The Center for Extended Magnetohydrodynamic Modeling
Progress, Plans, and Opportunities for Collaboration

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a SciDAC activity…

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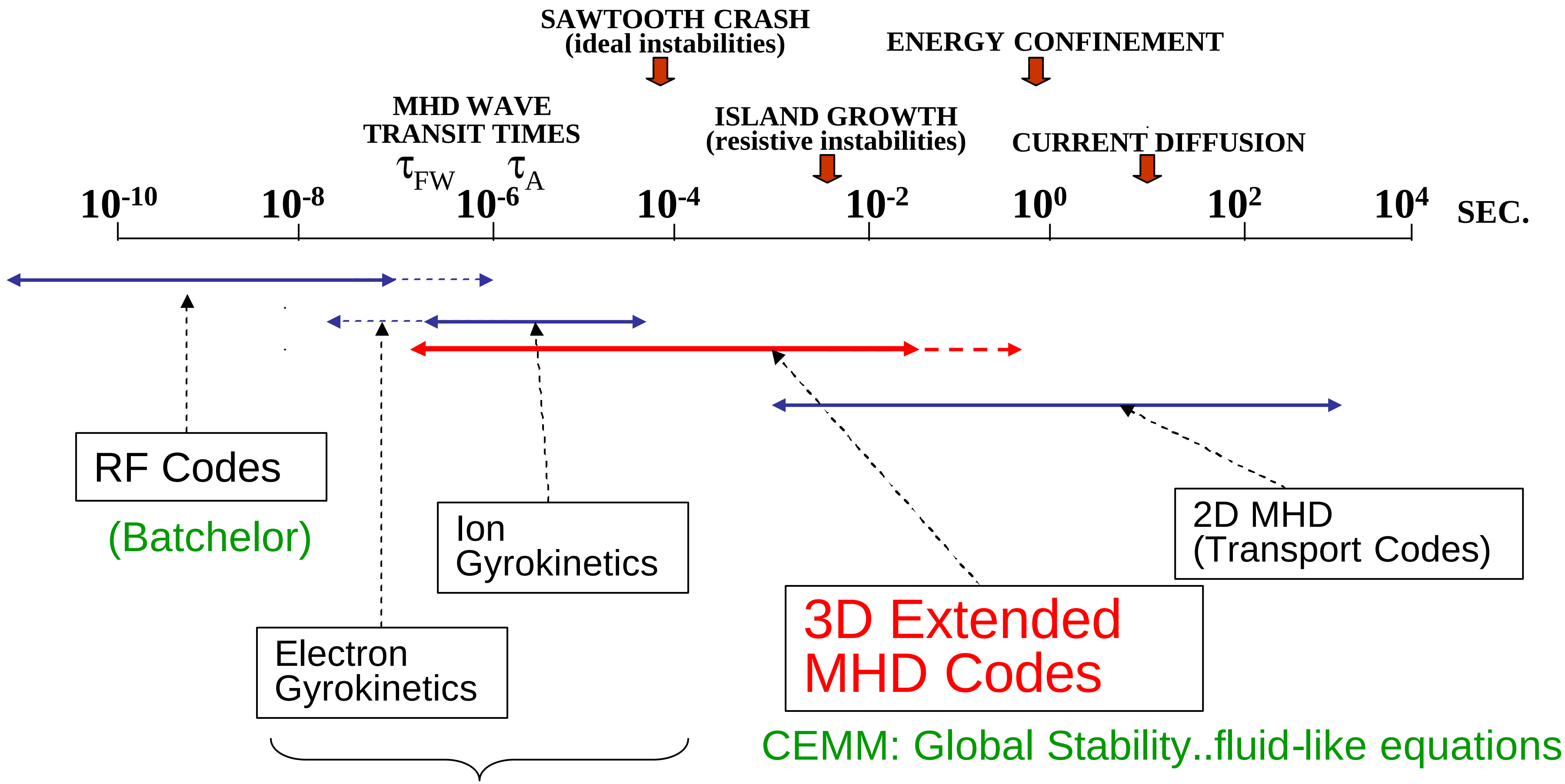
Time Scales a in “next step” ignition experiment: B = 10 T, R = 2 m, $n_e = 10^{14}$ cm^{-3}, T = 10 keV



PMP (Nevins): plasma micro-turbulence using kinetic equations

Also:
Bhattacharjee: basic reconnection
Pindzola: atomic physics

Present capability:

TSC (2D) simulation of an entire burning plasma tokamak discharge (FIRE)

Includes:

RF heating

Ohmic heating

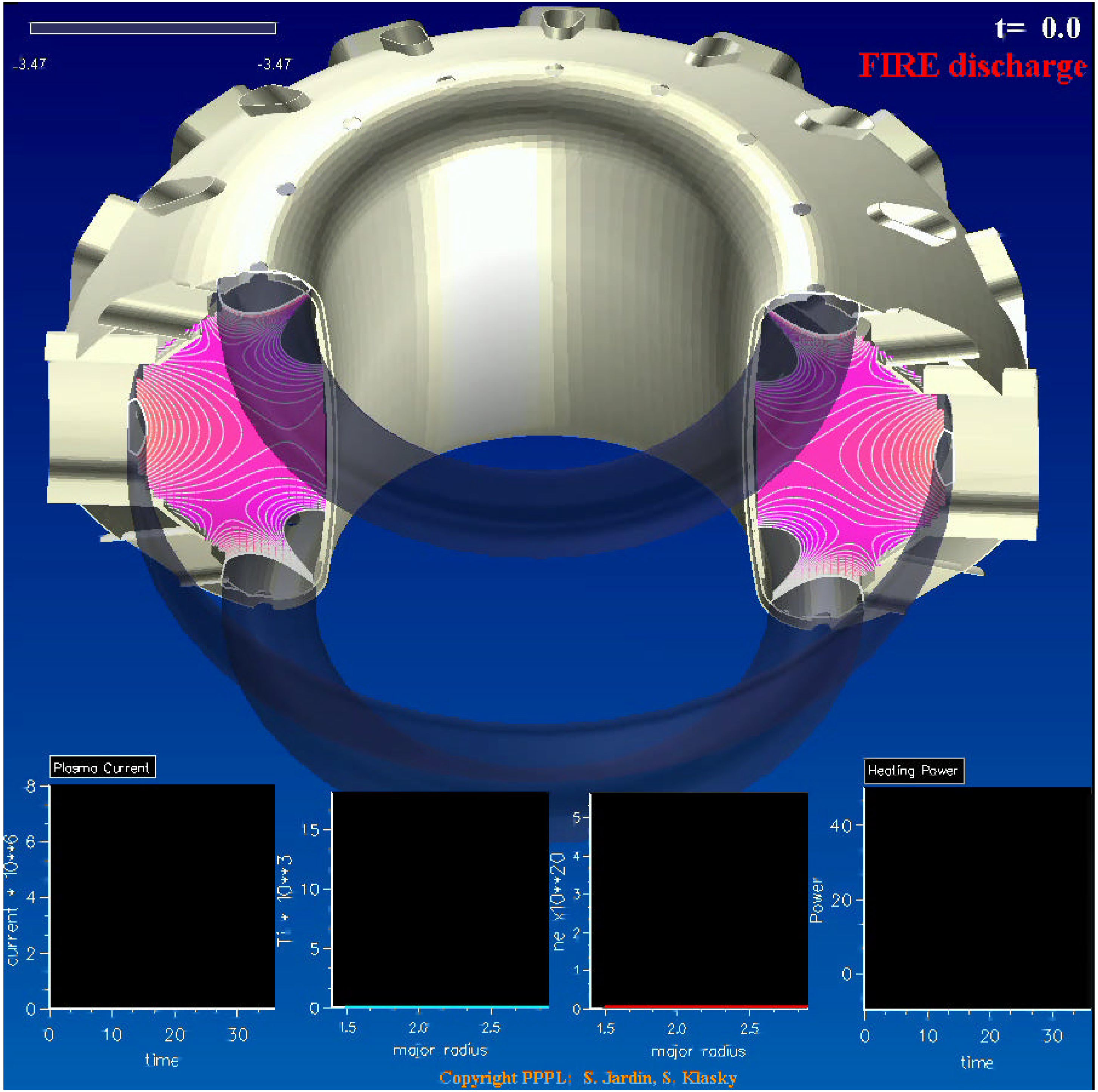
Alpha-heating

Microstability-based transport model

L/H mode transition

Sawtooth Model

Evolving Equilibrium with actual coils

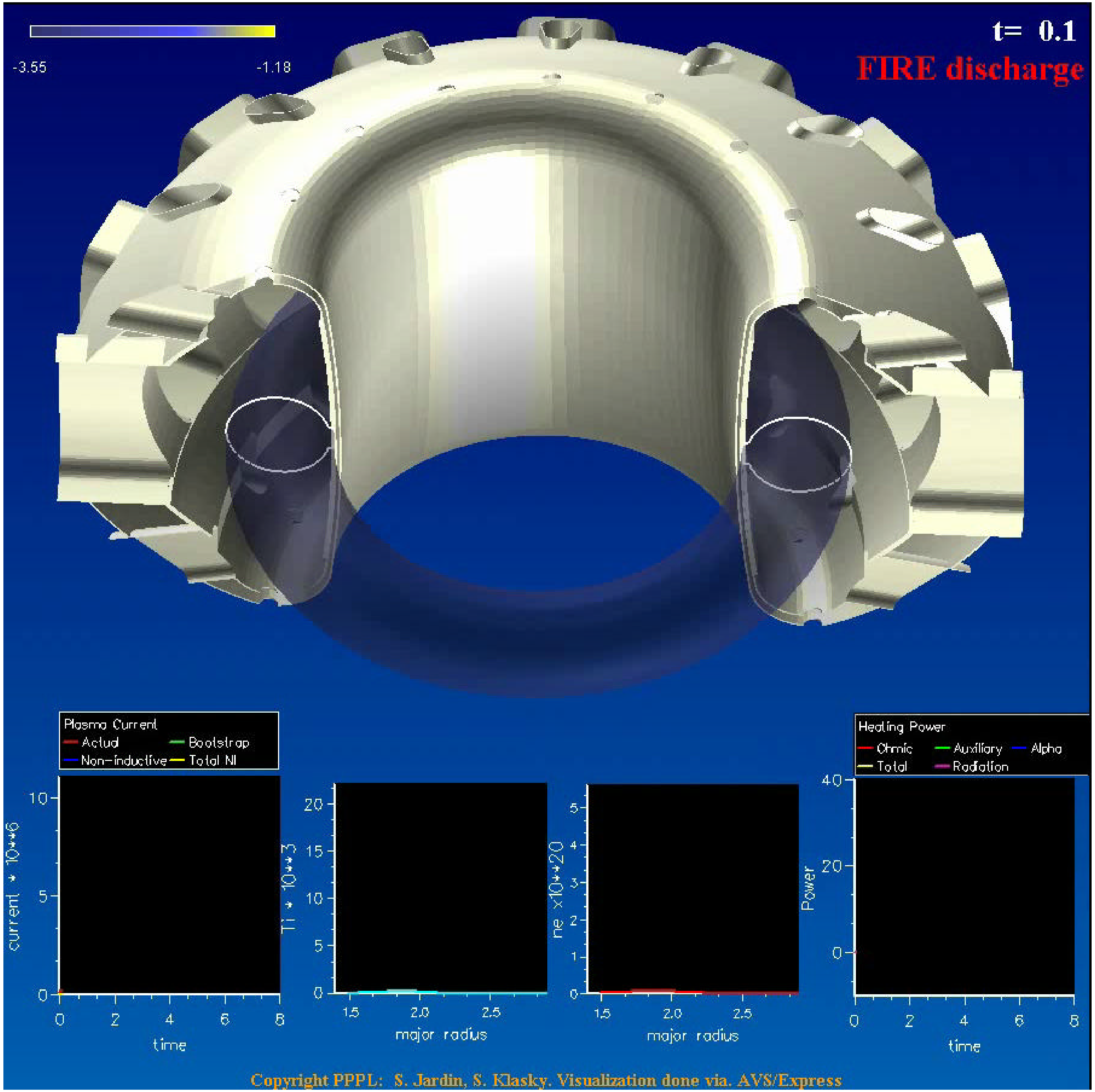


Even in 2D, things can go wrong:

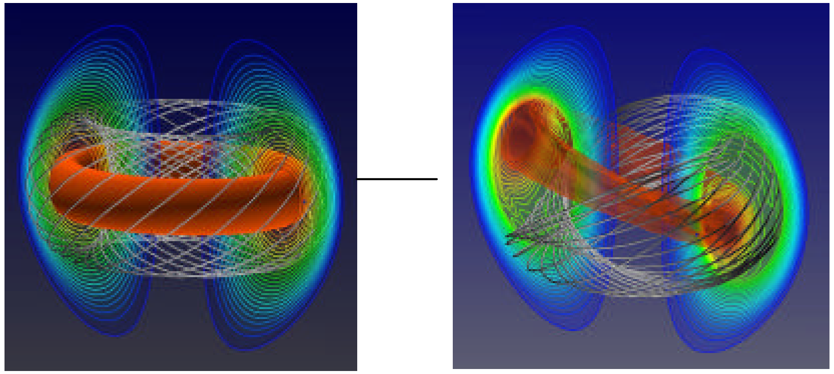
Vertical Displacement Event (VDE) results from loss of vertical control due to sudden perturbation

TSC simulation of an entire burning plasma discharge (FIRE)

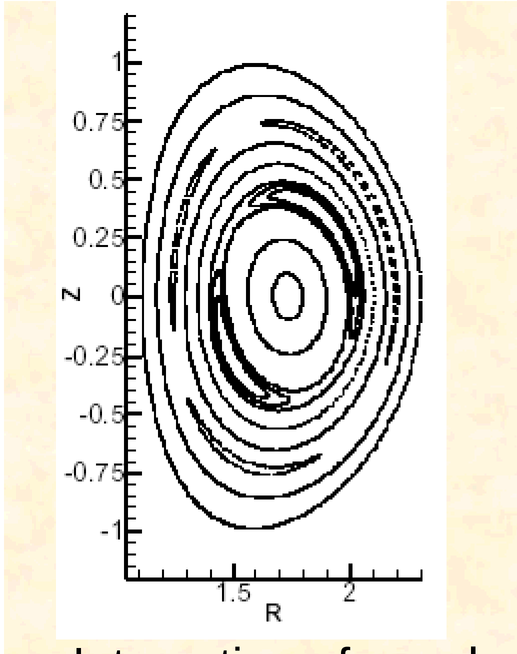
Starts out same as before…ends in a VDE



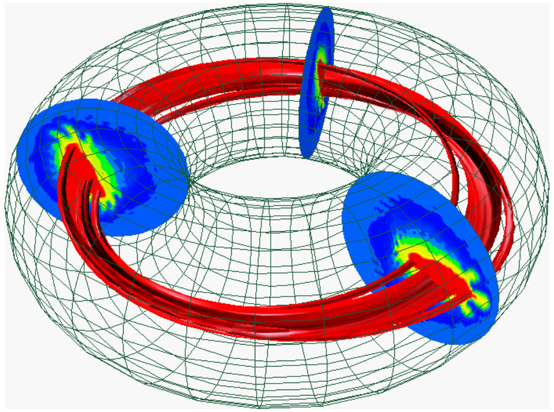
The need for 3D Tokamak models



Internal reconnection events or
“sawtooth oscillations”



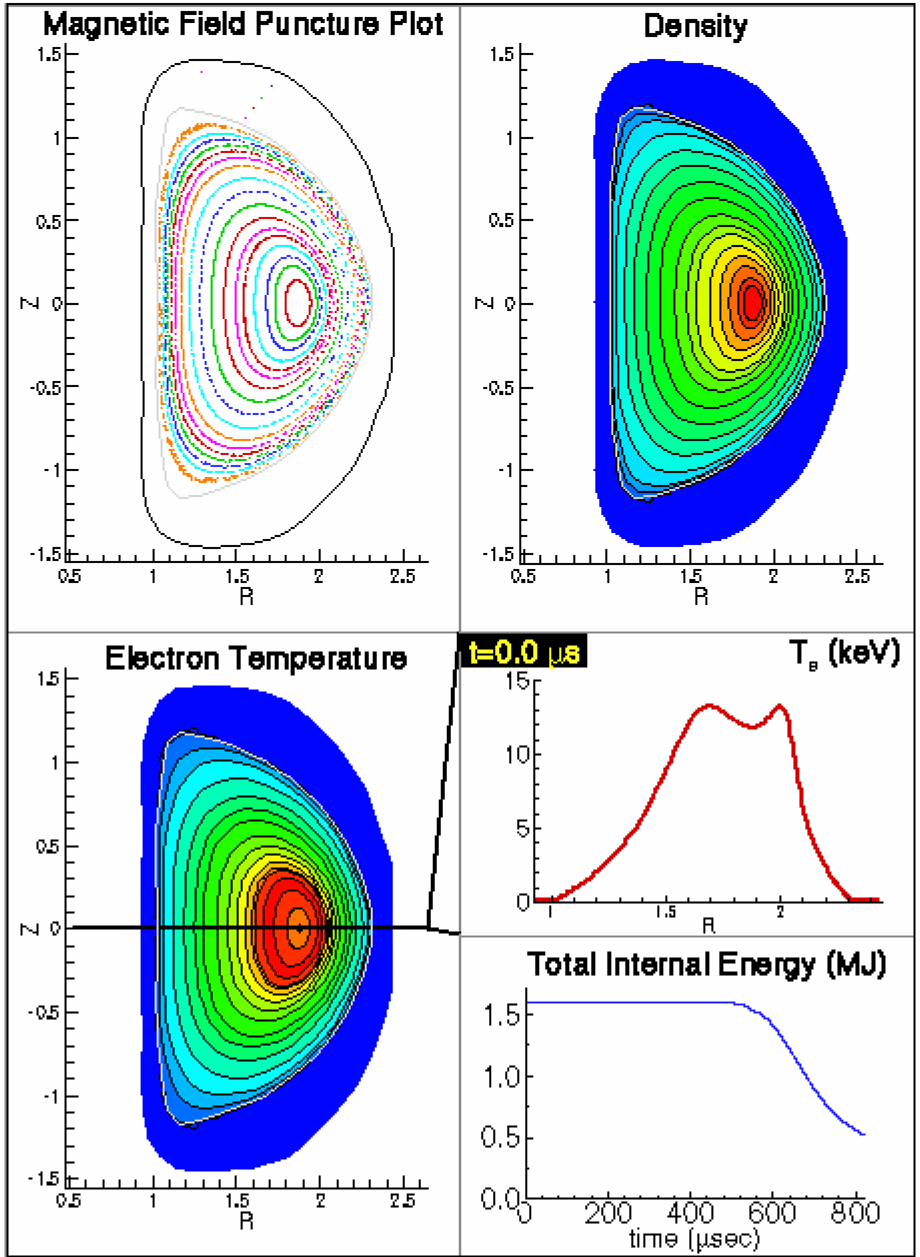
Interaction of coupled
island chains.



Short wavelength modes
interacting with helical structures.

NIMROD 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**



Plasma Models: XMHD

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

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

$$m_0 \vec{J} = \nabla \times \vec{B}$$

$$P = pI + \Pi$$

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

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

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

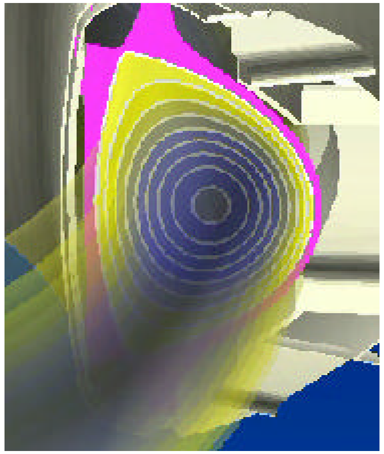
$$\frac{3}{2}\frac{\partial p_e}{\partial t} + \nabla \bullet \left(\vec{q}_e + \frac{5}{2} P_e \bullet \vec{V}_e\right) = \vec{J} \bullet \vec{E} + S_E$$

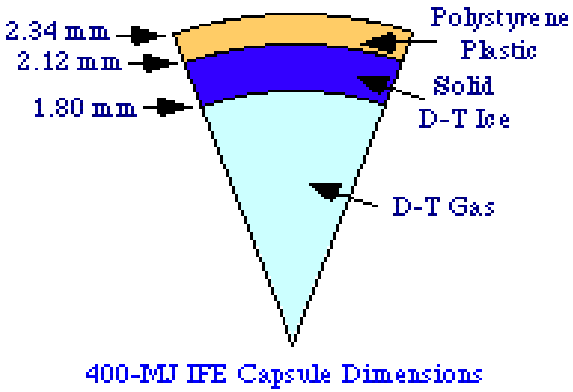
Two-fluid XMHD: define closure relations for P_i, P_e, $\mathbf{q_i}$, $\mathbf{q_e}$

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

Note that both IFE targets and MFE have similar equations, but the parameters and numerical challenges are totally different:

Lawson condition for Fusion $n\ (cm^{-3})\ \tau\ (sec) > 10^{14}$





MFE: $n = 10^{14}$, $\tau \sim 1$ sec

IFE: $n = 10^{25}$, $\tau \sim 10^{-11}$ sec

Multiple timescales	Multiple space-scales	Extreme anisotropy	Essential kinetic effects
Implicit methods and long running times	Adaptive meshing, unstructured meshes.	High-order elements, field aligned coordinates, artificial field method	Hybrid particle/fluid methods, integrate along characteristics

CEMM Simulation Codes:

	NIMROD	M3D	AMRMHD*
Poloidal discritization	Quad and triangular high order finite elements	Triangular linear finite elements	Structured adaptive grid
Toroidal discritization	pseudospectral	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 field method	Adaptive meshing
Libraries	AZTEC (Sandia)	PETSc (ANL)	CHOMBO (LBL)
Sparse Matrix Solver	Congugate Gradient	GMRES	Conjugate Gradient
Preconditioner	Line-Jacobi	Incomplete LU	Multigrid

*Exploratory project together with APDEC

M3D Scalar Equation time advance:

$$\frac{\partial Z}{\partial t} = -I\Delta^* \underline{I} - \Delta^* \underline{p} + \frac{m}{r}\nabla^2 \underline{Z}\ldots$$

$$\frac{\partial I}{\partial t} = -I\,\underline{Z} + h\Delta^* \underline{I}\ldots$$

$$\frac{\partial p}{\partial t} = -g\, p\,\underline{Z}\ldots$$

$$\frac{\partial C}{\partial t} = h\Delta^* \underline{C} + \ldots$$

$$\frac{\partial W}{\partial t} = \frac{m}{r}\nabla^2 \underline{W} + \ldots$$

$$\frac{\partial v_j}{\partial t} = \frac{m}{r}\nabla^2 \underline{v_j} \cdots$$

$$\frac{\partial d}{\partial t} = \ldots$$

$$\Delta^* c = Z$$

$$\Delta^\dagger U = W$$

$$\nabla_\perp^2 \Phi = \ldots$$

$$\nabla_\perp^2 f = -I/R$$

$$\Delta^* y = C$$

3 *coupled implicit time advance equations*

3 *uncoupled implicit time advance equations*

1 *explicit time advance*

5 *elliptic solves...but all 2D*

- **Only fast-wave, field diffusion, and viscosity terms are treated implicitly !**
- **Leads to fast convergence of iterative solvers, but time step still limited by Shear Alfven wave**

NIMROD Time Advance: greater degree of implicitness

The **numerical formulation** is derived through the differential approximation for an implicit time advance for ideal linear MHD with arbitrary time centering, θ.

$$\rho \frac{\partial \mathbf{V}}{\partial t} - \theta\,\Delta t \left[\frac{1}{\mu_0} \left(\nabla \times \frac{\partial \mathbf{B}}{\partial t} \right) \times \mathbf{B}_0 + \mathbf{J}_0 \times \frac{\partial \mathbf{B}}{\partial t} - \nabla \frac{\partial p}{\partial t} \right] = \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \mathbf{B}_0 + \mathbf{J}_0 \times \mathbf{B} - \nabla p$$

$$\frac{\partial \mathbf{B}}{\partial t} - \theta\,\Delta t \nabla \times \left(\frac{\partial \mathbf{V}}{\partial t} \times \mathbf{B}_0 \right) = \nabla \times (\mathbf{V} \times \mathbf{B}_0)$$

$$\frac{\partial p}{\partial t} + \theta\,\Delta t \left(\frac{\partial \mathbf{V}}{\partial t} \cdot \nabla p_0 + \gamma p_0 \nabla \cdot \frac{\partial \mathbf{V}}{\partial t} \right) = -(\mathbf{V} \cdot \nabla p_0 + \gamma p_0 \nabla \cdot \mathbf{V})$$

Using the alternative differential approximation,

$$\rho \frac{\partial \mathbf{V}}{\partial t} - \theta^2 \Delta t^2 \mathbf{L}(\partial \mathbf{V}/\partial t) = \frac{1}{\mu_0} (\nabla \times \mathbf{B}) \times \mathbf{B}_0 + \mathbf{J}_0 \times \mathbf{B} - \nabla p + 2\theta \Delta t \mathbf{L}(\mathbf{V})$$

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{V} \times \mathbf{B}_0)$$

$$\frac{\partial p}{\partial t} = -(\mathbf{V} \cdot \nabla p_0 + \gamma p_0 \nabla \cdot \mathbf{V})$$

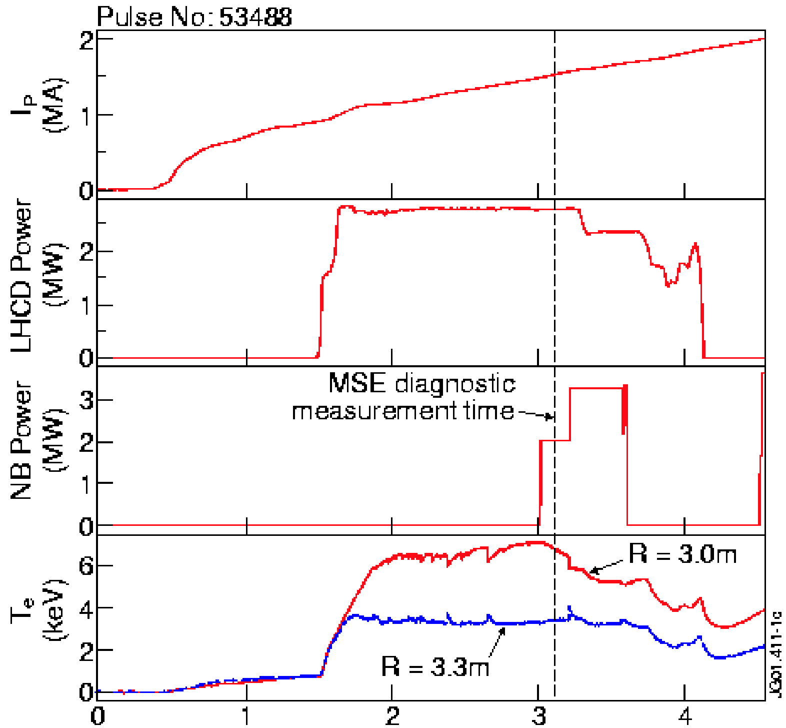
where $\mathbf{L}$ is the ideal MHD force operator. We may drop the Δt-term on the rhs to avoid numerical dissipation and arrive at a semi-implicit advance.

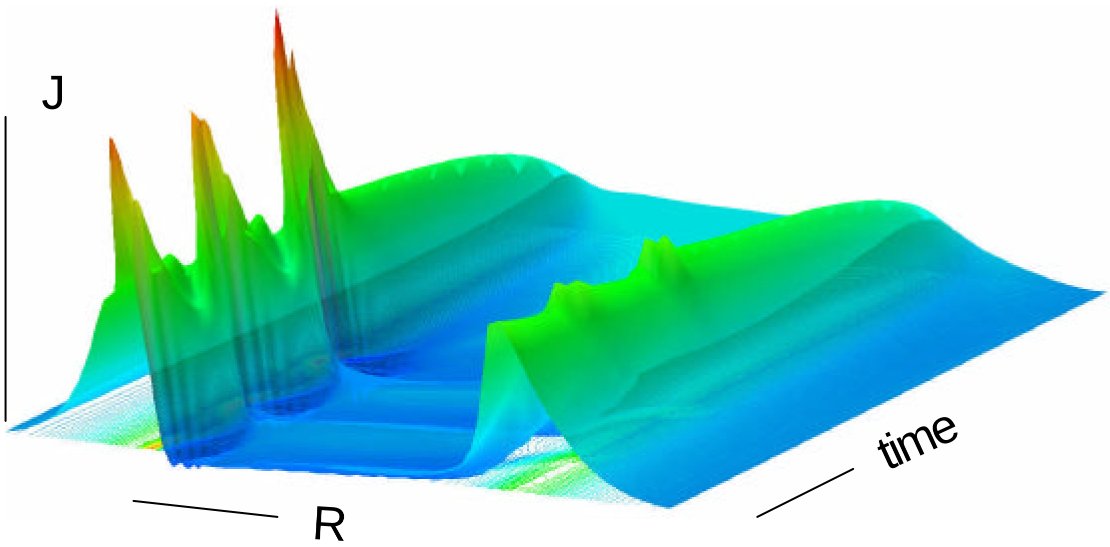
This approach requires solution of ill-conditioned linear systems at each step.

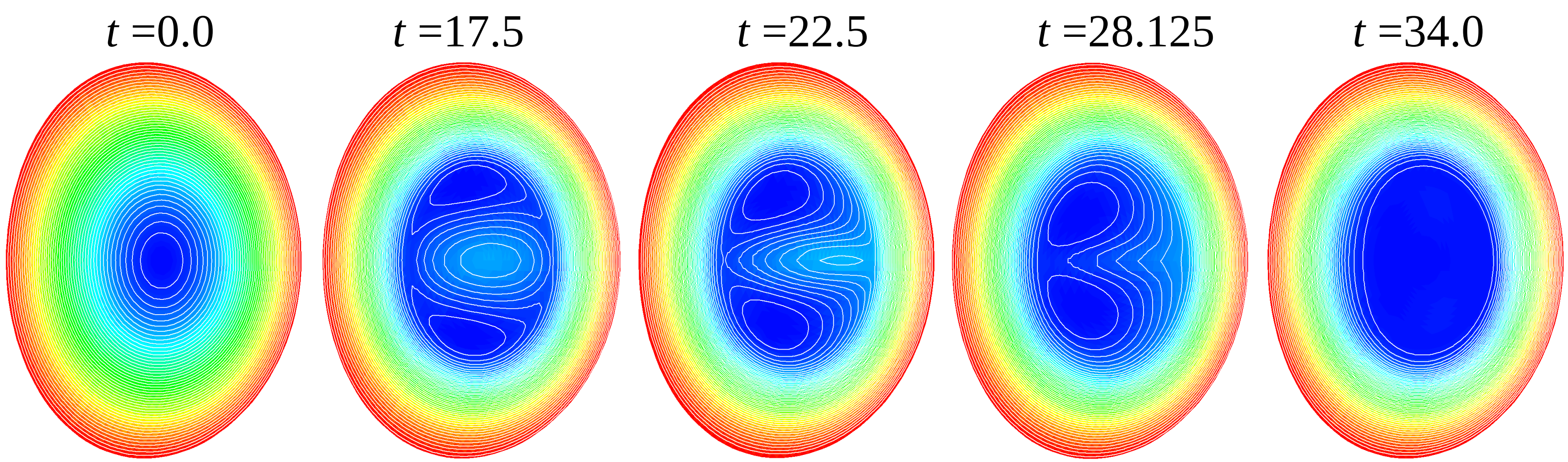
AMRMHD Time Advance:

- Implemented using the CHOMBO framework for AMR (http://www.seesar.lbl.gov/ANAG/chombo)
- Hyperbolic fluxes evaluated using explicit unsplit method (Colella JCP 90)
- Parabolic fluxes treated semi-implicitly
  - Helmholtz equations solved using Multi-grid on each level
  - TGA (Implicit Runge-Kutta) time integration
- Solenoidal B is achieved via projection
  - Solved using Multgrid on each level (union of rectangular meshes)
  - Coarser level provides Dirichlet boundary condition for f
- Both Helmholtz and Poisson equations multigrid solves involve
  - **O(h^3)** interpolation of coarser mesh f on boundary of fine level
  - a “bottom smoother” (conjugate gradient solver) is invoked when mesh cannot be coarsened
- Flux corrections at coarse-fine boundaries to maintain conservation
- Second order accurate in space and time

Recent Application: Interpretation of JET Current-Hole Experiments







Recent Application: Effect of anisotropic thermal conduction on island evolution

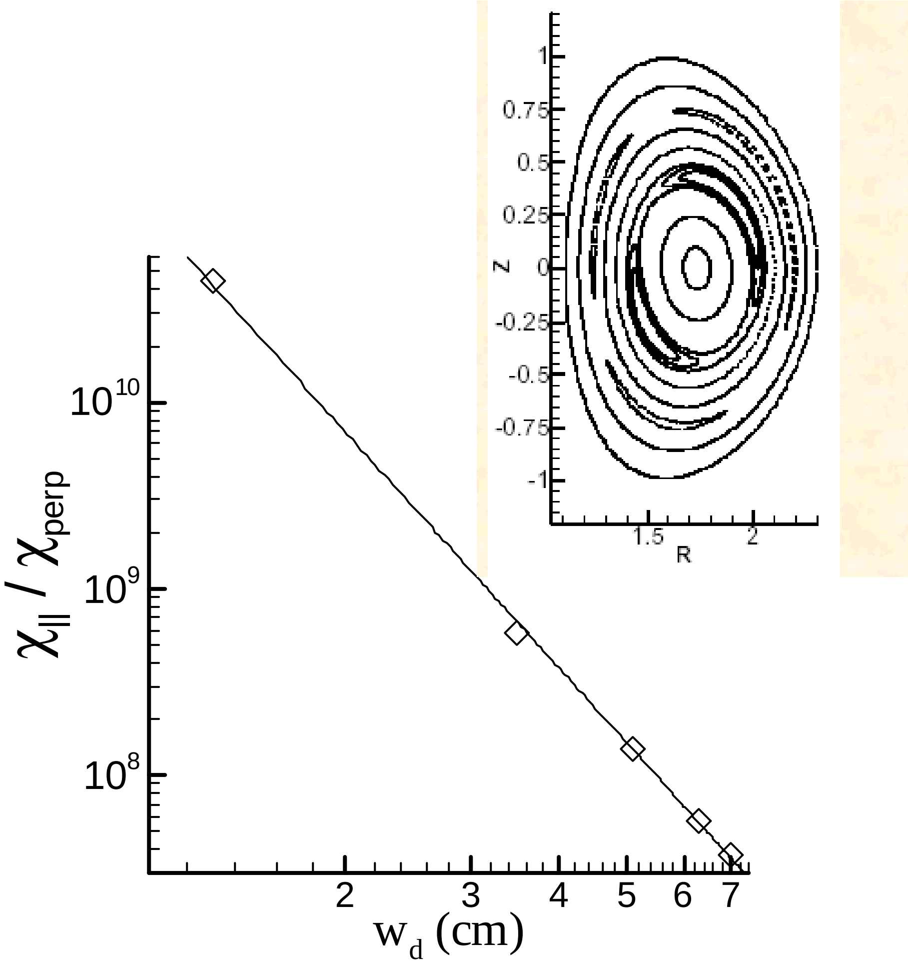
High order finite elements in NIMROD allows use of extreme values of thermal anisotropy.

• 5th order accurate biquartic finite elements

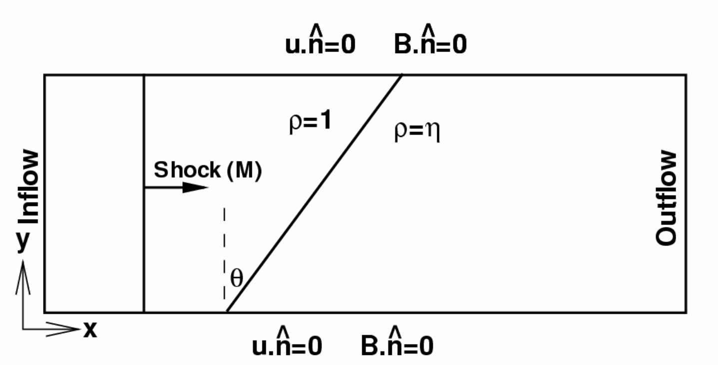
• Repeat calculations with different conductivity ratios and observe effect on flattening island temperature

• Result extends previous analytic result to toroidal geometry.

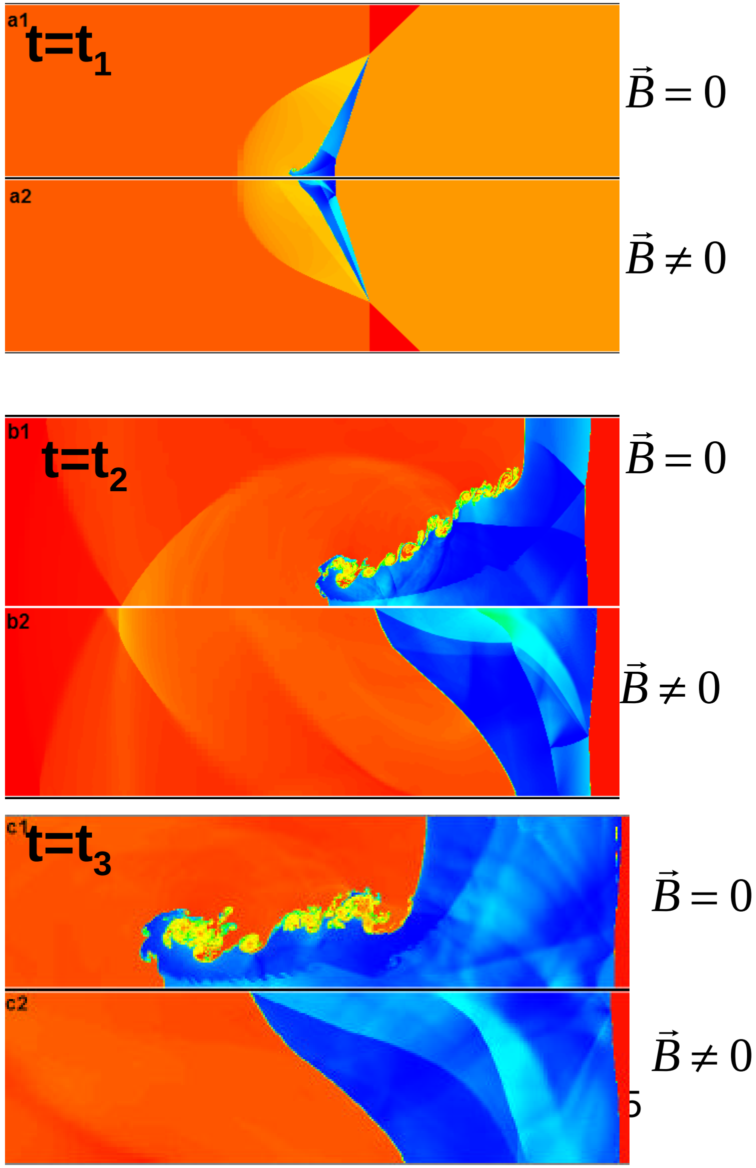
• 3D implicit thermal conduction is required to handle stiffness.



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



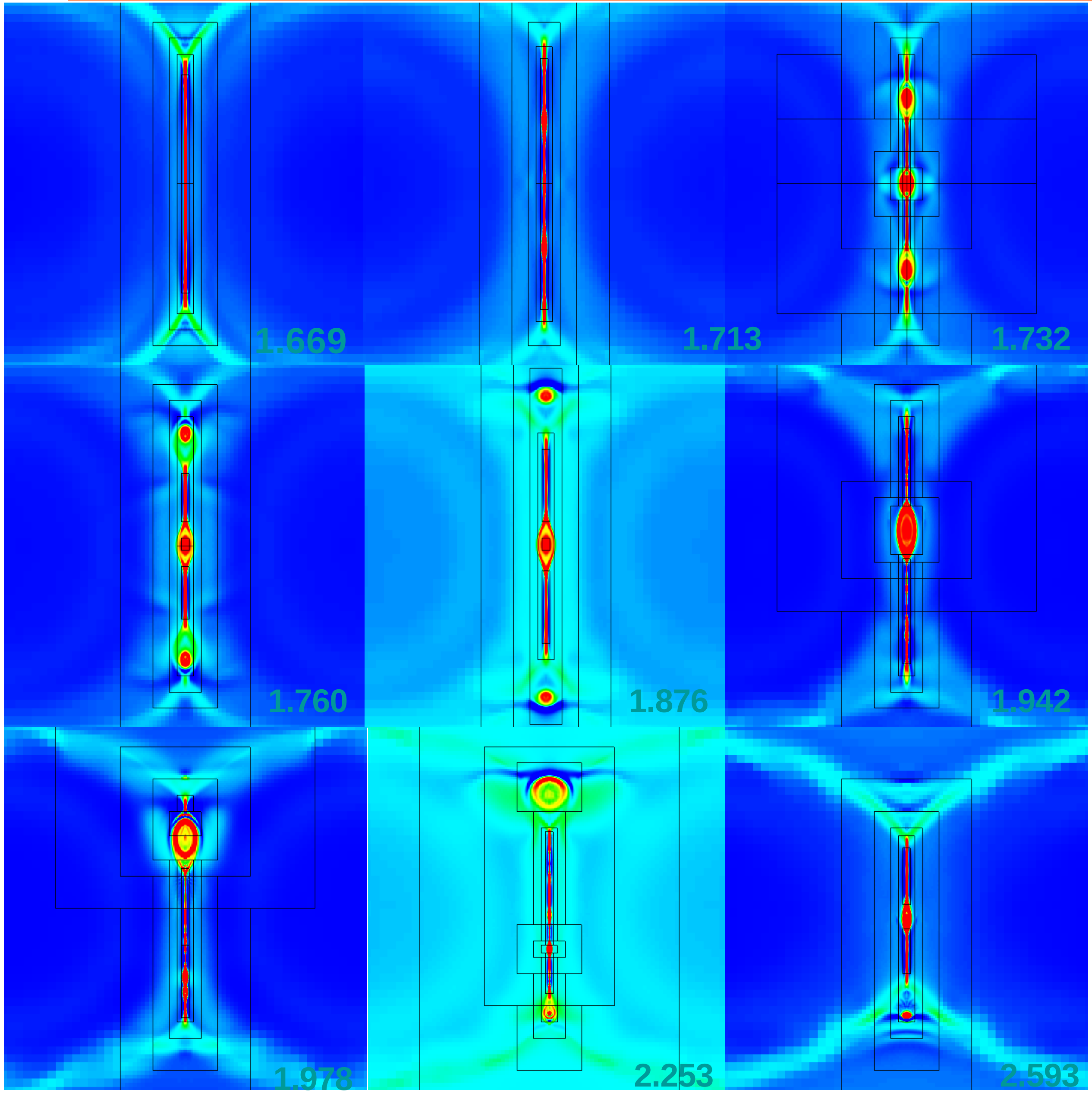
Recent Application: Current bunching and ejection during magnetic reconnection

New Physical Effect!

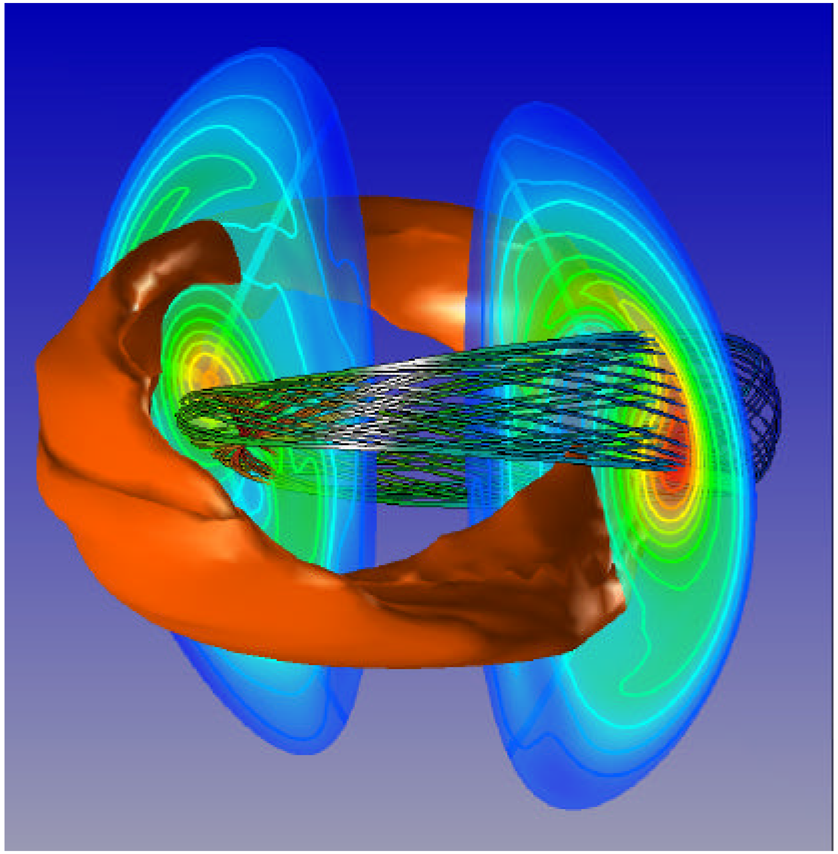
discovered by high-resolution enabled by AMR

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.



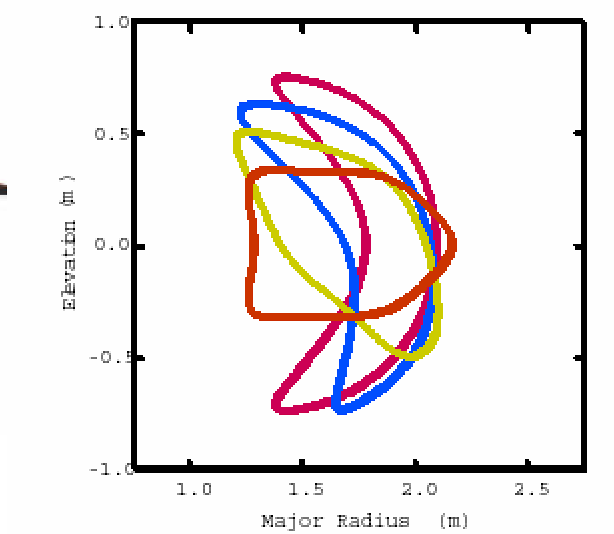
B Field line in the island
Density (Pressure) contours
Temperature isosurface

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.

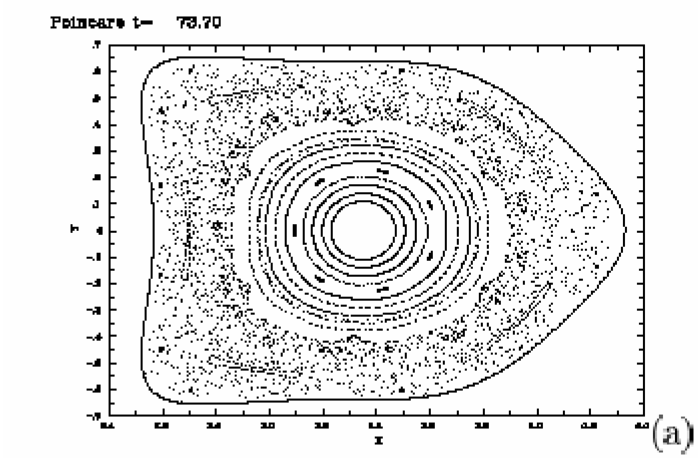
These simulations may account for phenomena recently observed in high-pressure discharges in the National Spherical Torus Experiment.

Recent Application: Diamagnetic Stabilization of Instabilities in Stellarators

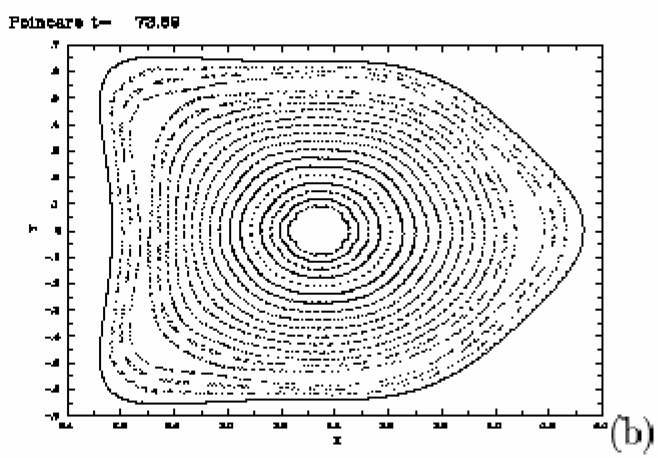


National Compact Stellarator Experiment

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.



Pure resistive MHD



Two-fluid MHD

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

Required Resources for future studies

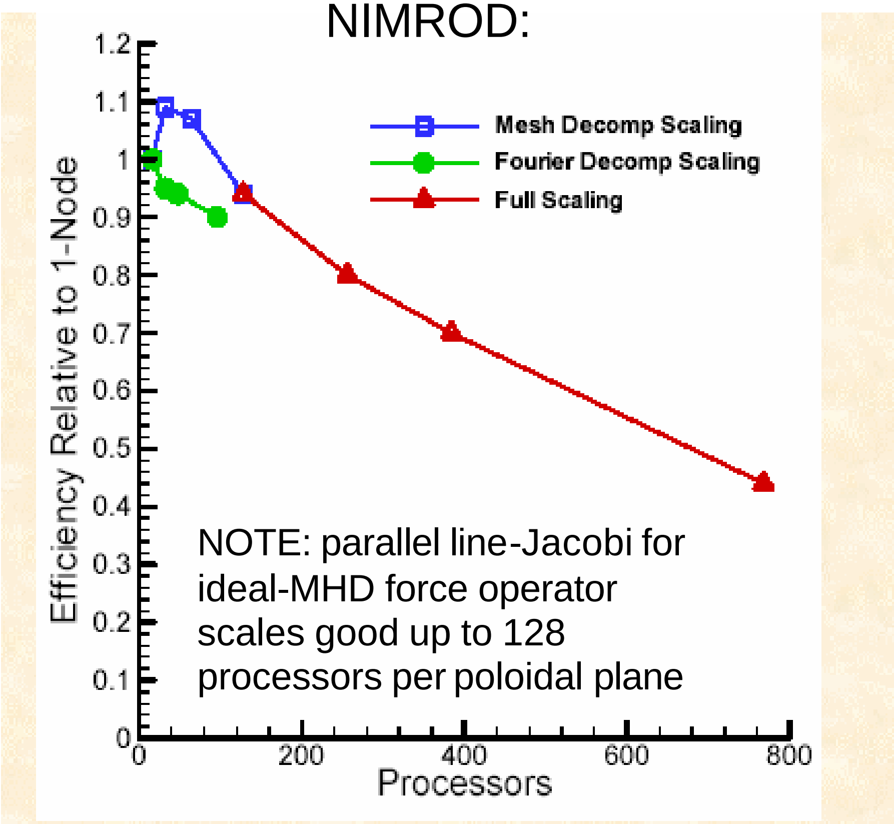
parameter	name	CDXU*	NSTX	CMOD	DIII-D	FIRE	ITER
R(m)	radius	0.3	0.8	0.6	1.6	2.0	5.0
Te[keV]	Elec Temp	0.1	1.0	2.0	2.0	10	10
β	beta	0.01	0.15	.02	0.04	0.02	0.02
$S^{1/2}$	Res. Len	200	2600	3000	6000	20000	60000
$(\rho^*)^{-1}$	Ion num	40	60	400	250	500	1200
$a/\lambda e$	skin depth	250	500	1000	1000	1500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

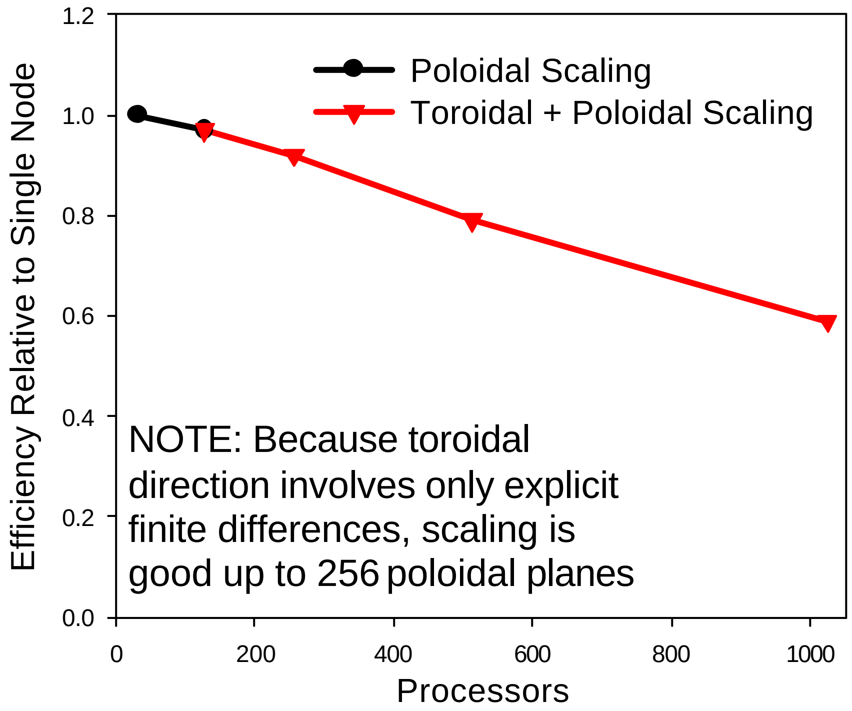
Both NIMROD and M3D exhibit strong scaling that begins to deteriorate at about 500-1000 p for typical problem sizes

NIMROD:



64 x 128 biquartic elements
6 toroidal harmonics

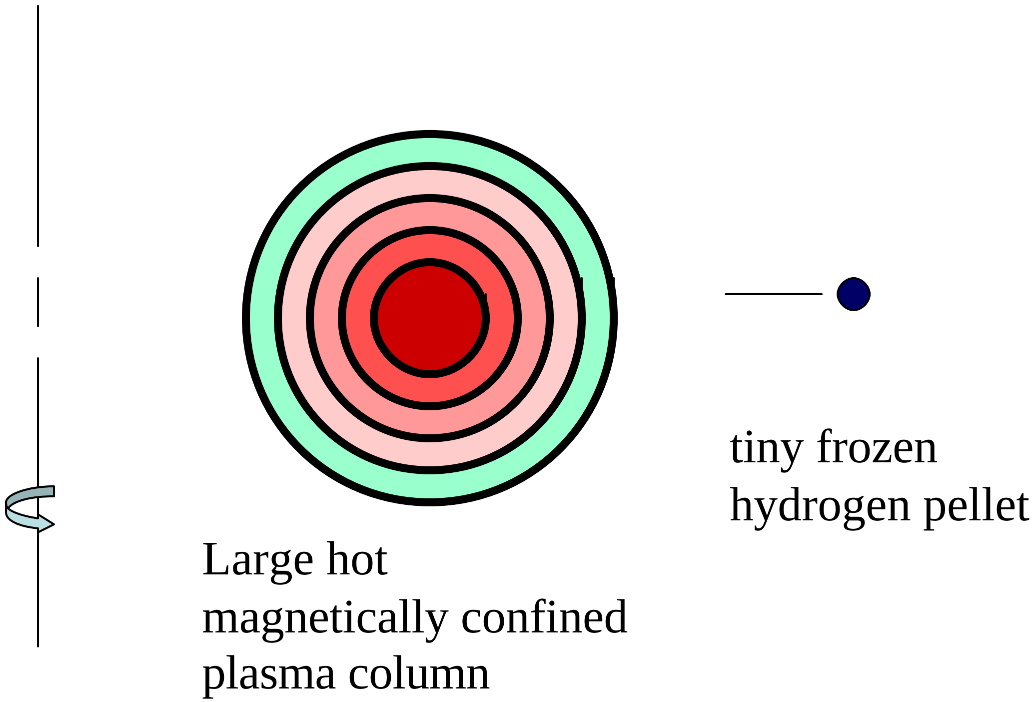
M3D

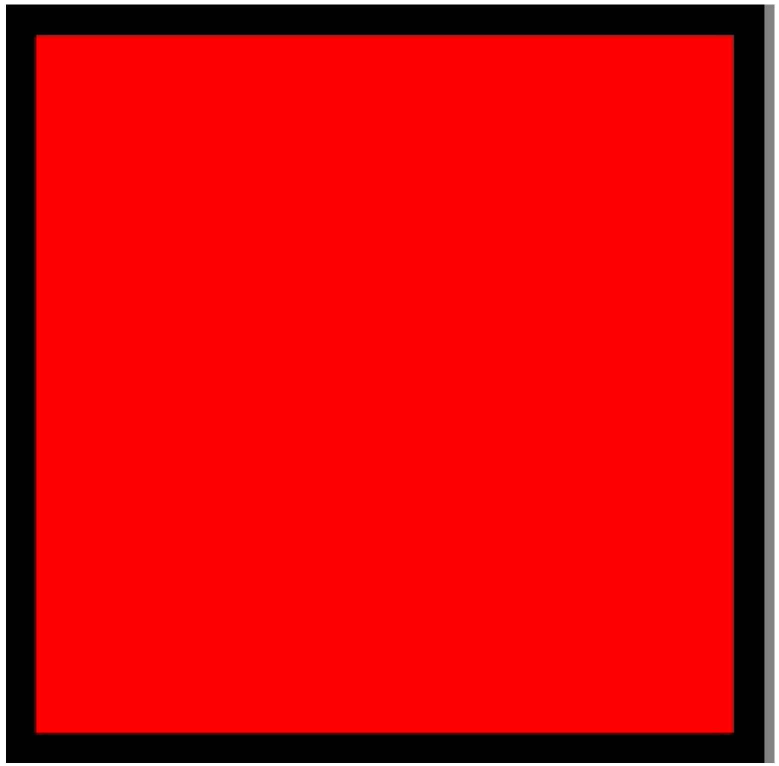


5000 linear poloidal elements
512 toroidal zones

Present 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, mass distribution





Present emphasis is on more complete (kinetic) Hybrid particle closure models

Field evolution equations are unchanged. Momentum equation replaced with "bulk fluid" and kinetic equations for energetic particles

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

or

$$r_b \frac{d\vec{V}_b}{dt} = -\nabla p_b + [\frac{1}{m_0}(\nabla \times \vec{B}) - \vec{J}_h] \times \vec{B} + q_h \vec{V}_b \times \vec{B}$$

ions are particles obeying guiding center equations

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

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

$$\dot{m} = 0$$

$(\vec{X}, U, m)$ *are gyrocenter coordinates*

$$\vec{B}^* = \vec{B} + \frac{m}{e} U \hat{b} \times (\hat{b} \bullet \nabla \hat{b})$$

This hybrid model describes the nonlinear interaction of energetic particles resonant with MHD waves

- small energetic to bulk ion density ratio
- 2 coupling schemes, pressure and current
- model includes nonlinear wave-particle resonances
- brings in essential new physics for burning plasmas with large alpha-particle component

CEMM Interests in ISIC centers

- Incorporation of “standard” grid generation and discretization libraries into M3D (and possibly 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)

Summary

- 2D modeling of fusion devices is fairly mature
- 3D Extended-MHD modeling of MFE fusion plasmas is proceeding: one of the most interesting and challenging problems in computational physics
- Wide range in time and space scales, extreme anisotropy, and essential kinetic effects differentiate this from other problems…requires new mix of techniques
- Much progress is being made: Many intrinsically 3D phenomena in laboratory plasmas have been modeled and understood in isolation.
- Current focus in on extending range of space and time scales (integrated modeling) and on incorporating kinetic physics on a routine basis….we need your help!

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