SCIDAC Center for Extended MHD Modeling

EXTENDED MHD MODELING: BACKGROUND, STATUS AND VISION

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OVERVIEW

- **The Extended MHD model**
- **The computational challenges:**
  - **Extreme separation of time scales**
  - **Extreme separation of spatial scales**
  - **Extreme anisotropy**
  - **Importance of geometry, boundary conditions**
  - **Causality: *can't parallelize over time!***

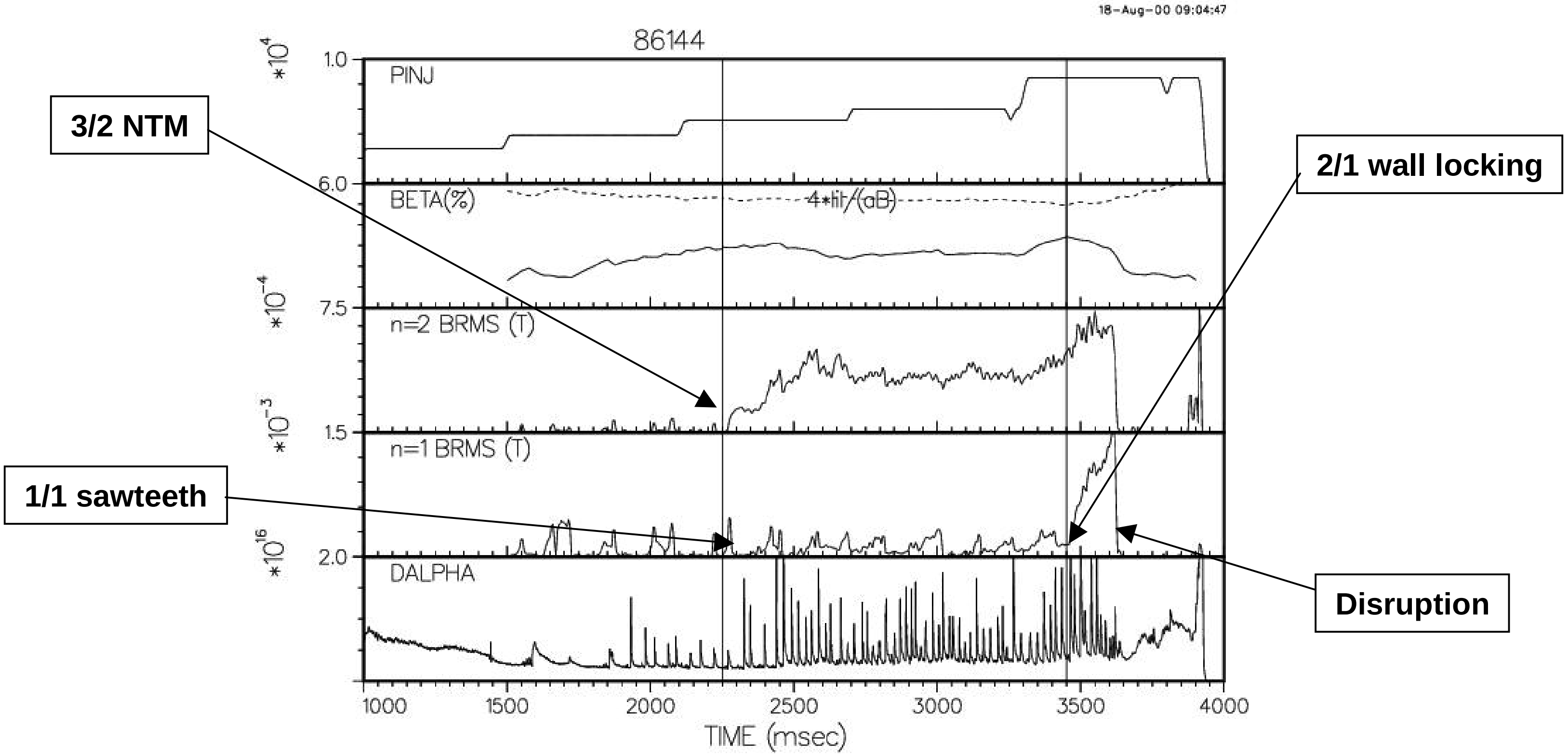
  At least as challenging as hydrodynamic turbulence!
- **Present computational approaches:**
  - **Implicit time differencing**
  - **Specialized spatial grids**
- **Status of present models**
- **Vision for integrated modeling**

DEFINITIONS

- *Hydrodynamics* - A mathematical model that describes the motion of a continuous, isotropic fluid
- *Magnetohydrodynamics* (MHD) - A mathematical model that describes the motion of a continuous, electrically conducting fluid in a magnetic field
  - Hydrodynamics and Maxwell equations coupled through Lorentz body force and Ohm's law
- *Ideal MHD* - the fluid has infinite electrical conductivity (zero resistivity)
- *Resistive MHD* - The fluid has finite conductivity and resistivity
- *Extended MHD* - additional effects of electron dynamics and/or non-Maxwellian species

MODERN TOKAMAKS ARE RICH IN MHD ACTIVITY

Example: DIII-D shot 86144



- **Sawtoothing discharge**
- **3/2 NTM triggered at 2250 msec**
- **2/1 locks to the wall**

MODELING REQUIREMENTS

- **Slow evolution**
  Nonlinear fluid model required
- **Plasma shaping**
  Realistic geometry required
- **High temperature**
  Large “Reynolds’ numbers”
- **Low collisionality**
  Extensions to resistive MHD required
- **Strong magnetic field**
  Highly anisotropic transport required
- **Resistive wall**
  Non-ideal boundary conditions required

APPROACHES

- **Quasi-equilibrium:**

$$\nabla p = \mathbf{J} \times \mathbf{B} \quad + \quad \text{constraints}$$

  - **"Magnetohydrostatics" (MHS?)**
  - **Eliminates all waves**
  - **Basis for 1-1/2 dimensional transport models**
  - **Extension to 3-D?**

- **Time dependent**
  - **Solve 2-fluid equations**
  - **Retain all normal modes**
  - **Focus of present SciDAC efforts**

FLUID MODELS

- **Kinetic models of plasmas based on distribution function for each charge species**
- **Satisfies *kinetic equation***

$$\frac{df_\alpha}{dt} = \sum_\beta C\left[f_\alpha, f_\beta\right]$$

$f_\alpha(\mathbf{x}, \mathbf{v}, t)$ **- six dimensions plus time**
- computationally impractical for time scales of interest

- ***Fluid models* derived by taking successive velocity moments of kinetic equation**
  - **Reduce dimensionality by 3**
- **Hierarchy of equations for *n*, v, *p*, Π, q, …….**
- **Equations truncated by closure relations**
  - **Express high order moments in terms of low order moments**
  - **Capture *kinetic effects* in these moments**
- **Result is *Extended MHD***

2-FLUID MODEL

- **Maxwell (no displacement current):**

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \quad , \qquad \nabla \times \mathbf{B} = \mu_0 \mathbf{J} \quad ,$$

- **Momentum, energy, and continuity for each species (*α* = *e*, *i*):**

$$m_\alpha n_\alpha \left(\frac{\partial \mathbf{v}_\alpha}{\partial t} + \mathbf{v}_\alpha \cdot \nabla \mathbf{v}_\alpha \right) = -\nabla \cdot \mathbf{P}_\alpha + q_\alpha n_\alpha (\mathbf{E} + \mathbf{v}_\alpha \times \mathbf{B}) + \sum_\beta \mathbf{R}_{\alpha\beta} + \mathbf{S}_\alpha^m$$

$$\frac{\partial p_\alpha}{\partial t} + \mathbf{v}_\alpha \cdot \nabla p_\alpha = -\frac{3}{2} p_\alpha \nabla \cdot \mathbf{v}_\alpha - \mathbf{P}_\alpha : \nabla \mathbf{v}_\alpha - \nabla \cdot \mathbf{q}_\alpha + \mathbf{Q}_\alpha$$

$$\frac{\partial n_\alpha}{\partial t} = -\nabla \cdot (n_\alpha \mathbf{v}_\alpha) + S_\alpha^n$$

- **Current and quasi-neutrality:**

$$\mathbf{J}_\alpha = n_\alpha q_\alpha \mathbf{v}_\alpha , \qquad n = n_e = Z n_i$$

SINGLE FLUID FORM

- **Add electron and ion momentum equations:**

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla\cdot\mathbf{P}' + \mathbf{J}\times\mathbf{B}$$

- **Subtract electron and ion momentum equations (Ohm's law):**

$$\mathbf{E} = -\underbrace{\mathbf{v}\times\mathbf{B}}_{Ideal\ \ MHD} + \underbrace{\eta\mathbf{J}}_{Resistive\ \ MHD} + \underbrace{\frac{1}{ne}\frac{1-\nu}{1+\nu}\mathbf{J}\times\mathbf{B}}_{Hall\ \ Effect}$$

$$-\underbrace{\frac{1}{ne\,(1+\nu)}\nabla\cdot\left(\mathbf{P}_e' - \nu\mathbf{P}_i'\right)}_{\substack{Diamagnetic\ \ Effects \\ and\ Closures}} + \underbrace{\frac{1}{\varepsilon_0\omega_{pe}^2\,(1+\nu)}\left[\frac{\partial \mathbf{J}}{\partial t} + \nabla\cdot\left(\mathbf{vJ}+\mathbf{Jv}\right)\right]}_{Electron\ \ Inertia}$$

All effects beyond resistivity constitute Extended MHD

COMPUTATIONAL CHALLENGES

- ***Extreme separation of time scales***
  - **Realistic "Reynolds' numbers"**
  - **Implicit methods**
- ***Extreme separation of spatial scales***
  - **Important physics occurs in internal boundary layers**
  - **Small dissipation cannot be ignored**
  - **Requires grid packing or adaption**
- ***Extreme anisotropy***
  - **Special direction determined by magnetic field**

  Accurate treatment of $\mathbf{B}\cdot\nabla$ ***operator is important***

  - **Requires specialized gridding**

SEPARATION OF TIME SCALES

$$\underbrace{\tau_A}_{Affvén\ transit\ time} < \underbrace{\tau_S}_{Sound\ transit\ time} << \underbrace{\tau_{evol}}_{MHD\ evolution\ time} << \underbrace{\tau_R}_{Resistive\ diffusion\ time}$$

Lundquist number: $S = \frac{\tau_R}{\tau_A} \sim 10^8 >> 1$

Explicit time step impractical:

$$\Delta t < \frac{\Delta x}{L}\tau_A \approx \frac{\tau_A}{N} <<<< \tau_{evol}$$

Require implicit methods

IMPLICIT METHODS

- **Partially implicit methods**
  - **Treat fastest time scales implicitly**
  - **Time step still limited by waves**
- **Semi-implicit methods**
  - **Treat linearized ideal MHD operator implicitly**
  - **Time step limited by advection**
  - **Many iterations**
- **Fully implicit methods**
  - **Newton-Krylov treatment of full nonlinear equations**
  - **Arbitrary time step**
  - **Still a research project**

LINEAR SOLVER REQUIREMENTS

- **Extremely large condition number : > 10^{10}!!**
  - **Specialized pre-conditioners**
  - **Anisotropy**
- **Ideal MHD is self-adjoint**
  - **Symmetric matrices**
  - **CG**
- **Advection and some 2-fluid effects (whistler waves) are not self-adjoint**
  - **Need for efficient non-symmetric solvers**
- **Everything must be efficient and scalable in parallel**
- **Should interface easily with F90**

SEPARATION OF SPATIAL SCALES

- Important dynamics occurs in internal boundary layers
  - Structure is determined by plasma resistivity or other dissipation
  - Small dissipation cannot be ignored
- Long wavelength along magnetic field
- Extremely localized across magnetic field:

$$\delta / L \sim S^{-\alpha} \ll 1 \text{ for } S \gg 1$$

- It is these long, thin structures that evolve nonlinearly on the slow evolutionary time scale

EXTREME ANISOTROPY

- **Magnetic field locally defines special direction in space**
- **Important dynamics are extended along field direction, very narrow across it**
- **Propagation of normal modes (waves) depends strongly on local field direction**
- **Transport (heat and momentum flux) is also highly anisotropic**

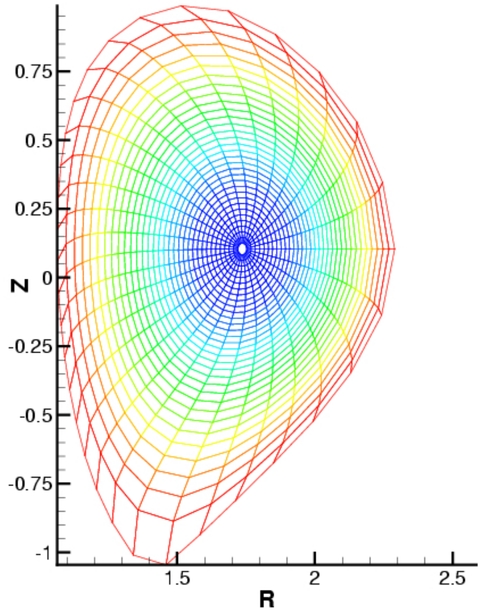
==> Requires accurate treatment of operator $\mathbf{B} \cdot \nabla$

Inaccuracies lead to "spectral pollution" and anomalous perpendicular transport

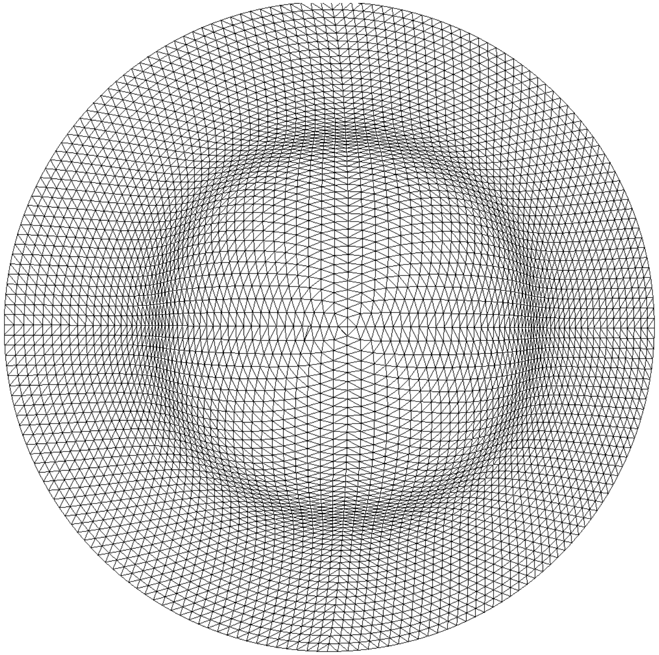
GRIDDING AND SPATIAL REPRESENTATION

- **Spatial stiffness and anisotropy require special gridding**
  - **Toroidal and poloidal dimensions treated differently**
- **Toroidal (ϕ, primarily along field)**
  - **Long wavelengths, periodicity => FFTs (finite differences also used)**
- **Poloidal plane (*R*,*Z*)**
  - **Fine structure across field direction**
  - **Grids aligned with flux surfaces (~ field lines)**
  - **Unstructured triangular grids**
  - **Extreme packing near internal boundary layers**
- **Finite elements**
  - **High order elements essential for resolving anisotropies**
- **Dynamic mesh adaption in research phase**

POLOIDAL GRIDS



DIII-D poloidal cross-section with flux aligned grid (NIMROD)



Circular poloidal cross-section with triangles and grid packing (M3D)

Poloidal grids from SciDAC development projects

BEYOND RESISTIVITY - EXTENDED MHD

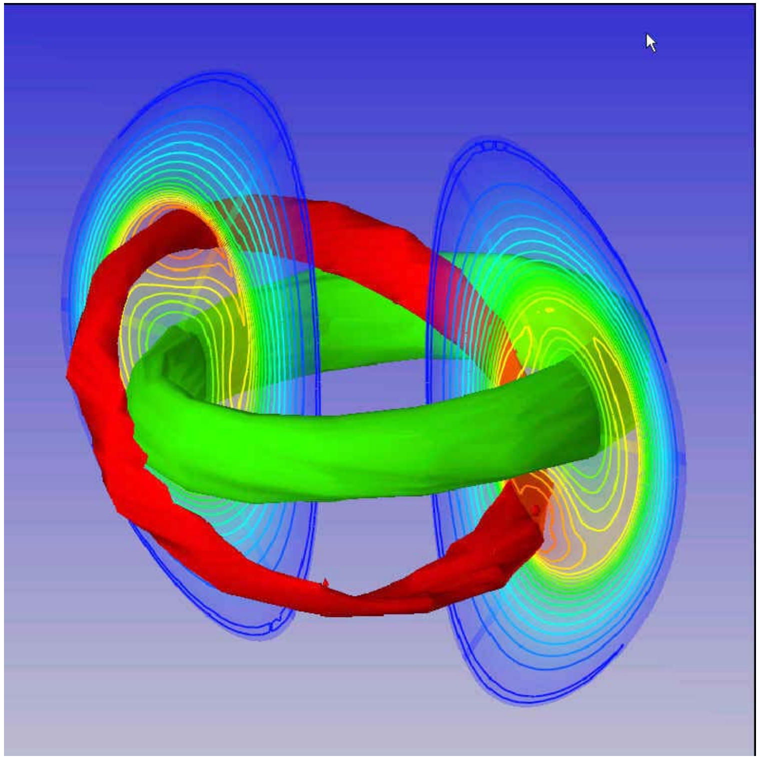
- **2-fluid effects**
  - **Whistler waves (Hall term) require implicit advance with non-symmetric solver**
  - **Electron inertia treated implicitly**
  - **Diamagnetic rotation may cause accuracy, stability problems**
- **Kinetic effects - influence of non-Maxwellian populations**
  - **Analytic closures**
    - **Seek *local* expressions for Π, q, etc.**
  - **Particle closures**
    - **Subcycle gyrokinetic δf calculation**
    - **Minority ion species - beam or α-particles**

STATUS

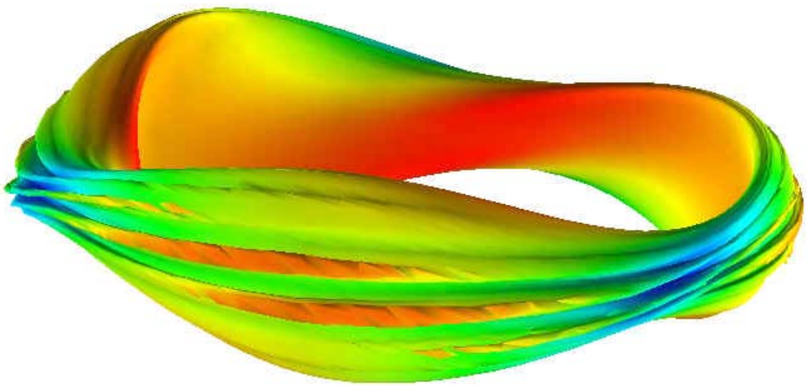
- **2 major SciDAC development projects for time-dependent models**
  - **M3D - multi-level, 3-D, parallel plasma simulation code**
    - **Partially implicit**
    - **Toroidal geometry - suitable for stellarators**
    - **2-fluid model**
    - **Neo-classical and particle closures**
  - **NIMROD - 3-D nonlinear extended MHD**
    - **Semi-implicit**
    - **Slab, cylindrical, or axisymmetric toroidal geometry**
    - **2-fluid model (evolving computationally)**
    - **Neo-classical closures**
    - **Particle closures being de-bugged**

  Both codes have exhibited good parallel performance scaling
- **Other algorithms are being developed in the fusion program**

STATUS - RESISTIVE MHD

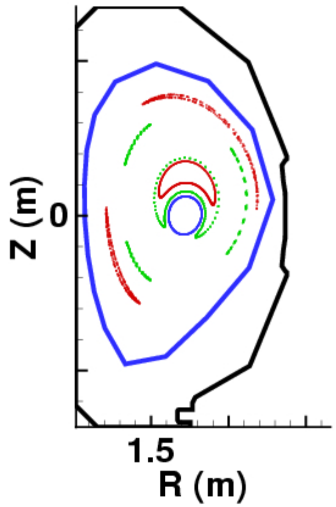


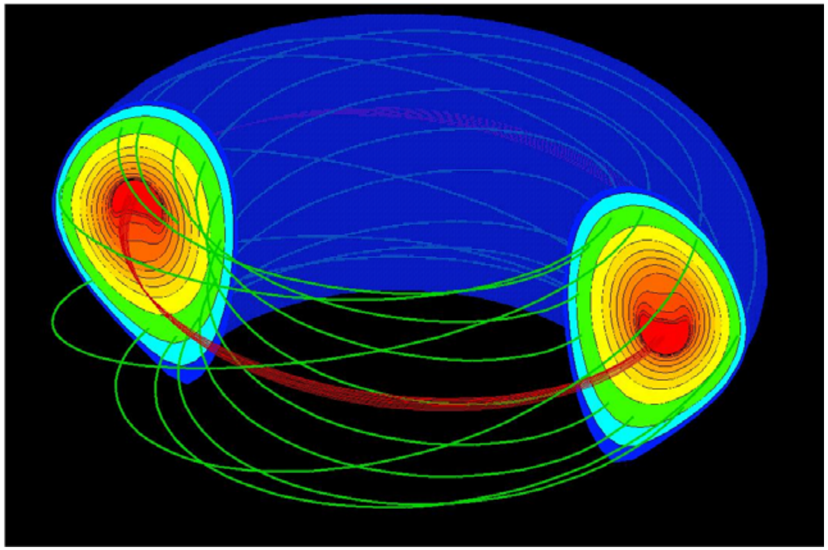
Sawtooth in NSTX computed by M3D

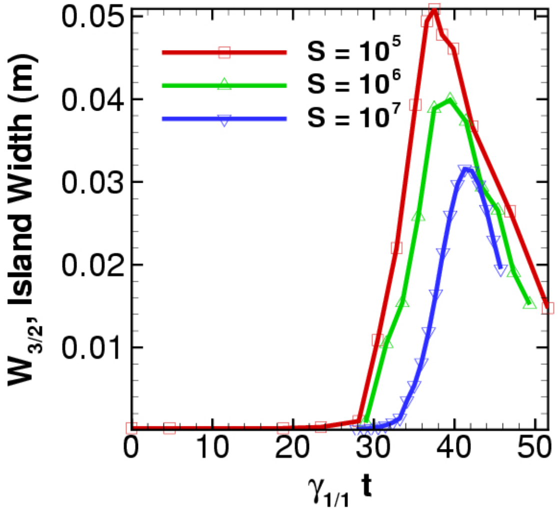


Stellarator ballooning mode computed by M3D

STATUS - RESISTIVE MHD



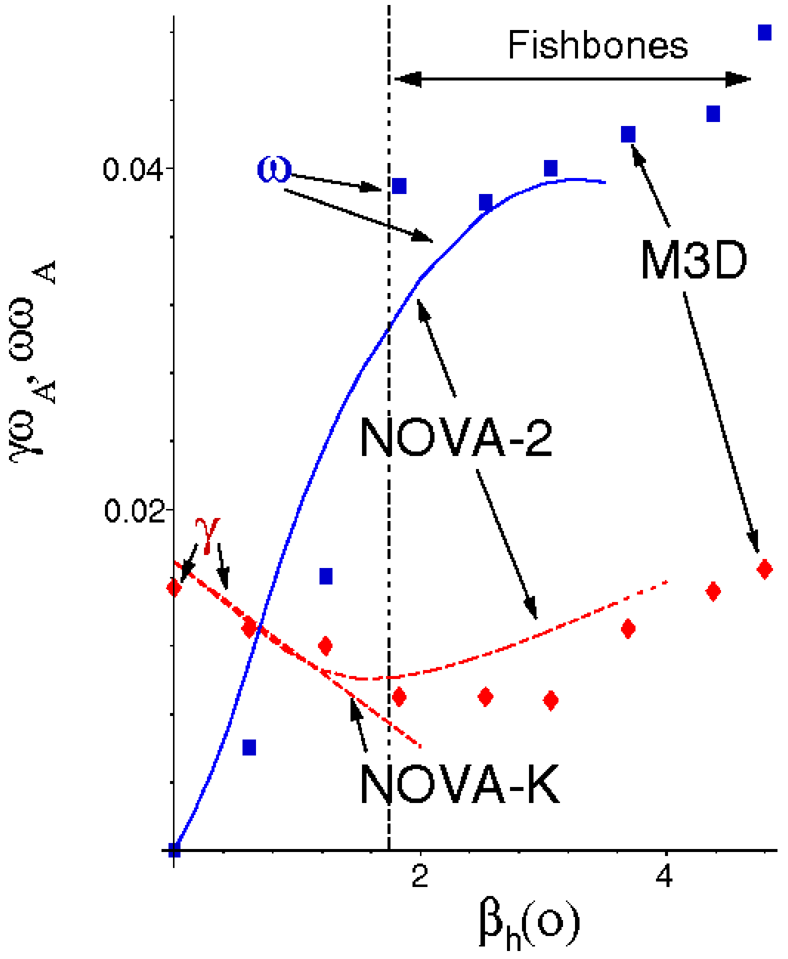




Secondary magnetic islands generated during sawtooth crash in DIII-D shot 86144 by NIMROD

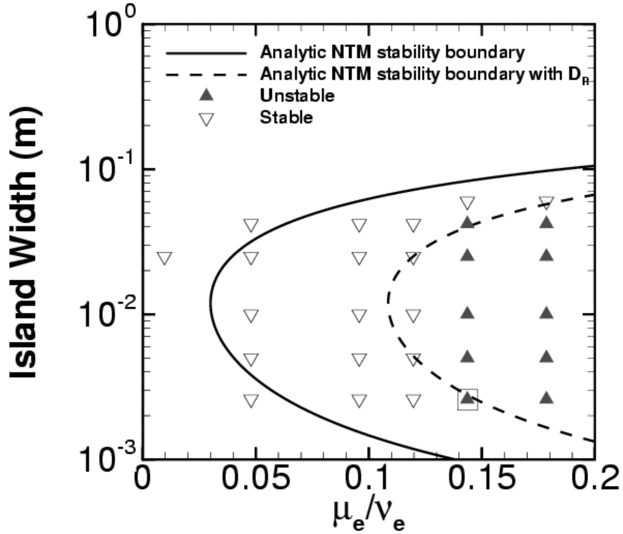
STATUS - EXTENDED MHD

- Effect of energetic particle population on MHD mode
- Subcycling of energetic particle module within MHD codes
- M3D agrees well with NOVA2 in the linear regime
- Energetic particles are being incorporated into NIMROD

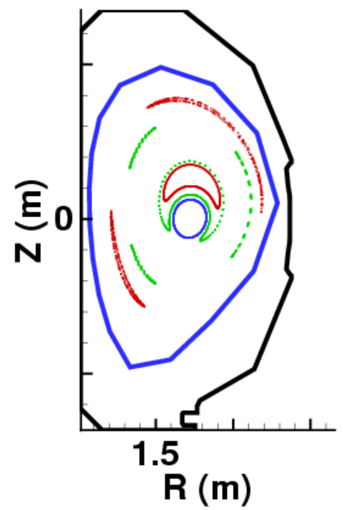


STATUS - EXTENDED MHD

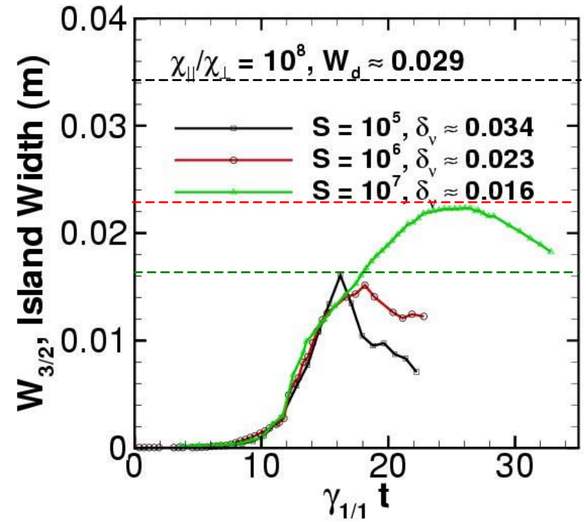
Neo-classical tearing modes with NIMROD using analytic closure



Computed NTM stability diagram



Sawtooth and secondary islands

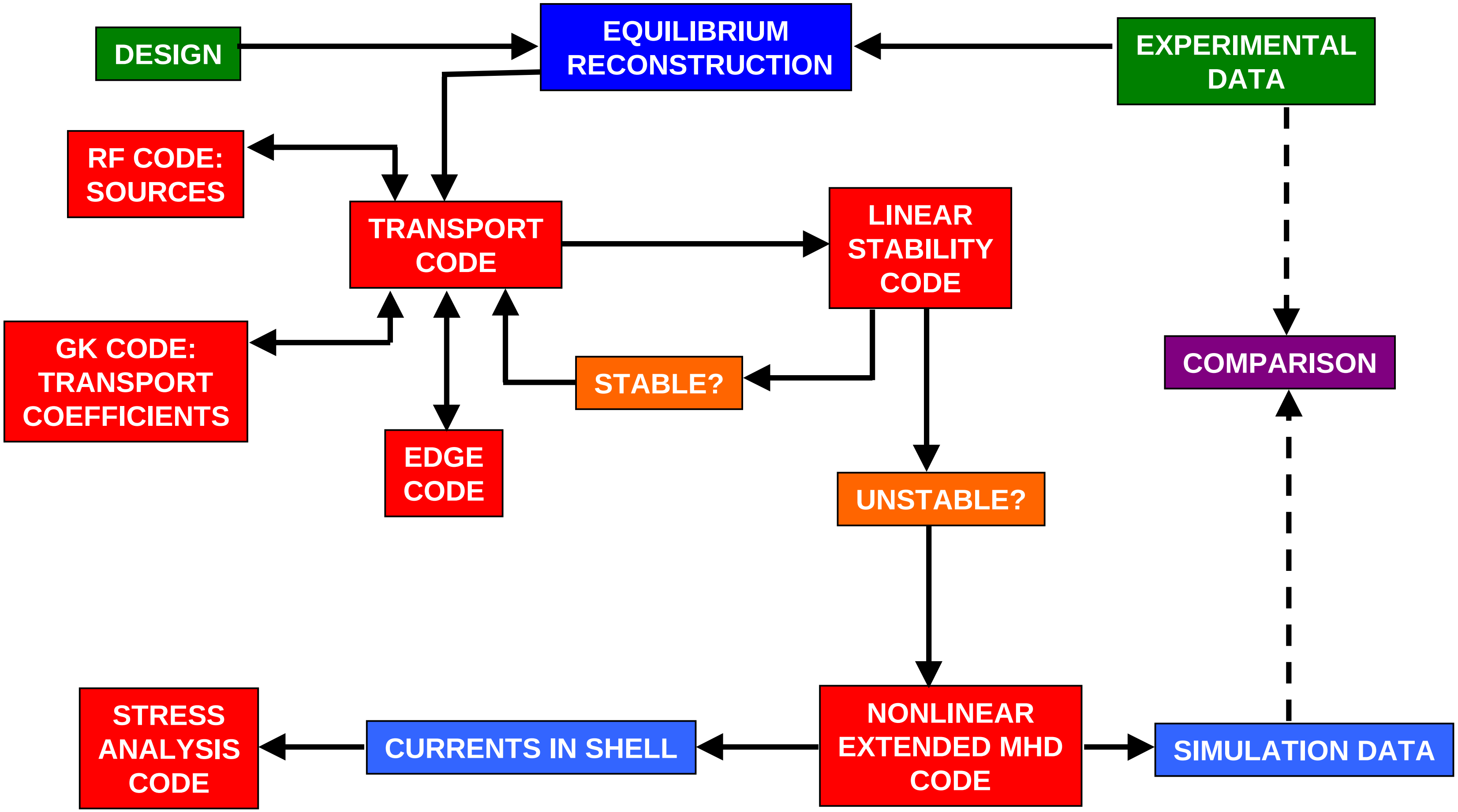


Secondary island growth Varying S

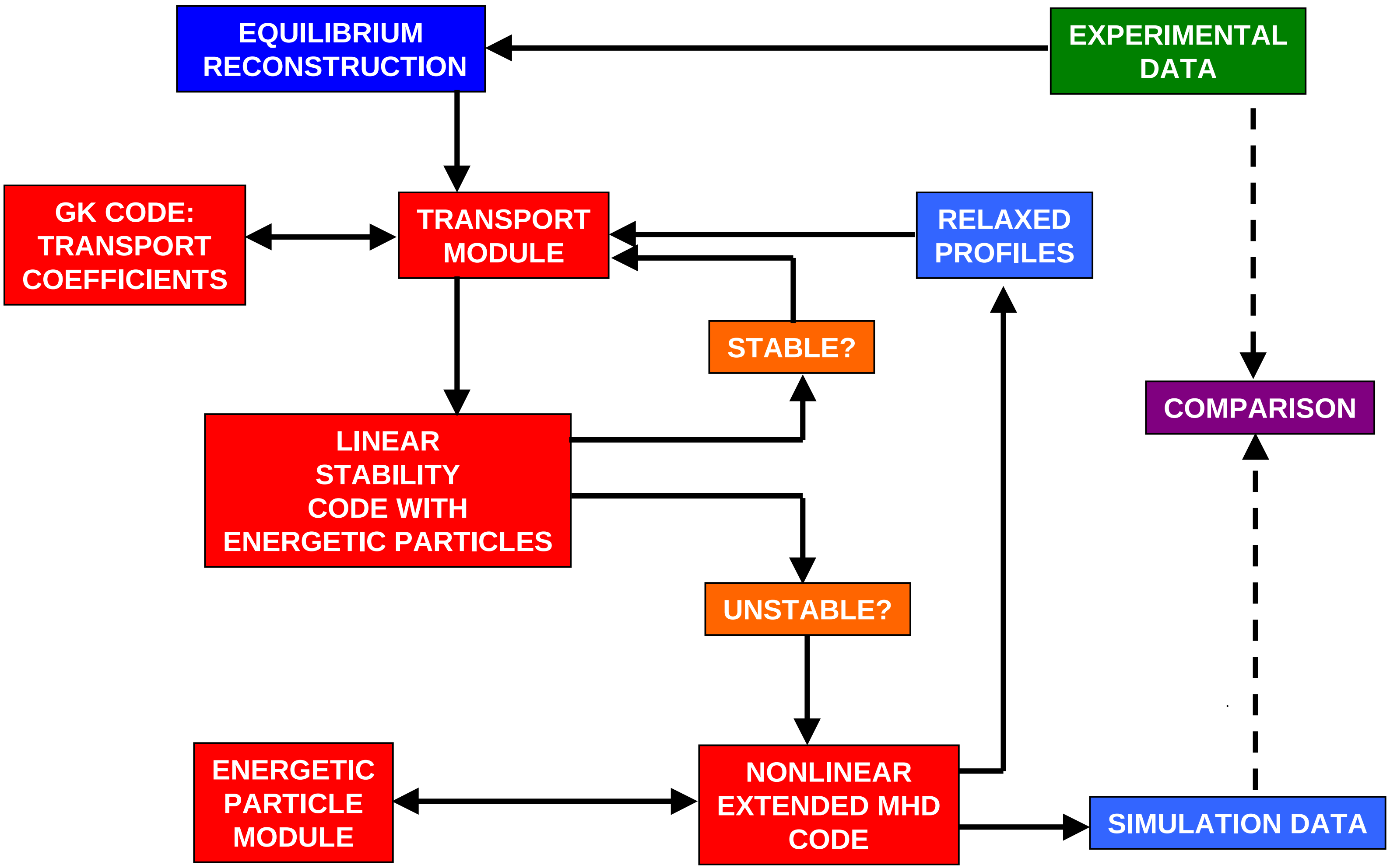
NEXT STEP - INTEGATED MODELING

- ***Non-local kinetic physics, MHD, and profile evolution are all inter-related***
  - **Kinetic physics determines transport coefficients**
  - **Transport coefficients affect profile evolution**
  - **Profile evolution can destabilize of MHD modes**
  - **Kinetic physics can affect nonlinear MHD evolution (NTMs, TAEs)**
  - **MHD relaxation affects profile evolution**
  - **Profiles affect kinetic physics**
- ***Effects of kinetic (sub grid scale) physics must be synthesized into MHD models***
  - **Extensions to Ohm's law (2-fluid models)**
  - **Subcycling/code coupling**
  - **Theoretical models (closures), possibly heuristic**
- ***Effects of MHD must be synthesized into transport models***
- ***Predictions must be validated with experimental data***

VISION: VDE EVOLUTION



VISION: SAWTOOTH CYCLE



ENABLING COMPUTER SCIENCE TECHNOLGIES

- *Largest, fastest computers!*
  - But intermediate computational resources often neglected, and…
  - *The computers will never be large or fast enough!*
- *Algorithms*
  - Parallel linear algebra
  - Gridding, adaptive and otherwise
- *Data structure and storage*
  - Adequate storage devices
  - Common treatment of experimental and simulation data
  - Common tools for data analysis
- *Communication and networking*
  - Fast data transfer between simulation site and storage site
  - Efficient worldwide access to data
  - Collaborative tools
  - Dealing with firewalls
- *Advanced graphics and animation*

SUMMARY

- ***Predictive simulation capability has 3 components***
  - **Code and algorithm development**
  - **Tightly coupled theoretical effort**
  - **Validation of models by comparison with experiment**
- ***Integration required for:***
  - **Coupling algorithms for disparate physical problems**
  - **Theoretical synthesis of results from different models**
  - **Efficient communication and data manipulation**
- ***Progress is being made with Extended MHD***
  - **Integration of energetic ion modules into 3-D MHD**
  - **Computationally tractable closures**
  - **Resistive wall modules**

Need to bring a broader range of algorithms and codes to bear for overall fusion problem