta t}=\kappa_\perp\nabla\cdot\left[\left(\mathbf{I}-\mathbf{bb}\right)\cdot\nabla T^{k+1}\right]-\nabla\cdot\mathbf{q}_\parallel\left(T,F\right)+G\left(T,F\right)$$

Kinetic heat flux calculated as moment of distribution function



Newton more costly than Picard iterations but can take larger time step

- 256 processors, 32x32 grid, polynomial degree=3
- Starting from MFE steady state, run an additional $10^{-5}\,\mathrm{s}$

	Δt	wall clock time to $t = 10^{-5}\,\mathrm{s}$	average GMRES iterations per step	time per iteration
Picard	$10^{-8}\,\mathrm{s}$	$75\,\mathrm{mins}$	5	$0.9\,\mathrm{s}$
Newton	$10^{-8}\,\mathrm{s}$	$200\,\mathrm{mins}$	4	$3\,\mathrm{s}$
Newton	$10^{-7}\,\mathrm{s}$	$49\,\mathrm{mins}$	52	$0.57\,\mathrm{s}$
Newton	$10^{-6}\,\mathrm{s}$	$42\,\mathrm{mins}$	723	$0.35\,\mathrm{s}$

- Need to implement parallelism over speed grid points for efficiency improvement.

Upcoming work

- Implement s-parallelism for simultaneous advance of T and F.
- Possibly speed-up Newton iterations
  (reuse preconditioning matrix, improved check for convergence)
- Adaptive time step
- Examine needed velocity grid for electron-ion collisions
- Use developed code in a tearing mode simulation
  with evolving $\mathbf{B}$, n, $\mathbf{V}$.