Center For Extended Magnetohydrodynamic Modeling

S. C. Jardin for the CEMM consortium

Presentation to the Fusion SciDAC PAC

August 3, 2001

PPPL

The CEMM Consortium:

GA: D.Schissel
LANL: (T. Gianakon, R. Nebel) ?
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NYU: H. Strauss
PPPL: J. Breslau, G. Fu, S. Hudson, S.Jardin , W. Park
SAIC: S. Kruger, D. Schnack
U. Colorado: C. Kim, S. Parker
U.Texas: F. Waelbroeck
U.Wisconsin: J. Callen, C. Hegna, C. Sovinec
Utah State: E. Held

Outline

- CEMM Background and Motivation
- PSACI Progress
- SciDAC Activity Areas
- CSET Partners
- Application Areas
- Resource Distribution and Task List

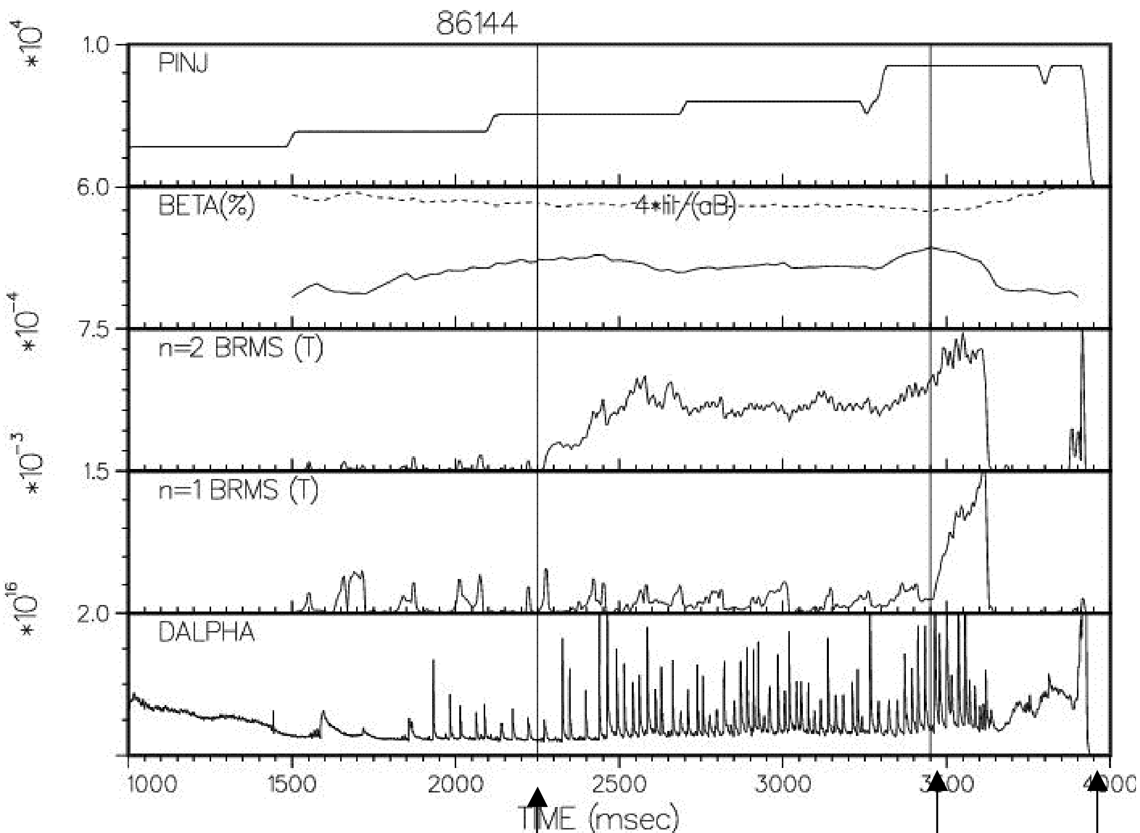
Background

"*…to* *develop* *and* *deploy* *predictive computational models for the study of low frequency, long wavelength fluid-like dynamics in the diverse geometries of modern magnetic fusion devices.*"

- High programmatic motivation:
  - disruptions, sawteeth, current, and beta limits
- Need for improved plasma models:
  - FLR, anisotropy, long MFP
- Need for improved computational techniques:
  - Extreme separation of time and space scales, and extreme anisotropy
  - Efficiency, visualization, data base management, code support

- **NIMROD** and **M3D** codes form basis: build on these assets

Experimental Observations



LaHaye

Neoclassical Tearing Mode growth begins

Disruption

Modes “lock” to wall

<u>Model Requirements</u>

- Realistic geometry
- Realistic parameters
- Long time-scales
- Realistic boundaries
- Anisotropic heat flux
- Neoclassical effects
- Two-fluid effects
- Kinetic extensions
- Energetic particles

Plasma Models: XMHD

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E}$$

$$\vec{E} + \vec{V} \times \vec{B} = \eta \vec{J} + \frac{1}{ne}\left[\vec{J} \times \vec{B} - \nabla \bullet P_e\right]$$

$$\mu_0 \vec{J} = \nabla \times \vec{B}$$

$$P = pI + \Pi$$

$$\rho\left(\frac{\partial \vec{V}}{\partial t} + \vec{V} \bullet \nabla \vec{V}\right) = \nabla \bullet P + \vec{J} \times \vec{B} + \mu \nabla^2 \vec{V}$$

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \vec{V}) = S_M$$

$$\frac{3}{2}\frac{\partial p}{\partial t} + \nabla \bullet \left(\vec{q} + \frac{5}{2} P \bullet \vec{V}\right) = \vec{J} \bullet \vec{E} + S_E$$

$$\frac{3}{2}\frac{\partial p_e}{\partial t} + \nabla \bullet \left(\vec{q}_e + \frac{5}{2} P_e \bullet \vec{V}_e\right) = \vec{J} \bullet \vec{E} + S_E$$

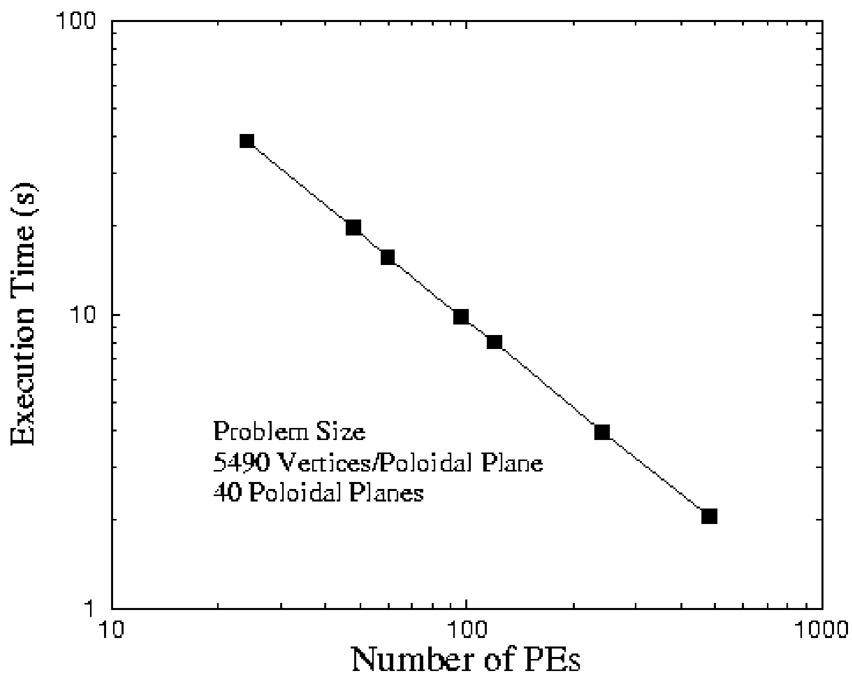
Two-fluid XMHD: define closure relations for $\mathbf{\Pi_i}$,$\mathbf{\Pi_e}$, $\mathbf{q_i}$, $\mathbf{q_e}$

Hybrid particle/fluid XMHD: model ions with kinetic equations, electrons either fluid or by drift-kinetic equation

Simulation Codes:

NIMROD: semi-implicit time integration, 2D quad and triangular finite elements+ pseudospectral, grid packing, AZTEC, MPI

M3D: quasi-implicit time integration, stream-function/potential representation, 3D Mesh, PETSc, MPI



Required Resources

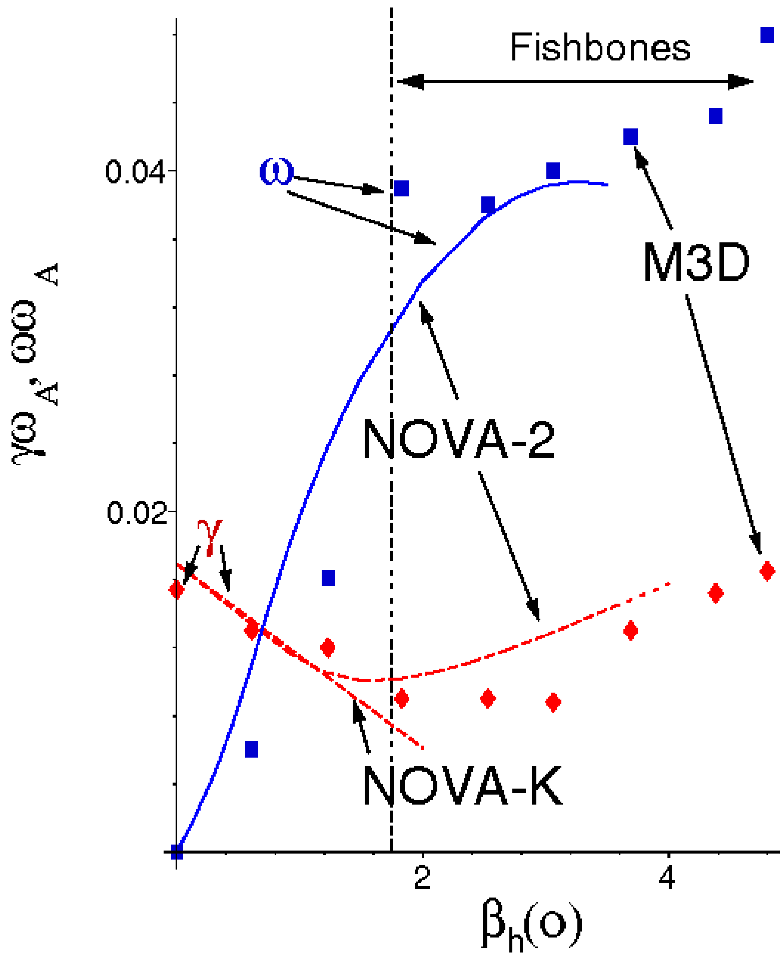
parameter	name	CDXU	NSTX	CMOD	DIII-D	FIRE	ITER
R(m)	radius	0.3	0.8	0.6	1.6	2.0	5.0
Te[keV]	Elec Temp	0.1	1.0	2.0	2.0	10	10
β	beta	0.01	0.15	.02	0.04	0.02	0.02
$S^{1/2}$	Res. Len	200	2600	3000	6000	20000	60000
$(\rho^*)^{-1}$	Ion num	40	60	400	250	500	1200
$a/\lambda e$	skin depth	250	500	1000	1000	1500	3000
P	Space-time	$\sim 10^{10}$	$\sim 10^{13}$	$\sim 10^{14}$	$\sim 10^{14}$	$\sim 10^{15}$	$\sim 10^{17}$

Estimate $P \sim S^{1/2} (a/\lambda e)^4$ for uniform grid explicit calculation. Adaptive grid refinement, implicit time stepping, and improved algorithms will reduce this.

Progress on PSACI Workscope:

- ✓ Series of Test Problems
  - Ideal MHD,
  - Resistive MHD,
  - 2-fluid,
  - Hot-Particle TAE
- ✓ Resistive Wall Mode
- ✓ Stellarator Physics
- ✓ Linear Solver Improvement
- ✓ Scaling to Large Processor Number
- ✓ Common Interfaces
- ✓ Data Management
- ✓ Visualization

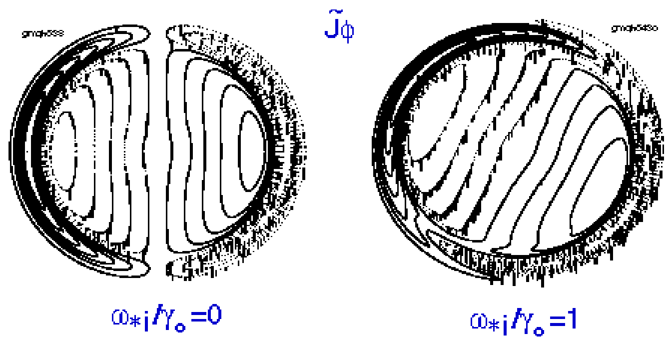
Hot Particle Test Case

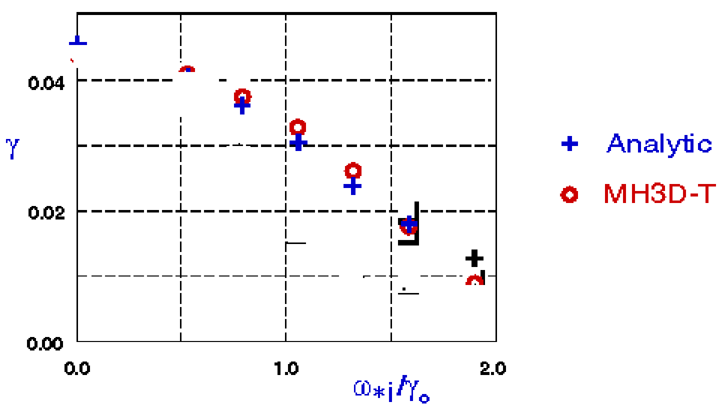


Fu

- M3D agrees well with NOVA-2 in linear regime
- NIMROD still adding hybrid-particle option
- Expect to have M3D/NIMROD comparison by APS

2-Fluid Test Case

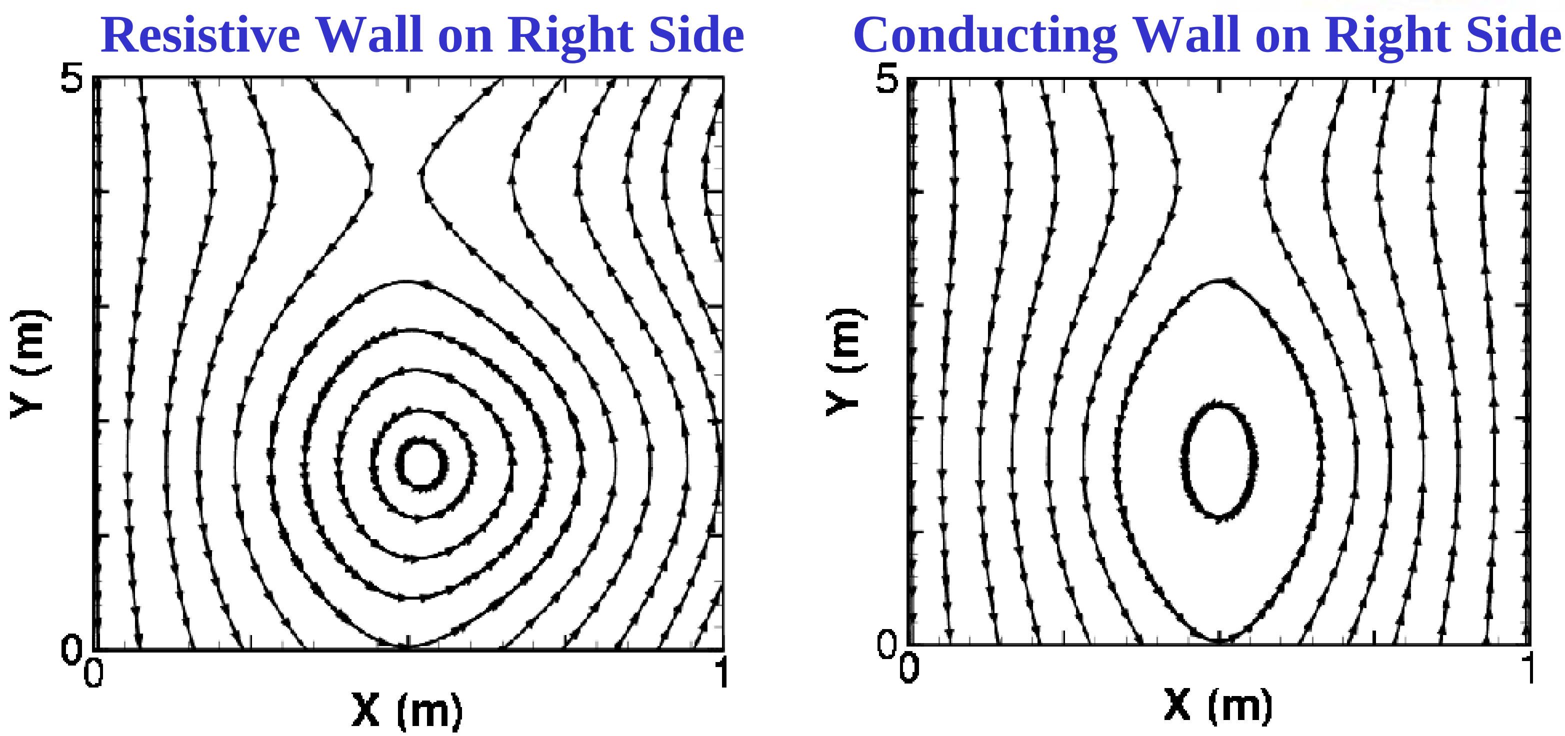




Sugiyama

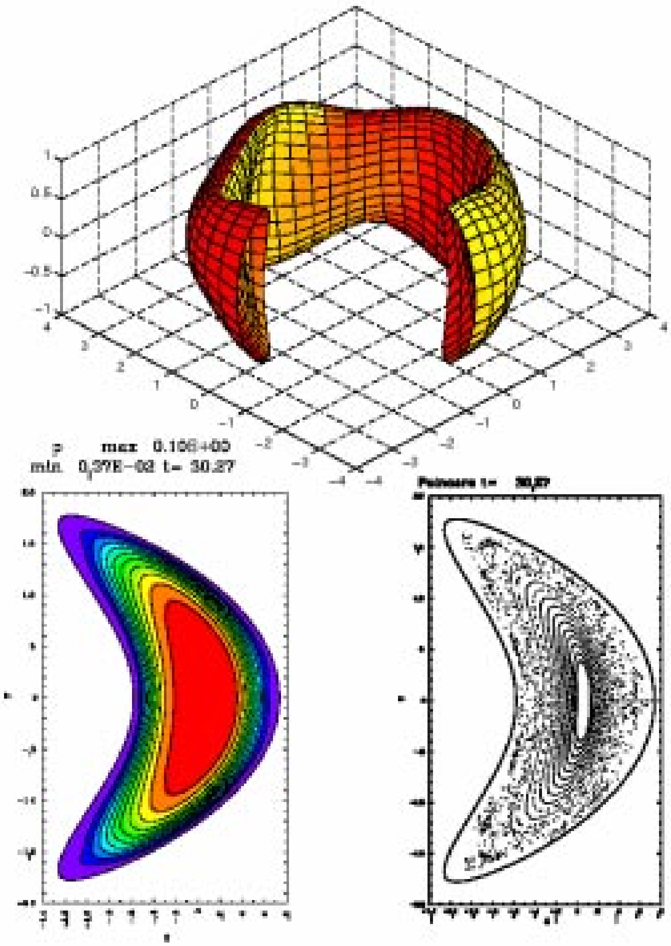
- M3D agrees with Zahkarov/Rodgers analytic model
- NIMROD getting different result – destabilizing rather than stabilizing
- Trying to isolate difference..model or bug?

Resistive Wall Modes:



- Resistive wall boundary conditions are being incorporated in both NIMROD and M3D using (same) GRIN module.
- Tearing mode unstable sheared slabs used for benchmarking saturate at a larger island width with the non-ideal (resistive) wall.

Stellarator Physics:



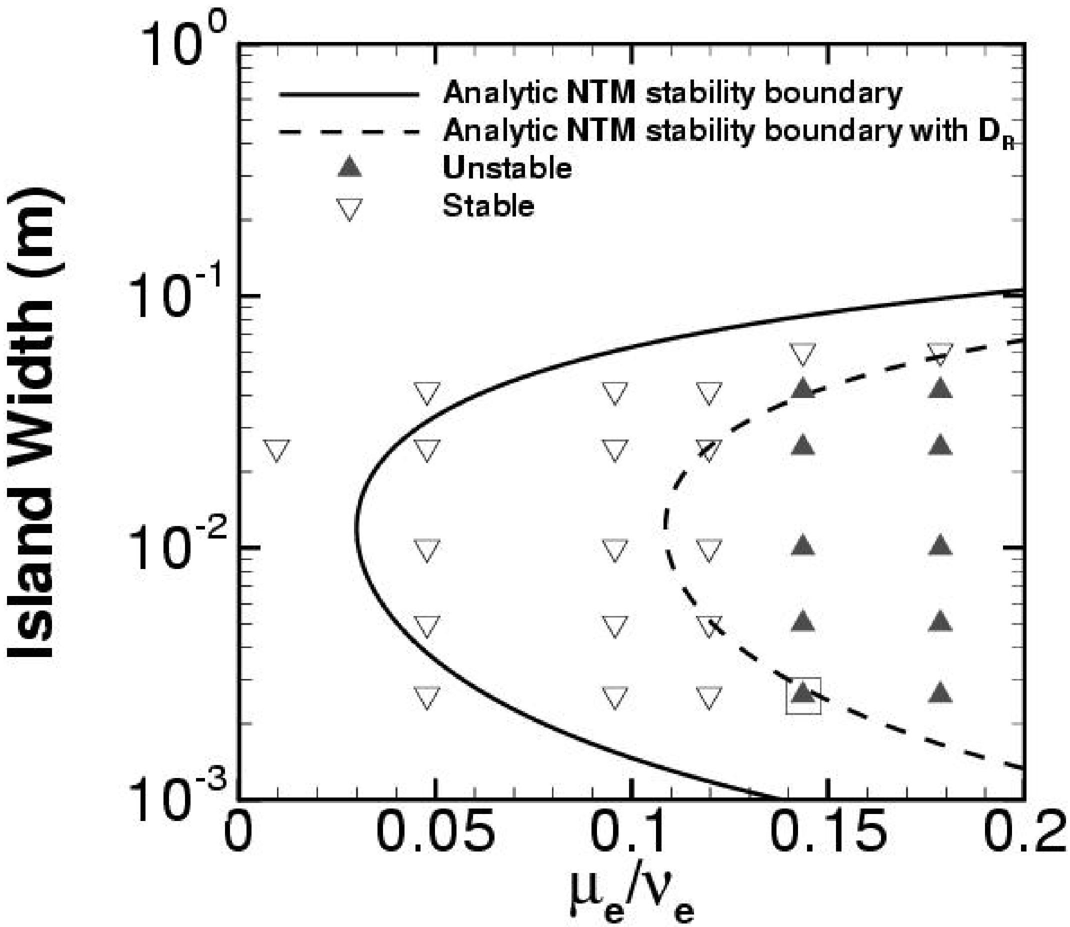
- NCSX design examined for flux surface quality and non-linear stability

- Issues associated with accuracy and resistive ballooning for D_R unstable configurations

- Stellarator capability now in MPP version

Strauss

Neoclassical Tearing Mode



- Analytic-based closure now in NIMROD ohms law
- Gives good agreement with theory for stability boundary
- Now concentrating on sawtooth trigger

Gianagon

CEMM Activity Areas:

- Code Development
- Model Development
- Visualization and Data Management
- CSET Collaborations
- Code Support
- Applications and Validations

Code Development

- Expanded use of Implicit Techniques
  - Implicit treatment of the Hall term and advective terms
  - Incorporate gyroviscosity free of time step restriction
  - Optimize parallel algorithms for elliptic terms
- Kinetic Closures for majority species
  - Trajectory tracking in non-uniform and unstructured mesh
  - Implementing δf /CEL closures into efficient time advance
- Improved and adaptive meshing
  - Improved and generalized mesh generation
  - Implement a field-aligned mesh
  - Implement mesh adaptivity

Model Development

- Kinetic Modeling Framework
  - δf with evolving Maxwellian
  - Simulation Particles or Chapman-Enskog-Like expansion
- Kinetic Modeling of Ions through Simulation Particles
  - Heat flux and stress tensor computed from particle moments
- Kinetic Modeling of Electrons through CEL closure
  - Basis functions used to solve gyro-averaged drift-kinetic equations
  - Small parameter is the small parallel gradients
  - Parallel integrations similar to simulation-particle tracking

Visualization and Data Management

- Evaluate, build-on, and expand pilot project started under PSACI funding
  - Store NIMROD and M3D data in MDSplus
  - Track runs using SQL server
  - AVS and IDL based visualization packages
  - Efficiency issues
- Develop higher dimensional data exploration tools
  - Find correlations
  - Visualize subspaces
  - Find data characterized by a particular formula

Computer Science Enabling Technology Partners

- Terascale Simulation Tools and Technologies (TSTT) **PI:** James Glimm
- Terascale Optimal PDE Simulations Center (TOPS) **PI:** David Keyes
- An Algorithmic and Software Framework for Applied Partial Differential Equations
  PI: Phil Collela
- National Fusion Collaboratory Pilot project
  PI: David Schissel

NOTE: also collaborations with major fusion experiments

Terascale Simulation Tools and Technology (TSTT)

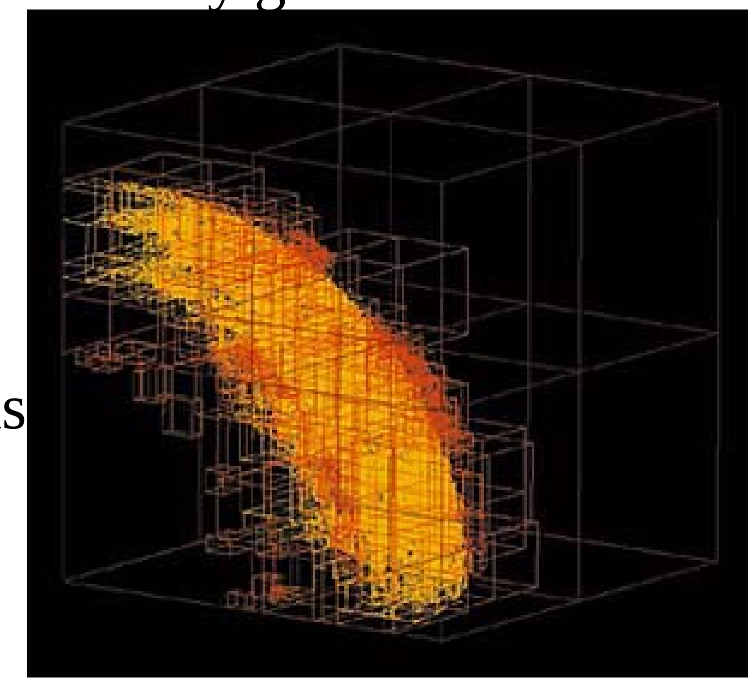
- Incorporation of “standard” grid generation and discretization libraries into M3D (and possibly NIMROD)
- Higher order and mixed type elements
- Explore combining potential and field advance equations
- Prof. Glimm visited PPPL in February
- Mark Shephard (Director of Renssalaer Scientific Computation Research Center), Joe Flaherty (now Dean of RPI School of Science), and Jean-Francois (RPI RA with MHD and fusion interest and experience) to visit PPPL Aug 6
- Tim Tautges (SNL/U.Wisconsin) participated in CEMM meeting Aug 1 in Madison

Terascale Optimal PDE Simulations (TOPS) Collaboration

- Extend the sparse matrix solvers in PETSc in several ways that will improve the efficiency of M3D
  - Develop multilevel solvers for stiff PDE systems
  - Addition of nonlinear Schwarz domain decomposition
  - Refinements in implementation to improve cache utilization
- David Keyes and Barry Smith primary contacts
- Keyes visited Princeton on June 6
- M3D team visited Smith at Argonne in January
- Jardin on TOPS "Advisory Council"
- Jardin to attend briefing on CEMM at Aug 20 meeting in Argonne

An Algorithmic and Software Framework for Applied Partial Differential Equations

- Implement and evaluate adaptive mesh refinement (AMR) for reconnection and localized instability growth
- Phil Colella, Project leader, visited PPPL in Spring
- Focus on adaptive mesh refinement
- Fusion one of three project areas
- New PPPL hire (with MICS SciDAC funds) from Cal Tech. CFD ASCI center
- Jardin on PAC



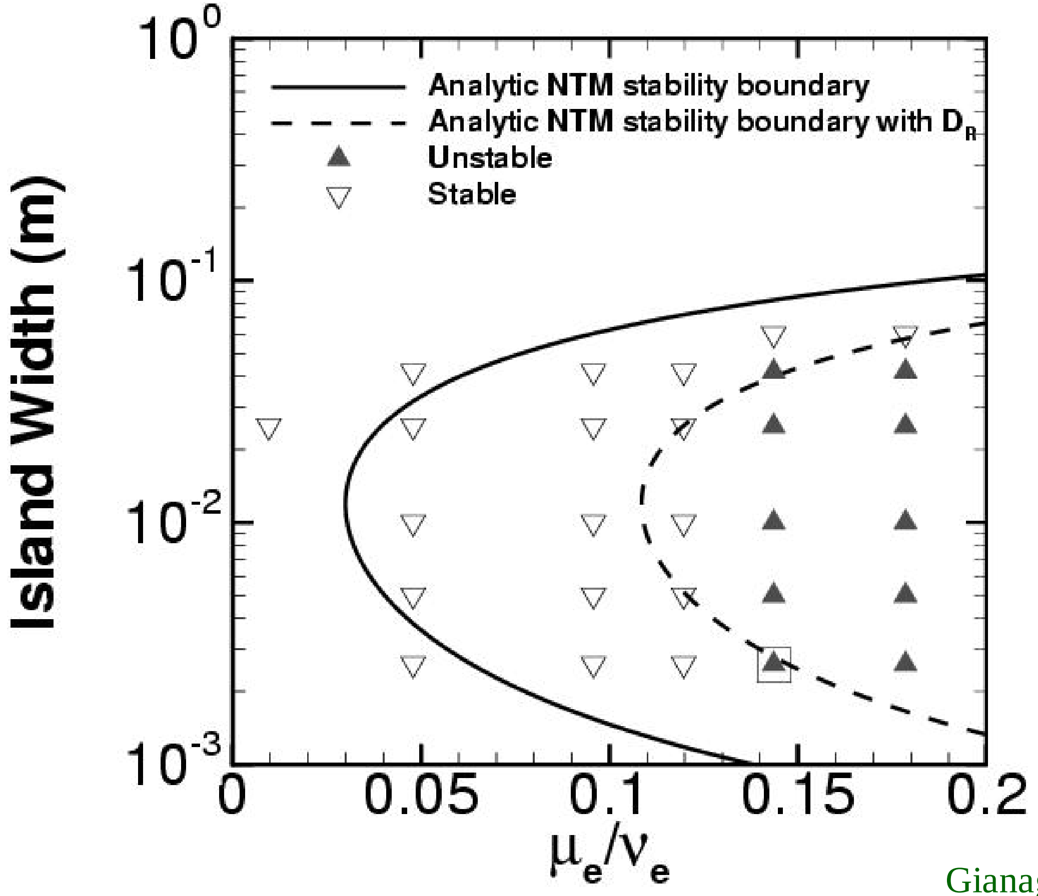
Fusion Collaboratory

- Develop more efficient integration of experiment and modeling
- Easier access to simulation codes
- Enhancements in communication capabilities for shared code development projects
- Scientific visualization, access grid, display wall
- D. Schissel , project director, also part of CEMM
- C. Sovinec (UW/NIMROD/CEMM) on oversight committee

Code Applications

- Neoclassical Tearing Modes in Tokamaks
  - Seed island, saturation level, active stabilization
- Edge Localized Modes
  - Predict nature of ELM for given parameters
- Burning Plasma MHD
  - m=1 (sawtooth), TAE and fishbone , NTM
- Relaxation in RFPs and Spheromaks
  - Effect of XMHD on relaxation processes
- Stellarator Stochasticity and Stability
  - Existance of surfaces, non-linear stability
- Basic-Physics Applications
  - Magnetic reconnection, accretion-disk, wave-particle interaction

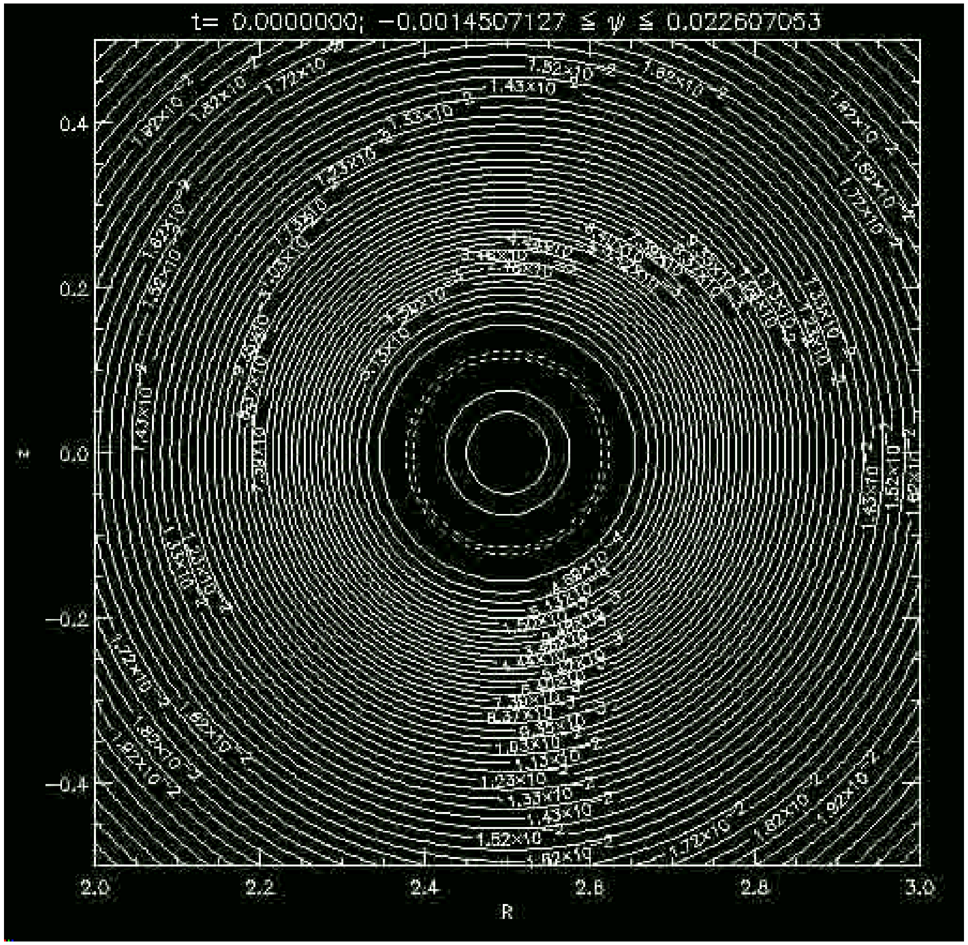
Neoclassical Tearing Modes in Tokamaks



Gianagon

- Build on PSACI work
- Seed Island
- Dependence of saturation level on model
- active stabilization

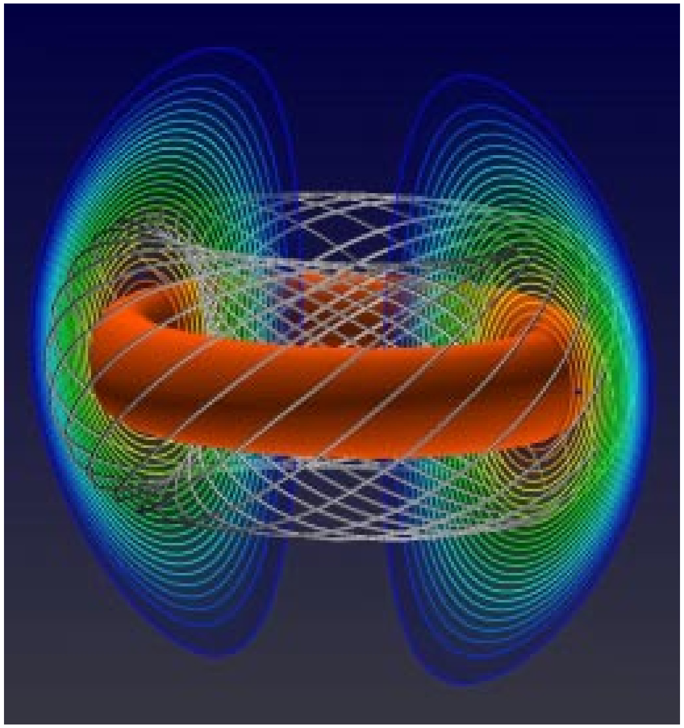
m=1 mode in hot plasmas

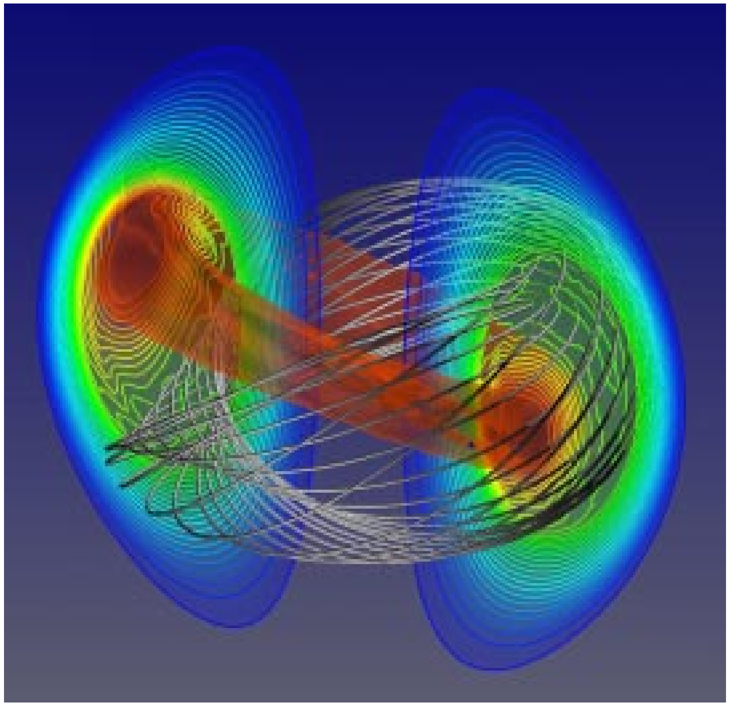


- better predictive model of m=1 mode is needed for burning plasma
- also a high priority issue for ST..can lead to IRE
- recent JET discharges with zero central current density show n=0,m=1

Breslau

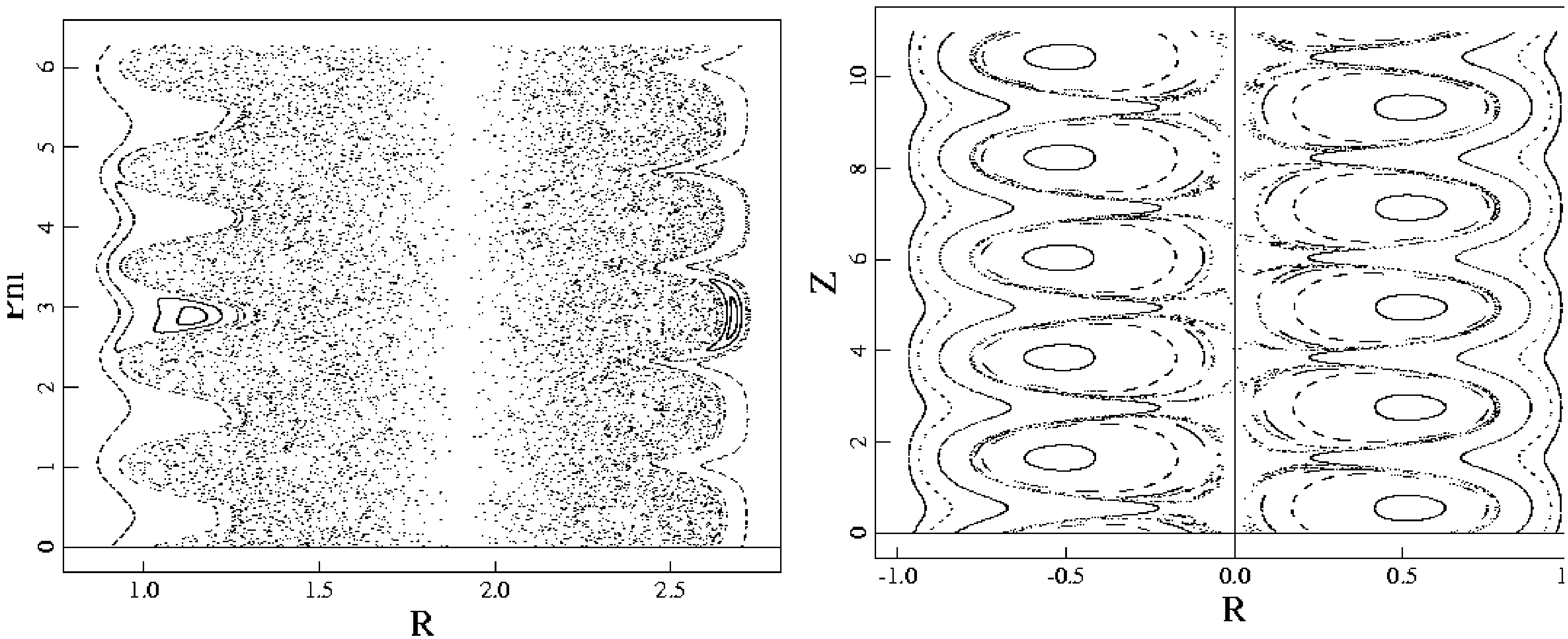
m=1 internal mode in NSTX agrees qualitatively with data





Park

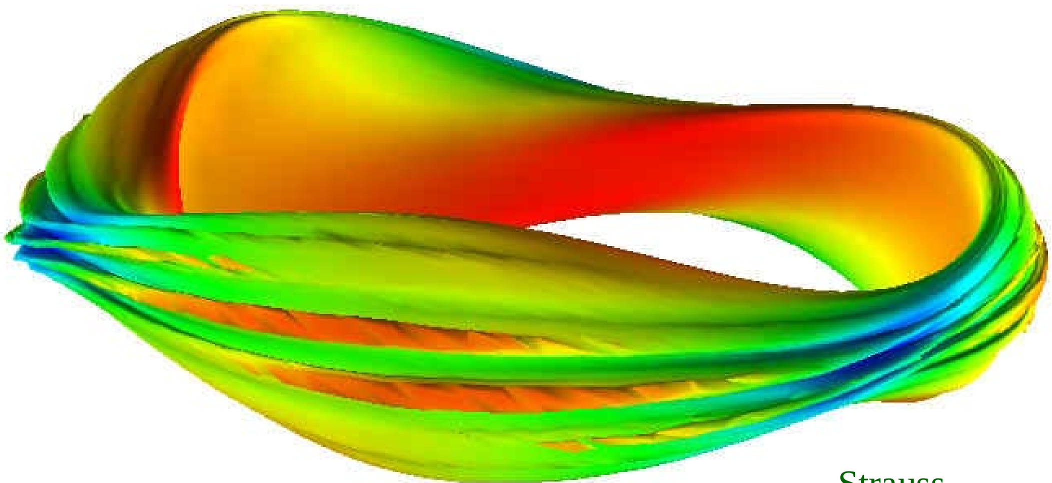
Application to RFP concentrating now on looking for coherent states



Results from a) toroidal geometry and b) periodic linear geometry with P_m=10, R/a=1.75, Θ=1.8.

Sovinec

Quasi-Axisymmetric Stellarator



Strauss

• Ballooning mode develops in li383 when design pressure exceeded

• nonlinear steepening of ribbons

• resistive ballooning also being studied for $D_R > 0$

Distribution of Resources

- $150 K SAIC
- $ 90 K University of Wisconsin
- $ 90 K PPPL
- $ 60 K University of Colorado
- $ 40 K MIT
- $ 40 K NYU
- $ 30 K GA
- ? LANL
- $ 0 K U. Utah
- $ 0 K U.Texas

Year 1 task list (in proposal):

- Move the M3D two-fluid/anisotropic pressure level to MPP architecture and apply to tokamaks and ST's.
- Develop MPP architecture energetic particle module for both M3D and NIMROD, and apply to TAE and fishbone modes in tokamaks and ST's.
- Implement parallel non-Hermitian matrix solves in NIMROD.
- Modeling efforts will resolve what form of gyroviscosity is most appropriate and develop the CEL-based stress tensor for electrons.
- Expand the M3D MPP mesh module by incorporating field-line-following mesh and carry out stellarator MHD simulations.

Year 2 task list (in proposal):

- Develop M3D MPP mesh for modeling separatrix and apply to ELMs.
- Continue development of two-fluid-level closure schemes for axisymmetric and non-axisymmetric systems; apply to neoclassical physics in stellarators.
- Apply energetic particle/MHD hybrid level to stellarators
- Implement majority ion δf computation and closure based on simulation particles.
- Implement the majority electron closures based on CEL.
- The Hall and gyroviscous advances in NIMROD will be changed to use the non-Hermitian matrix capability, improving the time advance algorithm.

Year 3 task list (in proposal):

- Work on adaptive mesh refinement methods and apply to global simulations that contain near-singular structures such as reconnection layers.
- Further development of multi-fluid closures, including higher order moments and parallel dynamics.
- Incorporate bulk ion particles in MPP: apply to tokamaks, ST, stellarators.
- Implement collisional effects in the simulation-particle δf to address distribution function filamentation.
- Analyze the efficacy of semi-implicit approaches used with CEL closures, addressing the stiffness associated with electron parallel
- Incorporate implicit advection for the fluid part of the algorithm.