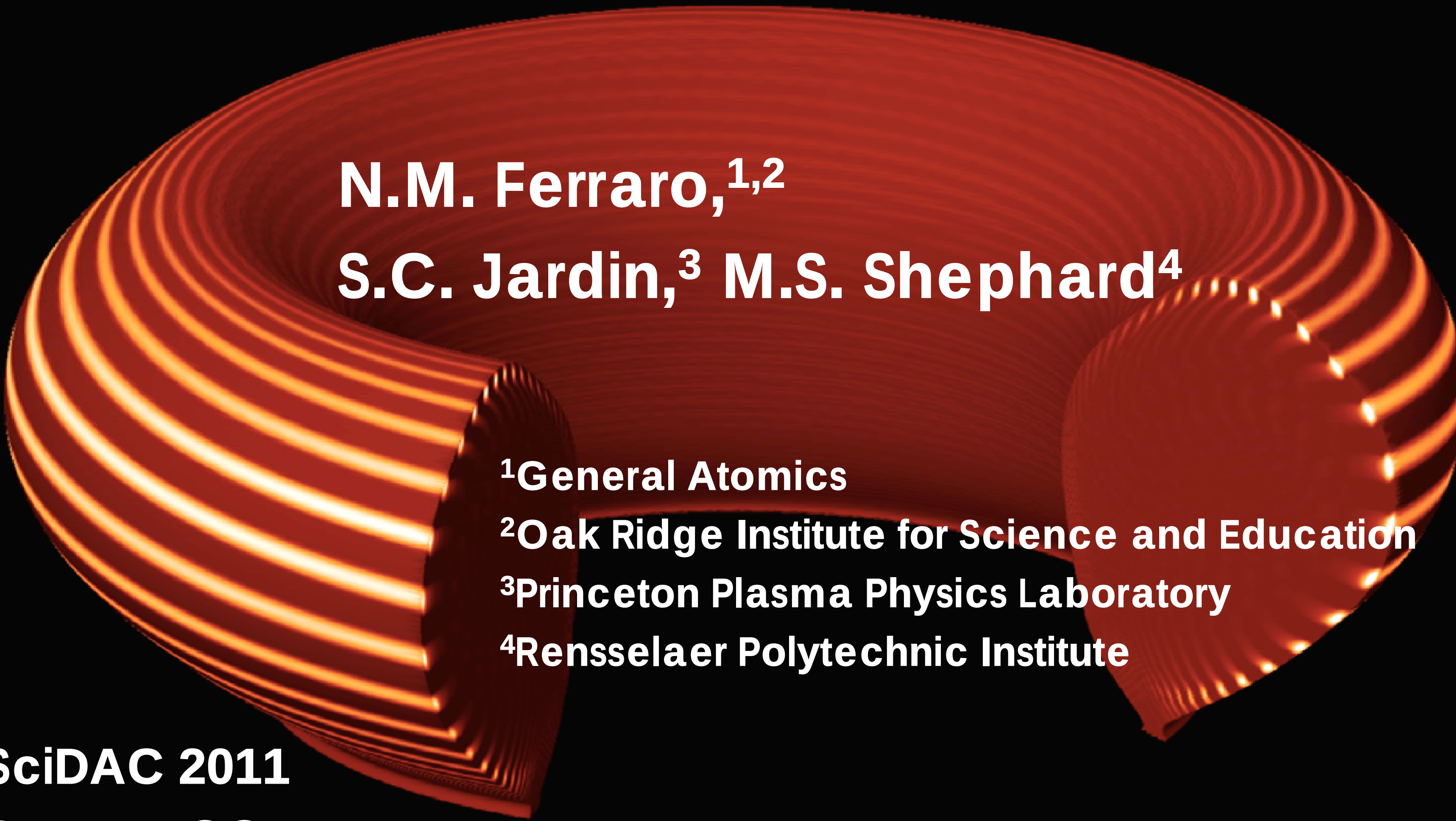
Fluid Modeling of Fusion Plasmas with M3D-C1



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Outline

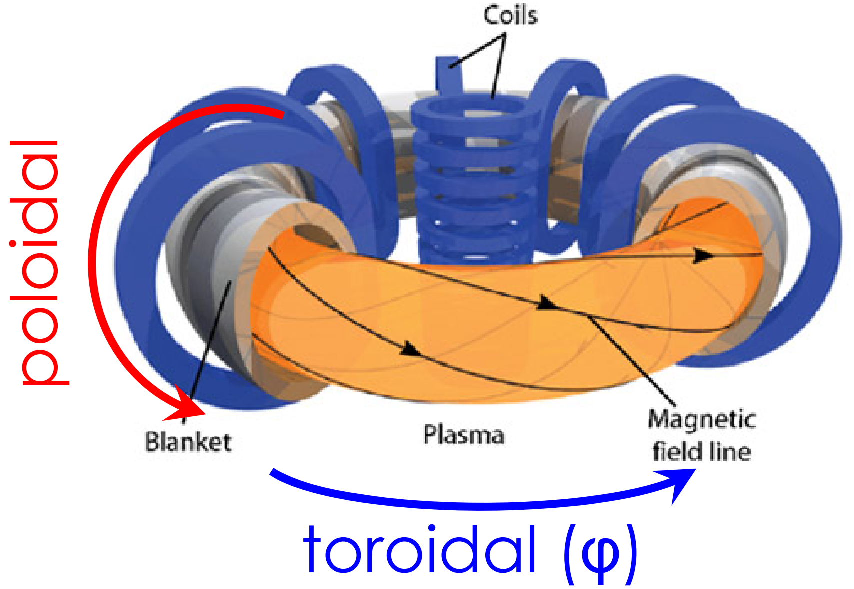
- **Fusion basics**

- **The M3D-C1 code**
  - Finite elements
  - Implicit time step
  - Flux/potential representation

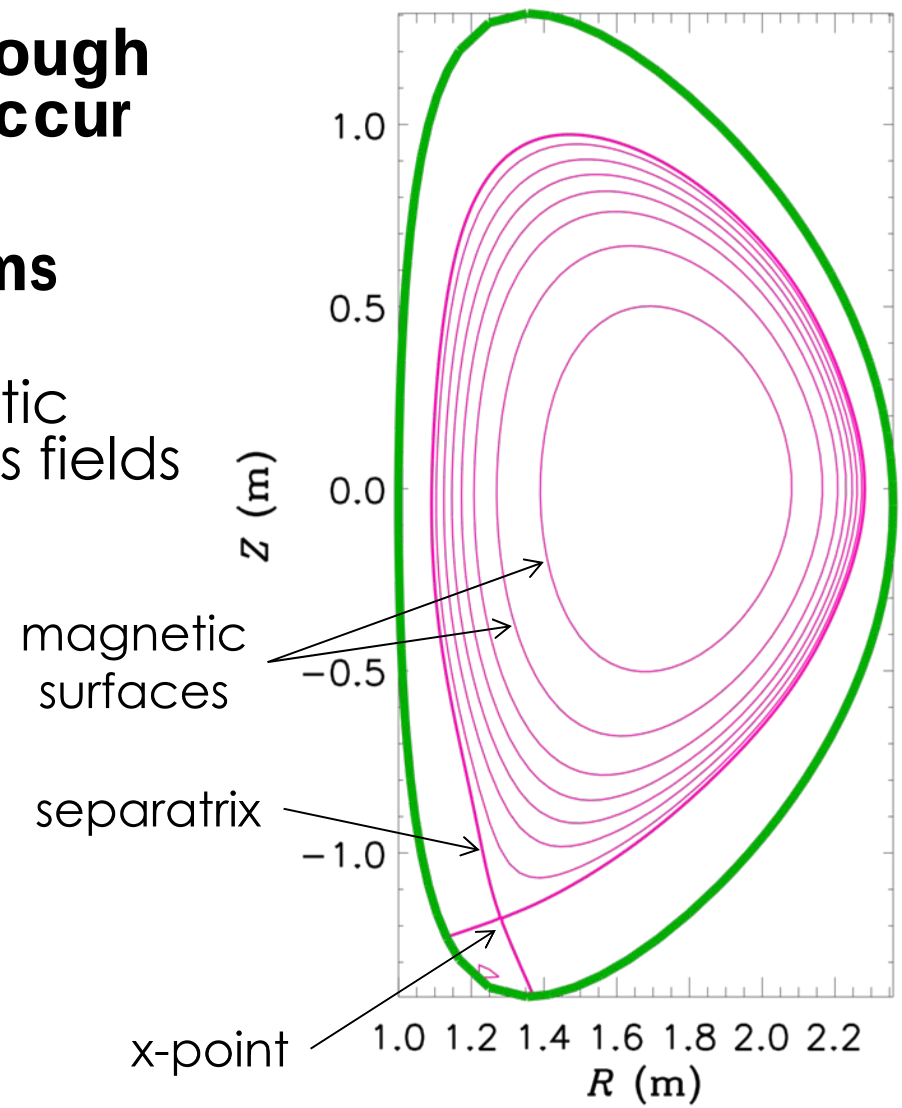
- **Results**
  - Edge localized modes (ELMs)
  - Sawtooth cycles

Magnetic Fusion Basics

- **Goal: to keep plasma hot enough in steady-state for fusion to occur**
- **Tokamak: magnetic field forms nested toroidal surfaces**
  - Particles travel along magnetic fields much faster than across fields



http://fusionforenergy.europa.eu/understandingfusion/



Scientific Challenges In Tokamaks

- **How can we heat the plasma and drive electrical currents in it?**
  - Radio frequency wave codes
  - CSWPI SciDAC

- **How can we minimize small-scale turbulence that causes heat to leak out?**
  - Gyrokinetic codes
  - CSPM, GSEP, GPS-TTBP SciDACs

- **How can we mitigate large-scale instabilities due to pressure gradients and currents?**
  - Fluid codes
  - CEMM SciDAC

MHD is a Fluid Description of Plasma

- **Magnetohydrodynamics (MHD) consists of:**
  - Conservation equations (for both ions and electrons)
  - Maxwell's equations
- **"Ideal MHD" excludes dissipative terms**

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0$$

Conservation of particles

$$n\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = \mathbf{J}\times\mathbf{B} - \nabla p - \boxed{\nabla\cdot\Pi}$$

Conservation of momentum (ions + electrons)

$$\mathbf{E} + \mathbf{v}\times\mathbf{B} = \boxed{\eta\mathbf{J}}$$

Conservation of momentum (electrons)

$$\frac{\partial p}{\partial t} + \mathbf{v}\cdot\nabla p = -\Gamma p \nabla\cdot\mathbf{v} - \boxed{(\Gamma - 1)\nabla\cdot\mathbf{q}}$$

Conservation of energy (ions + electrons)

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

Faraday's Law

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

Ampere's Law (minus displacement current)

Disparate Scales Make MHD Difficult

- **Ideal MHD contains a wide range of wave speeds**
  - Alfvén wave, Slow wave, Fast wave
- **Non-Ideal (dissipative) terms introduce new, much slower time scales**
  - Lundquist number = $\tau_R/\tau_A \sim 10^9$
- **Highly anisotropic thermal conductivity**
- **Many resonant surfaces and boundary layers**
  - Require localized regions of high resolution

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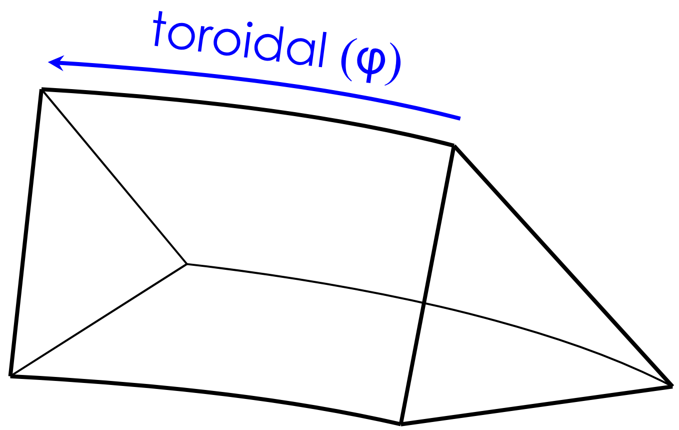
M3D-C^1 Uses Several Strategies to Improve Efficiency

- **High order, C^1 finite elements**
  - C^1: field values and derivative continuous everywhere
  - Allow up to 4th order weak derivatives
- **Unstructured mesh**
  - ITAPS meshing software
  - Higher resolution near boundary layers
- **Linear implicit time advance**
  - Split or unsplit methods
  - TOPS solvers (through PETSc)
- **Uses flux/potential representation of $\mathbf{B}$ and $\mathbf{u}$**
  - Increases accuracy of stability calculations
  - Improves conditioning of matrix

High-Order C^1 Finite Elements

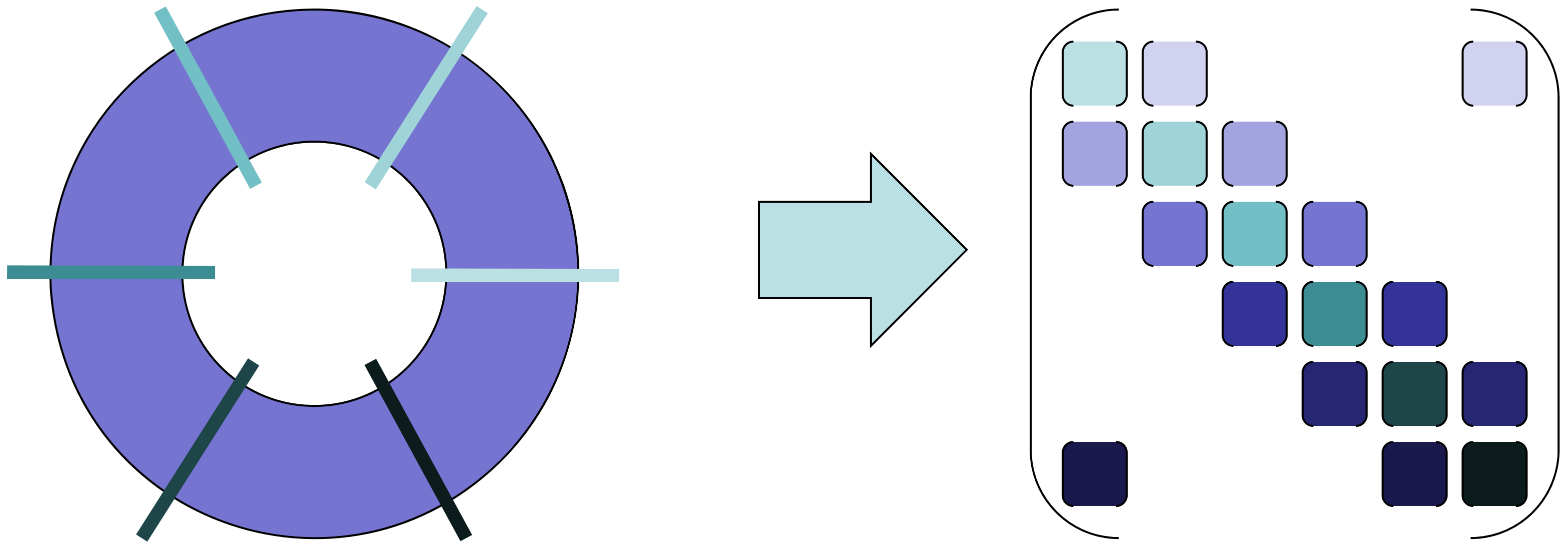
- **Elements are a tensor product**
  - Poloidally: 2D (triangular) reduced quintic elements
  - Toroidally: 1D cubic Hermite elements



- **High-order elements lead to more compact matrices**

- **C^1 in all directions**
  - Allows 4^{th} degree weak derivatives
  - Allows efficient use of flux/potential representation

Hermite Elements in Toroidal Direction Yields Block Cyclic Tridiagonal Matrix Structure



- **Each plane yields a diagonal block**
  - Only neighboring planes are coupled
  - Coupling is much stronger within planes than among planes (block diagonal dominant)

- **Block-Jacobi preconditioning is effective**
  - Diagonal block are factorized directly using SuperLU or MUMPS
  - This method is now available in PETSc (dev). Thanks H. Zhang!

Implicit Time Steps in M3D-C1

- **Two time-stepping methods are implemented**
  - θ-implicit method (Crank-Nicolson)
  - Split time step

- **θ-implicit method:**
  - Excellent convergence (with dt) properties
  - Very poorly conditioned matrices

- **Split time step:**
  - Smaller, better-conditioned matrices

Unsplit Time Step

- **Consider the simple equations:** $$\begin{pmatrix} \dot{\mathbf{v}} \\ \dot{\mathbf{B}} \end{pmatrix} = \begin{pmatrix} 0 & F \\ G & 0 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{B} \end{pmatrix}$$

- **Evaluate $\mathbf{u}$ and $\mathbf{B}$ at the θ-advanced time, and discretize:**

$$\mathbf{v} \to \mathbf{v}^n + \theta \, dt \, \dot{\mathbf{v}}$$

$$\dot{\mathbf{v}} = \left(\mathbf{v}^{n+1} - \mathbf{v}^n \right) / dt$$

$$\begin{pmatrix} 1 & -\theta \, dt \, F \\ -\theta \, dt \, G & 1 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{B} \end{pmatrix}^{n+1} = \begin{pmatrix} 1 & (1-\theta) \, dt \, F \\ (1-\theta) \, dt \, G & 1 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{B} \end{pmatrix}^{n}$$

- **Universally stable, second-order accurate when $\theta = ½$ (Crank-Nicolson)**

- **Matrix not diagonally dominant at large dt**

Split Time Step Obtained Via Block Gaussian Elimination

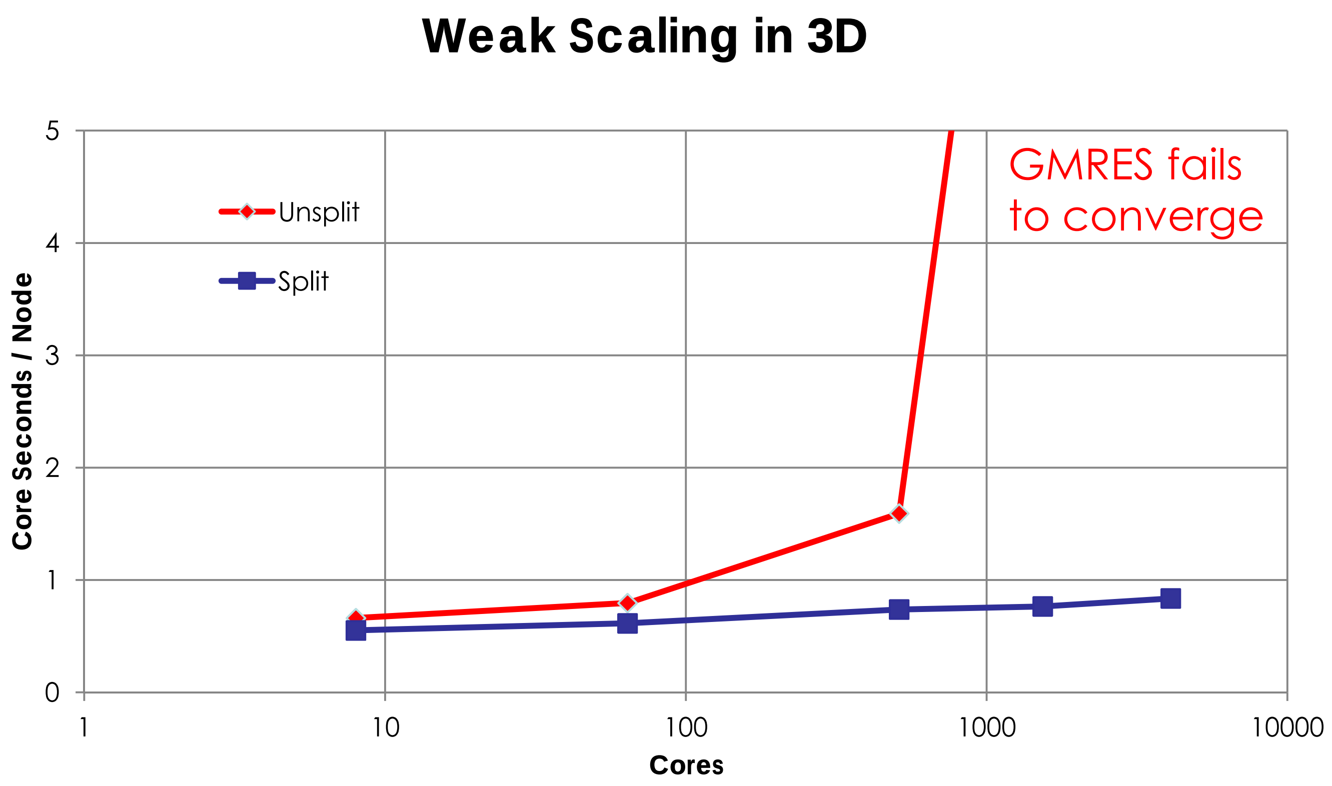
$$\begin{pmatrix} 1 & -\theta\, dt\, F \\ -\theta\, dt\, G & 1 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{B} \end{pmatrix}^{n+1} = \begin{pmatrix} 1 & (1-\theta)\, dt\, F \\ (1-\theta)\, dt\, G & 1 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{B} \end{pmatrix}^{n}$$

- **Use 2nd equation to eliminate $\mathbf{B}^{n+1}$ from 1st:**

$$\underset{\text{Schur complement}}{\longrightarrow} \begin{pmatrix} 1-\theta^2 dt^2 FG & 0 \\ -\theta\, dt\, G & 1 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{B} \end{pmatrix}^{n+1} = \begin{pmatrix} 1-\theta(\theta-1) dt^2 FG & dt\, F \\ (1-\theta)\, dt\, G & 1 \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{B} \end{pmatrix}^{n}$$

- **Matrix is lower-triangular → 1st equation can be solved independently of second**
  - Problem has been cut in half!
  - Same accuracy, stability properties as unsplit method

Split Method Scales Much Better Than Unsplit



- **Mesh resolution increased in all dimensions**
- **Core count increased accordingly**

Potential Representation

- **In neutral fluids, compression is highly stabilizing**
  - The most unstable mode will generally be incompressible
  - Discretization schemes not able to represent exactly incompressible modes will overestimate stability
  - This choice decouples U from compressible motion:

$$\mathbf{v} = \nabla U \times \nabla \varphi + R^2 \Omega \nabla \varphi + \nabla \chi$$

- **In a tokamak, compression of the magnetic field is highly stabilizing**
  - This choice decouples *U* from compression of the axisymmetric toroidal field

$$\mathbf{v} = R^2 \nabla U \times \nabla \varphi + R^2 \Omega \nabla \varphi + R^{-2} \nabla_{\perp} \chi$$

Vector Potential is Used to Represent Magnetic Field

$$\mathbf{A} = R^2 \nabla \varphi \times \nabla f + \psi \nabla \varphi$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

- **$\mathbf{B}$ is manifestly divergence-free**
- **$\mathbf{B}$ is represented using only two scalar fields**

- **Using subsets of scalar fields give physically meaningful systems**
  - (ψ, U) = "2-Field reduced MHD" (strong toroidal field, low pressure)
  - (ψ, U, f, Ω) = "4-Field reduced MHD" (low pressure)

- **Downside: requires high-order derivatives**
  - Obviated by use of C^1 elements

J.A. Breslau, N.M. Ferraro, and S.C. Jardin. *Phys. Plasmas* **16**:092503 (2009)

Annihilation Operators Decouple Waves

- **Scalar equations are obtained from split step velocity vector equation via three "annihilation" operators:**

$$\begin{pmatrix} \nabla\varphi\cdot\nabla\times \\ \nabla\varphi\cdot \\ \nabla_\perp\cdot \end{pmatrix}(\rho - s^2 L)\mathbf{v}$$

Schur complement

$$\mathbf{v} \sim \mathrm{Exp}[i\mathbf{k}\cdot\mathbf{x}]$$

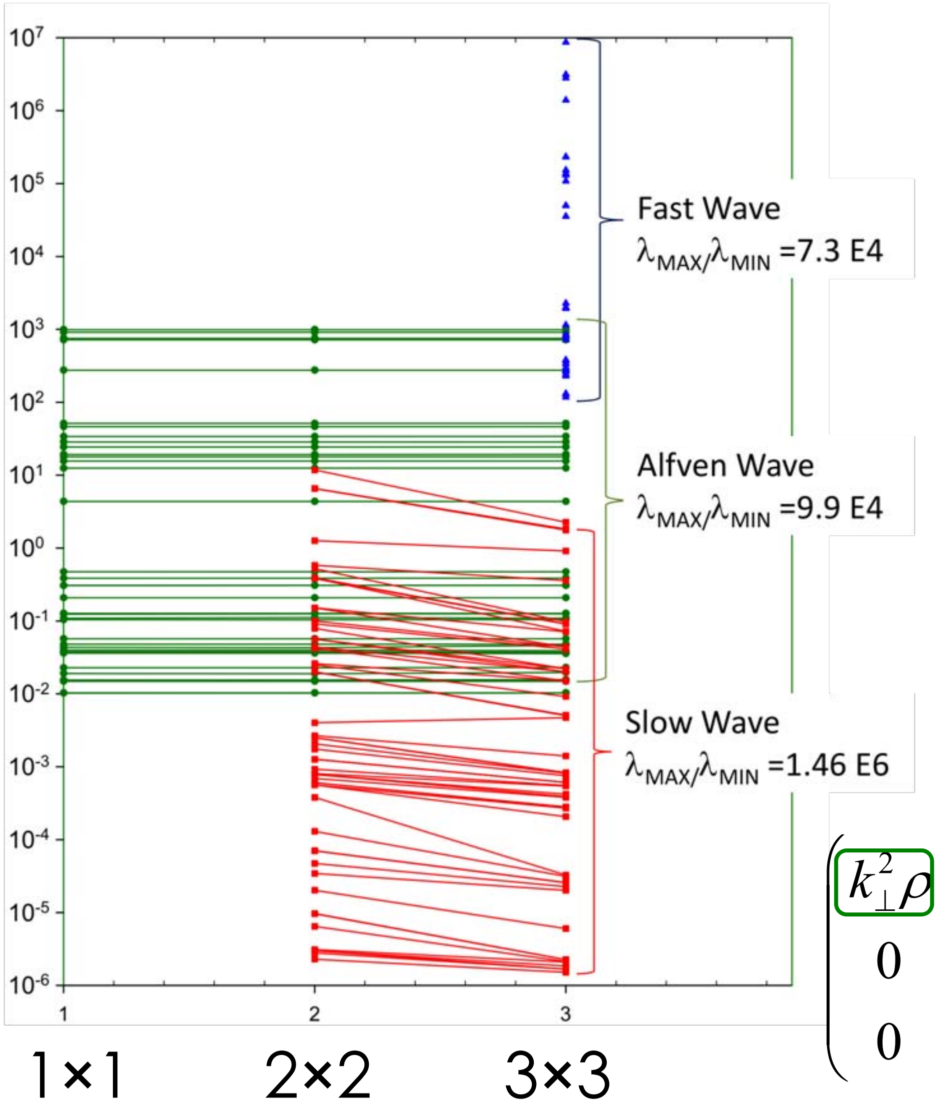
$$s^2 = \theta^2 dt^2$$

$$= \begin{pmatrix} k_\perp^2(\rho + s^2k_\parallel^2B^2) & 0 & 0 \\ 0 & \rho + s^2k_\parallel^2\Gamma p & s^2ik_\parallel k_\perp^2\Gamma p \\ 0 & s^2ik_\parallel k_\perp^2\Gamma p & -k_\perp^2\left[\rho + s^2k^2B^2 + s^2k_\perp^2\Gamma p)\right] \end{pmatrix}\begin{pmatrix} U \\ \Omega \\ \chi \end{pmatrix}$$

Alfvén wave Slow wave Fast wave

- **Since $k_\parallel$ is small in tokamaks, matrix is nearly diagonal**
  - The three waves are approximately decoupled

Diagonal Blocks Are Relatively Well-Conditioned



- **Different waves are weakly coupled**
- **The condition number of each block is much smaller than the condition number of the full matrix**

$$\begin{pmatrix} \boxed{k_\perp^2 \rho} & 0 & 0 \\ 0 & \boxed{\rho + s^2 k_\parallel^2 \Gamma p} & 0 \\ 0 & 0 & \boxed{-k_\perp^2 \left[\rho + s^2 k_\perp^2 (B^2 + \Gamma p)\right]} \end{pmatrix} \begin{pmatrix} U \\ \Omega \\ \chi \end{pmatrix}$$

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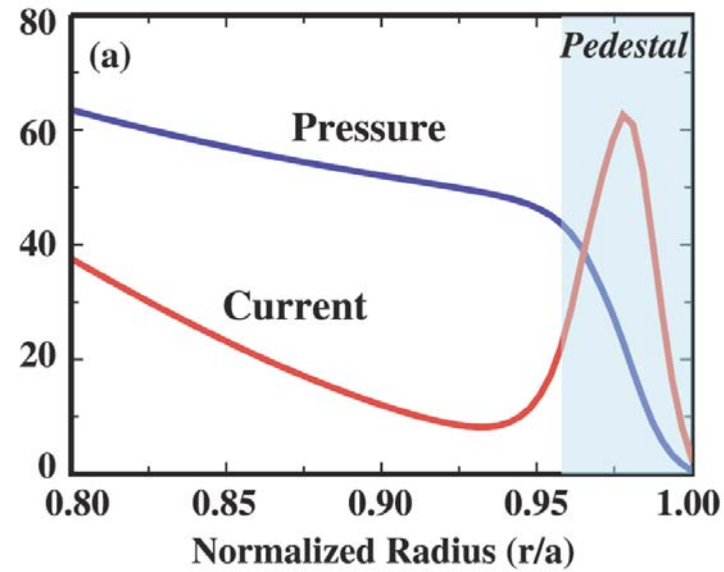
Edge Localized Modes (ELMs)

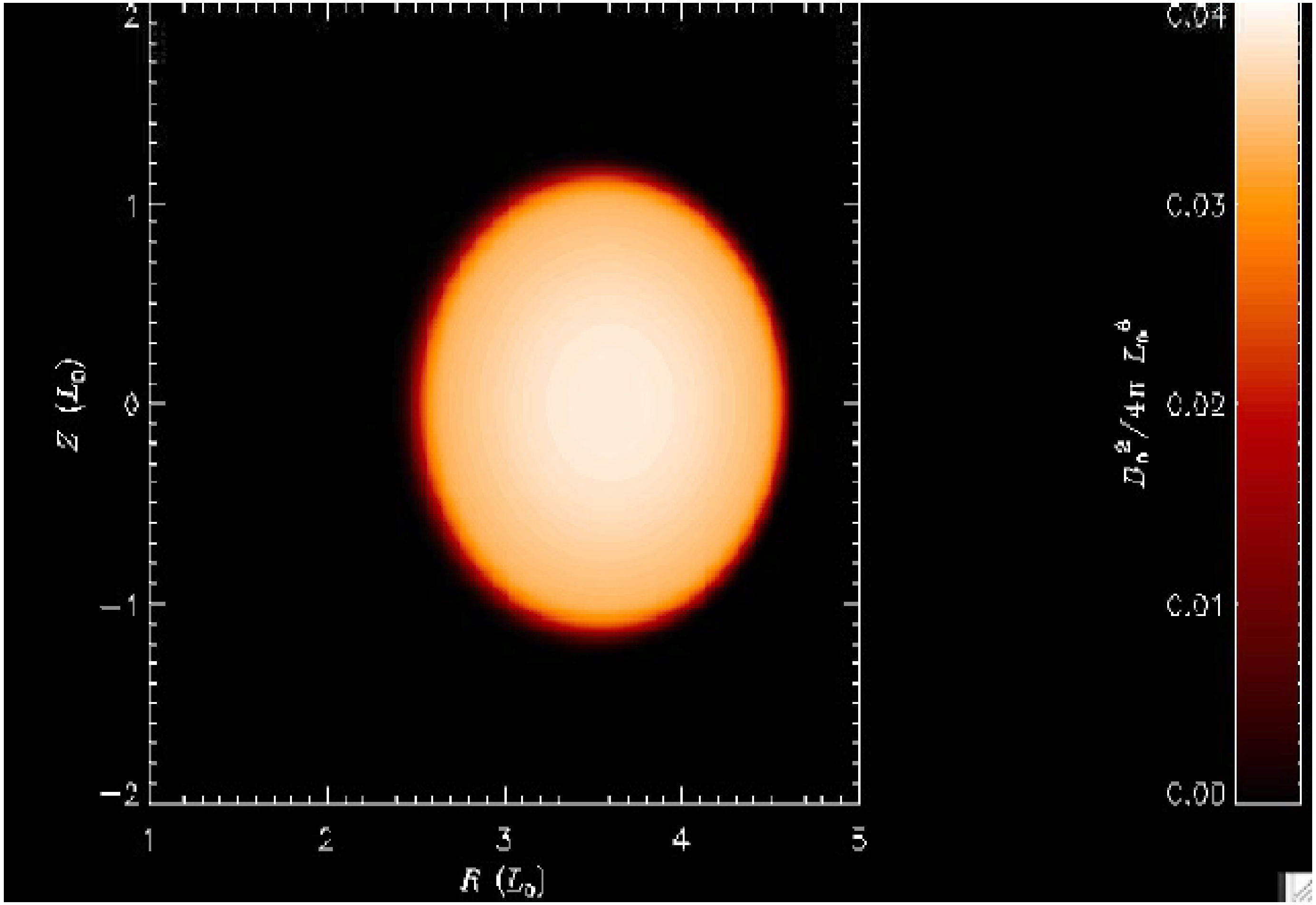
- **ELMs are periodic ejections of particles and energy**
- **Thought to be instabilities driven by currents and pressure gradients at the plasma edge**
- **May cause significant erosion in full-scale fusion reactor**



P.B. Snyder, et al. *Nucl. Fusion* **47**:961 (2007)

- **Questions:**
  - Are non-ideal effects important to stability? When?
  - How is energy deposited on wall?
- **Eigenfunction is difficult to calculate**
  - Sharp edge gradients
  - Singularity at x-point
  - Realistically small dissipation makes system extremely stiff

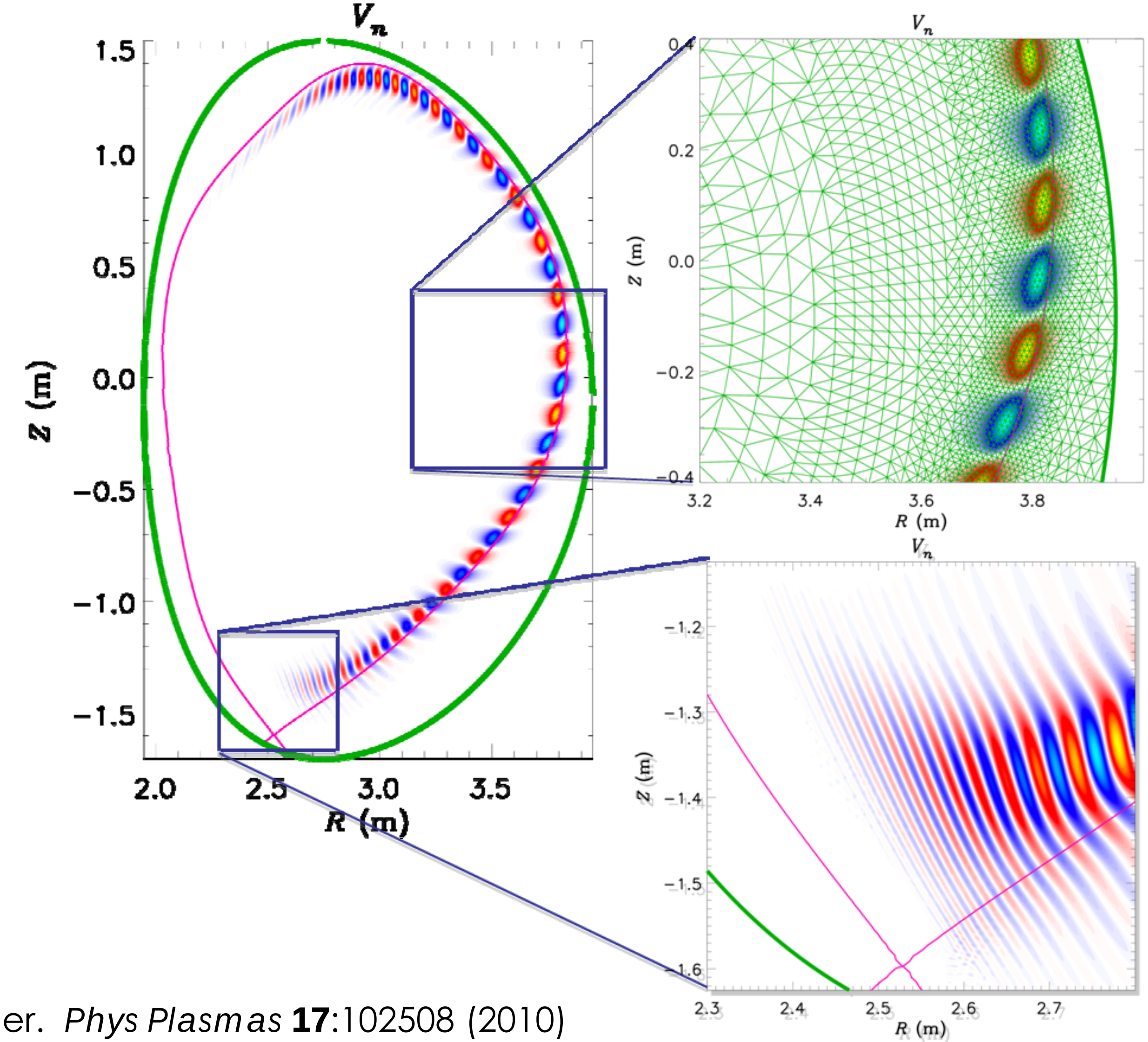
Nonlinear ELM Simulations Underway to Elucidate Energy Deposition



Calculated with realistic η, and $\mu=\kappa=0$!

Linear ELM Eigenfunctions Obtained For Realistic Equilbria

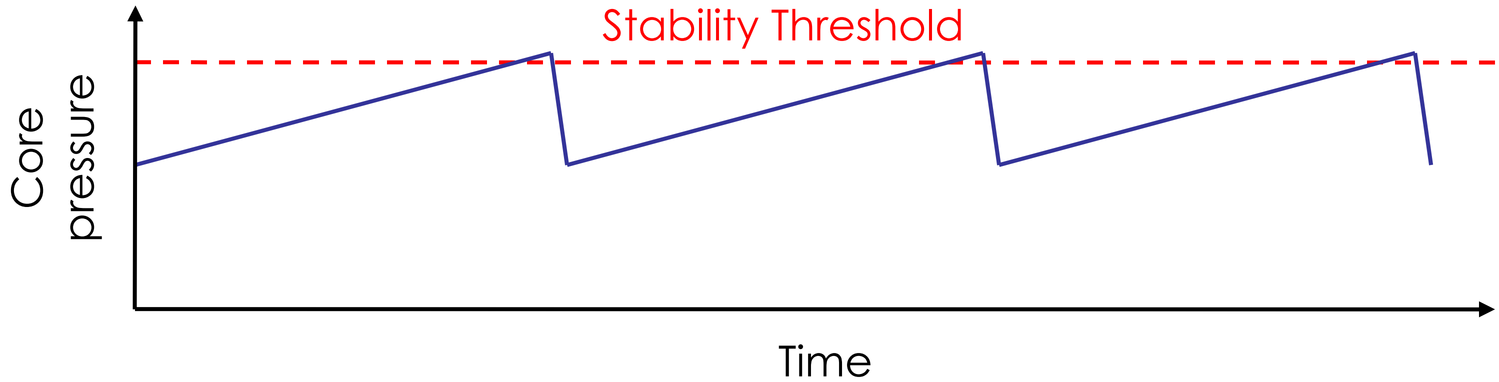
- **Non-ideal stability analysis of a realistic equilibrium (like this one) has not been successful until recently**
- **Non-ideal effects are found to be important:**
  - Edge resistivity
  - Gyroviscosity



N.M. Ferraro, S.C. Jardin, P.B. Snyder. *Phys Plasmas* **17**:102508 (2010)

Sawtooth Cycles

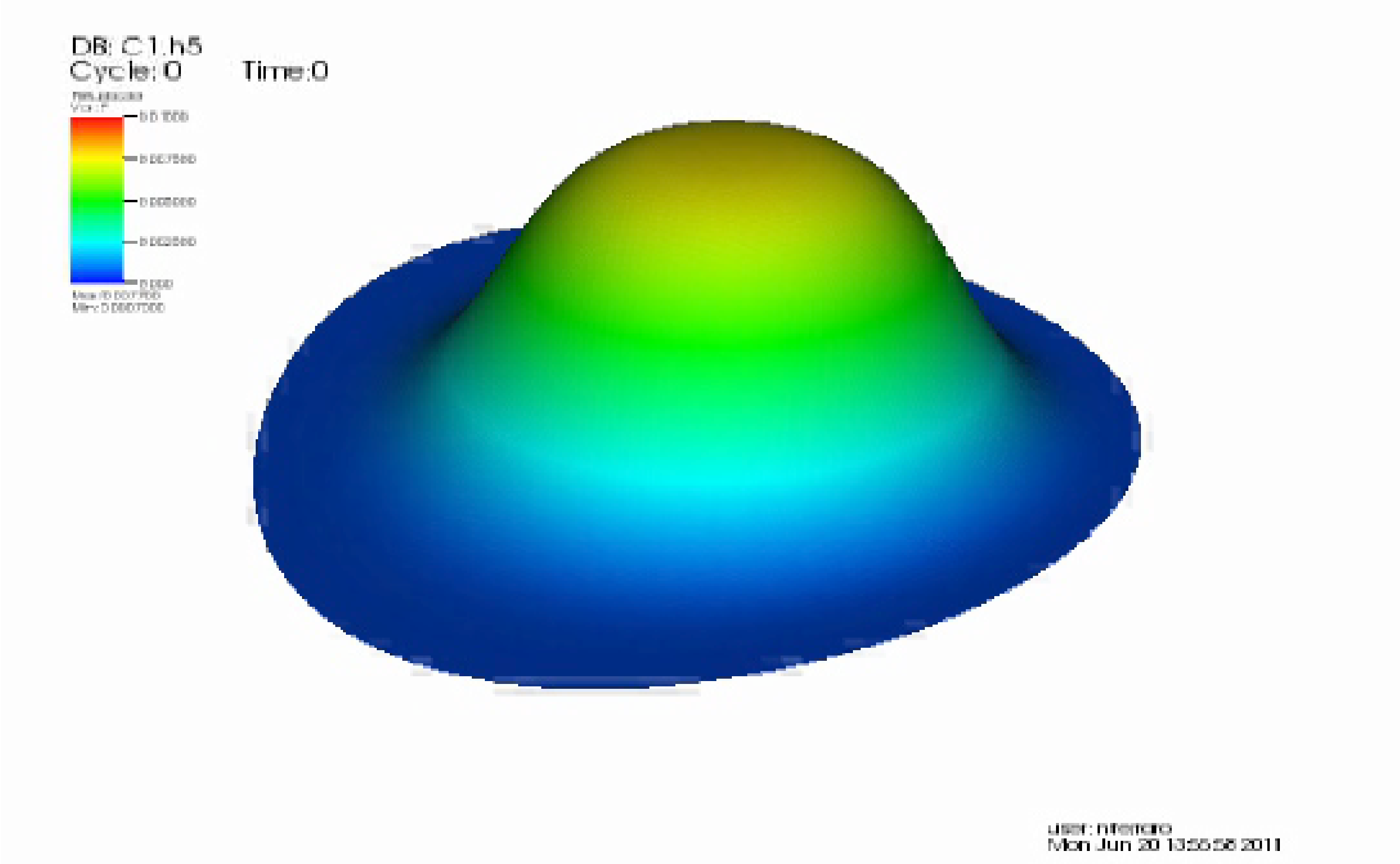
- **Tokamaks frequently exhibit "Sawtooth" cycles:**
  - Heating causes core pressure to rise slowly
  - Once stability threshold is passed, core pressure collapses rapidly



- **Questions:**
  - Where is the stability threshold?
  - How big is the collapse?

- **Disparate timescales make this cycle hard to simulate**

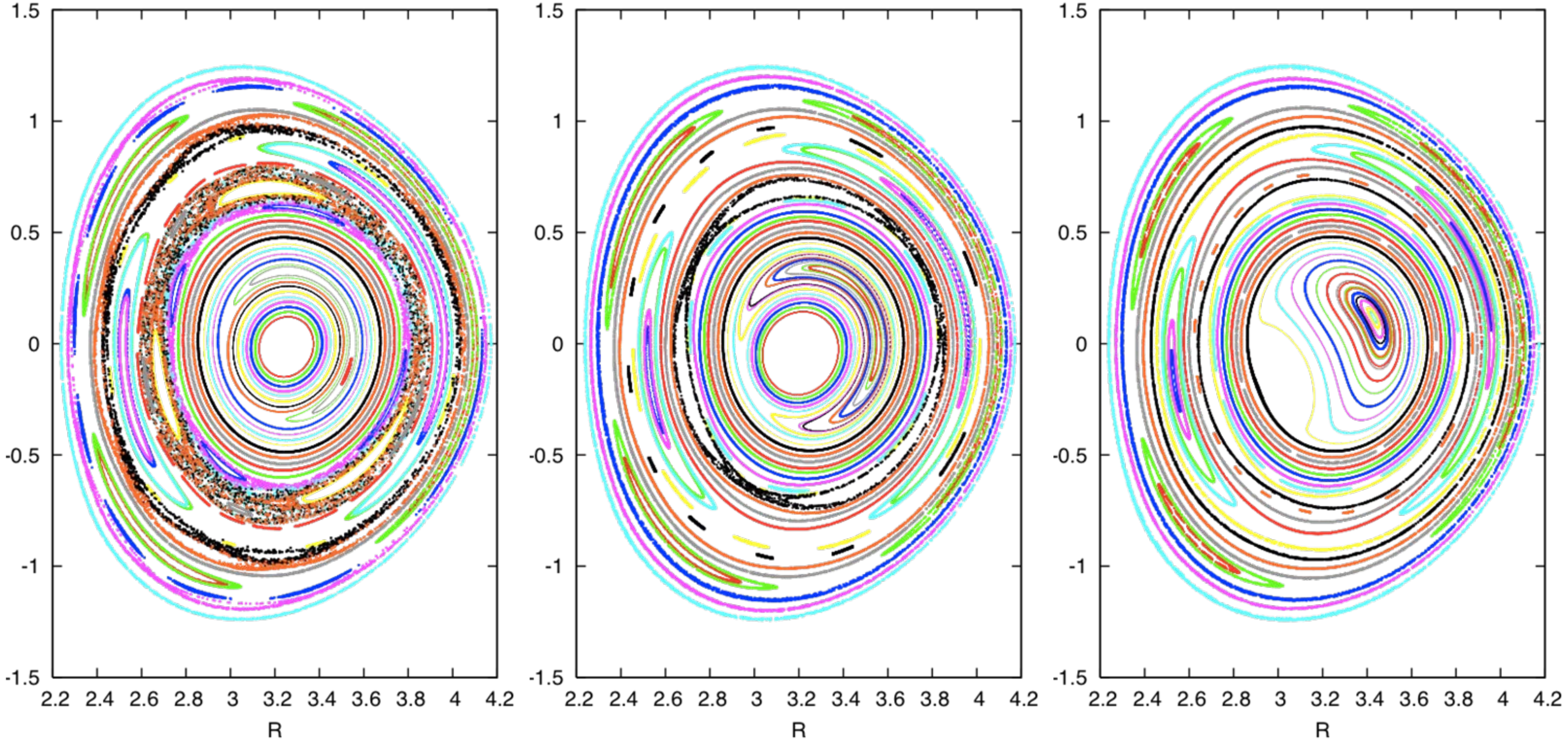
Sawtooth Causes Flattening of Pressure Profile



Movie made with **VisIt**
Special thanks to Allen Sanderson

Sawtooth Changes Magnetic Topology

- **Instability causes magnetic axis to shift and be replaced by new axis**



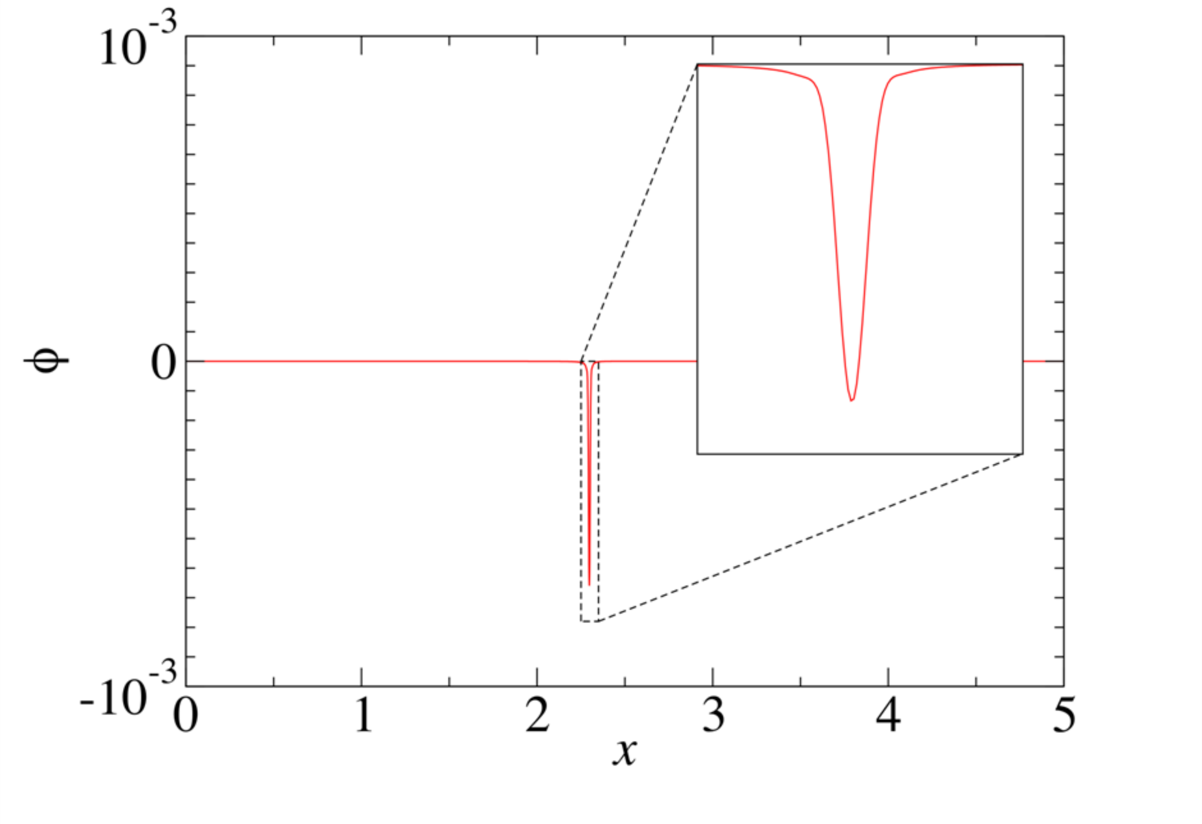
Summary

- **Several strategies are used to improve efficiency and matrix conditioning:**
  - High-order elements
  - Mesh packing
  - Split implicit time step
  - Flux/potential representation; annihilation operators
  - Block-Jacobi preconditioning
- **M3D-C1 is a collaborative effort that makes significant use of:**
  - Flexible Mesh DataBase (ITAPS)
  - PETSc (TOPS)
  - SuperLU (X. Li), MUMPS, GMRES
- **M3D-C1 has already yielded new physics results in areas of significant importance to magnetic fusion energy**

Extra Slides

Simple Test: 1D Resistive Layer

- **Simple equilibrium with one mode-rational surface**
- **Width of boundary layer determined by resistivity**
  - $\eta=10^{-9}$, $\Delta\phi\sim\eta^{1/3}$



Simple Test: 1D Resistive Layer

- **High-order elements give much better accuracy for a given solution time**