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, \( n_a, V_a, \) and \( T_a \)
▶ Kinetic equation governs kinetic distortion, \( F_a \)
▶ \( n_a, V_a, \) 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

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CEL method separates fluid and kinetic physics

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

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

where

\[
\mathbf{v}_{gc} = v_T s \xi \mathbf{b} + \frac{\mathbf{E} \times \mathbf{B}}{B^2} + \frac{Ts^2}{qB} \left( 1 + \xi^2 \right) \mathbf{b} \times \nabla \ln B
\]

\[
+ \frac{2Ts^2}{qB^2} \left[ \xi^2 (\mathbf{I} - \mathbf{b} \mathbf{b}) + \frac{1}{2} \left( 1 - \xi^2 \right) \mathbf{b} \mathbf{b} \right] \cdot \nabla \times \mathbf{B} + \frac{mv_T s \xi}{qB^2} \mathbf{b} \times \frac{\partial \mathbf{B}}{\partial t}
\]

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

\[
\dot{\xi} = \frac{1 - \xi^2}{2\xi} \left\{ -\xi^2 \frac{\partial \ln B}{\partial t} + (\mathbf{v}_\parallel + \mathbf{v}_c^*) \cdot \left( \frac{q \mathbf{E}}{Ts^2} - \nabla \ln B \right) + \xi^2 \frac{\mathbf{E} \times \mathbf{B}}{B^2} \cdot \nabla \ln B
\]

\[
- \frac{\xi^2}{B^2} [\mathbf{b} \mathbf{b} \cdot (\nabla \times \mathbf{B})] \cdot \mathbf{E} - 2 \frac{T s^2 \xi^2}{q} \mathbf{b} \cdot \nabla \left[ \frac{\mathbf{b} \cdot (\nabla \times \mathbf{B})}{B^2} \right] + \frac{mv_T s \xi}{qB} \nabla \cdot \left( \mathbf{b} \times \frac{\partial \mathbf{b}}{\partial t} \right)
\]

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

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

NIMROD’s **spatial representation**:

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

**Pitch-angle** discretization uses finite element method:

\[
F_{i, n} (s, \xi, t) = \sum_l F_{i, n, l} (s, t) P_l (\xi)
\]

**Speed** discretization uses collocation method with polynomial expansion:

\[
F_{i, n, l} (s, t) \equiv e^{-s^2} \sum_k F_{i, n, l, k} (t) L_k (s)
\]  

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

\[
\int_0^\infty ds L_k (s) L_{k'} (s) e^{-s^2} = \delta_{kk'}
\]

Challenges highlighted in kinetic thermal transport case studies

\[
\frac{3}{2} n \frac{\partial T}{\partial t} = \kappa \perp \nabla \cdot [(I - bb) \cdot \nabla T] - \nabla \cdot q_\parallel + Q
\]

Calculate parallel heat flux as moment of kinetic distortion

\[
q_\parallel = \frac{m}{2} \int d\nu v^2 v_\parallel F = \pi m v_T^6 \int_{-1}^{1} d\xi \int_{0}^{\infty} ds \left( s^5 \xi F \right)
\]

\[
\frac{\partial F}{\partial t} + v_\parallel \cdot \nabla F - \frac{1 - \xi^2}{2\xi} v_\parallel \cdot \nabla \ln B \frac{\partial F}{\partial \xi} - \frac{s}{2} \left( v_\parallel \cdot \nabla + \frac{\partial}{\partial t} \right) \ln T \frac{\partial F}{\partial s} = C + \left( \frac{5}{2} - s^2 \right) v_\parallel \cdot \nabla \ln T f^M + \frac{2}{3nT} \left( s^2 - \frac{3}{2} \right) \left( \nabla \cdot q_\parallel - Q \right) f^M
\]

(red terms have temperature dependence.)
Possible $\theta$-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**

\[
T(t^k) \rightarrow F(t^{k+\frac{1}{2}}) \rightarrow T(t^{k+1}) \rightarrow F(t^{k+\frac{3}{2}})
\]

\[
\Delta T - \theta \Delta t G_{\text{lin}}(\Delta T, F^{k+\frac{1}{2}}) = \Delta t G(T^k, F^{k+\frac{1}{2}})
\]

\[
\Delta F - \theta \Delta t H_{\text{lin}}(T^{k+1}, \Delta F) = \Delta t H(T^{k+1}, F^{k+\frac{1}{2}})
\]

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

\[
T(t^k), F(t^k) \rightarrow T(t^{k+1}), F(t^{k+1})
\]

\[
\Delta T - \theta \Delta t G(T^{k+1}, F^{k+1}) = (1 - \theta) \Delta t G(T^k, F^k)
\]

\[
\Delta F - \theta \Delta t H(T^{k+1}, F^{k+1}) = (1 - \theta) \Delta t H(T^k, F^k)
\]

GMRES fails to solve
Test case 1: Anisotropic thermal conduction

Step 1. Impose $\mathbf{E} = E_0 \cos (\pi x) \cos (\pi y) \hat{z}$ 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 $Q_{\text{ext}}$ 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: $\theta \Delta \mathbf{q}_\parallel \rightarrow \bar{\mathbf{q}}_\parallel \mathbf{b}$ where

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

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

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

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

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

Mixed finite element steady state

$q_{\parallel} \ [W/m^2]$
Review of Picard iterations

**Goal:** Integrate the nonlinear initial value problem

\[ x'(t) = g(x(t)), \quad x(t_0) = x_0 \]

Where formal integration gives

\[ x(t) = x_0 + \int_{t_0}^{t} g(x(s)) \, ds \]

Forward Euler method:

\[ x(t) = x_0 + \Delta t g(x_0) \]

Backward Euler method:

\[ x(t) = x_0 + \Delta t g(x(t)) \]

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

\[ x_{k+1} = x_0 + \Delta t g(x_k) \]
How to apply Picard and Newton methods to our set of differential equations?

Implicit advance of $F$:

$$\frac{F^{k+1} - F^k}{\Delta t} + \sqrt\frac{2T}{m} s\xi \left( \nabla_{\parallel} F^{k+1} - \frac{1 - \xi^2}{2\xi} \nabla_{\parallel} \ln B \frac{\partial F^{k+1}}{\partial \xi} \right) - \frac{s}{2T} \left( \sqrt\frac{2T}{m} s\xi \nabla_{\parallel} + \frac{\partial}{\partial t} \right) T \frac{\partial F^{k+1}}{\partial s}$$

$$= C\left(T, F^{k+1}\right) + \left[ \left( \frac{5}{2} - s^2 \right) \sqrt\frac{2}{mT} s\xi \nabla_{\parallel} T + \frac{2}{3nT} \left( s^2 - \frac{3}{2} \right) \left( \nabla \cdot q_{\parallel} \left(F^{k+1}, T\right) - G\right) \right] f^M(T)$$

Implicit advance of $T$:

$$\frac{3n}{2} T^{k+1} - T^k = \kappa_{\perp} \nabla \cdot \left[ (I - bb) \cdot \nabla T^{k+1} \right] - \nabla \cdot q_{\parallel} (T, F) + G$$
**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 \( A(x) = b \)

- Let \( f(x) = A(x) - b \), and choose initial guess, \( x_0 \).
- Let \( J_{ij}(x) = \frac{\partial f_i(x)}{\partial x_j}(x) = \frac{\partial A_i(x)}{\partial x_j}(x) \)
- Approximate \( f \) with hyper-plane:
  \[ y(x) = J(x_0) \cdot (x - x_0) + A(x_0) - b \]
- Find zeros of tangent lines, and iterate:
  \[ J(x_i) \cdot (x_{i+1} - x_i) = b - A(x_i) \quad \leftarrow \text{solved with preconditioned GMRES} \]
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 $10^{-5}$ s

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>Wall clock time to $t = 10^{-5}$ s</th>
<th>Average GMRES iterations per step</th>
<th>Time per iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Picard</td>
<td>$10^{-8}$ s</td>
<td>75 mins</td>
<td>5</td>
</tr>
<tr>
<td>Newton</td>
<td>$10^{-8}$ s</td>
<td>200 mins</td>
<td>4</td>
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<tr>
<td>Newton</td>
<td>$10^{-7}$ s</td>
<td>49 mins</td>
<td>52</td>
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<tr>
<td>Newton</td>
<td>$10^{-6}$ s</td>
<td>42 mins</td>
<td>723</td>
</tr>
<tr>
<td>Newton</td>
<td>$10^{-5}$ s</td>
<td>166 mins?</td>
<td>8207</td>
</tr>
</tbody>
</table>

- 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 $B$, $n$, $V$. 