SCIDAC Center for Extended MHD Modeling

ISSUES RELATED TO INTEGRATED MODELING IN FUSION SCIENCE

Dalton D. Schnack
Center for Energy and Space Science
Science Applications International Corp.
San Diego, CA

OVERVIEW

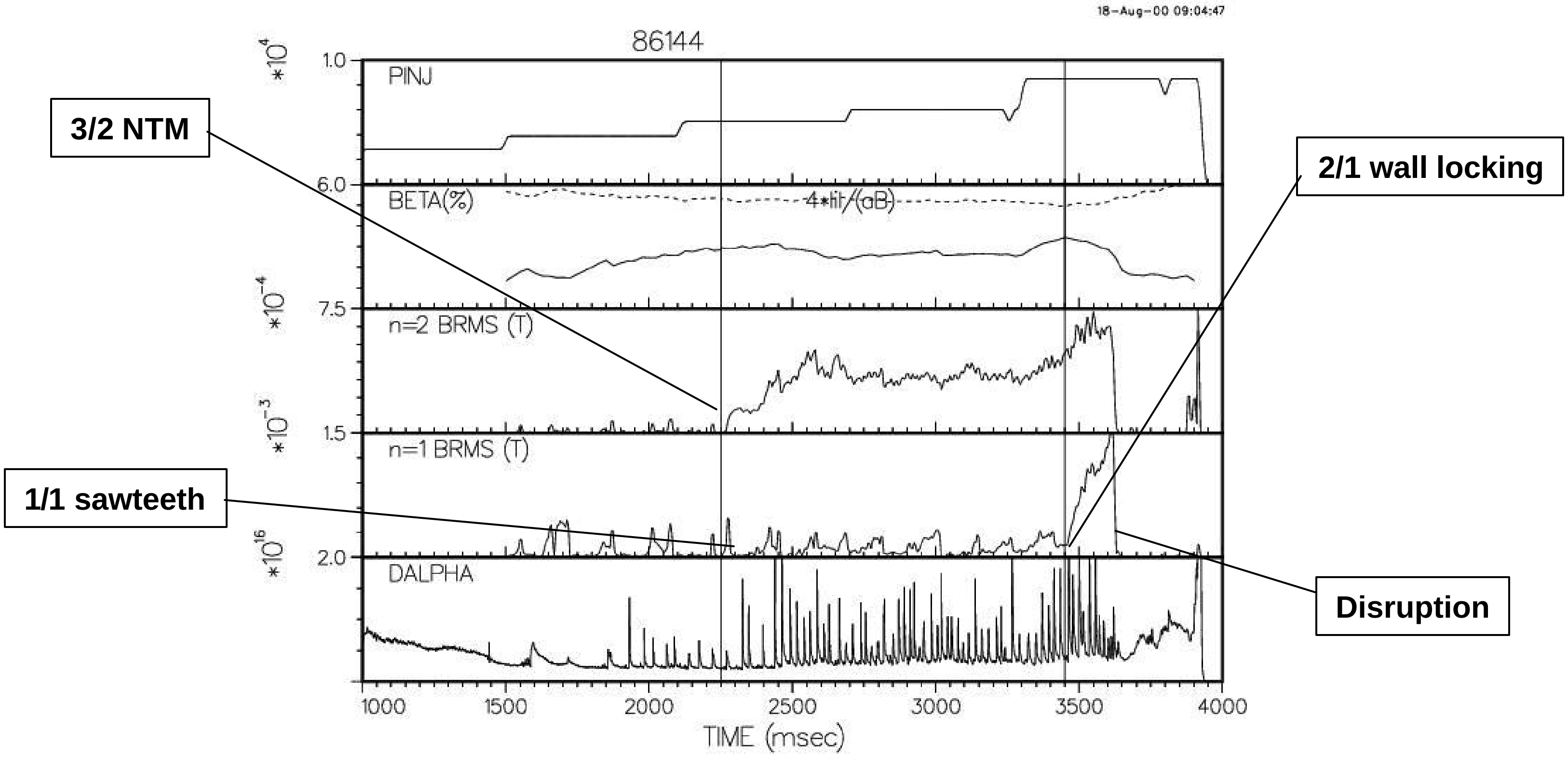
- **Goal of integrated modeling**
  - **A predictive simulation model of fusion plasma dynamics with realistic parameters and geometry**
- **Constraints imposed by physics, algorithms, and hardware**
  - **3-D fluid-based model is only practical approach**
  - **More detailed physics, longer time scale models must be integrated into this central module**
- **The computational challenges of fluid model:**
  - **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 a challenging as hydrodynamic turbulence!

- **Present computational approaches:**
  - **Implicit time differencing**
  - **Specialized spatial grids**
- **Status of present models**
- **Vision for integrated modeling**

DESIRED PREDICTABILITY: MODAL DYNAMICS

Example: DIII-D shot 86144


3/2 NTM

1/1 sawteeth

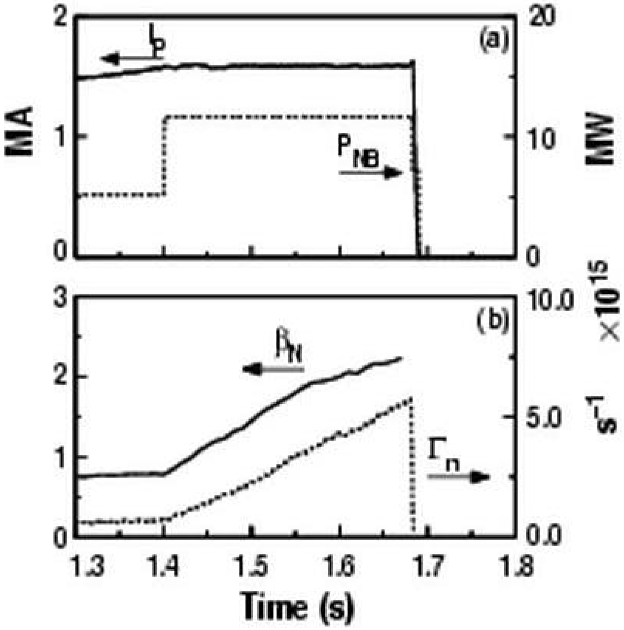
2/1 wall locking

Disruption

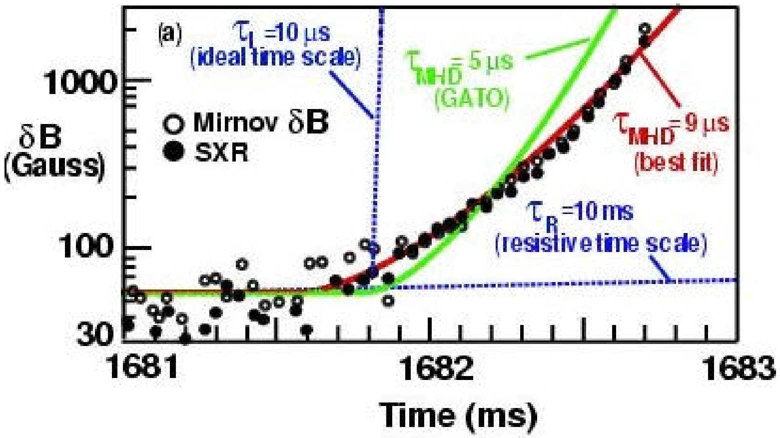
- **Sawtoothing discharge**
- **3/2 NTM triggered at 2250 msec**
- **2/1 locks to the wall**

DESIRED PREDICTABILITY: DISRUPTION

Example: DIII-D shot 87009



- **Increase in neutral beam power**
- **Plasma pressure increases**
- **Sudden termination (disruption)**



- **Time dependence at disruption onset**
- **Growing 3-D magnetic perturbation**
- **Nonlinear evolution?**
- **Effect on confinement?**
- **Can this be predicted?**

PREDICTIVE MODEL OF PLASMA DYNAMICS

- Magnetic perturbations
  Electromagnetic model
- Slow evolution
  1 msec. - 1 sec. problem time
- Plasma shaping
  Realistic geometry required
- High temperature
  Large “Reynolds’ numbers”
- Low collisionality
  Kinetic (velocity space) physics affects global evolution
- Strong magnetic field
  Dynamics are highly anisotropic
- Resistive wall
  Non-ideal boundary conditions
- Sources
  RF and beam interaction with plasma for heating, current drive
- Engineering calculations
  Heat loads, stresses, etc.

FUSION SCIENCE MODELS

- Source models (*fastest time scales; light waves*)
  - Interaction of RF waves or neutral beams with static 2-D background plasma
  - Sources of heat, mass, and electric field
- Global kinetic models (*first-principles; particle time scales*)
  - Solve kinetic (“gyrokinetic”) equations
  - 5 dimensional (3 space, 2 velocity) + time
  - Provide direct calculation of anomalous transport
- Fluid (MHD) models (*low frequency; no particles*)
  - 3 space dimensions *(realistic geometry*)
  - Single fluid (*lumped ions and electrons*)
  - Time dependent, temporally very stiff
  - No kinetic (particle) effects
- Extended fluid models (*fluid; non-conventional closures*)
  - Separate fluids for ions and electrons
  - Non-fluid effects through low dimensional or analytic “closures”
- Transport models (*long time scale; low dimensionality; no inertia*)
  - “1.5” dimensional, axisymmetric geometry
  - Time dependent, long time evolution
  - No waves: force balance + diffusion with sources

Disparate models must be “integrated” for predictive capability

A CONSTRAINT ON ALGORITHMS

Balance of algorithm performance and model requirements with available cycles

$$\frac{N^a Q}{\underbrace{\Delta t}_{\text{Algorithms}}} = 3\times10^7 \frac{eP}{\underbrace{CT}_{\text{Constraints}}}$$

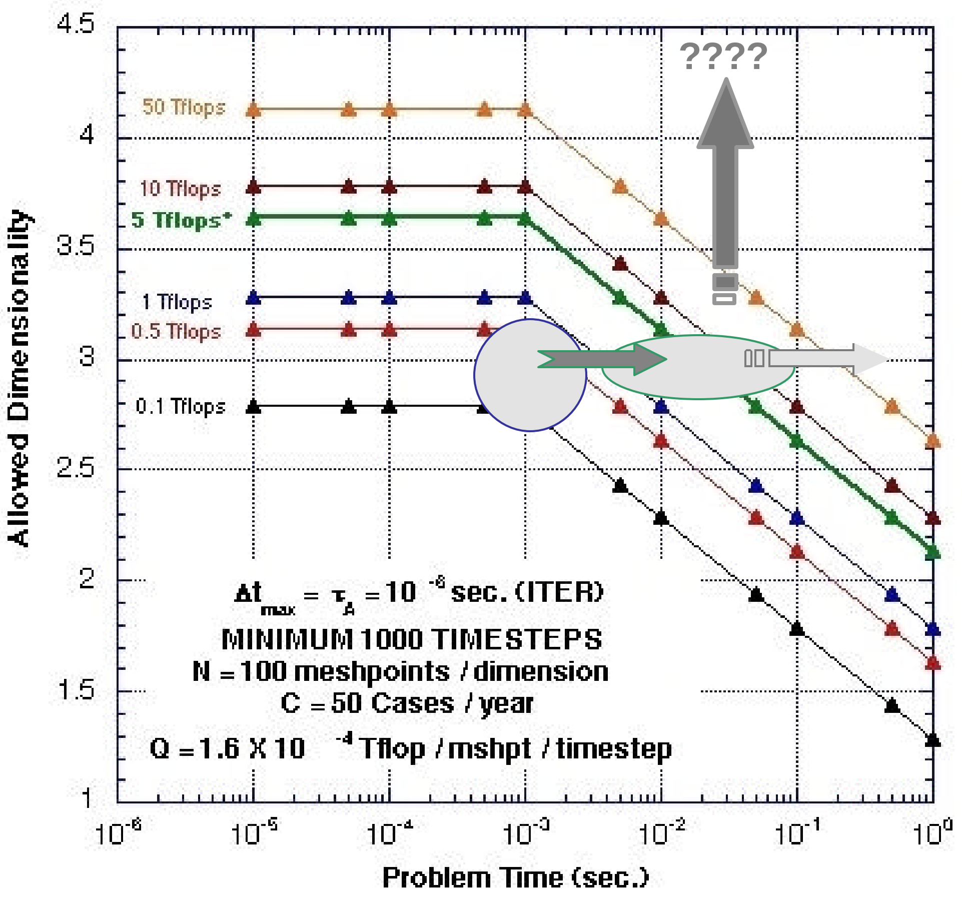
***Algorithms*:**

- ***N* - # of meshpoints for each dimension**
- ***a* - # of dimensions**
  - **1.5 - transport**
  - **3 (spatial) fluid**
  - **5-6 kinetic (spatial + velocity)**
- ***Q* - code-algorithm requirements (Tflop / meshpoint / timestep)**
- **D*t* - time step (seconds)**

***Constraints*:**

- ***P* - peak hardware performance (Tflop/sec)**
- ***e* - hardware efficiency**
  - ***eP* - delivered sustained performance**
- ***T* - problem time duration (seconds)**
- ***C* - # of cases / year**
  - **1 case / week ==> C ~ 50**

PERFORMANCE CONSTRAINTS



Assumptions:

- **Performance is *delivered***
- **Implicit algorithm**
- **Q ind. of Δt (!!)**

Requirements:

- **At least 3-D physics required**
- **Required problem time: 1 msec - 1 sec**

Conclusions:

- **3-D (i.e., fluid) calculations for times of ~ 10 msec within reach**
- **Longer times require next generation computers (or better algorithms)**
- **Higher dimensional (kinetic) long time calculations unrealistic**
- **Integrated kinetic effects must come through low dimensionality fluid closures**

3-D extended fluid calculation must form basis of integrated model

A 3-D FLUID BASED MODEL FOR INTEGRATION

- *Cannot afford higher dimensionality for experimental time scales!*
- Capture kinetic effects through 2-fluid closures
  - Analytic
  - Heuristic
  - Minority species (e.g., energetic ions)
- Can represent vacuums, realistic geometry and boundary conditions
- Produces data necessary for other integration components
  - *Edge models*
    - Details of specialized plasma regions
  - *Kinetic theory models*
    - First principles tests of closures and sub-grid scale physics
  - *Source models*
    - Details of heating and fueling
  - *Transport models*
    - Longer time scale evolution
  - *Engineering models*
    - Stresses on components, etc.

CLOSURES FOR FLUID MODELS

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

$$\frac{df_a}{dt} = \sum_b C\left[f_a, f_b\right]$$

$f_a(\mathbf{x},\mathbf{v},t)$ **- 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*, P, q, …….**
- **Equations truncated by closure relations**
  - **Express high order moments in terms of low order moments**
  - **Capture *kinetic effects* in these moments**

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*):**

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

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

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

- **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):**

$$\mathbf{E}=-\underbrace{\mathbf{v}\times\mathbf{B}}_{\textit{Ideal MHD}}+\underbrace{\eta\mathbf{J}}_{\textit{Resistive MHD}}+\underbrace{\frac{1}{ne}\frac{1-\nu}{1+\nu}\mathbf{J}\times\mathbf{B}}_{\textit{Hall Effect}}$$
$$-\underbrace{\frac{1}{ne(1+\nu)}\nabla\cdot\left(\mathbf{P}_e'-\nu\mathbf{P}_i'\right)}_{\substack{\textit{Diamagnetic Effects}\\ \textit{and Closures}}}+\underbrace{\frac{1}{\varepsilon_0\omega_{pe}^2(1+\nu)}\left[\frac{\partial\mathbf{J}}{\partial t}+\nabla\cdot(\mathbf{vJ}+\mathbf{Jv})\right]}_{\textit{Electron Inertia}}$$

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 adaptation
- *Extreme anisotropy*
  - Special direction determined by magnetic field

    Accurate treatment of $\mathbf{B} \cdot \nabla$ *operator is important*
  - Requires specialized gridding

At least as challenging as hydrodynamic turbulence!

1. SEPARATION OF TIME SCALES

$$\underbrace{t_A}_{Affv\acute{e}n\ \ transit\ \ time} \quad < \quad \underbrace{t_S}_{Sound\ \ transit\ \ time} \quad \ll \quad \underbrace{t_{evol}}_{MHD\ \ evolution\ \ time} \quad \ll \quad \underbrace{t_R}_{Resistive\ \ diffusion\ \ time}$$

Lundquist number: $S = \frac{t_R}{t_A} \sim 10^8 \gg 1$

Explicit time step impractical:

$$\Delta t < \frac{\Delta x}{L} t_A \approx \frac{t_A}{N} <<<< t_{evol}$$

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**

EXAMPLE: IDEAL MHD

$$\rho_0 \frac{\partial^2 \mathbf{v}}{\partial t^2} = \nabla \times \nabla \times (\mathbf{v} \times \mathbf{B}_0) \times \mathbf{B}_0$$

- **Linearized, ideal MHD wave equation**
- **Wide spectrum of normal modes**
- **Highly anisotropic spatial operator**
- **Basis of many implicit formulations**
- ***Not* a simple Laplacian**
- **Requires specialized pre-conditioners**

Challenge: find optimum algorithm for inverting this operator

with CFL ~ 1000

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

2. 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

3. 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**

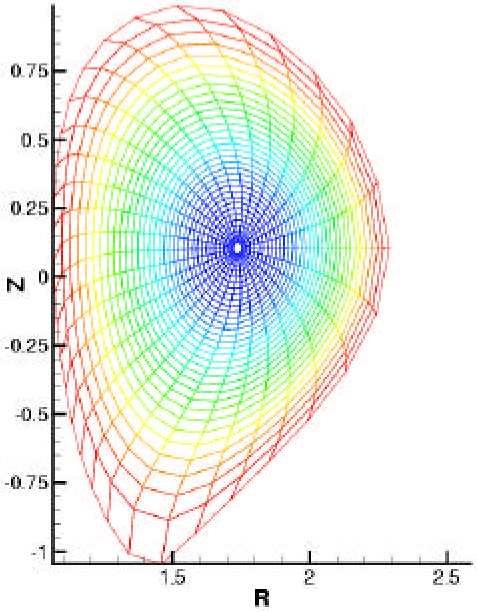
==> Requires accurate treatment of operator $\mathbf{B} \cdot \nabla$

Inaccuracies lead to “spectral pollution” and anomalous perpendicular transport

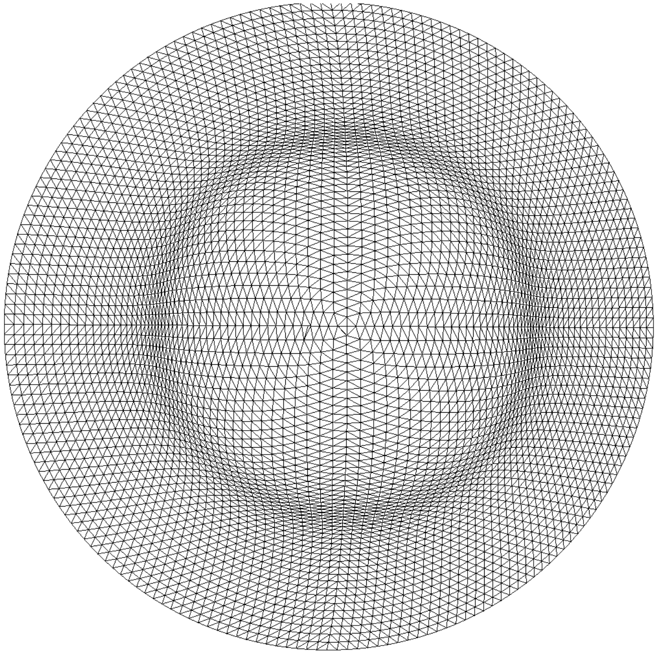
GRIDDING AND SPATIAL REPRESENTATION

- **Spatial stiffness and anisotropy require special gridding**
  - **Toroidal and poloidal dimensions treated differently**
- **Toroidal (f, 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 adaptation 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

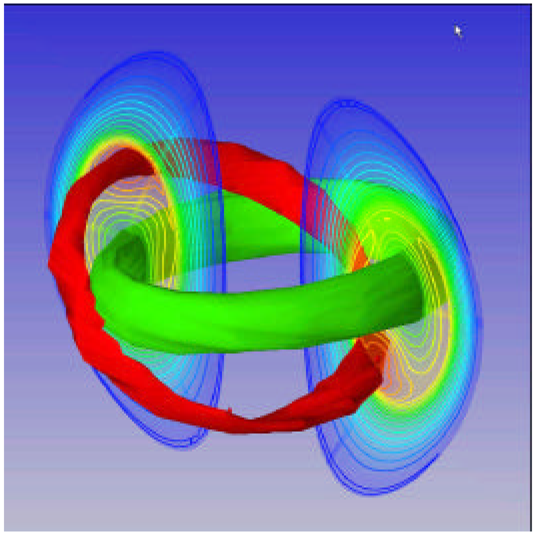
- **2-fluid effects**
  - **Whistler waves (Hall term) require implicit advance with non-symmetric solver**
  - **Electron inertia treated implicitly**
  - **Diamagnetic rotation may cause accuracy, stability problems**
- **Kinetic effects - influence of non-Maxwellian populations**
  - **Analytic closures**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

STATUS

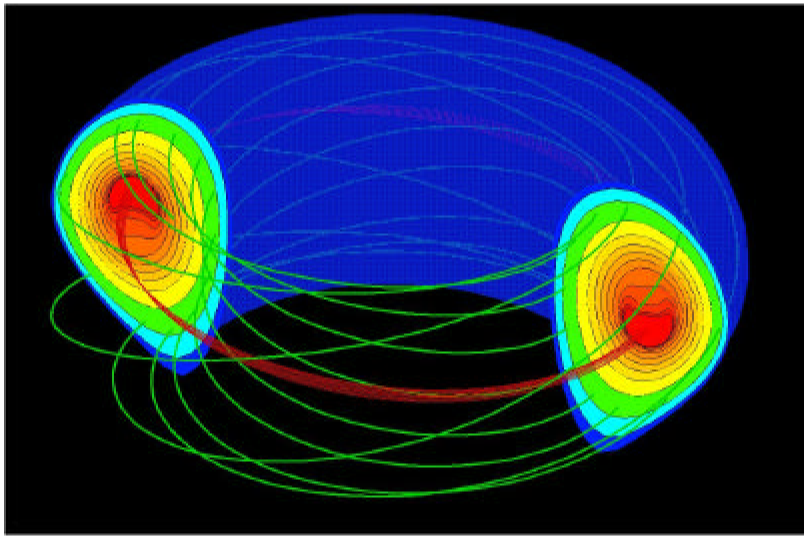
- 2 major SciDAC development projects for time-dependent models
  - M3D - multi-level, 3-D, parallel plasma simulation code
    - Partially implicit
    - Toroidal geometry - suitable for stellarators
    - 2-fluid model
    - Neo-classical and particle closures
  - NIMROD - 3-D nonlinear extended MHD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

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

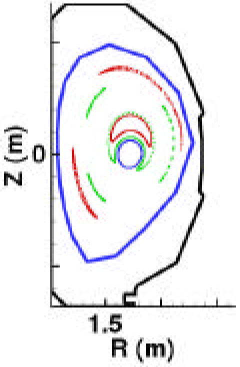
STATUS - RESISTIVE MHD



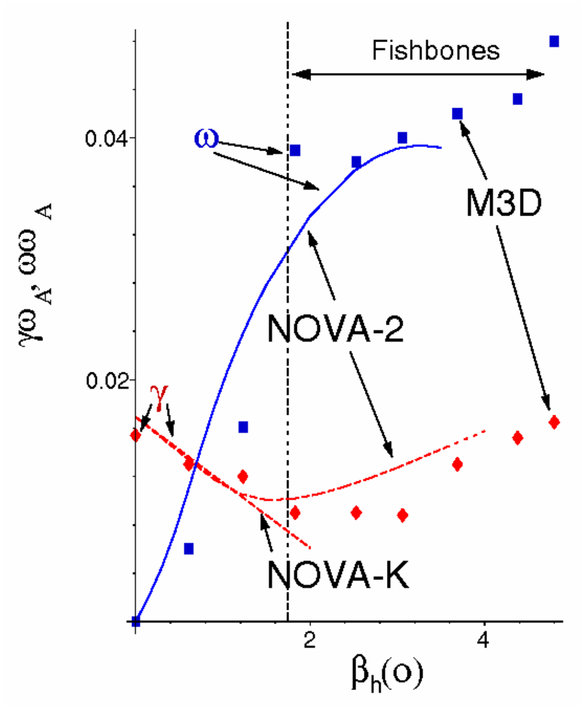
Sawtooth in NSTX computed by M3D

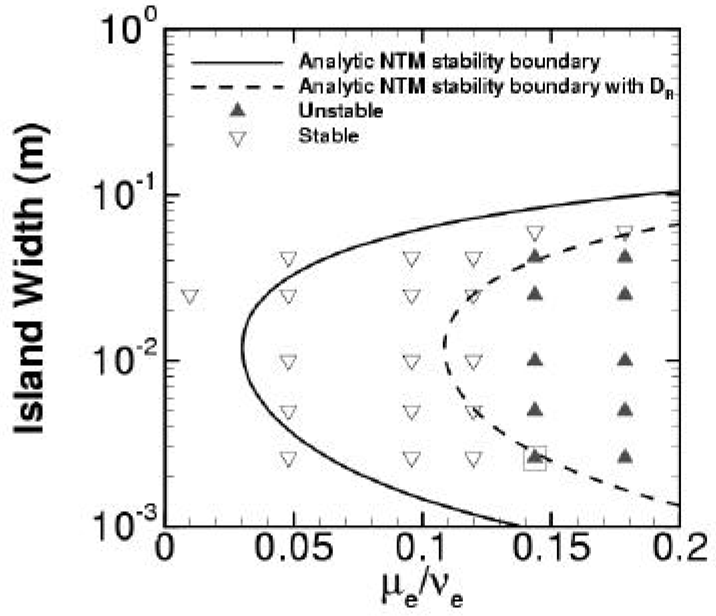


Secondary magnetic islands generated during sawtooth crash in DIII-D shot 86144 by NIMROD



STATUS - EXTENDED MHD





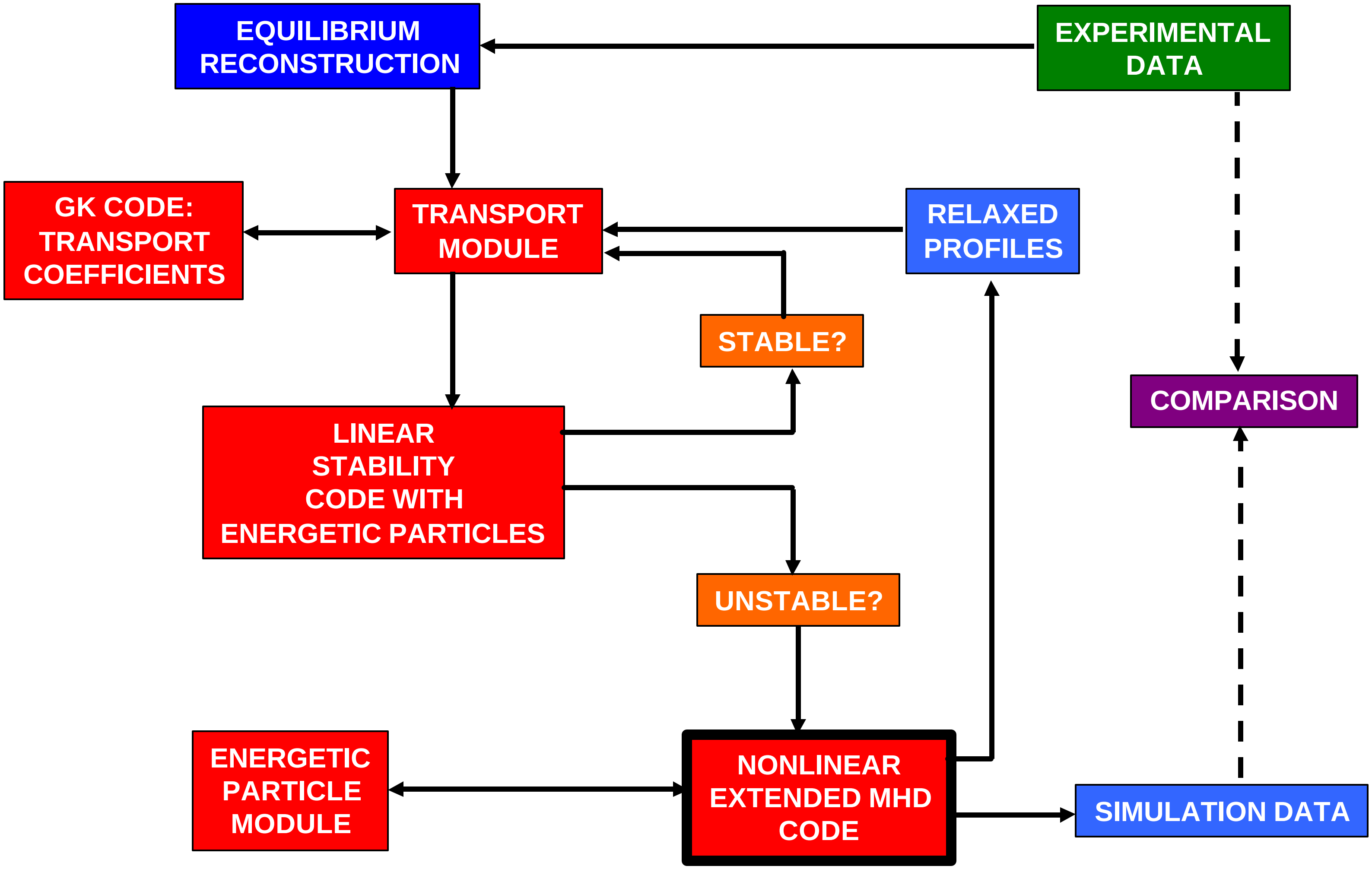
- Effect of energetic particles on MHD instability
- Subcycling of kinetic calculation

- Effect of trapped electrons and ions on resistive stability
- Analytic/heuristic fluid closure

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: SAWTOOTH CYCLE



EQUILIBRIUM RECONSTRUCTION

EXPERIMENTAL DATA

GK CODE: TRANSPORT COEFFICIENTS

TRANSPORT MODULE

RELAXED PROFILES

STABLE?

COMPARISON

LINEAR STABILITY CODE WITH ENERGETIC PARTICLES

UNSTABLE?

ENERGETIC PARTICLE MODULE

NONLINEAR EXTENDED MHD CODE

SIMULATION DATA

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**
- ***Extended MHD is the only practical central element for integrated modeling***
  - **Only model that can address realistic geometry and time scales with foreseeable resources**
- ***Progress is being made in Extended MHD***
  - **Integration of energetic ion modules into 3-D MHD**
  - **Computationally tractable closures**

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