Continuum Drift Kinetic Computations in
NIMROD

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Status of integral closures in NIMROD.

• Integral forms for electron and ion parallel heat flow (CEL and higher-order moment approach) and parallel ion stress (CEL approach) implemented in NIMROD.
  - computations are costly although method of fitting $T$ and $V$ drives greatly speeds up closure calculation (John James thesis),
  - improved parallel scaling using separate groups of processors devoted to closure calculation (scaling talk this afternoon),
  - further improvements include efforts to reuse closure data along field line to minimize number of integrations; also considering mapping techniques.

• Existing implementation uses local, diffusive forms for semi-implicit stabilization.
  - mixed finite element approach used to improve spatial accuracy of semi-implicit operator,
  - continuum closure computation could also be used to improve semi-implicit stabilization of integral closures which are treated explicitly.
Mixed finite-element method (MFEM) treats $q_{||}$ as fundamental variable.

- Solve expanded system for $T$ and auxiliary scalar, $q_{||}$:

$$\frac{3}{2} n \Delta T + \kappa_0 \sqrt{\theta} \Delta t \vec{B} \cdot \vec{\nabla} q_{||} = \ldots,$$

$$\frac{\kappa_0^2 B^2}{\kappa_{||} - \kappa_{\perp}} q_{||} + \kappa_0 \sqrt{\theta} \Delta t \vec{B} \cdot \vec{\nabla} \Delta T = -\kappa_0 \sqrt{\frac{\Delta t}{\theta}} \vec{B} \cdot \vec{\nabla} T^n$$

- Term “mixed” loosely implies treating flux, $q_{||}$, as expanded quantity.

- Formulation has symmetric treatment of $q_{||}$ and $T$.

- Constant, $\kappa_0$, used for scaling. Constant, $\theta$, is centering parameter.

- Implementation solves either for $(\Delta T, q_{||})$ or $(T^{n+1}, q_{||})$. 
Error reduced considerably in JCP anisotropic test problem (Sovinec et al., JCP 2004).
Applied to heat transport problem in cylindrical geometry (Hölzl et al., POP 2008).

2/1 island stuck into zero pressure, cylindrical eq. Heat source finite for $r < 0.2$ and zero outside. Core $T$ accurate in MFEM case with only 4 grid points and bi-quadratic polynomials.
Motivate continuum solution to closure problem.

- Using NIMROD's infrastructure can easily
  - test different representations of velocity space basis functions including 2D finite elements,
  - handle time dependence in fully implicit manner,
  - incorporate $|\mathbf{B}|$ and accelerations effects, and
  - allows for multiple parallelization strategies.

- This work will aid implementation of higher-order moment equations as well.
Apply MFEM approach in continuum solution.

- Solve for fully implicit $q_\parallel$ closure from lowest order Chapman-Enskog-like drift kinetic equation (CEL-DKE):

$$\frac{\partial F}{\partial t} + v_\parallel \hat{b} \cdot \vec{\nabla} F - C (F + f_M) = \text{thermodynamic drives.}$$

- Expanding $F = \sum F_i (x,v,t) P_i (v_\parallel / v)$ yields:

$$\frac{\partial \tilde{F}}{\partial t} + A v \hat{b} \cdot \vec{\nabla} \tilde{F} - B v (\hat{b} \cdot \vec{\nabla} \ln B) \tilde{F} - C \tilde{F} = \text{drives},$$

- Matrices $A$, $B$, and $C$ represent free-streaming, $|B|$ and collisional couplings, respectively.
Fully implicit solution for coefficients, \( F_n \), couples to \( T \) advance through \( q_{\parallel} \).

- Ignoring nonlinearities, treating \( T \) drive only and evaluating remaining speed dependence at \( v = v_T \) yields coupled system:

\[
\frac{3}{2} n \Delta T + \Delta t \nabla \cdot q_{\parallel} \hat{b} = \ldots ,
\]

\[
( a_{i,i} + \theta \Delta t \nu_0 c_{i,i} ) \Delta \hat{F}_i / v_T + \theta \Delta t \hat{b} \cdot \nabla [ a_{i,i+1} \Delta \hat{F}_{i+1} + a_{i,i-1} \Delta \hat{F}_{i-1} + \delta_{i,i} a_{i,i} \Delta T ] + \theta \Delta t ( \hat{b} \cdot \nabla \ln(B) ) [ b_{i,i+1} \Delta \hat{F}_{i+1} + b_{i,i-1} \Delta \hat{F}_{i-1} ] = \ldots ,
\]

\[
q_{\parallel} = -T \int d \vec{v} \nu_{\parallel} L^{3/2}_1 P_1 \left( \frac{\nu_{\parallel}}{v} \right) F_1 , \text{ with } \hat{F}_i = F_i / (L^{3/2}_1 f_M).
\]
Apply continuum solution to Hölzl problem.

- T profiles as function of flux show flattening across 2/1 island.
- All cases used 3 Fourier modes and 10 x 10 grid.
- Predicted T from continuum solution accurate even for lower-order finite elements, pd = 2.

pd=2, continuum solution using $F_1$ and $F_2$.

T flattening across island.
Solve separated equations for expansion coefficients of $F$ and stagger from $T$.

- First solve for $\Delta F$ (actually $\Delta f_i = f_i^{k+1} - f_i^k$) using $T^{k+1/2}$:

$$
\left[ 1 + \theta \Delta t \left( \frac{\gamma_L}{2} + \gamma_i \nu \hat{b} \cdot \vec{\nabla} \right) \right] \Delta f_i = \Delta t \left( \frac{\gamma_L}{2} + \gamma_i \nu \hat{b} \cdot \vec{\nabla} \right) f_i^k + \Delta t \ W_{il}^{-1} L_1^{3/2} \nu \left( \hat{b} \cdot \vec{\nabla} \ln T^{k+1/2} \right) f_{\text{Max}}^{k+1/2}
$$

- Then solve for $\Delta T = T^{k+3/2} - T^{k+1/2}$ using centered $f^{k+1}$:

$$
\left[ 1 + \theta \Delta t \vec{\nabla} \cdot \kappa_\perp \vec{\nabla} \right] \Delta T = \theta \Delta t \vec{\nabla} \cdot \kappa_\perp \vec{\nabla} T^{k+1/2} - \Delta t \vec{\nabla} \cdot q_\parallel^{k+1},
$$

where $q_\parallel^{k+1} = -T \int d\vec{v} \nu_\parallel L_1^{3/2} \ P_1 \sum_i W_{1i} f_i^{k+1}$.
Solving on speed grid expands system. Can keep nonlinearities.

- Solve coupled systems at particular $\nu$.

\[
\frac{3}{2} n \Delta T + \Delta t \vec{\nabla} \cdot q_\parallel \hat{b} = \ldots, \\
\theta \Delta t \hat{b} \cdot \vec{\nabla} \left[ a_{i,i+1} \Delta F_{i+1} + a_{i,i-1} \Delta F_{i-1} + \delta_{i1} a_{i,i} \Delta T \right] + \\
\theta \Delta t (\hat{b} \cdot \vec{\nabla} \ln (B)) \left[ b_{i,i+1} \Delta F_{i+1} + b_{i,i-1} \Delta F_{i-1} \right] = g(\nu_j),
\]

\[
q_\parallel = - T 2 \pi \int_{-1}^{1} d \xi \sum_j w_j \nu_\parallel L_1^{3/2} P_1(\nu_\parallel / \nu) F_1(x, t, \nu_j).
\]
Generalize velocity space basis to include 2-D finite elements.

- Solve for fully implicit $q_\parallel$ closure from lowest order Chapman-Enskog-like drift kinetic equation (CEL-DKE):

$$\frac{\partial F}{\partial t} + v_\parallel \hat{b} \cdot \vec{\nabla} F - C(F + f_M) = \text{thermodynamic drives.}$$

- Expand $F = \Sigma F_i \phi_i(\xi, \mu)$, where $\xi$ is pitch-angle variable and $\mu$ is magnetic moment and compute integrals of form

$$\int d\tilde{x} \int d\tilde{v} \phi_j (\phi_i \frac{\partial F_i}{\partial t} + \phi_i \hat{b} \cdot \vec{\nabla} F_i - F_i C(\phi_i) = \text{drives,})$$

- Use NIMROD finite element and Gaussian quadrature machinery to compute velocity integrals.
Choose from various basis functions for velocity variables.

- Legendre functions for pitch-angle with simple grid in speed, $v$, is easiest.
- Can also use 2D finite elements with packed grids.

$$(\xi, \mu)$$.space pack near RF resonance in $v$

$$(v, \cos^{-1}(\xi))$$.space pack in speed and angle for slowing down of hot particles
Future work.

- Test convergence as Legendre polynomials and grid points in speed are added.
- Test staggered advance against simultaneous, fully implicit solution for $T$ and $F$.
- Apply 3-D iterative solves in continuum solution of CEL-DKE and/or higher order moment equations.
- Include flow and collisional (beyond Lorentz pitch-angle scattering) drives.
- At present, can compute full matrix that arises from spatial coupling and solve for $F_i(x,t)$ on grid in $v$ using SuperLU.
- Use recent improvements to 3-D preconditioning for non-symmetric systems.