Application of continuum drift kinetics to parallel heat transport*

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Continuum kinetic physics have been incorporated into NIMROD

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

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

*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).

Discretization based on NIMROD's spatial and novel velocity representation*

NIMROD's **spatial representation**:

$$F\left(R,Z,\phi,s,\xi,t\right)=\sum_{i}F_{i,n=0}\left(s,\xi,t\right)\alpha_{i,n=0}+2\Re e\left[\sum_{i,n>0}F_{i,n}\left(s,\xi,t\right)\alpha_{i,n}\right]$$

Pitch-angle discretization uses finite element method:

$$F_{i,n}\left(s,\xi,t\right)=\sum_{l}F_{i,n,l}\left(s,t\right)P_{l}\left(\xi\right)$$

Speed discretization uses collocation method with polynomial expansion:

$$F_{i,n,l}\left(s,t\right)\equiv\mathrm{e}^{-s^{2}}\sum_{k}F_{i,n,l,k}\left(t\right)L_{k}\left(s\right) \tag{1}$$

where collocation points and polynomials, $L_{k}\left(s\right)$, are abscissa and polynomials of non-standard quadrature scheme with weight function $\mathrm{e}^{-s^{2}}$ and orthogonality :

$$\int_{0}^{\infty}dsL_{k}\left(s\right)L_{k'}\left(s\right)\mathrm{e}^{-s^{2}}=\delta_{kk'}$$

*E. D. Held, *et al*, Phys Plasmas **22**, 032511 (2015).

Challenges highlighted in kinetic thermal transport case studies

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

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

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

complex nonlinear combinations of T and F

- Staggered advance

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

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

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

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

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

GMRES fails to solve

Test case 1: Anisotropic thermal conduction*

Step 1. Impose $\mathbf{E} = E_0 \cos(\pi x) \cos(\pi y)\, \hat{\mathbf{z}}$ on high density plasma resulting in low flow and $\mathbf{B}$ field with field lines along contours of $|\mathbf{E}|$.
Step 2. Rescale n, fix $\mathbf{B}$ and evolve T:

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

where Q_{ext} has same spatial dependence as $|\mathbf{E}|$.
The resulting steady state has

$$\mathbf{B} \cdot \nabla T = 0$$

- Standard Fourier conduction: $\mathbf{q}_\parallel = -\kappa_\parallel (\mathbf{b} \cdot \nabla T)\, \mathbf{b}$
- Mixed finite element: $\theta \Delta \mathbf{q}_\parallel \to \bar{q}_\parallel \mathbf{b}$ where

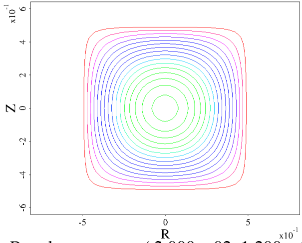
$$\bar{q}_\parallel + \theta \kappa_\parallel \mathbf{b} \cdot \nabla \Delta T = -\kappa_\parallel \mathbf{b} \cdot \nabla T^n$$

- Kinetic heat flux: $\mathbf{q}_\parallel = \frac{m}{2} \int d\mathbf{v} v^2 v_\parallel F$

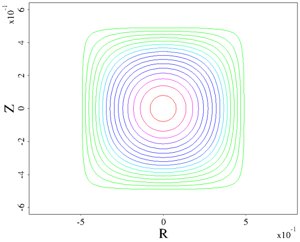
*C.R. Sovinec, *et al,* J. Comput. Phys. **195** (2004) 355–386

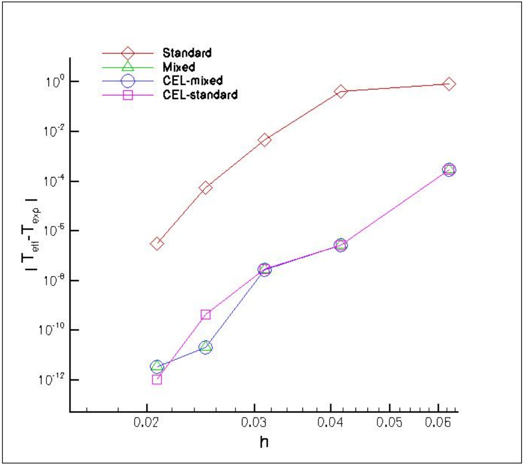
Staggered advance to steady state illustrates kinetic closure akin to mixed finite element

Poloidal flux, extrema=(-5.063e-02, 1.583e-16)



Re tele, extrema=(2.000e+02, 1.200e+03)

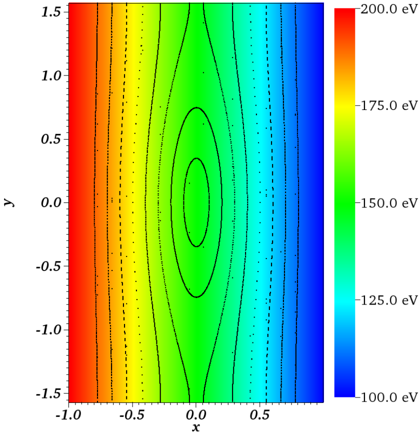




Test case 2: thermal transport in magnetic island

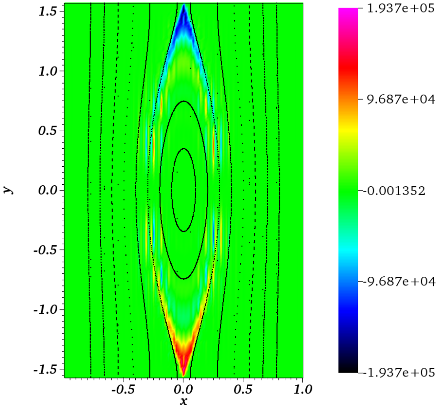
Kinetic parallel thermal transport across magnetic island in slab geometry

- $n = 9.5175 \times 10^{18}\,\mathrm{m}^{-3}$, $\mathbf{V} = 0$
- 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



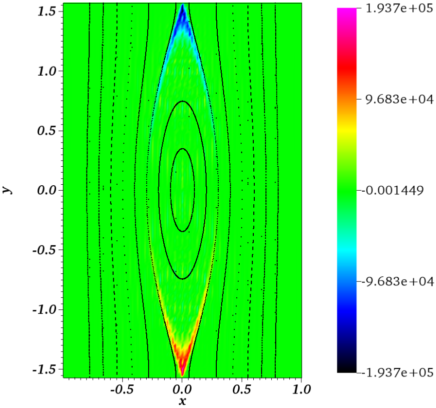
Initial temperature is a linear gradient that flattens across island as T evolves

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

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

Review of Picard iterations

Goal: Integrate the nonlinear initial value problem

$$\mathbf{x}'(t) = \mathbf{g}(\mathbf{x}(t)), \qquad \mathbf{x}(t_0) = \mathbf{x}_0$$

Where formal integration gives

$$\mathbf{x}(t) = \mathbf{x}_0 + \int_{t_0}^{t} \mathbf{g}(\mathbf{x}(s))\, ds$$

Forward Euler method:

$$\mathbf{x}(t) = \mathbf{x}_0 + \Delta t \mathbf{g}(\mathbf{x}_0)$$

Backward Euler method:

$$\mathbf{x}(t) = \mathbf{x}_0 + \Delta t \mathbf{g}(\mathbf{x}(t))$$

Picard iterations: solve explicit equation iteratively to converge on solution to implicit equation

$$\mathbf{x}_{k+1} = \mathbf{x}_0 + \Delta t \mathbf{g}(\mathbf{x}_k)$$

How to apply Picard and Newton methods to our set of differential equations?

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:

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

Review of Newton's method

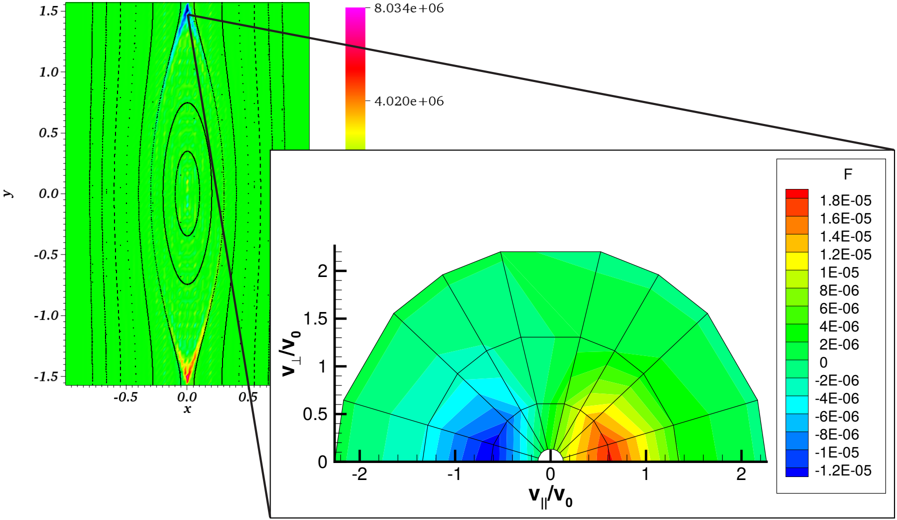
Goal: find zero of nonlinear $f(x)$ near x_0

- Approximate function with tangent line:
  $y(x) = f'(x_0)(x - x_0) + f(x_0)$
- Find zero of tangent line, and iterate:
  $f'(x_i)(x_{i+1} - x_i) = -f(x_i)$

Goal: find solution to nonlinear system $\mathbf{A}(\mathbf{x}) = \mathbf{b}$

- Let $\mathbf{f}(\mathbf{x}) = \mathbf{A}(\mathbf{x}) - \mathbf{b}$, and choose initial guess, $\mathbf{x}_0$.
- Let $J_{ij}(\mathbf{x}) = \partial f_i / \partial x_j (\mathbf{x}) = \partial A_i / \partial x_j (\mathbf{x})$
- Approximate $\mathbf{f}$ with hyper-plane:
  $\mathbf{y}(\mathbf{x}) = \mathbf{J}(\mathbf{x}_0) \cdot (\mathbf{x} - \mathbf{x}_0) + \mathbf{A}(\mathbf{x}_0) - \mathbf{b}$
- Find zeros of tangent lines, and iterate:
  $\mathbf{J}(\mathbf{x}_i) \cdot (\mathbf{x}_{i+1} - \mathbf{x}_i) = \mathbf{b} - \mathbf{A}(\mathbf{x}_i) \longleftarrow \text{solved with preconditioned GMRES}$

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	$0.35\,\mathrm{s}$
Newton	$10^{-5}\,\mathrm{s}$	$166\,\mathrm{mins?}$	8207	$1.2\,\mathrm{s}$?

- Unoptimized algorithm leaves room for improvement

Upcoming work

- Implement s-parallelism for simultaneous advance
- Possibly speed-up Newton iterations
  (reuse preconditioning matrix, improve 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, $\mathbf{V}$.