Hybrid Kinetic-MHD simulations with NIMROD

Charlson C. Kim
and
the NIMROD Team

Plasma Science and Innovation Center
University of Washington

CSCADS Workshop
July 18, 2011

NIMROD

C.R. Sovinec, *JCP*, **195**, 2004

- 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
  - U. Wisc, U. Wash, Utah S., Tech-X, GA, CU-Boulder
- **model fusion relevant experiments** - **DOE/OFES**

NIMROD's Extended MHD Equations

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \kappa_{divb}\nabla(\nabla \cdot \mathbf{B})$$

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

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

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

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

$$\frac{n_\alpha}{\Gamma - 1}\left(\frac{\partial T_\alpha}{\partial t} + \mathbf{V}_\alpha \cdot \nabla T_\alpha\right) = -p_\alpha \nabla \cdot \mathbf{V}_\alpha - \nabla \cdot q_\alpha + Q_\alpha - \Pi_\alpha : \nabla \mathbf{V}_\alpha$$

- 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:

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

  - b, h denote bulk plasma and hot particles
  - $\rho, \mathbf{U}$ for **entire plasma**, both bulk and hot particle
- steady state equation $\mathbf{J}_0 \times \mathbf{B}_0 = \nabla p_0 = \nabla p_{b0} + \nabla p_{h0}$
  - p_{b0} is scaled to accomodate hot particles
  - assumes equilibrium hot particle pressure is isotropic
- alternative $\mathbf{J}_h$ current coupling possible

PIC in FEM - Nontrivial

- particles pushed in real space (R, Z) **but** field quantities evaluated in logical space (η, ξ)
- requires particle coordinate (R_i, Z_i) to be inverted to logical coordinates (η_i, ξ_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 δf PIC-MHD model

- advance particles and δf[1]

$$\mathbf{z}_i^{n+1} = \mathbf{z}_i^n + \dot{\mathbf{z}}(\mathbf{z}_i)\Delta t$$
$$\delta f_i^{n+1} = \delta f_i^n + \dot{\delta f}(\mathbf{z}_i)\Delta t$$

- 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

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

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

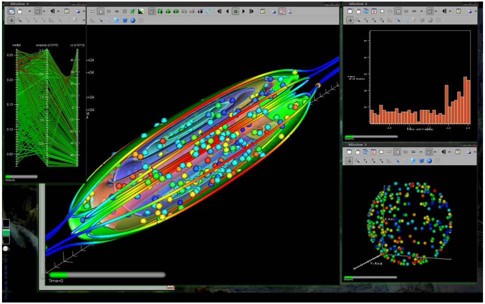
Computational Methods

- **F90/MPI** based code
- 2D FE plane spatial domain decomposed
- axisymmetric direction spectral decomposition[2]
- 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 seperate 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 $(v_{\|}, \mu)$, Lorentz force $(\vec{\mathbf{v}})$
- 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 $f(\mathbf{z})$ PIC
  - numeric representation of $f_{eq}(\vec{\mathbf{x}}, \vec{\mathbf{v}})$
    - e.g. load experimental phase space profiles
    - for evolution of δf
  - kinetic closure

Overview of PIC method

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

$$f(\mathbf{x}, \mathbf{v}, t) \simeq \sum_{i=1}^{N} g_i(t) S(\mathbf{x} - \mathbf{x}_i(t)) \delta(\mathbf{v} - \mathbf{v}_i(t))$$

  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 $[\mathbf{x}_i(t), \mathbf{v}_i(t)]$ along equations of motion
  - deposit moment of g_i on grid using $S(\mathbf{x} - \mathbf{x}_i)$
  - solve for fields from deposition
- PIC is noisy, limited by $1/\sqrt{N}$

The δf PIC method reduces noise

S. E. Parker, *PFB*, 1993, A. Y. Aydemir, *PoP*, 1994

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

- split phase space distribution into steady state and evolving perturbation $f = f_{eq}(\mathbf{z}) + \delta f(\mathbf{z},t)$ - control variates
- substitute f in Vlasov Equation to get δf evolution equation along characteristics $\dot{\mathbf{z}}$

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

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

- apply PIC to $\delta f(\mathbf{z},t) \Rightarrow \delta f_i(t)$, sample f_{eq} - importance sampling

Drift Kinetic Equation of Motion

- follows gyrocenter in limit of zero Larmour radius
- reduces $6D$ to $4D+1$ $\left[\mathbf{x}(t), v_{\|}(t), \mu = \frac{\frac{1}{2}mv_{\perp}^2}{\|\mathbf{B}\|}\right]$
- drift kinetic equations of motion

$$\dot{\mathbf{x}} = v_{\|}\hat{\mathbf{b}} + \mathbf{v}_D + \mathbf{v}_{E\times B}$$

$$\mathbf{v}_D = \frac{m}{eB^4}\left(v_{\|}^2 + \frac{v_{\perp}^2}{2}\right)\left(\mathbf{B}\times\nabla\frac{B^2}{2}\right) + \frac{\mu_0 m v_{\|}^2}{eB^2}\mathbf{J}_{\perp}$$

$$\mathbf{v}_{E\times B} = \frac{\mathbf{E}\times\mathbf{B}}{B^2}$$

$$m\dot{v}_{\|} = -\hat{\mathbf{b}}\cdot(\mu\nabla B - e\mathbf{E})$$

δf and the Lorentz Equations

- Lorentz equations of motion

$$\dot{\mathbf{x}} = \mathbf{v}$$
$$\dot{\mathbf{v}} = \frac{q}{m}\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)$$

- for Lorentz equations use[3]

$$f_{eq} = f_0(\mathbf{x}, v^2) + \frac{1}{\omega_c}\left(\mathbf{v} \cdot \mathbf{b} \times \nabla f_0\right)$$

- weight equation is

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

[3] M. N. Rosenbluth and N. Rostoker "Theoretical Structure of Plasma Equations", Physics of Fluids **2** 23 (1959)