Recent Progress and Plans for High Order Finite Element Full Orbit (HOFEFO) PIC in NIMROD

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PSI Center Kinetic Group

- **Objective:** develop the capability to model full orbit energetic minority species in NIMROD
  - necessary for energetic particles in novel fields of ICC devices
  - may be necessary for very energetic particles
- Current Status (working in rectangular mesh)
  - Lorentz force equations of motion have been implemented
  - timestepping $\rightarrow$ orbit averaging implemented
  - high order field eval implemented
  - uniform shape high order deposition to grid is implemented
- Left to be done
  - implement polynomial shape function $S \propto \left[1 - \left(\frac{r}{R}\right)^2\right]^\alpha$
  - new grid grid structure and communicator will be necessary
  - generalize to general geometries

General Outline

- brief overview of hybrid kinetic-MHD
- sketch of PIC in Finite Element Grids
- details of implementation
- things left to do

The δf PIC method [a] [b]

- PIC is a Lagrangian simulation of phase space $f(\mathbf{x}(\mathbf{t}), \mathbf{v}(\mathbf{t}))$
- typically PIC is noisy, can't beat $1/\sqrt{N}$
- δf PIC reduces the discrete particle noise associated with conventional PIC
- derivation begins with Vlasov Equation

$$\frac{\partial f(\mathbf{z})}{\partial t} + \dot{\mathbf{z}} \cdot \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} = 0$$

  $\mathbf{z}$ is the phase coordinate

- split phase space distribution into steady state and evolving perturbation:

$$f = f_{eq}(\mathbf{z}) + \delta f(\mathbf{z}, t)$$

[a] S. E. Parker and W. W. Lee, 'A fully nonlinear characteristic method for gyro-kinetic simulation', *Physics of Fluids B*, **5**, 1993

[b] G. Hu and J. A. Krommes, "Generalized weighting scheme for δf particle simulation method", *Physics of Plasmas*, **1**, 1994

- δf evolves along the characteristics $\dot{\mathbf{z}}$(equation of motion)

$$\dot{\delta f} = -\tilde{\mathbf{z}} \cdot \frac{\partial f_{eq}}{\partial \mathbf{z}}$$

  using $\mathbf{z} = \mathbf{z}_{eq} + \tilde{\mathbf{z}}$ and $\dot{\mathbf{z}}_{eq} \cdot \frac{\partial f_{eq}}{\partial \mathbf{z}} = 0$

- choice of f_{eq} is critical to success of δf
- fields computed from moments of δf, this is a sum in PIC

The Hybrid Kinetic-MHD Equations[a]

- in the limit $n_h \ll n_0$, $\beta_h \sim \beta_0$, quasi neutrality, only modification of MHD equations is addition of the hot particle pressure tensor in the momentum equation:

$$\rho \left(\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} \right) = \mathbf{J} \times \mathbf{B} - \nabla p_b - \nabla \cdot \underline{\mathbf{p}}_h$$

  the subscripts b, h denote the bulk plasma and hot particles

- the steady state equation

$$\mathbf{J}_0 \times \mathbf{B}_0 = \nabla p_0 = \nabla p_{b0} + \nabla p_{h0}$$

- evolved momentum equation is ($\mathbf{U}_s = 0$)

$$\rho_s \frac{\partial \delta \mathbf{U}}{\partial t} = \mathbf{J}_s \times \delta \mathbf{B} + \delta \mathbf{J} \times \mathbf{B}_s - \nabla \cdot \delta \underline{\mathbf{p}}_b - \nabla \cdot \delta \underline{\mathbf{p}}_h$$

[a] C.Z.Cheng,'A Kinetic MHD Model for Low Frequency Phenomena', *J. Geophys. Rev* **96**, 1991

PIC in Finite Element Grids

- PIC models phase space distribution function $f(\mathbf{z})$ by sampling the phase space with particles (Lagrangian simulation)
- moments of distribution become sums over the particles
- moments used to calculate the field
- fields used to advance particles
- two grid interactions
  - gather of fields to particle
  - scatter of moments to grid
  - for Finite Element grid, this is a little involved

PIC in FEM

- gather/scatter require logical coordinates
- FE representation for (R, Z) need to be inverted

$$R = \sum_j R_j N_j(\eta, \xi), \quad Z = \sum_j Z_j N_j(\eta, \xi),$$

- Use Newton method to solve for (η, ξ) given (R, Z)

$$\left\{ \begin{array}{c} \eta^{k+1} \\ \xi^{k+1} \end{array} \right\} = \left\{ \begin{array}{c} \eta^{k} \\ \xi^{k} \end{array} \right\} + \frac{1}{\Delta_k} \left(\begin{array}{cc} \frac{\partial Z}{\partial \xi} & -\frac{\partial R}{\partial \xi} \\ -\frac{\partial Z}{\partial \eta} & \frac{\partial R}{\partial \eta} \end{array} \right)_k \left\{ \begin{array}{c} R - R^k \\ Z - Z^k \end{array} \right\}$$

  where Δ_k is the determinant and k denotes iteration

- sorting required for parallelization
  - may be able to use sorted list to reduce cache thrashing
- may need some development for general high order geometry

High Order Field Gather

- add routine for fast evaluation of finite element shapes functions
- polynomials are evaluated in standard form

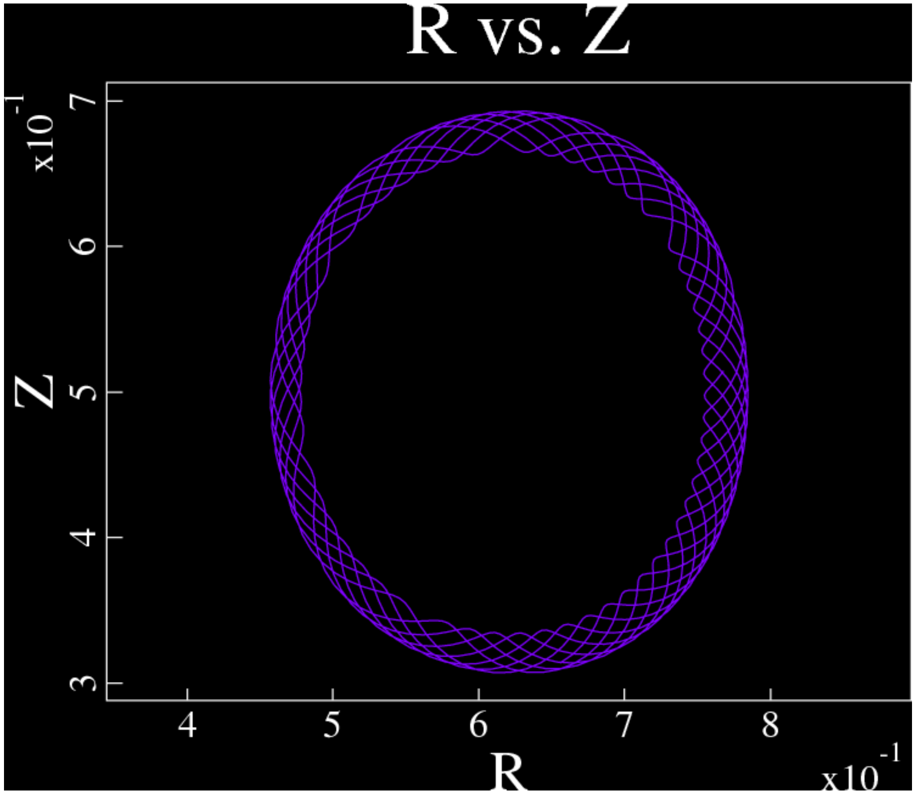
$$N^i(x) = \sum a_n^i x^n$$

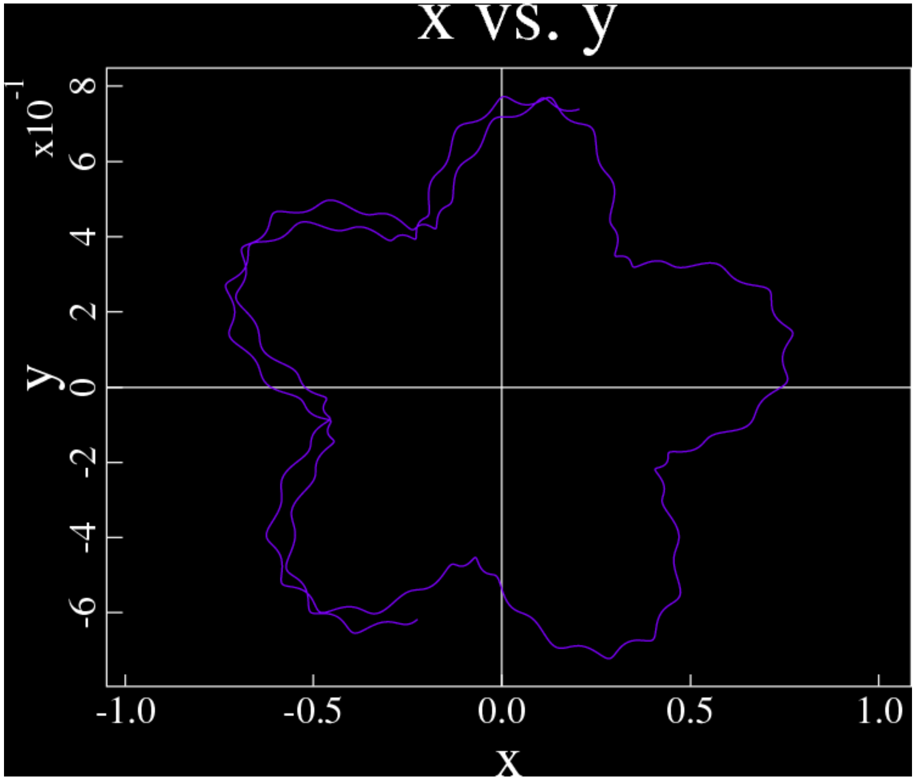
- table of coefficients up to $pd = 5$

```
      REAL(r8) :: ulcf4(1:4,1:5)
      DATA ulcf4/-25,  70, -80,  32,
     $            48,-208, 288,-128,
     $           -36, 228,-384, 192,
     $            16,-112, 224,-128,
     $            -3,  22, -48,  32/
      REAL(r8) :: uldn4=3
```

- about $\times 5$ faster - no IF evaluation
- still room for improvements in performance

Particle Trace in Bessel Function Spheromak in a tuna can





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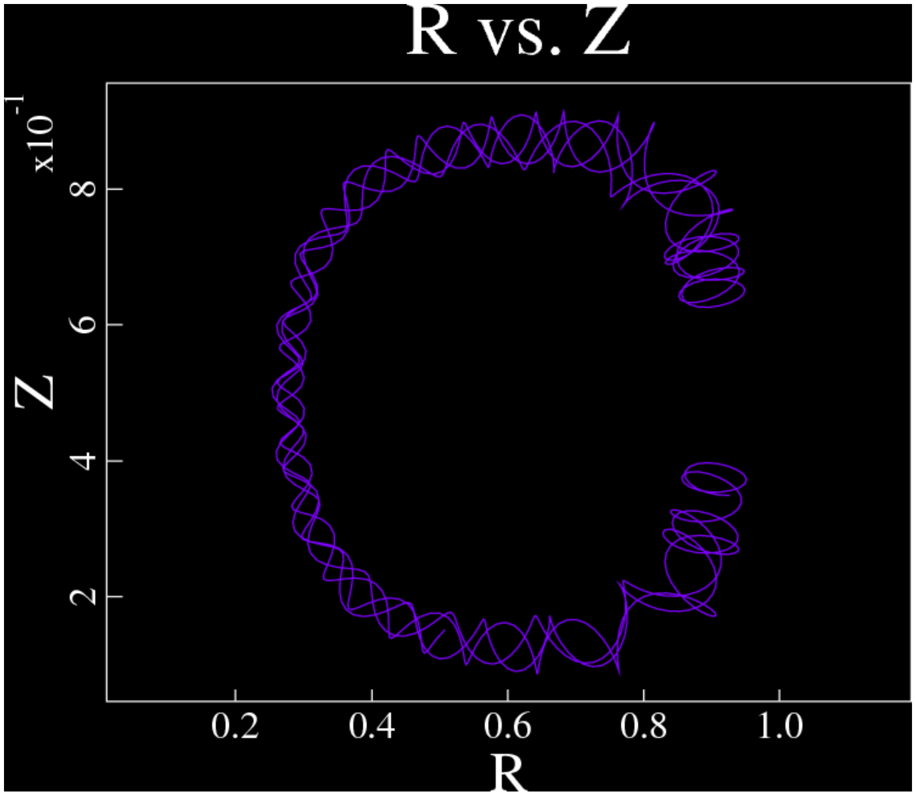
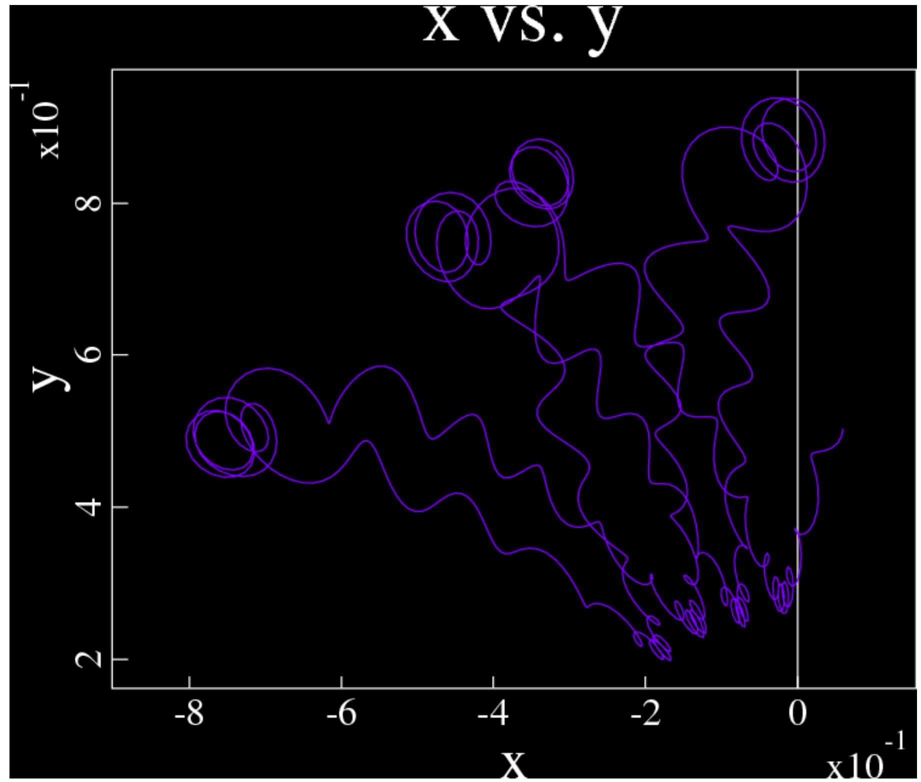


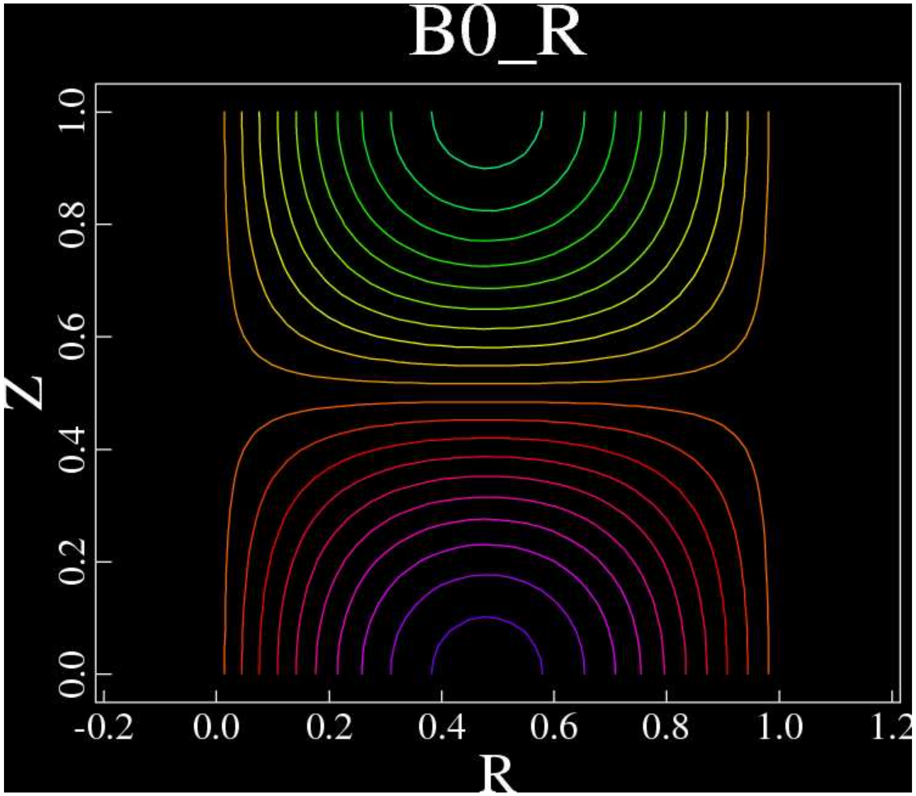


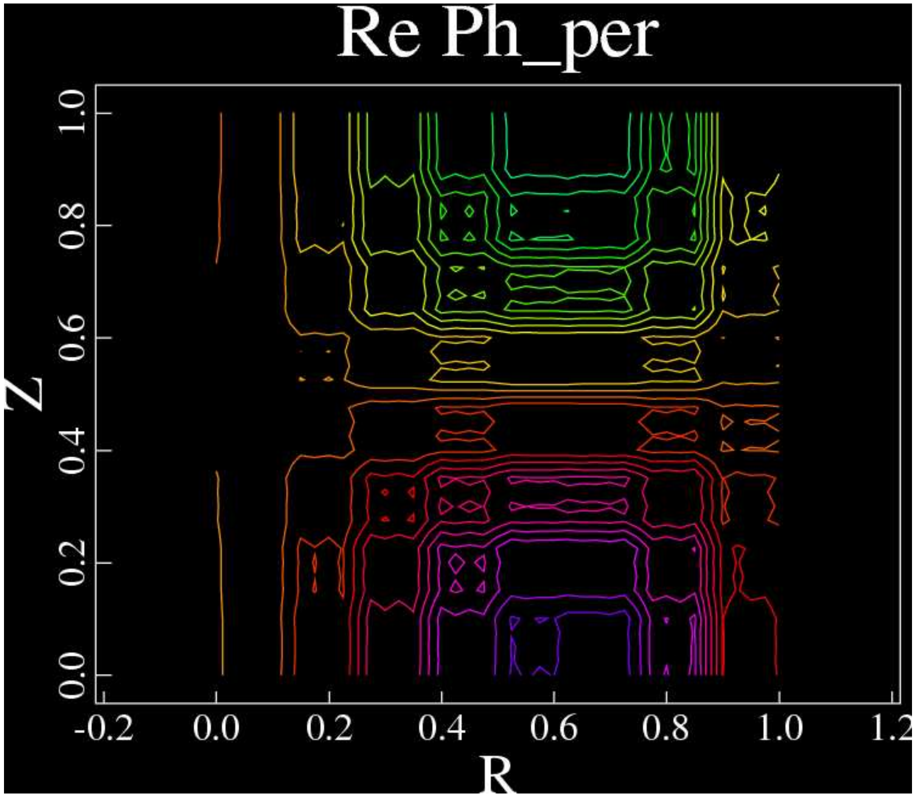
Preliminary Particle deposition is done

- deposit onto quadrature point
- probably will invert mass matrix and a quadrature eval
- conjecture that this will give some smoothing
- need to implement particle shape function

Particle representation of Br

- grid is 8x8x5, 10K particles





Shape function remains

- use shape function[a]

$$S \propto \left[1 - \left(\frac{r}{R}\right)^2\right]^\alpha$$

where r is distance from particle, R is distance of influence, and α is shaping parameter to fiddle with

- this will dictate which quadrature points get scattered PIC moment
- initial implementation will use global grid and allreduce
- for domain decomposition will need to implement ghost cells and new communications (this part will probably suck)
- will be best to use poloidal decomp independent of the fluid decomp

[a] G. B. Jacobs and J. S. Hesthaven, 'High-order nodal discontinuous Galerkin PIC method on unstructured grids', *JCP*, **214**, 2006

Whats required for general geometry?

- ?
- it may already be there
- remains to be seen
- turn on the full energetic pressure tensor