Magnetic Fusion Application:

Center For
Extended Magnetohydrodynamic Modeling

presented by S. C. Jardin
for the CEMM consortium

SciDAC Kickoff Meeting
January 15-17
Hyatt Regency Reston, VA
www-unix.mcs.anl.gov/discovery/kickoff.html

The CEMM Consortium:

GA:	D.Schissel
LANL:	T. Gianakon, R. Nebel
MIT:	L. Sugiyama
NYU:	H. Strauss
PPPL:	J. Breslau, J. Chen, G. Fu, S.Jardin* ,W.Park, R. Samtaney
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

*PI

Outline:

1. **CEMM objectives and goals**

2. Computational and mathematical challenges

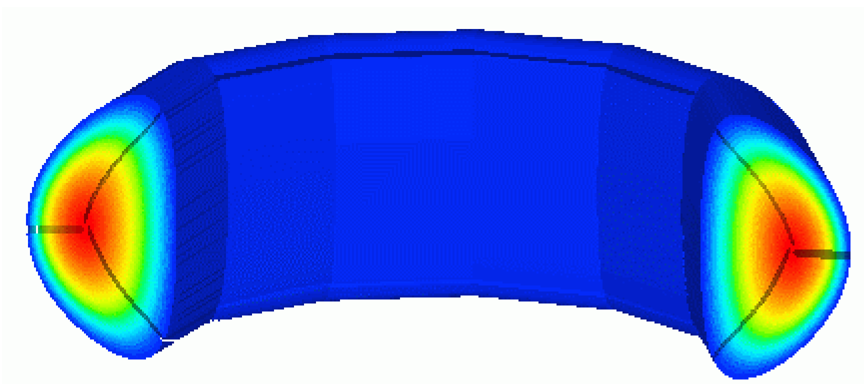
3. Typical applications..current state of the art

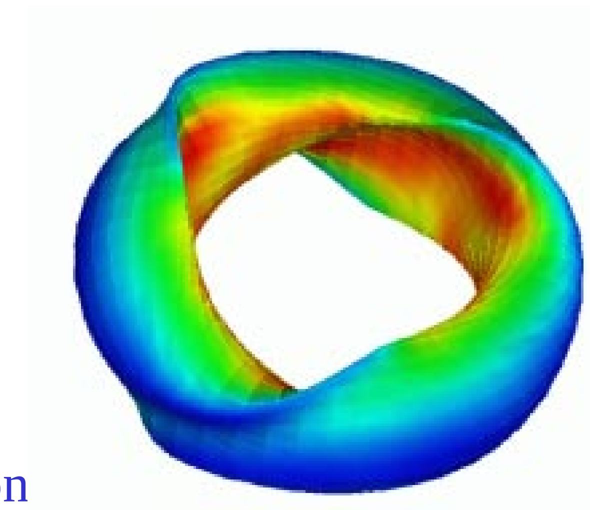
4. Possible significant results and breakthroughs

5. Interactions between CEMM and ISIC centers

CEMM Objectives:

"*…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.*"





- Improved physics models and better resolution
- Large scale instabilities –not turbulence.
- Toroidal devices…tokamak, stellarator, FRC, RFP,…

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

Outline:

1. CEMM objectives and goals
2. **Computational and mathematical challenges**
3. Typical applications..current state of the art
4. Possible significant results and breakthroughs
5. Interactions between CEMM and ISIC centers

The computational challenges:

- temporal stiffness, or multiplicity of time scales,

$$\frac{\partial \vec{U}}{\partial t} + \overleftrightarrow{A} \bullet \frac{\partial \vec{U}}{\partial \vec{x}} = \ldots \quad \frac{\lambda_A^{\max}}{\lambda_A^{\min}} >> 1 \ \ (\sim 100), \qquad S = \frac{\tau_{RESISTIVE\ DIFFUSION}}{\tau_{ALFVEN\ WAVE\ TRANSIT}} >> 1 \quad (\sim 10^8)$$

- large differences in spatial scales lengths
  - internal reconnection layers develop with steep gradients
  - typical reconnection length scale $\dfrac{\delta}{L} \sim S^{-1/2}$

- anisotropy introduced by the strong magnetic field

$$\vec{q}_{||} \gg \vec{q}_{\perp}$$

Less complex model, valid for high-collisionality, strong fields, long times

More computationally demanding. Required to describe many important but subtle phenomena.

Single Fluid Resistive MHD	Two Fluid MHD (electrons and ions)	Two Fluid MHD plus energetic gyro-particles	Gyro-particle ions and fluid electrons	Full orbit particle ions and fluid electrons
External kink modes	**Neoclassical tearing mode (including rotation)** **m =1 mode**	**MHD modes destabilized by wave-particle resonance with energetic species**	**Kinetic stabilization of internal MHD modes by ions**	**Tilting and interchange modes in FRC**

Several variations of the Extended-MHD model exist.

Plasma Models: XMHD

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

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

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

$$\overleftrightarrow{P} = p\overleftrightarrow{I} + \overleftrightarrow{\Pi}$$

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

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

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

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

Two-fluid XMHD: define closure relations for Π_i ,Π_e, q_i, q_e

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

Simplest 2-fluid Closure for ions and electrons

$$\rho\left(\frac{\partial \vec{V}_i}{\partial t} + \left((\vec{V}_i - \vec{V}_*)\bullet\nabla\right)\vec{V}_i\right) + \nabla P = \vec{J}\times\vec{B}$$

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

$$\vec{E} + \vec{V}_i\times\vec{B} = \eta\vec{J} + \frac{1}{ne}\left(\underline{\vec{J}\times\vec{B}} - \nabla p_e\right)$$

"Hall Term" in Ohm's Law brings in essential new physics in 2-fluid equations

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

$$\vec{V}_* \equiv \vec{B}\times\nabla p_i \big/ enB^2$$

$$P = p_e + p_i$$

$$\nabla\times\vec{B}=\nabla P=\vec{V}=0$$

2-fluid zero-pressure dispersion relation:

$$\left[\frac{\omega^2}{V_A^2}-(k_x^2+k_z^2)\right]\left[\frac{\omega^2}{V_A^2}-k_z^2\right]-\frac{\omega^2}{V_A^2}\left(\frac{V_A^2}{\Omega^2}\right)k_z^2(k_x^2+k_z^2)=0$$

$$\vec{B}_0=(0,0,B),$$

$$\vec{k}=(k_x,0,k_z)$$

the Hall modified fast wave (+) and shear Alfven wave (-) are given by:

$$\omega^2/V_A^2=\frac{1}{2}\left[k_x^2+2k_z^2+\frac{V_A^2}{\Omega^2}k_z^2\left(k_x^2+k_z^2\right)\right]$$

$$\pm\frac{1}{2}\left[k_x^4+2\frac{V_A^2}{\Omega^2}\left(k_x^2+2k_z^2\right)k_z^2\left(k_x^2+k_z^2\right)+\frac{V_A^4}{\Omega^4}k_z^4\left(k_x^2+k_z^2\right)^2\right]^{1/2}$$

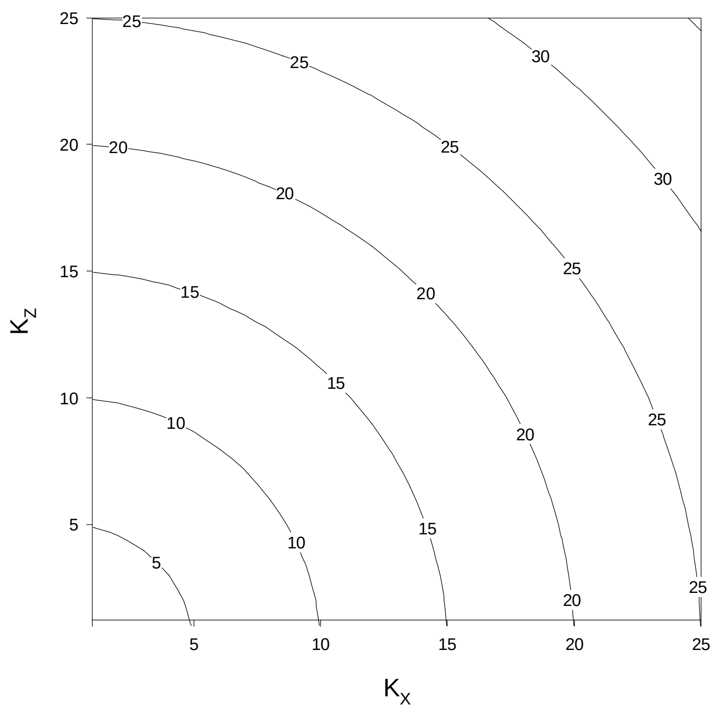
large k limit:

$$k^2\gg\left(\frac{V_A^2}{\Omega^2}\right)^{-1}$$

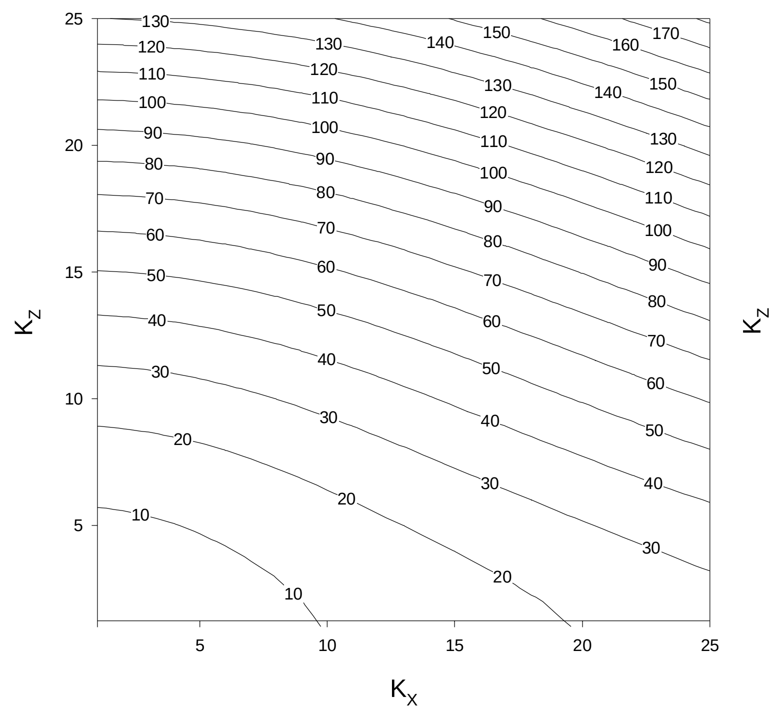
$$\frac{\omega^2}{V_A^2}\sim\left(1+\frac{V_A^2}{\Omega^2}k_z^2\right)\left(k_x^2+k_z^2\right)+\ldots$$ Fast wave

$$\frac{\omega^2}{V_A^2}\sim\left(\frac{V_A^2}{\Omega^2}\right)^{-1}-\left(\frac{V_A^2}{\Omega^2}\right)^{-2}\frac{\left(k_x^2+2k_z^2\right)}{k_z^2\left(k_x^2+k_z^2\right)}+\ldots$$ Shear Alfven

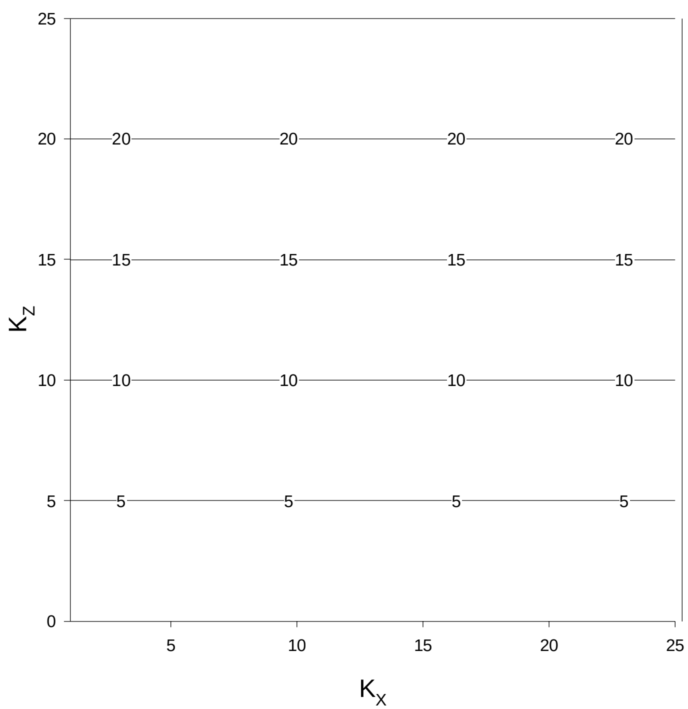
ω^2/V_A^2 for Fast Wave with $(V_A^2/\Omega^2=0)$



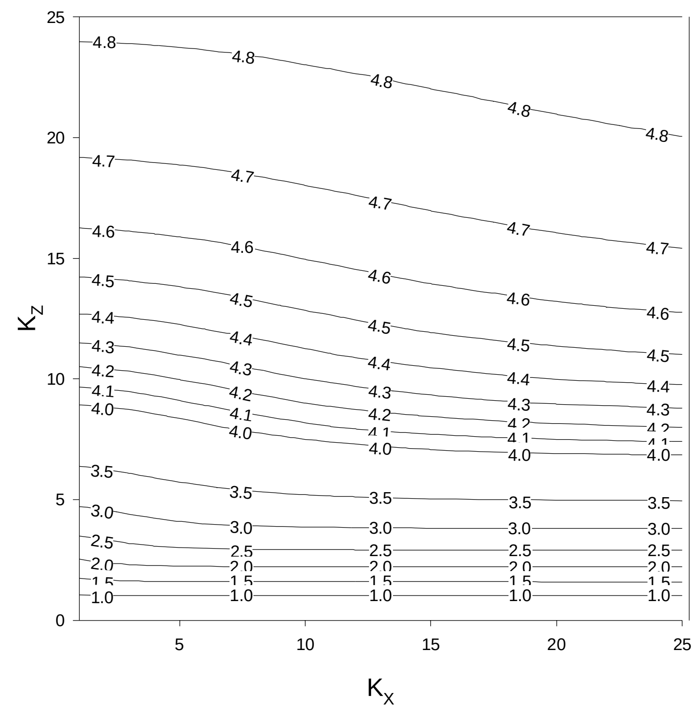
ω^2/V_A^2 for Hall modified Fast Wave with $(V_A^2/\Omega^2=0.04)$



ω^2/ V_A^2 for Alfven Wave with $(V_A^2/\Omega^2=0)$



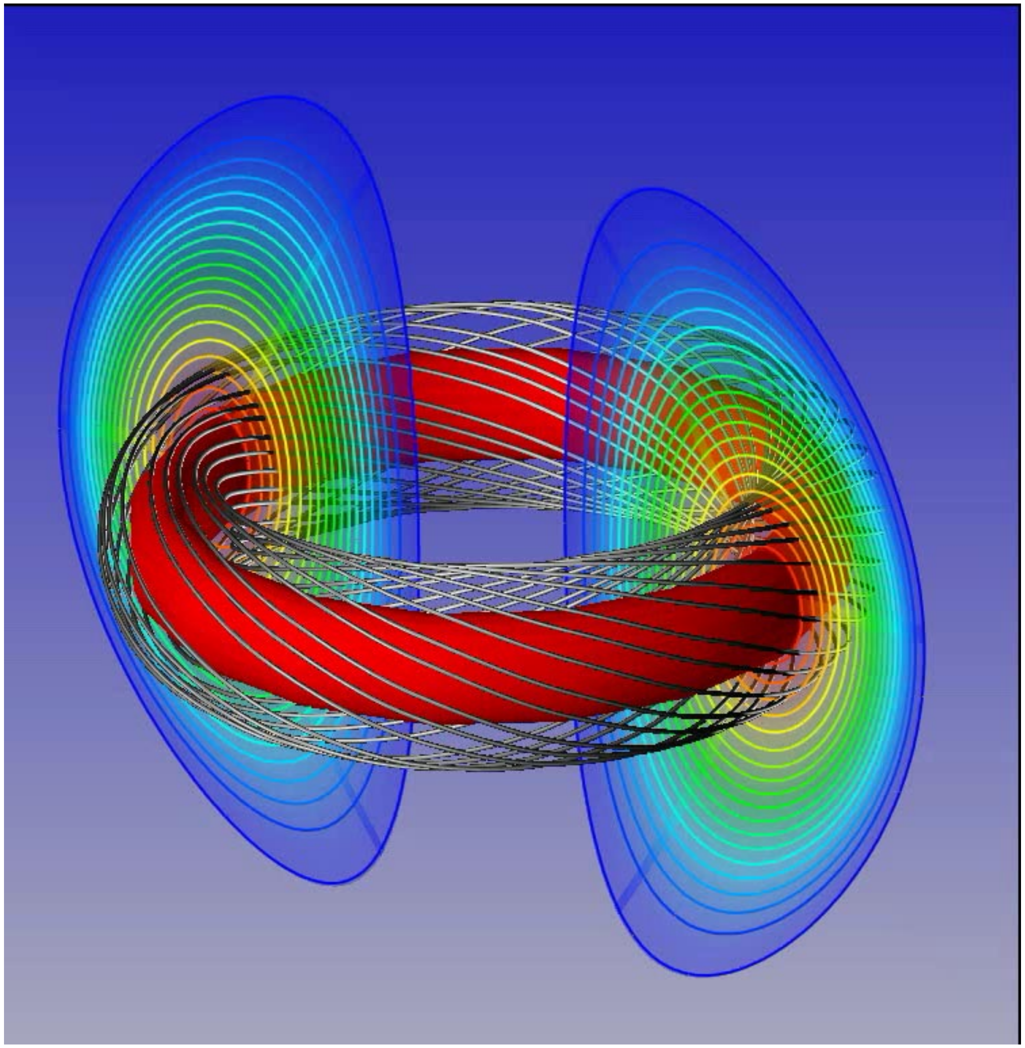
ω^2/ V_A^2 for Hall modified Alfven Wave with $(V_A^2/\Omega^2=,04)$



Outline:

1. CEMM objectives and goals
2. Computational and mathematical challenges
3. **Typical applications..current state of the art**
4. Possible significant results and breakthroughs
5. Interactions between CEMM and ISIC centers

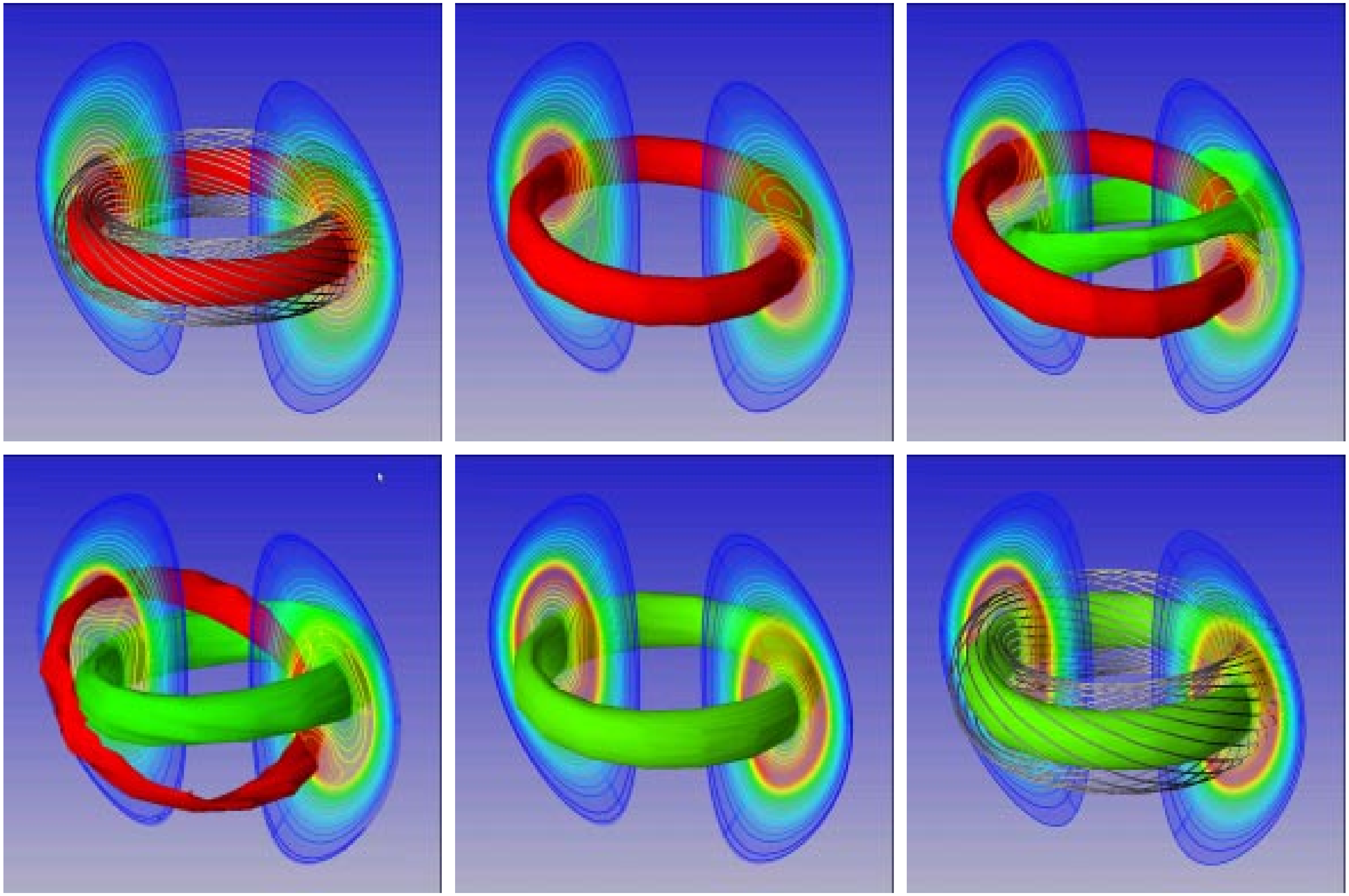
m=1 mode (sawtooth) in tokamak is high priority objective



- caused by tendency of plasma current to peak in center and become unstable
- involves reconnection layer, 2-fluid, hot-particles
- better predictive model of m=1 mode is needed for next step tokamak burning plasma
- benign self-regulating event or plasma termination?

Shown are constant pressure surfaces and some magnetic field lines

Hot inner region interchanges with colder outer region via magnetic reconnection

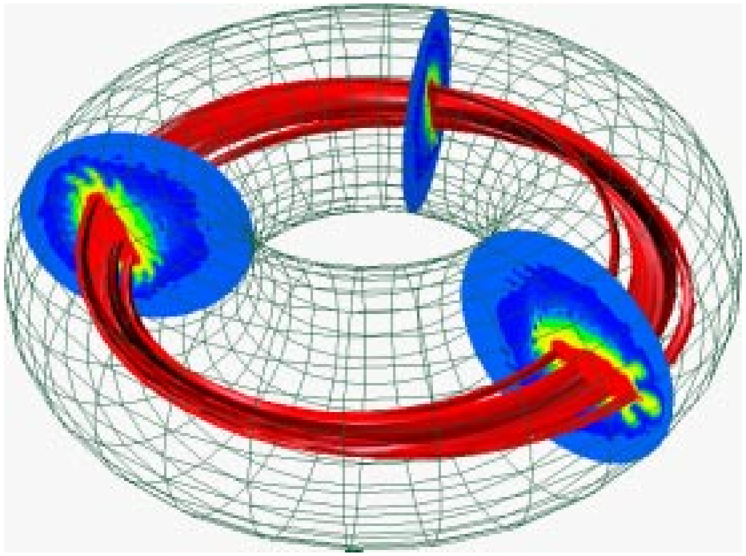


m=1 mode can also destablize short wavelength modes and lead to plasma termination

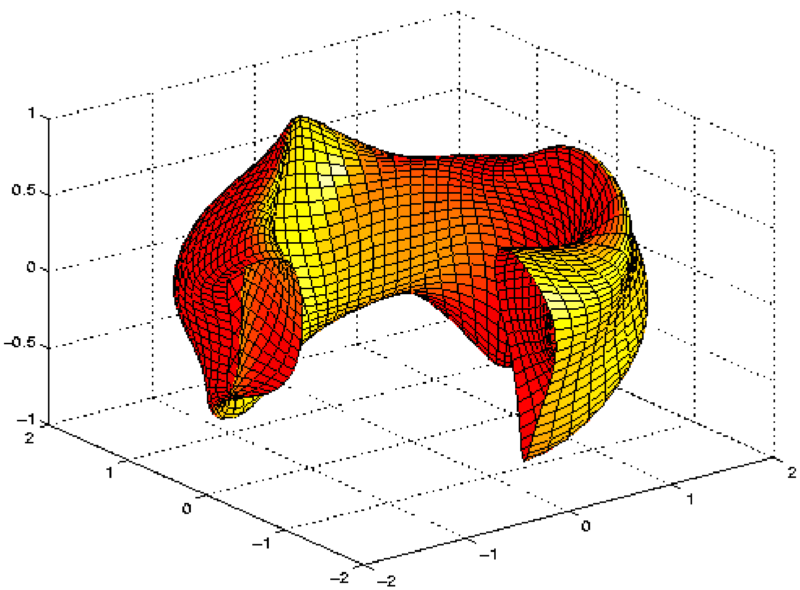
- If plasma pressure is already high and near stability limit, m=1 helical distortion can make it locally unstable to pressure-driven-modes

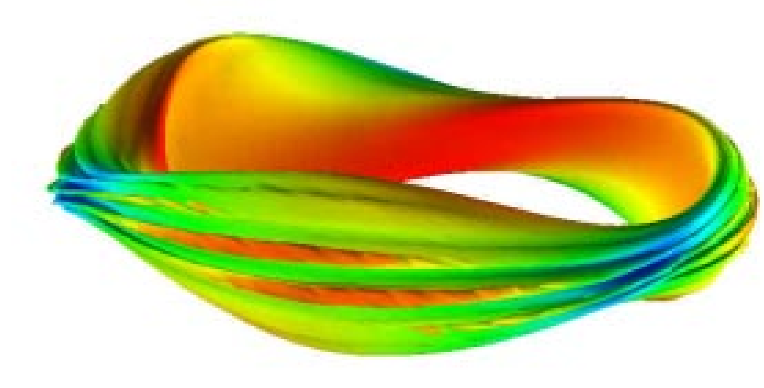
- These modes steepen nonlinearly in a ribbon like structure driving field line stochasticity and leading to plasma termination.

- The plasma termination event in the record making 10 MW fusion power DT TFTR discharge has been explained by this mechanism



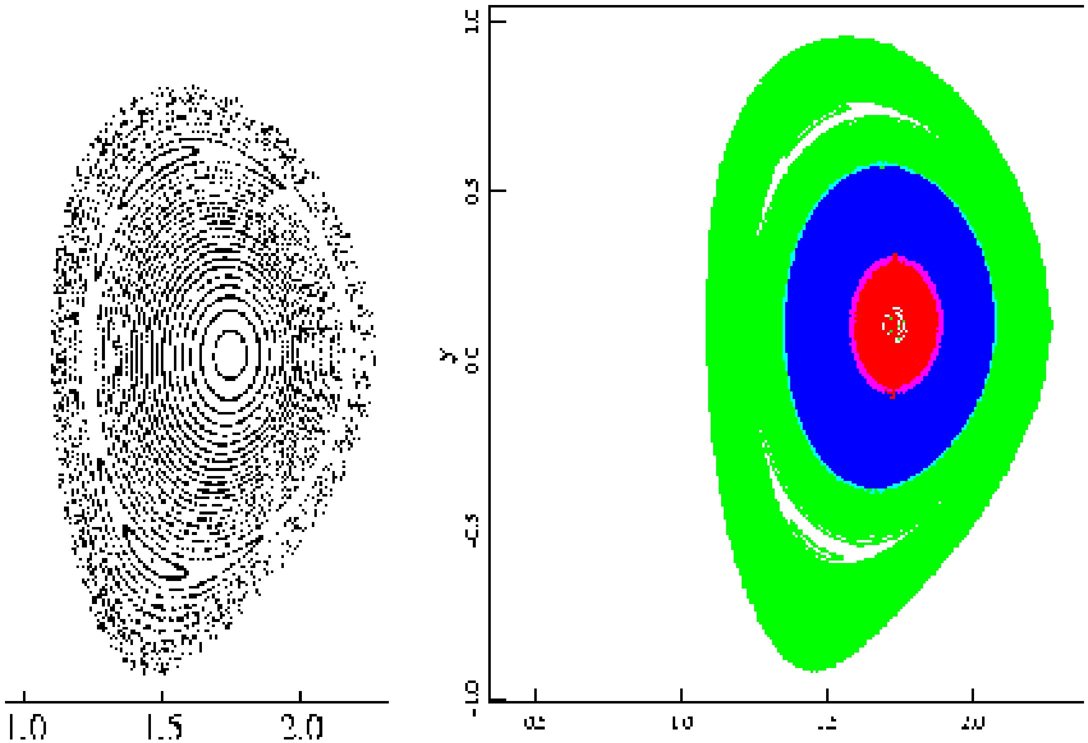
Quasi-Axisymmetric Stellarator NCSX now being designed





- **Stellarator has “twisted” outer surface formed by 3D coil set…does not need to carry net plasma current like tokamak**
- **No sawtooth modes…but instabilities can be excited when the pressure locally exceeds stability limit**
- **Instabilities cause high pressure areas to further steepen nonlinearly …consequence ?**

Spontaneous development of Magnetic Islands (tearing modes)



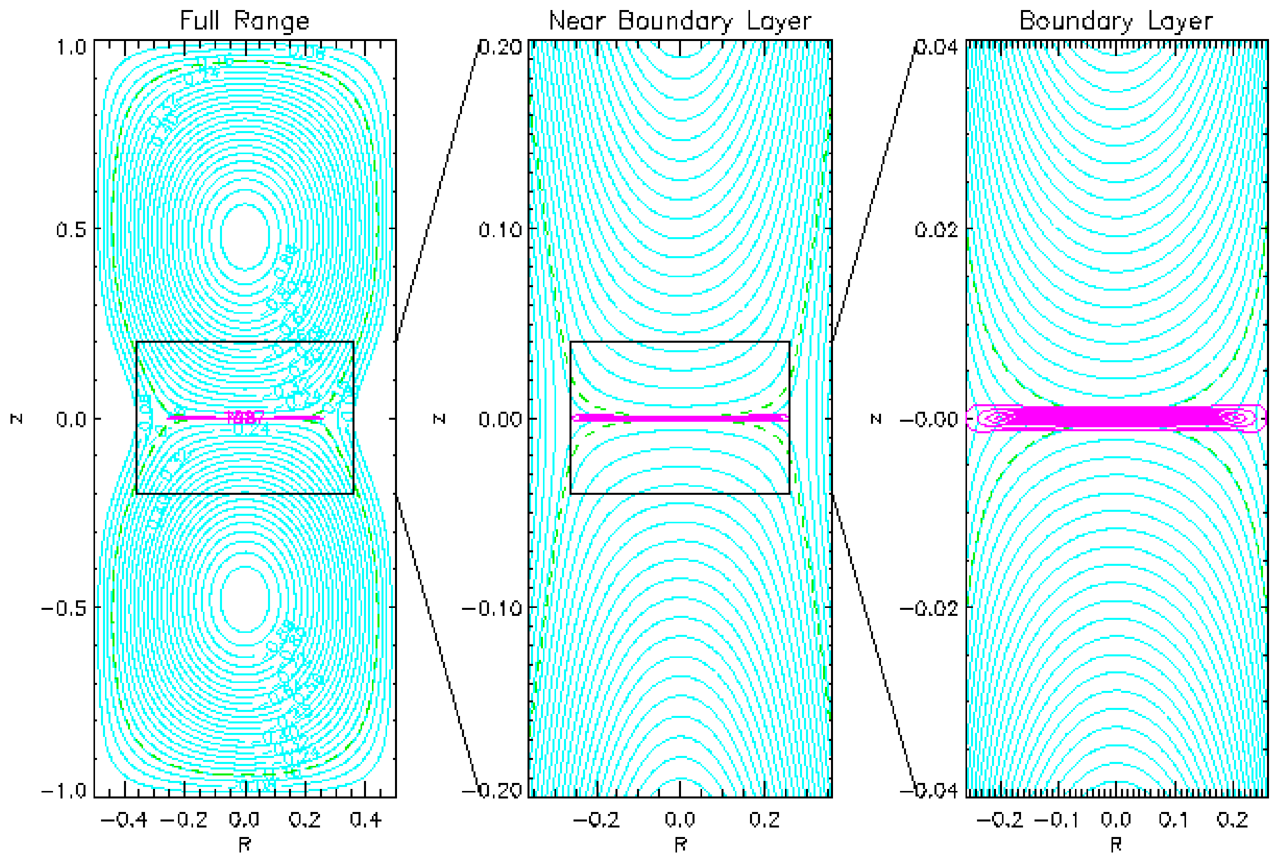
NIMROD

• “neo-classical tearing modes” driven by small differences in the plasma current-carrying capability inside the islands

• comparing results 3 different fluid closures with exp. data

Model 2D problem: merging spheromaks with 2-fluid MHD equations, high-resolution

$\eta = 10^{-5}$

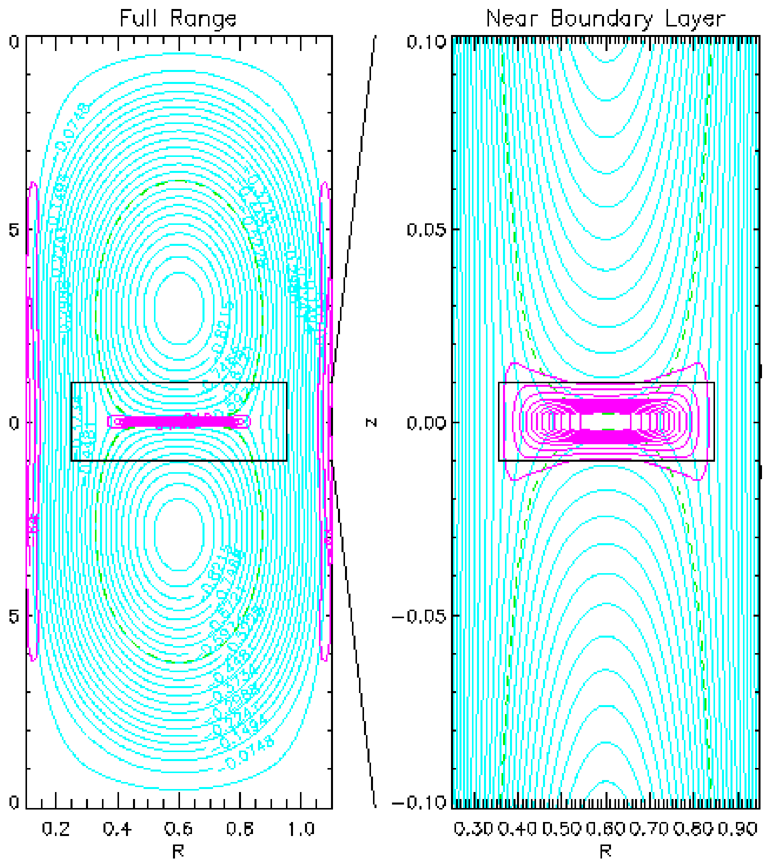


- Variable resolution grid allows resolution of <u>disparate space scales.</u>
- note: cyan: flux purple: current

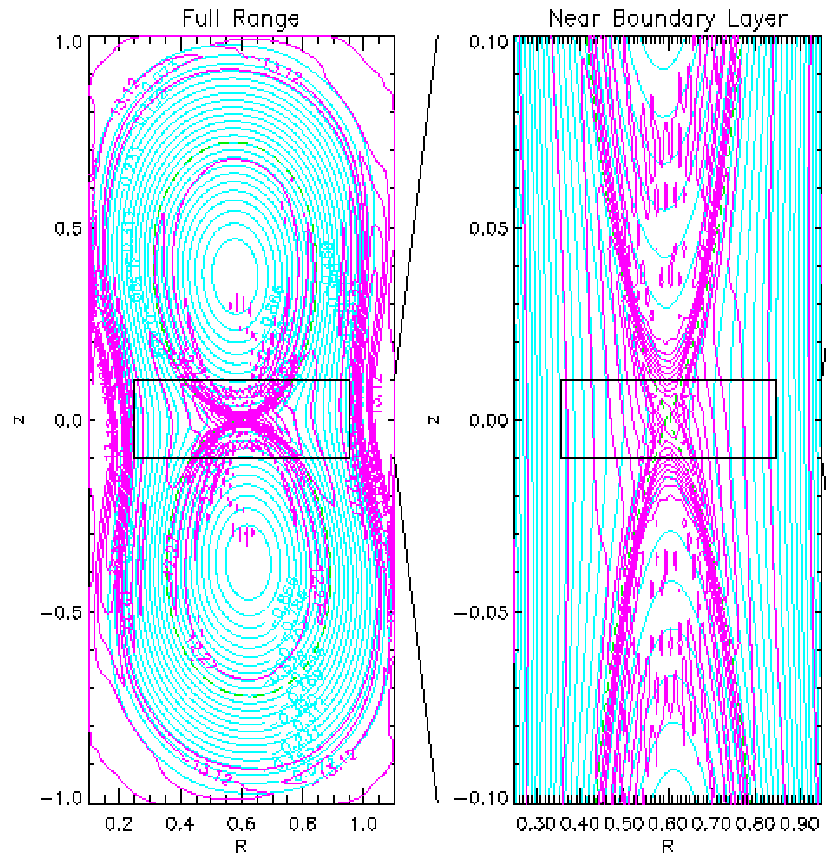
Breslau

More complete physics (two-fluid) can change he qualitative nature of the reconnection physics

$\chi = 0$ (resistive MHD)



$\chi = 0.2$ (2-fluid MHD)



reconnection rate with 2-fluid MHD ($\chi > 0$) can increase reconnection rate by order of magnitude..or more!

Outline:

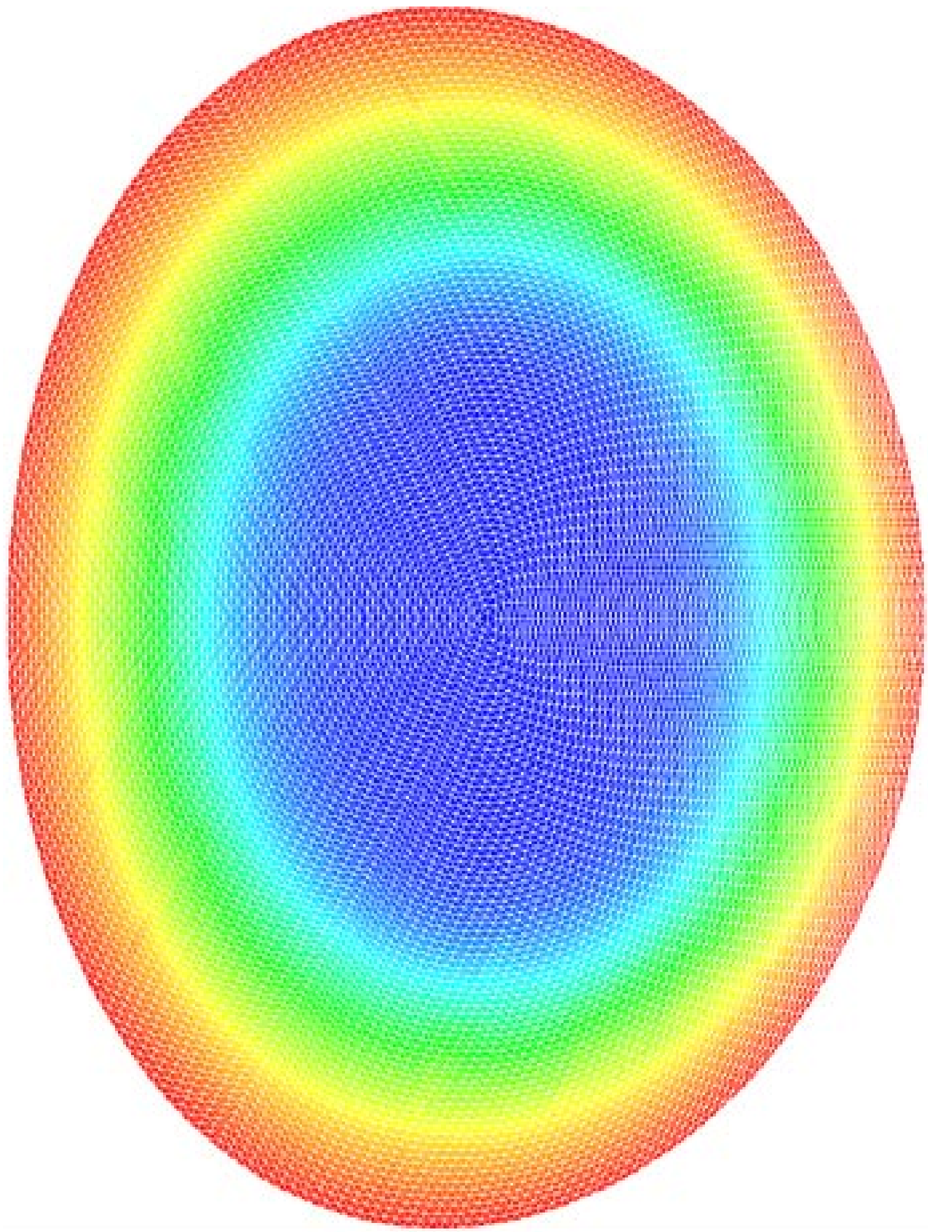
1. CEMM objectives and goals

2. Computational and mathematical challenges

3. Typical applications..current state of the art

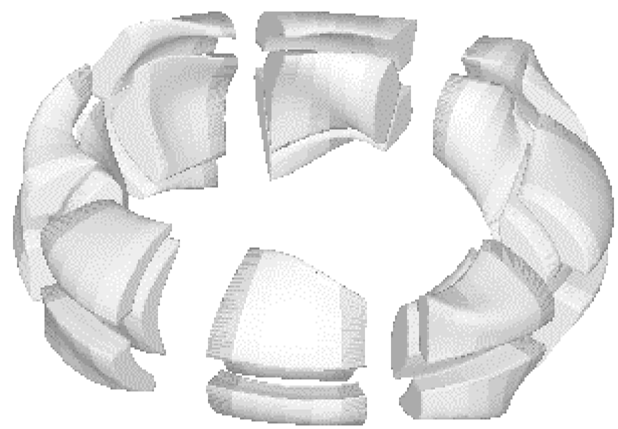
4. **Possible significant results and breakthroughs**

5. Interactions between CEMM and ISIC centers



Typical M3D Mesh in Poloidal Plane

- Unstructured
- Not adaptive



Relation of APDEC Activity to Baseline

M3D
• quasi-implicit (Krylov)
• stream function/ potential
• triangular finite elements in poloidal plane
• domain decomposition in poloidal plane using MPI
• Finite difference in toroidal direction
• scales good on 256-512 processors on T3E & SP2
• resistive MHD, two-fluid (Hall term) & hybrid/particles
• uses PETSC framework

NIMROD:
• strongly implicit (Krylov)
• uses B and V
• triangular and quad finite elements in poloidal plane
• domain decompositon in poloidal plane using MPI
• pseudo-spectral (FFT) in toroidal direction
• scales good on 256-512 processors on T3E & SP2
• resistive MHD, two-fluid (Hall term) & hybrid/particles

APDEC Activity:
• adaptive mesh
• structured mesh with embedded boundary
• evaluate generalized upwind FD methods

Must eventually dea with
• partially implicit solve
• Hall term in Ohm's la
• Anisotropic heat conduction
• hybrid particle/fluid description
• must interface with existing code(s)

Outline:

1. CEMM objectives and goals

2. Computational and mathematical challenges

3. Typical applications..current state of the art

4. Possible significant results and breakthroughs

5. **Interactions between CEMM and ISIC centers**

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)

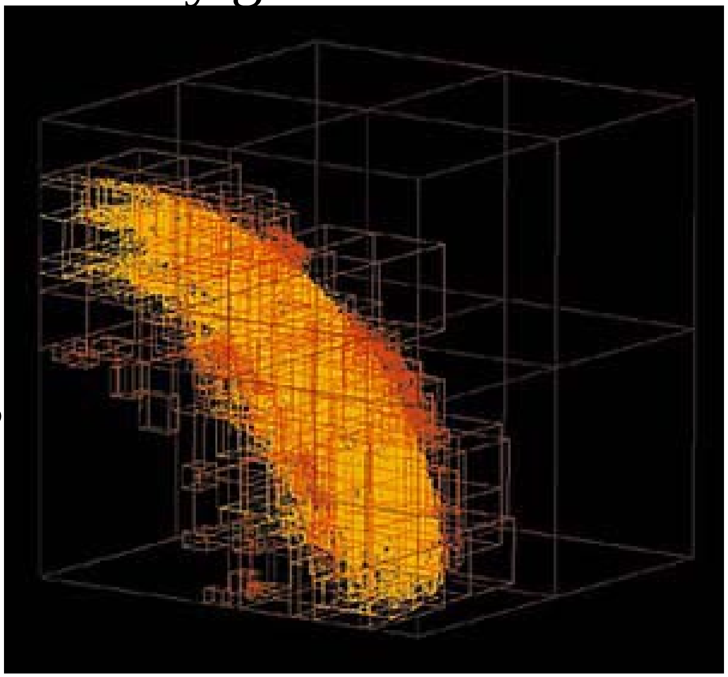
- Incorporation of “standard” grid generation and discretization libraries into M3D (and possibly NIMROD)
- Higher order and mixed type elements
- Explore combining potential and field advance equations
- Prof. Glimm visited PPPL in February
- Mark Shephard (Director of Renssalaer Scientific Computation 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

Summary:

1. CEMM objectives and goals
2. Computational and mathematical challenges
3. Typical applications..current state of the art
4. Possible significant results and breakthroughs
5. Interactions between CEMM and ISIC centers