Application of continuum drift kinetics to parallel heat transport*

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Abstract

The Chapman-Enskog like electron drift kinetic equation* provides kinetic closure of fluid equations and extends to the long mean free path regime of magnetized plasmas. In this work we discuss the application of a continuum numerical solution to this equation to provide closures for the NIMROD code. Accuracy of the solution is aided by expressing the equation in velocity coordinates using pitch-angle and speed normalized by the thermal speed. This tightly couples the temperature to the kinetic distortion, and demands a careful treatment of the time-centering to implicitly advance both over large time steps. Comparisons are presented for three approaches: 1) leapfrog integration, 2) Picard iteration, and 3) simultaneous semi-implicit integration. Comparisons are made of computational efficiency and required velocity space resolution. Results are presented for applications involving equilibration along field lines which leads to temperature flattening across magnetic islands in slab, cylindrical and toroidal geometry.

*J. J. Ramos, Phys Plasmas **17**, 082502 (2010).

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

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

*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 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

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

Calculate parallel heat flux as moment of kinetic distortion

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

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

(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

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

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

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

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

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

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:

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

where $Q_{\rm ext}$ 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: $\theta \Delta \mathbf{q}_\parallel \rightarrow \bar{q}_\parallel \mathbf{b}$ where

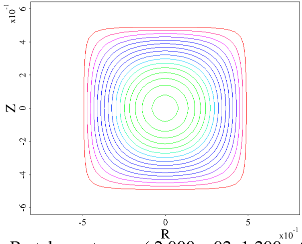
$$\bar{q}_\parallel + \theta \kappa_\parallel \mathbf{b} \cdot \nabla \Delta T = -\kappa_\parallel \mathbf{b} \cdot \nabla T^n$$

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

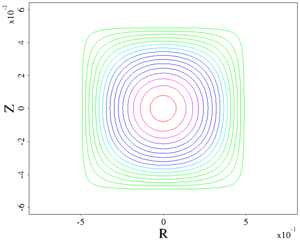
*C.R. Sovinec, *et al,* J. Comput. Phys. **195** (2004) 355–386

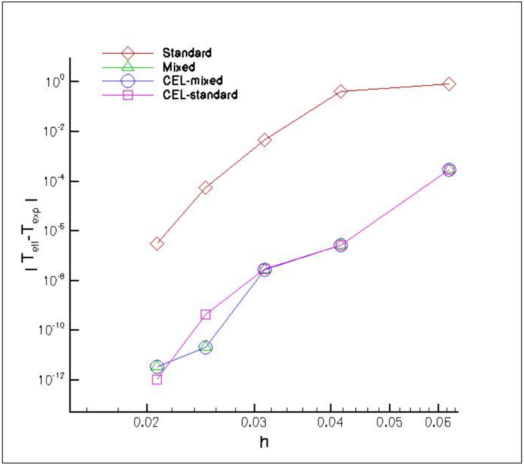
Staggered advance to steady state illustrates kinetic closure akin to mixed finite element

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



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

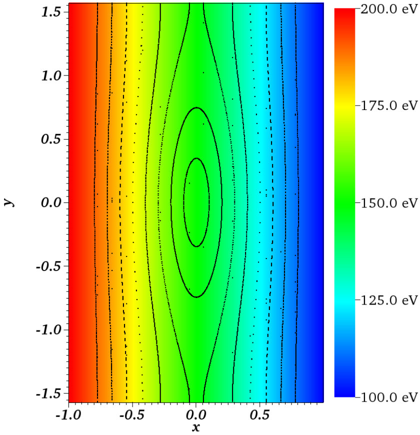




Test case 2: thermal transport in magnetic island

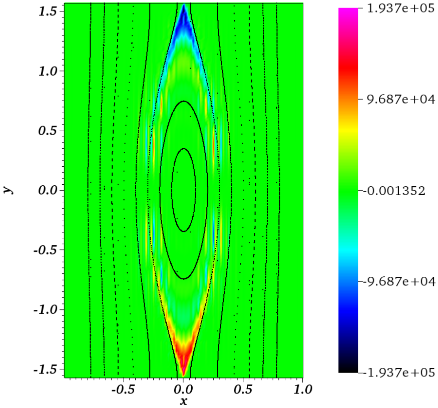
Kinetic parallel thermal transport across magnetic island in slab geometry

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



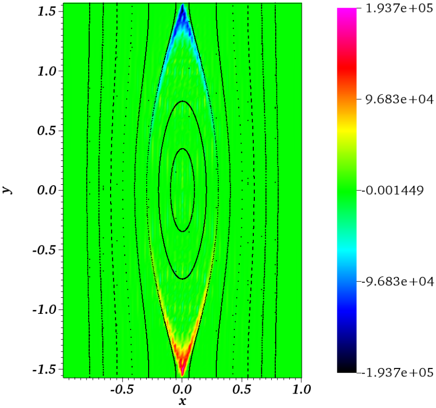
Initial temperature is a linear gradient that flattens across island as T evolves

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

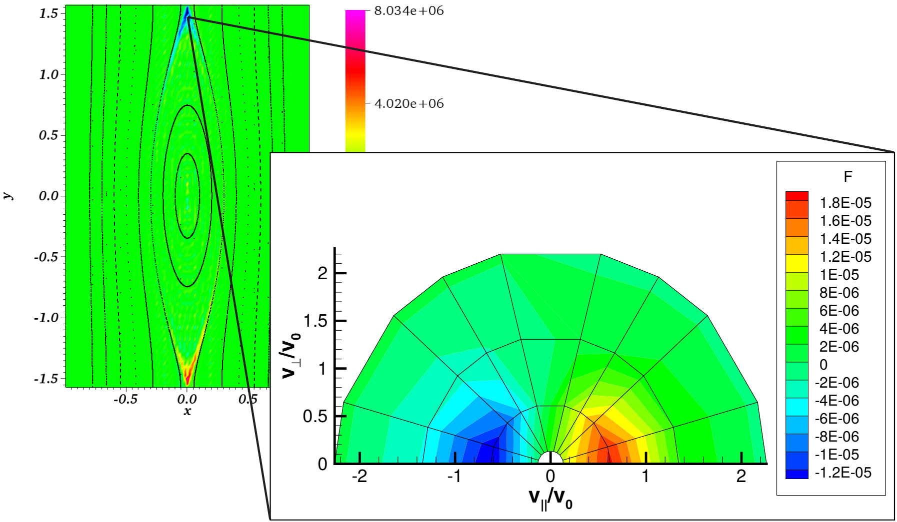
Goal: find zero of nonlinear $f(x)$ near x_0

- 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	$0.35\,\mathrm{s}$

- Need to implement parallelism over speed grid points for efficiency 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, $\mathbf{V}$.