

# Grungy details for continuum kinetics in NIMROD

## NIMROD Team Meeting, Madison, WI

E. Held<sup>1</sup>   S. Kruger<sup>2</sup>   J. King<sup>2</sup>   NIMROD Team

<sup>1</sup>Department of Physics  
Utah State University

<sup>2</sup>Tech-X Corp.

April 2, 2016

# Electron, ion and hot particle DKEs in NIMROD

- Hazeltine's form for the first-order drift kinetic equation in energy,  $\varepsilon$ , and magnetic moment,  $\mu$ , variables:

$$\frac{\partial f}{\partial t} + (\mathbf{v}_{\parallel} + \mathbf{v}_D) \cdot \nabla f + \left( \mu \frac{\partial B}{\partial t} + e(\mathbf{v}_{\parallel} + \mathbf{v}_D) \cdot \mathbf{E} \right) \frac{\partial f}{\partial \varepsilon} = C(f)$$

- Transforming to  $\xi = v_{\parallel}/v$  and  $s = v/v_0$  yields

$$\begin{aligned} \frac{\partial f}{\partial t} + (\mathbf{v}_{\parallel} + \mathbf{v}_D) \cdot \left[ \nabla f - \frac{1-\xi^2}{2\xi} \nabla \ln B \frac{\partial f}{\partial \xi} - \frac{s}{2} \nabla \ln T_0 \frac{\partial f}{\partial s} \right] - C(f) + \\ \frac{1-\xi^2}{2\xi} \left[ -\xi^2 \frac{\mathbf{b}}{B} \cdot \frac{\partial \mathbf{B}}{\partial t} + \frac{q}{s^2 T_0} (\mathbf{v}_{\parallel} + \mathbf{v}_D) \cdot \mathbf{E} + \xi^2 \frac{\mathbf{E} \times \mathbf{B}}{B^2} \cdot \nabla \ln B \right] \frac{\partial f}{\partial \xi} + \\ \frac{s}{2} \left[ -(1-\xi^2) \frac{\mathbf{b}}{B} \cdot \frac{\partial \mathbf{B}}{\partial t} + \frac{q}{s^2 T_0} (\mathbf{v}_{\parallel} + \mathbf{v}_D) \cdot \mathbf{E} + (1+\xi^2) \frac{\mathbf{E} \times \mathbf{B}}{B^2} \cdot \nabla \ln B \right] \frac{\partial f}{\partial s} = 0 \end{aligned}$$

where

$$\mathbf{v}_D = \frac{\mathbf{E} \times \mathbf{B}}{B^2} + \frac{T_0 s^2}{q B^2} \left[ (1+\xi^2) \mathbf{b} \times \nabla B + 2\xi^2 \mu_0 \mathbf{J}_{\perp} + (1-\xi^2) \mu_0 \mathbf{J}_{\parallel} \right] + \frac{m v_0 s \xi}{q B^2} \mathbf{b} \times \frac{\partial \mathbf{B}}{\partial t}.$$

# Use NIMROD's spatial representation and efficient 2D velocity space representation.

Distribution functions expanded as

$$f(R, Z, \phi, \xi, s, t) = \sum_i f_{i,n=0}(\xi, s, t) \alpha_{i,n=0} +$$

$$\sum_{i,n>0} f_{i,n}(\xi, s, t) \alpha_{i,n} + f_{i,n}^*(\xi, s, t) \alpha_{i,n}^*,$$

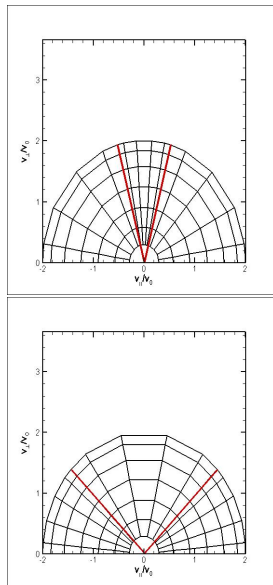
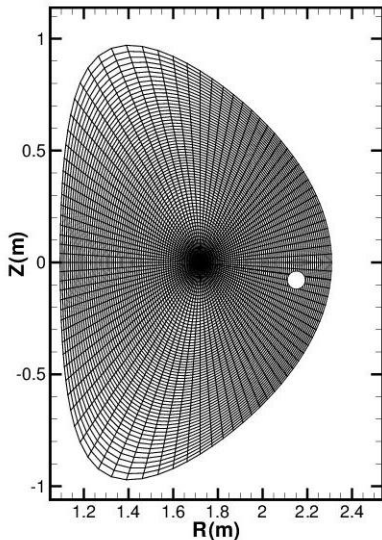
where  $\alpha_{i,n} \equiv \psi_i(x, y) \exp(in\phi)$  and for 2D velocity space

$$f_{i,n}(\xi, s, t) = \sum_l \sum_{k=0}^{N_s-1} f_{i,n,l,k}(t) P_l(\xi) \delta(s - s_k).$$

$P_l(\xi)$  are 1D FE in a pitch-angle type variable,  $\xi$ , and DKEs are solved at  $N_s$  collocation points in normalized speed,  $s$ .

Vertex nodes in  $\xi$  grid at  $\pm\xi_t(\psi)$  may help convergence.

t/p bnd varies in poloidal plane



# Correct streaming term with trapped/passing grids.

- Started with  $(\mathbf{v}_{||} + \mathbf{v}_D) \cdot \nabla|_{\mu,w,t} f$ .
- Rewrote as  $(\mathbf{v}_{||} + \mathbf{v}_D) \cdot (\nabla|_{\xi,s,t} + \nabla\xi\partial/\partial\xi + \nabla s\partial/\partial s) f$ .
- Finally transform from  $\xi$  to logical pitch-angle variable  $\eta$ :  
 $(\mathbf{v}_{||} + \mathbf{v}_D) \cdot (\nabla|_{\eta,s,t} + \nabla|_{\xi}\eta\partial/\partial\eta) f$
- Second term needed when distribution functions vary in pitch-angle and  $\nabla|_{\xi}\eta = \nabla R\partial\eta/\partial R + \nabla Z\partial\eta/\partial Z$ .
- In negative passing space mapping is  $\xi = -\cos(\theta_{tp}\eta/m)$   
where  $\theta_{tp} = \theta_{tp}(R, Z)$

## Can also interpret as 3D FE method.

- Basis functions:  $\alpha = \alpha(R(x, y), Z(x, y), \xi(x, y, \eta))$

- 3D Jacobian:  $J_{3D} = \left( \frac{\partial R}{\partial x} \frac{\partial Z}{\partial y} - \frac{\partial R}{\partial y} \frac{\partial Z}{\partial x} \right) \frac{\partial \xi}{\partial \eta}$

$$\frac{\partial}{\partial R} = J_{2D}^{-1} \left( Z_y \frac{\partial}{\partial x} - Z_x \frac{\partial}{\partial y} \right) + J_{3D}^{-1} \left( Z_x \xi_y - Z_y \xi_x \right) \frac{\partial}{\partial \eta}$$

$$\frac{\partial}{\partial Z} = J_{2D}^{-1} \left( R_x \frac{\partial}{\partial y} - R_y \frac{\partial}{\partial x} \right) + J_{3D}^{-1} \left( R_y \xi_x - R_x \xi_y \right) \frac{\partial}{\partial \eta}$$

$$\frac{\partial}{\partial \xi} = \frac{\partial \eta}{\partial \xi} \frac{\partial}{\partial \eta}$$

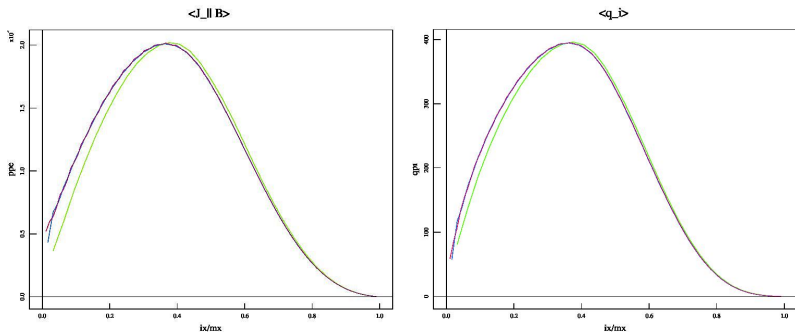
- Both approaches were implemented as a check. They yield the same results.

# Velocity space coefficients coupled explicitly in integrands.f90.

- Field comps type routines construct coupling array, vpn.
- Implicit streaming terms for trapped/passing pitch-angle grids is

```
IF (gridshape_v(5:7) == 'tpb') THEN
  int(jq,iq,:,jv,iv) = int(jq,iq,:,jv,iv) + SUM(
    dt*fcel*alpha(:, :, iv)*alpha(:, :, jv)*
    (vpn(1,il+n,il+m, :, :) * tpr(1, :, :)
    + vpn(2,il+n,il+m, :, :) * tpz(1, :, :)) , 1)
ENDIF
```

# Revisit high-beta NEO/NIMROD benchmark case.



- Local trapped/passing boundary used throughout poloidal plane, implementation no longer assumes grid alignment with flux surfaces.
- Can now test convergence properties of trapped/passing grids.
- Improved equilibria with resolve of GS equation help.
- Alternate solves for  $F_i$  and  $F_e$  speeds up computation.



# Full linearized Coulomb collision operator important.

- Implemented full, linearized collision operator using 1D finite-elements in pitch angle and non-classical, orthogonal speed polynomials.
- Expand  $F = \sum_l F_l(\mathbf{x}, s, t) P_l(\xi) = \sum_{lk} F_{lk}(\mathbf{x}, t) L_k(s) P_l(\xi)$  and use in

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

where  $\mathcal{L} = \partial_\xi(1 - \xi^2)\partial_\xi$  and  $g$  and  $h$  are Rosenbluth potentials.

# Issues with Lorentz operator?

- Weak form of Lorentz operator with “surface” term is

$$-\int_{-1}^1 d\xi \frac{\partial \alpha'}{\partial \xi} (1 - \xi^2) \frac{\partial F}{\partial \xi} + \int_{-1}^1 d\xi \frac{\partial}{\partial \xi} [\alpha' (1 - \xi^2) \frac{\partial F}{\partial \xi}]$$

- Considering that pitch-angle basis functions are in  $C^0$ , should jump conditions be kept at t/p boundaries?

$$\Delta [\alpha' (1 - \xi^2) \frac{\partial F}{\partial \xi}] |_{-\xi_t} + \Delta [\alpha' (1 - \xi^2) \frac{\partial F}{\partial \xi}] |_{+\xi_t}$$

# Could static condensation in pitch-angle speed up nonlinear solves? Timing results from NEO/NIMROD benchmark.

Timing statistics:

	CPU secs	% of loop
Iteration time	= 4.15608E+02	3.42237E+01
Factoring time	= 2.94936E+02	2.42868E+01
SuperLU time	= 4.15697E+02	3.42310E+01
FFT time	= 6.08556E-02	5.01122E-03
FE_matrix time	= 1.31587E+00	1.08357E-01
FE_vector time	= 2.71233E+02	2.23350E+01
Static_con time	= 3.35868E+00	2.76574E-01
CEL_comp time	= 1.21408E+03	9.99746E+01
	CPU secs	% of total
Loop time	= 1.21439E+03	9.48839E+01
Setup time	= 6.54791E+01	5.11609E+00
Total time	= 1.27987E+03	1.00000E+02

# Is static condensation in pitch-angle worth the effort?

- Preconditioning for nonlinear solves uses matrices that are diagonal in speed variable,  $s$ .
- Full coupling in pitch angle, however, seems wasteful with 3 FE cells and very high-order polynomials,  $pdxi = 5, \dots, 15$ .
- Majority of nodes are interior and could be eliminated prior to preconditioning.
- Reduce matrix memory by improving storage scheme?
- All of this would likely require developing routines for matrix manipulation.