

# 3D Extended MHD Calculations of Magnetically Confined Plasmas

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Island Ballroom B  
11:00-11:25 am

# 3D Extended MHD Calculations of Magnetically Confined Plasmas

We discuss the status of the SciDAC Center for Extended Magnetohydrodynamic Modeling (CEMM). This center is focused on using advanced computing methods to evaluate the global stability of magnetic fusion confinement configurations. A combination of the very wide range in time and space scales, extreme anisotropy, and essential kinetic effects, makes this problem **one of the most challenging in computational physics.**

# The Center for Extended Magnetohydrodynamic Modeling (Global Stability of Magnetic Fusion Devices)

**GA:** D. Schissel

**MIT:** L. Sugiyama

**NYU:** H. Strauss

**LANL:** R. Nebel

**PPPL:** J. Breslau, G. Fu, S. Klasky, S. Jardin, W. Park, R. Samtaney

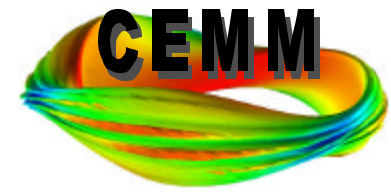
**SAIC:** S. Kruger, D. Schnack

**U. Colorado:** C. Kim, S. Parker

**U. Texas, IFS:** F. Waelbroeck

**U. Wisconsin:** J. Callen, C. Hegna, C. Sovinec

**Utah State:** E. Held



*a SciDAC activity...*



## Present capability:

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

Includes:

RF heating

Ohmic heating

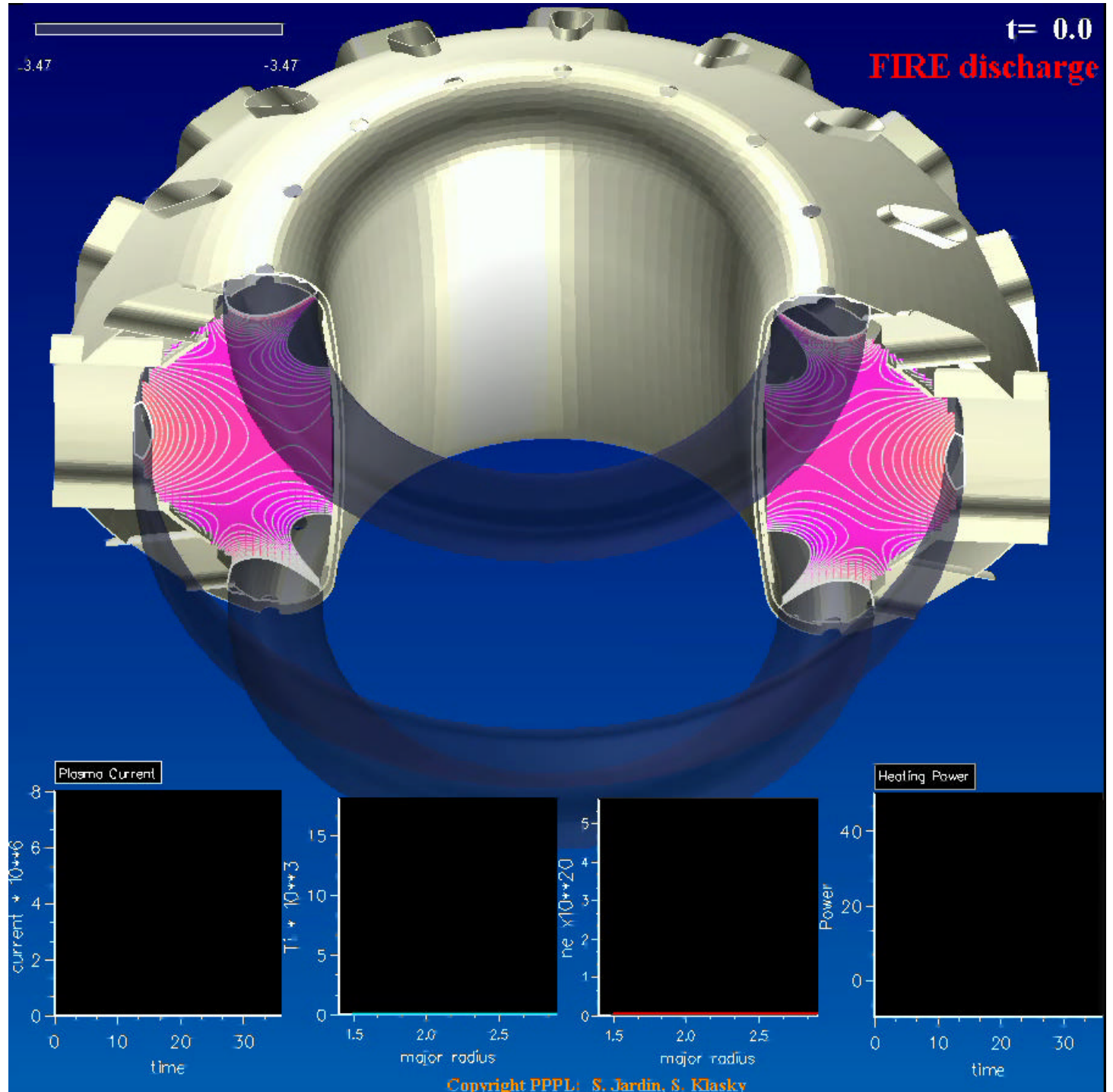
Alpha-heating

Microstability-based  
transport model

L/H mode transition

Sawtooth Model

Evolving Equilibrium  
with actual coils



Even in 2D, things  
can go wrong:

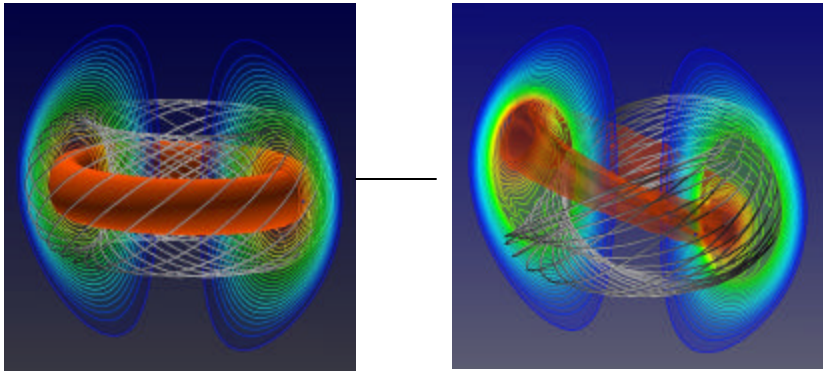
Vertical  
Displacement Event  
(VDE) results from  
loss of vertical  
control due to  
sudden perturbation

TSC simulation of  
an entire burning  
plasma discharge  
(FIRE)

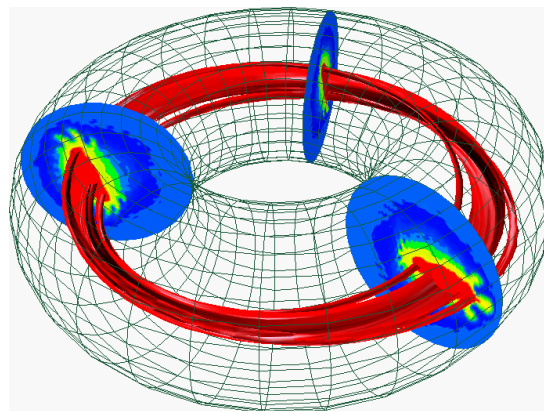
Starts out same as  
before...ends in a  
VDE



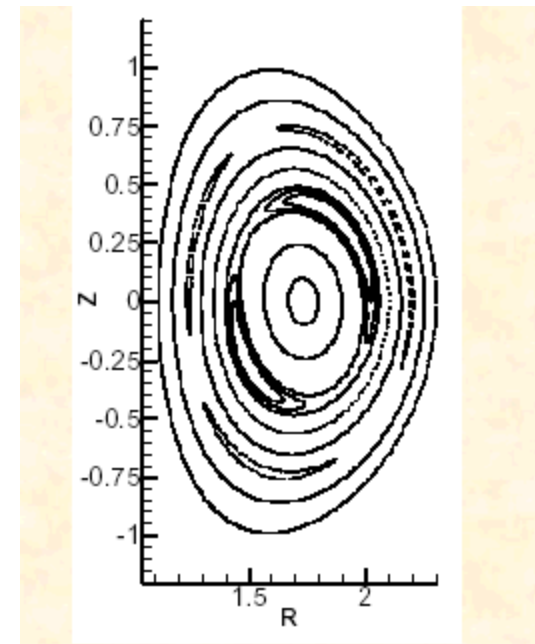
# The need for 3D Tokamak models



Internal reconnection events or “sawtooth oscillations”



Short wavelength modes interacting with helical structures.



Interaction of coupled island chains.

# Plasma Models: XMHD

$$\begin{aligned}
 \frac{\partial \vec{B}}{\partial t} &= -\nabla \times \vec{E} & \mathbf{r} \left( \frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} \right) &= \nabla \cdot P + \vec{J} \times \vec{B} + m \nabla^2 \vec{V} \\
 \vec{E} + \vec{V} \times \vec{B} &= \mathbf{h} \vec{J} & \frac{\partial \mathbf{r}}{\partial t} + \nabla \cdot (\mathbf{r} \vec{V}) &= S_M \\
 &+ \frac{1}{ne} \left[ \vec{J} \times \vec{B} - \nabla \cdot P_e \right] & \frac{3}{2} \frac{\partial p}{\partial t} + \nabla \cdot \left( \vec{q} + \frac{5}{2} P \cdot \vec{V} \right) &= \vec{J} \cdot \vec{E} + S_E \\
 m_0 \vec{J} &= \nabla \times \vec{B} & \frac{3}{2} \frac{\partial p_e}{\partial t} + \nabla \cdot \left( \vec{q}_e + \frac{5}{2} P_e \cdot \vec{V}_e \right) &= \vec{J} \cdot \vec{E} + S_E \\
 P &= pI + \Pi & &
 \end{aligned}$$

**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

# Difficulties in 3D MHD Modeling of Magnetic Fusion Experiments

Multiple timescales

Implicit methods and long running times

Multiple space-scales

Adaptive meshing, unstructured meshes, and implicit methods

Extreme anisotropy

High-order elements, field aligned coordinates, artificial field method

Essential kinetic effects

Hybrid particle/fluid methods, integrate along characteristics



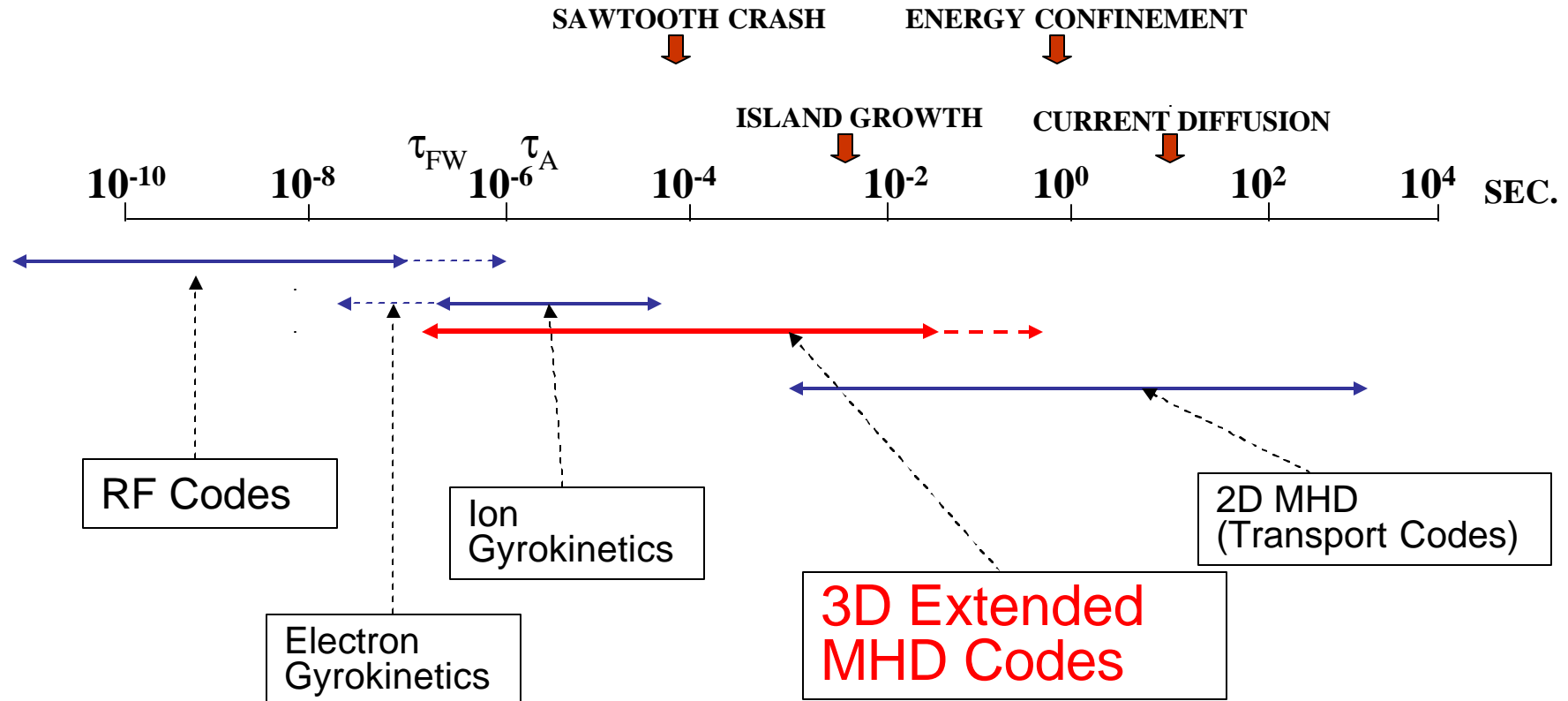
# CEMM Simulation Codes:

	NIMROD	M3D	AMRMHD*
Poloidal discretization	Quad and triangular high order finite elements	Triangular linear finite elements	Structured adaptive grid
Toroidal discretization	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
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

Multiple timescales

# Time Scales in FIRE: $B = 10 \text{ T}$ , $R = 2 \text{ m}$ , $n_e = 10^{14} \text{ cm}^{-3}$ , $T = 10 \text{ keV}$



## M3D Scalar Equation time advance:

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

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

$$\frac{\partial p}{\partial t} = -\mathbf{g} p \underline{Z} \dots$$

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

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

$$\frac{\partial v_j}{\partial t} = \frac{\mathbf{m}}{\mathbf{r}} \nabla^2 \underline{v}_j \dots$$

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

$$\Delta^* \mathbf{c} = Z$$

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

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

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

$$\Delta^* \mathbf{y} = C$$

*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 Alfvén 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,  $\theta$ .

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

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

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

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  $\Delta t$ -term on the rhs to avoid numerical dissipation and arrive at a semi-implicit advance.

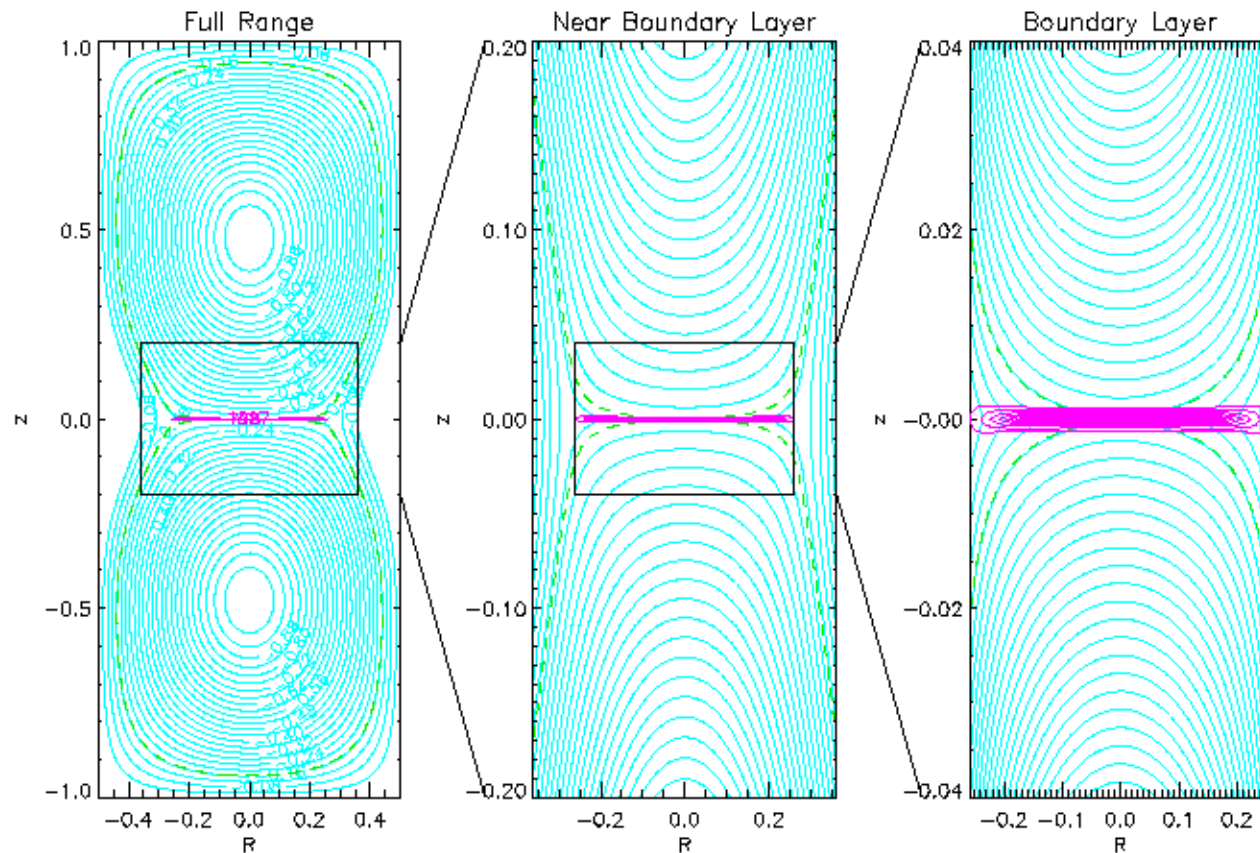
**This approach requires solution of ill-conditioned linear systems at each step.**

## 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

Model problem: merging plasma columns with full resistive MHD equations, high-resolution

$$\eta = 10^{-5}$$



- Variable resolution grid allows resolution of disparate space scales.

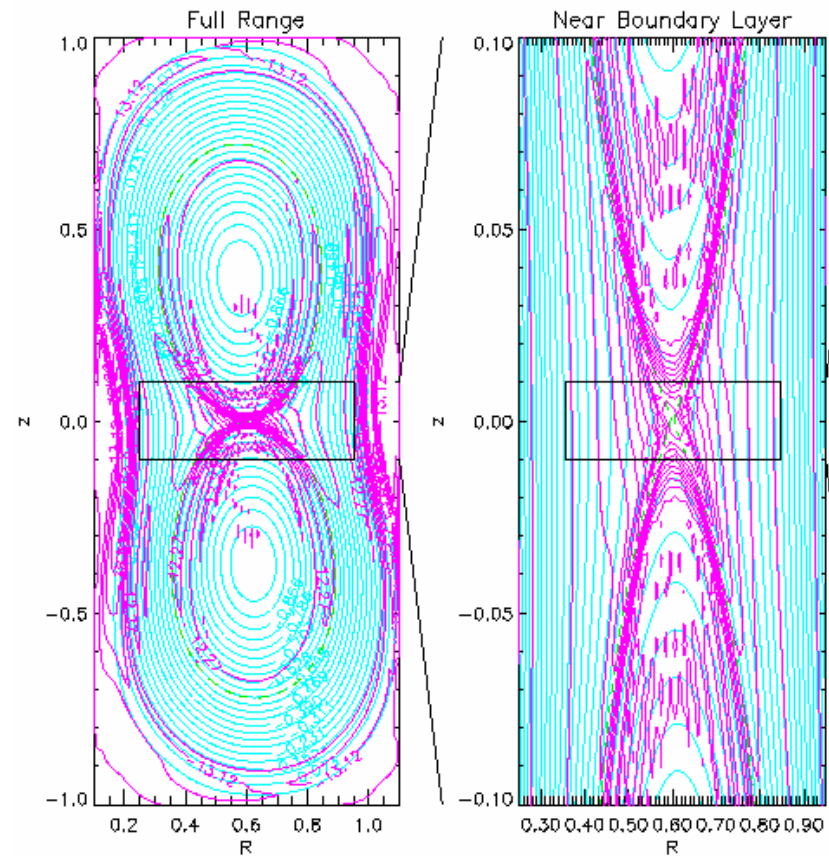
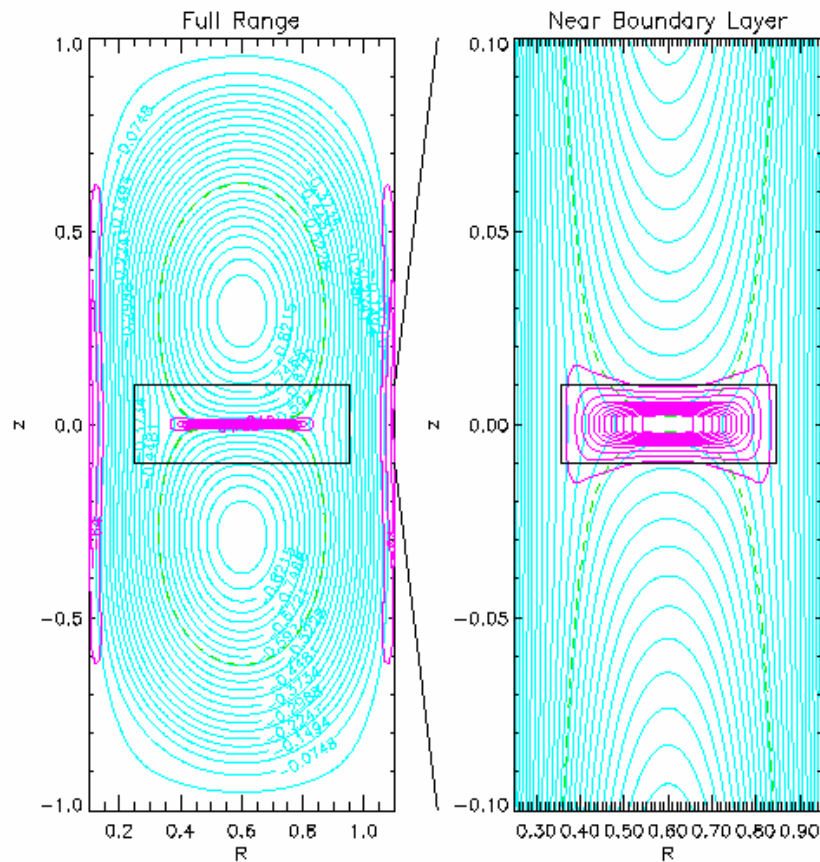
- note: cyan: flux purple: current

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

$\chi = 0$  (resistive MHD)

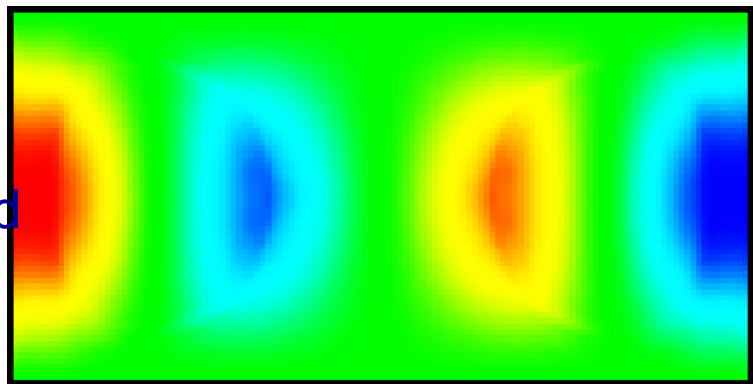
$\eta = 10^{-4}$

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

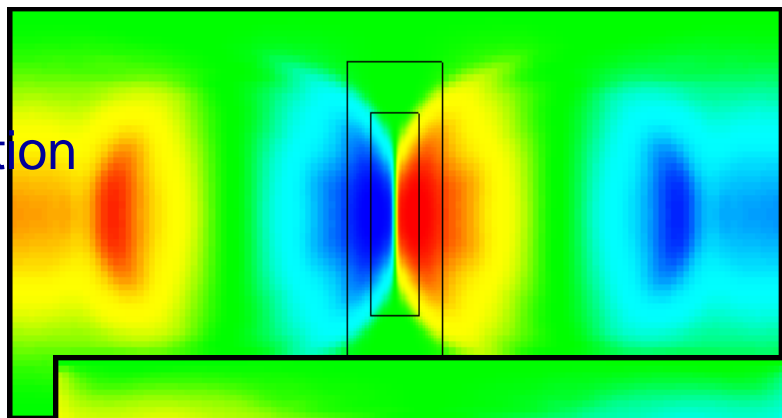


# AMRMHD: Reconnection $\eta = 10^{-3}$

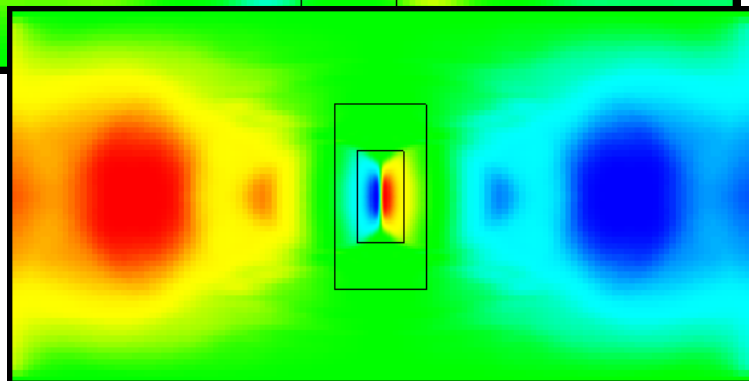
Stage 1  
Middle island  
decays



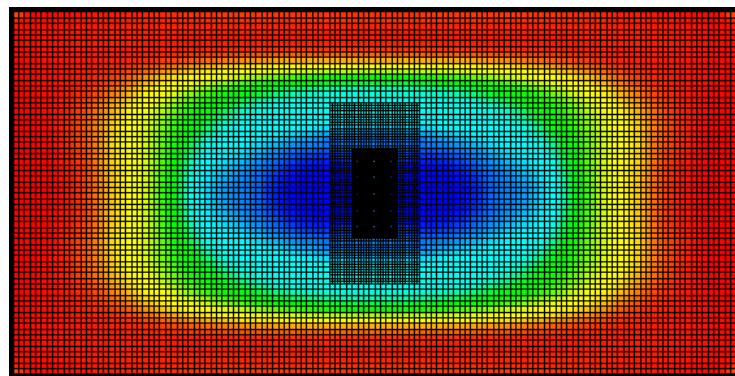
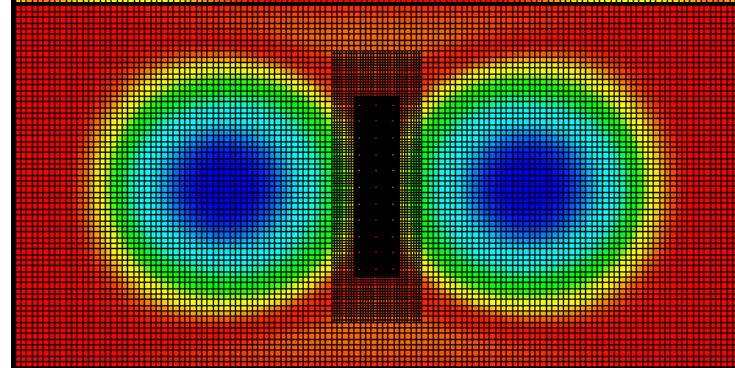
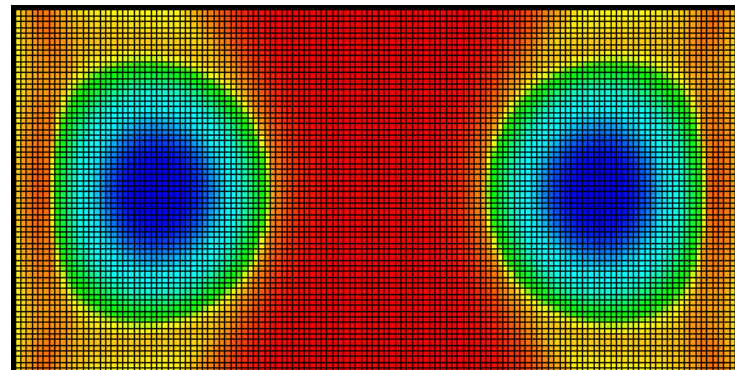
Stage 2  
Reconnection



Stage 3  
Decay



$B_y$



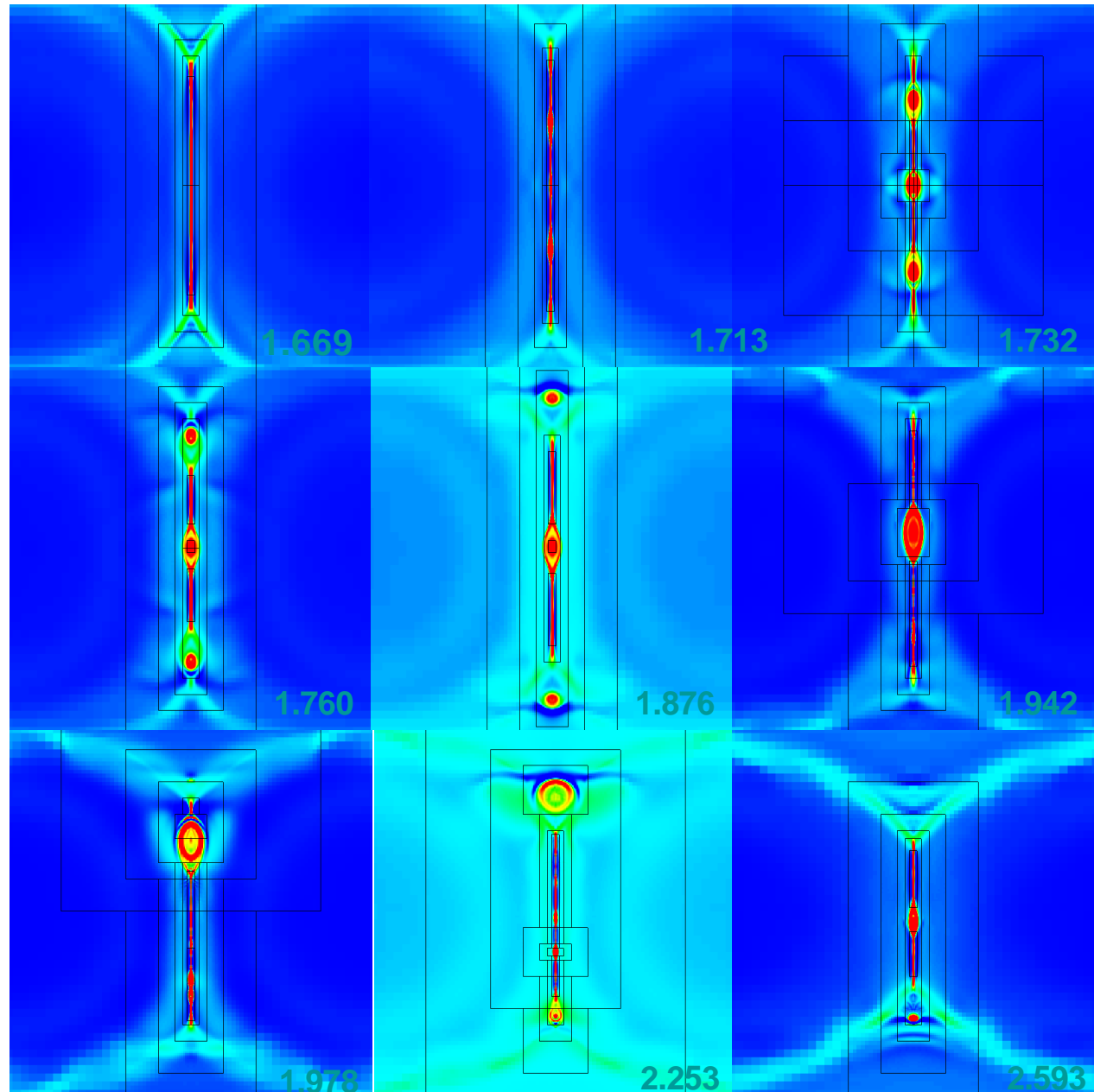
$B_z$



# Current: Reconnection $\eta = 10^{-4}$

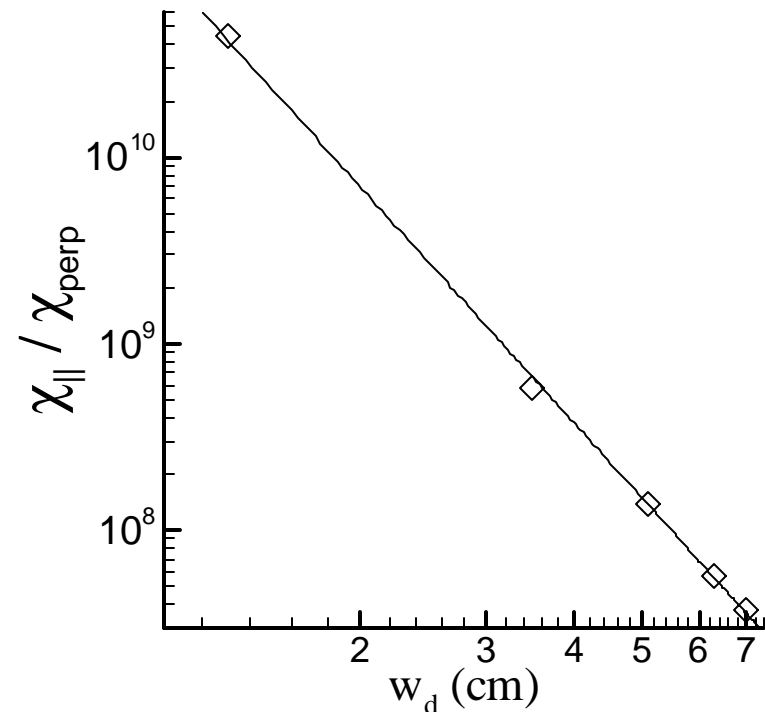
New Physical Effect!

Time sequence of current ( $J_z$ )  
Thin current layer bunches, then  
“clumps”  
followed  
by asymmetric plasma ejection



## High order finite elements 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.
- **Implicit thermal conduction is required to handle stiffness.**



## Hybrid particle closure models

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

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

or

$$\mathbf{r}_b \frac{d\vec{V}_b}{dt} = -\nabla p_b + \left[ \frac{1}{\mathbf{m}_0} (\nabla \times \vec{B}) - \vec{J}_h \right] \times \vec{B} + q_h \vec{V}_b \times \vec{B}$$

*ions are particles obeying guiding center equations*

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

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

$$\dot{\mathbf{m}} = 0$$

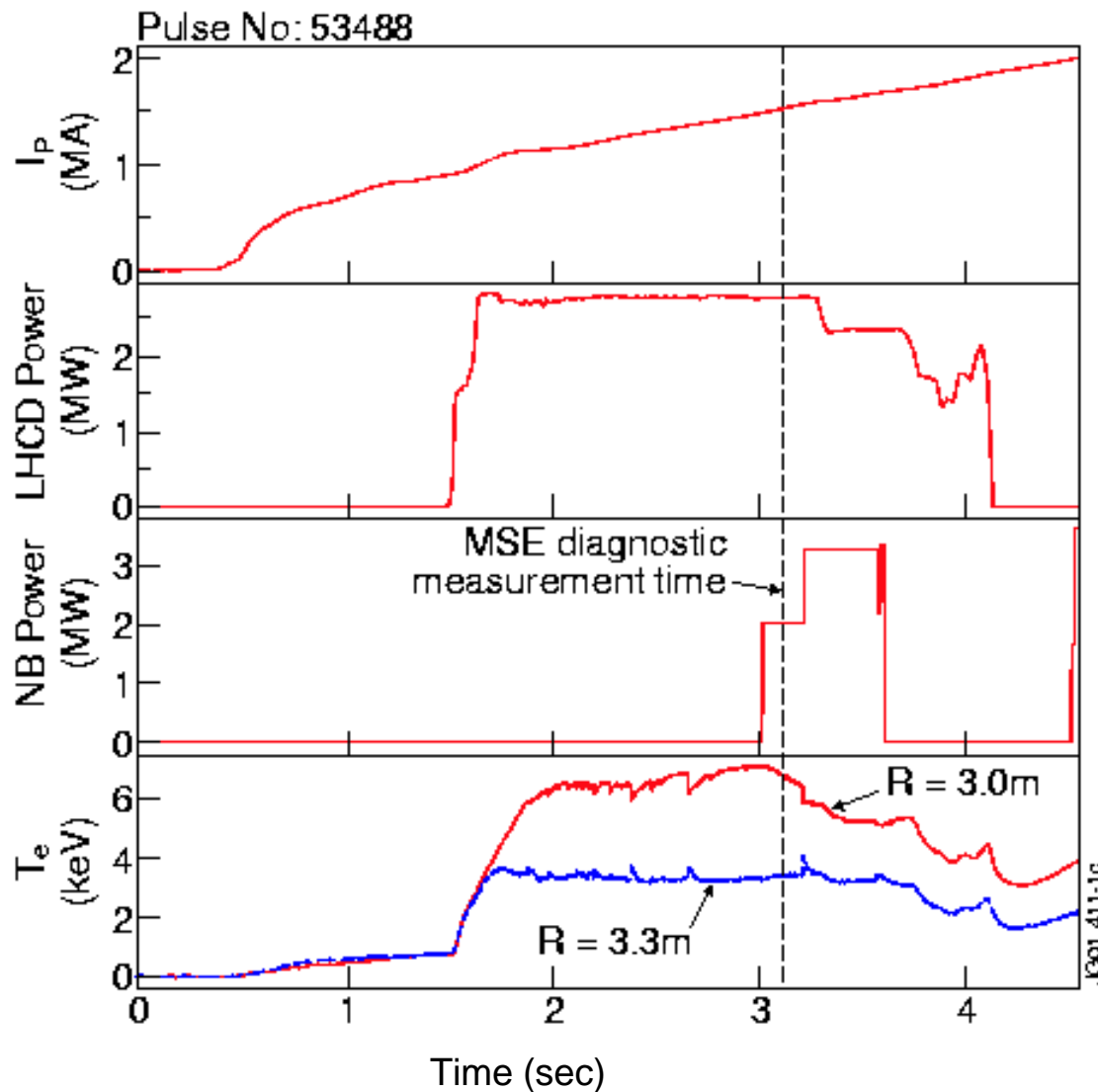
$(\vec{X}, U, \mathbf{m})$  are gyrocenter coordinates

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

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

- small energetic to bulk ion density ratio
- 2 coupling schemes, pressure and current
- model includes nonlinear wave-particle resonances

# Recent Application: Interpretation of JET Current-Hole Experiments

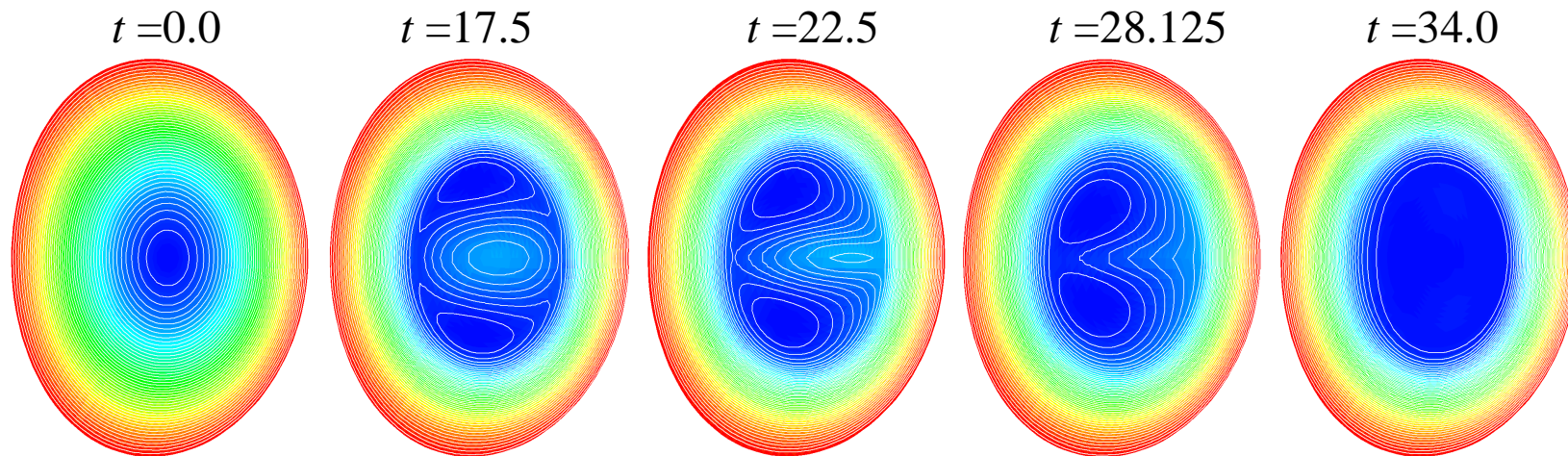


- External current drive (LHCD) during current rampup **should drive central current negative** according to 1D transport codes
- Careful measurements with MSE showed **central current was zero**...but not negative
- This was explained by CEMM calculation which showed an **axisymmetric reconnection** event clamps current at zero

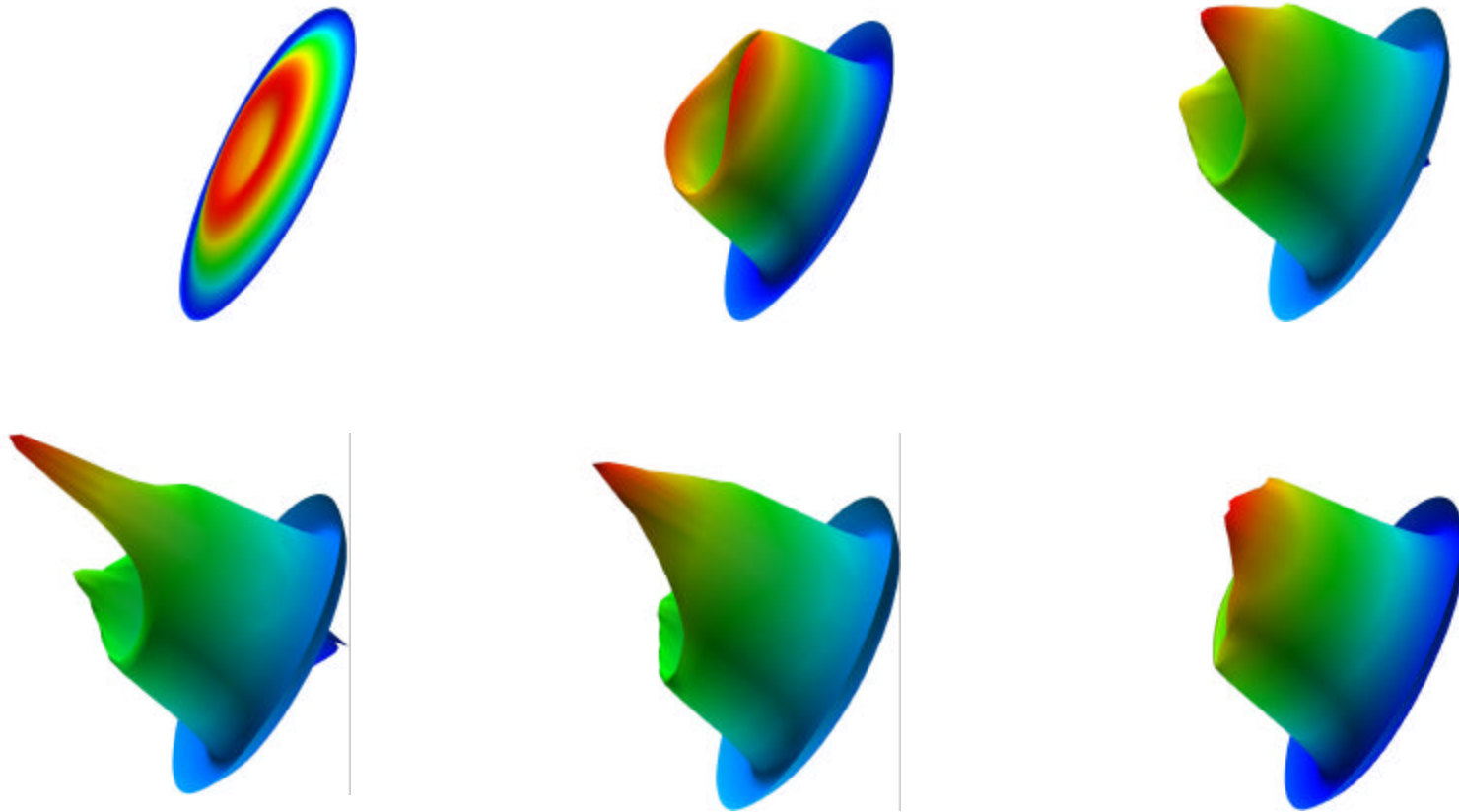
# M3D Study of Current hole

Result:  $n=0$  reconnection (axisymmetric sawtooth).

Poloidal flux contours:

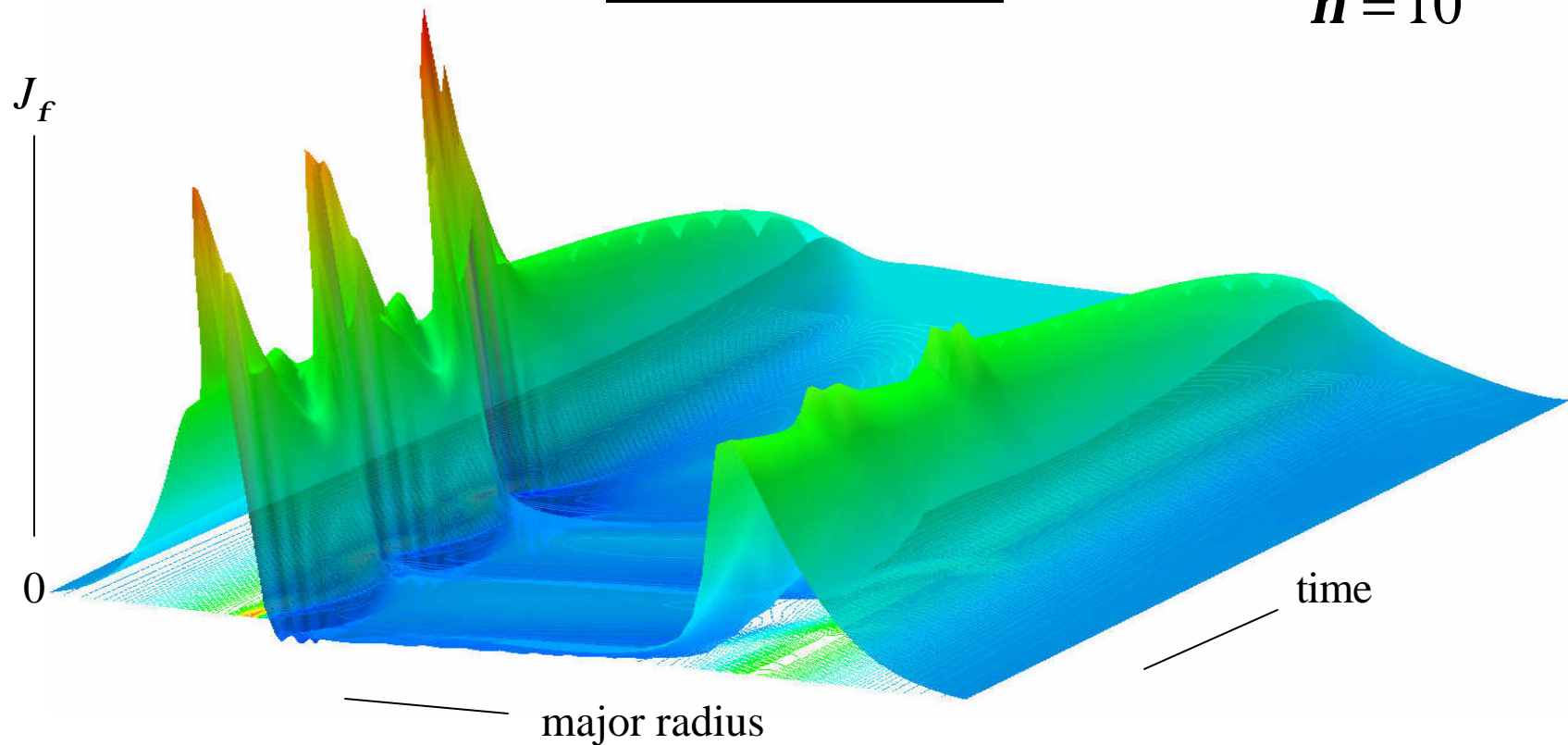


Toroidal current density during the sawtooth cycle shows sharp peaking in the reconnection region



# Current Density History at Midplane

$$h = 10^{-4}$$



- Repeated reconnection events keep current flat in center

# 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
$\beta$	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
<b>P</b>	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.



# 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 is one of the most interesting and challenging in computational physics
- Wide range in time and space scales, extreme anisotropy, and essential kinetic effects all require state-of-the-art techniques
- Current focus is on extending range of space and time scales...(new integrated modeling initiative to be described in FSP session on Tuesday Morning)

Please visit our web site at [w3.pppl.gov/CEMM](http://w3.pppl.gov/CEMM)