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Progress on the development of a scalable fully-implicit stabilized unstructured FE capability for resistive MHD.

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Outline

- **Motivation: MHD Systems and Multiple-time-scale Multi-physics Nonlinear Systems**
- **Brief Outline of Stabilized FE Formulation for Resistive MHD**
- **Some Representative Verification Results**
- **Why Newton-Krylov Methods?**
    - **Fully-implicit and Steady-state Solution Methods**
    - **Characterization of Complex Solution Spaces: Hydromagnetic Rayleigh-Bernard**
    - **PDE Constrained Optimization**
- **Representative Solution Algorithm Performance**
    - **Additive Schwarz DD and Algebraic Multi-level Preconditioners**
- **Conclusions**

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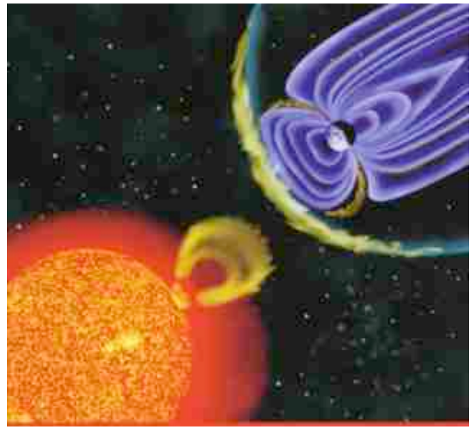
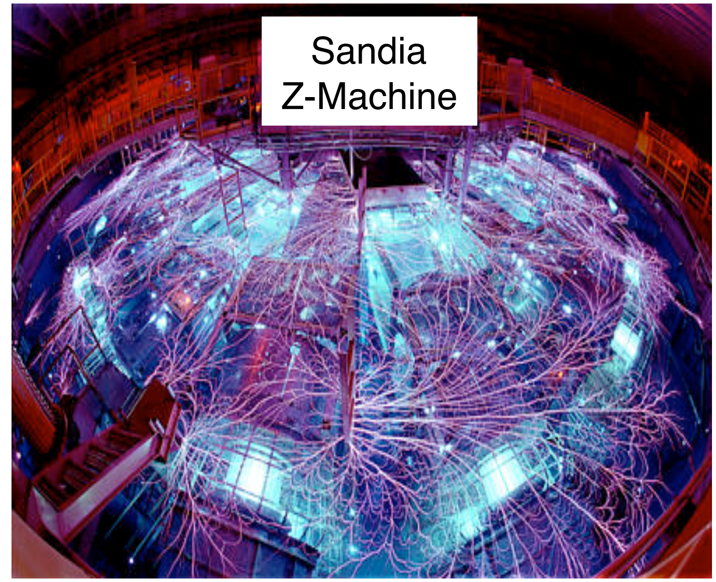
Scientific Motivation

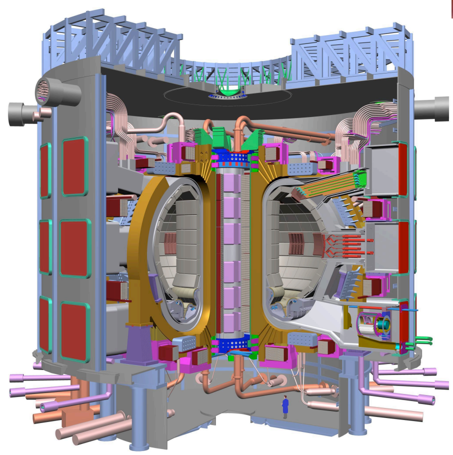
- **Resistive and extended MHD models a variety of important plasma physics**
  - Astrophysics: Solar flares, sunspots, reconnection
  - Geophysics: Earth's magnetospheric sub-storms, geo-dynamo
  - Fusion: Magnetic confinement (ITER - Tokamak), Inertial conf. (NIF, Z-pinch)
  - Technology/Engineering: Plasma Reactors, MHD Pumps, ..
  - …

<u>Mathematical / Computational Motivation:</u> Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multi-physics PDE Systems



Magnetosphere
Credit: Steele Hill/NASA





ITER

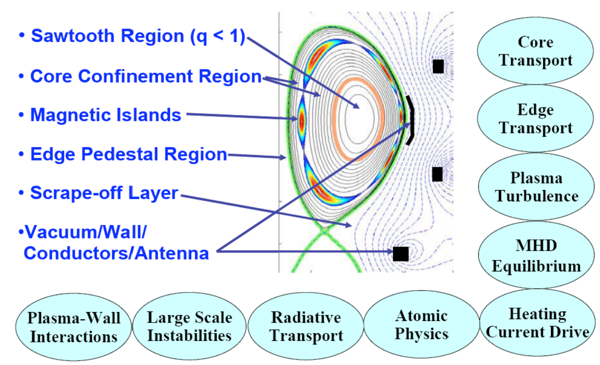


Fig. 2: Illustration of the interacting physical processes within a tokamak discharge.

FSP Report

<u>Mathematical / Computational Motivation:</u> Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multi-physics PDE Systems

What are multi-physics systems? (A multiple-time-scale perspective)

These systems are characterized by a myriad of complex, interacting, nonlinear multiple time- and length-scale physical mechanisms.

These mechanisms can balance to produce:

- **steady-state behavior,**
- **nearly balance to evolve a solution on a dynamical time scale that is long relative to the component time scales,**
- **or can be dominated by one, or a few processes, that drive a short dynamical time scale consistent with these dominating modes.**

e.g. Nuclear Fusion / Fission Reactors; Astrophysics; Conventional /Alternate Energy Systems

Our approach - pursue new applied math/algorithms to develop robust, accurate, scalable, and efficient implicit formulations and fully-coupled Newton-Krylov methods with integrated optimization/UQ tools for predictive simulation technologies for complex coupled multi-physics systems.

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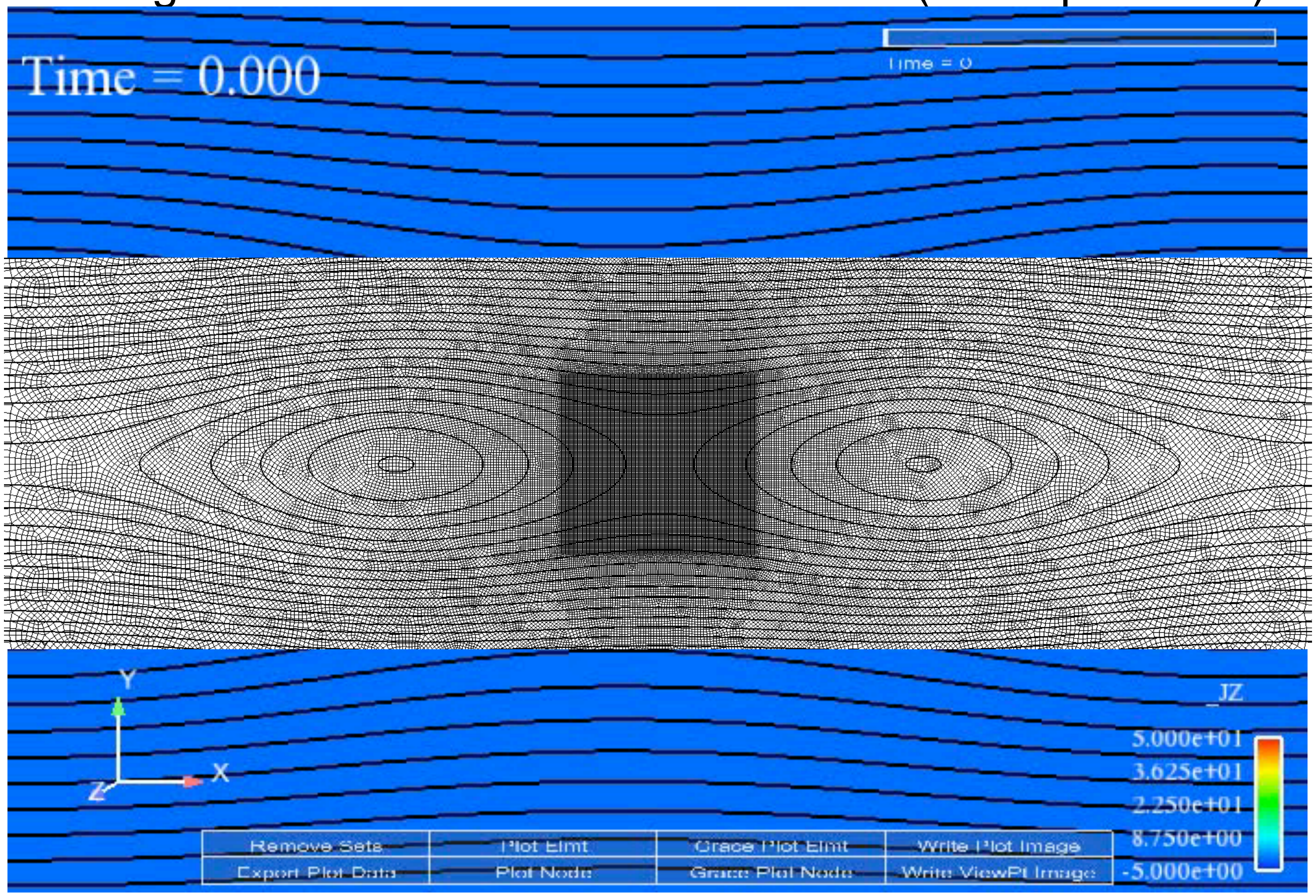
Multiple-time-scale systems: E.g. Driven Magnetic Reconnection with a Magnetic Island Coalescence Problem (Incompressible)

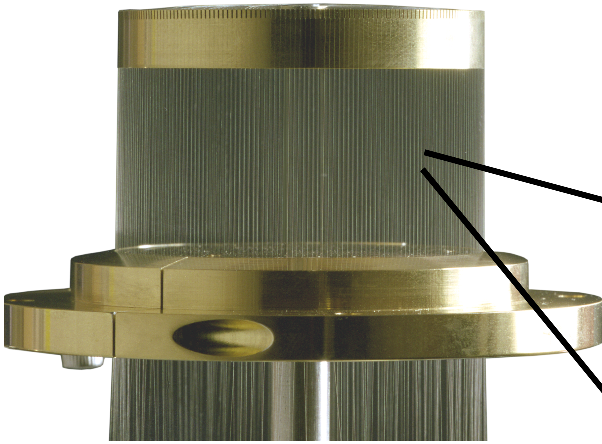


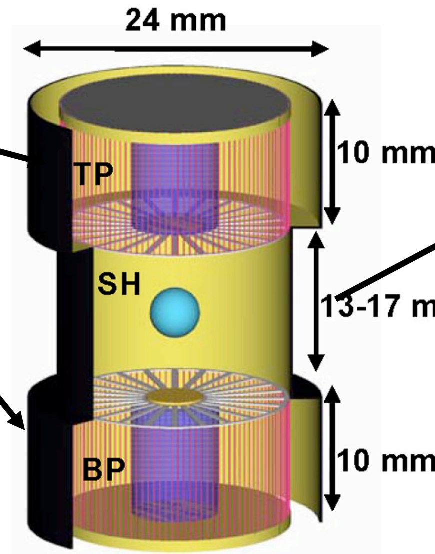
<u>Approx. Computational Time Scales:</u>

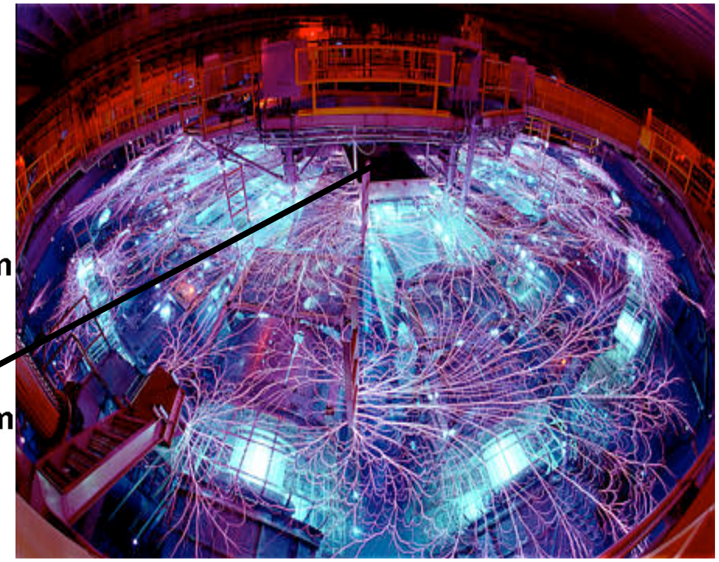
- **Ion Momentum Diffusion: 10^{-7} to 10^{-3}**
- **Magnetic Flux Diffusion: 10^{-7} to 10^{-3}**

- **Ion Momentum Advection: 10^{-4} to 10^{-2}**
- **Alfven Wave** $\left(\tau_A = \frac{h\sqrt{\rho\mu_0}}{B_O}\right)$ **: 10^{-4} to 10^{-2}**
- **Whistler Wave** $\left(\tau_w = \frac{h^2}{V_A d_i}\right)$ **: 10^{-7} to 10^{-1}**
- **Magnetic Island Sloshing: 10^0**
- **Magnetic Island Merging: 10^1**

Z-pinch Double Hohlraum Schematic







<u>Z Machine (Approximate Ranges)</u>

100ns current rise time for 20 MA Electrical Current

250 ns plasma shell collapse and stagnation

10-30 ns X-ray power pulse ~280 TW power

<u>Computational Stability Constraints:</u>

Hyperbolic Operators: $\Delta t < \Delta x/2c$
- **Alfven waves**
- **Magneto-sonic waves**
- **Material transport**
- **Radiation transport**

Parabolic Operators: $\Delta t < \Delta x^2/D$
- **Magnetic Diffusion**
- **Heat Conduction**

Hall Physics: Whistler waves
-> $\Delta t < \Delta x^2/(V_A d_i)$

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Extended MHD Equations

Extended MHD Model in Residual Form

$$\mathbf{R_m} = \frac{\partial(\rho\mathbf{v})}{\partial t} + \nabla \cdot [\rho\mathbf{v}\otimes\mathbf{v} - \mathbf{T}] - \mathbf{J}\times\mathbf{B} = \mathbf{0}\ ; \quad \mathbf{T} = -\left(P + \frac{2}{3}\mu(\nabla\bullet\mathbf{u})\right)\mathbf{I} + \mu[\nabla\mathbf{u} + \nabla\mathbf{u}^T]$$

$$R_p = \frac{\partial(\rho)}{\partial t} + \nabla\cdot[\rho\mathbf{v}] = 0$$

$$R_e = \frac{\partial(\rho e)}{\partial t} + \nabla\cdot[\rho\mathbf{v}e + \mathbf{q}] - \mathbf{T} : \nabla\mathbf{v} - \eta\|\mathbf{J}\|^2 + Q^{rad} + Q = 0$$

$$\mathbf{R_B} = \frac{\partial\mathbf{B}}{\partial t} + \nabla\times\mathbf{E} = 0 \quad \mathbf{J} = \frac{1}{\mu_0}\nabla\times\mathbf{B} \quad \mathbf{E} = -\mathbf{v}\times\mathbf{B} + \eta\mathbf{J} + \underbrace{\frac{1}{en}(\mathbf{J}\times\mathbf{B} - \nabla\mathbf{P_e})}_{\text{Hall}}$$

Involution: $\nabla\cdot\mathbf{B} = \mathbf{0}$

Divergence Conservation Form

$$\frac{\partial\mathbf{U}}{\partial t} + \nabla\bullet\mathbf{F} + \mathbf{S} = \mathbf{0}$$

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho\mathbf{v} \\ \Sigma_{tot} \\ \mathbf{B} \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} \rho\mathbf{v} \\ \rho\mathbf{v}\otimes\mathbf{v} - \frac{1}{\mu_0}\mathbf{B}\otimes\mathbf{B} - \mathbf{T} + \frac{1}{2\mu_0}\|\mathbf{B}\|^2\mathbf{I} \\ \rho E\mathbf{v} - \mathbf{T}\cdot\mathbf{v} + \mathbf{E}\times\mathbf{B} + \mathbf{q} \\ \mathbf{v}\otimes\mathbf{B} - \mathbf{B}\otimes\mathbf{v} - \frac{\eta}{\mu_0}\left(\nabla\mathbf{B} - \nabla\mathbf{B}^T\right) \end{bmatrix} \quad \mathbf{S} = \begin{bmatrix} 0 \\ \mathbf{0} \\ Q^{rad} + Q \\ \mathbf{0} \end{bmatrix}$$

$$\Sigma_{tot} = \rho E + \frac{1}{2\mu_0}\|\mathbf{B}\|^2 \qquad E = e + \frac{1}{2}\|\mathbf{v}\|^2$$

Involution: $\nabla\cdot\mathbf{B} = \mathbf{0}$

General Case a Strongly Coupled, Multiple Time- and Length-Scale, Nonlinear, Nonsymmetric System with Parabolic and Hyperbolic Character

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Magnetic Vector Potential Formulation (2D)

$$\mathrm{B} = \nabla \times \mathbf{A} \rightarrow \nabla \cdot \mathrm{B} = \nabla \cdot \nabla \times \mathbf{A}$$

Solenoidal involution is automatically satisfied provided that the discrete differential operator enforces $\nabla \cdot \nabla \times \mathbf{A} = 0$ to machine accuracy.

$$\mathbf{E} = -\nabla\Phi - \frac{\partial \mathbf{A}}{\partial t} \longrightarrow \frac{\partial \mathbf{A}}{\partial t} - \mathbf{v} \times (\nabla \times \mathbf{A}) + \frac{\eta}{\mu_0} \nabla \times \nabla \times \mathbf{A} = -\nabla\Phi.$$

Select a Coulomb-type Gauge and in 2D

$$\Phi + \frac{\eta}{\mu_0} \nabla \cdot \mathbf{A} = 0 \longrightarrow \frac{\partial A_z}{\partial t} + \mathbf{v} \cdot \nabla A_z - \frac{\eta}{\mu_0} \nabla^2 A_z = 0$$

Remarks:

- Convection/Diffusion/Reaction equation → can use SUPG Stabilization.
- On interior of Elements Div B = 0; Only weakly divergence free however

Summary of Initial Stabilized FE Weak form of Equations
for Low Mach Number MHD System;

Governing Equation	**Stabilized FE Residual** (following Hughes et. al., Shakib - Navier-Stokes; Salah et. al. 99 & 01, Codina et. al. 2006 -Magnetics)
Momentum	$F_{m,i} = \int_{\Omega} \Phi R_{m,i} d\Omega + \sum_e \int_{\Omega^e} \rho \tau_m (\mathbf{u} \bullet \nabla \Phi) R_{m,i} d\Omega + \sum_e \int_{\Omega^e} \nu_{m,i} \nabla \Phi \bullet \mathbf{G}^c \nabla u_i d\Omega$
Total Mass	$F_P = \int_{\Omega} \Phi R_P d\Omega + \sum_e \int_{\Omega^e} \rho \tau_m \nabla \Phi \bullet \mathbf{R_m} d\Omega$ $\sum_e \int_{\Omega^e} \rho \tau_m \nabla \Phi \cdot \left[\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v}] + \nabla P - \nabla \cdot \Pi - \mathbf{J} \times \mathbf{B} \right] d\Omega$
Thermal Energy	$F_T = \int_{\Omega} \Phi R_T d\Omega + \sum_e \int_{\Omega^e} \rho \hat{C}_P \tau_T (\mathbf{u} \bullet \nabla \Phi) R_T d\Omega + \sum_e \int_{\Omega^e} \nu_T \nabla \Phi \bullet \mathbf{G}^c \nabla T d\Omega$
Magnetics (Vector Potential)	$F_{A_z} = \int_{\Omega} \Phi R_{A_z} d\Omega + \sum_e \int_{\Omega^e} \rho \tau_{A_z} (\mathbf{u} \bullet \nabla \Phi) R_{A_z} d\Omega + \sum_e \int_{\Omega^e} \nu_{A_z} \nabla \Phi \bullet \mathbf{G}^c \nabla A_z d\Omega$

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Summary of Structure of Linear Systems Generated in Newton's Method

Galerkin FE (Mixed interpolation FEM):

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{v}} \\ \dot{\mathbf{P}} \end{bmatrix} + \begin{bmatrix} \mathbf{A} & -\mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \mathbf{P} \end{bmatrix} \qquad \mathbf{v} = (\mathbf{u}, T, A_z)$$

Stabilized FE (Hughes et. al)
Q1/Q1 V-P elements, SUPG like terms and
Discontinuity Capturing type operators

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{N} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{v}} \\ \dot{\mathbf{P}} \end{bmatrix} + \begin{bmatrix} \mathbf{A} & -\mathbf{B}^T \\ (\mathbf{B} + \mathbf{L}) & \mathbf{K} \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \mathbf{P} \end{bmatrix}$$

$$\mathbf{K} = \sum_e \int_{\Omega^e} \rho \tau_m \nabla\Phi \bullet \nabla\Phi \, d\Omega$$

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Lagrange Multiplier Form. (Dedner et. al. 2002, Codina 2006, …)

$$\frac{\partial(\rho\mathbf{v})}{\partial t} + \nabla \cdot \left[\rho\mathbf{v} \otimes \mathbf{v} - \frac{1}{\mu_0}\mathbf{B} \otimes \mathbf{B} + \left(P + \frac{1}{2\mu_0}\|\mathbf{B}\|^2\right)\mathbf{I} - \mathbf{\Pi}\right] = \mathbf{0}$$

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

$$\frac{\partial\mathbf{B}^*}{\partial t} + \nabla \cdot \left[\mathbf{v} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{v} - \frac{\eta}{\mu_0}\left(\nabla\mathbf{B}^* - (\nabla\mathbf{B}^*)^T\right)\right] = \quad - \nabla\psi \quad = \mathbf{0}$$

$$\nabla \cdot \mathbf{B} = \mathbf{0}$$

Remarks:

- Only weakly divergence free in FE implementation
- VMS formulation for convection & coupling effects under development
- Elliptic constraint used to enforce divergence free condition.
- Can show relationship with a projection method (e.g. Brackbill and Barnes 1980) when a 1st order-split integration is used

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Lagrange Multiplier Form. (contd.)

Stabilization to circumvent inf-sup (LBB) condition(s):

$$F_p = \int_\Omega \Phi R_P d\Omega + G(\mathbf{v}, \mathbf{B}, p; \Phi)$$

Consistent residual-based stabilization: Hughes et. al.

$$\sum_e \int_{\Omega^e} \rho \tau_m \nabla \Phi \cdot \left[\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v}] + \nabla P - \nabla \cdot \Pi - \mathbf{J} \times \mathbf{B} \right] d\Omega$$

Filtering type: Dohrmann-Bochev-Gunzburger

$$\int_\Omega \frac{1}{\mu} (P - \pi P)(\Phi - \Pi \Phi) d\Omega$$

$$F_\psi = \int_\Omega \Phi R_\psi d\Omega + G(\mathbf{v}, \mathbf{B}, \psi; \Phi)$$

Consistent residual-based stabilization: Hughes et. al.

$$\sum_e \int_{\Omega^e} \tau_{\mathbf{B}} \nabla \Phi \cdot \left[\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot \left[\mathbf{v} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{v} - \frac{\eta}{\mu_0} \left(\nabla \mathbf{B} - \nabla \mathbf{B}^T \right) \right] - \nabla \psi \right] d\Omega$$

Filtering type

$$\int_\Omega \frac{\mu_0}{\eta} (\psi - \pi \psi)(\Phi - \Pi \Phi) d\Omega$$

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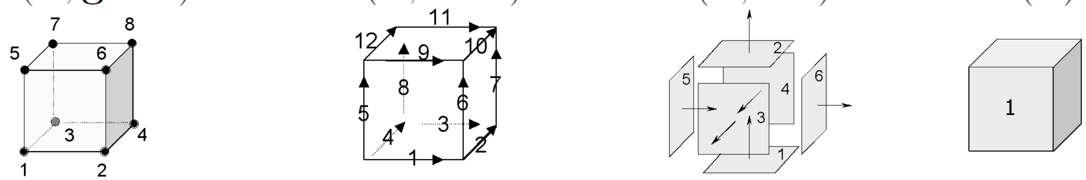
Advanced Discretizations

Intrepid: *Trilinos* **toolbox for discretizations** (**Bochev**, Ridzal, Peterson, Pawlowski).

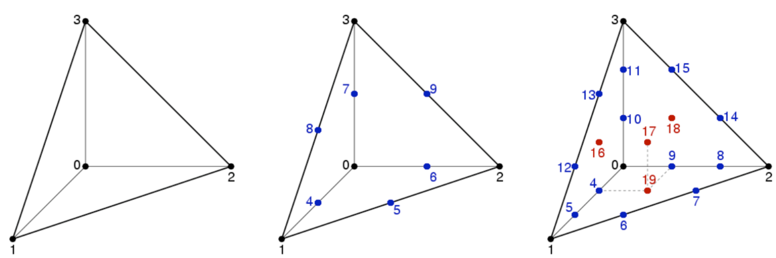
- allows access to finite element, finite volume, and finite difference methods via a common API
- compatible node-, edge-, face-, and cell-based discretizations

$$H(\Omega, \mathbf{grad}) \xrightarrow{\nabla} H(\Omega, \mathbf{curl}) \xrightarrow{\nabla\times} H(\Omega, \mathrm{div}) \xrightarrow{\nabla\cdot} L^2(\Omega)$$

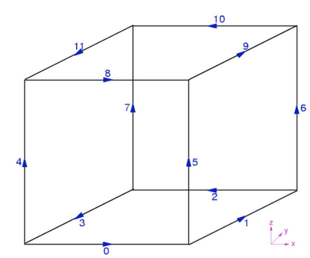


- enables hybrid discretizations (FE, FV, FD) on unstructured grids
- reference-map-based low- and high-order FE discretizations on standard cells
- “direct” low-order FV and FD discretizations on arbitrary polyhedral cells

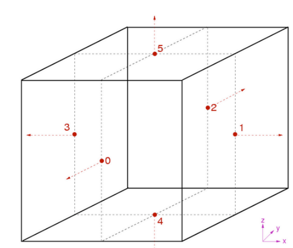
Completed development of **basic finite element** reconstruction operators (Bochev, Ridzal):



Lagrange elements of order 1,2,3



Nedelec element



Raviart-Thomas element

Stable, Accurate, Scalable, and Efficient xMHD Unstructured FE Solution Methods

Currently:

- Variable density and Low Flow-Mach-Number compressible Resistive MHD
- Initial MHD Formulations (weak divergence free):
  - 2D Vector Potential
  - 2D & 3D B field Projection and

    Lagrange Multiplier Method;
- Fully-implicit: 1^{st}-5^{th} variable order BDF (Rhythmos) & TR;
- 2D & 3D Unstructured Stabilized FE [$(\Delta x)^2$ & $(\Delta x)^3$]
- Automatic Diff. Enabled Implementation (Saccado);
- Direct-to-Steady-State (NOX); Continuation, Linear Stability and Bifurcation (LOCA / Anasazi), PDE Constrained Optimization (Moocho)
- Efficient Parallel Newton-Krylov Solution Methods
  - Additive Schwarz DD w/ Var. Overlap; (AztecOO)
  - Aggressive Coarsening Graph Based Block Multi-level [AMG] for Systems (ML);
  - Initial Physics Based Preconditioning

In Development & Implementation:

- Extended MHD
- High-resolution Hyperbolic Solver (FE-TVD/FCT)
- Physics Compatible Discretizations (e.g. Div B = 0)

  [e.g De Rham complex, Nodal, Edge, Face, volume elements (Intrepid)]

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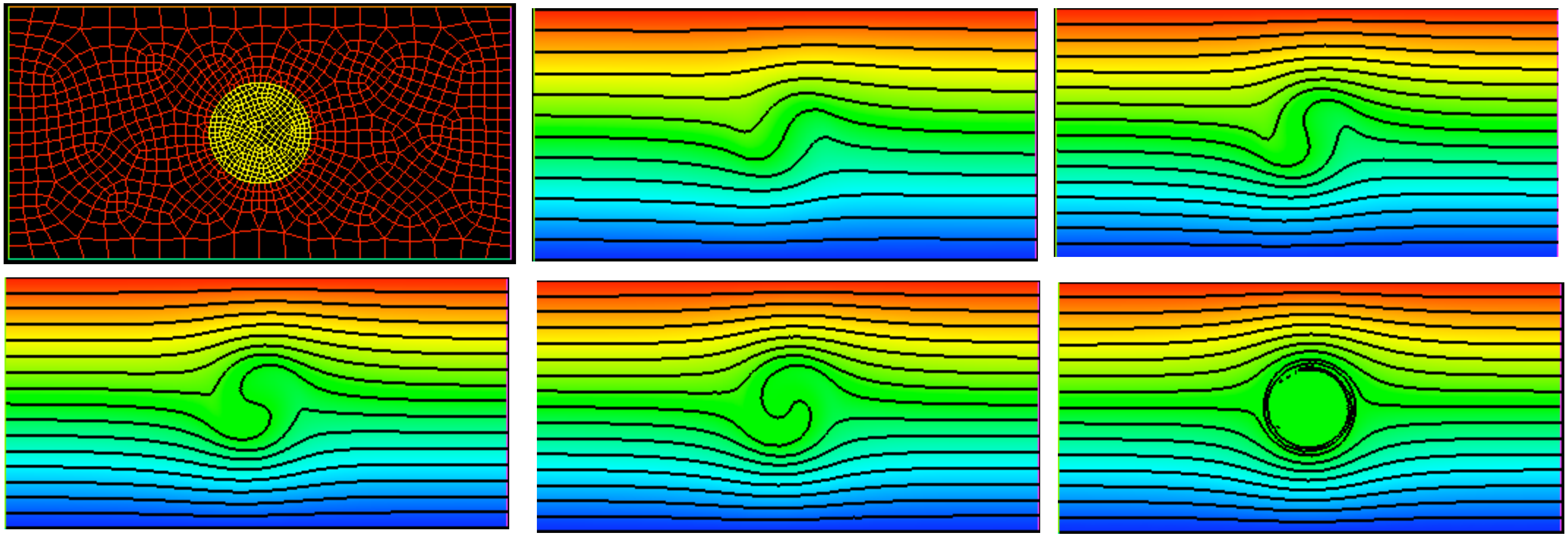
Flux Expulsion
(Unstructured Mesh)



Analytic Solution: $Az = Im[B_0 f(r) e^{ie}]$

$$f(r) = DJ_1(pr), r \leq r_0$$

$$f(r) = r + \frac{c}{r}, r < r_0$$

$$D = \frac{2}{pJ_0(pr_0)}$$

$$C = \frac{r_0[2J_1(pr_0) - pr_0 J_0(pr_0)]}{pJ_0(pr_0)}$$

$$k_0 = \frac{\sqrt{Re_m}}{r_0}$$

$$p = \frac{(1-i)k_0}{\sqrt{2}}$$

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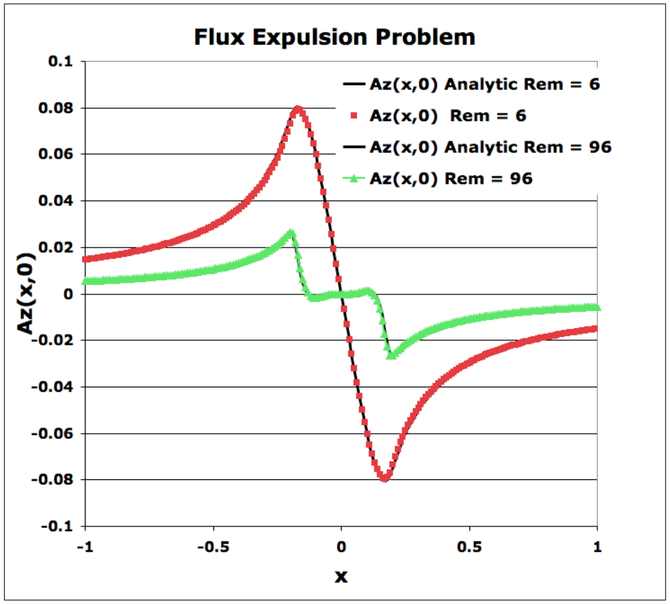
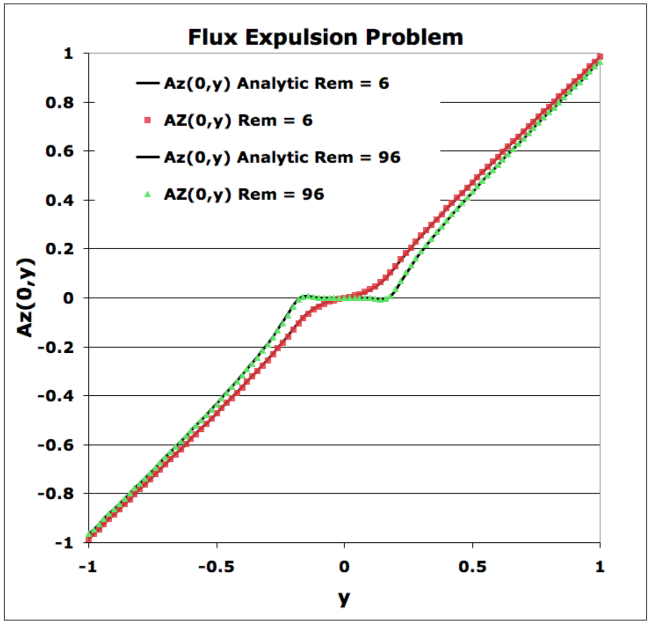
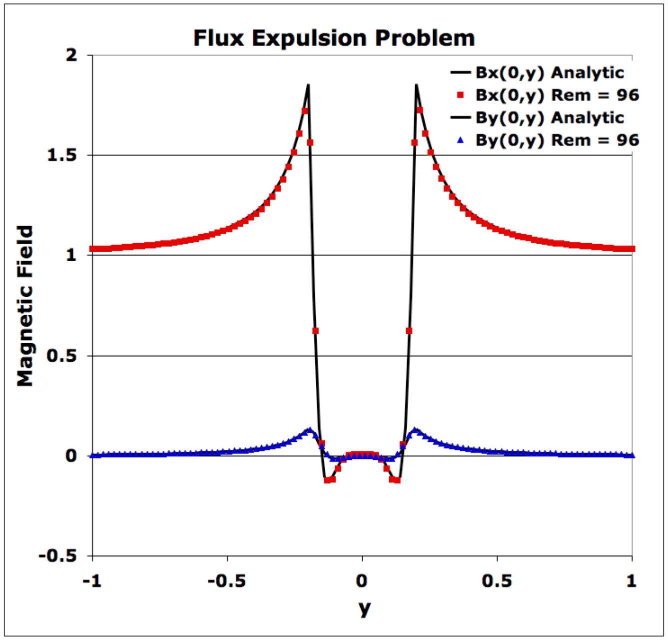
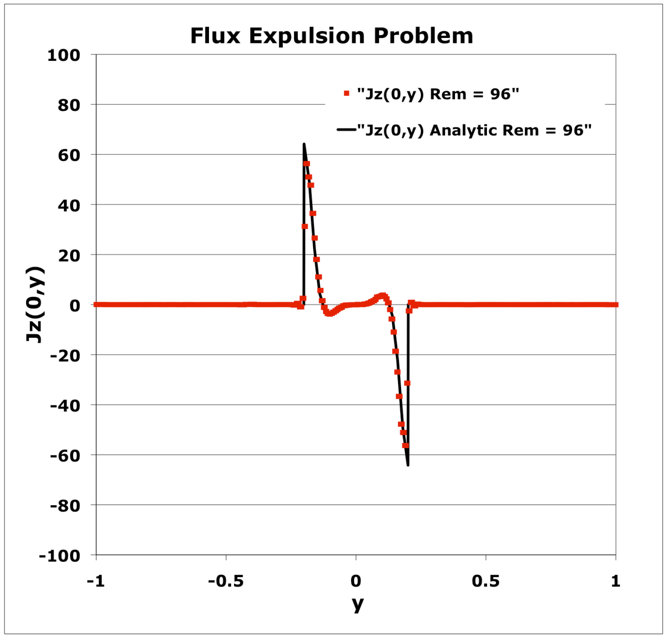
Flux Expulsion (Unstructured Mesh)









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MHD Rayleigh Flow and Alfven Wave (Transient w/ Analytic Solution)

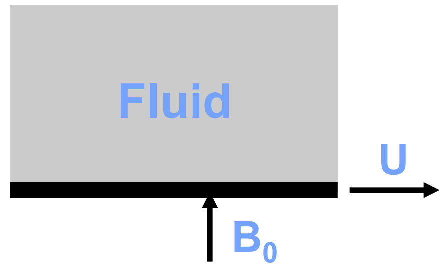
Analytic Solution:

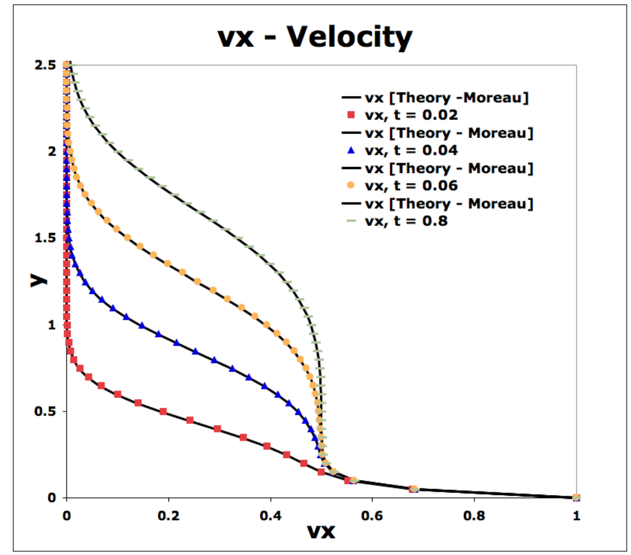
$$v_x = \frac{1}{4}U\left[e^{-\frac{A_0 y}{d}}\left(1-erf\left(\frac{y-A_0 t}{2\sqrt{dt}}\right)\right) - erf\left(\frac{y-A_0 t}{2\sqrt{dt}}\right)\right]$$
$$+\frac{1}{4}U\left[e^{\frac{A_0 y}{d}}\left(1-erf\left(\frac{A_0 t+y}{2\sqrt{dt}}\right)\right) - erf\left(\frac{A_0 t+y}{2\sqrt{dt}}\right)+2\right]$$

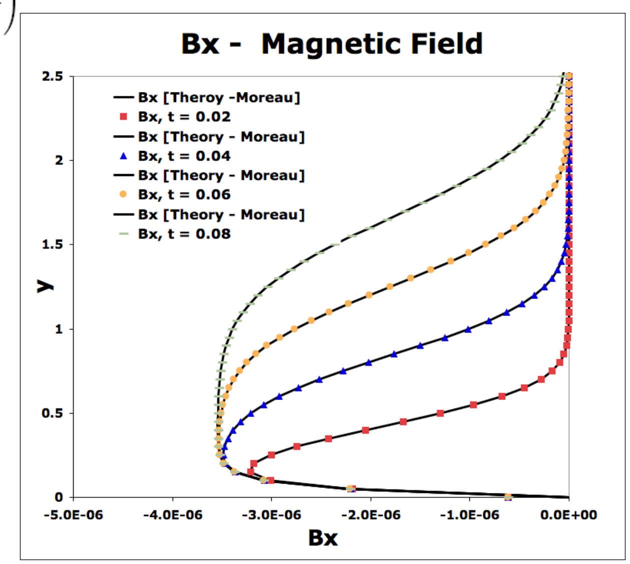
$$B_x = -\frac{1}{4}e^{-\frac{A_0 y}{d}}\left(-1+e^{\frac{A_0 y}{d}}\right)U\sqrt{\mu\rho}\left(erfc\left(\frac{y-A_0 t}{2\sqrt{dt}}\right)+e^{\frac{A_0 y}{d}}erfc\left(\frac{A_0 t+y}{2\sqrt{dt}}\right)\right)$$

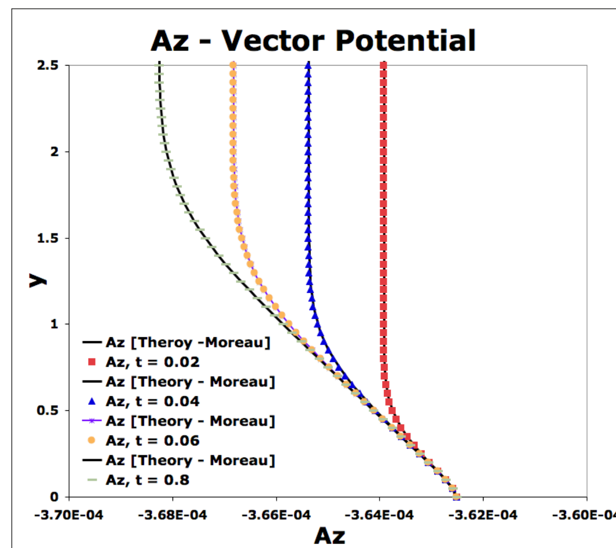
$$A_z = -B_0\, x + \frac{U\sqrt{dt}\sqrt{\mu\rho}}{2\sqrt{\pi}}\left(e^{-\frac{(y-A_0 t)^2}{4dt}} - e^{-\frac{(y+A_0 t)^2}{4dt}}\right)$$
$$+\frac{U}{4}\frac{\sqrt{\mu\rho}}{A_0}\left(d+{A_0}^2\, t\right)\left(erf\left(\frac{A_0 t-y}{2\sqrt{dt}}\right)-erf\left(\frac{A_0 t+y}{2\sqrt{dt}}\right)\right)$$
$$-\frac{U}{4}\frac{\sqrt{\mu\rho}}{A_0}e^{\frac{-A_0 y}{d}}\left(d+A_0 e^{\frac{A_0 y}{d}}y\right)erfc\left(\frac{y-A_0 t}{2\sqrt{dt}}\right)$$
$$-\frac{U}{4}\frac{\sqrt{\mu\rho}}{A_0}\left(de^{\frac{A_0 y}{d}}-A_0 y\right)erfc\left(\frac{A_0 t+y}{2\sqrt{dt}}\right)$$

$$E_z^0 = \frac{B_0\, U}{2}$$

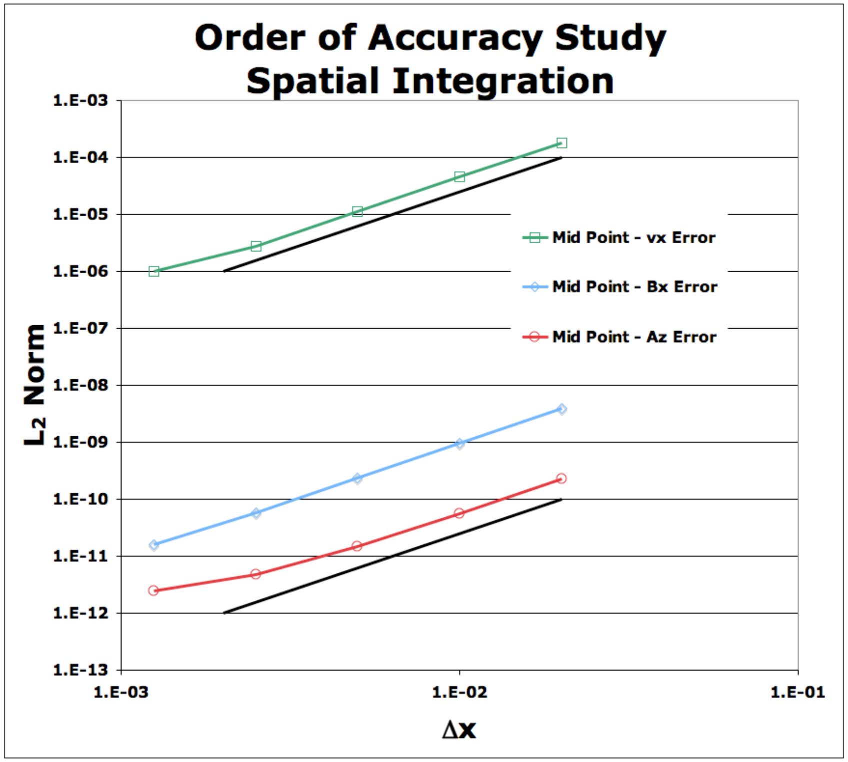


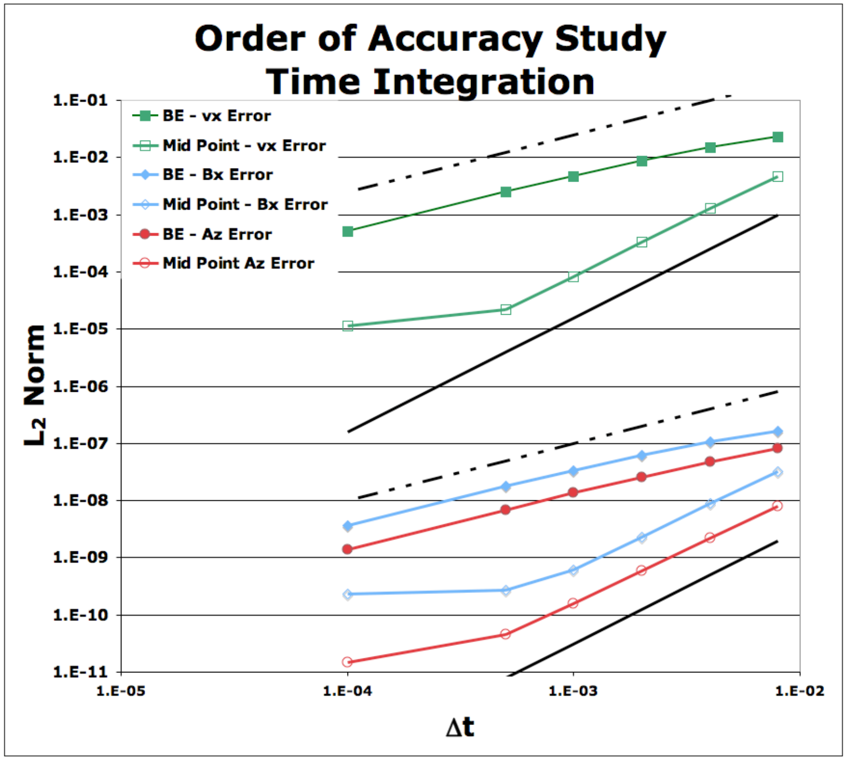






MHD Rayleigh Flow and Alfven Wave





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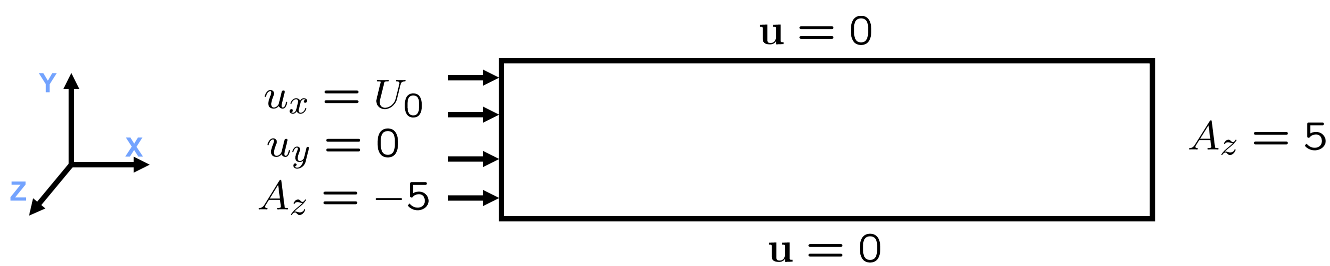
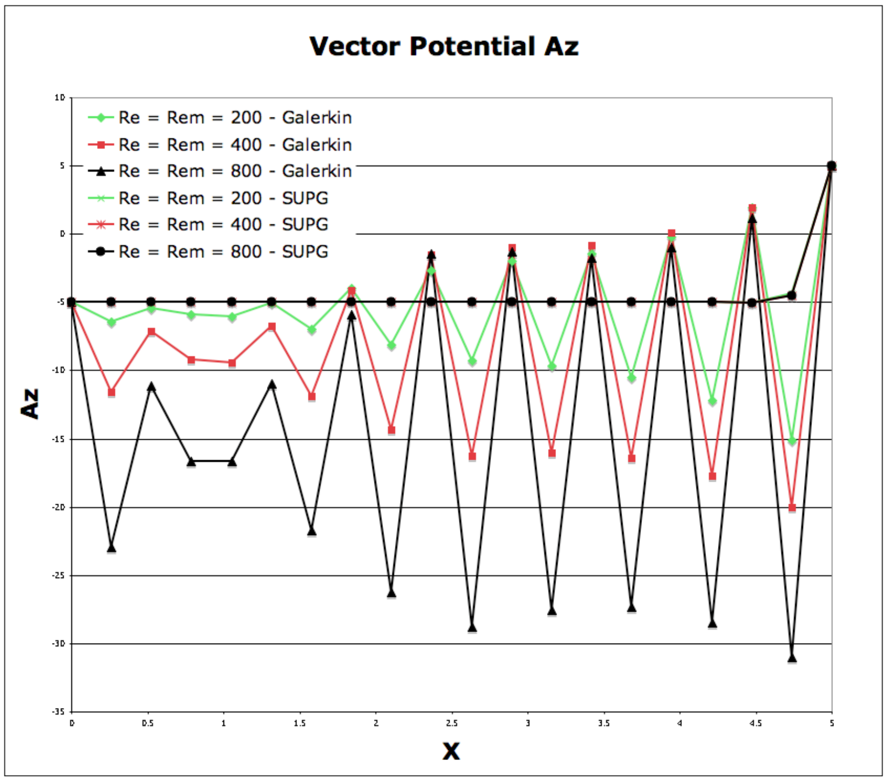
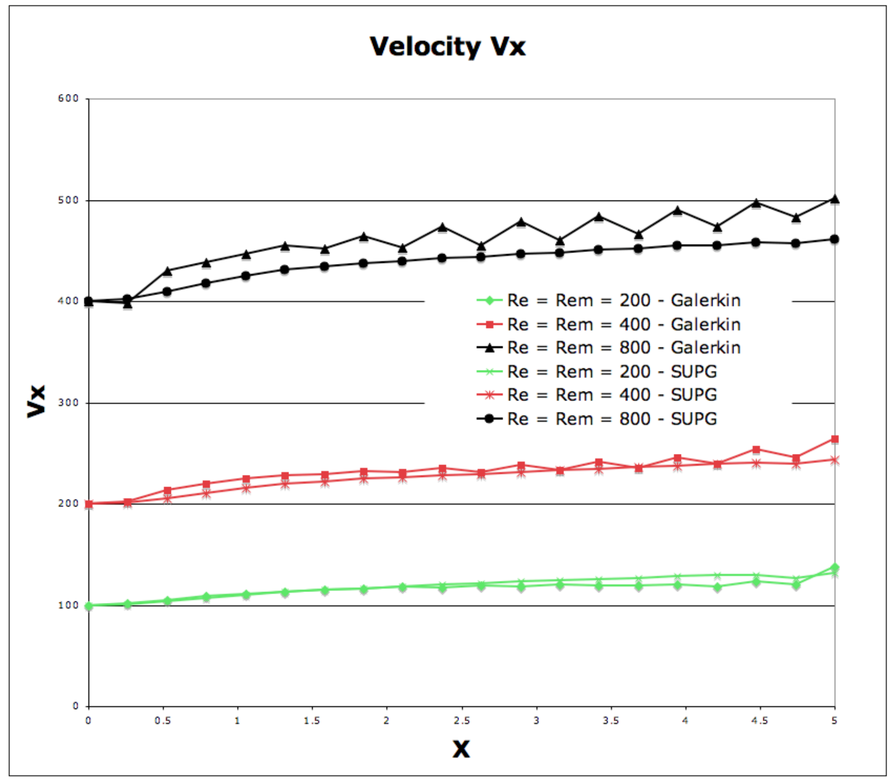
MHD Duct Flow Test for SUPG Stabilization







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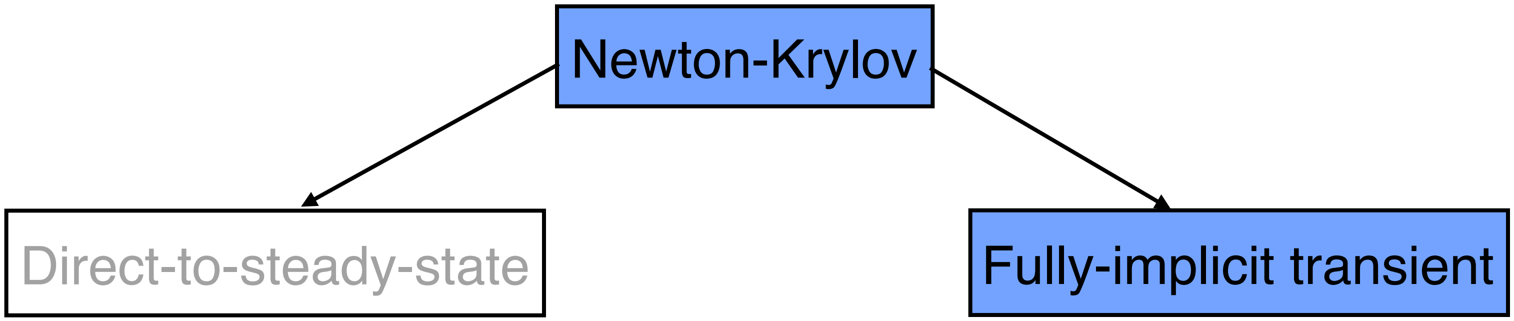
Why Newton-Krylov Methods?



$$\mathbf{F}(\dot{\mathbf{x}},\mathbf{x},\lambda_1,\lambda_2,\lambda_3,..)=\mathbf{0}$$

e.g.

$$\left.\frac{\partial c}{\partial t}\right|^{n+1} + \nabla\bullet\left(\left[\rho c\mathbf{u}\right]^{n+1}\right) - \nabla\bullet\left[D^{n+1}\nabla c^{n+1}\right] + S_c^{n+1} = 0$$

<u>Stability and Accuracy Properties</u>

- Stable (stiff systems)
- High order methods
- Variable order techniques
- Local and global error control possible
- Can be stable and accurate run at the dynamical time-scale of interest in multiple-time-scale systems (e.g. Knoll et. al., Brown & Woodward., Chacon and Knoll)

Why Newton-Krylov Methods?

Newton-Krylov

→ Direct-to-steady-state

→ Fully-implicit transient

<u>Convergence properties</u>

• Strongly coupled multi-physics often requires a strongly coupled nonlinear solver

• Quadratic convergence near solutions (backtracking, adaptive convergence criteria)

• Often only require a few iterations to converge, if close to solution, independent of problem size

$$\mathbf{F}(\mathbf{x}, \lambda_1, \lambda_2, \lambda_3, ..) = \mathbf{0}$$

<u>Inexact Newton-Krylov</u>

$$\text{Solve } \mathbf{J}\mathbf{p}_k = -\mathbf{F}(\mathbf{x}_k); \quad \text{until } \frac{\left\|\mathbf{J}\mathbf{p}_k + \mathbf{F}(\mathbf{x}_k)\right\|}{\left\|\mathbf{F}(\mathbf{x}_k)\right\|} \leq \eta_k$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \Theta \mathbf{p}_k$$

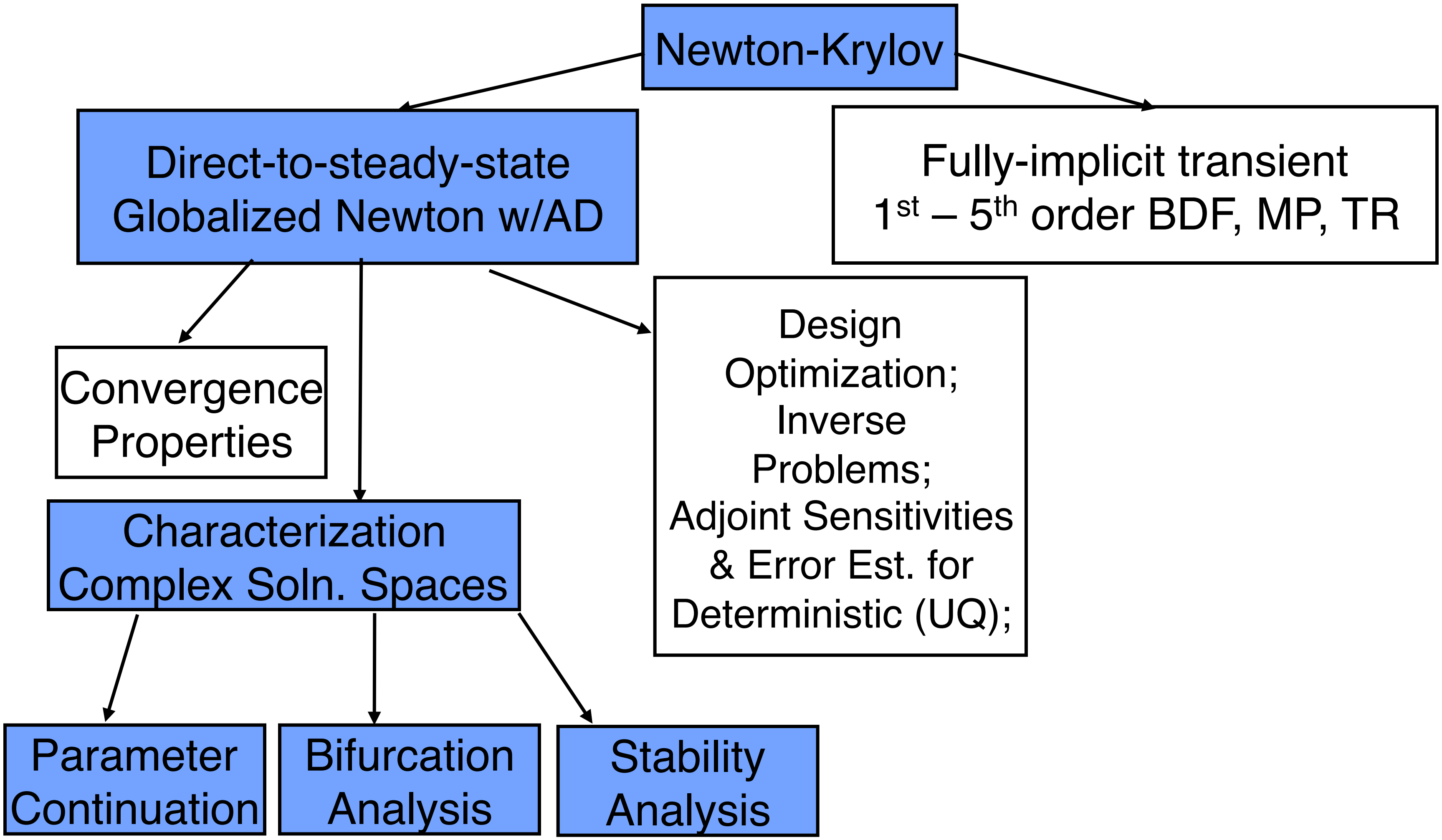
<u>Jacobian Free N-K Variant</u>

$$\mathbf{M}\mathbf{p}_k = \mathbf{v}$$

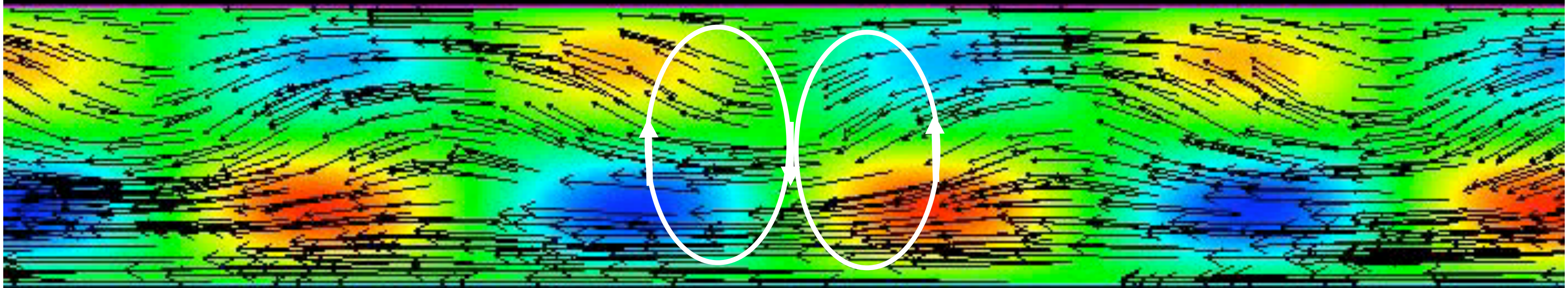
$$\mathbf{J}\mathbf{p}_k = \frac{\mathbf{F}(\mathbf{x} + \delta \mathbf{p}_k) - \mathbf{F}(\mathbf{x})}{\delta}\ ; \text{ or by AD}$$

See e.g. Knoll & Keyes, JCP 2004

Why Newton-Krylov Methods?



Vx



Stable Fields/Flow at Ra = 4000, Q = 81

Hydro-Magnetic Rayleigh-Bernard Stability

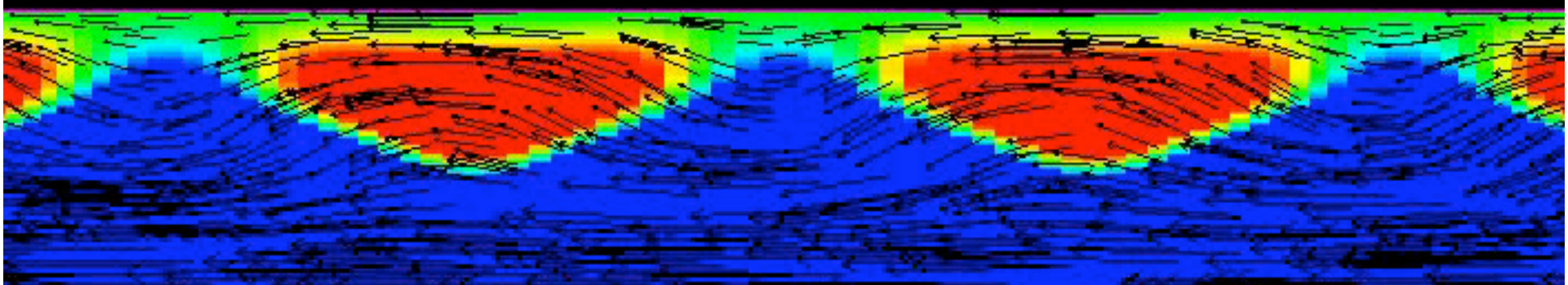
$$Ra = \frac{g\beta}{\nu\alpha}\Delta T d^3 \quad and \quad Q = \frac{B_0^2 d^2}{\mu_0 \rho \nu \eta}$$

$$Pr = \frac{\nu}{\alpha}$$

$$Pr_m = \frac{\nu}{\eta}$$

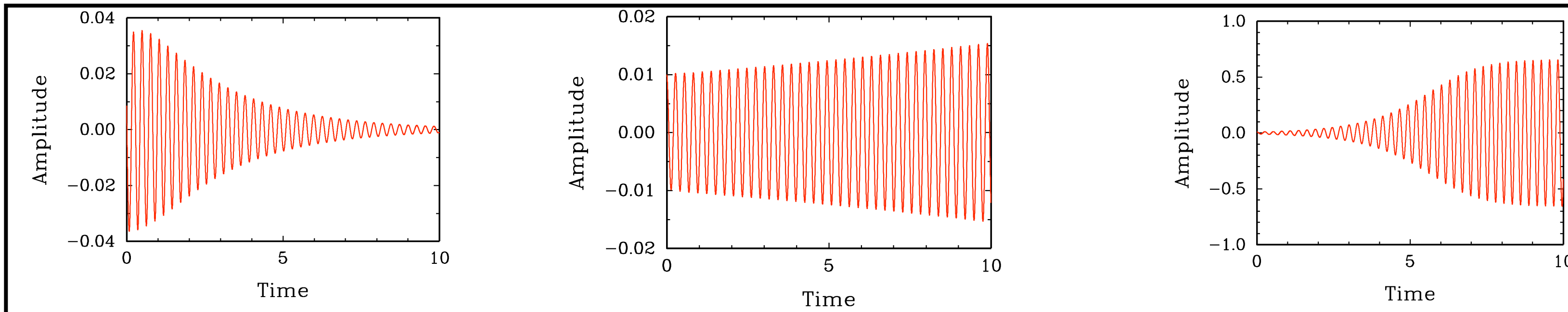
Unstable Flow at Ra = 4000, Q = 144

Jz



Y

Characterizing Complex Nonlinear Solution Spaces with a Transient Code is Difficult

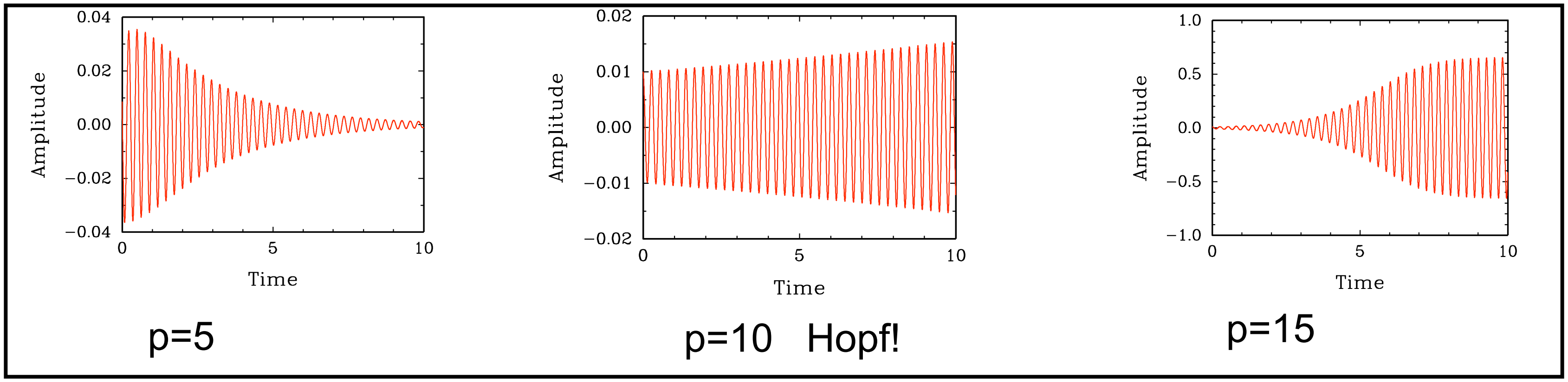


p=5 p=10 Hopf Bifurcation? p=15

Various discrete time integration methods:

- **can produce “spurious” stable and unstable steady solutions and limit cycles**
- **can stabilize unstable solutions of the ODE/PDE**
- **can produce very different dynamics and bifurcation behavior than ODE/PDE**

Characterizing Complex Nonlinear Solution Spaces with a Transient Code is Difficult



Various discrete time integration methods: **(can also be said of discrete spatial approx)**

- **can produce "spurious" stable and unstable steady solutions and limit cycles**
- **can stabilize unstable solutions of the ODE/PDE**
- **can produce very different dynamics and bifurcation behavior than ODE/PDE**

In addition:

- **turn a BVP -> IBVP with unknown initial data (basin of attraction of solutions)**
- **require very long time integration near critical points**
- **require a detailed sampling of parameter space to characterize a solution space**
- **produce complex interactions between temporal and spatial discretizations**
- **cannot be used to efficiently "track" location of critical points with multiple parameters**

e.g. Helen Yee - Very nice study of these issues

Yee, Sweby, IJCFD, 4, 1995

Yee, Sweby, RIACS Tech. Rept. 1997

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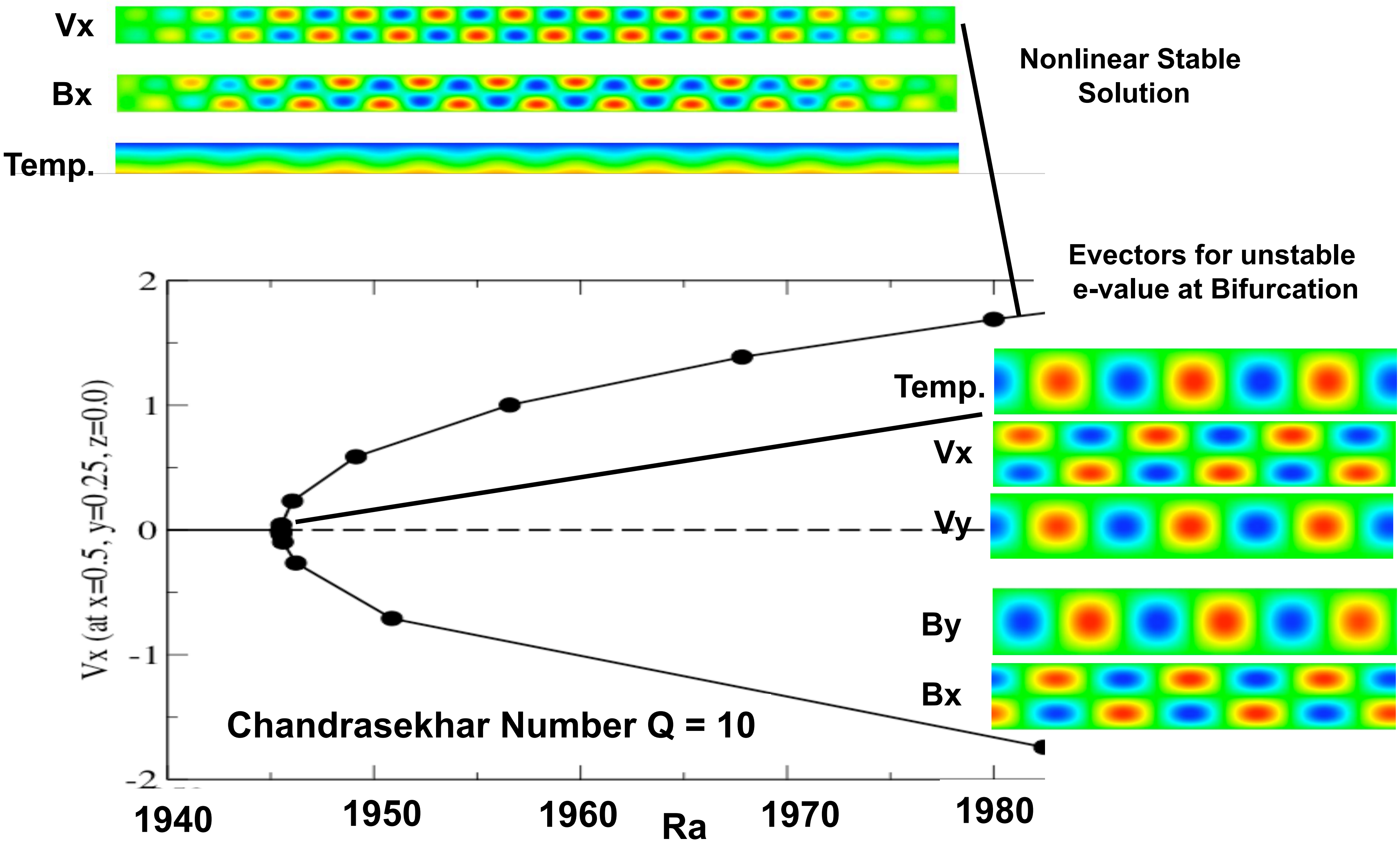
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Linear Stability and Nonlinear Equilibrium Solutions (Steady State Solves)



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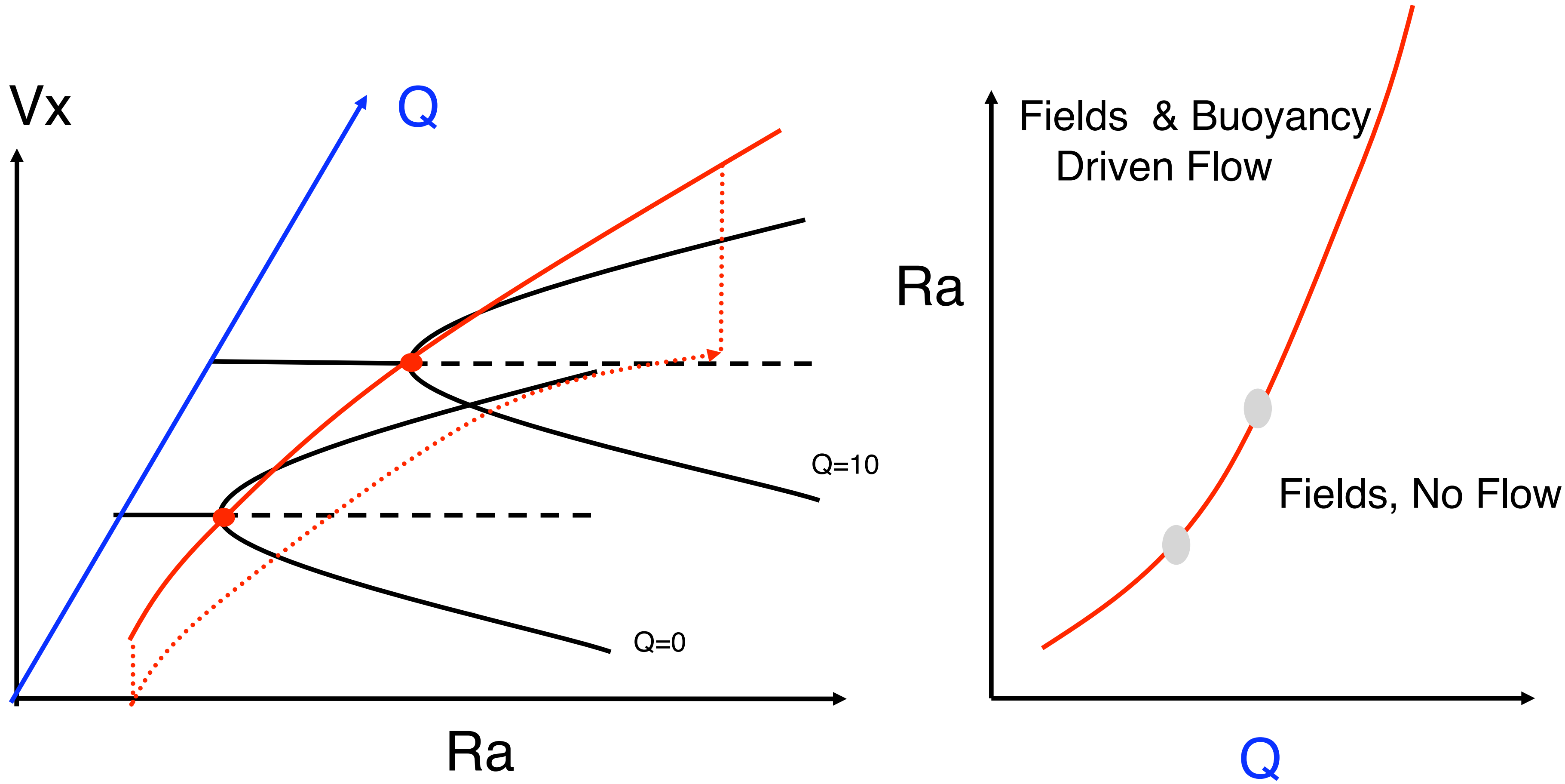
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Linear Stability and Nonlinear Equilibrium Solutions (Steady State Solves)

Q	Ra*	Ra_{cr} [Chandrasekhar[]]	% error
0	1707.77	1707.8	0.002
10^1	1945.78	1945.9	0.006
10^2	3756.68	3757.4	0.02

- 2 Direct-to-steady-state solves at a given Q
- Arnoldi method using Cayley transform to determine approximation to 2 eigenvalues with largest real part
- Simple linear interpolation to estimate Critical Ra*

Bifurcation / Stability (Two-Parameter) Diagram



- "No flow" does not equal "no-structure" – pressure and magnetic fields must adjust/balance to maintain equilibrium.
- LOCA can perform multi-parameter continuation

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Hydro-Magnetic Rayleigh-Bernard: Directly Determining Critical Stability and Critical Points

Linear Stability of Computational Solution by Normal Mode Analysis

$$\sigma_i \mathbf{B}\mathbf{q}_i = \mathbf{F}^{'}\mathbf{q}_i$$

$$(\mathbf{F}^{'} - \eta_c \mathbf{B})^{-1}(\mathbf{F}^{'} - \mu_c \mathbf{B})\mathbf{w} = \nu \mathbf{w}$$

Approximately invert by ML preconditioned Krylov solve

Turning Point Tracking:

$$\mathbf{F}\left(\mathbf{x}, Ra^*, Q^*\right) = \mathbf{0}$$

$$\mathbf{F}^{'}\mathbf{v} = \mathbf{0}$$

$$\mathbf{\Gamma}^{\mathbf{T}}\mathbf{v} - 1 = 0$$

Solve extended system with Newton's method

Moore-Spence

- Turning point formulation:

$$f(x,p) = 0$$
$$Jn = 0$$
$$\phi \cdot n - 1 = 0$$

- Newton's method (2N+1):

$$\begin{bmatrix} J & 0 & f_p \\ (Jn)_x & J & J_p n \\ 0 & \phi^T & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta n \\ \Delta p \end{bmatrix} = \begin{bmatrix} -f \\ -Jn \\ 1 - \phi^T \cdot n \end{bmatrix}$$

- 4 linear solves per Newton iteration:

$$Ja = -f$$
$$Jb = -f_p$$
$$Jc = -(Jn)_x a - Jn$$
$$Jd = -(Jn)_x b - J_p n$$
$$\Delta p = (1 - \phi \cdot n - \phi \cdot c)/(\phi \cdot d)$$
$$\Delta n = c + \Delta p d$$
$$\Delta x = a + \Delta p b$$

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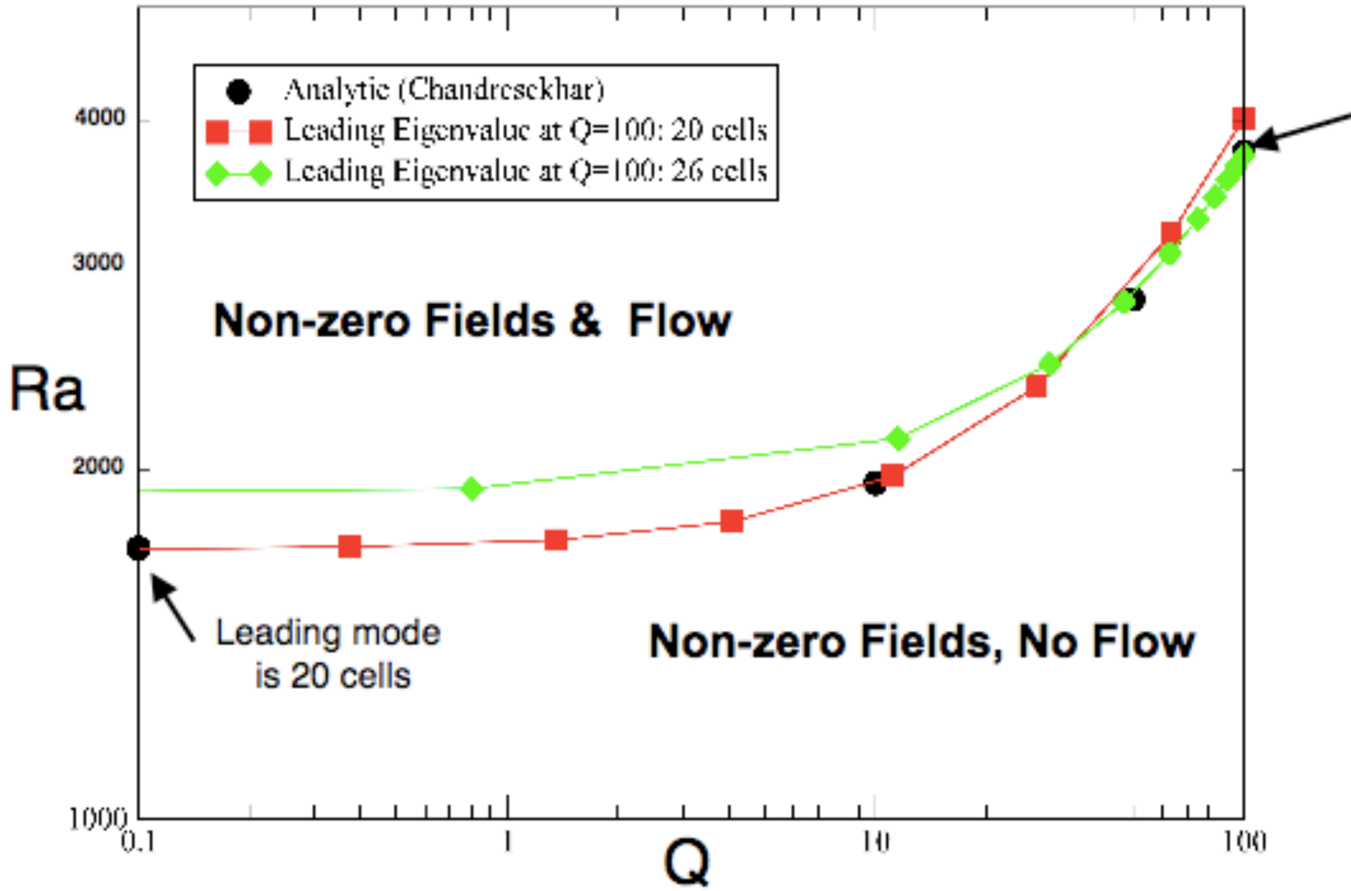
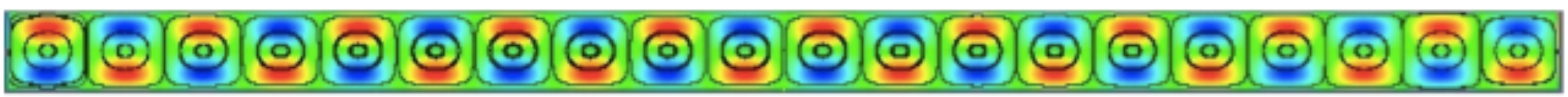
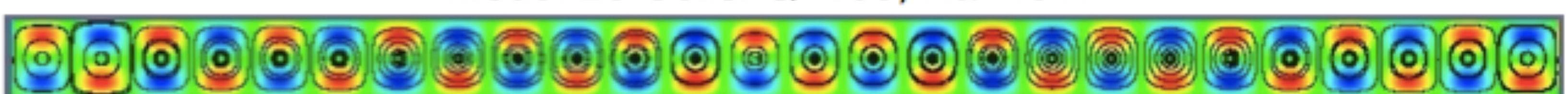
Direct Determination of Bifurcation Points (Ra*, Q*) (multiple steady state solves)

Magnetic Field Compresses Most Unstable Mode as Q Increases





Mode: 20 Cells: Q=100, Ra=4017



Mode: 26 Cells: Q=100, Ra=3757

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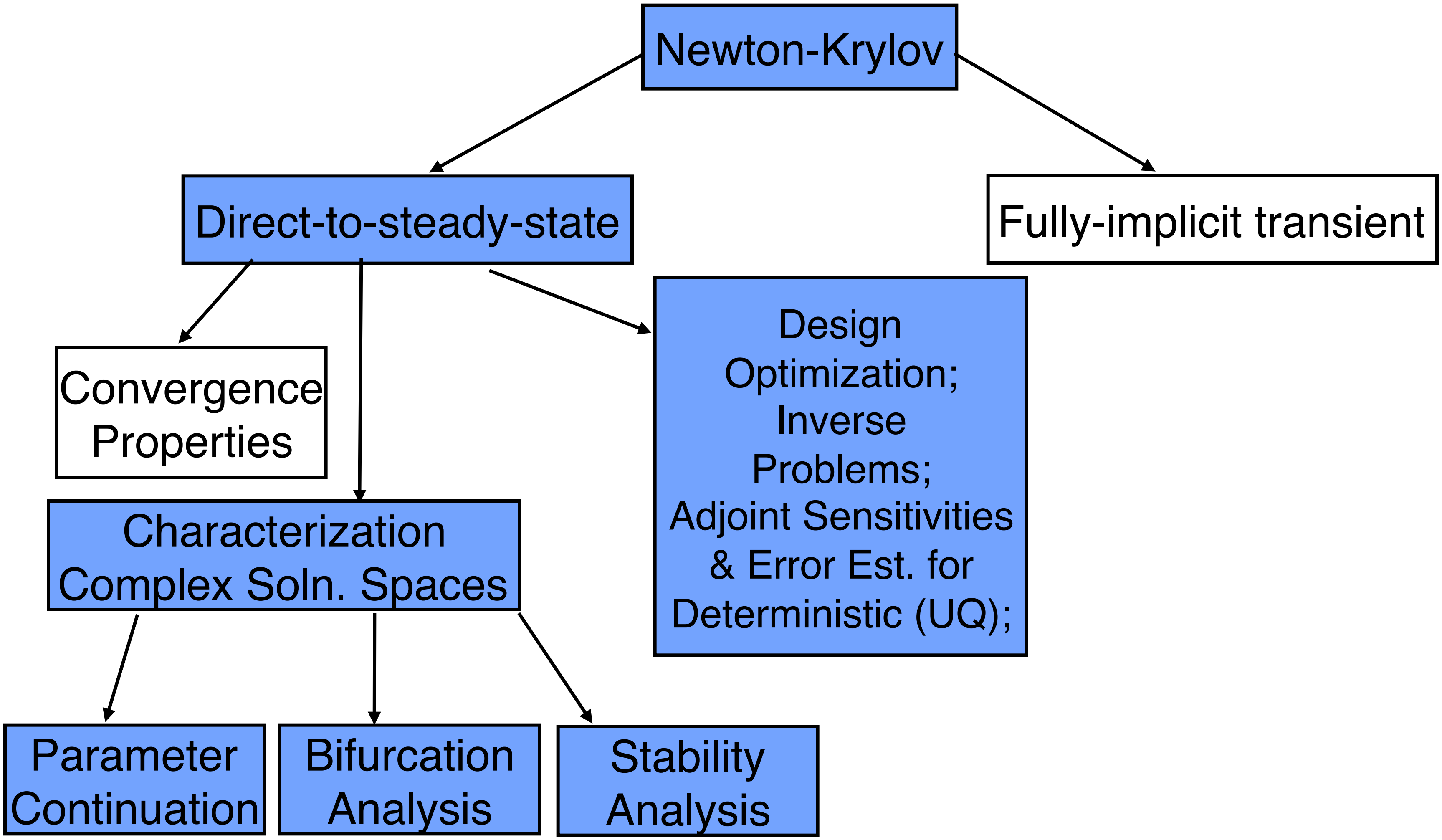
Why Newton-Krylov Methods?



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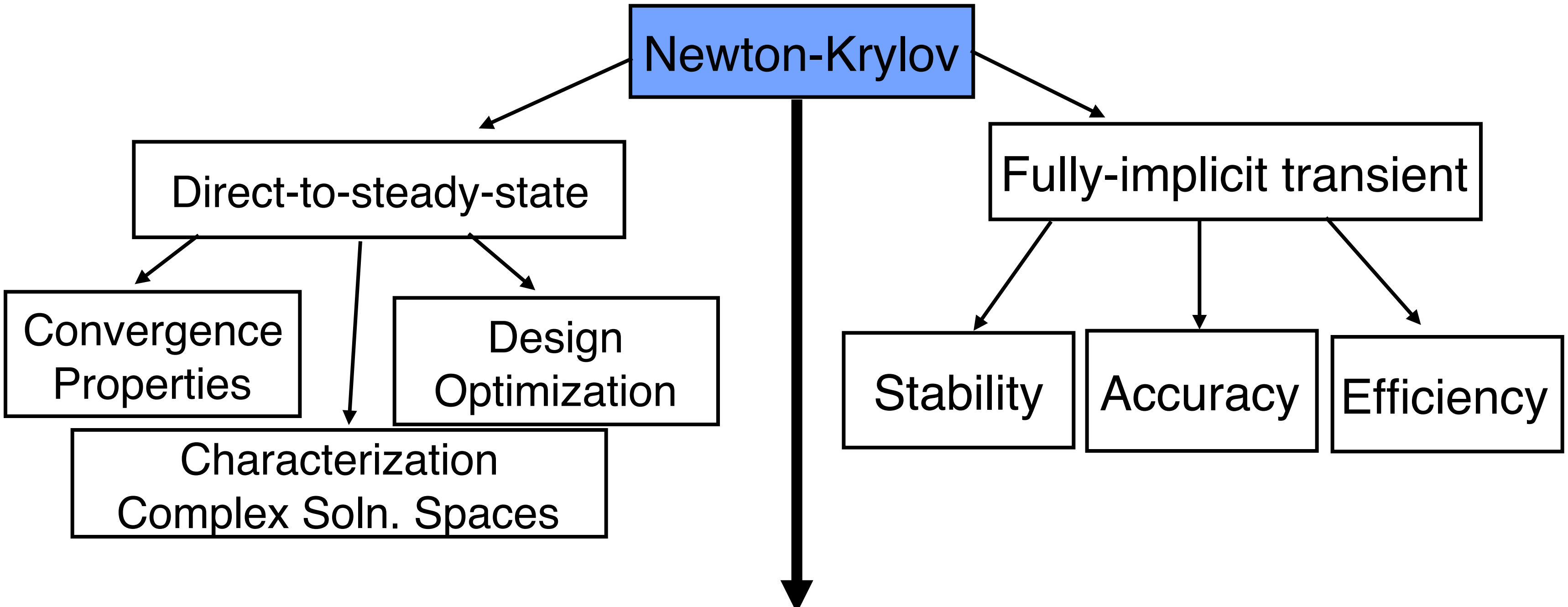
Why Newton-Krylov Methods?



Very Large Problems -> Parallel Iterative Solution of Sub-problems

Krylov Methods - Robust, Scalable and Efficient Parallel Preconditioners

- Approximate Block Factorizations
- Physics-based Preconditioners
- Multi-level solvers for systems and scalar equations

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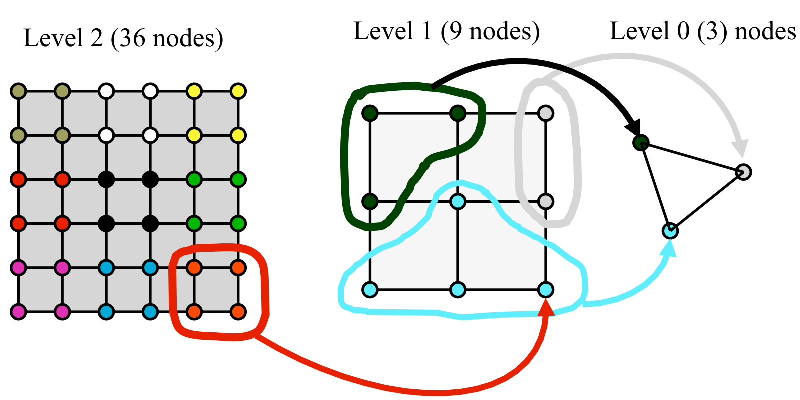
ML library: Multilevel Preconditioners

(R. Tuminaro, M. Sala (BMW-Sauber), J. Hu, C. Siefert, M. Gee (UT Munich))

2-level and N-level Aggressive Coarsening Graph-based Block AMG

- Aggregation is used to produce a coarse operator
  - **Create graph where vertices are block nonzeros in matrix A_k**
  - **Edge between vertices i and j included if block $B_k(i,j)$ contains nonzeros**
  - **Decompose graph into aggregates (subgraphs) [Metis/ParMetis]**
- Construction of simple restriction/interpolation operators (e.g. piecewise constants on agg.)
- Construction of A_{k-1} as $A_{k-1} = R_{k-1} A_k I_{k-1}$

- Galerkin and Petrov-Galerkin Projections
- Nonsmoothed & smoothed aggregation
- Smoothers: domain decomposition smoothers (sub-domain GS and ILU(k))
- Coarse grid solver can use fewer processors than for fine mesh solve (direct/approximate/iterative)



Visualization of effect of partition of matrix graph on mesh

Aggregation based Multigrid:
- **Vanek, Mandel, Brezina, 1996**
- **Vanek, Brezina, Mandel, 2001**

Aggregation used in DD:
- **Paglieri, Scheinine, Formaggia, Quateroni, 1997**
- **Jenkins, Kelley, Miller, Kees, 2000**
- **Toselli, Lasser, 2000**
- **Sala, Formaggia, 2001**

Choice of Prolongation/Restriction

- Non-smoothed aggregation and a Galerkin Projection (simple choice, good stability, more optimal for hyperbolic operators)

$$\hat{P}(i,\alpha) = \begin{cases} 1 & \text{if} \quad i \in \text{agg}(\alpha) \\ 0 & \text{if} \quad \text{otherwise} \end{cases} ; \qquad R = \hat{P}^T$$

- Smoothed aggregation and a Galerkin projection. Damped Jacobi a typical choice for smoothing prolongator in smoothed aggregation (optimal smoothing parameters for Laplace, etc.)

$$P_i = (I - \omega_i D^{-1} A)\hat{P}_i$$
$$R = P^T$$

$\hat{P}_i$: tentative prolongator
$D = diag(A)$
ω_i: damping parameter

- Petrov-Galerkin type smoothed aggregation preconditioner for nonsymmetric linear systems [Sala and Tuminaro, SISC 2008]

$$P_i = (I - \omega_i D^{-1} A)\hat{P}_i$$
$$R_i = \hat{P}_i^T (I - A D^{-1} \omega_i^{(r)})$$

  + Perform restriction smoothing
  + Restriction operator does not correspond to transpose of prolongator for nonsymmetric problems
  + Rather than use a single damping parameter, calculate values to minimize P_i and R_i

- Sub-domain decomposition smoothers (sub-domain GS and ILUT, ILU(k), LU)
- Coarse grid solver can use fewer processors than for fine mesh solve (sparse direct (KLU, SuperLU) / approximate (ILUT) / iterative

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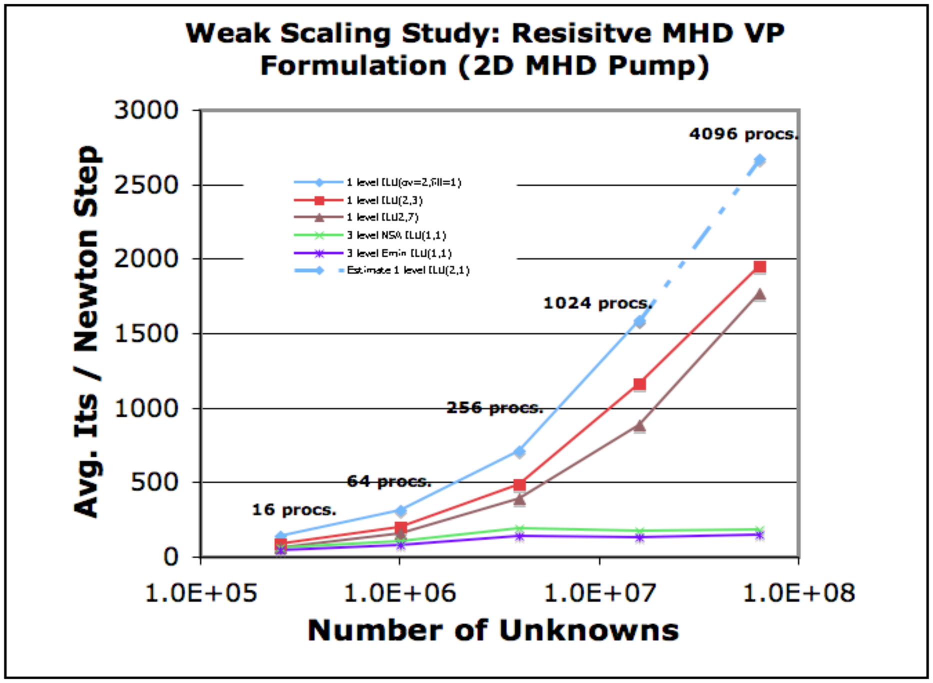
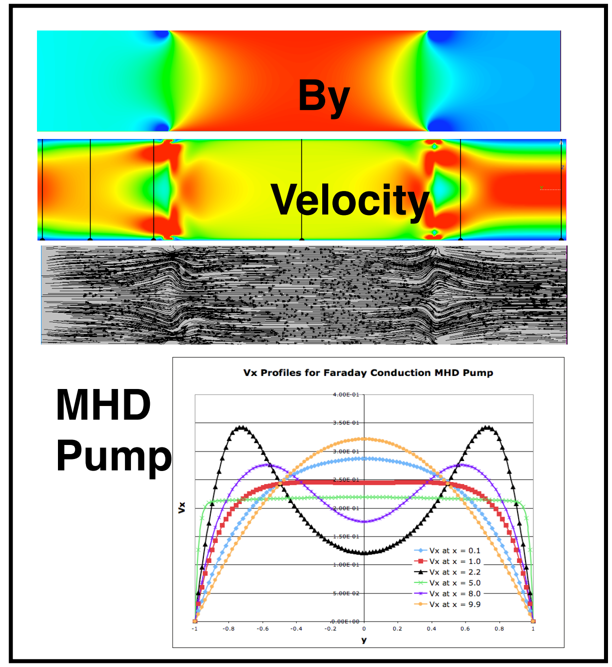
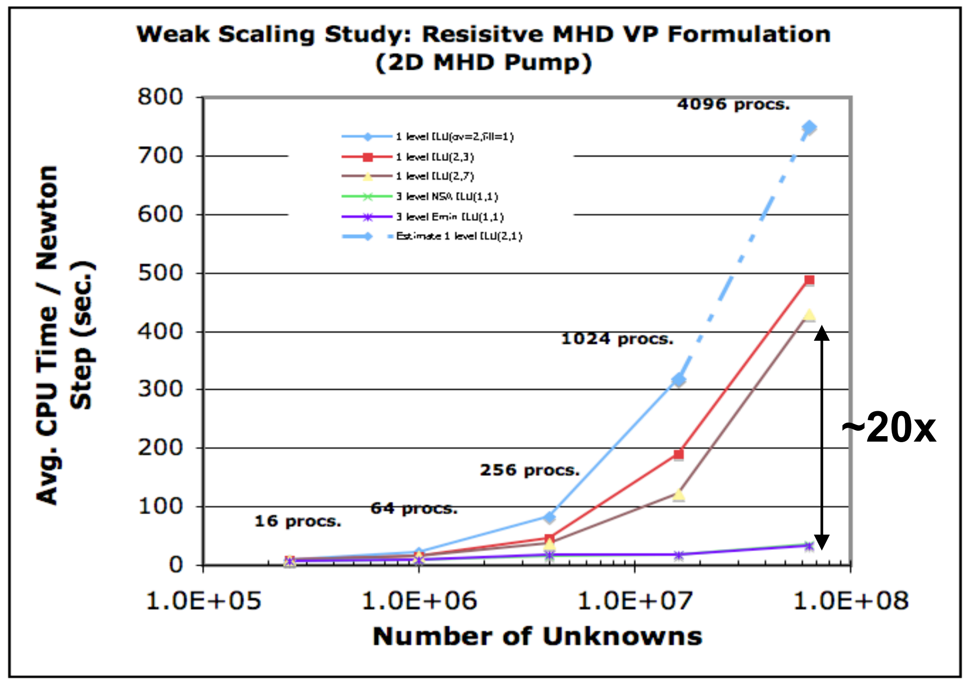
Scaling Performance for Fully-coupled Resistive MHD/ Block AMG - Cray XT3/4

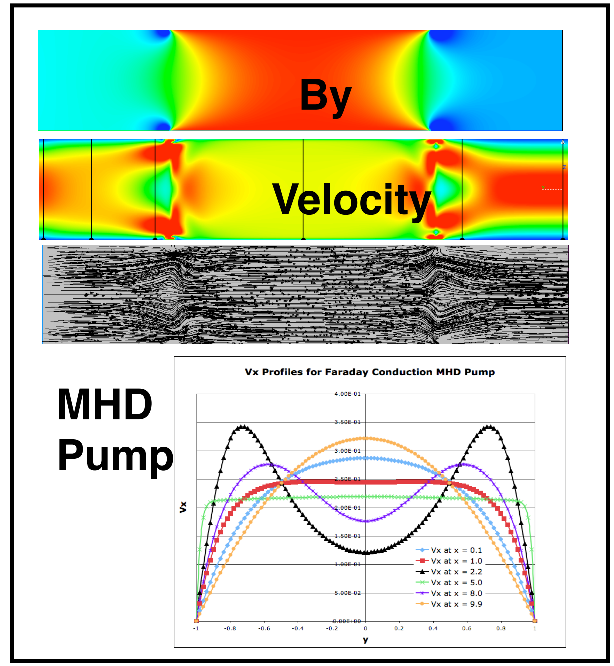






Multicore Performance of Fully-coupled Resistive MHD Simulations - Cray XT3/4

Nodes	Cores	Compute Jac +Prec		Linear Solve		Total	
		Time (sec)	η (%)	Time (sec)	η (%)	Time (sec)	η (%)
4096	1	16.9	---	4.3	---	21.2	---
2048	2	18.2	93	4.5	95	22.6	94
1024	4	17.7	95	4.9	88	22.6	94



Our Largest Fully-coupled Direct-to-steady-state Simulation to Date:

1+ Billion unknowns
250 Million Quad elements
24,000 cores Cray XT3/4

Newton-GMRES / ML: PG-AMG 4 level
18 Newton steps
86 Avg. No. Linear Its. / Newton step
33 min. for solution

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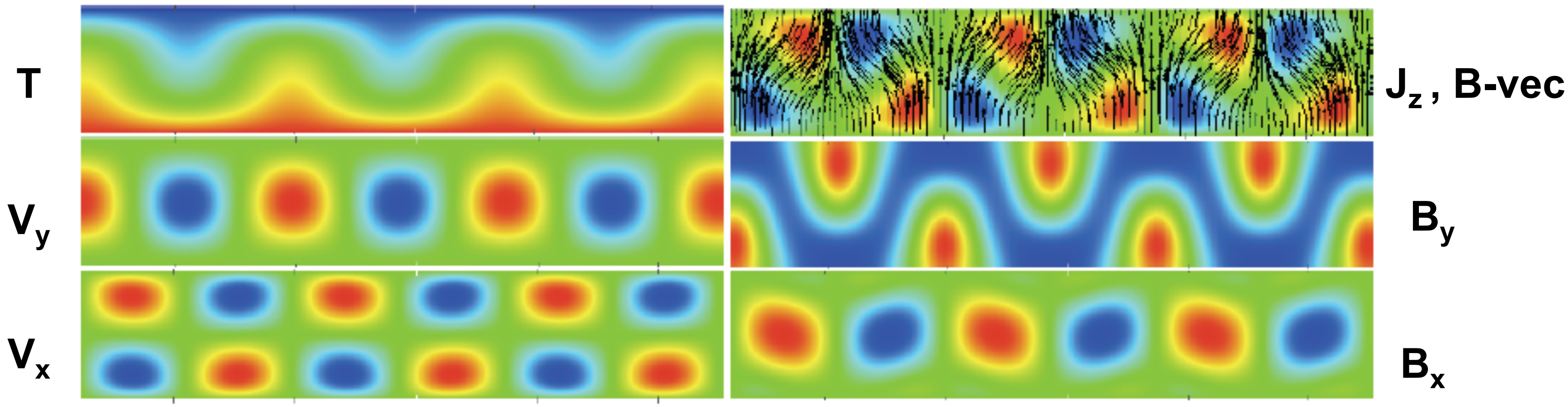
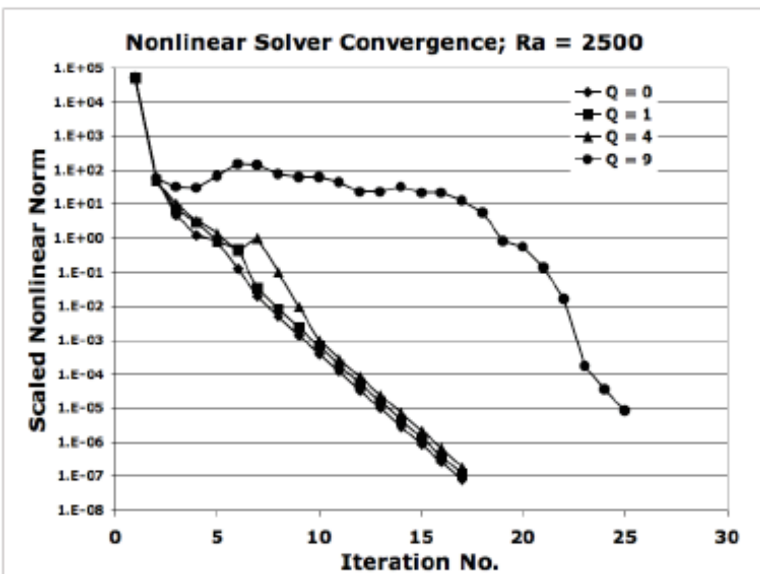
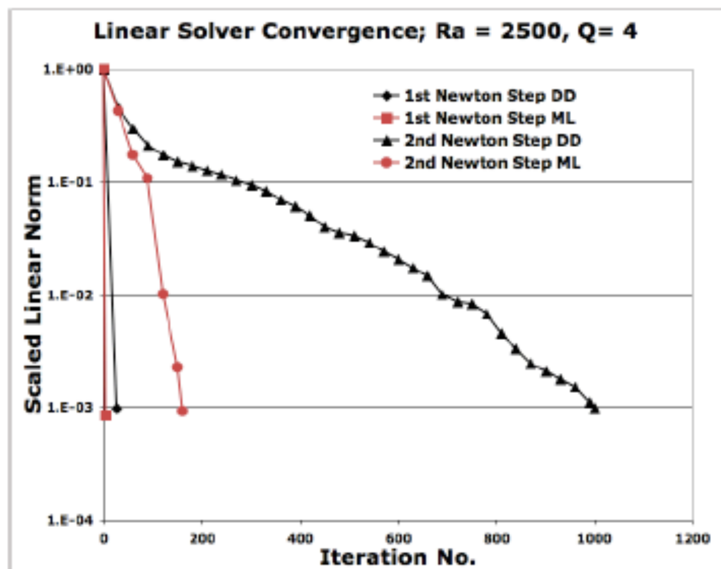
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Nonlinear Equilibrium Solutions (Steady State Solves, Ra = 2500)







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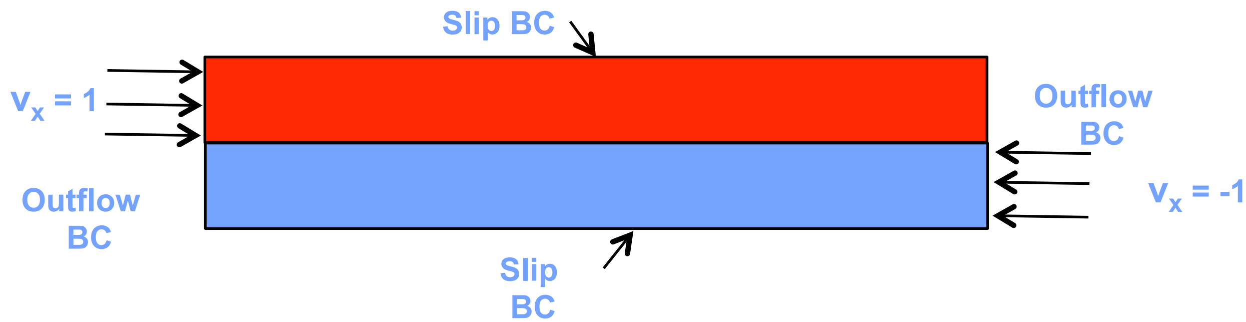
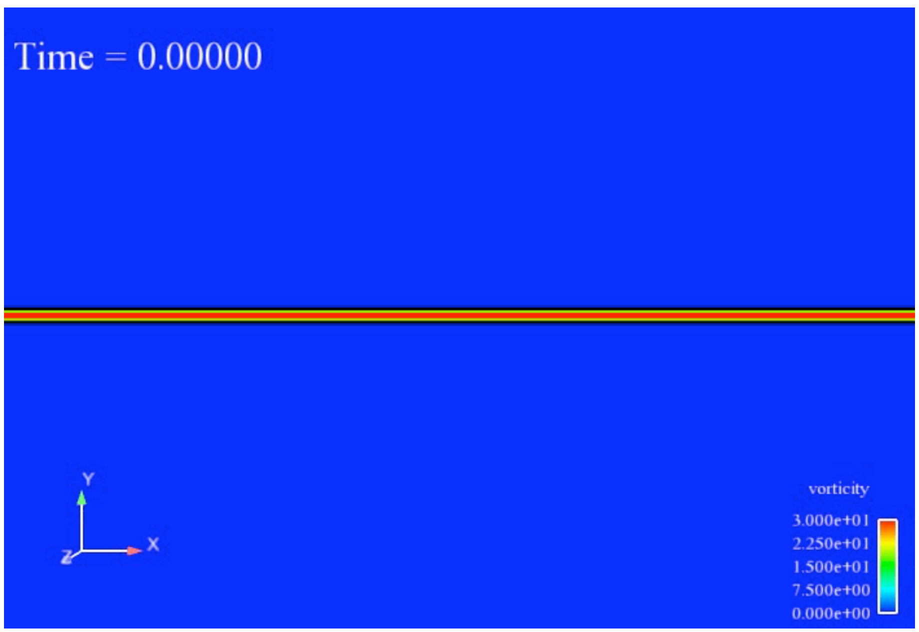
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Nonlinear Equilibrium Solutions (Steady State Solves, Ra = 2500)

Robustness and Efficiency of DD and Multilevel Preconditioners

proc	fine grid size	fine grid unknowns	1-level ILU		3-level V(1,1) ILU-ILU-KLU			
			avg its/ Newt step	time (sec)	medium unkns size	coarse unkns size	avg its/ Newt step	time (sec)
2048	500x5000	12.5M	1910[40]	> 7200*	412450	13745	115[17]	226

(initial) Kelvin-Helmholtz





Re = 10,000

Re = 1,000

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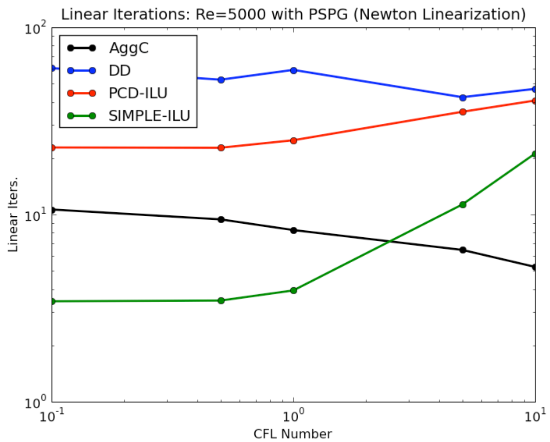
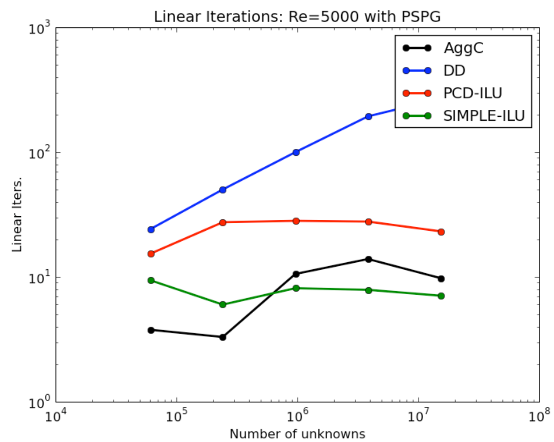
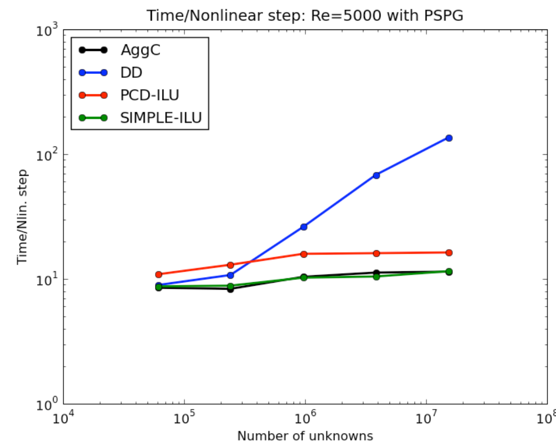
Transient Kelvin-Helmholtz







Kelvin Helmholtz: Re=5000, Weak scaling at CFL=2.5

- **Run on 1 to 256cores**
- **Pressure - PSPG, Velocity - SUPG (residual and Jacobian)**

1. **SIMPLEC strongly dependent on CFL**
2. **Block methods scale as well as AggC**

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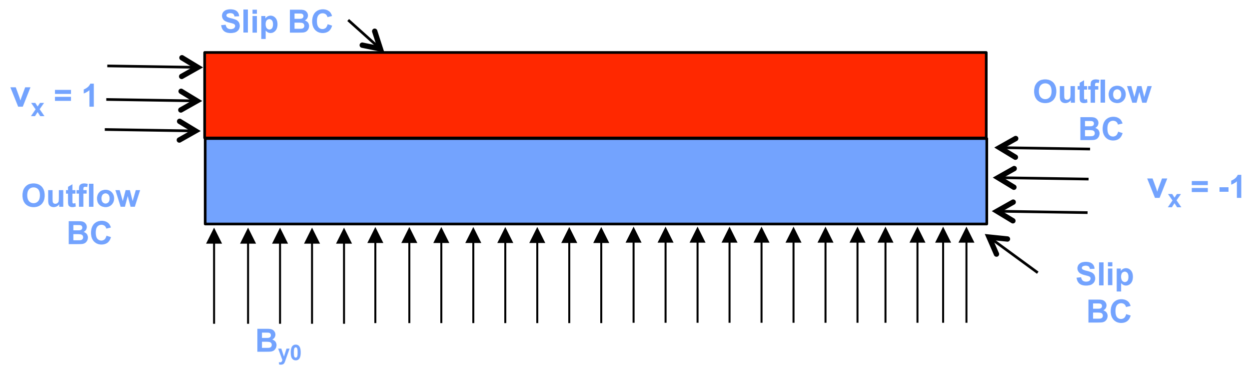
(initial) Hydro-magnetic Kelvin-Helmholtz

$Re = Re_m = 1{,}000;$



$Q = 10{,}000;$

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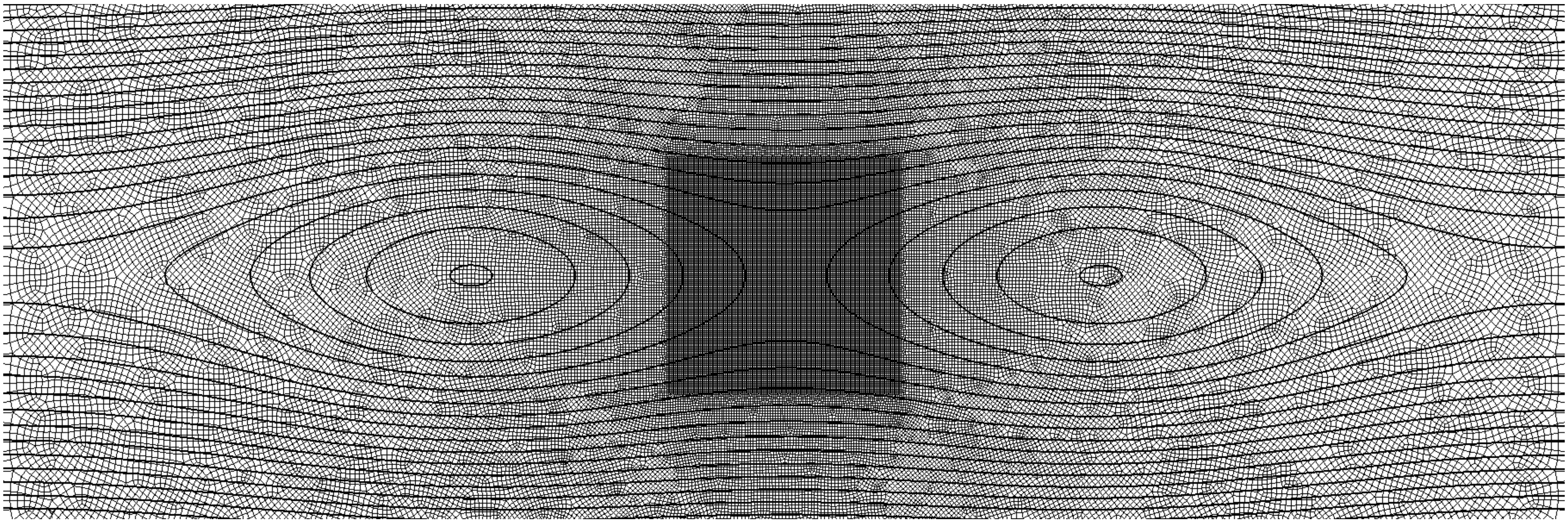
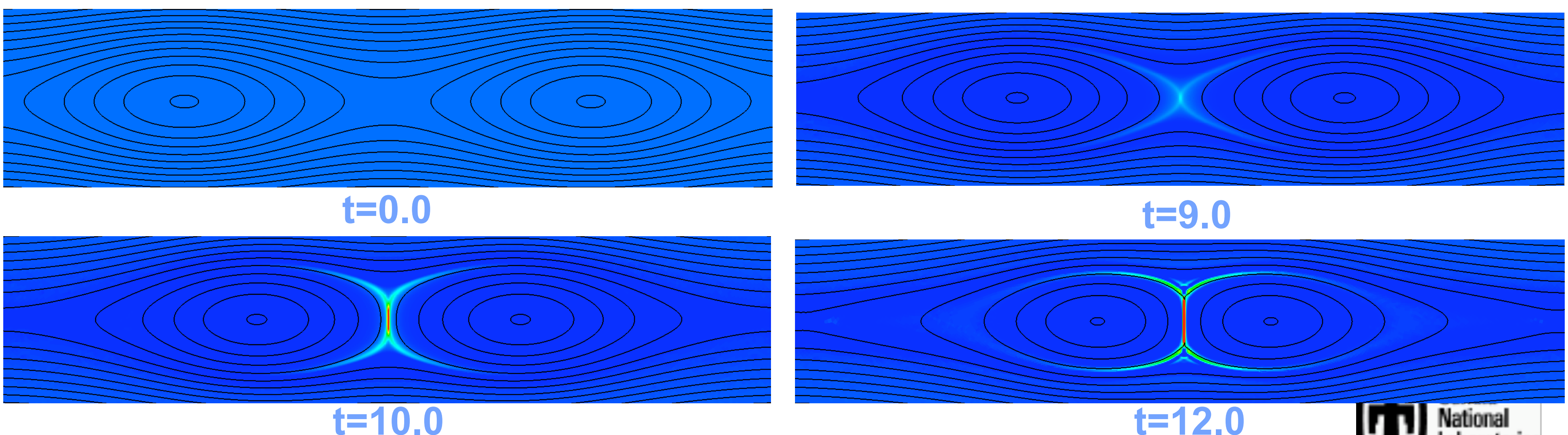
Multiple-time-scale systems: E.g. Driven Magnetic Reconnection with a Magnetic Island Coalescence Problem (Incompressible – resistive MHD)





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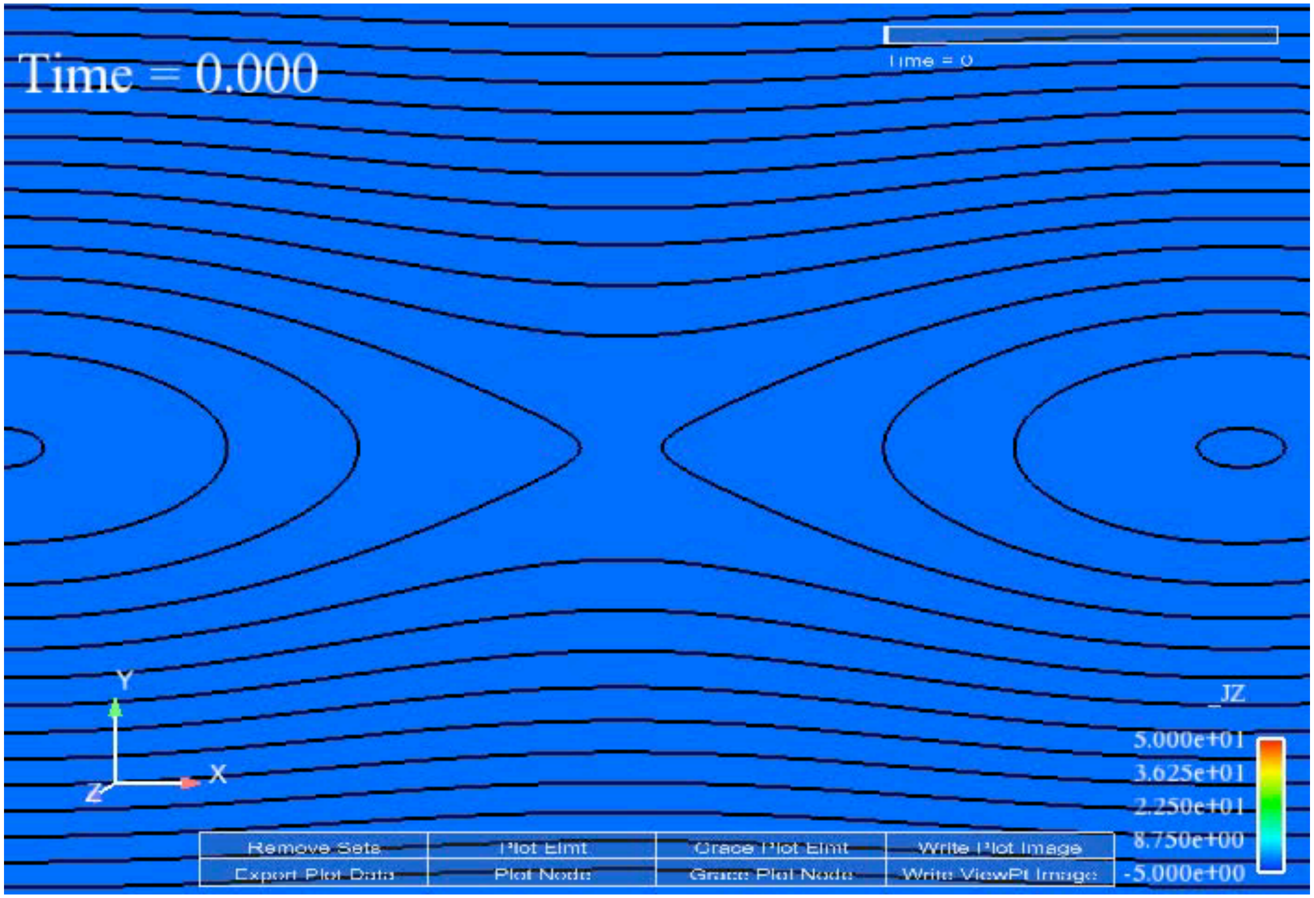
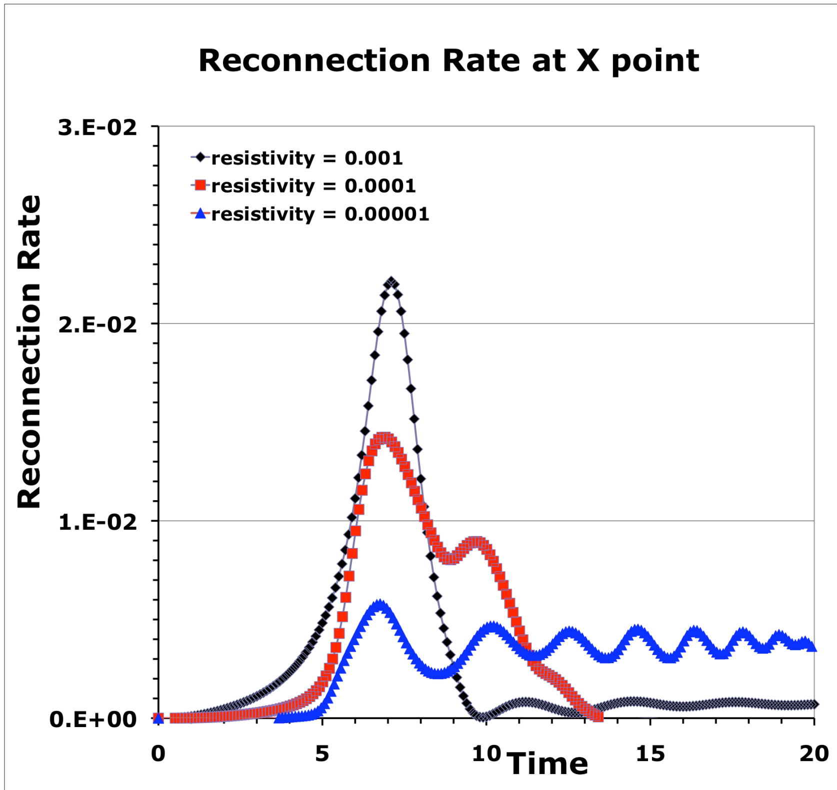
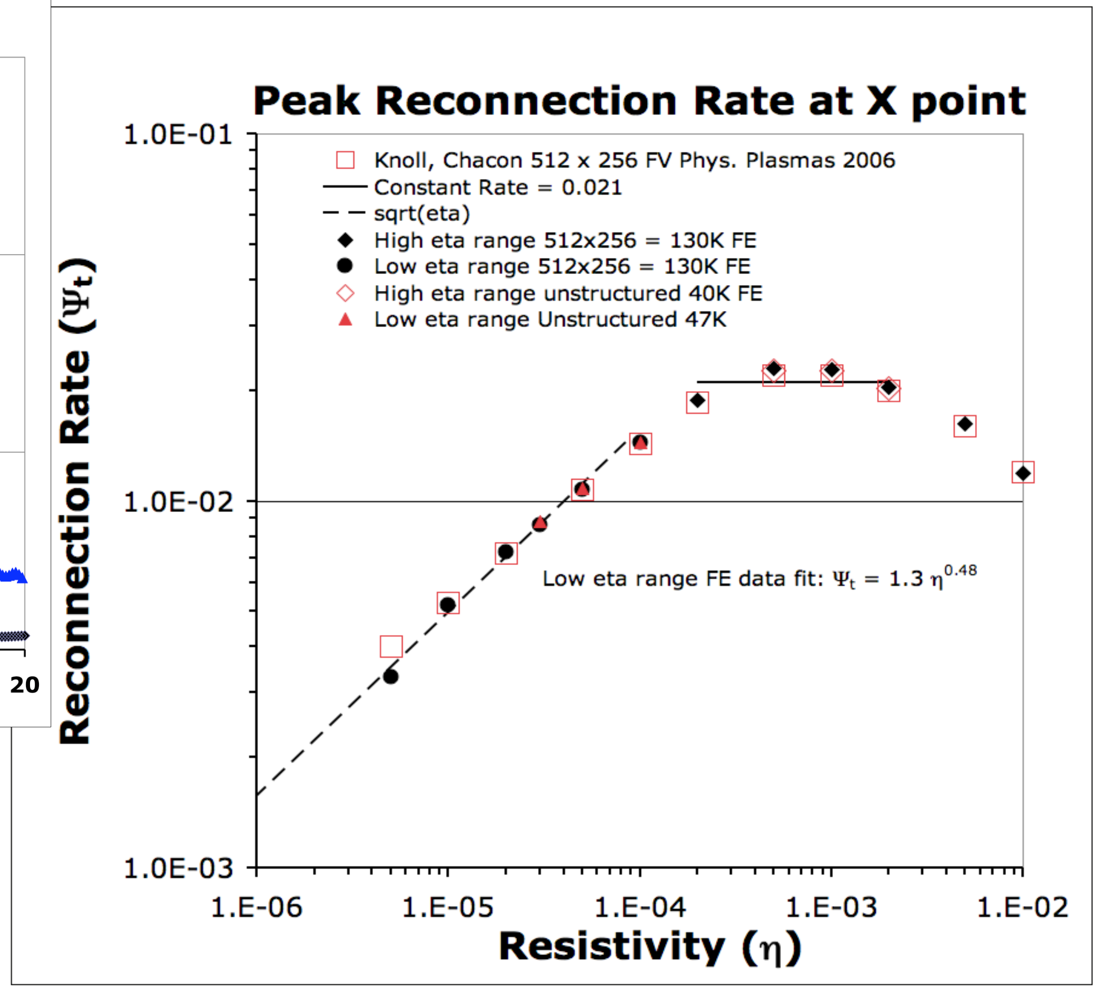


<u>Approx. Computational Time Scales:</u>

- **Ion Momentum Diffusion: 10^{-7} to 10^{-3}**
- **Magnetic Flux Diffusion: 10^{-7} to 10^{-3}**
- **Ion Momentum Advection: 10^{-4} to 10^{-2}**
- **Alfven Wave** $\left(\tau_A = \frac{h\sqrt{\rho\mu_0}}{B_O}\right)$ **: 10^{-4} to 10^{-2}**
- **Whistler Wave** $\left(\tau_w = \frac{h^2}{V_A d_i}\right)$ **: 10^{-7} to 10^{-1}**
- **Magnetic Island Sloshing: 10^{0}**
- **Magnetic Island Merging: 10^{1}**

Sloshing in Resistive MHD:
Island Coalescence problem (FE MHD)





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Preliminary Weak Scaling Results on Island Coalescence Problem (@resistivity η=1.0e-3)

Charon_xmhd, FE

Procs	Mesh	# Unk	Newton / $\Delta\tau$	Gmres / Newton	Time / Newton	Gmres / $\Delta\tau$	Time / $\Delta\tau$	Est. Serial Time	Ratio
1	64x64	16K	3.9	4.4	2.1	17.2	8.1	810	3.6486
4	128x128	64K	4.6	5.8	2.6	26.7	11.9	4760	4.379
16	256x256	.25M	4.9	6.3	2.9	30.9	14.2	22720	3.8944
64	512x512	1M	6.2	8.8	4	54.6	24.6	157440	5.7502

Grid	Newton	GMRES/dt	CPU(s)
64x64	3.3	3.3	222
128x128	4	4.5	1087
256x256	4.5	6.2	5834
512x512	4.7	8.3	27380

Chacon & Knoll, FV Physics-based Prec.

Only ~4-5 times slower, considering...

- Research code – no investment in efficiency (coming soon)
- Unstructured FE vs Structured FV solver: no leveraging of mesh structure.
- No physics based preconditioning (Block - AMG)
- Need faster and lower memory physics based approach for transients and lower resistivity.

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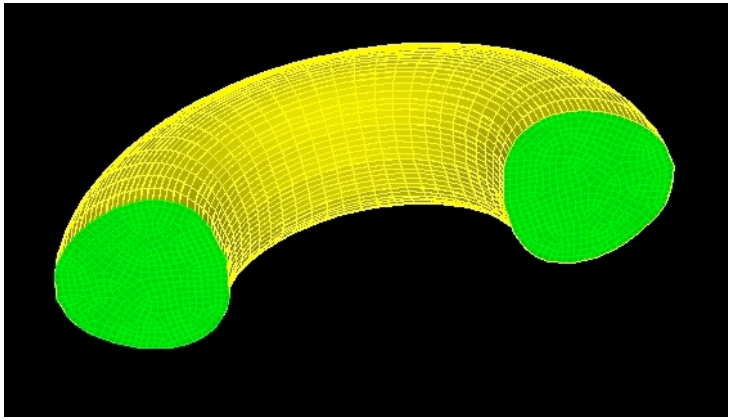
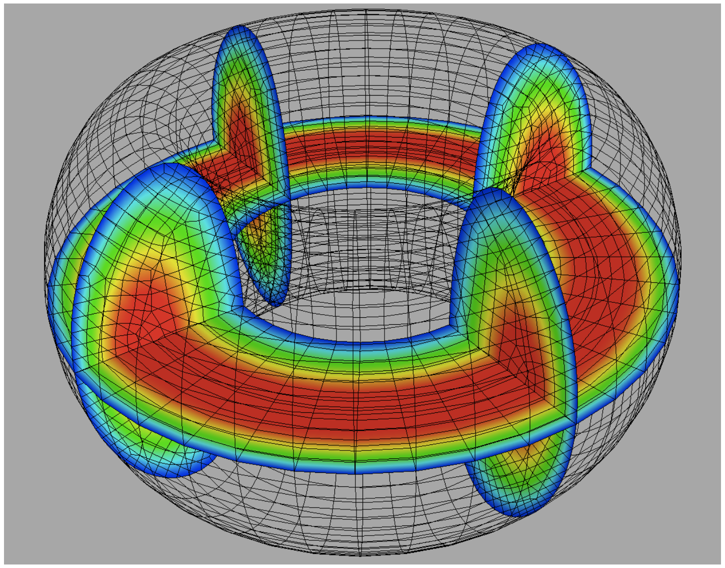
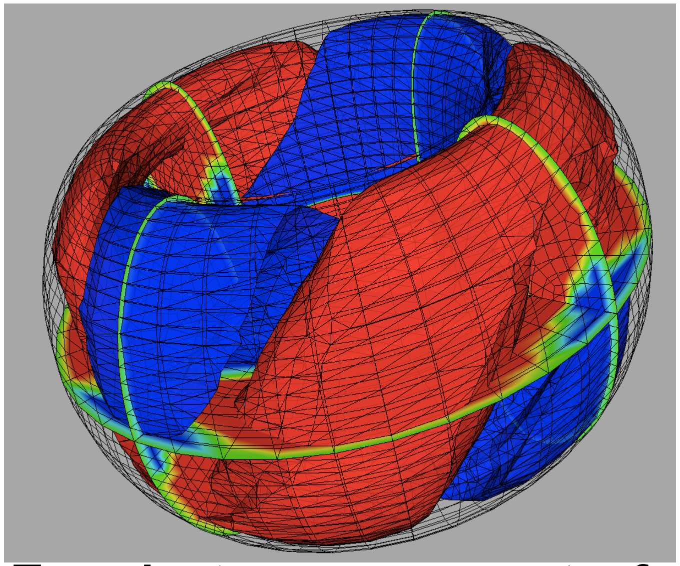
Towards simulation of a 3D Ideal Kink Instability in Tokamak Geometry (Solov’ev equilibrium) [B field solver – Lagrange multiplier method.]



Unstructured FE mesh for tokamak geometry. Kappa = 1



A representative Solov’ev equilibrium pressure field.
Kappa = 2



Transient rearrangement of a pressure field.
Kappa = 2

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Conclusions

- Initial results for stabilized FE formulation of low Mach number resistive MHD system is encouraging

- Newton-Krylov /block AMG methods can provide a very effective, robust and flexible solution technology for analysis and characterization of complex nonlinear solution spaces.

- Parallel multilevel preconditioners have shown promising results for algorithmic scalability and CPU time performance for initial MHD solutions.

(Issues: Hyperbolic operators, FE aspect ratios for multilevel methods)

- For transient simulations physics based preconditioners are required for fast solutions. Use block AMG as sub-system solvers.

- Next 3D formulations, physics-based preconditioners, new Schur complement approximations, and tokamak geometries

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Trilinos: Full Vertical Solver Coverage
(Part of DOE: TOPS SciDAC Effort)

Optimization Unconstrained: Constrained:	Find $u \in \Re^n$ that minimizes $g(u)$ Find $x \in \Re^m$ and $u \in \Re^n$ that minimizes $g(x, u)$ s.t. $f(x, u) = 0$	Sensitivities (Automatic Differentiation: Sacado)	MOOCHO
Bifurcation Analysis	Given nonlinear operator $F(x, u) \in \Re^{n+m}$ - For $F(x, u) = 0$ find space $u \in U \ni \frac{\partial F}{\partial x}$ s		LOCA
Transient Problems DAEs/ODEs:	Solve $f(\dot{x}(t), x(t), t) = 0$ $t \in [0, T], x(0) = x_0, \dot{x}(0) = x_0'$ for $x(t) \in \Re^n, t \in [0, T]$		Rythmos
Nonlinear Problems	Given nonlinear operator $F(x) \in \Re^m \rightarrow \Re$ Solve $F(x) = 0 \quad x \in \Re^n$		NOX
Linear Problems Linear Equations: Eigen Problems:	Given Linear Ops (Matrices) $A, B \in \Re^{m \times n}$ Solve $Ax = b$ for $x \in \Re^n$ Solve $A\nu = \lambda B\nu$ for (all) $\nu \in \Re^n, \quad \lambda \in$		AztecOO Belos Ifpack, ML, teko Anasazi
Distributed Linear Algebra Matrix/Graph Equations: Vector Problems:	Compute $y = Ax; A = A(G); A \in \Re^{m \times n}, G \in \Im^{m \times n}$ Compute $y = \alpha x + \beta w; \alpha = \langle x, y \rangle; x, y \in \Re^n$		Epetra Tpetra