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

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- **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 $\delta f$ PIC method a b

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

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

$z$ is the phase coordinate

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

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

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b G. Hu and J. A. Krommes, ”Generalized weighting scheme for $\delta f$ particle simulation method”, *Physics of Plasmas*, 1, 1994
\( \delta f \) evolves along the characteristics \( \dot{z} \)(equation of motion)

\[ \dot{f} = -\tilde{z} \cdot \frac{\partial f_{eq}}{\partial z} \]

using \( z = z_{eq} + \tilde{z} \) and \( \dot{z}_{eq} \cdot \frac{\partial f_{eq}}{\partial z} = 0 \)

• choice of \( f_{eq} \) is critical to success of \( \delta f \)

• fields computed from moments of \( \delta f \), this is a sum in PIC
The Hybrid Kinetic-MHD Equations

- 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:

\[
\rho \left( \frac{\partial U}{\partial t} + U \cdot \nabla U \right) = J \times B - \nabla p_b - \nabla \cdot p_h
\]

the subscripts \( b, h \) denote the bulk plasma and hot particles

- the steady state equation

\[
J_0 \times B_0 = \nabla p_0 = \nabla p_{b0} + \nabla p_{h0}
\]

- evolved momentum equation is (\( U_s = 0 \))

\[
\rho_s \frac{\partial \delta U}{\partial t} = J_s \times \delta B + \delta J \times B_s - \nabla \cdot \delta p_b - \nabla \cdot \delta p_h
\]

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**PIC in Finite Element Grids**

- PIC models phase space distribution function $f(z)$ 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 \((\eta, \xi)\) given \((R, Z)\)

\[
\begin{bmatrix}
\eta^{k+1} \\
\xi^{k+1}
\end{bmatrix} = \begin{bmatrix}
\eta^{k} \\
\xi^{k}
\end{bmatrix} + \frac{1}{\Delta_k} \begin{pmatrix}
\frac{\partial Z}{\partial \xi} & -\frac{\partial R}{\partial \xi} \\
-\frac{\partial Z}{\partial \eta} & \frac{\partial R}{\partial \eta}
\end{pmatrix}_k \begin{bmatrix}
R - R^k \\
Z - Z^k
\end{bmatrix}
\]

where \(\Delta_k\) 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

\[ N^i(x) = \sum a^n x^n \]

- table of coefficients up to \( pd = 5 \)

```plaintext
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

R vs. Z

X vs. Y

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Particle Trace in Bessel Function Spheromak in a tuna can
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

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

where \( r \) is distance from particle, \( R \) is distance of influence, and \( \alpha \) 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

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What's required for general geometry?

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