M3D-C^1-K

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NSTX-U Results Review

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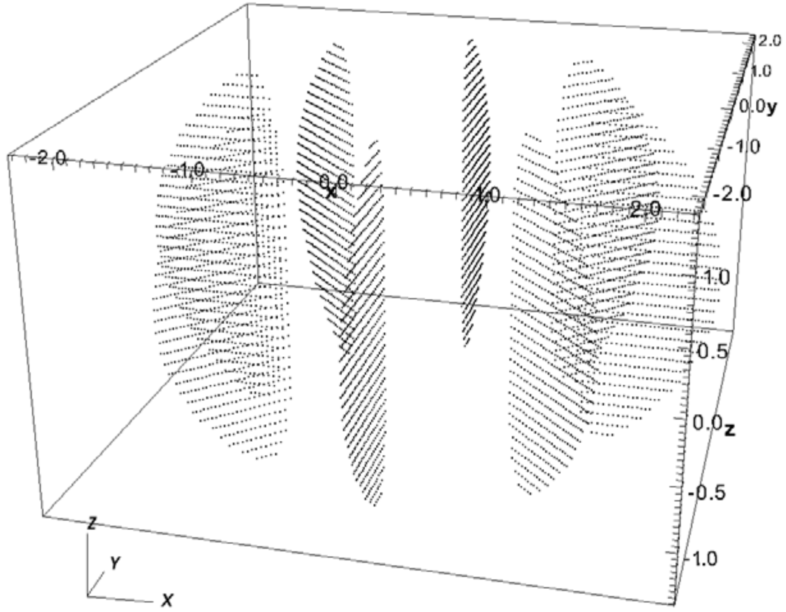
Background & Motivation

- M3D-C[1] is a mature nonlinear extended MHD code that has superseded the old M3D code for most tokamak applications because of its
  - Efficient, high-accuracy 5th-order-polynomial finite-element field representation with C^1 continuity
  - Fully implicit time advance scheme
  - More accurate model of gyroviscous stress and Hall terms, etc.
  - Fast 2D-complex mode of operation for linear problems
  - Finite-thickness resistive wall capability and in-mesh coils
  - Clean, modern Fortran programming paradigm

- A key remaining step to achieving feature parity with M3D-K is the development of a hybrid kinetic capability for energetic ions.

Particle loading

- Physical space initialization: uniform over (R,φ,z) cube with Jacobian to ensure uniformity over d^3x. Particles outside mesh rejected.
- Velocity space initialization: use Jacobian to initialize distribution uniformly on d^3v, with $0<|\mathbf{v}|<\mathrm{sqrt}(2E_{max}/m)$.
- Uniform particle weights.



Sample spatial distribution over four-partition KSTAR mesh:
5840 / 8192 = 32 x 8 x 32
particles deposited.

Particle push

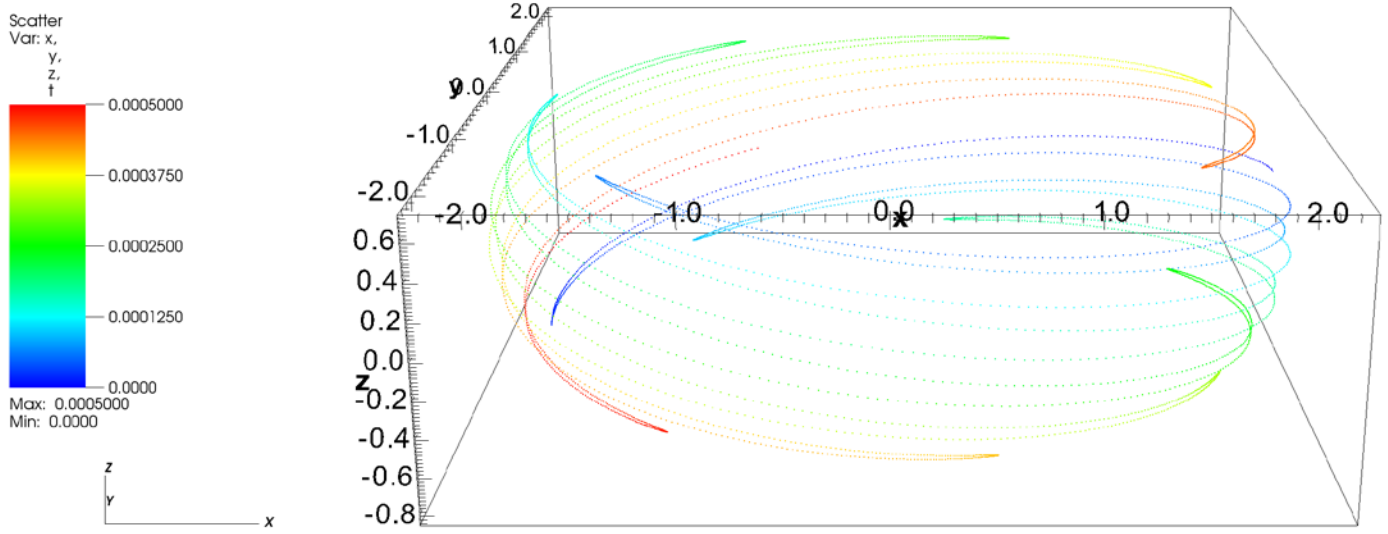
- Particles advance by a specified time increment between fluid steps, using given 2D (real or complex) or 3D fields, subcycling as necessary.

- Hierarchical organization of particles by element, element ensemble, OMP thread, and MPI/mesh partition allows good optimization.

- 4th- and 5th-order Runge-Kutta ODE integration have been implemented; both show good energy, P_φ conservation over many time steps.

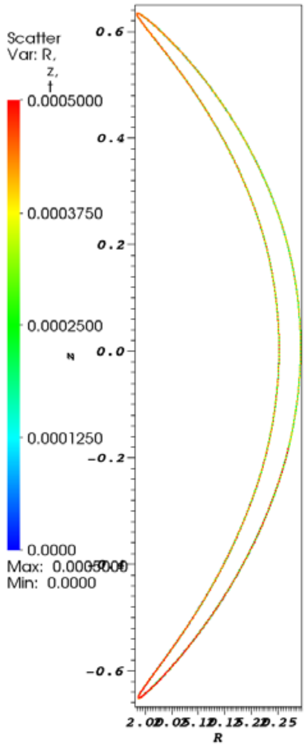
Sample trapped orbit ($\lambda_0 = 3\pi/5$)

- 5000 steps, dt (drift-kinetic)=10^{-7} s ≈ 5 gyroperiods.
- Initial KE=9.9995e+03 eV; final=9.9990e+03.
- Initial P_φ=-0.476633; final=-0.476630.



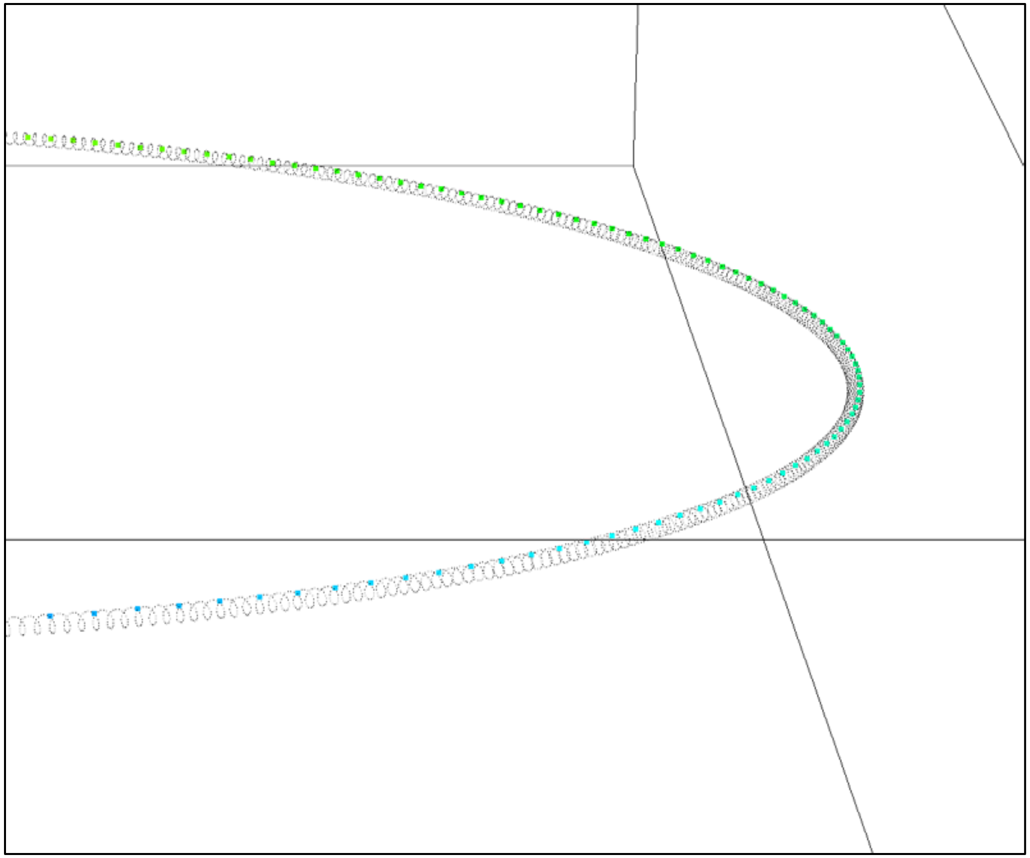
Colors indicate advancing time.

R-z plane projection



Drift-kinetic/full-orbit comparison

- Full-orbit: 20,480 steps, dt=10^{-10} s $\approx$ 0.005 gyroperiods.



Detail

- KE conservation for full-orbit is good, but angular momentum conservation is relatively poor.
- A drift-kinetic step is about twice as fast as a full-orbit step, and can be around 1600x larger for comparable accuracy.

Pressure deposition

- RHS vectors for $p_{||}$, $p_{\perp}$ computed by integrating over particle delta functions within each element.

- LHS vectors computed by mass matrix inversion for each component.
  - Very fast (time is independent of particle count).

Fluid coupling

- In progress!
- Plan: pressure coupling, i.e.,

$$n\left(\frac{\partial \mathbf{V}}{\partial t}+\mathbf{V}\bullet\nabla\mathbf{V}\right)=\mathbf{J}\times\mathbf{B}-\nabla p-\nabla\bullet\Pi_{visc}-\nabla\bullet\Pi_{hot} \tag{1}$$

where

$$\Pi_{hot}\equiv\left(p_{\|}-p_{\perp}\right)\hat{\mathbf{b}}\hat{\mathbf{b}}+p_{\perp}\mathbf{I} \tag{2}$$

so that if $\delta p \equiv p_{||}\text{-}p_{\perp}$, then

$$\nabla\bullet\Pi_{hot}=\left[\nabla\left(\delta p\right)\bullet\hat{\mathbf{b}}\right]\hat{\mathbf{b}}+\delta p\nabla\bullet\left(\hat{\mathbf{b}}\hat{\mathbf{b}}\right)+\nabla p_{\perp} \tag{3}$$

Fluid coupling, continued

- All terms in (3) are projected to the M3D-C^1 velocity representation with appropriate operators integrated by parts:

$$U : \iint d^2 R R^2 \nabla_\perp \nu_i \times \nabla \varphi \bullet ,$$

$$\omega : \iint d^2 R \nu_i R^2 \nabla \varphi \bullet ,$$

$$\chi : \iint d^2 R R^{-2} \nabla_\perp \nu_i \bullet ,$$

e.g.

$$R^2 \nabla \varphi \bullet \left[\nabla \bullet \left(\delta p \; \hat{\mathbf{b}}\hat{\mathbf{b}} \right) \right] = \frac{F}{B} \left(\hat{\mathbf{b}} \bullet \nabla \delta \mathbf{p} \right) + R \delta p \hat{\varphi} \bullet \nabla \bullet \left(\hat{\mathbf{b}}\hat{\mathbf{b}} \right)$$

I/O & Diagnostics

- The particle_test() subroutine writes out the entire trajectory of a predetermined subset of particles, tracking KE and P_φ .

- Subroutine hdf5_write_particles() uses parallel HDF5 to dump the entire particle distribution at a given time, including positions, velocities, and weights.
  - Utilities exist to extract position data from these to a text file, enabling comparisons and plotting with VisIt.
  - Utilities to visualize velocity distributions, pressure tensor components are now being developed.

- Checkpointing of particle distribution will be based on HDF5.

Summary

- Particle initialization, full-*f* push, pressure deposition, and I/O now working, tested and optimized for 2D complex version.
- Weight evolution, fluid coupling in progress.
- First linear validation tests on fishbone mode to be conducted in October.