Coulomb Collision Operator in NIMROD Continuum Kinetic Calculations

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DKEs solved in NIMROD

For electrons, thermal ions and energetic ions can evolve

$$
\begin{aligned}
&\partial_t f + (\mathbf{v}_{||} + \mathbf{v}_D) \cdot \nabla f \\
&\quad + \frac{s}{2}\Big[-(\mathbf{v}_{||} + \mathbf{v}_D) \cdot \nabla \ln T_0 - (1-\xi^2)\frac{\mathbf{b}}{B} \cdot \nabla \times \mathbf{E} + \\
&\quad \frac{e}{s^2 T_0}(\mathbf{v}_{||} + \mathbf{v}_D) \cdot \mathbf{E} + (1+\xi^2)\frac{\mathbf{E} \times \mathbf{B}}{B^2} \cdot \nabla \ln B\Big]\frac{\partial f}{\partial s} \\
&\quad + \frac{1-\xi^2}{2\xi}\Big[-(\mathbf{v}_{||} + \mathbf{v}_D) \cdot \nabla \ln B + \xi^2 \frac{\mathbf{b}}{B} \cdot \nabla \times \mathbf{E} + \\
&\qquad \frac{e}{s^2 T_0}(\mathbf{v}_{||} + \mathbf{v}_D) \cdot \mathbf{E} + \xi^2 \frac{\mathbf{E} \times \mathbf{B}}{B^2} \cdot \nabla \ln B\Big]\frac{\partial f}{\partial \xi} = C(f)
\end{aligned}
$$

Existing $C(f)$ implementation issues I

Continuum approach in NIMROD uses 1D FE in pitch angle $\xi = v_{||}/v$ and grid in normalized speed $s = v/v_T$:

$$f(\mathbf{x}, t, \xi, s) \quad = \quad \sum_{l} f^{li}(\mathbf{x}, t, s_i)\phi_l(\xi).$$

Linearized Coulomb collision operator expressed using moments is

$$C^1_{ab} \quad = \quad \sum_{lk} \frac{f_{0a}}{\sigma^l_k} P_l(v_{||}/v) \left[\nu^{lk,0}_{ab}(s_a) M^{lk}_{||a}(\mathbf{x}, t) + \nu^{0,lk}_{ab}(s_a) M^{lk}_{||b}(\mathbf{x}, t) \right].$$

Moment definition is

$$M^{lk}_{||} \quad \equiv \quad \frac{l!}{(2l-1)!!} \frac{v_T^{l+2k}}{n} \int d\mathbf{v} L_k^{l+1/2}(s^2) s^l P_l(v_{||}/v) f.$$

Existing $C(f)$ implementation issues II

Projection on to moments done using quadrature

$$
\begin{aligned}
M_{||}^{lk} &= 2\pi \frac{l!}{(2l-1)!!} \frac{v_T^{l+2k+3}}{n} \int_0^\infty ds s^{l+2} L_k^{l+1/2} \int_{-1}^{1} d(v_{||}/v) P_l \sum_{l'} f^{l'm}(\mathbf{x}, t, s_m)\phi_{l'} \\
&= 2\pi \frac{l!}{(2l-1)!!} \frac{v_T^{l+2k+3}}{n} \sum_m w_m s_m^{l+2} L_k^{l+1/2}(s_m^2) \sum_{l'} p_{ll'} f^{l'm}(\mathbf{x}, t, s_m).
\end{aligned}
$$

- Care must be taken in choosing an appropriate number of moments.
- Legendre polynomials (over whole ξ domain) struggle to represent boundary layers between trapped and passing space.
- Finite-element nodes at trapped/passing boundary aid convergence in velocity space.
- Non-classical polynomials associated with speed grid may also help.

Start with TR potentials and Coulomb collision operator.

Using Trubnikov-Rosenbluth potentials:

$$
\begin{aligned}
g_b(\mathbf{v},\mathbf{x},t) &\equiv \int d\mathbf{v}' f_b(\mathbf{v}',\mathbf{x},t)\,|\mathbf{v}-\mathbf{v}'| \\
h_b(\mathbf{v},\mathbf{x},t) &\equiv \int d\mathbf{v}' f_b(\mathbf{v}',\mathbf{x},t)\,|\mathbf{v}-\mathbf{v}'|^{-1},
\end{aligned}
$$

the Coulomb collision operator may be written

$$
C_a = -\nabla\cdot\sum_b \Gamma_{ab}\left(\frac{m_a}{m_a+m_b} f_a \frac{\partial h_b}{\partial \mathbf{v}} - \frac{1}{2}\frac{\partial f_a}{\partial \mathbf{v}}\cdot\frac{\partial^2 g_b}{\partial \mathbf{v}\partial \mathbf{v}}\right),
$$

where $\Gamma_{ab} = \frac{4\pi q_a^2 q_b^2 \Lambda_{ab}}{m_a^2}$.

Expand distribution functions.

Gyroaveraged distribution functions in $s = v/v_T$ and $\xi = v/v_{||}$ expanded as

$$\begin{aligned} f &= \sum_l f^l(s, \mathbf{x}, t)\phi_l(\xi) \\ &= \sum_{lk} f^{lk} L_{lk}(s) f_0(s)\phi_l(\xi) \end{aligned}$$

For Legendre polynomials: $\phi_l = P_l$, $f_0(s) = e^{-s^2}$, and $L_{lk}(s) = s^l \bar{L}_k^{l+1/2}(s^2)$ satisfy $\int_0^\infty ds s^{2l+1} \bar{L}_k^{l+1/2} \bar{L}_j^{l+1/2} e^{-s^2} = \delta_{kj}$.

For a finite-elements: ϕ_l are nodal FE basis functions, $f_0(s) = e^{-s^2}$, and $L_{lk}(s) = L_k(s)$ satisfy $\int_0^\infty ds s^2 L_k L_j e^{-s^2} = \delta_{kj}$.

Nonlinear Collision Operator

In v and ξ variables, nonlinear collision operator for species a colliding with species b is

$$
\begin{aligned}
C_{ab} \;=\; & \Gamma_{ab}\{\frac{1}{2v^4}((vf_v - \xi f_\xi)\mathcal{L}(g) + (vg_v - \xi g_\xi)\mathcal{L}(f)) + \\
& (\frac{1}{v^2}g_v f_v - \frac{\xi^2}{v^4}g_\xi f_\xi) - \frac{1}{2v^4}(1-\xi^2)^2 g_{\xi\xi} f_{\xi\xi} + \\
& \frac{1-\xi^2}{v^2}(g_{v\xi} - \frac{1}{v}g_\xi)(f_{\xi v} - \frac{1}{v}f_\xi) + \frac{1}{2}g_{vv}f_{vv} + \\
& (1 - \frac{m_a}{m_b})(f_v h_v + \frac{1-\xi^2}{v^2}f_\xi h_\xi) + \frac{m_a}{m_b}4\pi f_a f_b\}.
\end{aligned}
$$

Linearized Collision Operator

Expanding about lowest order distribution functions that do not depend on ξ yields

$$
\begin{aligned}
C_{ab}^{test} &= \Gamma_{ab}\{\frac{1}{2v^3}g_v^0\mathcal{L}(f) + \frac{1}{v^2}g_v^0 f_v + \frac{1}{2}g_{vv}^0 f_{vv} + (1-\frac{m_a}{m_b})h_v^0 f_v + \frac{m_a}{m_b}4\pi f_b^0 f_a\} \\
C_{ab}^{field} &= \Gamma_{ab}\{\frac{1}{2v^3}f_v^0\mathcal{L}(g) + \frac{1}{v^2}f_v^0 g_v + \frac{1}{2}f_{vv}^0 g_{vv} + (1-\frac{m_a}{m_b})f_v^0 h_v + \frac{m_a}{m_b}4\pi f_a^0 f_b\}.
\end{aligned}
$$

where $\mathcal{L} = \partial_\xi(1-\xi^2)\partial_\xi$.

Write TR potentials in v and ξ.

For velocity distributions that depend only on ξ and v

$$
\begin{aligned}
h_b(v,\xi) &= \int_0^\infty dv' v'^2 \int_{-1}^{1} d\xi' \int_0^{2\pi} d\phi' \frac{f_b(v',\xi')}{|\mathbf{v}-\mathbf{v}'|} \\
g_b(v,\xi) &= \int_0^\infty dv' v'^2 \int_{-1}^{1} d\xi' \int_0^{2\pi} d\phi' f_b(v',\xi')|\mathbf{v}-\mathbf{v}'|.
\end{aligned}
$$

where $\mathbf{v} = v\cos\theta\mathbf{b} + v\sin\theta\mathbf{x}$ and

$\mathbf{v}' = v'\cos\theta'\mathbf{b} + v'\sin\theta'\cos\phi'\mathbf{x} + v'\sin\theta'\sin\phi'\mathbf{y}$ with

$|\mathbf{v}-\mathbf{v}'| = \sqrt{v^2 + v'^2 - 2vv'\xi\xi' - 2vv'\sqrt{1-\xi^2}\sqrt{1-\xi'^2}}.$

Integration over ϕ' yields

Write TR potentials in v and ξ.

$$h_b(v,\xi) = 4v^2 \int_0^\infty d\bar{v}\,\bar{v}^{3/2} \int_{-1}^{1} d\xi' f_b \frac{K(k)}{\sqrt{\bar{v}+\bar{v}^{-1}-2(\xi\xi'-\sqrt{1-\xi^2}\sqrt{1-\xi'^2})}}$$

$$g_b(v,\xi) = 4v^4 \int_0^\infty d\bar{v}\,\bar{v}^{5/2} \int_{-1}^{1} d\xi' f_b E(k) \sqrt{\bar{v}+\bar{v}^{-1}-2(\xi\xi'-\sqrt{1-\xi^2}\sqrt{1-\xi'^2})},$$

where $k \equiv 4\sqrt{1-\xi^2}\sqrt{1-\xi'^2}/\sqrt{\bar{v}+\bar{v}^{-1}-2(\xi\xi'-\sqrt{1-\xi^2}\sqrt{1-\xi'^2})}$
with $\bar{v} \equiv v'/v$.

K and E are elliptic integrals

$K(k) \equiv \int_0^{\pi/2} d\theta/\sqrt{1-k^2\sin^2\theta}$

$E(k) \equiv \int_0^{\pi/2} d\theta\sqrt{1-k^2\sin^2\theta}$ for $0 \le k < 1$.

Evaluate for finite-element basis.

For FE expansion using nodal basis functions

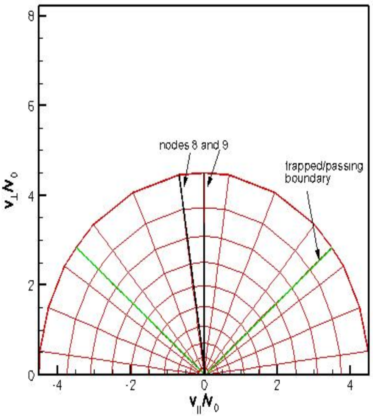
$$h_b^l(v) \;=\; 4v^2 \int_0^\infty d\bar{v}\,\bar{v}^{3/2} \sum_{l'} f_b^{l'} K_{ll'}(\bar{v})$$

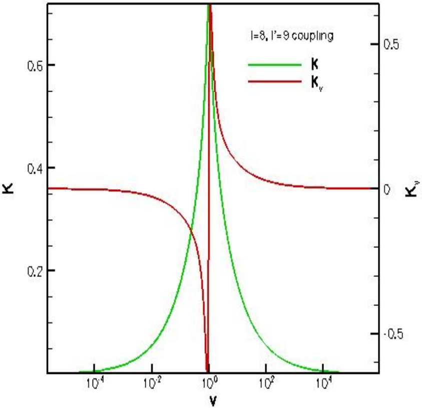
$$g_b^l(v) \;=\; 4v^4 \int_0^\infty d\bar{v}\,\bar{v}^{5/2} \sum_{l'} f_b^{l'} E_{ll'}(\bar{v}).$$

$K_{ll'}(\bar{v})$ and $E_{ll'}(\bar{v})$ vary rapidly near $\bar{v} = 1$ for overlapping basis.
Final integral evaluated using $f_b^l = \sum_k f_b^{lk} L_k(s) f_0(s)$ and high-order, Gauss-Legendre quadrature in domains $\bar{v} \epsilon [0, 1)$ and $\bar{v} \epsilon (1, \infty)$.
Also need derivatives of $K_{ll'}(\bar{v})$ and $E_{ll'}(\bar{v})$ with respect to v and ξ.

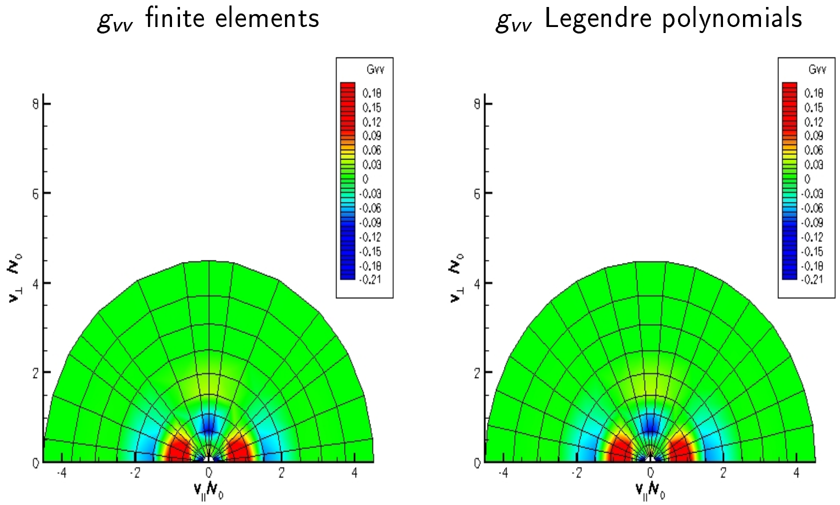
Example of FE couplings in $K_{ll'}$ and $\partial_v K_{ll'}$.

FE grid with polynomial degree 4, 1 cell in positive and negative passing space and 2 cells in trapped space.



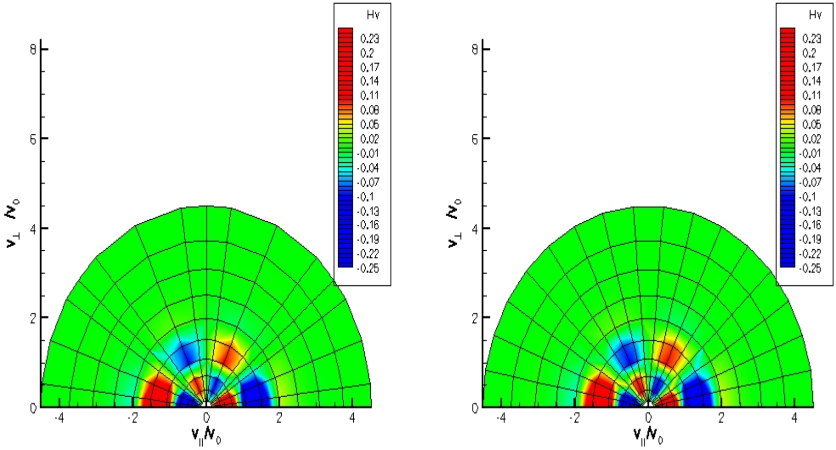


Comparison for $f = s^2 L_3^{2+1/2}(s^2) exp(-s^2) P_2(\xi)/v_T^3$.



Comparison for $f = s^3 L_4^{3+1/2}(s^2) exp(-s^2) P_3(\xi)/v_T^3$.

h_v finite elements | h_v Legendre polynomials



Future Work

- Implement new formulation of linearized operator in NIMROD.
- Finish benchmark with NEO.
- Implement nonlinear collision terms in NIMROD.
- Continue other continuum kinetic work including:
    1. energetic and thermal ion effects on RSAEs, ITGs and Giant Sawteeth.
    2. NTMs with RF quasilinear diffusion operator in electron DKE.