Hybrid Kinetic-MHD Simulation in General Geometry

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The dynamics of fusion plasmas lead to instabilities that can spontaneously erupt and degrade confinement and sometimes lead to catastrophic disruptions of the entire plasma itself. These instabilities occur in a broad range of spatial and temporal scales, spanning many orders of magnitude, often resulting from nonlinear interactions. Computational simulations are crucial to understanding these phenomena.

NIMROD(NonIdeal MHD with Rotation - Open Discussion)[1] is a massively parallel three dimensional magnetohydrodynamic simulation utilizing finite elements (**FE**) to represent the poloidal plane and a fourier decomposition in the toroidal direction. The use of finite elements allows flexibility in the representation of the simulation domain. The ability to model experimental shots with NIMROD provides a platform to test new ideas of plasma behavior. To expand the physics capabilities of NIMROD, kinetic effects have been added to NIMROD by the addition of δf PIC(Particle in Cell) module. The addition of kinetic particle effects captures essential wave-particle interactions important in the saturation of various MHD instabilities such as the internal kink mode, sawtooth and fishbone instabilities, and toroidal Alfven eigenmodes. Particle simulation capabilities in NIMROD can also be extended to simulate various phenomena such as neutral beam injection, ion cyclotron resonance heating, and anomalous loss mechanisms. In addition, this hybrid kinetic-MHD technique lays the foundations for a kinetic closure to the MHD equations.

This poster will briefly introduce NIMROD and δf PIC in general, then detail the development of PIC in finite elements and their implementation and present preliminary results.

[1] C. R. Sovinec et al,"Nonlinear Magnetohydrodynamic Simulation using High-Order Finite Elements", *to appear in Journal of Computatioal Physics*

Kinetic

- described by phase space continuity equation

  $\rightarrow$Vlasov Equation
- fast time scales - $\{\Omega_i^{-1}, \tau_t\}$
- small spatial scales - $\{\rho_i, \sim 100\rho_i\}$
- plasma described by abstract 6-D phase space
- equations are fundamental

Fluid-MHD

- described by velocity moment of Vlasov Equation

  $\rightarrow$MHD Equations
- long time scales - $\{\tau_A, \tau_r\}$
- global spatial scales
- plasma described by physical quantities - $\{n, \mathbf{V}, p\}$
- many assumptions made

Hybrid Kinetic-MHD Bridges the Two

- captures kinetic effects lost in MHD equations
- kinetic effects strongly effect MHD instabilities
  - fishbone
  - sawtooth
  - TAE
- can simulate real fusion plasma experiments
  - α particles effects
  - neutral beam injection
  - ICRF heated ions
- ultimate of ultimates : kinetic closures

Kinetic MHD Equations[2]

Starting from Vlasovs equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0$$

and take the first velocity moment ($\int m\mathbf{v}\,[\cdot]\,d\mathbf{v}$) with $f = f_b + f_h$ and $E_\parallel = 0$.

$$mn\frac{d\mathbf{U}}{dt} + m\frac{\partial n_h \mathbf{V}_h}{\partial t} = -\nabla p_b - \nabla \cdot \mathbf{P}_h + \mathbf{J} \times \mathbf{B}$$

where $\mathbf{P}_h = \int \mathbf{v}\mathbf{v} f_h d\mathbf{v}$

assume $v_{\parallel h} \gg v_{\perp h}$

$$mn\frac{d\mathbf{U}}{dt} + m\frac{\partial n_h \mathbf{V}_{\parallel h}}{\partial t} = -\nabla p_b - \nabla \cdot \mathbf{P}_h + \mathbf{J} \times \mathbf{B}$$

momentum equation for hot particles is

$$m\frac{\partial n_h \mathbf{V}_h}{\partial t} = -\nabla \cdot \mathbf{P}_h + \mathbf{J}_h \times \mathbf{B}$$

subtract parallel component

$$mn\frac{d\mathbf{U}}{dt} = -\nabla p_b - \left(\nabla \cdot \mathbf{P}_h\right)_\perp + \mathbf{J} \times \mathbf{B}$$

[2] W. Park, et al, "Three-dimensional hybrid gyrokinetic- magnetohydrodynamic simulation", *Physics of Fluids B*, **4**, 1992

Kinetic Equation and δf-method[3]

Vlasov Equation

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

where $f(\mathbf{z})$ is the 6 dimensional phase space distribution and $\mathbf{z}$ is the phase coordinate.

Typically (in the fusion community), kinetic equations are implemented as particle-in-cell(PIC) simulations using the δf-method.

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

$$f = f_0(\mathbf{z}) + \delta f(\mathbf{z}, t)$$

- put into Vlasov Equation:

$$\frac{\partial \delta f}{\partial t} + \dot{\mathbf{z}} \cdot \frac{\partial \delta f}{\partial \mathbf{z}} = -\mathbf{z}_1 \cdot \frac{\partial f_0}{\partial \mathbf{z}}$$

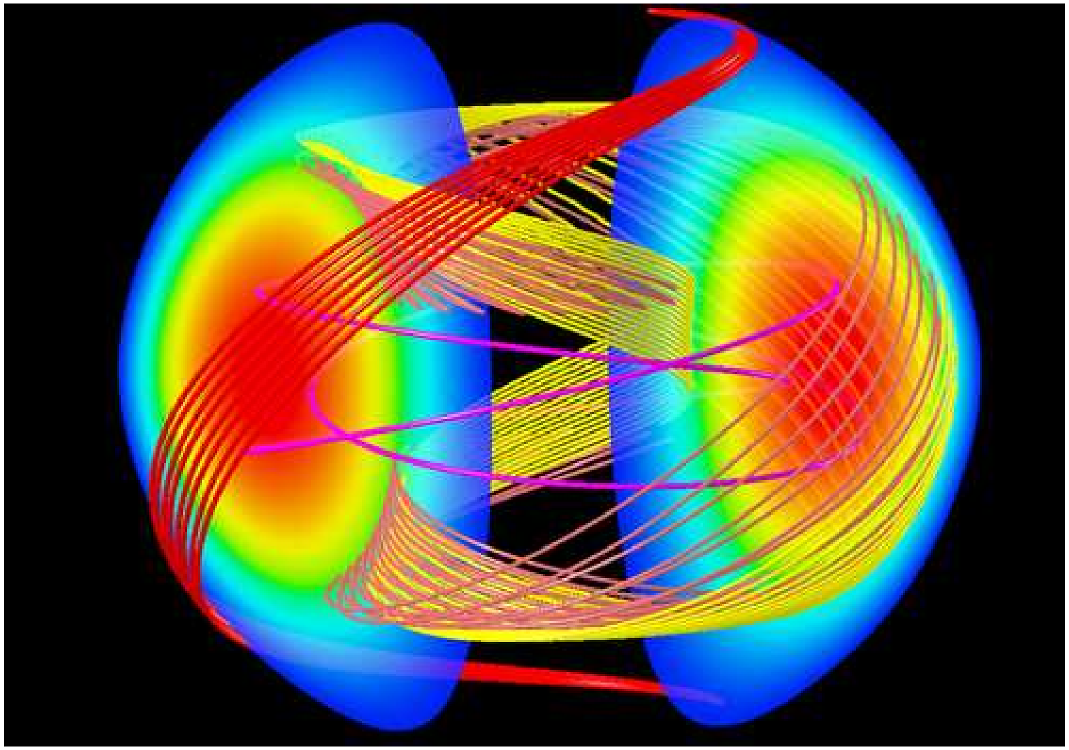
  using $\mathbf{z} = \mathbf{z}_0 + \mathbf{z}_1$ and $\dot{\mathbf{z}}_0 \cdot \frac{\partial f_0}{\partial \mathbf{z}} = 0$

- along the characteristics $\dot{\mathbf{z}}$

$$\dot{\delta f} = -\mathbf{z}_1 \cdot \frac{\partial f_0}{\partial \mathbf{z}}$$

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

Characteristic Equations of Motion



Use the drift kinetic equations of motion.

$$\dot{\mathbf{x}} = v_\parallel \hat{\mathbf{b}} + \frac{m}{eB^4}\left(u^2 + \frac{v_\perp^2}{2}\right)\left(\mathbf{B} \times \nabla \frac{B^2}{2}\right) + \frac{\mathbf{E} \times \mathbf{B}}{B^2}$$

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

‘Like NIMROD, the mighty hunter before the Lord’

NIMROD(NonIdeal MHD with Rotation - Open Discussion)

- massively parallel 3-D MHD simulation
- domain decomposition in poloidal plane and fourier modes
- utilizes Lagrange type finite element
- can handle extreme anisotropies, $\frac{\chi_\parallel}{\chi_\perp} \gg 1$
- flexibility to model general geometry $\longrightarrow$ real experiments
- model experiment relevant parameters, $S > 10^7$
- semi-implicit advance, not restricted by magnetosonic CFL condition

NIMROD equations

NIMROD evolves the extended MHD equations

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

where the heat flux is

$$\mathbf{q} = -n\left[\chi_{\|}\hat{\mathbf{b}}\hat{\mathbf{b}} + \chi_{\perp}(1 - \hat{\mathbf{b}}\hat{\mathbf{b}})\right] \cdot \nabla T$$

recall $\frac{\chi_{\|}}{\chi_{\perp}} \gg 1$

Q is a source term

$$Q = \eta\mathbf{J}^2 + \nu mn\nabla\mathbf{U}^T : \nabla\mathbf{U}$$

from Ohmic and viscous heating.

plasma obeys the ideal gas law, $p = nT$.

Spatial representation in NIMROD

The perturbed NIMROD fields are in FE-Fourier representation

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

where

$$\alpha_{j,n} = N_j(p,q)\exp(in\phi)$$

(p,q) are logical coordinates

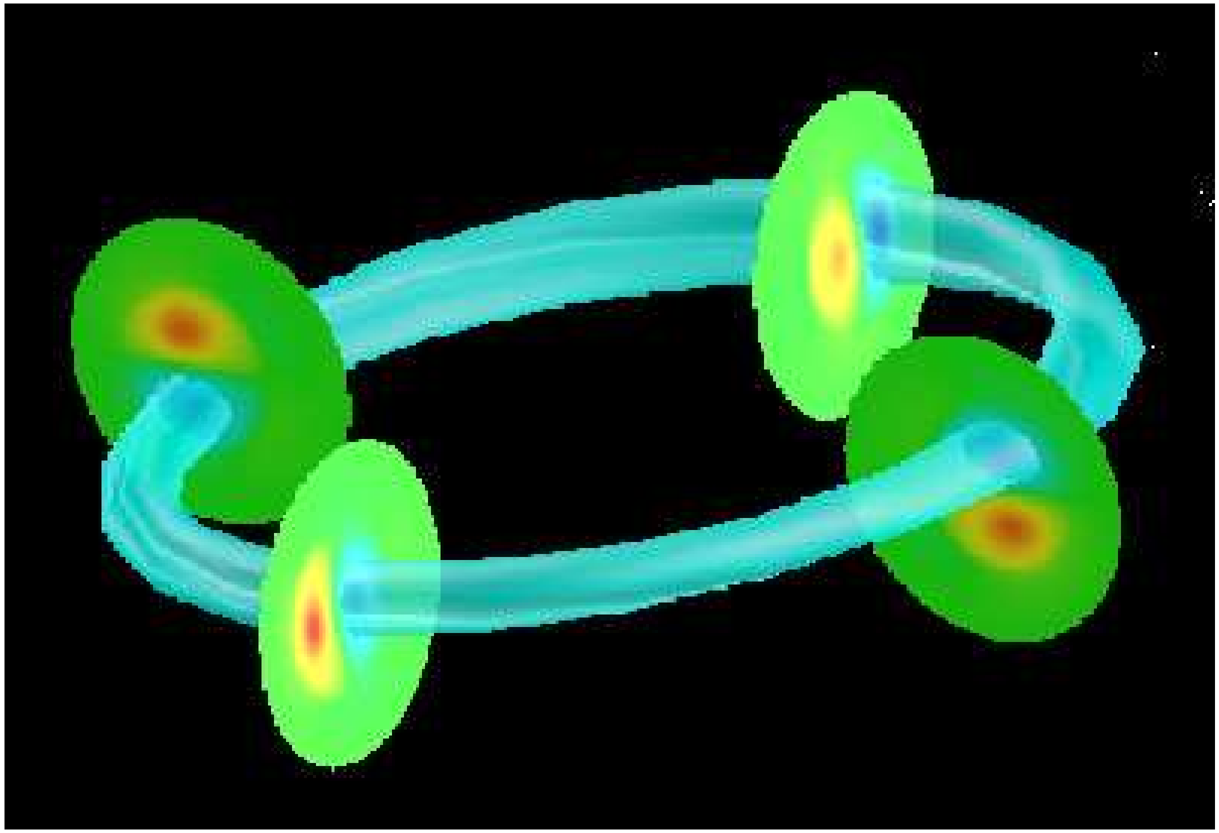
The Lagrange type elements are composed of polynomials of the form:

$$l_j^m(\eta) = \frac{\prod_{b=1_{b\neq a}}^m (\eta - \eta_b)}{\prod_{b=1_{b\neq a}}^m (\eta_a - \eta_b)}$$

such that

$$N_k(p,q) = l_i(p)l_j(q)$$

(1,1) internal kink eigenmode from NIMROD



Formulation of PIC in FEM

Particles in a finite element grid have the added complication of an irregular grid.

- nontrivial shape functions associated with the gather and scatter process
- a more complicated search algorithm
- added complications of parallelization

Shape function used for gather and scatter:

$$A_p = \sum_i N_i(p,q) A_i, \quad M_j = \sum_e \sum_p N_j(p,q) m_p J_p$$

Need to determine logical coordinates (p, q) of each particle to evaluate shape functions

Solving for the p's&q's

Express particle coordinates in finite element fashion:

$$R_p = \sum_{i=1}^{m^2} R_i N_i(p,q), \quad Z_p = \sum_{i=1}^{m^2} Z_i N_i(p,q),$$

(p,q) must be solved for in an iterative fashion due to the nonlinear nature of the relevent equations.

Invert this relation using Newton-Raphson method.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{f(\mathbf{x}_k)}{f'(\mathbf{x}_k)}$$

where the $\mathbf{x} = (p,q)$

More explicitly

$$\left\{ \begin{array}{c} p^{k+1} \\ q^{k+1} \end{array} \right\} = \left\{ \begin{array}{c} p^{k} \\ q^{k} \end{array} \right\} + f'^{-1} \left\{ \begin{array}{c} R_p - R_p^k \\ Z_p - Z_p^k \end{array} \right\}$$

$$f'^{-1} = \begin{pmatrix} \frac{\partial p}{\partial R} & \frac{\partial p}{\partial Z} \\ \frac{\partial q}{\partial R} & \frac{\partial q}{\partial Z} \end{pmatrix}$$

Invoke the Inverse Function Theorem

$$f_k'^{-1} = \begin{pmatrix} \frac{\partial R}{\partial p} & \frac{\partial R}{\partial q} \\ \frac{\partial Z}{\partial p} & \frac{\partial Z}{\partial q} \end{pmatrix}^{-1} = \frac{1}{\Delta_k} \begin{pmatrix} \frac{\partial Z}{\partial q} & -\frac{\partial R}{\partial q} \\ -\frac{\partial Z}{\partial p} & \frac{\partial R}{\partial p} \end{pmatrix}_k$$

where Δ_k is the determinant

Inserting the definitions for the shapefunctions

$$\begin{pmatrix} \frac{\partial R}{\partial p} & \frac{\partial R}{\partial q} \\ \frac{\partial Z}{\partial p} & \frac{\partial Z}{\partial q} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{m^2} R_i l'(p) l(q) & \sum_{i=1}^{m^2} R_i l(p) l'(q) \\ \sum_{i=1}^{m^2} Z_i l'(p) l(q) & \sum_{i=1}^{m^2} Z_i l(p) l'(q) \end{pmatrix}$$

Iterate until

$$\sqrt{(R - R_p^k)^2 + (Z - Z_p^k)^2} < \epsilon$$

If $-1 \le p, q \le 1$ is <u>not</u> true, then the particle is not in this element, and another element needs to be searched. The new element to be searched is determined by the value of (p, q), left if $p < -1$, right if $p > 1$, down if $q < -1$, up if $q > 1$, and combinations thereof.

Particle Sorting

- Sorting is important because:
  - sorting makes domain decomposition of particles trivial
  - cache thrashing is minimized
- Each processor does a 'bucket' sort of it's own assigned particles
- Particles are sorted wrt the finite element grid
- Particles with a logical coordinate outside of the processor sub-domain are passed to their appropriate processor
- A locally sorted list of particles is finally tabulated on each processor

Parallel performance

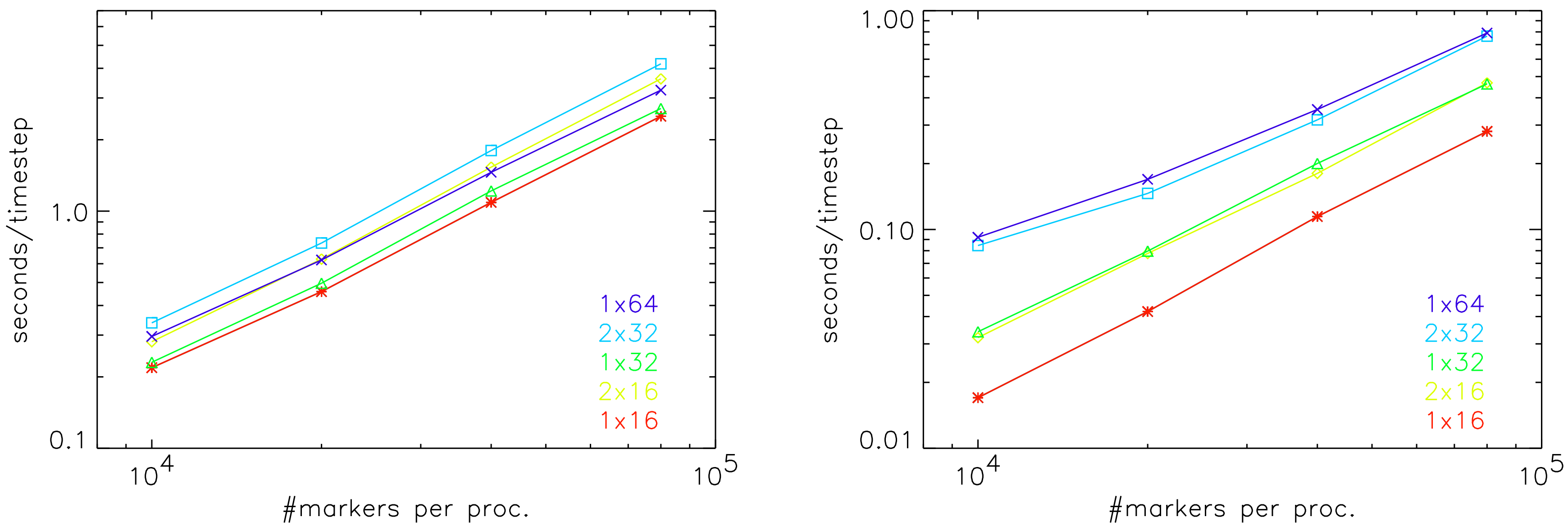
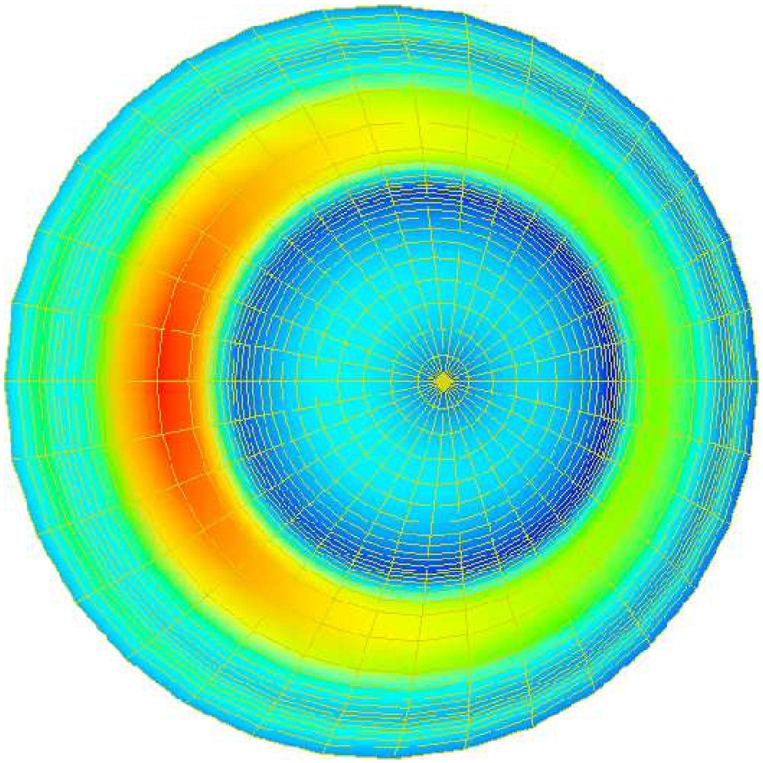
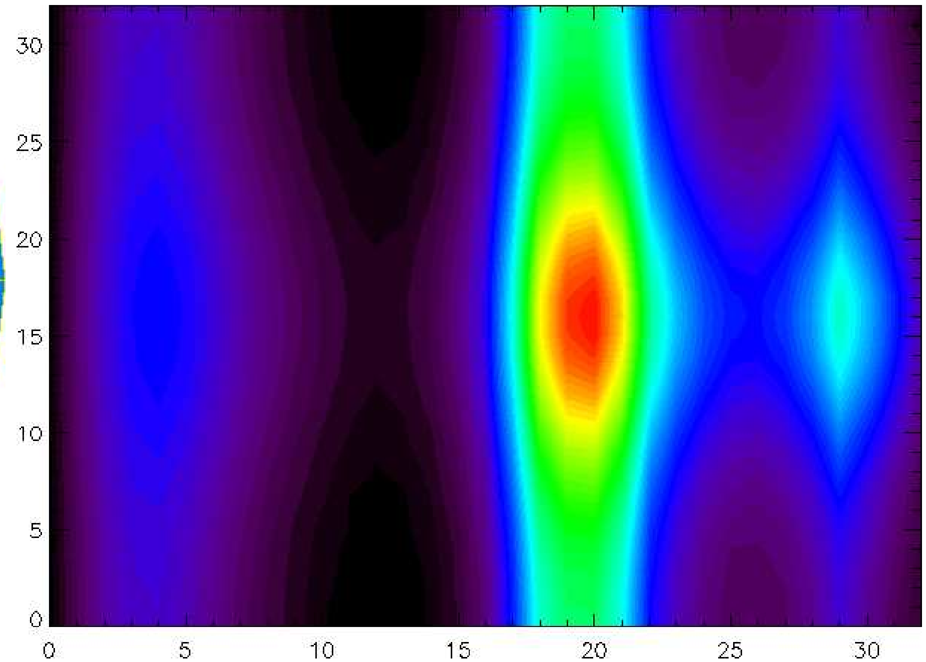


Figure 1: scaling of total time and sorting time wrt #processors and particle number

- Algorithm is scalable, total cpu time $\propto \frac{1}{\#procs}$
- search algorithm shows strong dependence on the number of processors degrading scalability

Load Balancing Issues





Nonuniform grid causes dramatic load balancing problem.

Current solution is to restrict domain decomposition to poloidal direction.

CGL Pressure Tensor

The Kinetic MHD momentum equation is

$$mn\left(\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U}\cdot\nabla\mathbf{U}\right) = \mathbf{J}\times\mathbf{B} - \nabla p - \left(\nabla\cdot\mathbf{P}_{hot}\right)_{\perp}$$

where

$$\mathbf{P}_{hot} = \int m\mathbf{v}\mathbf{v}\delta f \; d\mathbf{v}$$

for CGL pressure tensor we have

$$\mathbf{P} = \begin{pmatrix} p_{\perp} & 0 & 0 \\ 0 & p_{\perp} & 0 \\ 0 & 0 & p_{\parallel} \end{pmatrix}$$

where $p_{\perp} = \int \mu B\delta f \; d\mathbf{v}$ and $p_{\parallel} = \int mv_{\parallel}^2\delta f \; d\mathbf{v}$ so

$$\left(\nabla\cdot\mathbf{P}_{hot}\right)_{\perp} = \nabla_{\perp}p_{\perp}$$

Slowing Down Distribution

Assume an energetic minority ion species resulting from beams or α particles with uniform initial energy. Through collisions with electrons, the monoenergetic distribution becomes the slowing down distribution

$$f_0 = \frac{P_0 \exp(\frac{P_\zeta}{\psi_0})}{\varepsilon^{3/2} + \varepsilon_0^{3/2}}$$

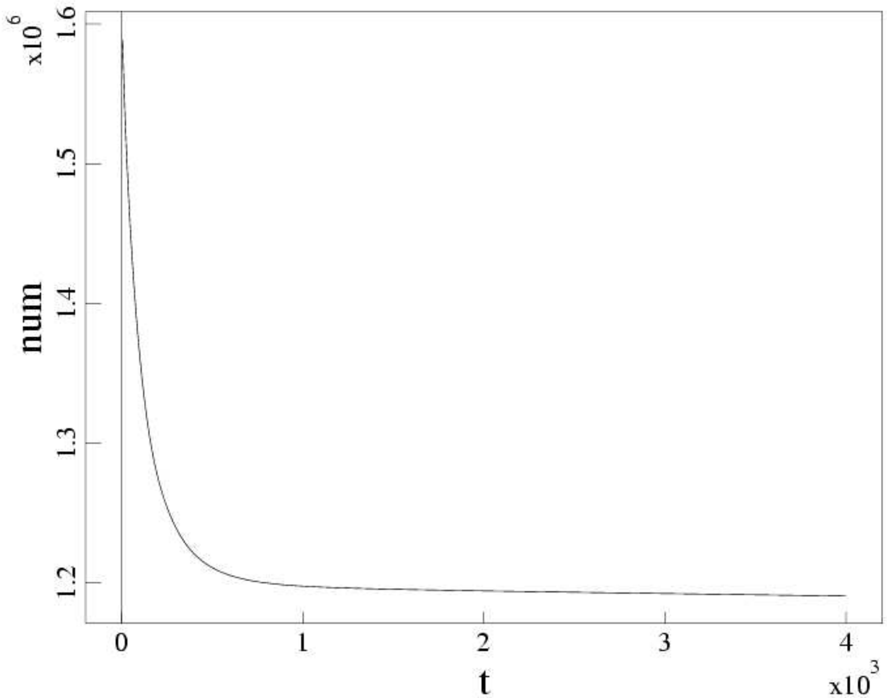
where $P_\zeta = g(\psi_p)\rho_\parallel - \psi_p$

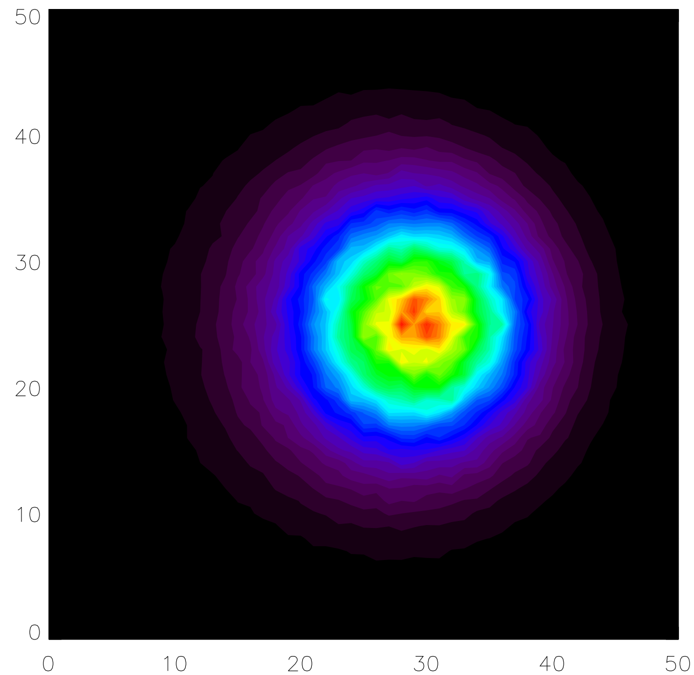
$$\begin{aligned} \dot{\delta f} &= f_0 \left\{ \frac{mg}{e\psi_0 B^3} \left[\left(v_\parallel^2 + \frac{v_\perp^2}{2} \right) \delta\mathbf{B} \cdot \nabla B \right] \right. \\ &\left. + \frac{\mathbf{v}_1 \cdot \nabla\psi_p}{\psi_0} + \frac{3}{2} \frac{e\varepsilon^{1/2}}{\varepsilon^{3/2} + \varepsilon_0^{3/2}} \mathbf{v}_D \cdot \mathbf{E} \right\} \end{aligned}$$

$$\begin{aligned} \mathbf{v}_D &= \frac{m}{eB^3} \left(v_\parallel^2 + \frac{v_\perp^2}{2} \right) (\mathbf{B} \times \nabla B) \\ \mathbf{v_1} &= \frac{\mathbf{E} \times \mathbf{B}}{B^2} + \mathbf{v}_\parallel \cdot \frac{\delta\mathbf{B}}{B} \end{aligned}$$

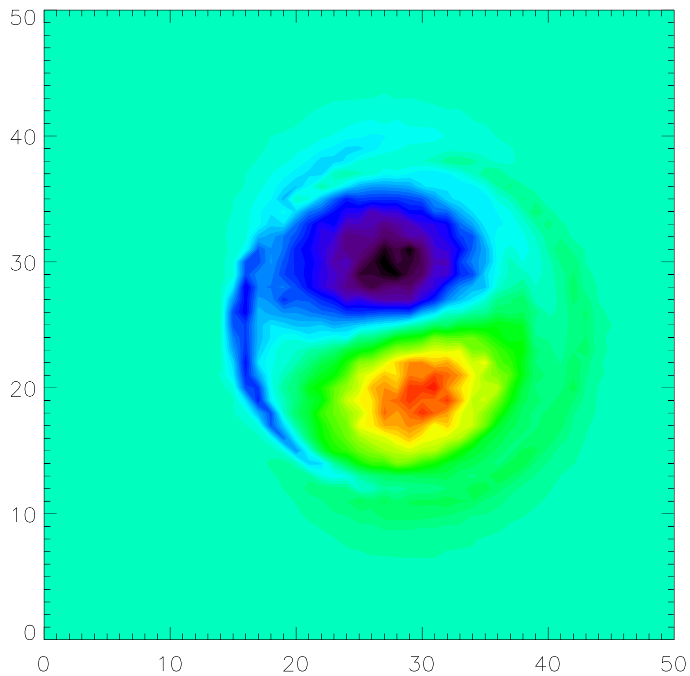
Particle Equilibration

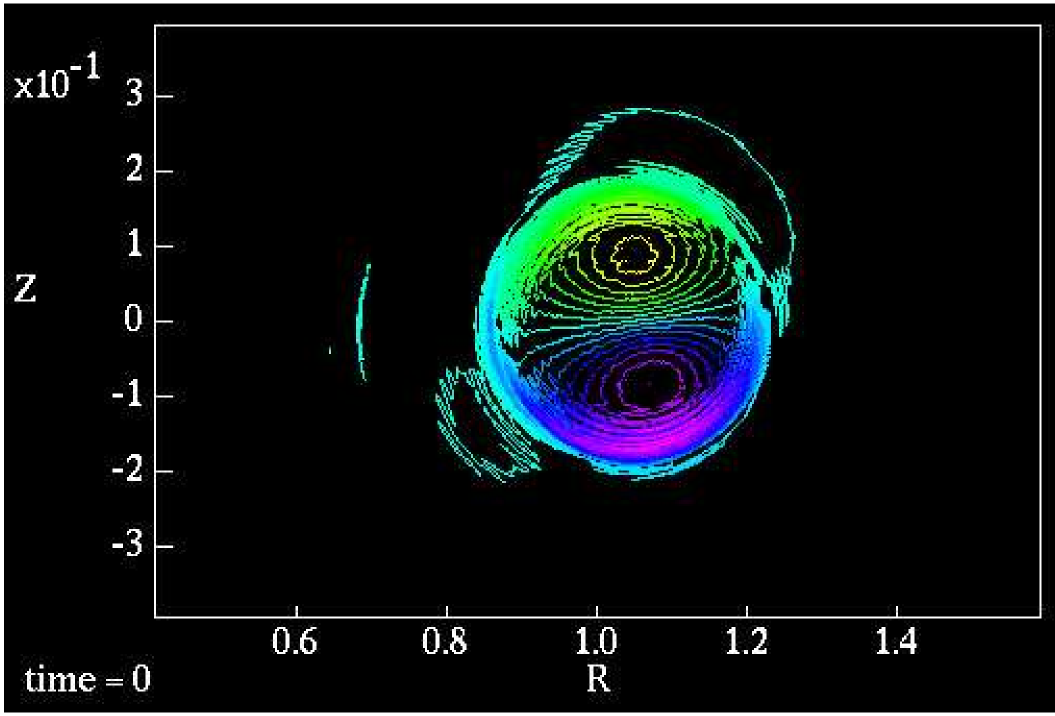
Within a few transit times, the simulation particle distribution settles



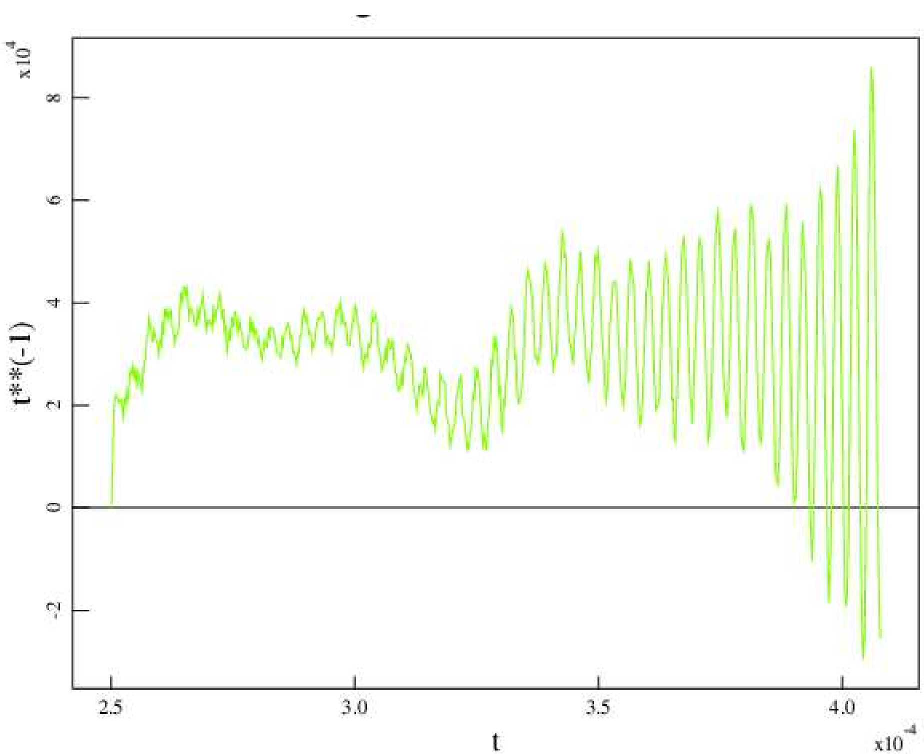


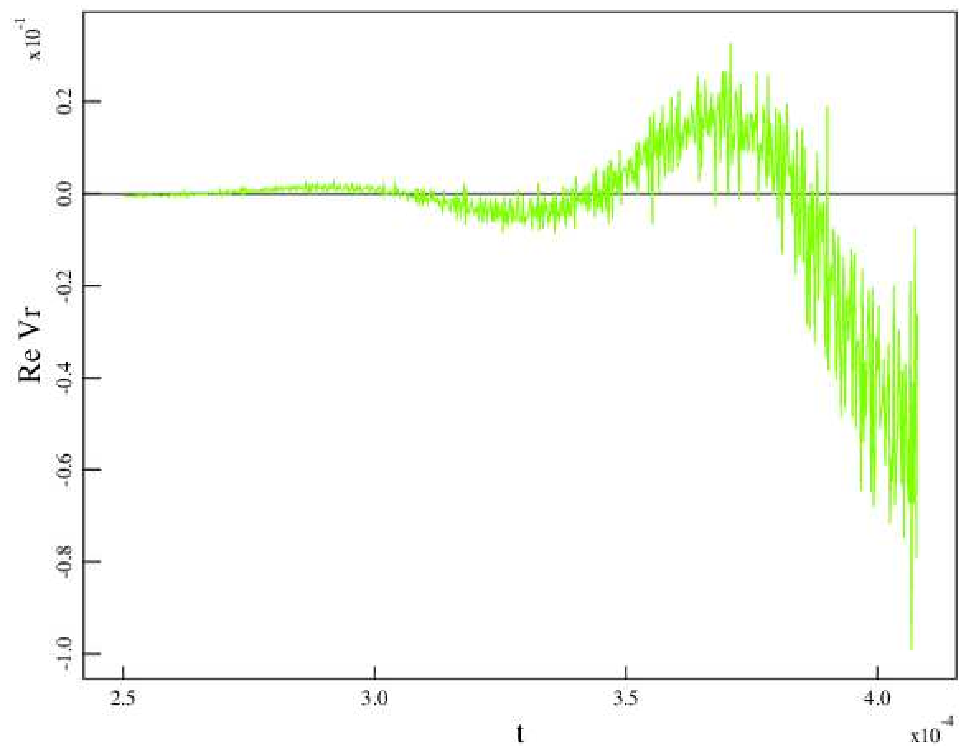
P_{hot} shows Eigenfunction Formation



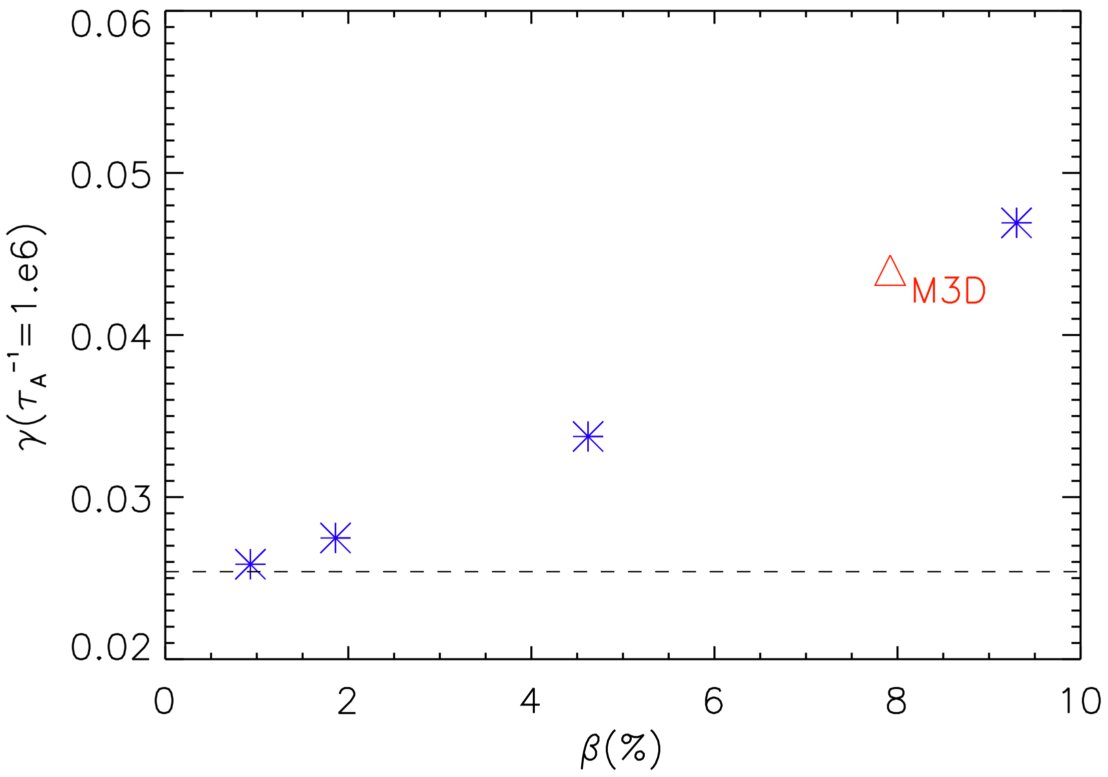


Growth rate and time history of V_r





CEMM Energetic Particle Benchmark



Summary

- develop PIC algorithm suitable for FEM
- parallelization scales well for small number of processors
- sorting is nonscaling and strongly dependent on the number of processors
- load balancing an issue
- particle noise must be reduced
- particle orbits accurately calculated
- P_{hot} picks up NIMROD eigenmode
- inclusion of kinetic effects drives instability
- linear results agree with competing simulation (M3D) for $\beta_h = 0$ and $\beta_h = 8\%$