Extension of Drift Kinetic Hot Particles to Full Orbits in NIMROD

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Objective: develop the capability to model full kinetic minority species in NIMROD

The Plan
- implement full kinetic orbits for particles
- test different coupling schemes ($J$ vs. $P$)
- improve timestepping $\rightarrow$ orbit averaging
- implement collisions with background\(^a\)
- implement multiple ‘species’ e.g. some full kinetic particles some drift
- explore issues concerning open boundary conditions\(^b\)
- explore running fluid electrons and kinetic ions

\(^{a}\) Y. Chen and R. B. White, ‘Collisional $\delta f$ method’, Physics of Plasmas 4 3591 (1997)

\(^{b}\) ibid
Outline

- Motivation
- the full kinetic equations of motion
- hybrid kinetic MHD model
- $\delta f$ PIC
- brief description of NIMROD and Extended MHD equations
- finite elements and PIC in the finite element method
- benchmark of hybrid kinetic MHD model
- summary and future plans
Full Orbit Particles are Necessary for ICC devices

- capture kinetic effects lost in MHD approximation
- lost kinetic effects can **significantly** affect MHD instabilities
  - fraction of plasma executes non-trivial orbits
- experiments show that FRCs are stable to MHD tilt modes, attributed to FLR effects
- recent simulations have shown this is a possible mechanism\textsuperscript{a}
- kinetic effects are believed ubiquitous in ICC devices

Full Orbit Equations Well Studied

• equations of motion are Lorentz force equations

\[ \dot{v} = \frac{q}{m} (E + v \times B) \]

• Buneman (1967)
  – subtracts off \( v_{E \times B} \)
  – separates \( \parallel, \perp \) motion
  – rotation of \( v_{\perp} \)

• Boris (1970) - this is what we have initially implemented
  – limited in timestep by \( \omega_c \Delta t < 0.35 \)
Description of the Boris Algorithm

- Boris push utilizes leap frog time centering
- half step push of electric field $\mathbf{v}^- = \mathbf{v}_{t-\Delta t/2} + \frac{q\mathbf{E}}{m} \frac{\Delta t}{2}$
- increment $\mathbf{v}^-$ to $\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \tilde{\omega}_c \frac{\Delta t}{2}$ where $\tilde{\omega}_c = \frac{qB}{m}$

- rotate $\mathbf{v}^-$ to $\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times s\tilde{\omega}_c$ where $s = \frac{\Delta t}{1 + \omega_c^2 \frac{\Delta t^2}{4}}$ s.t. $|\mathbf{v}^+| = |\mathbf{v}^-|$
- remainder of half step push of electric field $\mathbf{v}_{t+\Delta t/2} = \mathbf{v}^+ + \frac{q\mathbf{E}}{m} \frac{\Delta t}{2}$
Full Ion Orbits in Tokamak

full orbits has marginal consequences for overall trajectory in tokamaks

nontrivial orbits in ICCs
The $\delta f$ PIC method

- PIC is a Lagrangian simulation of phase space $f(x, v)$
- PIC evolves $f(x(t), v(t))$
- spatial grid is not inherently necessary, but very convenient!
- in principle, $f(x(t), v(t))$ contains everything
- typically PIC is noisy, can’t beat $1/\sqrt{N}$
- $\delta f$ PIC reduces the discrete particle noise associated with conventional PIC
- 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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• $\delta f$ evolves along the characteristics $\dot{z}$ (control variates MC$^b$)

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

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

• the particle characteristics are taken form the equations of motion

• as particle algorithm advances, may be useful to compare $\delta f$ PIC implementation with full PIC

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The Hybrid Kinetic-MHD Equations\textsuperscript{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:

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

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

- the steady state equation

$$\mathbf{J} \times \mathbf{B} = \nabla \cdot \mathbf{p} = \nabla \cdot \mathbf{p}_b + \nabla \cdot \mathbf{p}_h$$

- evolved momentum equation is

$$\delta \rho \mathbf{U}_s \cdot \nabla \mathbf{U}_s + \rho_s \left( \frac{\partial \delta \mathbf{U}}{\partial t} + \mathbf{U}_s \cdot \nabla \delta \mathbf{U} + \delta \mathbf{U} \cdot \nabla \mathbf{U}_s \right) =$$

$$\mathbf{J}_s \times \delta \mathbf{B} + \delta \mathbf{J} \times \mathbf{B}_s - \nabla \cdot \delta \mathbf{p}_b - \nabla \cdot \delta \mathbf{p}_h$$

NIMROD\textsuperscript{a} (NonIdeal MHD with Rotation - Open Discussion)

- massively parallel 3-D MHD simulation
- finite elements in poloidal plane and Fourier modes in toroidal direction → axisymmetric geometry
- utilizes Lagrange type finite element
- can handle extreme anisotropies, \( \frac{\chi_\parallel}{\chi_\bot} \gg 1 \)
- flexibility to model general geometry → real experiments
- model experiment relevant parameters, \( S > 10^7 \)
- semi-implicit advance, not restricted by magnetosonic CFL condition
- assumes a steady state background and evolves perturbed quantities
  \( \rightarrow A(x, t) = A_s(x) + \delta A(x, t) \)
NIMROD equations

- NIMROD evolves the extended MHD equations

\[
\begin{align*}
\frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \mathbf{E} \\
\nabla \times \mathbf{B} &= \mu_0 \mathbf{J} \\
\mathbf{E} &= -\mathbf{U} \times \mathbf{B} + \eta \mathbf{J} + \frac{1}{ne} \mathbf{J} \times \mathbf{B} \\
&\quad + \frac{m_e}{ne^2} \left[ \frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot (\mathbf{JU} + \mathbf{UJ}) \right] \\
&\quad + \sum_{\alpha} \frac{q_\alpha}{m_\alpha} \left( \nabla p_\alpha + \nabla \cdot \Pi_\alpha \right) \\
\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{U}) &= \nabla \cdot D \nabla n \\
mn \left( \frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} \right) &= \mathbf{J} \times \mathbf{B} - \nabla p - \nabla \cdot \Pi - \nabla \cdot \mathbf{p_h} \\
\frac{n_\alpha}{\gamma - 1} \left( \frac{\partial T_\alpha}{\partial t} + \mathbf{U}_\alpha \cdot \nabla T_\alpha \right) &= -\nabla \cdot q_\alpha + Q_\alpha \\
&\quad - p_\alpha \nabla \cdot \mathbf{U}_\alpha - \Pi_\alpha : \nabla \mathbf{U}_\alpha
\end{align*}
\]
Finite Element representation of NIMROD

- the perturbed NIMROD fields are in FE-Fourier representation

\[
\delta A(x, t) = \sum_j A_{j,0}(t)\alpha_{j,0} + \sum_j \sum_n (A_{j,n}(t)\alpha_{j,n} + c.c.)
\]

where

\[
\alpha_{j,n} = N_j(\eta, \xi) \exp(in\phi)
\]

(\eta, \xi) are logical coordinates

- PIC becomes nontrivial in FE
**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
- load balancing tricky
Deposition of $\delta p_h$ onto Finite Element grid

- assume CGL-like form $\delta p_h = \begin{pmatrix} p_\perp & 0 & 0 \\ 0 & p_\perp & 0 \\ 0 & 0 & p_{\parallel} \end{pmatrix}$

- evaluate pressure moment at a position $\mathbf{x}$ is

$$\delta p(x) = \int m(v - V_h)^2 \delta f(x, v)d^3v$$

$$= \sum_{i=1}^{N} m(v_i - V_h)^2 g_0 w_i \delta^3(x - x_i)$$

where sum is over the particles, $m$ mass of the particle, $g_0 w_i$ is the perturbed phase density, and $V_h$ is the hot flow velocity

- discretize to the poloidal plane by performing a Fourier transform, \(a\)

$$\delta p_n(R, Z) = \sum_{i=1}^{N} m(v_i - V_h)^2 g_0 w_i \delta(R - R_i) \delta(Z - Z_i) e^{-in\phi_i}$$

\(a\)for large $n$ runs, a conventional $\phi$ deposition with a FFT is performed
• express \( \delta p_n(R, Z) \) in the finite element basis,

\[
\delta p_n(R, Z) = \sum_k \delta p_n^k N^k(\eta, \xi)
\]

where sum \( k \) is over the basis functions and \( (\eta, \xi) \) are functions of \( (R, Z) \)

• project onto the finite element space by casting in weak form:

\[
\int N^l \sum_k \delta p_n^k N^k d^3 x = \int N^l \sum_{i=1}^N m(v_i - V_h)^2 g_0 w_i \delta(R - R_i) \delta(Z - Z_i) e^{-in\phi_i} d^3 x
\]

\[
\mathbf{M}\delta p_n^k = \sum_{l \in k} \sum_{i=1}^N m(v_i - V_h)^2 g_0 w_i e^{-in\phi_i} N^l(\eta_i, \xi_i)
\]

\( \mathbf{M} \) is the finite element mass matrix

• gather is done using the same shape functions

\[
A(x_i) = \sum_l A^l N^l(\eta_i, \xi_i)
\]

for some field quantity \( A \)
Drift Kinetic Benchmark with M3D

- transition from internal kink mode to fishbone\(^a\)
- monotonic \(q\), \(q_0 = .6\), \(q_a = 2.5\), \(\beta_0 = .08\), circular tokamak \(R/a=2.76\)
- \(dt=1e-7\), \(\tau_A = 1.e6\)

Summary and Future Plans

- Lorentz equation of motion has been implemented as Boris push
- can push particles multiple times per MHD time step
- orbits calculated for FRC equilibrium
- implement orbit averaged pressure deposition and couple to MHD
- explore alternative coupling schemes
- investigate implementation of collisions and sources/sinks for open b.c.