The Center for Extended Magnetohydrodynamic Modeling
Progress, Plans, and Collaborations

Presentation to the
OFES SciDAC PAC
June 5, 2003
Princeton Plasma Physics Laboratory

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CEMM

a SciDAC activity…

Math ISIC partners:
TOPS
TSTT
APDEC

CEMM Simulation Codes:

	NIMROD	M3D	AMRMHD*
Poloidal discritization	Quad and triangular high order finite elements	Triangular linear finite elements	Structured adaptive grid
Toroidal discritization	Pseudo-spectral	Finite difference	Structured adaptive grid
Time integration	Semi-implicit	Partially implicit	Partially implicit and time adaptive
Enforcement of $\nabla\cdot\mathbf{B} = 0$	Divergence cleaning	Vector Potential	Projection Method
Anisotropic Heat conduction	Implicit solve using high order elements	Artificial sound method	Adaptive meshing
Libraries	AZTEC (Sandia) (optional)	PETSc (ANL)	Chombo (LBL)
Sparse Matrix Solver	Congugate Gradient	GMRES	Conjugate Gradient
Preconditioner	Line-Jacobi	Incomplete LU	Multigrid

*Exploratory project together with APDEC

Parts of the Presentation

(1) how we have responded to the 2002 PAC recommendations and made progress on achieving scientific targets;

(2) how super-computing resources have enabled the achievement of the targeted scientific goals;

(3) what role have collaborative interactions within each project and also with other SciDAC activities played; and

(4) what is the vision/scientific roadmap for the next 3-year phase

Part 1:

How have we responded to the 2002 PAC recommendations and made progress on achieving scientific targets;

2002 PAC recommendations:

1. Publish more
2. More Synergy with CMR
3. Perform nonlinear test problem

Scientific Progress:

1. Simulation of high-beta disruption in DIIID
2. Simulation of current hole in JET
3. Effect of anisotropic heat conduction on island evolution
4. Magnetic stabilization of Richtmyer-Meshkov instability
5. Current bunching and ejection during 2D reconnction
6. The effect of strong sheared toroidal flow on reconnecting modes in toroidal systems
7. Diamagnetic stabilization of instabilities in stellarators
8. Hybrid Simulations of unstable Toroidal Alfven Eigenmodes in NSTX

#1. CEMM Publications and Reports in 2002-2003:

(1) C. R. Sovinec, T. A. Gianakon, E. D. Held, et al, "NIMROD: a computational laboratory for studying nonlinear fusion magnetohydrodynamics", Phys. Plasmas **10** 1727 (2003);

(2) C. R. Sovinec, D. C. Barnes, T. A. Gianakon, et al, "Nonlinear Magnetohydrodynamics Simulation Using High-Order Finite Elements", submitted to J. Comp. Phys (2003);

(3) J. A. Breslau and S. C. Jardin, "A parallel algorithm for global magnetic reconnection studies", Comp. Phys. Comm. **151** pp 8-24 (2003);

(4) J. A. Breslau and S. C. Jardin, "Global Extended MHD Studies of Fast Magnetic Reconnection", Phys. Plasmas **10** 1291 (2003);

(5) J. A. Breslau, S.C. Jardin, and W. Park, "Simulation Studies of the Role of Reconnection in the 'Current Hole' experiments in JET", Phys. Plasmas **10** 1665 (2003);

(6) D. P. Brennan, et al, "A Mechanism for Tearing Mode Onset Near Ideal Stability Boundaries", **10** 1643 Phys. Plasmas (2003);

(7) T. A. Gianakon, S. E. Kruger, and C. C. Hegna, "Heuristic closures for numerical simulations of neoclassical tearing modes", Phys. Plasmas **9**, 536 (2002);

(8) S. E. Kruger, D. D. Schnack, D. P. Brennan, T. A. Gianakon, and C. R. Sovinec, "Nonlinear MHD dynamics of tokamak plasmas on multiple time scales", submitted to Nuclear Fusion (2002);

(9) R. H. Cohen, H. L. Berk, B. I. Cohen, et al, "Theoretical investigation of field-line quality in a driven spheromak", submitted to Nuclear Fusion (2002);

(10) P. Martin, L. Marrelli, G. Spizzo, et al, "Overview of quasi-single helicity experiments in reversed field pinches, submitted to Nuclear Fusion (2002);

(11) B. C. Stratton, J. A. Breslau, R. V. Budny, et al, "The Role of Axisymmetric Reconnection Events in JET Discharges with Extreme Shear Reversal", Plasma Phys. Control. Fusion **44** (2002) 1127;

(12) W. Park, J. Breslau, J. Chen, et al, "Nonlinear Simulation Studies of Tokamaks and STs", IAEA-CN-94/TH5-1(19th IAEA Fusion Energy Conf., Lyon, France) to appear in Nuclear Fusion (2002);

(13) H. Strauss, G. Fu, W. Park, et al, "Nonlinear MHD and Energetic Particle Modes in Stellarators", IAEA-CN-94/TH/P2-12(19th IAEA Fusion Energy Conf. Lyon, France) submitted to Nuclear Fusion (2002)

(14) R. Samtaney, " Suppression of the Richtmyer-Meshkov Instability in the Presence of a Magnetic field", PPPL-3794 to appear in Phys. Fluids (2003)

#2. More synergy with the Center for Magnetic Reconnection

- Following up on the recommendations of the PAC, we held a joint meeting of the CEMM and the Center for Magnetic Reconnection,
  - held at General Atomics on August 19-21, 2002.
  - excellent exchange of ideas and results on both computational algorithms and magnetic reconnection physics.
  - It was also attended by members of the SciDAC TOPS team who are now partnering with both CEMM and CMR in a very synergistic way.

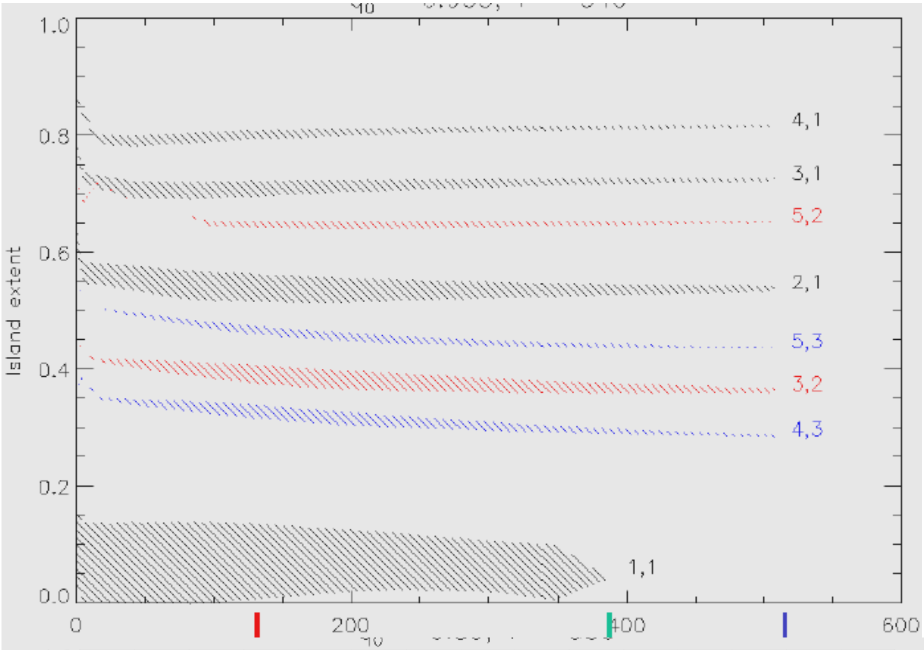
#3. Benchmarking for a nonlinear problem, such as the n=1 sawtooth crash:

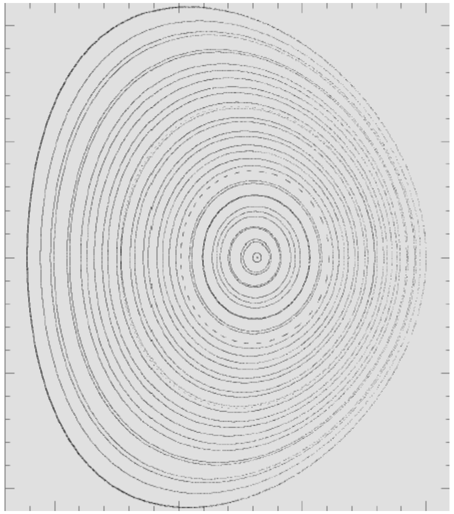
- 3-way nonlinear test problem involving the M3D and NIMROD codes and the CDX-U experiment agreed to at August 2002 workshop
- Rationale is that the size and parameters of CDX-U allow us to consider modeling the entire discharge using the real parameters of the device without the need for scaling.
- Initial comparison results presented Nov 2002 CEMM meeting (see http://w3.pppl.gov/CEMM/APS2002/index.htm)
- There were many similarities between the two codes and the experiment, but the exercise highlighted the need for more careful comparisons.
  - (1) resolve the difference in the linear growth rates between NIMROD and M3D,
  - (2) quantify through a sequence of runs (and new diagnostics) what the conditions for developing stochasticity are,
  - (3) compare relative mode amplitudes between the two codes,
  - (4) examine a number of cases starting with different q_0 values,
- Second round of comparison results presented at April CEMM meeting (see http://w3.pppl.gov/CEMM/Sherwood2003/index.htm
  - Followup discussions specified all details of initial equilibrium, sources, and boundary conditions for future runs
- We are also preparing another non-linear benchmark involving an energetic particle species, but this is waiting final internal benchmarking of this option.

M3D: Magnetic Island Structure vs time for 2-initial conditions

CDX-U

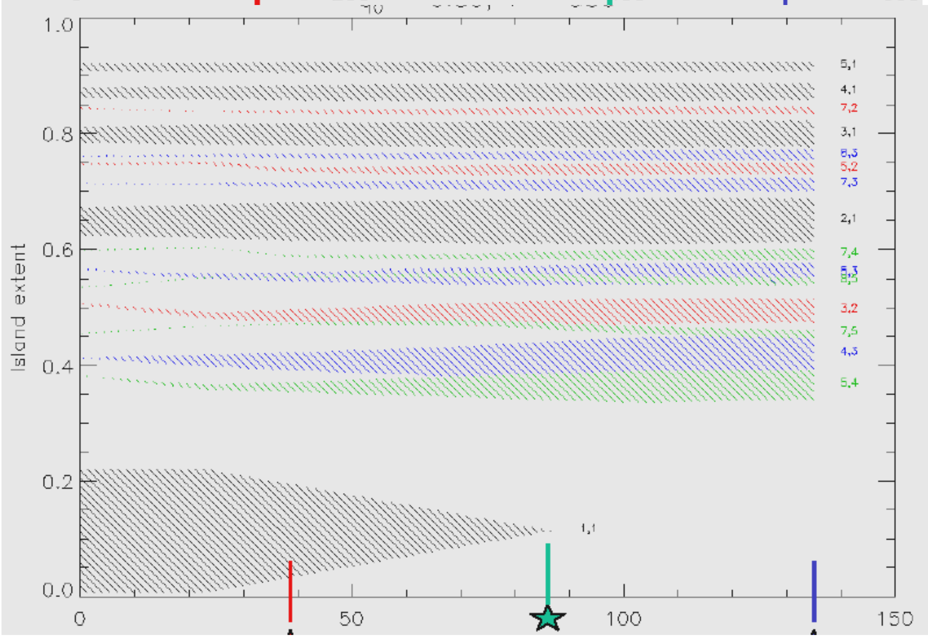
$q_0 = .95$

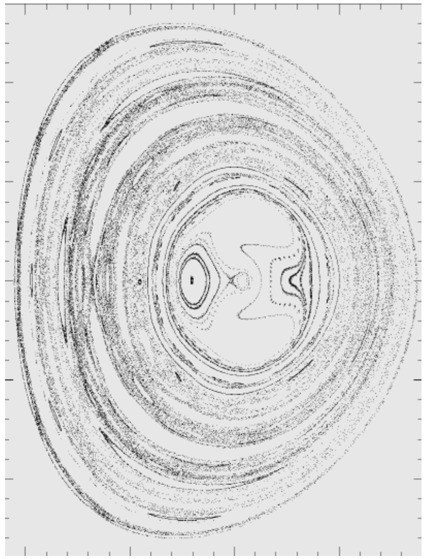




Restored axisymmetry

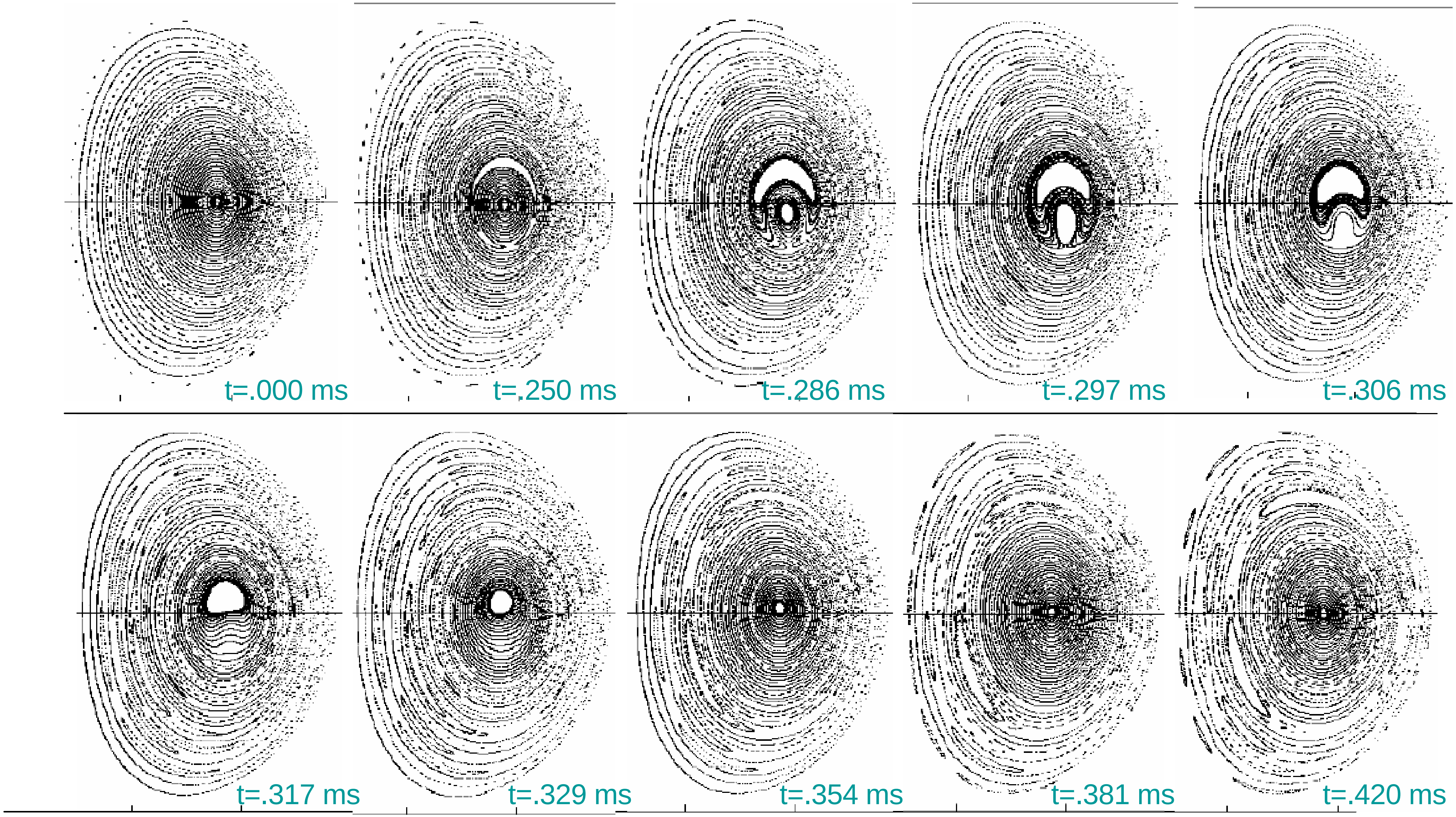
$q_0 = .89$



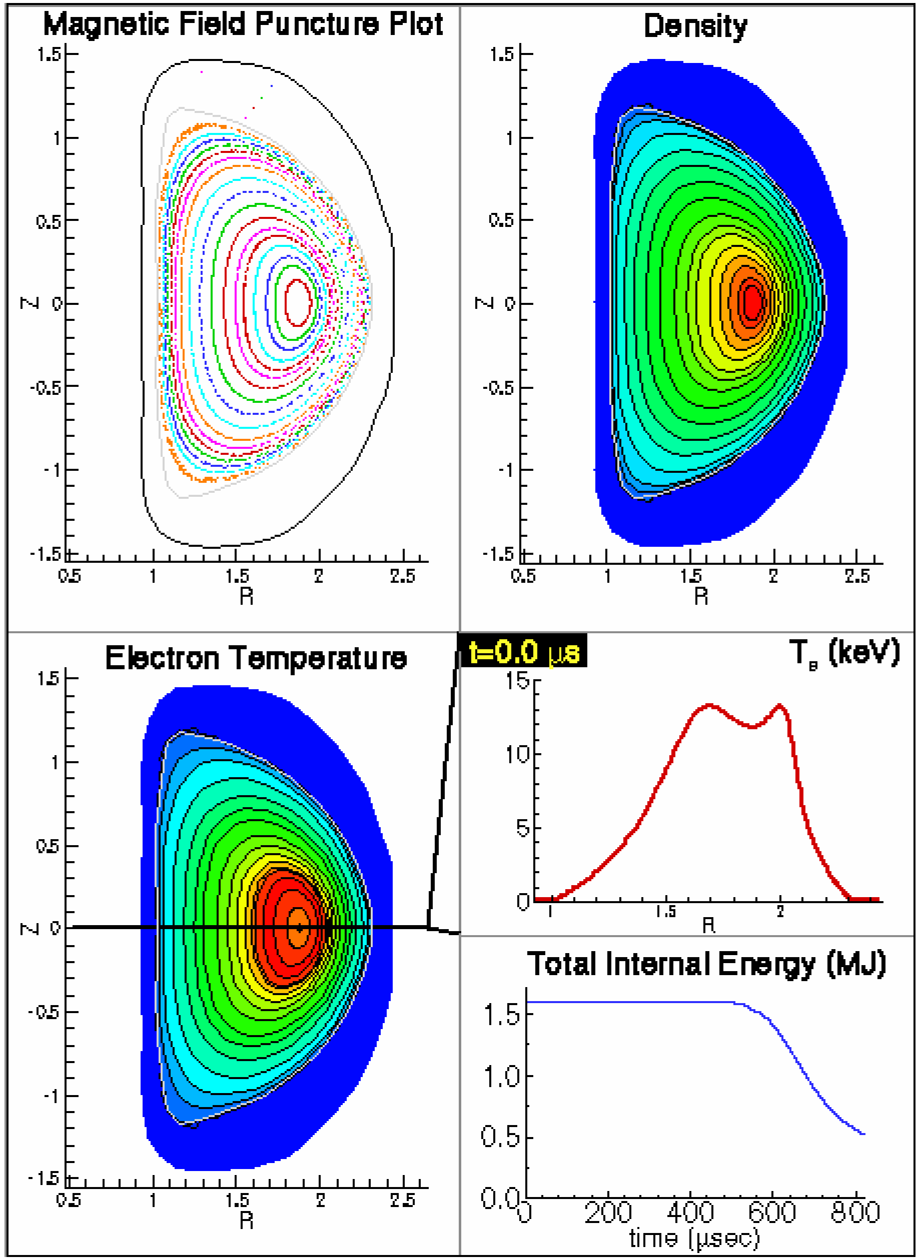


Disruption

Nimrod: Initial equilibrium with $q_0 = 0.97$

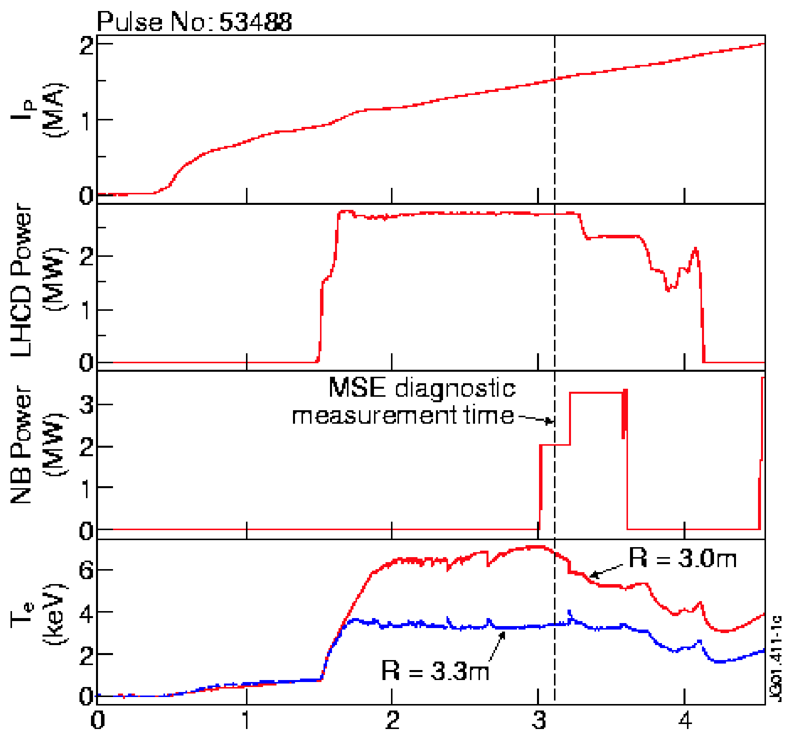


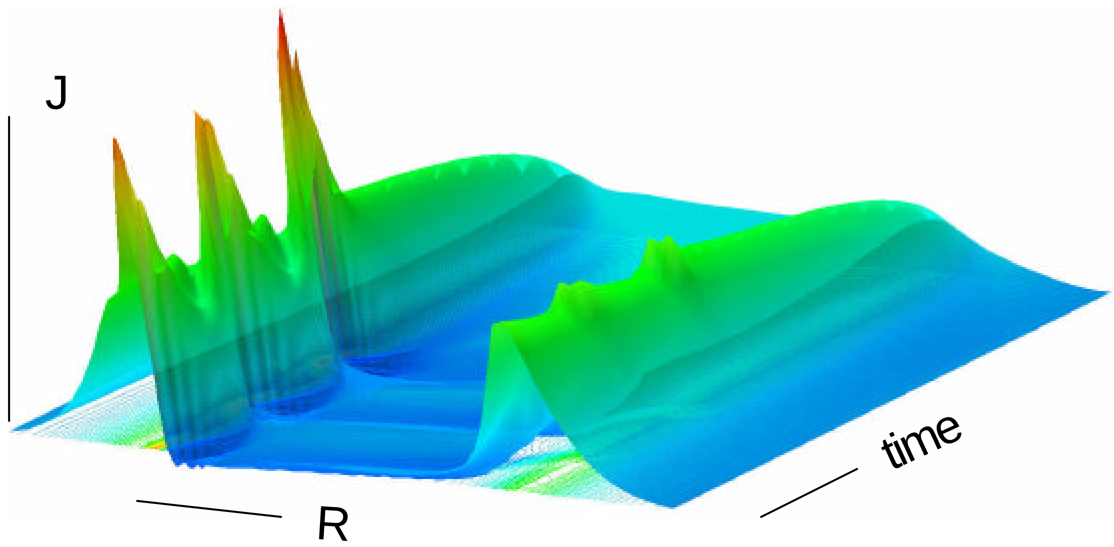
Recent Application: Simulation of a High-b Disruption in DIII-D

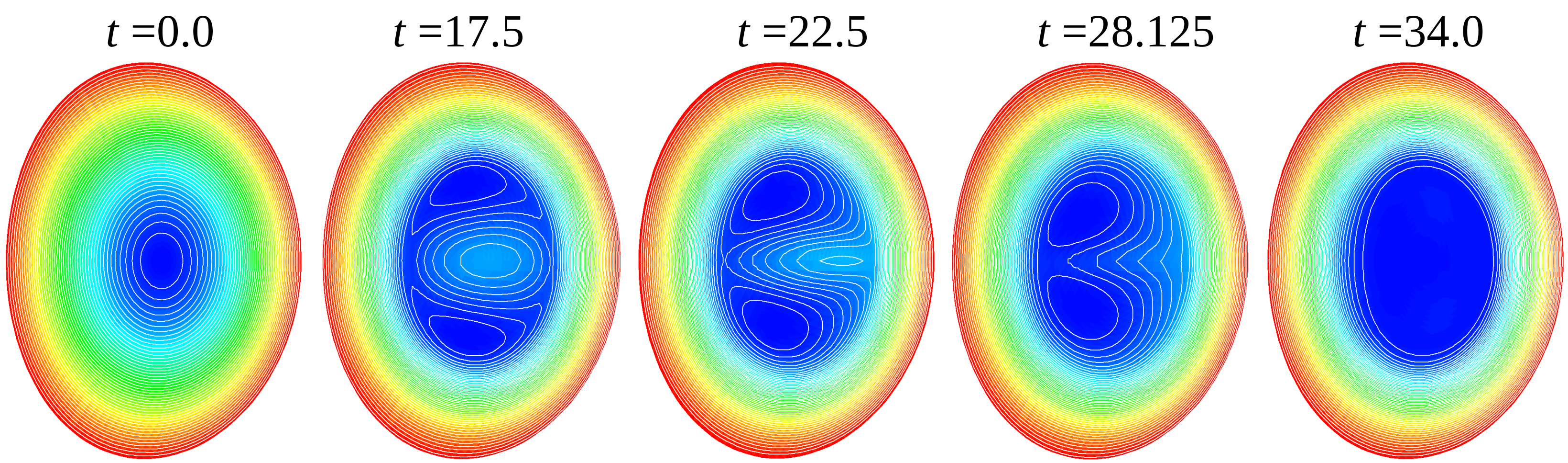


- Simulation includes 3 toroidal harmonics n = 0, 1, 2
- Anisotropic heat conduction
- Vacuum region
- Evolution at single toroidal cross section
- Ideal modes grow with finite resistivity ($S = 10^5$)
- Magnetic field becomes stochastic
- Heat lost to wall preferentially at divertor
- Time for crash ~ 200 msec.
- Power ~ 5 GW

Recent Application: Interpretation of JET Current-Hole Experiments







Recent Application: Effect of anisotropic thermal conduction on island evolution

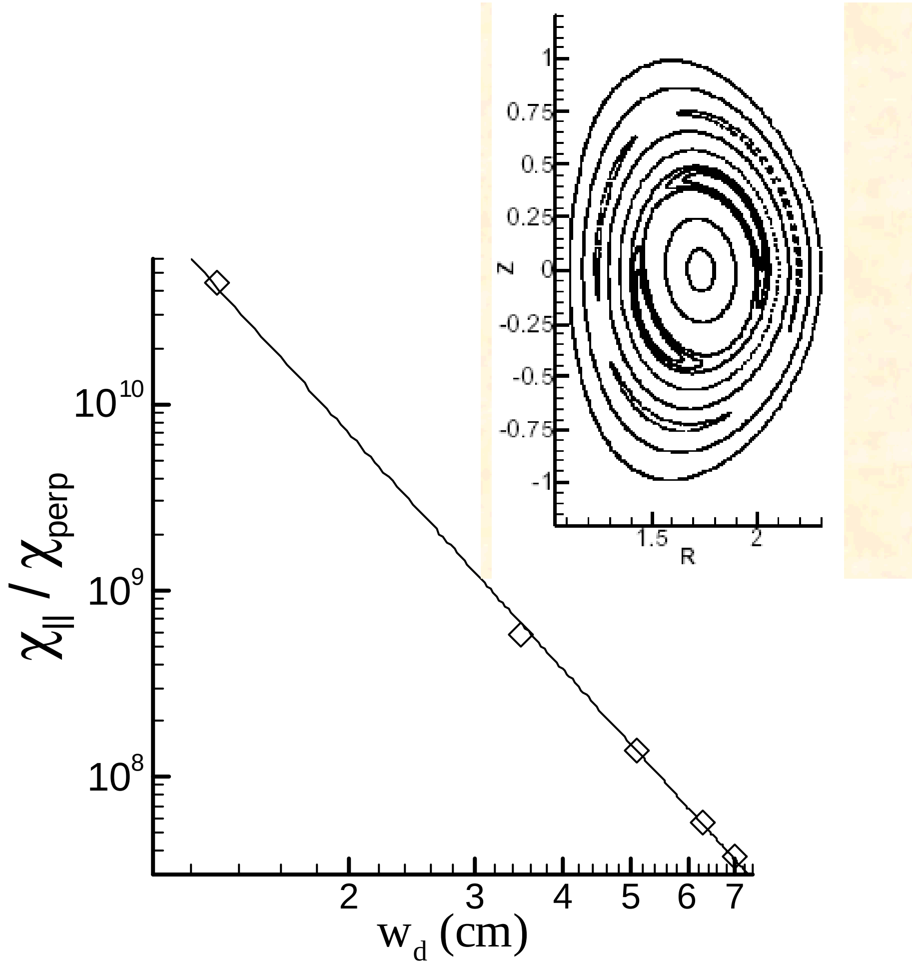
High order finite elements in NIMROD allows use of extreme values of thermal anisotropy.

- 5th order accurate biquartic finite elements

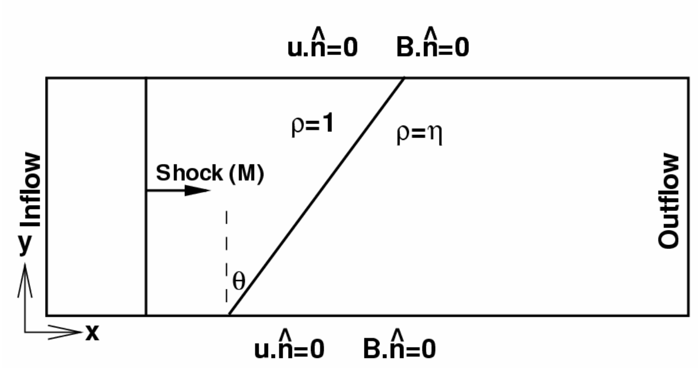
- Repeat calculations with different conductivity ratios and observe effect on flattening island temperature

- Result extends previous analytic result to toroidal geometry.

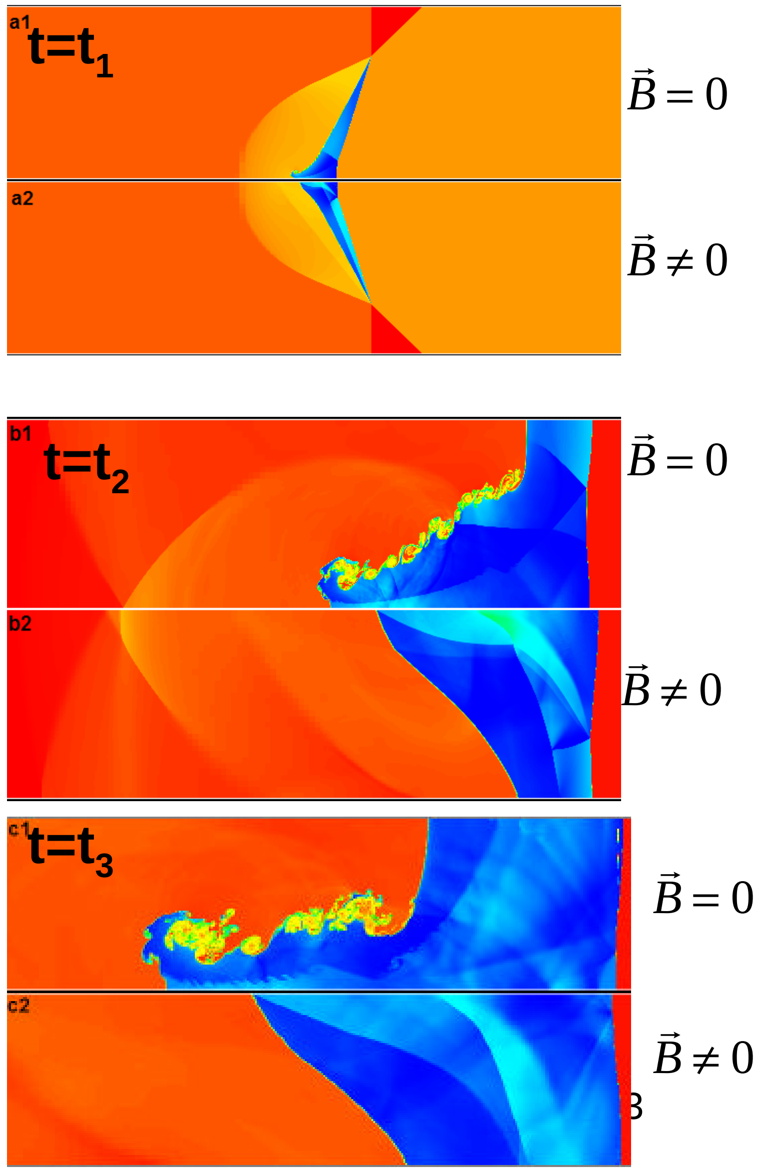
- 3D implicit thermal conduction is required to handle stiffness.



Recent Application: Stabilization of Richtmyer Meshkov Instability by a magnetic field



- By adapting an existing Adaptive Mesh Refinement (AMR) code to the MHD equations, we have been the first to show that a magnetic field can stabilize the Richtmyer-Meshkov Instability (RMI) when a strong shock is incident on a material interface
  - Results are shown for an effective mesh of 16384x2048 points which took approximately 150 hours on 64 processors on NERSC.
  - Speedup of over a factor of 25 compared to a non-AMR code
  - collaboration between CEMM and APDEC centers



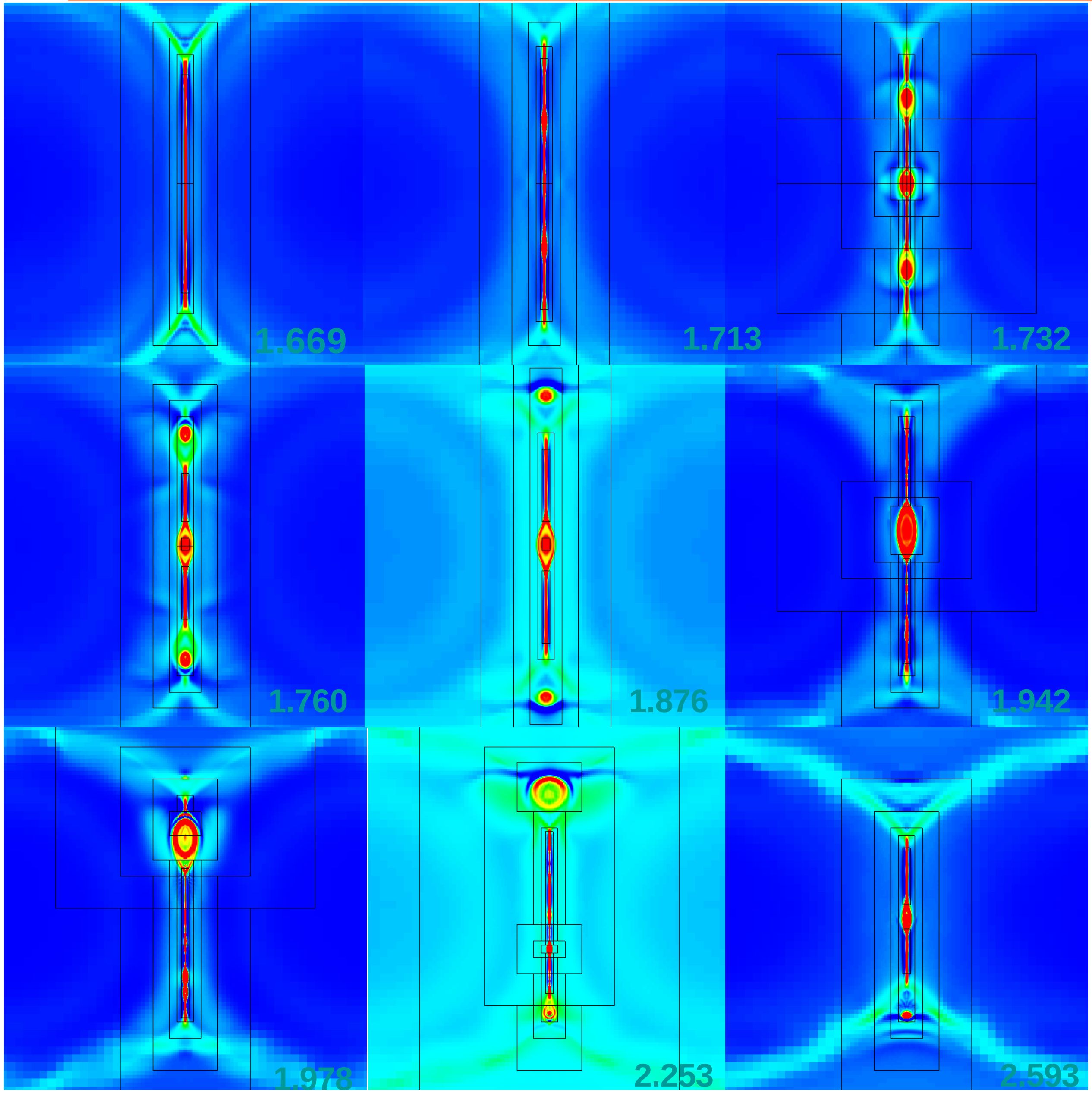
Recent Application: Current bunching and ejection during magnetic reconnection

New Physical Effect!

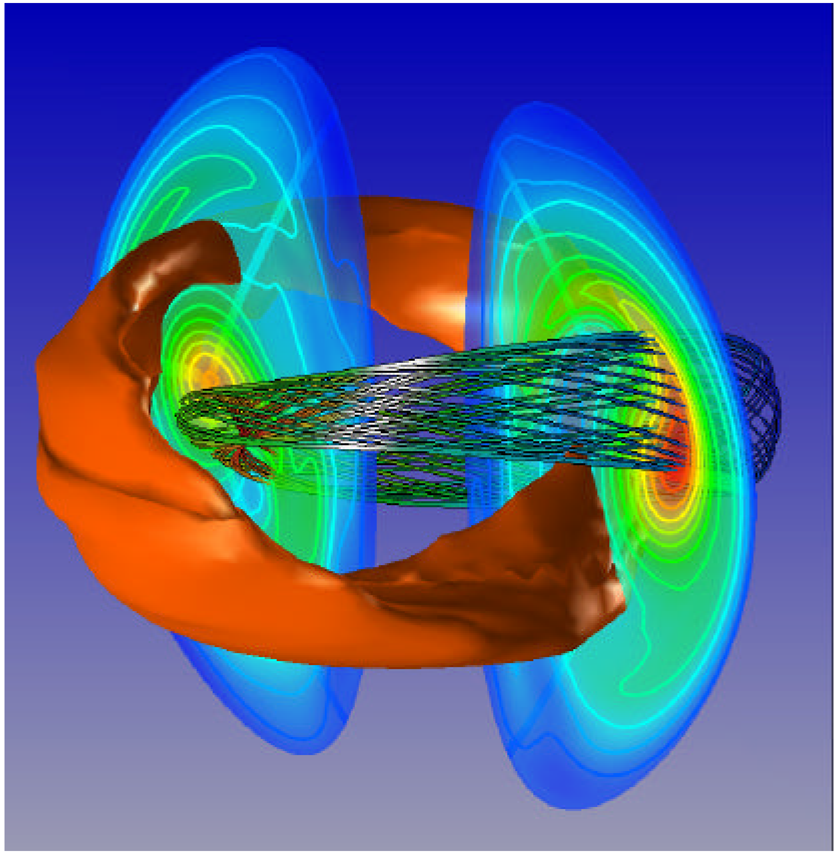
discovered by high-resolution enabled by AMR

Time sequence of current (J_z)

Thin current layer bunches, then "clumps" followed by asymmetric plasma ejection



Recent Application: Strong sheared toroidal flows will cause reconnection modes to saturate.



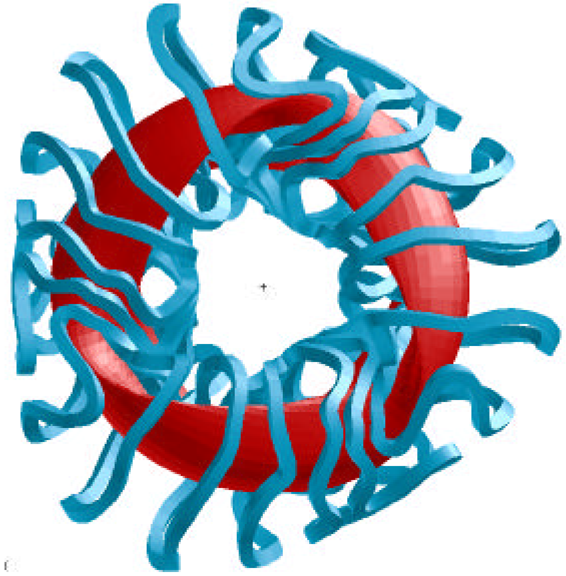
B Field line in the island
Density (Pressure) contours
Temperature isosurface

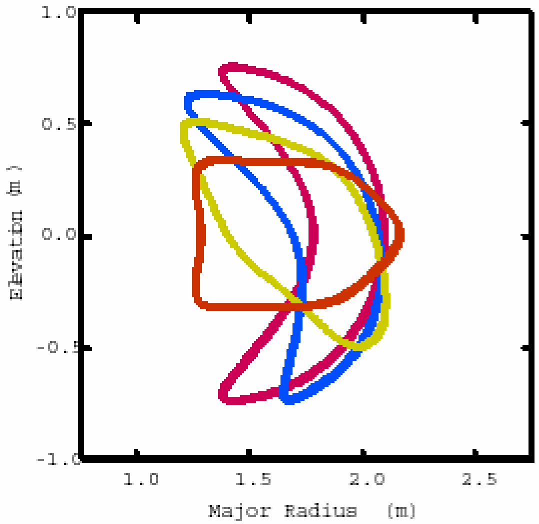
Pressure peaks inside the island together with shear flow causes the mode saturation.

The sheared toroidal flow can have a strong stabilizing effect nonlinearly and, as shown, can cause saturation of otherwise unstable modes if the rotation profile is maintained.

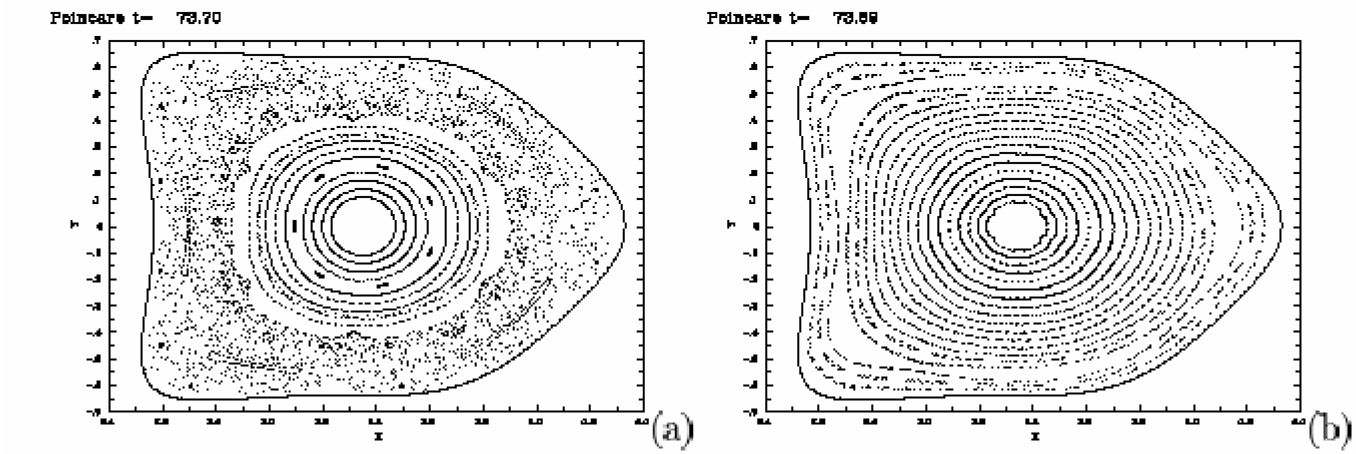
These simulations may account for phenomena recently observed in high-pressure discharges in the National Spherical Torus Experiment.

Recent Application: Diamagnetic Stabilization of Instabilities in Stellarators





National Compact Stellarator Experiment



Pure resistive MHD

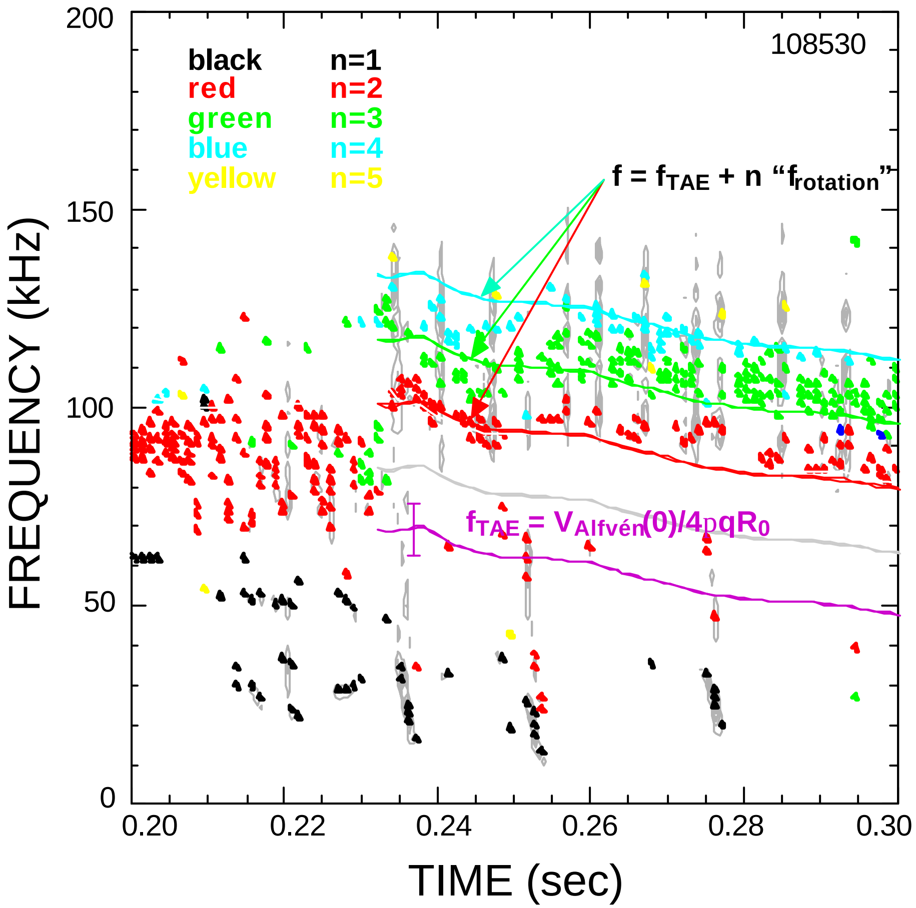
Two-fluid MHD

Extending the MHD description to the 2-fluid model has been shown to be essential in predicting the stabilization of an important class of localized instabilities in stellarators.

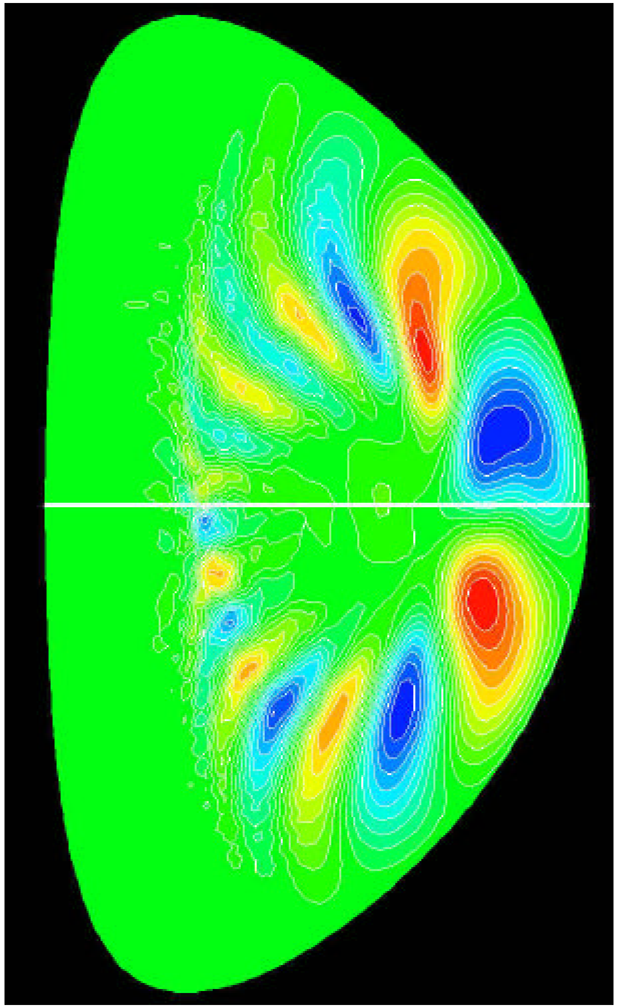
The more complete plasma model generates self-consistent large-scale (diamagnetic) plasma flows that stabilize the localized instabilities.

Recent Application: Hybrid Simulations of unstable Toroidal Alfven Eigenmodes in NSTX

Computed frequencies are consistent with measurements for modes with toroidal mode numbers 1,2,3,4.



n=4 TAE



Part 2:

How super-computing resources have enabled the achievement of the targeted scientific goals;

1. All the studies presented make use of supercomputers
   - 2,877,000 MPP hours at NERSC used by M3D/NIMROD in FY2003
2. We need the ability to calculate many more space-time points in order to model real parameters of fusion experiments of interest
3. M3D and NIMROD scale adequately to thousands of processors.

Required Resources for future studies

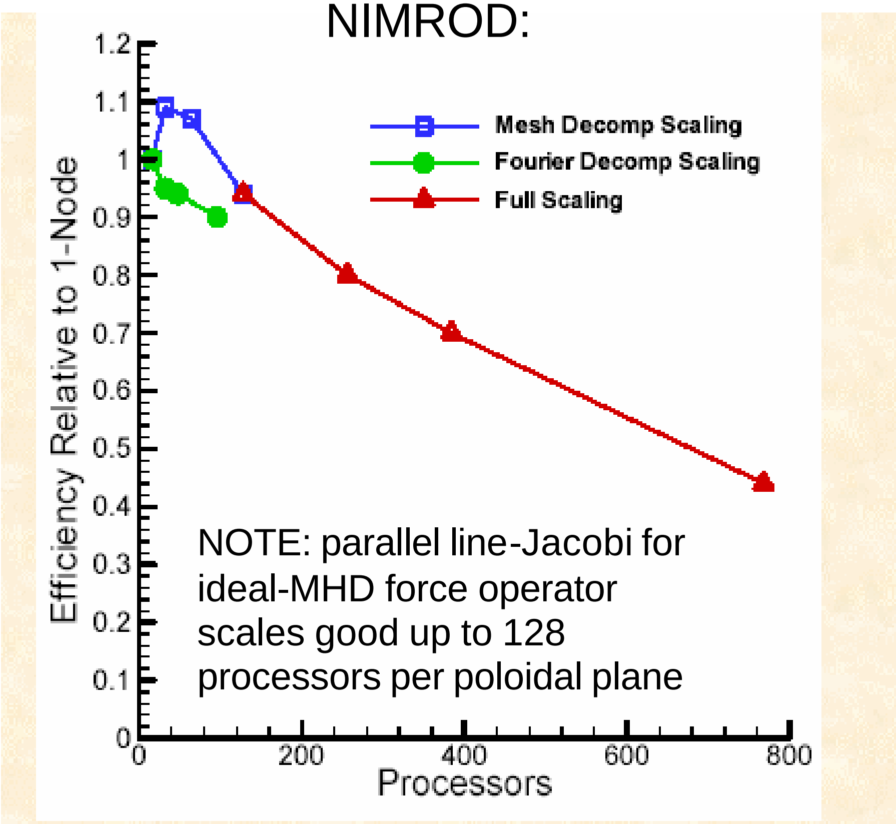
parameter	name	CDXU*	NSTX	CMOD	DIII-D	FIRE	ITER
R(m)	radius	0.3	0.8	0.6	1.6	2.0	5.0
Te[keV]	Elec Temp	0.1	1.0	2.0	2.0	10	10
β	beta	0.01	0.15	.02	0.04	0.02	0.02
$S^{1/2}$	Res. Len	200	2600	3000	6000	20000	60000
$(\rho^*)^{-1}$	Ion num	40	60	400	250	500	1200
$a/\lambda e$	skin depth	250	500	1000	1000	1500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

*Possible today

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.

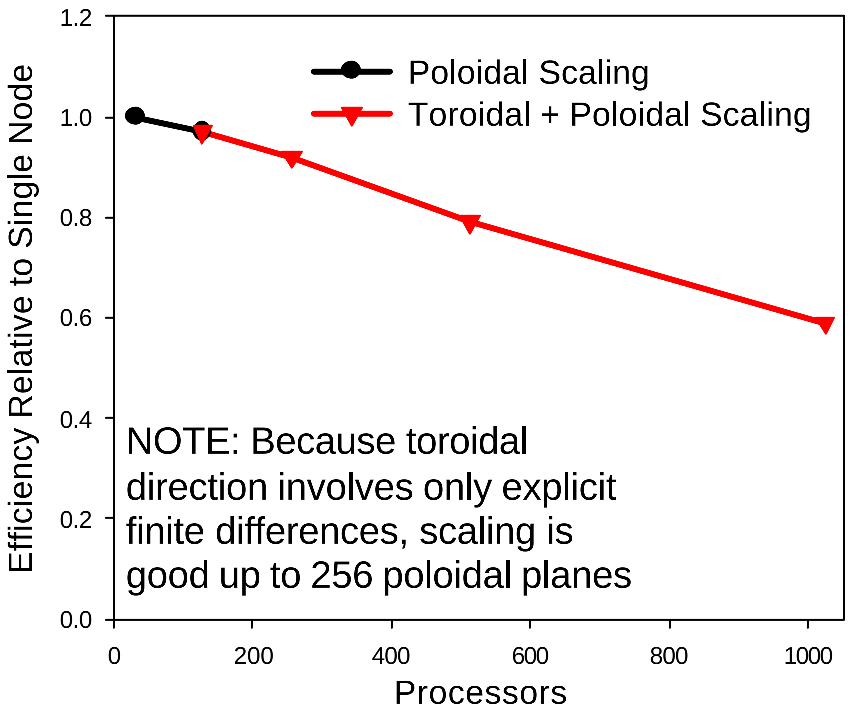
Both NIMROD and M3D exhibit strong scaling that begins to deteriorate at about 500-1000 p for typical problem sizes

NIMROD:



64 x 128 biquartic elements
6 toroidal harmonics

M3D



5000 linear poloidal elements
512 toroidal zones

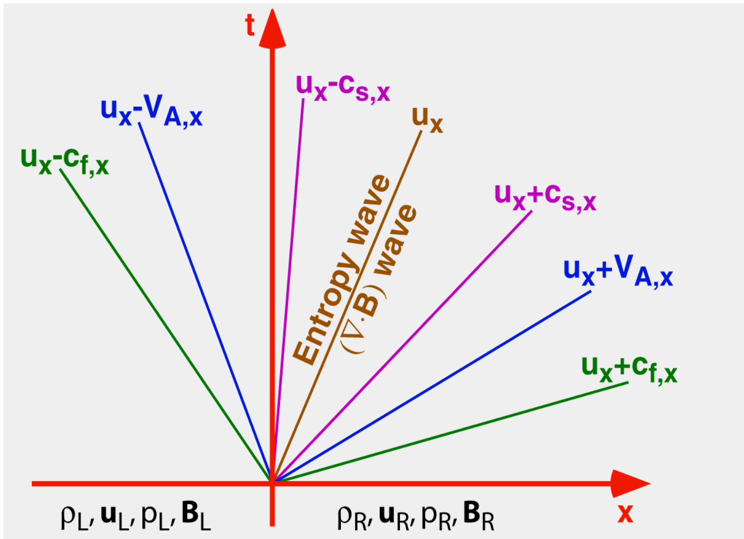
Part 3:

What role have collaborative interactions within each project and also with other SciDAC activities played;

1. CEMM: Test problems
   - Series of linear benchmarks
   - Nonlinear m=1 study relies on the M3D/NIMROD comparison
   - Nonlinear energetic-particle benchmark in progress
2. CMR: Fruitful collaboration on reconnection processes
3. APDEC: Development of AMR MHD code
   - Magnetic reconnection
   - Richtmyer-Meshkov instability
   - 3D pellet injection and mass redistribution in tokamaks
4. TOPS: improved efficiency of M3D linear solvers via hypre
   - Beginning discussions on non-linear solvers
   - Initial results with direct solvers in NIMROD look very promising
5. TSTT: high-order finite elements, mesh generator
   - Developing fusion-specific evaluation criteria: anisotropy, multiple space-scales, multiple time-scales: “CEMM Challenge Problems”

New code for solving the MHD equations was developed with APDEC center using Chombo AMR framework

- MHD Equations written in symmetrizable near-conservative form (Godunov, Numerical Methods for Mechanics of Continuum Media, 1, 1972, Powell et al., J. Comput. Phys., vol 154, 1999).
  - Deviation from total conservative form is of the order of Ñ×**B** truncation errors
- The symmetrizable MHD equations lead to the 8-wave method.
  - The fluid velocity advects both the entropy and Ñ× **B**
- Finite volume approach. Hyperbolic fluxes determined using the unsplit upwinding method (Colella, J. Comput. Phys., Vol 87, 1990)
  - Predictor-corrector.
  - Fluxes obtained by solving Riemann problem
  - Good phase error properties due to corner coupling terms
- $\nabla \cdot B=0$ ensured by projecting the face-centered B from Riemann problem solutions.



BERKELEY LAB

High-Order Adaptive Finite Element Methods for Magnetohydrodynamics

J.E. Flaherty, S. Lankalapalli, K. Pinchedez and M. S. Shephard
Scientific Computation Research Center, Rensselaer Polytechnic Institute
joint research with
J. Breslau, J. Chen, S. Jardin and H. Strauss
Princeton Plasma Physics Lab (PPPL)

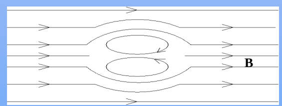
Terascale Simulation Tools and Technology (TSTT), Department of Energy (DoE) sponsored Scientific Discovery through Advanced Computing (SciDAC) Project

Magnetohydrodynamics (MHD)

- Study of plasmas in the presence of magnetic fields
- Physical system exhibits a characteristic two way coupling:
  - Fluid motion induces an electromotive force that will modify existing electromagnetic field
  - Presence of an electric current, together with magnetic field will exert a mechanical force on fluid particles
- Applications in Plasma Physics:
  - fusion power generation

Example: Tilt Instability

- Initial equilibrium consists of two oppositely directed currents embedded in a constant magnetic field
- Initial magnetic field (B) is a dipole vortex :



- When perturbed, vortices turn and get expelled
- Kinetic energy grows like exp(γt)

Current Research

- Implement higher order methods in the Multilevel 3D Project (M3DP) code to simulate MHD flows of plasmas
- Solve the coupled system of Navier-Stokes and Maxwell's equations
- Adaptivity based on:
  - Error Estimation
  - Space-time adaptivity with
    - h-refinement
    - p-refinement

Numerical Method

- Stream functions formulation :

$$\mathbf{B} = \left(\frac{\partial y}{\partial y}, -\frac{\partial y}{\partial x}\right) \text{where} \quad y \text{ is magnetic flux}$$

$$\mathbf{v} = \left(\frac{\partial f}{\partial y}, -\frac{\partial f}{\partial x}\right) \text{ where} \quad f \text{ is the velocity flux}$$

$$\text{Vorticity,} \quad O = \Delta f \;; \quad \text{Current,} \quad C = \Delta y$$

- Streamline Upwind Petrov-Galerkin(SUPG) stabilization
- Time discretization by Backward Euler
- Equations solved successively by retarding variables with an inner iteration

Incompressible MHD Equations

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B})$$

$$r \frac{\partial \mathbf{v}}{\partial t} = -r(\mathbf{v}.\nabla)\mathbf{v} + (\nabla \times \mathbf{B}) \times \mathbf{B} + rm \Delta \mathbf{v}$$

$$\nabla . \mathbf{v} = 0$$

$$\nabla . \mathbf{B} = 0$$

where :

$\mathbf{B}$ is magnetic field $\quad r$ is density

$\mathbf{v}$ is velocity $\quad m$ is viscosity

Results

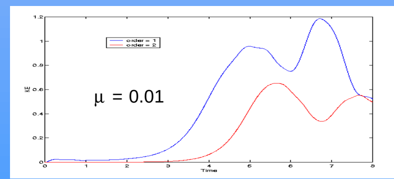
- Obtained on a square domain of size [6x6] with :
  - Initial conditions :

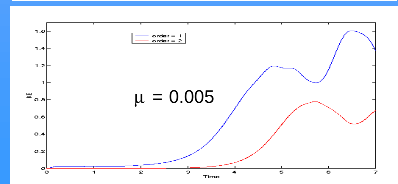
$$y_0 = \begin{cases} \frac{2}{kJ_0(k)} J_1(kr)\, Cos\, q, & r < 1 \\ \left(r - \frac{1}{r}\right) Cos\, q, & r > 1 \end{cases} \qquad \Omega_0 = 0$$

$$J_1(k) = 0$$

  - Boundary conditions : *f = 0; C = 0*
  - Triangular elements with Lagrange basis of orders 1 and 2

Kinetic Energy

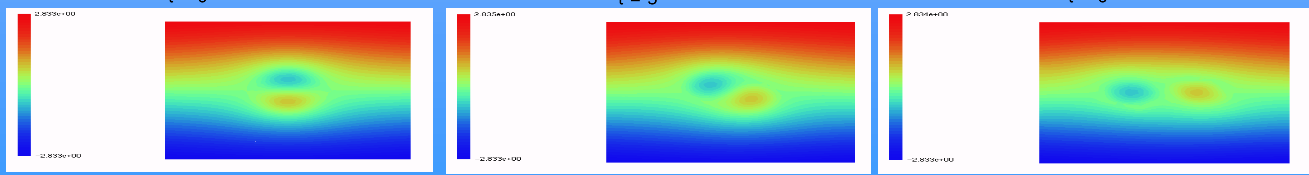




Magnetic Flux (y)

μ= 0.005, order = 2 and mesh of 924 elements

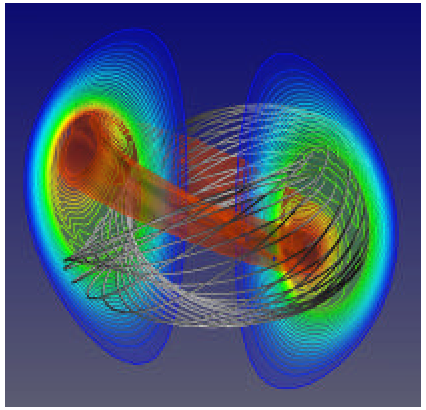
t = 0 t = 5 t = 6



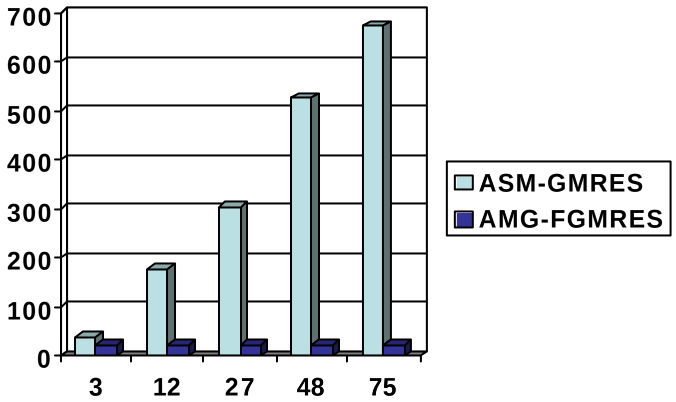
MSERC Rensselaer

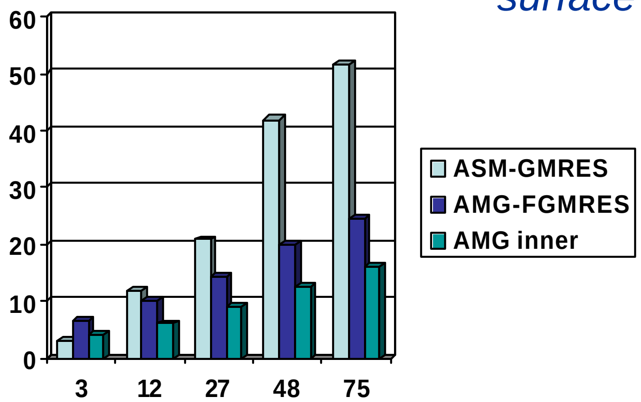
We are speeding up tokamak simulations through PETSc-*hypre* combo

- CEMM's M3D code is built upon PETSc's distributed data structures
- *hypre*'s AMG solver (via PETSc) is now speeding up simulations
  - **Perfect iteration scaling**
  - **Still performance issues to resolve**
  - **Time is halved or better for large runs**



NSTX sawtooth, showing pressure contours and surface with some B-lines





From TOPS review (R. Falgout)

TOPS
Terascale Optimal PDE Simulations

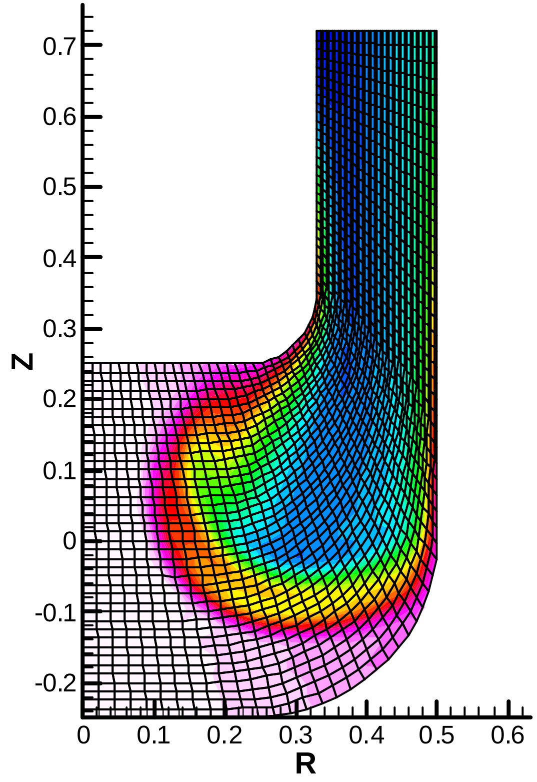
Part 4:

What is the vision for the next 3-years ?

1. Exploratory projects
   - High-order and adaptive elements
   - Non-linear implicit time advance to allow large timesteps
2. Incremental improvement of M3D and NIMROD
   - Improved Physics Models
   - Improved numerical representation/methods
3. New Physics Applications: focus on burning plasma issues
   - Sawtooth Phenomena
   - Tearing and Neoclassical Tearing Modes
   - Energetic Particle Modes
   - Edge Localized Modes
   - Forces due to disruptions
   - The physics of pellet fueling
   - Resistive wall mode control
4. Integrated Modeling
   - Kinetic/fluid integration
   - RF MHD integration

CEMM Future Interests in ISIC centers

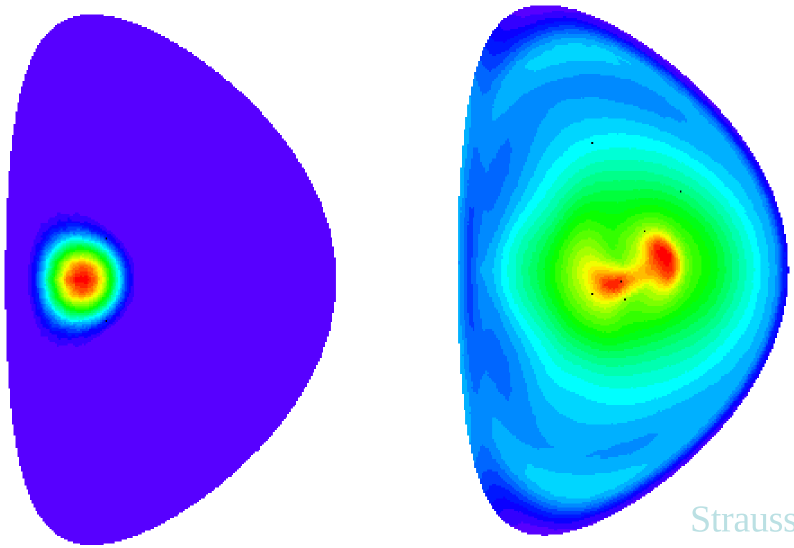
- Incorporation of "standard" grid generation and discretization libraries into M3D and NIMROD
- Higher order and mixed type elements into M3D
- Explore combining separate elliptic solves in M3D
- Extend the sparse matrix solvers in PETSc in several ways that will improve the efficiency of M3D
  - Develop multilevel solvers for stiff PDE systems
  - Take better advantage of previous timestep solutions
  - Refinements in implementation to improve cache utilization
  - Optimized versions for Cray X1 and NEC SX-6
- Implicit hyperbolic methods for adaptive mesh refinement (AMRMHD)
- Nonlinear Newton-Krylov time advance algorithms
- Efficient iterative solvers that can handle NIMROD non-symmetric matrices (needed for 2-fluid and strong flow problems)
- Initial investigation of direct solvers in NIMROD look very promising (Super-LU_DIST courtesy TOPS)



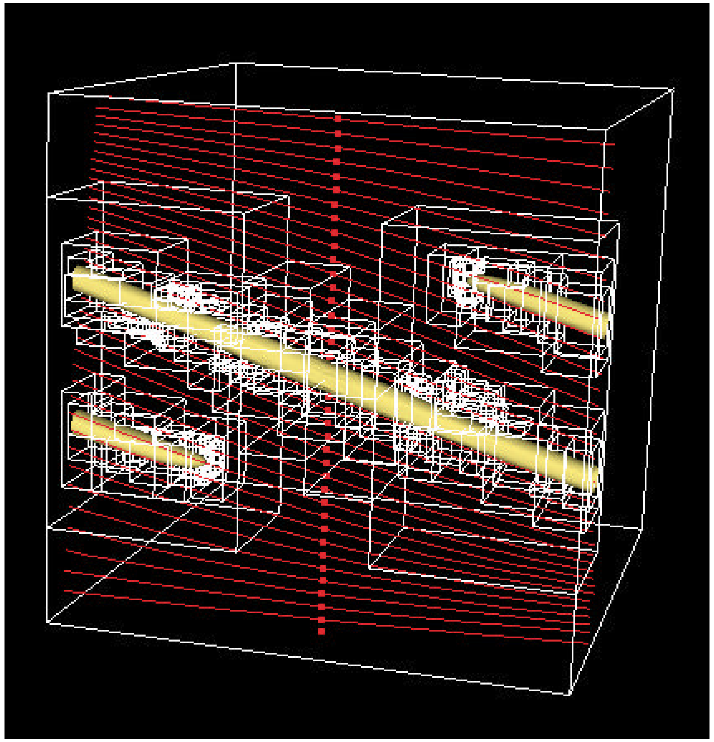
SSPX mesh using CUBIT (courtesy TSTT)

New focus of AMR work is to provide a quantitative description of pellet fueling of fusion plasmas

- Experimentally, it is known that injection of pellet can cause localized MHD instabilities that have large effect on fuelling efficiency,



Initial M3D calculations (1998) showed essential physics, but at low resolution

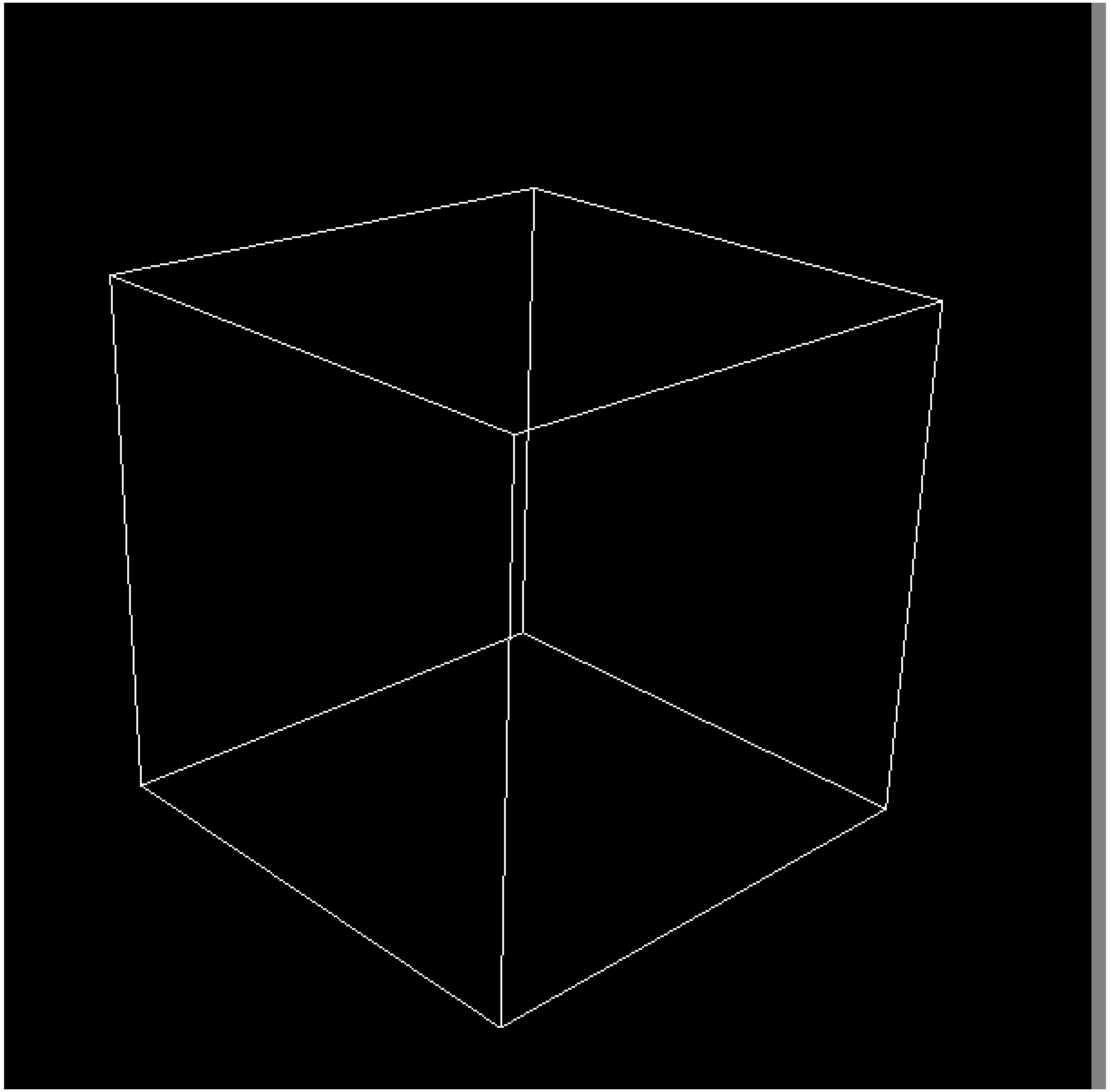


Initial AMR simulations of pellet injection in periodic cylinder illustrate that high resolution is possible; now being extended to torus.

AMR continued….

Pellet injection simulations show density equilibrating along field lines to equilibrate on surfaces, and these can become unstable due to localized high pressure causing interchange instabilities.

Essential toroidal effects now being addded



Present model development emphasis is on more complete (kinetic) Hybrid particle closure and Integral heat-flow closures

For Hybrid method, field evolution equations are unchanged. Momentum equation replaced with "bulk fluid" and kinetic equations for energetic particles

$$r_b \frac{d\vec{V}_b}{dt} = -\nabla p_b - (\nabla \bullet \vec{P}_h)_\perp + \vec{J} \times \vec{B}$$

ions are particles obeying guiding center equations

$$\dot{\vec{X}} = \frac{1}{B}\left[\vec{B}^* U + \hat{b} \times (m \nabla B - \vec{E}) \right],$$

$$\dot{U} = -\frac{1}{B} \vec{B}^* \bullet \left(m \nabla B - \frac{e}{m} \vec{E} \right),$$

- The hybrid model describes the nonlinear interaction of energetic particles resonant with MHD waves
- brings in essential new physics for burning plasmas with large alpha-particle component

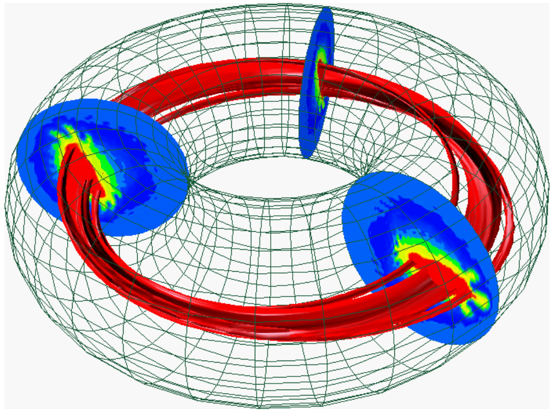
Integral closure retains free-streaming and collisional effects

$$q_{||}(L') = \int^{L'} dL \left[T(L' - L) - T(L' + L) \right] \frac{\partial K}{\partial (\ln L)}$$

$$K(L) = n_0 v_{th} s^3 \left(s^2 - \tfrac{5}{2} \right)^2 \sum_{i=0}^{N} a_i e^{-(s^2 + \bar{k}_i L)}$$

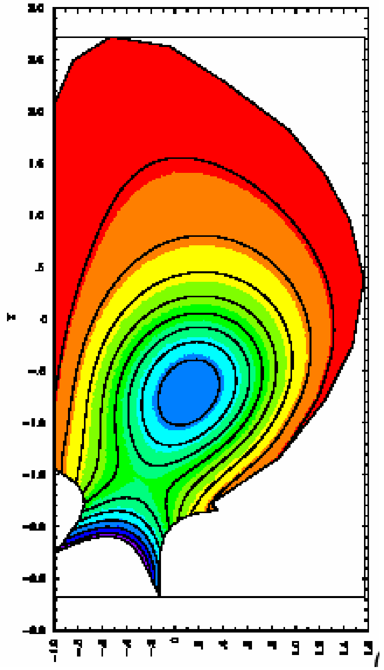
- Here, the parameters a_i and k_i are generated in the solution of the drift kinetic equation
- Provides non-local thermal conductivity valid in long mean free path regime
- massively parallel implementation allows incorporation in NTM simulation

Prediction of the Cause and Effect of Disruptions



One mechanism for the Disruption:
Short wavelength modes interacting with helical structures.

Park

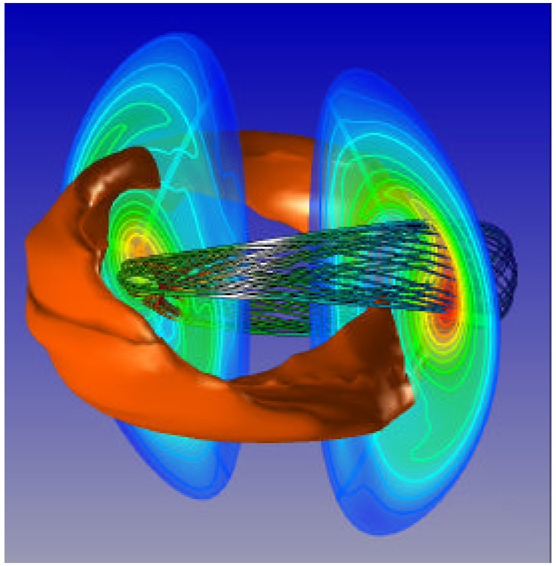


Strauss et al

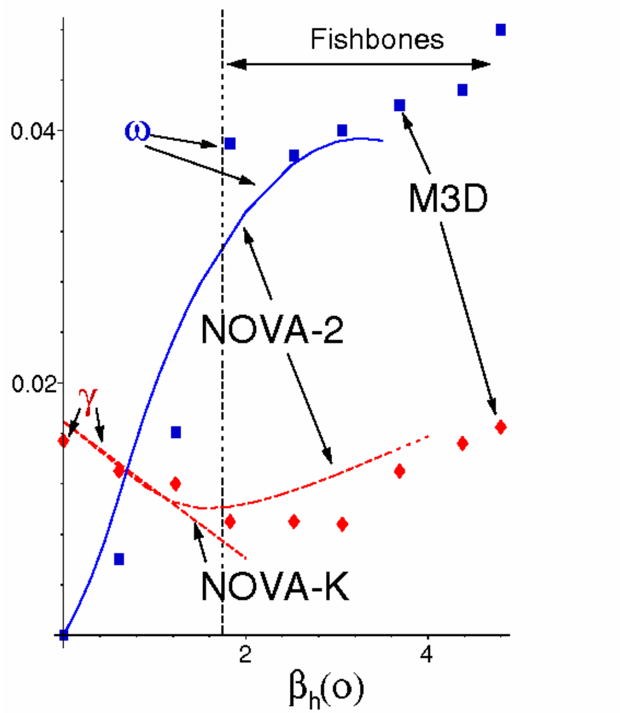
Non-axisymmetric Disruption Forces being computed by M3D

Long term goal is to identify all sequences of events that can lead to plasma disruptions, and to identify relatively "disruption free" regimes of operation, and to accurately predict peaking factor of halo-currents.

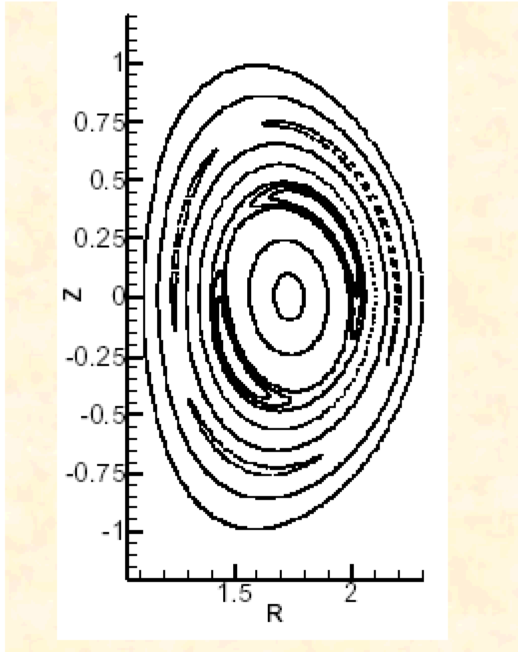
Beta limiting MHD modes



Internal reconnection events, including plasma flow



Energetic particle modes are beta and profile dependent.



Interaction of coupled island chains, NTMs.

Park, Fu, Gorelenkov, Kruger

Goal is to develop a complete, predictive, reliable model for determining beta limits in a burning plasma

Summary

- Scientific & Technical Merit,
  - Several APS Invited talks, IAEA papers, refereed publications, Colloquia
  - Current nonlinear m=1 test problem is rich in physics and will likely lead to new discovery.   Nonlinear kinetic test problem even richer.
  - CEMM codes represent a unique capability worldwide
  - Now addressing many of the key issues for a tokamak burning plasma as identified by ITER and FIRE
  - Fundamental work in reconnection and in Richtmyer-Meshkov stabilization
- Readiness for Terascale Computing,
  - Codes routinely run on 100s (or 1000s) of processors at NERSC
  - Working with ORNL to evaluate M3D and NIMROD on Cray-X1
  - NIMROD NTM application with integral heat flow has been chosen as NERSC "Big Splash" based on competitive review
  - Working with math ISICs to further optimize (TOPS, TSTT, APDEC)
- Potential for Impact on Other Scientific Disciplines
  - Magnetic stabilization of Richymyer-Meshkov motivating analytical and possible experimental investigations
  - Many spinoffs possible to astrophysical and space plasmas

Please visit our web site at w3.pppl.gov/CEMM