CEMM Meeting Agenda

9:00	S. Jardin	News, Proposal Review discussion, and old milestone review
9:15	S. Jardin	M3D-C^1 update and plans / reconnection update
9:30	Josh Breslau	CDX-U new Equilibrium, new M3D results / Error field calculations
10:00	Carl Sovinec	NIMROD CDX-U update and other NIMROD Developments
10:30		Break
10:45	Alan Glasser	Preconditioning and Scalability with FETI-DP
11:15	Valorie Izzo	Disruption Calculations
11:45	Ping Zhu	FLR stabilization in extended MHD
12:15		Lunch – (on your own)
1:30	Nate Ferraro	2-Fluid equilibrium with flow
2:00	Hank Strauss	Spectral Elements in M3D
2:30	Guo-Yong Fu,	Energetic Particle Update and Plans
3:00	Scott Parker	Low Moment Kinetic MHD
3:30		Break
3:45	Alexei Pankin	NIMROD ELM modeling
4:15	L. Sugiyama	ELM Modeling and Toroidal effects on Gyrokinetic and fluid models
4:45	Scott Kruger	RMP simulations using NIMROD
5:15	D. Schnack	SWIM Slow MHD Campaign
5:45	Eric Held	LMP Closures
6:15	Jesus Ramos	Fluid-Kinetic Parallel Closures and Discussion of Model problems
6:45	all	Planning and review of new milestones
7:00		adjourn --- discussions can be continued over drinks and dinner

Center for Extended Magnetohydrodynamic Modeling

Rosen Centre Hotel, Salon 11

Orlando, FL

November 11, 2007

Reviewer Comments (strengths)

- research team has excellent qualifications in computational plasma physics, and has made excellent progress in recent years: publications and workshops
- state-of-the art techniques being applied to key problems
- NIMROD and M3D effectively use DOE HPC capability
- building on established framework, but proposing significant advances
- comparing with experimental results
- have effective ties with physics community and with some applied math and CS. project will enhance productive interaction between exp, theory, CS
- benchmarking vs analytic results
- benchmarking the two codes against each other is very powerful
- educational benefits are substantial (Grad Students, Postdocs)
- spin-offs demonstrated to space and astrophysics

Reviewer Comments (weaknesses)

- deficiencies in composition of research team and research methodology
  - case for spectral elements not made
  - did not discuss conservation properties of discretization scheme
  - discussion of time integration very unsophisticated. do not consider global long time accuracy
  - V&V discussion very weak. Comparing results from two codes or from a code to an experiment without some analysis of uncertainty is meaningless. Need to go beyond “picture-norm” and manufactured solutions.
- did not put proposal in context of what other groups are doing
- Overly ambitious. Would rank ELMs, NTM physics, RWM issues highest
- Should consider modeling NB or ICRH stabilized sawteeth
- NTM studies should include such things as ion polarization current, and how these effects scale to ITER parameters
- Can we include 3D wall in RWM studies? Coupling of RWM and ELMs.
- Present discretizations may not be ideal for newer closures.
- Should include TAE modes and impact on energetic alpha transport.

Workshop Planning

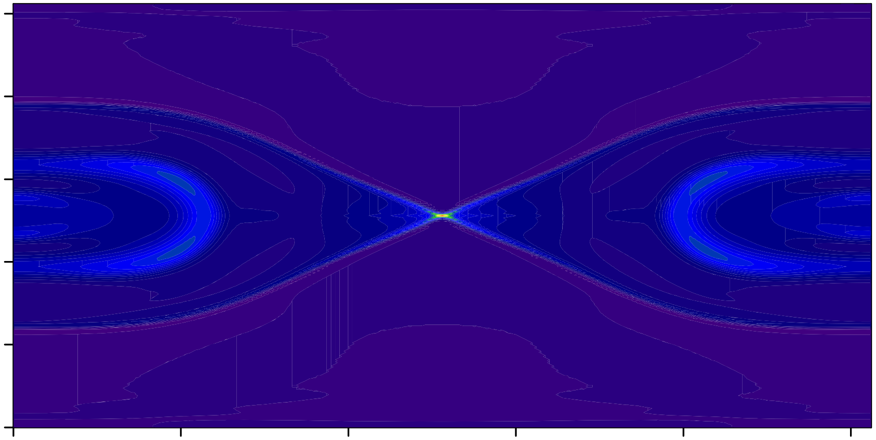
- Should we sponsor a workshop next summer?

- Possible topics
  - implicit time advance methods for MHD
  - validation and verification of physics codes
  - computational modeling of ELMs/RWMs
  - RMP physics
  - Closures -2
  - other

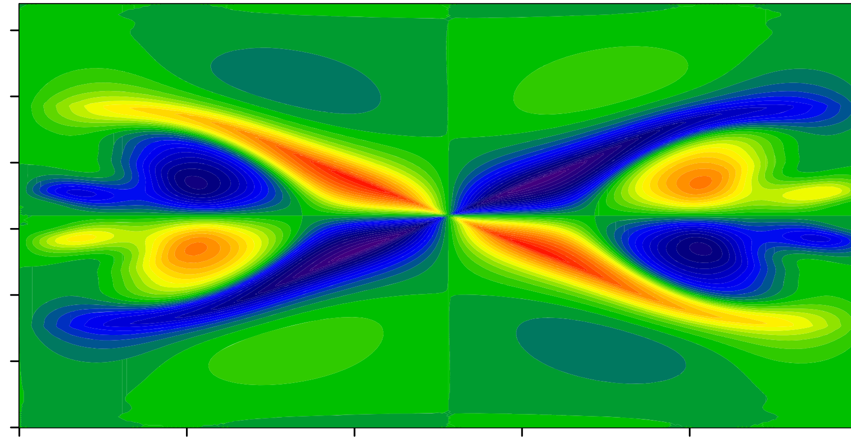
M3D-C^1 update

- new time advance
  - improved numerical stability (very high resolution cases now stable!)
  - improved convergence in Δt (especially in steady state...see Ferraro)
- 2D code now toroidal, with fully unstructured triangular elements
  - uses RPI tools to hide parallelism and mesh functions, adaptivity
- 2D code restructured to use SuperLU via PETSc
  - can now easily compare different solvers, natural extension to 3D
- toroidal 2F equilibrium with flow (Ferraro)
- 2D magnetic reconnection with GF
  - now shows good energy conservation
  - initial comparison with NIMROD shows GF inhibits GEM reconnection
  - exploring parameter regime: $\delta \ll \rho_S \ll c/\omega_{Pi}$
- 3D linear and nonlinear equations for matrix elements derived
  - With Breslau, Ferraro, M3D team (50 pages)
  - option being added for complex matrices (3D linear) results by Jan 1?
  - 3D nonlinear iterative solve being implemented

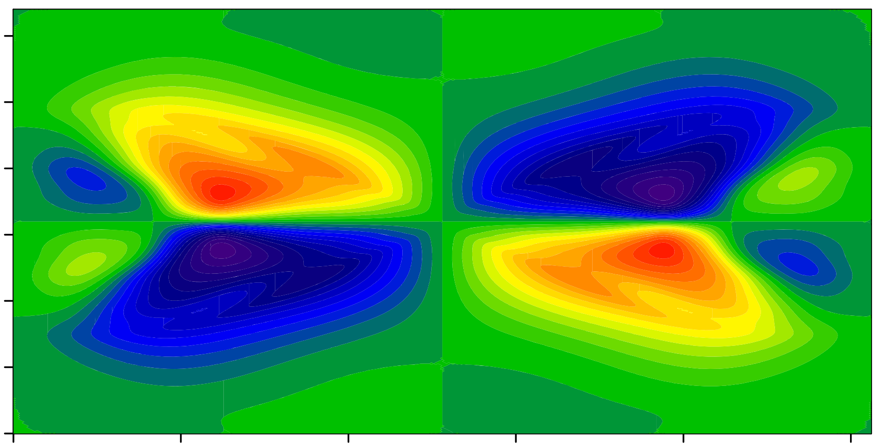
2F GEM Reconnection snapshot at time of maximum velocity (200^2 nodes)



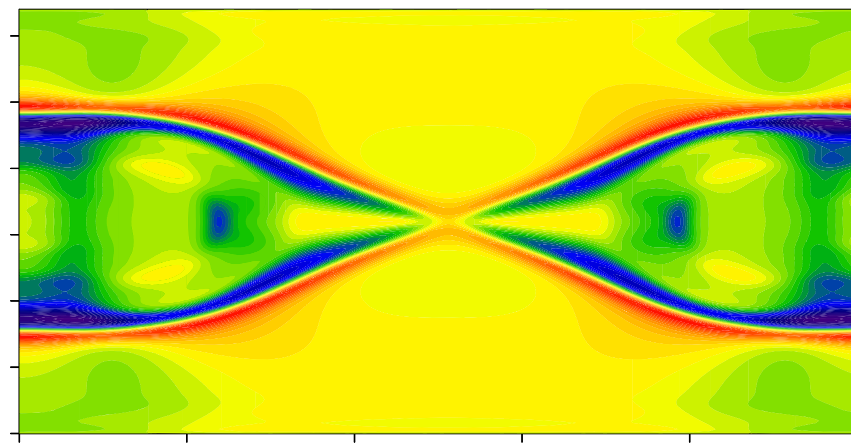
out-of-plane current



out-of-plane magnetic field



vorticity field



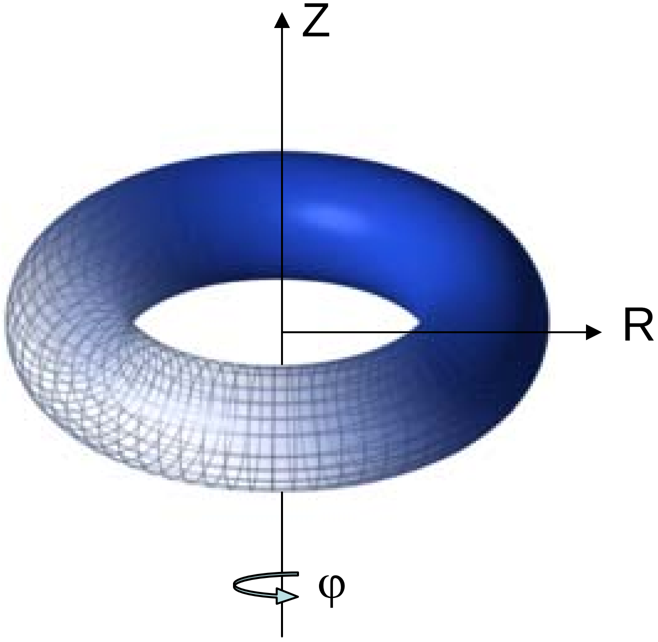
velocity divergence

Energy conservation to 1 in 10^3, flux conservation exact.

$$\mathbf{M} \equiv \left\{\rho - \theta^2 (\delta t)^2 L\right\} \mathbf{V}^{n+1} - \left\{\rho - \theta^2 (\delta t)^2 L\right\} \mathbf{V}^{n} + \delta t \left\{ \nabla p - \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \mathbf{B} \right\} = 0$$

3D M3D-C^1

$$L\{\mathbf{V}\} = \frac{1}{\mu_0} \left\{ \nabla \times \left[\nabla \times \left(\mathbf{V} \times \mathbf{B} \right) \right] \right\} \times \mathbf{B} + \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \left[\nabla \times \left(\mathbf{V} \times \mathbf{B} \right) \right]$$
$$+ \nabla \left(\mathbf{V} \bullet \nabla p + \gamma p \nabla \bullet \mathbf{V} \right)$$



$$\mathbf{V} = \nabla U \times \nabla \varphi + \nabla_{\perp} \chi + v \nabla \varphi$$

$$\mathbf{A} = R^2 \nabla \varphi \times \nabla f + \psi \nabla \varphi \qquad p, p_e, \rho$$

- 8- scalar 3D variables + gauge condition
- 2D triangular C^1 finite elements, FD in φ

$$-\iint dRdZRv_i R^2 \nabla \varphi \bullet \nabla \times \mathbf{M} = 0$$

$$\iint dRdZRv_i R^2 \nabla \varphi \bullet \mathbf{M} = 0$$

$$\iint dRdZRv_i \nabla_{\perp} \bullet \mathbf{M} = 0$$

$\theta(\theta - 1) \rightarrow \theta^2$

new gauge for **A**

- turn crank for 50 pages

Solver Strategy

- In 2D, solve efficiently with direct solver up to $(200)^2$ nodes
- In 3D, leads to block triangular structure

$$
\begin{bmatrix}
\mathbf{B}_1 & \mathbf{C}_1 & & & & & & \mathbf{A}_1 \\
\bullet & \bullet & \bullet & & & & & \\
 & \bullet & \bullet & \bullet & & & & \\
 & & \mathbf{A_j} & \mathbf{B_j} & \mathbf{C_j} & & & \\
 & & & \bullet & \bullet & \bullet & & \\
 & & & & \bullet & \bullet & \bullet & \\
 & & & & & \bullet & \bullet & \bullet \\
\mathbf{C_N} & & & & & & \mathbf{A_N} & \mathbf{B_N}
\end{bmatrix}
\bullet
\begin{bmatrix}
x_1 \\ . \\ x_{j-1} \\ x_j \\ x_{j+1} \\ . \\ . \\ x_N
\end{bmatrix}
=
\begin{bmatrix}
y_1 \\ . \\ y_{j-1} \\ y_j \\ y_{j+1} \\ . \\ . \\ y_N
\end{bmatrix}
$$

Block Jacobi preconditioner corresponds to multiplying each row by $\mathbf{B}_\mathbf{j}^{\mathbf{-1}}$

2-variable (reduced MHD) subset in 3D

$$\Delta^* \dot{U} = -R^2 \left[\frac{\Delta^* \dot{U}}{R^2}, U \right] + R^2 \left[\frac{\Delta^* \psi}{R^2}, \psi \right] + \frac{F}{R^2} \Delta^* \psi' + \left(\frac{F}{R^2}, \psi' \right)$$

$$\nabla \bullet \frac{1}{R^2} \nabla_\perp \dot{\psi} = -\nabla \bullet \frac{1}{R^2} \nabla_\perp [\psi, U] + \nabla \bullet \frac{1}{R^2} \nabla_\perp \eta \Delta^* \psi + \nabla \bullet \frac{1}{R^2} \left[\frac{F}{R^2} \nabla_\perp U' + \eta \frac{1}{R^2} \nabla_\perp \psi'' \right]$$

$$[a,b] = \nabla a \times \nabla b \bullet \nabla \varphi$$

$$(a,b) = \nabla_\perp a \bullet \nabla_\perp b$$

$$\nabla_\perp a = a_R \hat{r} + a_Z \hat{z}$$

$$(\ )' \equiv \frac{\partial}{\partial \varphi} (\ )$$

$$\Delta^* \equiv R^2 \nabla \bullet \frac{1}{R^2} \nabla_\perp$$

- energy theorem

$$\iiint \frac{1}{R^2} (\psi, \dot{\psi}) + \frac{1}{R^2} \left(U, \dot{U} \right) = -\frac{\eta}{R^2} \left[(\Delta^* \psi)^2 + \frac{1}{R^2} (\psi', \psi') \right]$$

- solving in linear (~ $e^{in\varphi}$) and nonlinear (FD in φ) codes as warm-up
- *F* = constant for reduced MHD (uniform TF0

FY07 Milestones

- Perform new linear and nonlinear m=1 mode comparison with analytic equilibrium
- ELM studies: detailed comparison between ideal, resistive MHD, 2F
- GEM nonlinear reconnection with guide field
- Scaling studies with NIMROD and M3D beyond 10,000 processors

Table I: Physics Model Development Milestones

Topic	Year 1	Year 2	Year 3
Analytic test problems	- Define critical tests for 2F equilibrium with flow (FC,PP) -Define 2-fluid slab drift tearing test case (FC,EP,PP)	-Detailed comparison of 2F equilibria with flow with analytic results. (FC,PP) -Define simplified m=1 2F test problem (FC,EP,PP) -Convergence studies of drift tearing (FC,EP,PP)	- Complete 2F drift-tearing and m=1 mode analytic studies and numerical benchmarks (FC,EP,PP)
Stochastic Transport	-Develop chaotic-coordinate technique (PP)	-Compare chaotic-coordinate with non-local conduction in model problem (PP,US)	- Implement chaotic-co-ordinate method in M3D (PP)
Implicit Electron Stress	- Implement the terms that allow non-uniform electron viscosity profiles(EP)	-Implement non-linear terms and begin testing stability (EP,US)	-Evaluate bootstrap current and test for NTM behavior in fluid model (EP, US)
Kinetic-Ion MHD	-Verify the kinetic ion MHD closure model against linear kinetic theory of Alfven, whistler, and ion Landau damping of ion acoustic waves.(UC)	-Compare current closure and pressure closure models for linear and non-linear simulations. Test energy conservation (UC)	-Study ion kinetic effects on the nonlinear evolution of a magnetic island. (UC,US) - Comparison with nonlocal parallel closures. (UC,US)
Nonlocal Parallel Closures	-Apply steady-state, parallel heat flow closure in heat transport studies. (US)	- Develop time-dependent, continuum solution of Chapman-Enskog-like, drift kinetic (CEL-DKE) equ. in NIMROD. (US)	Test solution of CEL-DKE by comparing with kinetic-ion MHD closure for ion Landau damping and 2F simulations and theory for drift tearing modes. (US,UC)

Table II: Code and Algorithmic Development Milestones

Topic	**Year 1**	**Year 2**	**Year 3**
Spectral elements in M3D	-fully implement Spectral Elements in M3D (PP,NY)	-Evaluate and optimize parallel scaling (PP,NY)	-Integrate Spectral Elements with new more implicit time advance in M3D (PP,NY)
M3D-C^1 development	-Calculate accurate toroidal equilibrium with flow in toroidal geometry (PP)	-Calculate linear 3D stability with spectral expansion (PP)	-Test full 3D implicit solve using block relaxation method. (PP)
M3D Vacuum	- Add Lust-Martinson terms to VACUUM (PP)	-Install VACUUM in M3D (PP)	- Install VACUUM in M3D-C^1 (PP)
Parallel Scalability	-Implement FETI-DP on 2D structured grid (LA) -Remove the static condensation steps within NIMROD to test SuperLU scaling with larger work-loads per processor (EP)	-Port FETI-DP to other 2D grids (LA) -Assist and evaluate SAP efforts with an incomplete-factorization version of SuperLU. (EP)	-Test FETI-DP in 3D (LA) - Investigate multi-grid (through PETSc) as an alternative preconditioner for poloidal coupling in NIMROD (EP)
NIMROD Basis Functions	-Continue tests of MHD interchange in comparison with analytical results. (EP) -Formulate implementation of additional DOF for vector fields.(EP)	-Implement new basis functions for vector fields and compare interchange behavior with original (EP)	-Verify two-fluid drift stabilization of interchange using the new basis functions.(EP)
NIMROD Preconditioning	-Formulate preconditioning for toroidal coupling in the implicit Hall advance. (EP) -Begin implementation of new algebraic systems with existing preconditioners (EP)	-Complete implementation and test in different computations. (EP) -Test use of the new algebraic systems as an additive pre-conditioning step.(EP)	-Implement algebraic systems for preconditioning toroidal coupling in the flow-velocity and temperature advances.(EP)
Newton-Krylov (NK) Solves and Time-centered Advance in NIMROD	-NK evaluation in 2D (TX) - Modify NIMROD to provide nonlinear iterations to achieve time-centering and compare with the existing semi-implicit algorithm. (EP)	-Initial NK in simplified 3D (TX) -Modify NIMROD to compute the residual of a state vector for matrix-free Newton-Krylov. (EP)	-Full NK in toroidal geometry (TX) -Implement the matrix-free NK method using PETSc to test preconditioning based on NIMROD's existing advance. (EP)

Table III. Application Milestones

Topic	Year 1	Year 2	Year 3
Sawtooth	-M3D/NIMROD benchmark with CDX-U boundary conditions and parameters (TX,EP,PH,PP)	-Study of 2-fluid effects on sawtooth (TX, EP, PH, PP)	-2-fluid simulations at large S and with energetic particles (TX, EP, PH, PP)
Neoclassical Tearing Mode	-Setup and test equilibrium and closures for neoclassical tearing mode simulations(US (TX,EP,PH,US)	-Begin simulations using nonlocal closures for parallel heat flow and electron stress.(TX,EP,PH,US)	-Continue massively parallel NTM simulations with nonlocal closures (TX,EP,PH,US)
Edge Localized Modes (ELMs)	-Continue verification of M3D and NIMROD with ELITE and extend to 2F and nonlinear (TX,NY,GA)	-Perform nonlinear simulations in ITER geometry (NY,GA)	-Study nonlinear effect of RMP on ELMs (NY,GA) - Incorporate nonlocal parallel closures (US) .
Resistive Wall	- Setup of ITER double wall in VACUUM (TX,PP,NY)	- Benchmark 2F with MARS (TX,PP,NY)	-Nonlinear simulations in ITER geometry (TX,PP,NY)
Error Field (EF) Studies	Plan and define error field studies for NSTX (PP)	Begin systematic study of EF studies in NSTX (PP)	Produce a publication on EF studies in NSTX (PP)
Disruption Mitigation Studies	Run Argon and Helium simulations for C-Mod (GA)	Complete DIII-D simulations for sym vs. non-sym fueling (GA)	Compare mitigated and unmitigated DIII-D free-boundary disruptions(GA)

Institutions

- (PP) PPPL,
- (NS) MIT-LNS,
- (FC)-MIT-PSFC,
- (NY)-NYU, (
- EP)-U. Wisc. Engin. Phys.,
- (LA) LANL,
- (US) Utah State U.,
- (GA) General Atomics,
- (TX) Tech-X,
- (UC) U. Colorado,
- (PH) U. Wisc. Physics.