Gyrokinetic δf particles in NIMROD

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Coupling Particles to FE fields

- assume that the density of hot particles is negligible compared to the bulk MHD density
- **but** allow $\beta_{hot} \sim \beta_{bulk}$.
- particles coupled to the fields through $\mathbf{\Pi}_{hot}$

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{V}\cdot\nabla\right)\mathbf{V} = \mathbf{J}\times\mathbf{B} - \nabla\cdot\mathbf{\Pi} - \nabla\cdot\mathbf{\Pi}_{hot}$$

where

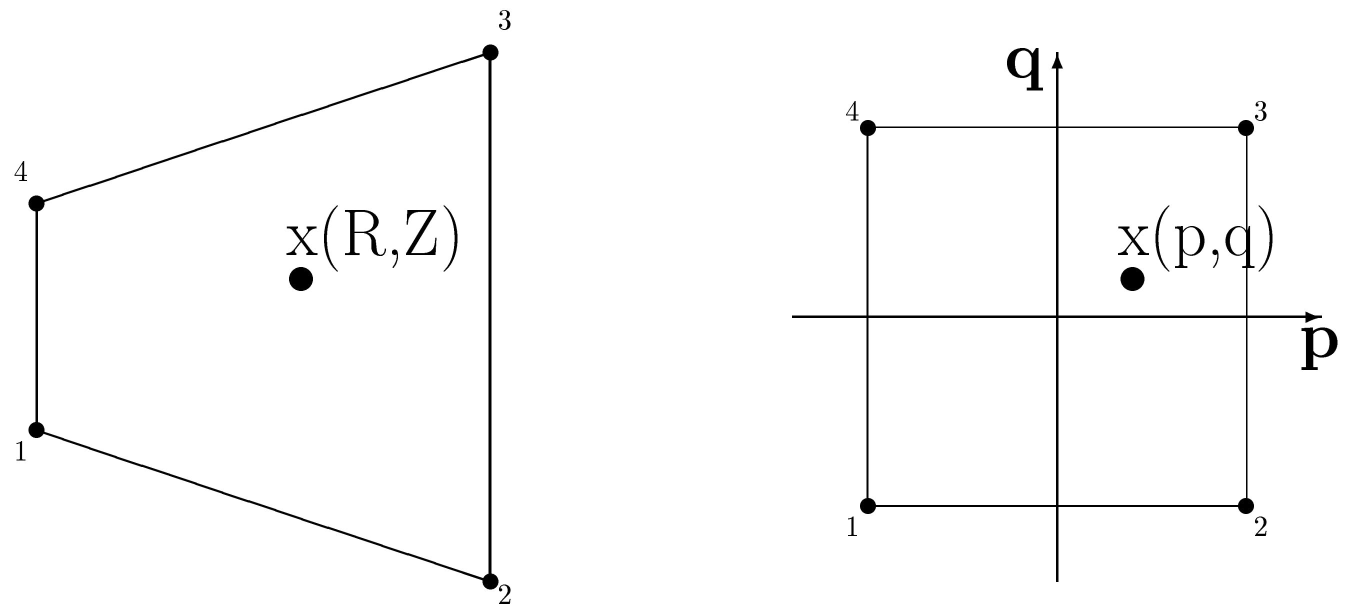
$$\mathbf{\Pi}_{hot} = \int m\mathbf{v}'\mathbf{v}'\delta f\ d\mathbf{v}$$
$$\mathbf{v}' = \mathbf{v} - \mathbf{V}$$

- also can couple through $\mathbf{J}$

Define shape functions in logical space (p, q) [1]

$$N_1(p,q) = \frac{1}{4}(1-p)(1-q) \quad N_2(p,q) = \frac{1}{4}(1+p)(1-q)$$

$$N_3(p,q) = \frac{1}{4}(1+p)(1+q) \quad N_4(p,q) = \frac{1}{4}(1-p)(1+q)$$



[1] Alejandro Allievi and Rodolfo Bermejo, JCP, 132, (1997)

where $-1 \leq p, q \leq 1$

Use Newton method to solve for (p, q) given (R, Z)

$$\begin{Bmatrix} p^{k+1} \\ q^{k+1} \end{Bmatrix} = \begin{Bmatrix} p^{k} \\ q^{k} \end{Bmatrix} + \frac{1}{\Delta^k} \begin{bmatrix} b_2 + b_3 p^k & -a_2 - a_3 p^k \\ -b_1 - b_3 q^k & a_1 + a + 3q^k \end{bmatrix} \begin{Bmatrix} R_p - R_p^k \\ Z_p - Z_p^k \end{Bmatrix}$$

where

$$R_p^k = \sum_{i=1}^{4} R_i N_i(p^k, q^k), \quad Z_p^k = \sum_{i=1}^{4} Z_i N_i(p^k, q^k),$$

$$a_1 = \frac{1}{4}(R_2 - R_1 + R_3 - R_4), \quad b_1 = \frac{1}{4}(Z_2 - Z_1 + Z_3 - Z_4),$$
$$a_2 = \frac{1}{4}(R_3 - R_1 + R_4 - R_2), \quad b_2 = \frac{1}{4}(Z_3 - Z_1 + Z_4 - Z_2),$$
$$a_3 = \frac{1}{4}(R_1 - R_2 + R_3 - R_4), \quad b_3 = \frac{1}{4}(Z_1 - Z_2 + Z_3 - Z_4),$$

$$\Delta^k = (a_1 b_2 - a_2 b_1) + (a_1 b_3 - a_3 b_1) p^k + (a_3 b_2 - a_2 b_3) q^k$$

- matrix on **rhs** is inverse of the Jacobian relating the logical coordinates to the real coordinates

$$\frac{1}{\Delta^k}\begin{bmatrix} b_2 + b_3 p^k & -a_2 - a_3 p^k \\ -b_1 - b_3 q^k & a_1 + a + 3q^k \end{bmatrix} = \begin{pmatrix} \frac{\partial R}{\partial p} & \frac{\partial R}{\partial q} \\ \frac{\partial Z}{\partial p} & \frac{\partial Z}{\partial q} \end{pmatrix}^{-1}$$

- this is used in computation of derivatives on the finite elements.
- iterate until $\sqrt{(R_p - R_p^k)^2 + (Z_p - Z_p^k)^2} < \epsilon$
- if $-1 \leq p, q \leq 1$ is <u>not</u> true, then the particle is not in this element, and another element needs to be searched
- new element to be searched is determined by the value of (p, q), left if $p < -1$, right if $p > 1$, down if $q < -1$, up if $q > 1$, and combinations thereof.

Equations of motion

$$
\begin{aligned}
m\frac{d\mathbf{u}}{dt} &= -\hat{b}\cdot(\mu\nabla B + e\nabla\psi) \\
\frac{d\mathbf{x}}{dt} &= \mathbf{u} + \frac{m}{eB^4}\left(u^2 + \frac{v_\perp^2}{2}\right)\left(\mathbf{B}\times\nabla\frac{B^2}{2}\right) + \frac{\mathbf{E}\times\mathbf{B}}{B^2} \\
\frac{dw}{dt} &= -\dot{z}_1\cdot\nabla f_0 \\
&= -\tilde{v}_D\left(\frac{\nabla n}{n} + \frac{\nabla T}{T}\left(\frac{3}{2} - \frac{v^2}{v_{th}^2}\right)\right) + \frac{2q\tilde{E}v}{mv_{th}^2}
\end{aligned}
$$

- need gradient quantities
- take the derivative of the shape functions

$$
\frac{\partial B}{\partial R} = \sum_{i=1}^{4} B_i \frac{\partial N_i(p,q)}{\partial R} = \sum_{i=1}^{4} B_i \left(\frac{\partial N_i}{\partial p}\frac{\partial p}{\partial R} + \frac{\partial N_i}{\partial q}\frac{\partial q}{\partial R}\right)
$$

- similarly for Z.

- from the inverse function theorem

$$\begin{bmatrix} \frac{\partial p}{\partial R} & \frac{\partial p}{\partial Z} \\ \frac{\partial q}{\partial R} & \frac{\partial q}{\partial Z} \end{bmatrix} = \begin{bmatrix} \frac{\partial R}{\partial p} & \frac{\partial R}{\partial q} \\ \frac{\partial Z}{\partial p} & \frac{\partial Z}{\partial q} \end{bmatrix}^{-1}$$

- right hand matrix is easy to compute if one recalls that

$$R = \sum_{i=1}^{4} R_i N_i(p,q)$$

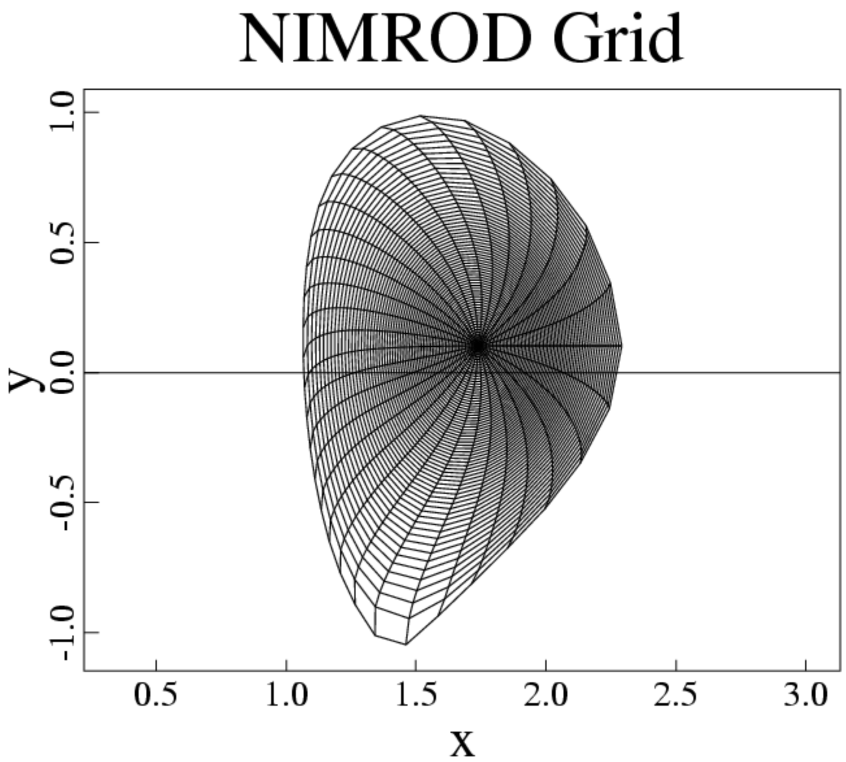
$$\frac{\partial R}{\partial p} = \sum_{i=1}^{4} R_i \frac{\partial N_i}{\partial p} \quad \frac{\partial R}{\partial q} = \sum_{i=1}^{4} R_i \frac{\partial N_i}{\partial q}$$

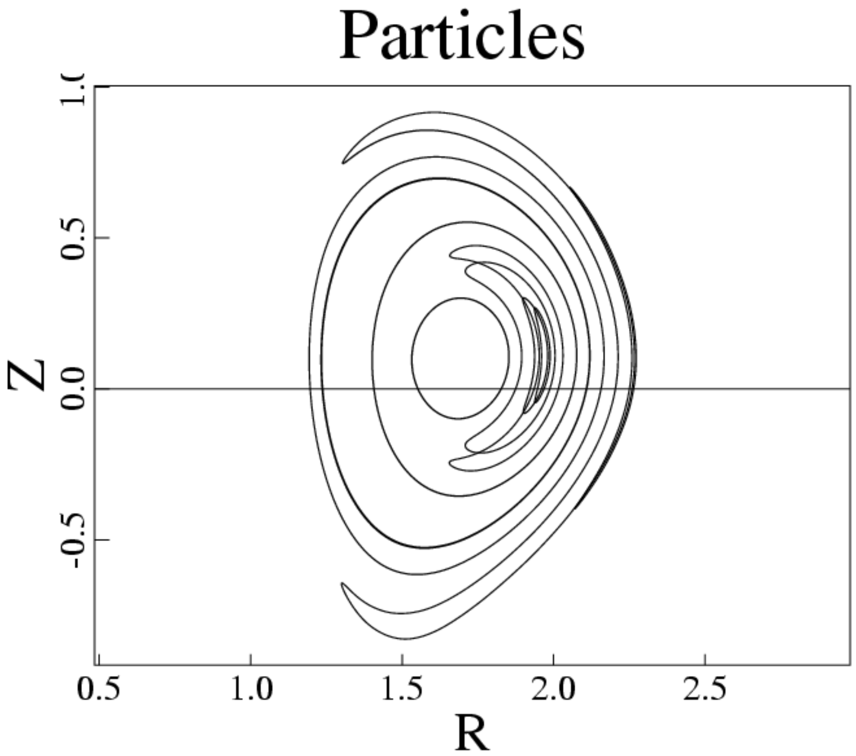
$$\frac{\partial Z}{\partial p} = \sum_{i=1}^{4} Z_i \frac{\partial N_i}{\partial p} \quad \frac{\partial Z}{\partial q} = \sum_{i=1}^{4} Z_i \frac{\partial N_i}{\partial q}$$

- already computed for Newton Method

Test Case

Particles trace field lines and execute bounce motion for the simplified test case.



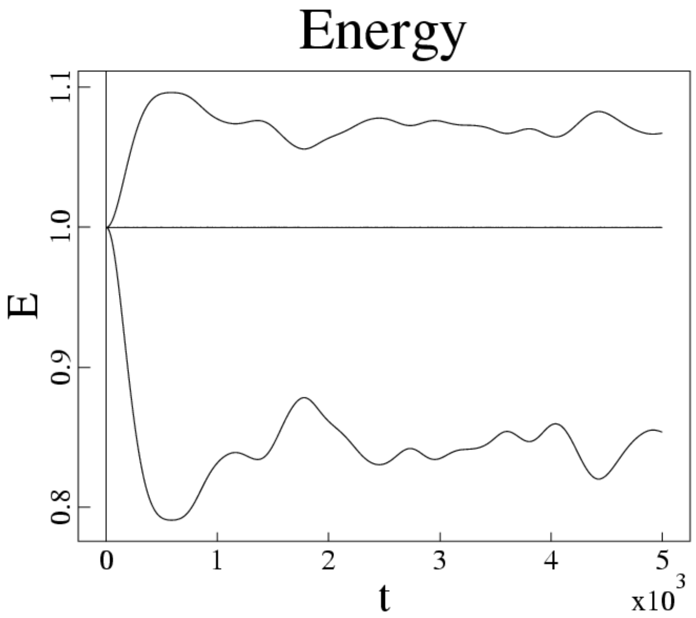


To test the method, a reduced equation of motion is used,

$$
\begin{aligned}
m\dot{\mathbf{u}} &= -\frac{\mu}{B}\left(B_R\frac{\partial B}{\partial R} + B_Z\frac{\partial B}{\partial Z}\right) \\
\dot{R} &= \mathbf{u}\cdot\hat{R} + v_D(-B_\phi)\frac{\partial B}{\partial Z} \\
\dot{Z} &= \mathbf{u}\cdot\hat{Z} + v_D(-B_\phi)\frac{\partial B}{\partial R} \\
\dot{\phi} &= \mathbf{u}\cdot\hat{\phi} + v_D\left(B_R\frac{\partial B}{\partial Z} - B_Z\frac{\partial B}{\partial R}\right),
\end{aligned}
$$

where $v_D = \frac{m}{eB^3}\left(u^2 + \frac{v_\perp^2}{2}\right)$, assume axisymmetry, cylindrical geometry, and no $\mathbf{E}$-field.

For the simple test case, energy conservation is excellent, to a few parts in 10^4 or better depending on ϵ, the stopping criterion. The performance is 10's of μs per particle, per timestep. This also varies with ϵ.



Parallelization

- two levels of parallelization - fourier layers and rblocks
- for fourier layer, use domain cloning
  - divide particles evenly among fourier layers
  - each layer evolves own set of particles
  - global sum required to gather particle information
  - particles are never passed between layers
- rblocks is domain decomposition
  - generate map from global grid to rblock-decomposed grid
  - sort particles on global grid
  - use map to pass particles to appropriate rblock
  - sorting allows optimization by reducing field evalution

Sorted PIC

- sort particles into respective cell
- gather/scatter done cell by cell instead of particle by particle
- reduce field evaluation to once per cell instead of once per particle
- allows for alternative particle deposition

Minimal Implementation

- assume some κ profile
- for a single linear mode use energy conservation to observe effects of kinetic particles

$$(\delta W_{MHD}^{n+1} - \delta W_{MHD}^{n}) + (\delta W_{KE}^{n+1} - \delta W_{KE}^{n}) = 0$$

- scale amplitude of δW_{MHD} to maintain energy conservation

$$\delta W_{MHD}^{n+1} = \alpha \delta W_{MHD}^{n}$$

- solve for α

$$\alpha \delta W_{MHD}^{n} - \delta W_{MHD}^{n} + \delta W_{KE}^{n+1} - \delta W_{KE}^{n} = 0$$

$$\alpha = 1 + \frac{\delta W_{KE}^{n} - \delta W_{KE}^{n+1}}{\delta W_{MHD}^{n}}$$