

Status and Plans for δf PIC-MHD in NIMROD

Charlson C. Kim

Plasma Science and Innovation Center
University of Washington, Seattle

PSI-Center Meeting 2010
University of Washington
August 17, 2010

Outline

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 - PIC overview
 - Hybrid Kinetic MHD
 - PIC in FEM
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 - Lorentz particle traces in FRC
 - initial linear simulations
- 3 future directions
 - overview of future directions
 - performance improvements
 - algorithm improvements
 - future applications
- 4 conclusion

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 Hybrid Kinetic-MHD Equations

C.Z.Cheng, *JGR*, 1991

- $n_h \ll n_0$, $\beta_h \sim \beta_0$, quasi neutrality, MHD momentum equation modified by addition of 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 accommodate hot particles
- assumes equilibrium hot particle pressure is isotropic

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 \mathbf{V}_h is COM velocity of particles

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** moment $\delta p(\mathbf{x}) = \sum_{i=1}^N \delta f_i m (v_i - V_h)^2 S(\mathbf{x} - \mathbf{x}_i)$ on FE grid

- **advance** NIMROD field equations with hybrid Kinetic-MHD momentum equation

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

- particle dynamics augment fluid dynamics

PIC in FEM - nontrivial

- particles pushed in real space (R, Z) **but** field quantities in logical space (η, ξ)
- particle coordinate (R_i, Z_i) needs to be **inverted** to logical coordinates

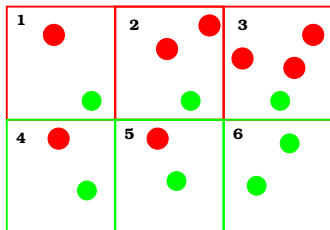
$$R = \sum_j R_j N_j(\eta, \xi), \quad Z = \sum_j Z_j N_j(\eta, \xi),$$

- iterative process
- sorting and parallelization done at same time
- sorting done by a bucket sort
- computationally most demanding - greatest room for performance increase

Particle Sorting

- Sorting is important because:
 - essential to domain decomposition
 - cache thrashing is minimized
- use “bucket” sort
- particles are sorted on global FE grid
- particles outside of processor sub-domain (rblock) are passed to their appropriate processor

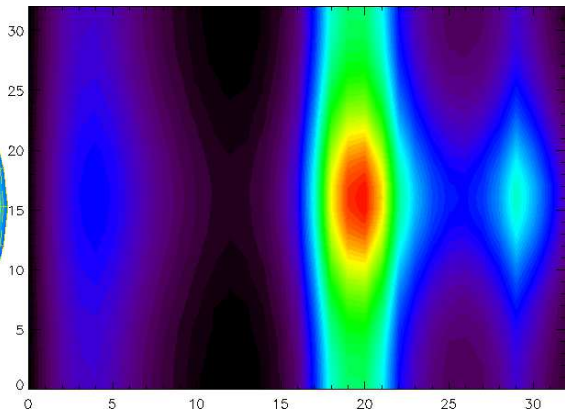
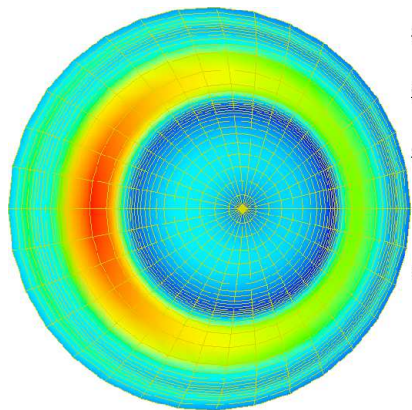
Bucket Sort



cell number	1	2	3	4	5	6
red count	1	2	3	1	1	0
green count	1	1	1	1	1	2
total count	2	3	4	2	2	2
local displacement	2	5	9	2	4	6

- number of particles in each element is tabulated (**red count**, **green count**)
- **total count** gives number of particles in each element
- displacement array is calculated from **total count** - bucket size is determined
- pass particles outside of subdomain (**red particle** to **green cells** and **green particles** to **red cells**)
- using displacement array, sorted particle list is filled

Nonuniform grid causes load balancing issues



PIC options

- two equations of motion available
 - drift kinetic equations of motion
 - full Lorentz force equations of motion
- eventually provide capability of direct comparison
- several distribution functions are available
 - slowing down distribution
 - Maxwellian
 - monoenergetic
 - monoenergetic, no v_{\parallel}
- several spatial profiles are available
 - proportional to MHD profile
 - uniform
 - peaked gaussian
- room for growth

δf and the Lorentz Equations

- Lorentz equations of motion

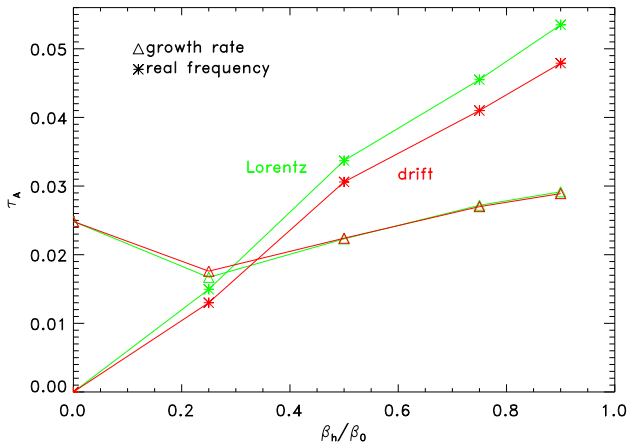
$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{v} \\ \dot{\mathbf{v}} &= \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B})\end{aligned}$$

- use Boris push
- weight equation is

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

Full orbit recovers drift kinetic

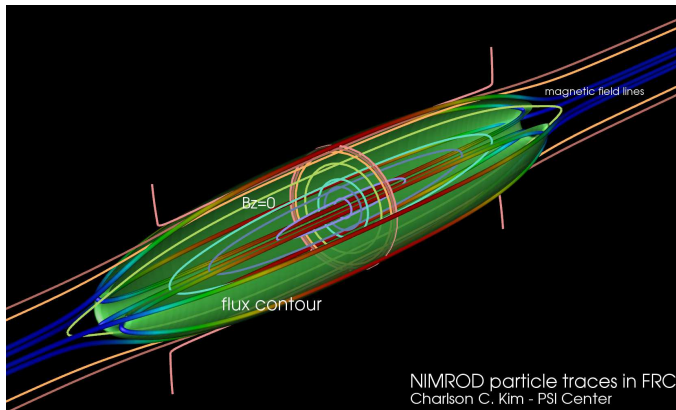
β_{frac} scan of (1, 1) benchmark kink



3 categories of orbits based on v_{phi} , λ at midplane

- thermal energy
 - mostly obeys $\rho \ll L$
 - mostly dominated by drift motion
 - long time orbit probably volume filling
- mid energy
 - classic “betatron” orbits
 - small integer “clover” orbit pattern
 - crosses the null
 - never reaches the axis
 - long time orbit usually traces a cylindrical annulus
- high energy
 - orbit pattern mode number $n = [0, 1]$
 - confined to outboard side of FRC
 - never crosses null
 - long time orbit traces a cylindrical shell

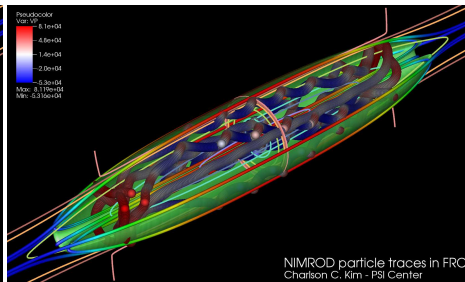
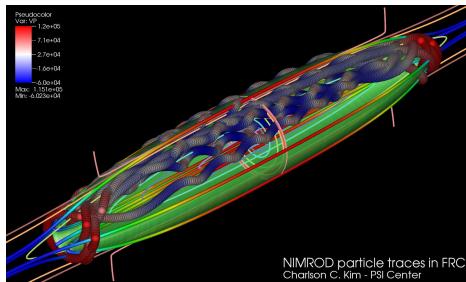
Lorentz particle traces in FRC



- examine particles orbits in equilibrium axisymmetric FRC field
- $|B|_{max} \simeq .1T$, $R_s = .4m$, $L = 4m$
- gradient is stronger outboard (vs. inboard)

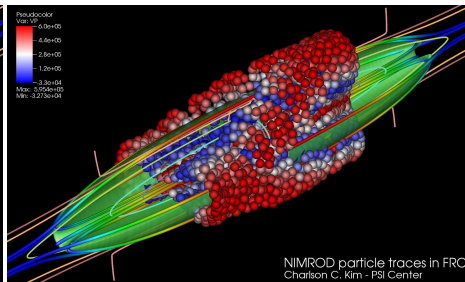
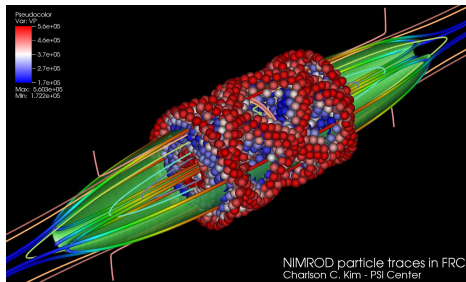
Lorentz particle traces in FRC

Low energy particles exhibit drifting cyclotron motion



- mostly gyromotion and drift motion (from ∇B drift) are apparent
 - particles are colored with v_ϕ
 - orbits are probably volume filling but on a **very** long time scale
- !!! demagnetizes at cusp

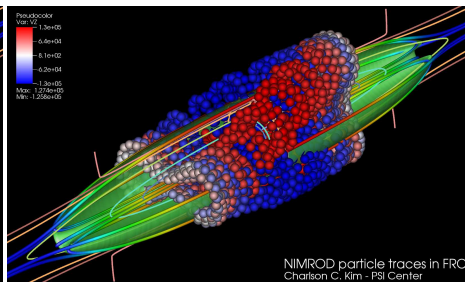
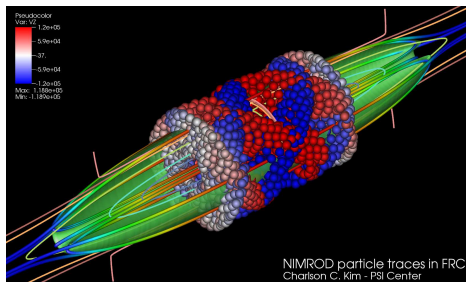
Mid-energy particles exhibit betatron



- betatron orbits with commensurate v_z form interesting structures
- both pictured orbits are $n \simeq 2$ “clover” pattern
- different “resonance” with v_z
- both orbits exhibit more structure than a cylindrical annulus

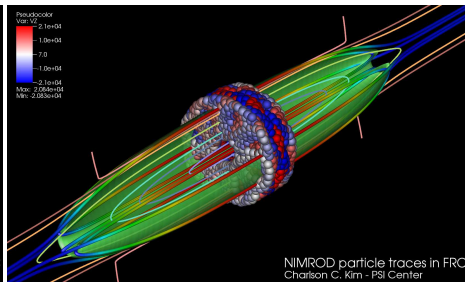
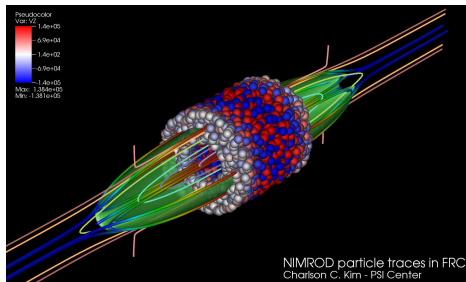
Lorentz particle traces in FRC

Mid-energy particles colored by v_z show even more structure



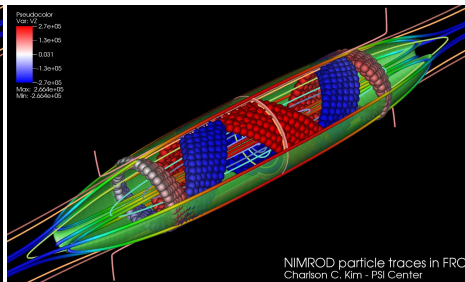
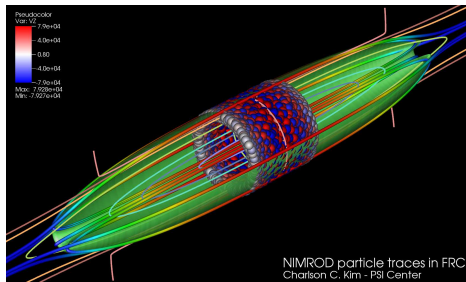
- bands of positive and negative v_z
- some orbits show a crystalline structure

More typical mid-energy particle orbit



- non-commensurate v_ϕ, v_z
- more typical mid-energy orbits $n \simeq 2, n \simeq 3$
- fills up the cylindrical annulus
- particular $n \simeq 3$ orbit has low v_z
- higher n penetrates deeper towards axis

Highest energy particle orbit entirely outboard

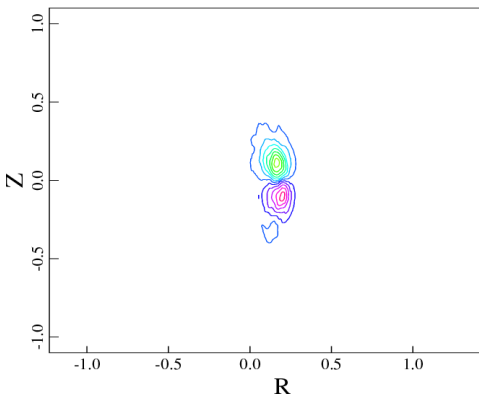
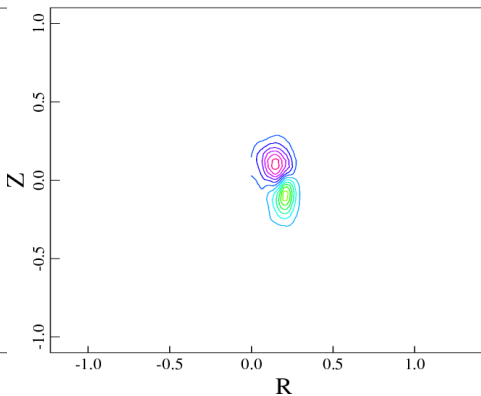


- orbit characterized by $n = 0, 1$
- $n = 0$ axisymmetric orbit, shell has no width
- $n = 1$ offset orbit, shell of small but finite width
- commensurate (wrt v_z) and non-commensurate orbits exist
- highest energy particles confined to outboard midplane!

Initial Linear Simulations

- working mechanically
- particles damp growth rate
- particles excite real frequency
- parity of particle pressure troubling → sign error?

Re P

Re Ph_{RR}

Future Directions

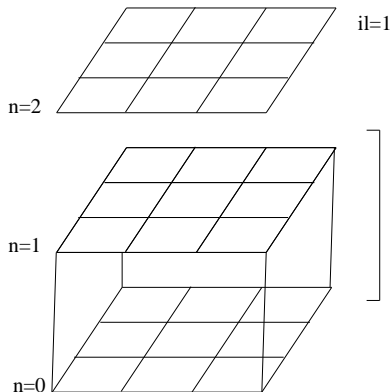
- improve performance
 - improve parallelization - decomposition with `nlayer`, domain cloning, asynchronous
 - improve efficiency - utilize sorted particle list, try type of arrays data structure
- improve algorithms
 - improve interpolation/deposition
 - full f option, hybrid nonlinear mode, multi-species, current coupling
- applications - details tomorrow
 - continue FLR tearing in RFP's
 - $m = 0$ edge mode (V. Mirnov, MST)
 - FRC applications and other ICC's (LDX, Bellan, SSX)
 - ? TAE's

Improvements to Parallelization

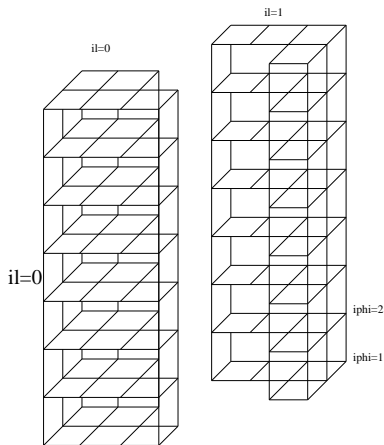
- decomposition with `nlayer`
 - work with NIMROD's domain decomposition (next slide)
 - forces deposition in real space
 - particles reside in `nlayer` subdomain of `rblocks`
- improve load balancing
 - particle based domain partitioner
 - decouple particle domain from field domain for better load balance
- domain cloning
 - redundant field solves (clone NIMROD domain)
 - increase particle statistics
 - rolloff at $n_{clones} \sim 10$
- asynchronous mpi calls - interleave communication and computation

Domain Decomposition with $n_{layer} > 1$

Normal Decomp



Configuration-space Decomp.



Improvements to Efficiency

- use exact solver for getting (η, ξ)
- use sorted list to decrease cache thrashing
- datatype - type of arrays
- advanced integrators

Improvements to Algorithms

- improve gather/scatter
 - H.O.F.E.
 - quadrature interpolation
 - advanced shape functions
- couple through current instead of pressure
 - better for zero β simulations
- full f PIC option
- hybrid nonlinear mode
- multi PIC species
- numeric f_0

Future Applications

stay tuned - tomorrow

Concluding Remarks

- work continues on δf Lorentz hybrid kinetic-MHD in NIMROD
- preliminary FRC kinetics are very interesting
- CEMM is funded
 - should free enough \$\$\$ for graduate student dedicated to FRC-PIC
 - allow focus on algorithm development
- visit with S. Parker to discuss
 - kinetic closures
 - sources
 - collisions