Advances in Analysis of Hybrid Kinetic-MHD Simulations

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Outline

1. Hybrid Kinetic MHD in NIMROD
   - NIMROD
   - Hybrid Kinetic-MHD model
2. (1,1) Phase Space Analysis
   - (1,1) internal kink benchmark
   - $n = 1$ Δp_h and δf
   - increasing the maximum energy
3. New Analysis Tools
   - VisIt
   - H5Part/FastBit
   - PIC Visualization Tools
4. Conclusions and Future Develoment

motivation - why hybrid kinetic-MHD

- captures kinetic effects absent in MHD equations
- some parts of the plasma are very kinetic
  - α particles effects
  - neutral beam injection
  - ICRF heated ions
- kinetic effects can significantly alter MHD instabilities
  - kink
  - tearing
- kinetic effects can excite non-MHD instabilities
  - fishbone/giant sawtooth
  - TAE/EPM
- ultimate of ultimates : kinetic closures

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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
- model experimental geometry and physical parameters
  - semi-implicit and implicit operators
  - $\frac{\chi_{\parallel}}{\chi_{\perp}} \gg 1,\ S \sim 10^7,\ Pr < 1$
  - extensive **V&V**
- active developer and user base
- continually expanding capabilities

NIMROD's Extended MHD Equations

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

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

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

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

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

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

red, blue, and green terms comprise the extensions to resistive MHD, Hall and 2-fluid effects, Braginski and beyond closures, and the energetic particles, respectively.

The 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
  - ρ, $\mathbf{U}$ 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

The Hybrid δf PIC-MHD model

- advance particles and δf

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

- deposit $\delta p(\mathbf{x}) = \sum_{i=1}^{N} \delta f_i m(v_i - V_h)^2 S(\mathbf{x} - \mathbf{x}_i)$ on FE grid
- advance NIMROD hybrid kinetic-MHD momentum equation

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

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

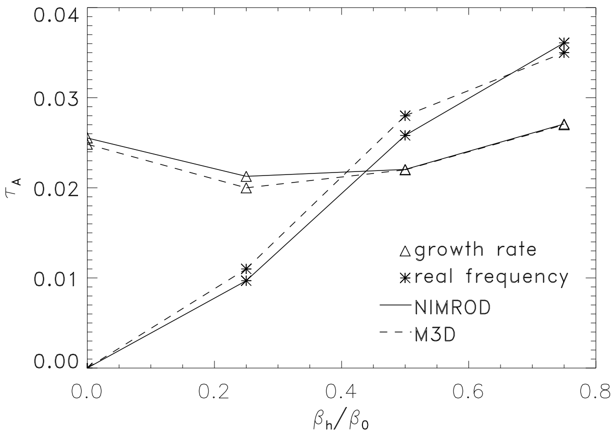
PIC options

- 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
  - 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

Outline

Analysis of Drift kinetic $(1,1)$ kink benchmark

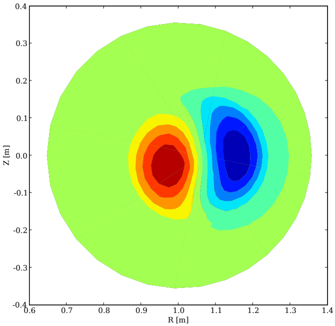
C. C. Kim, *PoP* **15** 072507 (2008)



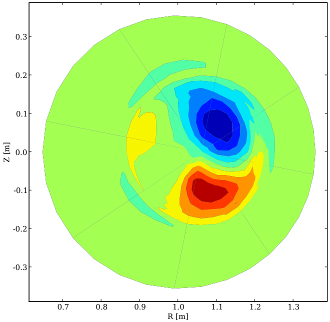
circular,
monotonic q,
$q_0 = .6, \; q_a = 2.5$,
$\beta_0 = .08$,
$R/a = 2.76$,
$E_{hmax} = 10KeV$,
dt=1e-7, $\tau_A = 1.e6$

$\Delta p_h = p_{h\|} - p_{h\perp}$ is dominant Energetic Particle effect

$n = 1$ $p_{h\perp}$



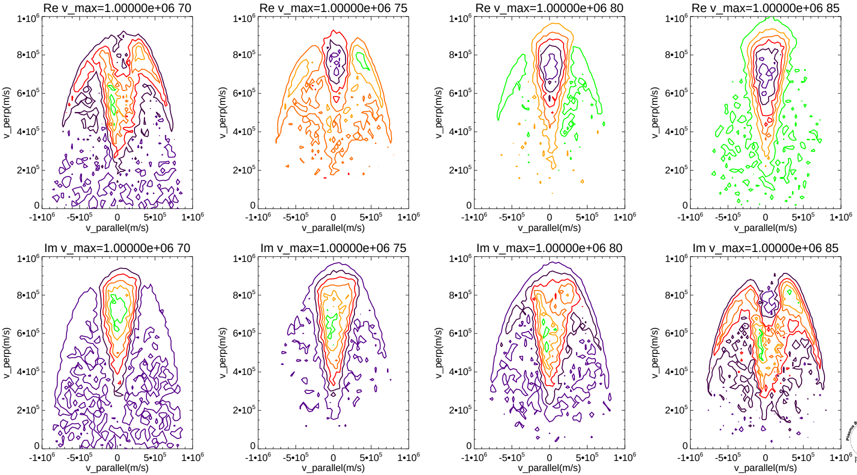
$n = 1$ Δp_h



- without anisotropy, reproduce ideal MHD γ within 10%
  - slowing down not Maxwellian
- no real frequency!

$\delta f_{n=1}$ concentrated in trapped cone and passing "wings"

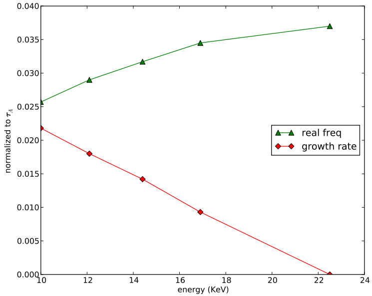
$$\delta f_{n=1} = \int_{n=1} \exp(in\phi) \times \delta f(v_{\|}, v_{\perp}) d^3x$$



Increasing $E_{h\ max}$ stabilizes $(1,1)$

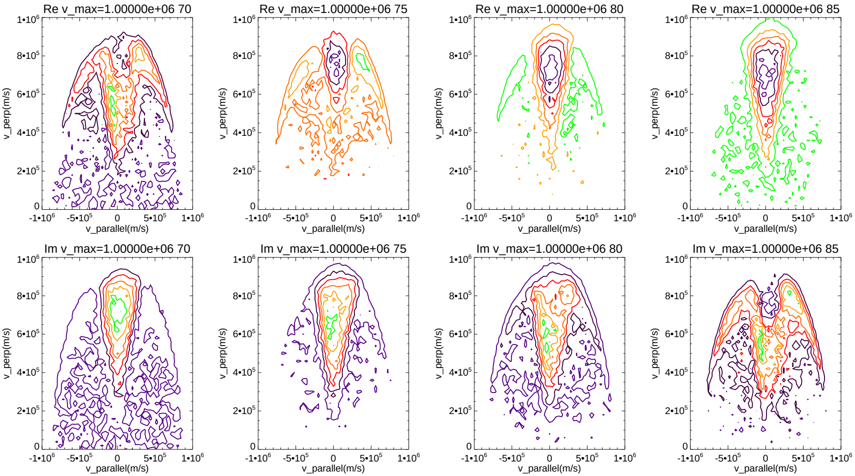
- benchmark $(1,1)$ performed with $E_{h\ max} = 10KeV$
- increasing $E_{h\ max}$ stronger stabilization, larger frequency

fixed
$\beta_h = 50\%\beta$



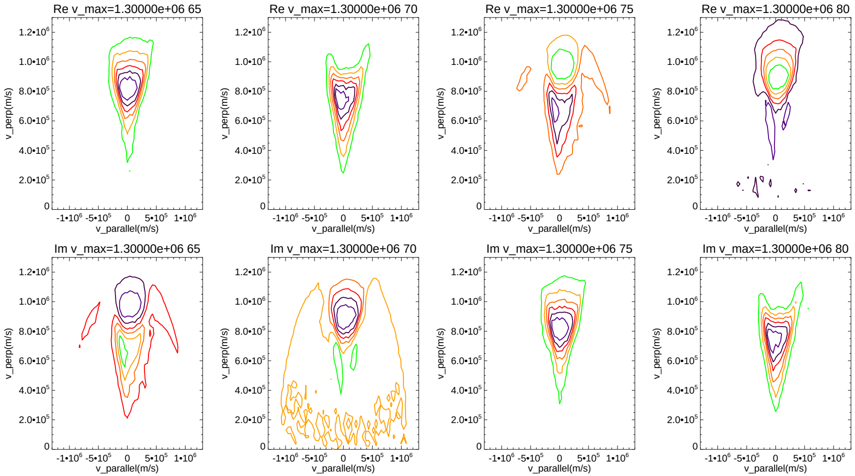
- fixed β_h - $\Uparrow$increase in energy range, $\Downarrow$ decrease in density
  - $\Rightarrow$ **fewer particles are doing more!**
  - $\Rightarrow$ increase in real frequency

$E_{h\,max} = 10KeV$ activity around $v \simeq v_{max}$



$\delta f_{n=1}$ at $v_{max} = 1.0 \times 10^6 \mathrm{m/s}$

$E_{h\ max} = 17KeV$ less activite $v \simeq v_{max}$ "wings"



$$\delta f_{n=1} \text{ at } v_{max} = 1.3 \times 10^6 \text{m/s}$$

Examination of $\delta f_{n=1}$ in phase space

- higher energy particles drive higher frequency
- comparison of $E_{h\ max} = (10KeV, 17KeV)$ shows
  - concentration of $\delta f_{n=1}(v_{||}, v_{\perp})$ activity to trapped cone
  - passing “wing” amplitude decreased
  - decreased growth rate (stabilized?)
  - excites higher frequency
- trend agrees with theory predictions
- temporally evolving coherent structures

Examination of $\delta f_{n=1}$ leaves questions

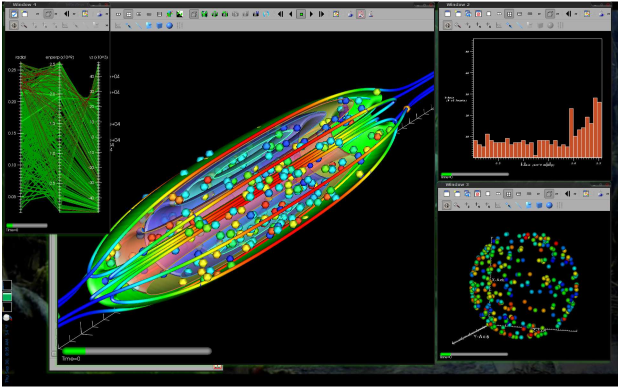
- role of the asymmetry
  - role of P_ζ and orbit loss (mostly for edge modes)
  - co-/counter NB, i.e. $V_h \neq 0$
  - what is the nature of the structure in $\delta f_{n=1}$ and its relation to e.g. Δp_h
- role of trapped vs. passing particles
  - what is going on in the "wings"
  - what is the structure in the trapped cone
  - what is the nature of the oscillation
- **which particles are doing what where and when**

Outline

VisIt - https://wci.llnl.gov/codes/visit/

- active and responsive development - (VACET, A. Sanderson)
  - Tuesday JO4.00002 : Analysis Tools for Fusion Simulations
- best interactive 3D visualization software
  - supports most data formats (e.g. HDF5,Silo,VTK)
  - open source, scriptable in Python
  - allows plotting of multiple scalar and vector quantities (contours, volumes, vectors, streamlines)
  - intuitive GUI
- allows manipulation of data and visualization
  - built in mathematical operators
  - slicing, clipping, projection
  - query tools
  - many more
- visually correlate and analyze volumetric data
- **integrated environment to explore the data**

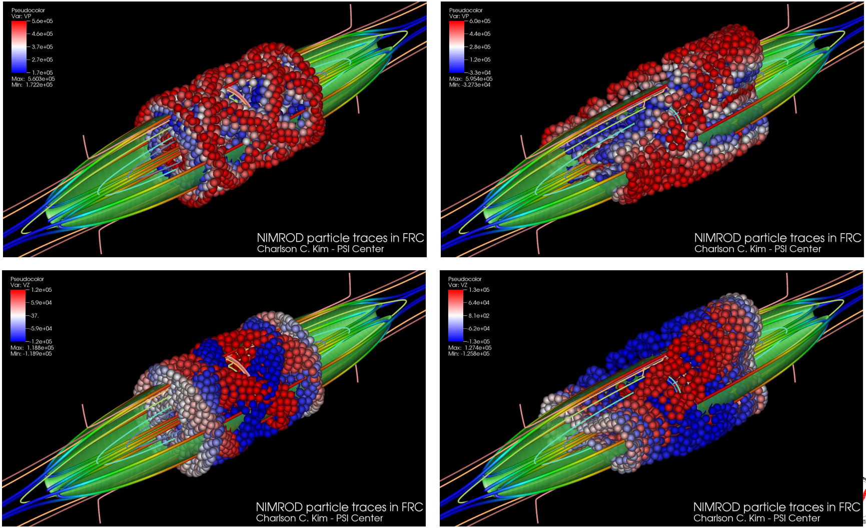
H5Part/FastBit enables interactive PIC analysis



- PIC - high volume, high dimensionality
- H5Part is HDF5 data schema tailored for PIC
- VisIt supports H5Part/FastBit

- FastBit augments HDF5 data files with bitmap index
  - fast multidimensional "semantic indexing"
  - *e.g.* get $v_\phi \in [5e5, 7e5]$ AND $r \in [.3, .55]$

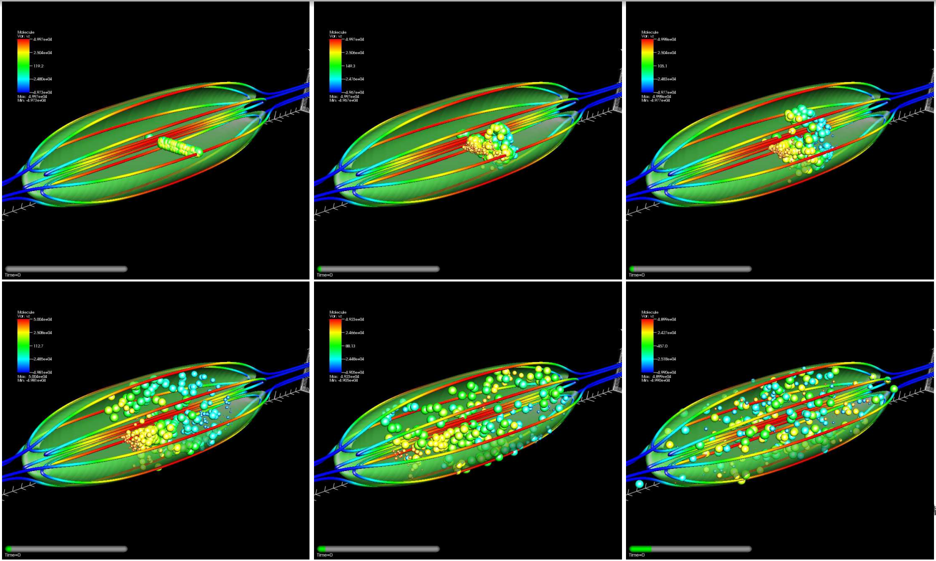
3+1D Pseudocolor Plot reveals structure



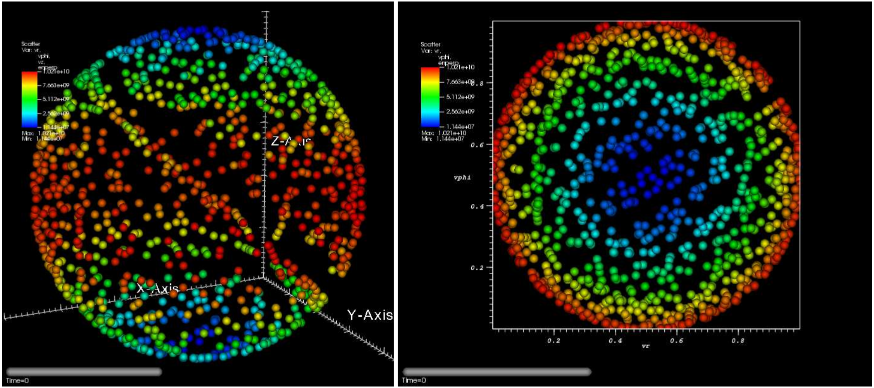
V_ϕ

V_Z

3+2D Molecule Plot - **YouTube:***charlsonification*

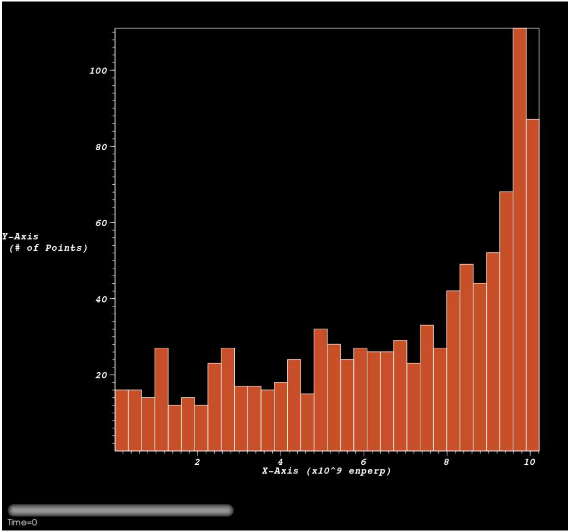


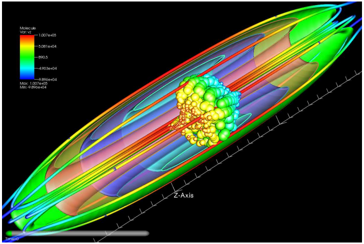
Supports Plots in arbitrary coordinate - e.g. $\vec{v}$



- pseudo-color/molecule plot
- suitable postprocessing can construct phase space field data
- *What is the distribution?*

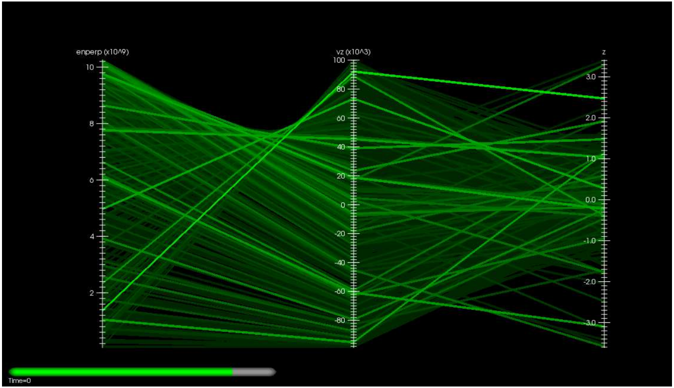
Histograms fundamental to PIC analysis





- histograms are easily digestable
- expand capabilities to higher dimension, e.g. $\delta f_{n=1}(v_{\|}, v_{\perp})$
- means of generating phase space field

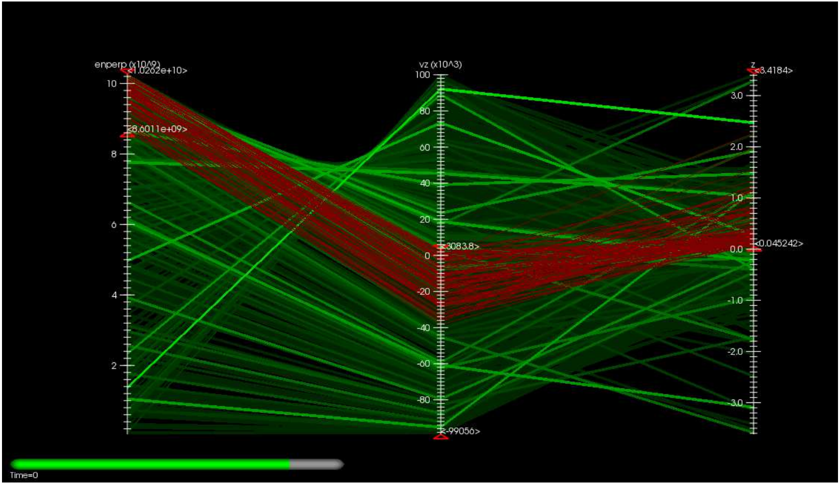
Parallel Coordinate tool correlates histograms



- visualize correlations in n-dimensional data using n parallel axes and polylines

- data is binned and polylines are drawn
- “connect-the-dot” histogram
- appropriate choice of coordinates critical

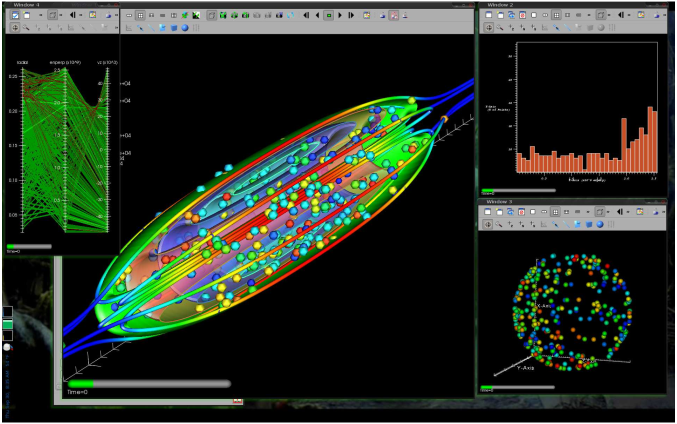
Parallel Coordinate is a key selection tool



- selection propogates to all plots

Outline

NIMROD is outfitted with basic set of visualization tools



- first primitive applications
- beginning to explore 6D plasma phase space $f(\vec{\mathbf{x}}, \vec{\mathbf{v}})$
- need to apply and refine

related APS-DPP presentations

1. **BP9.00098** Hybrid Kinetic-MHD Studies of FRC's using Lorentz δf PIC in Finite Elements
2. **BP9.00126** Comparison of energetic particles effects on $m/n = 3/2$ and $m/n = 2/1$ modes in DIII-D
3. **BP9.00107** MHD and 2-Fluid Stability of DIII-D Shot #96043 using the NIMROD Code
4. **BP9.00127** Toroidal Coupling of Tearing Modes in RFP
5. **UO4.00004** Extrapolating the kinetic effects of energetic particles on resistive MHD stability to ITER
6. **JO4.00002** Analysis Tools for Fusion Simulations

Next steps

- NIMROD continues to improve and grow
- hybrid kinetic-MHD continues to develop
  - developing multispecies option
  - full $f(\vec{\mathbf{z}})$ PIC
  - numeric representation of $f_{eq}(\vec{\mathbf{x}}, \vec{\mathbf{v}})$
    - for loading
    - for evolution of δf
- new computing tools on the horizon
  - massively parallel machines (10^5)
  - hybrid processors GPU, Cell, other?
  - 3D graphics processors and displays
  - pervasive ethernet - cloud computing
- larger scale simulations of greater detail
  - larger volumes of data
  - need for more interaction with simulation and data
- hybrid kinetic-MHD is equipped with tools to handle simulation and data

Outline

5. appendix
   - Hybrid kinetic-MHD momentum equation
   - Drift Kinetic and Lorentz equations
   - Passing vs. Trapped Particles
   - f_0 and f_{ss}

Linearized Momentum Equation and $\delta \underline{\mathbf{p}}_h$

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

- CGL-like $\delta \underline{\mathbf{p}}_h = \begin{pmatrix} \delta p_\perp & 0 & 0 \\ 0 & \delta p_\perp & 0 \\ 0 & 0 & \delta p_\parallel \end{pmatrix}$
- evaluate pressure moment at $\mathbf{x}$

$$\delta \underline{\mathbf{p}}(\mathbf{x}) = \int m \langle \mathbf{v} - \mathbf{V}_h \rangle \langle \mathbf{v} - \mathbf{V}_h \rangle \delta f(\mathbf{x}, \mathbf{v}) d^3 v$$

δf is perturbed phase space density, m mass of particle, and V_h is COM velocity of particles

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

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

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

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

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

Slowing Down Distribution for Hot Particles

- slowing down distribution function $f_{eq} = \dfrac{P_0 \exp(\frac{P_\zeta}{\psi_0})}{\varepsilon^{3/2} + \varepsilon_c^{3/2}}$
- $P_\zeta = g\rho_\parallel - \psi$ canonical toroidal momentum, ε energy, ψ_p poloidal flux, ψ_0 gradient scale length, ε_c critical energy

$$\dot{\delta f} = f_{eq}\left\{\frac{mg}{e\psi_0 B^3}\left[\left(v_\parallel^2 + \frac{v_\perp^2}{2}\right)\delta\mathbf{B}\cdot\nabla B - \mu_0 v_\parallel \mathbf{J}\cdot\delta\mathbf{E}\right] + \frac{\delta\mathbf{v}\cdot\nabla\psi_p}{\psi_0} + \frac{3}{2}\frac{e\varepsilon^{1/2}}{\varepsilon^{3/2}+\varepsilon_c^{3/2}}\mathbf{v}_D\cdot\delta\mathbf{E}\right\}$$

$$\mathbf{v}_D = \frac{m}{eB^3}\left(v_\parallel^2 + \frac{v_\perp^2}{2}\right)(\mathbf{B}\times\nabla B) + \frac{\mu_0 m v_\parallel^2}{eB^2}\mathbf{J}_\perp$$

$$\delta\mathbf{v} = \frac{\delta\mathbf{E}\times\mathbf{B}}{B^2} + \mathbf{v}_\parallel\cdot\frac{\delta\mathbf{B}}{B}$$

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[1]

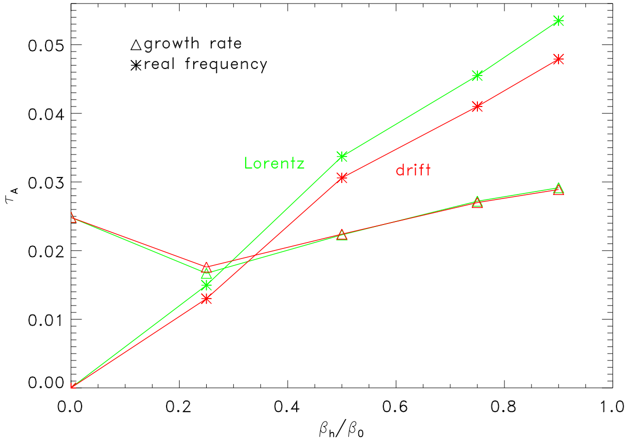
$$f_{eq} = f_0(\mathbf{x}, v^2) + \frac{1}{\omega_c}\left(\mathbf{v} \cdot \mathbf{b} \times \nabla f_0\right)$$

- weight equation is

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

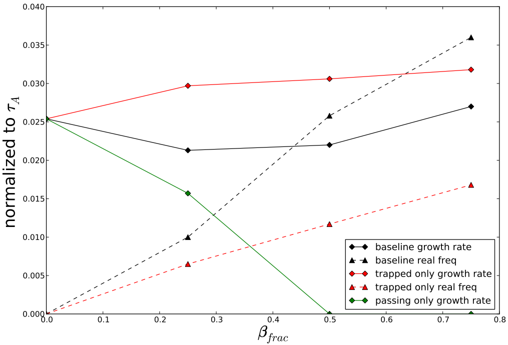
[1] M. N. Rosenbluth and N. Rostoker "Theoretical Structure of Plasma Equations", Physics of Fluids **2** 23 (1959)

Full orbit recovers drift kinetic result



β_{frac} scan of $(1,1)$ benchmark kink with drift and Lorentz particles

Isolated populations display suprising effects

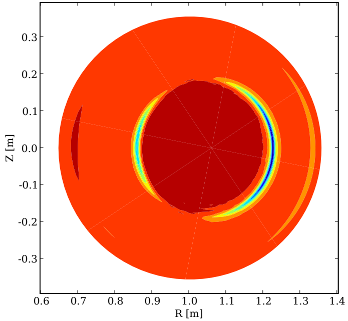


- trapped particles destabilize precessional fishbone
- passing particles stabilize kink
- primarily "barely" passing particles

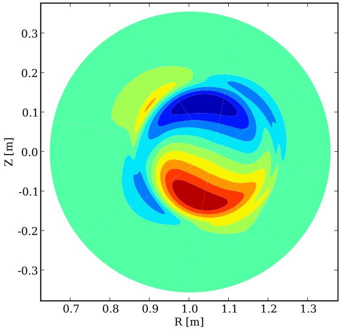
- passing particles do NOT excite real frequency
- suprising synergistic effect of passing particles
  - decreases growth rate of fishbone
  - ! enhance fishbone frequency

Trapped Particle excite Precessional Fishbone

$n = 1 V_\phi$ with passing particles

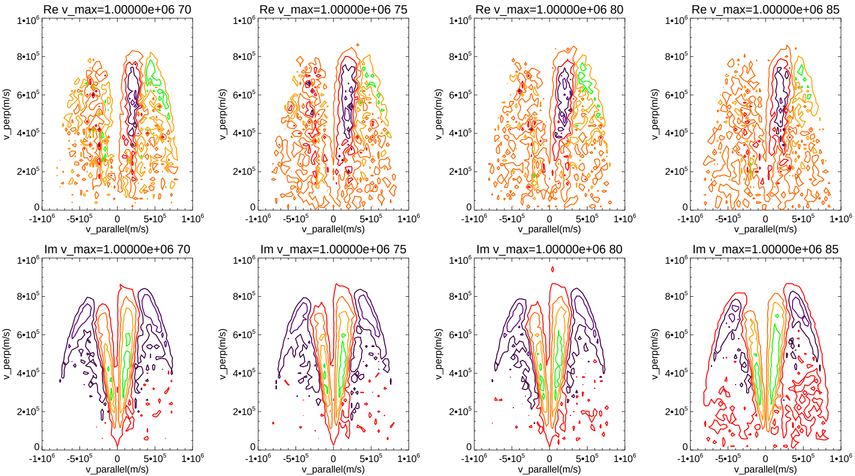


$n = 1 V_\phi$ with trapped particles



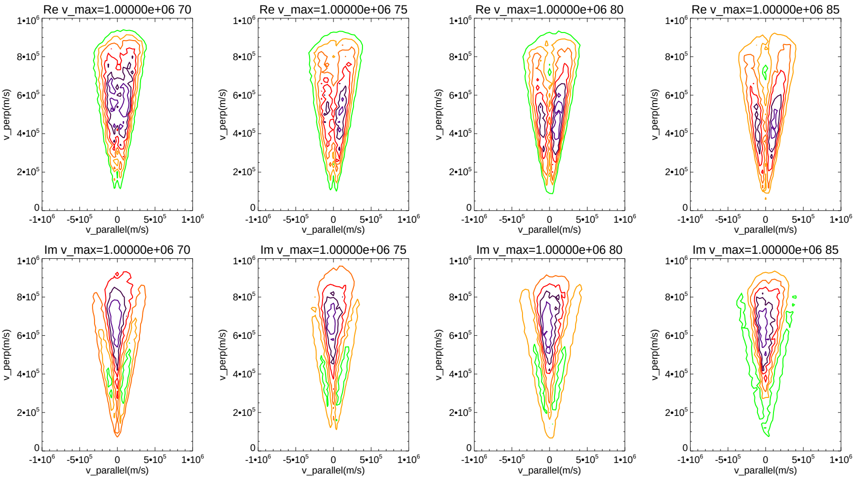
- simulations with only passing particles stabilize but do not change V_ϕ mode topology
- precessional fishbone mode has global topology

Passing Only Dominated by Barely Passing Particles



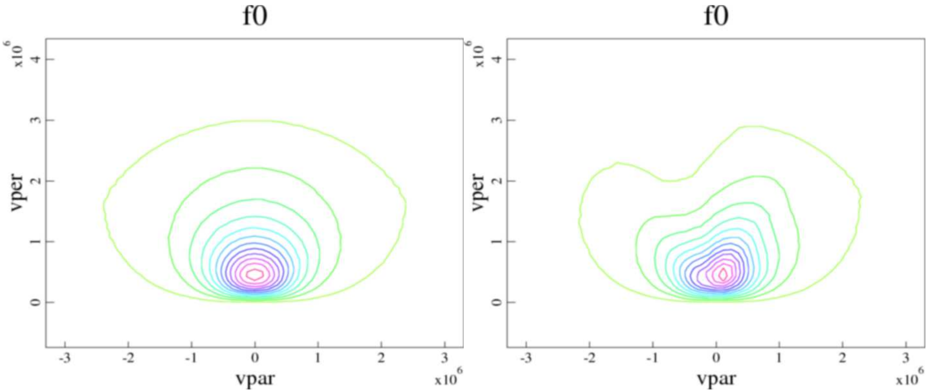
structure is stationary

Passing Only Dominated by Barely Passing Particles



displays more structure than all particle case

Finite Orbits lead to Particle Loss



- orbit loss in outer minor radius
- results in net flow $\Rightarrow$?impact on equilibrium?
- hot ion current!