Hybrid Kinetic-MHD simulations with NIMROD

Charlson C. Kim
and
the NIMROD Team

Plasma Science and Innovation Center
University of Washington

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parallel, 3-D, initial value extended MHD code
2D high order finite elements + Fourier in symmetric direction
linear and nonlinear simulations
semi-implicit and implicit time advance operators
simulation parameters approaching fusion relevant conditions
sparse, ill conditioned matrices
large and growing V&V
active developer and user base with continually expanding capabilities

model fusion relevant experiments - DOE/OFES
NIMROD’s Extended MHD Equations

\[
\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \kappa \text{div} \nabla (\nabla \cdot \mathbf{B})
\]

\[
\mathbf{J} = \frac{1}{\mu_0} \nabla \times \mathbf{B}
\]

\[
\mathbf{E} = -\mathbf{V} \times \mathbf{B} + \eta \mathbf{J}
\]

\[
+ \frac{m_e}{n_e e^2} \left[ \frac{e}{m_e} (\mathbf{J} \times \mathbf{B} - \nabla p_e) + \frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot (\mathbf{J} \mathbf{V} + \mathbf{V} \mathbf{J}) \right]
\]

\[
\frac{\partial n_\alpha}{\partial t} + \nabla \cdot (n\mathbf{V})_\alpha = \nabla \cdot D \nabla n_\alpha
\]

\[
\rho \left( \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) = \mathbf{J} \times \mathbf{B} - \nabla p
\]

\[
+ \nabla \cdot \rho \nu \nabla \mathbf{V} - \nabla \cdot \Pi - \nabla \cdot p_h
\]

\[
\frac{n_\alpha}{\Gamma - 1} \left( \frac{\partial T_\alpha}{\partial t} + \mathbf{V}_\alpha \cdot \nabla T_\alpha \right) = -p_\alpha \nabla \cdot \mathbf{V}_\alpha
\]

\[
- \nabla \cdot q_\alpha + Q_\alpha - \Pi_\alpha : \nabla \mathbf{V}_\alpha
\]

- resistive MHD
- Hall and 2-fluid
- Braginski and beyond closures
- energetic particles
Hybrid Kinetic-MHD Equations
C.Z. Cheng, JGR, 1991

- \( n_h \ll n_0, \beta_h \sim \beta_0 \), quasi-neutrality \( \Rightarrow n_e = n_i + n_h \)
- momentum equation modified by hot particle pressure tensor:

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

- \( b, h \) denote bulk plasma and hot particles
- \( \rho, U \) for entire plasma, both bulk and hot particle
- steady state equation \( J_0 \times B_0 = \nabla p_0 = \nabla p_{b0} + \nabla p_{h0} \)
- \( p_{b0} \) is scaled to accommodate hot particles
- assumes equilibrium hot particle pressure is isotropic
- alternative \( J_h \) current coupling possible
particles pushed in *real space* \((R, Z)\) *but* field quantities
evaluated in *logical space* \((\eta, \xi)\)
requires particle coordinate \((R_i, Z_i)\) to be *inverted* to logical
coordinates \((\eta_i, \xi_i)\)

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

\((R_i, Z_i)^{-1} \Rightarrow (\eta_i, \xi_i)\) performed with sorting/parallel
communications

*algorithmic bottleneck*
Schematic of Hybrid $\delta f$ PIC-MHD model

- **advance** particles and $\delta f^1$

  \[
  z_i^{n+1} = z_i^n + \dot{z}(z_i)\Delta t \\
  \delta f_i^{n+1} = \delta f_i^n + \dot{\delta f}(z_i)\Delta t
  \]

- **deposit** $\delta p(\eta) = \sum_{i=1}^{N} \delta f_i m(v_i - V_h)^2 S(\eta - \eta_i)$ on FE logical space

- **advance** NIMROD hybrid kinetic-MHD with modified momentum equation

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

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Computational Methods

- **F90/MPI** based code
- 2D FE plane spatial domain decomposed
- axisymmetric direction spectral decomposition
- particles share domain decomposition (*my expertise*)
- full spectrum of computers
  - laptops to DOE computing centers
- SLU for linear systems and preconditioning
- GMRES for 3D nonlinear solves (*outside my expertise*)
  - better scalable solvers actively researched
- fluid - reasonable weak scaling to 10K procs
- PIC - reasonable scaling to \( \sim 1K \) procs
- typically 100’s used

\(^2\)3D operations performed in real space, auxiliary load balancing performed
I/O and Visualization

- Fortran binary checkpoint file, written by root
- particles write separate checkpoint file (each proc)
- extensive use of VisIt

- auxiliary VTK, silo, HDF5, H5part files
- python, matlab, tecplot, xdraw
Goals

- room for improvement in particle parallelization
  - utilize sorted list
  - switch from array of types to types of arrays
  - implement domain decomposition in 3rd dimension
- better checkpointing for particles (H5Part?)
- scale particles to $10K+$
- minimal use of profile/performance analysis tools
- totalview is a pain to use
Summary of PIC Capabilities

- tracers, linear, (nonlinear)
- two equations of motion
  - drift kinetic ($v_\parallel, \mu$), Lorentz force ($\vec{v}$)
- multiple spatial profiles - loading in $x$
  - proportional to MHD profile, uniform, peaked gaussian
- multiple distribution functions - loading in $v$
  - slowing down distribution, Maxwellian, monoenergetic
- room for growth
  - developing multispecies option, e.g. drift+Lorentz
  - full $f(z)$ PIC
  - numeric representation of $f_{eq}(\vec{x}, \vec{v})$
    - e.g. load experimental phase space profiles
    - for evolution of $\delta f$
- kinetic closure
Overview of PIC method

- PIC is a Lagrangian simulation of phase space \( f(x, v, t) \)
- PIC is a discrete sampling of \( f \)

\[
f(x, v, t) \approx \sum_{i=1}^{N} g_i(t) S(x - x_i(t)) \delta(v - v_i(t))
\]

- \( N \) is number of particles, \( i \) denotes particle index, \( g_i \) is phase space volume, \( S \) is shape function
- all dynamics are in particle motion
- PIC algorithm
  - advance \([x_i(t), v_i(t)]\) along equations of motion
  - deposit moment of \( g_i \) on grid using \( S(x - x_i) \)
  - solve for fields from deposition
- PIC is noisy, limited by \( 1/\sqrt{N} \)
The $\delta f$ PIC method reduces noise


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

- split phase space distribution into steady state and evolving perturbation $f = f_{eq}(z) + \delta f(z, t)$ - control variates
- substitute $f$ in Vlasov Equation to get $\delta f$ evolution equation along characteristics $\dot{z}$
  $$\dot{\delta f} = -\delta \dot{z} \cdot \frac{\partial f_{eq}}{\partial z}$$
  using $\dot{z} = \dot{z}_{eq} + \delta \dot{z}$ and $\dot{z}_{eq} \cdot \frac{\partial f_{eq}}{\partial z} = 0$
- apply PIC to $\delta f(z, t) \Rightarrow \delta f_i(t)$, sample $f_{eq}$ - importance sampling
Drift Kinetic Equation of Motion

- follows gyrocenter in limit of zero Larmour radius
- reduces $6D$ to $4D + 1$
- drift kinetic equations of motion

\[
\dot{x} = v_\parallel \hat{b} + v_D + v_{E \times B}
\]

\[
v_D = \frac{m}{eB^4} \left( v_\parallel^2 + \frac{v_\perp^2}{2} \right) \left( B \times \nabla \frac{B^2}{2} \right) + \frac{\mu_0 m v_\parallel^2}{eB^2} J_\perp
\]

\[
v_{E \times B} = \frac{E \times B}{B^2}
\]

\[
mv_\parallel = -\hat{b} \cdot (\mu \nabla B - eE)
\]
$\delta f$ and the Lorentz Equations

- Lorentz equations of motion

\[
\begin{align*}
\dot{x} &= v \\
\dot{v} &= \frac{q}{m} (E + v \times B)
\end{align*}
\]

- for Lorentz equations use\(^3\)

\[
f_{eq} = f_0(x, v^2) + \frac{1}{\omega_c} (v \cdot b \times \nabla f_0)
\]

- weight equation is

\[
\dot{\delta f} = - \frac{\delta E + v \times \delta B}{B} \cdot b \times \nabla f_0 - \frac{2q}{m} \delta E \cdot v \frac{\partial f_0}{\partial v^2}
\]

\(^3\)M. N. Rosenbluth and N. Rostoker “Theoretical Structure of Plasma Equations”, Physics of Fluids 2 23 (1959)