SAND2013-5447C

Performance of an Implicit Finite Element Resistive MHD Solver for High Rayleigh Number Thermal Convection in Rotating Systems with Magnetic Fields

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Resistive MHD Equations

Resistive MHD Model in Residual Notation

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

$$R_P = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \mathbf{T_M} = \frac{1}{\mu_0}\mathbf{B} \otimes \mathbf{B} - \frac{1}{2\mu_0}\|\mathbf{B}\|^2 \mathbf{I}$$

$$R_e = \frac{\partial(\rho e)}{\partial t} + \nabla \cdot [\rho \mathbf{v} e + \mathbf{q}] - \mathbf{T} : \nabla \mathbf{v} - \eta \| \frac{1}{\mu_0} \nabla \times \mathbf{B} \|^2 = 0$$

$$\mathbf{R_B} = \frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u} \times \mathbf{B}) + \nabla \times (\frac{\eta}{\mu_0} \nabla \times \mathbf{B}) = \mathbf{0}.$$

2D →

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

$$R_{A_z} = \frac{\partial A_z}{\partial t} + \mathbf{u} \cdot \nabla A_z - \frac{\eta}{\mu_0} \nabla^2 A_z + E_z^0 = 0.$$

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

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B Field Lagrange Multiplier Formulation
(Dedner et. al. 2002, Codina et. al. 2006, 2011; …)

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

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

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

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

Remarks:

- Elliptic constraint used to enforce divergence involution.
    - Only weakly divergence free in FE implementation (stabilization)
- Can show relationship with a projection method (e.g. Brackbill and Barnes 1980) when a 1st order-split integration is used.
- Issue for using C^0 FE for domains with reentrant corners / soln singularities (Costabel et. al. 2000, 2002, Codina, 2011)

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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	$F_{m,i} = \int_{\Omega} \Phi R_{m,i}\, d\Omega + \sum_e \int_{\Omega^e} \rho \tau_m \left(\mathbf{u} \bullet \nabla\Phi\right) R_{m,i}\, d\Omega + \sum_e \int_{\Omega^e} \nu_{m,i} \nabla\Phi \bullet \mathbf{C}^c \nabla u_i\, d\Omega$
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	$F_T = \int_{\Omega} \Phi R_T\, d\Omega + \sum_e \int_{\Omega^e} \rho C_P \tau_T \left(\mathbf{u} \bullet \nabla\Phi\right) R_T\, d\Omega + \sum_e \int_{\Omega^e} \nu_T \nabla\Phi \bullet \mathbf{C}^c \nabla T\, d\Omega$
Magnetics (Vector Potential)	$F_{A_z} = \int_{\Omega} \Phi R_{A_z} d\Omega + \sum_e \int_{\Omega^e} \rho \tau_{A_z} \left(\mathbf{u} \bullet \nabla\Phi\right) R_{A_z} d\Omega + \sum_e \int_{\Omega^e} \nu_{A_z} \nabla\Phi \bullet \mathbf{C}^c \nabla A_z d\Omega$

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

Galerkin FE (e.g. Mixed Q2/Q1 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 Q1/Q1 V-P elements, SUPG like terms and Discontinuity Capturing type operators

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

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

Comments on Formulations, Solution Algorithms and Underlying Software Arch.

Drekar: Low flow Mach number CFD & resistive MHD with coupled multiphysics

- Multiple Momentum, Energy, Mass Transport/reaction eqns.
- Fully-implicit: 1st-5th order BDF; IRK; MP; (Rythmos),
  & Semi-implicit with BDF compatible extrapolation.
- 2D & 3D Unstructured FE (Intrepid)
  - Stabilized FE (VMS),
  - Mixed FE e.g. Q2/Q1,
  - Physics Compatible Discretizations (edge, face, …)
  - High-resolution Positivity-preserving in dev.
- Software Arch.:
  - Massively Parallel: Currently MPI-only (>128K cores); Exploring kernels on GPUs;
  - Solvers/Linear Alg. tools based on Trilinos packages
  - Template-based Generic Programming with Automatic Differentiation [AD] (Sacado)
  - Asynchronous dependency graphs for multiphysics complexity management (Phalanx)
- Fully Coupled Globalized Newton-Krylov Solver
  - Residuals are Programed and AD generates Jacobian/derivatives for NK, JFNK, Sensitivities, Adjoints, SGE -UQ, etc.
  - GMRES and Block Krylov (AztecOO, Belos)
  - Scalable Preconditioners: Fully-coupled system AMG (ML), Physics-based with AMG (Teko)

- Advanced Outer Loop Solvers
  - Direct-to-Steady-State (NOX),
  - Parameter Continuation, Linear Stability and Bifurcation (LOCA),
  - PDE Constrained Optimization & Parameter Inversion is Possible (Moocho)
- UQ Tools
  - Initial Adjoint formulations for Error Estimation and Sensitivity Analysis (Panzer)
  - Initial Stochastic Galerkin Expansions for UQ capability
  - Trikota blackbox interface to Dakota

[Drekar: Shadid, Pawlowski, Cyr, Smith, Wildey, Weber]

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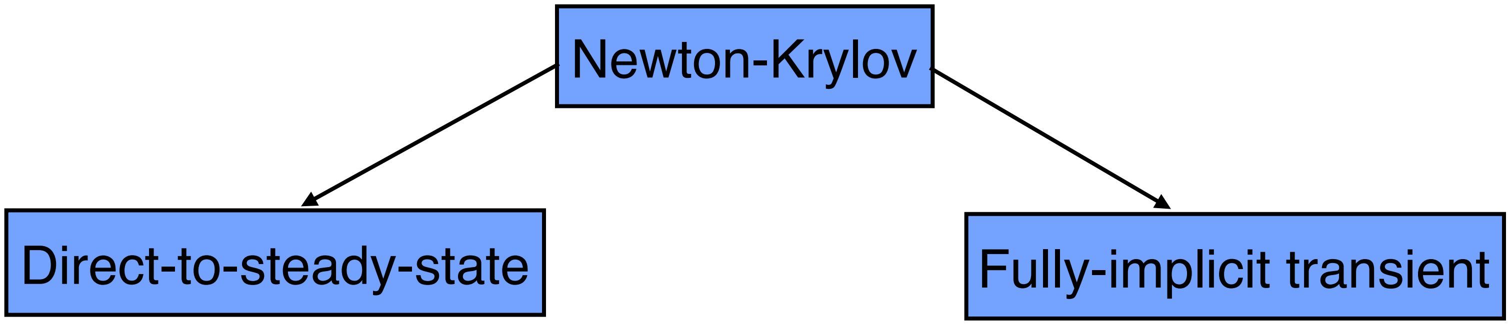
Why Newton-Krylov Methods?



Robustness, Convergence and Flexibility

- **Strongly coupled multi-physics often requires a strongly coupled nonlinear solver**
- **Quadratic convergence near solutions**
- **Enables bifurcation, stability, optimization, integrated adjoint error estimation, sensitivity and UQ**

Stability, Accuracy and Efficiency

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

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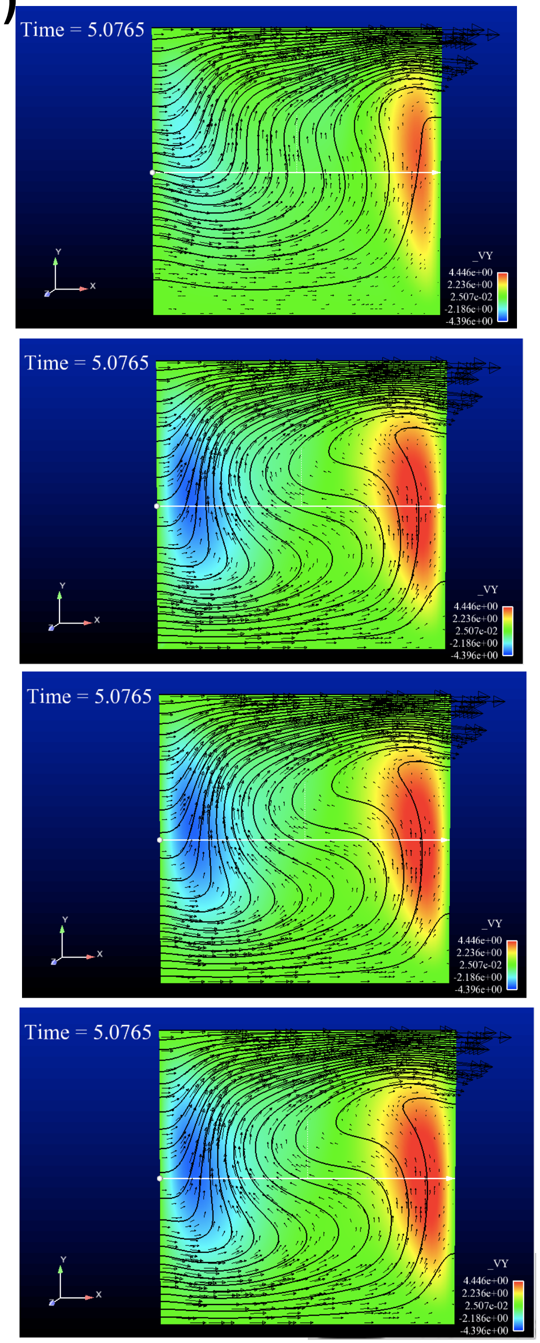
Equations of State (& e.g. HydroMagnetic Thermal Cavity)



Constant Density - Strictly incompressible

$$\rho = \rho_0 = \text{ constant}$$

Boussinesq Approximation

$$\rho \approx \rho_0 + \frac{\partial \rho}{\partial T}\Big|_0 (T - T_0) \text{ in momentum body force term}$$

$$\rho = \rho_0 \text{ and everywhere else}$$

Variable density Formulations

Low Flow Mach Number Approximation

$$P_{th} = f(\rho, T, Y_i) \text{ where } P_{th} \text{ is thermodynamic}$$
$$\text{not hydrodynamic pressure (P)}$$

Anelastic Approximation

$$P = f(\rho, T, Y_i) \text{ and } \frac{\partial \rho}{\partial t} = 0 \text{ in continuity eq.}$$

Compressible Fluid

$$P = f(\rho, T, Y_i)$$

Adjoint methods have been well studied and demonstrated for parabolic PDEs.
[e.g. Rannacher, Oden, C. Johnson, Estep, Bangerth, Barth, Suli, Braack, …..]

1) E.g. Steady Navier-Stokes Re = 1000 channel flow (Analytic sol.). QoI point value of x-vel.

$U_x = U_x^h$ + err. est.

$U_x = 123.85 + 0.20833 \sim 124.05833$

$U_{exact} = \quad = 124.05896$

QofI	Re	Estimated Value	Estimated Error	Effectivity Ratio
1	10	8.3125E-1	2.0833E-3	1.000
2	10	1.2385E+0	2.0779E-3	0.997
3	10	8.3125E-1	2.0833E-3	1.000
1	1000	8.3125E+1	2.0833E-1	1.000
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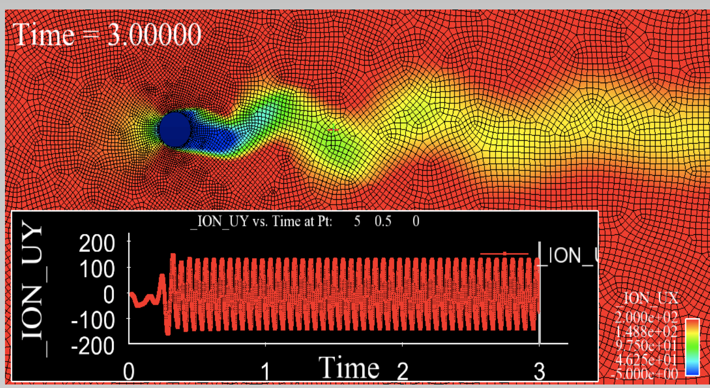
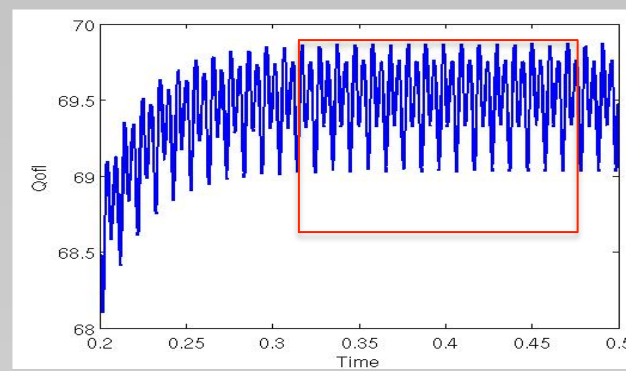
2) E.g Transient Navier-Stokes, vortex shedding behind Cylinder; QoI time-averaged drag

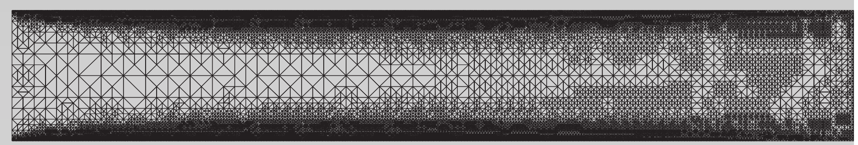




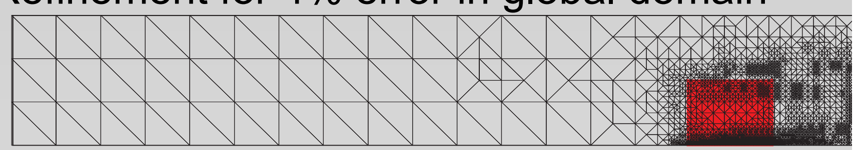
C_D^h = 69.4

Error Est. = 4.2%

3) Useful for error est. leading to mesh refinement (Conv./Diff. example)

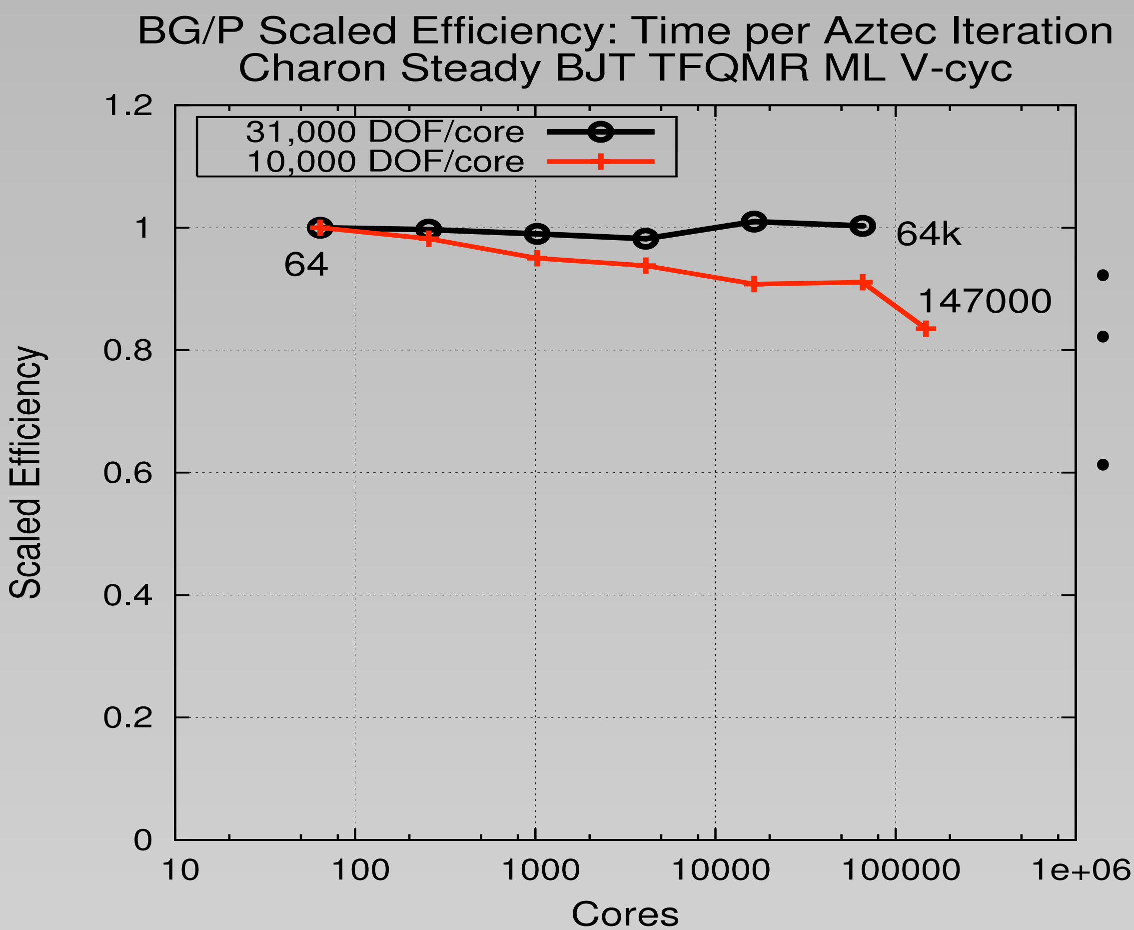


Refinement for 4% error in global domain



Refine for 4% error in localized region (QoI)

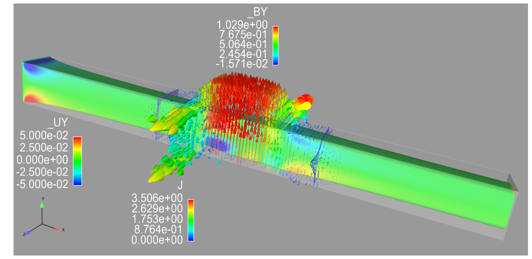
Comments on Formulations, Solution Algorithms and Underlying Software Arch.

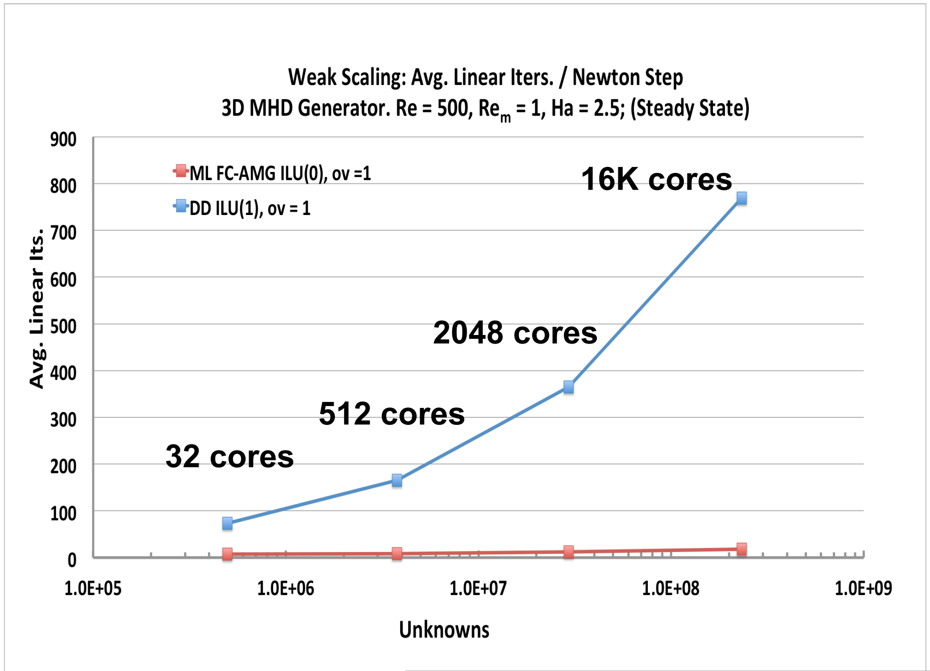


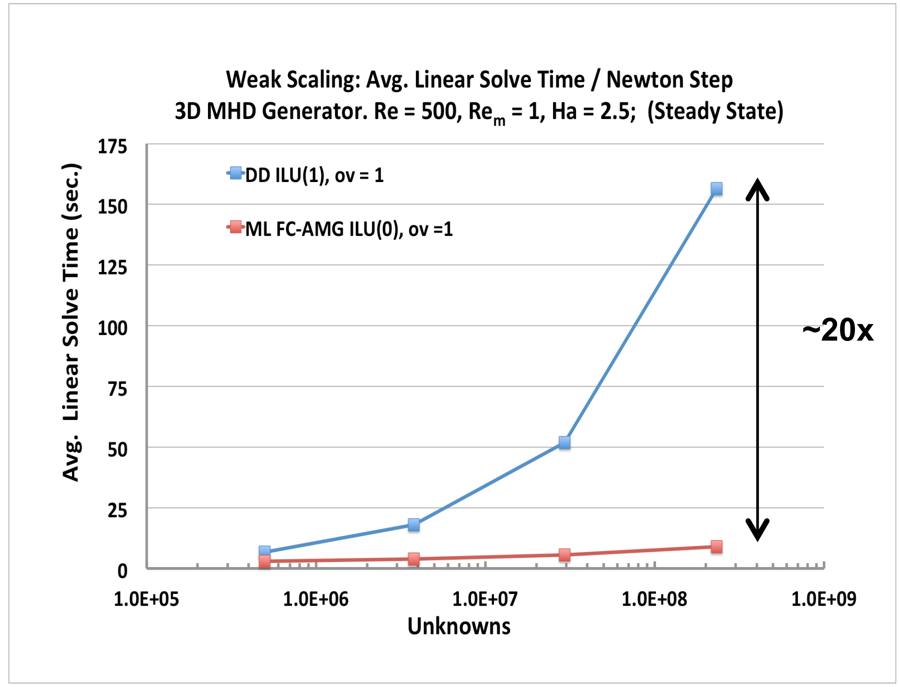
Scaling of Critical Solver Kernel used in Implicit FE MHD: Krylov solver and AMG V-cycle (Drift-Diffusion application*) [ML – Tuminaro, Hu, et. al.; *P.T. Lin IJNME, 91 (9) 2012]

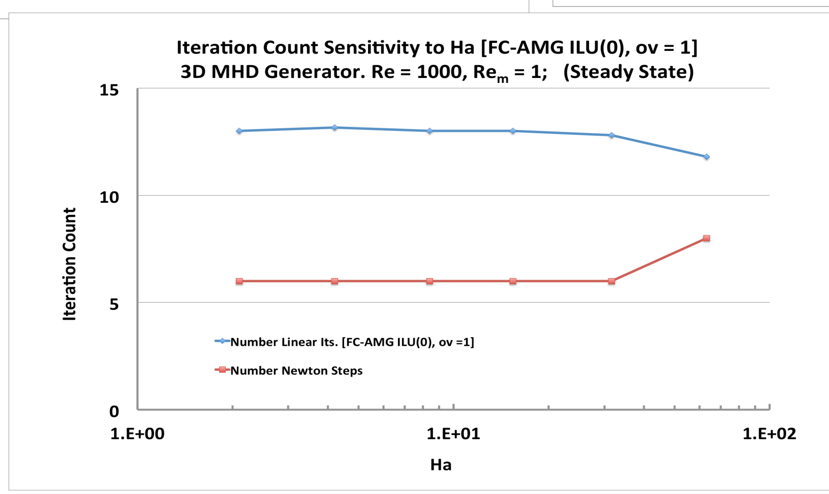
- **V-cycle scaling is very good.**
- **Now working on preconditioner construction**
- **Overall efficiency ~50% at this point for 1K processor count increase > 64K cores.**

Weak Scaling Gmres/FC-AMG ILU(0), ov = 1; V(3,3)
3D MHD Generator
Initial Titan (Cray XE7). [Re = 500, Ha = 2.4]









Scaling of Avg. Linear Its with Hartmann No.

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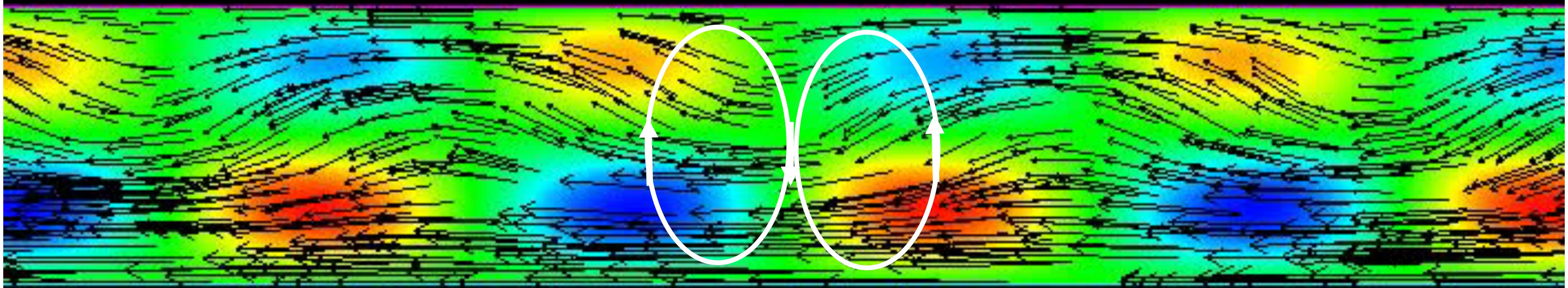
Vx



Hydro-Magnetic Rayleigh-Bernard Stability

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

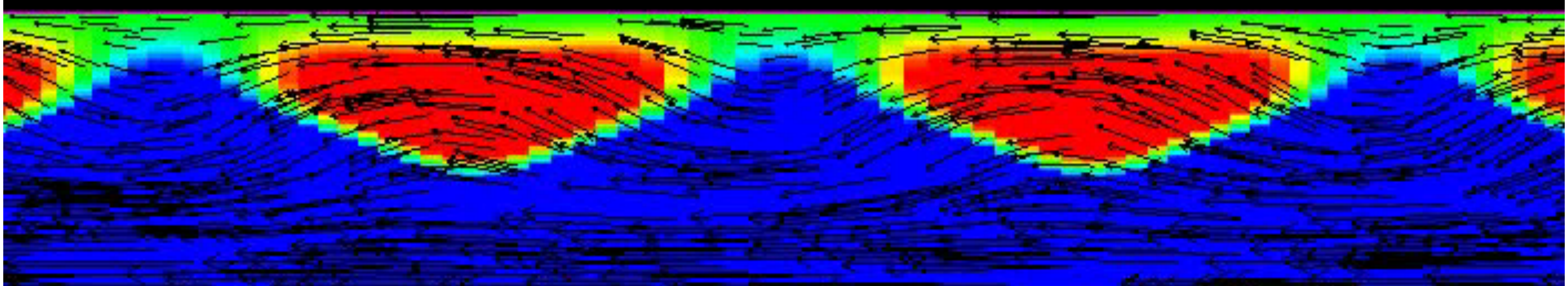
$$Pr = \frac{\nu}{\alpha}$$

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

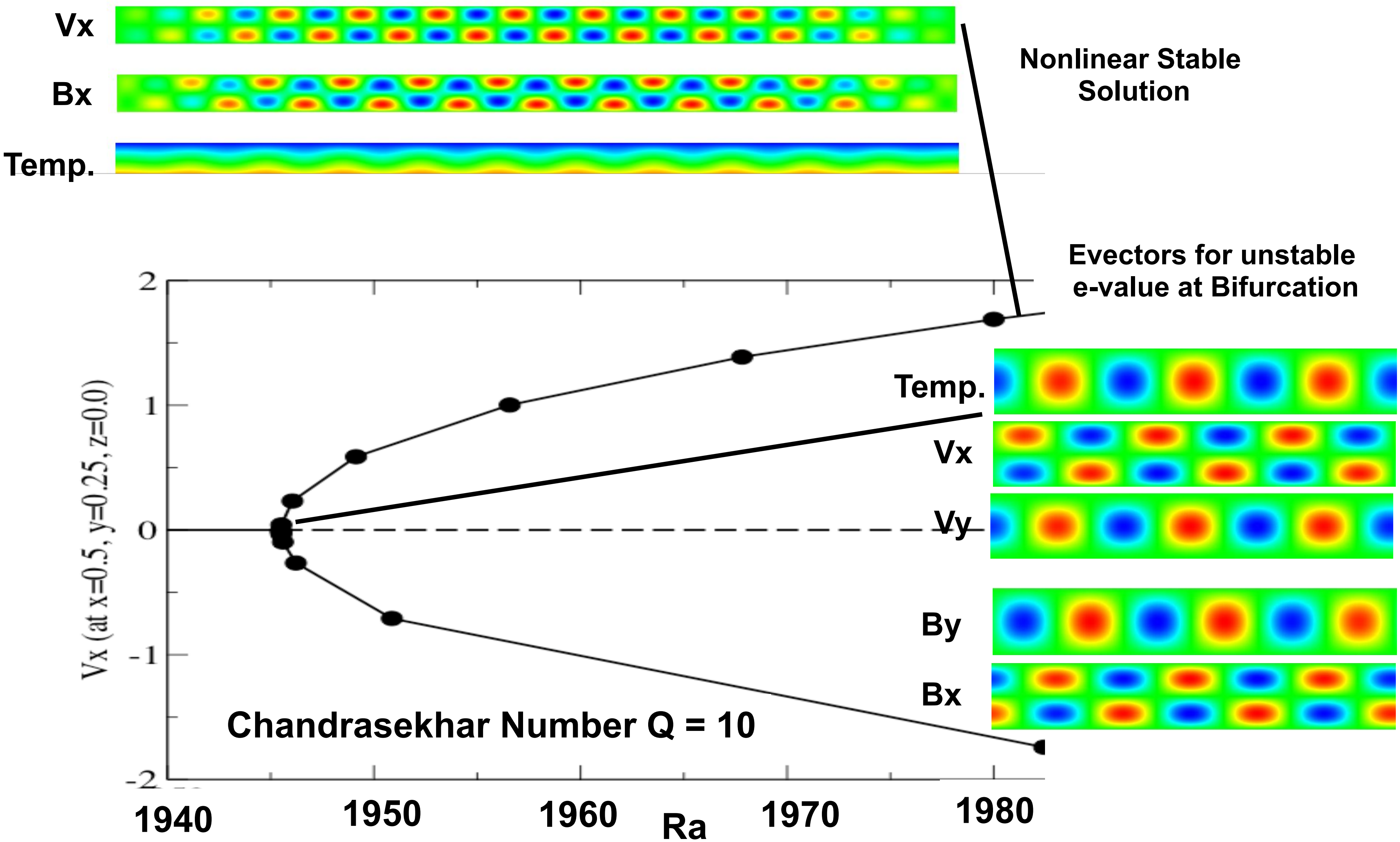
Stable Fields/Flow at Ra = 4000, Q = 81

Unstable Flow at Ra = 4000, Q = 144

Jz



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*

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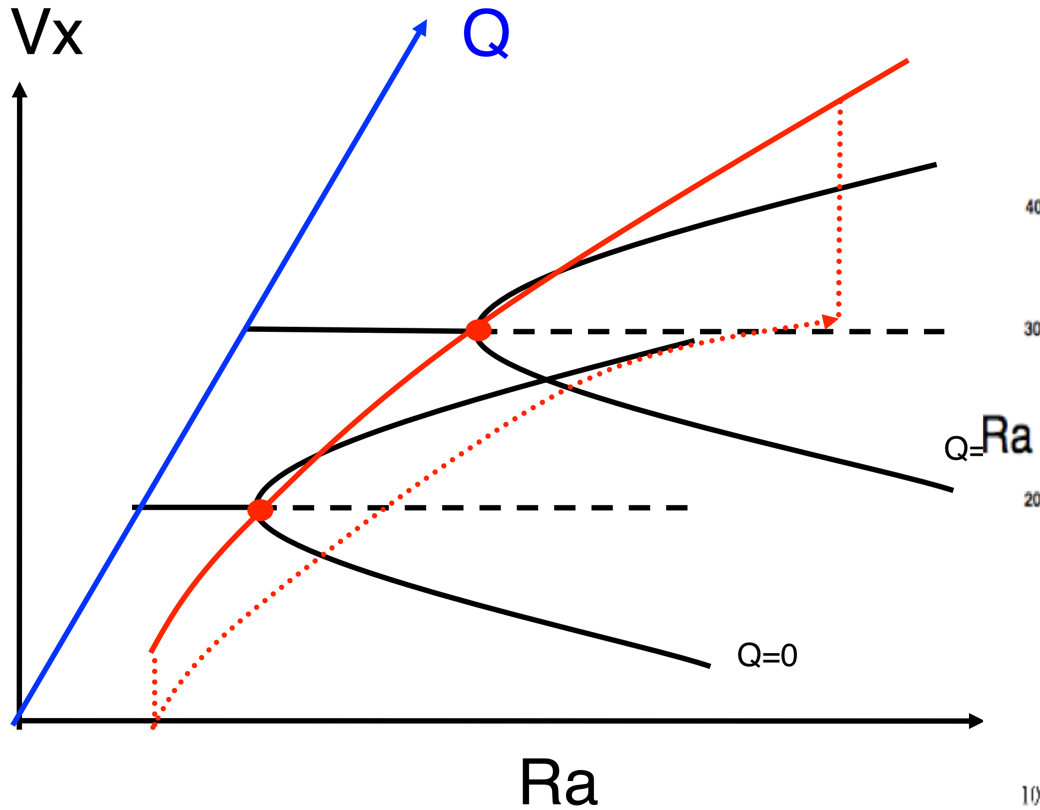
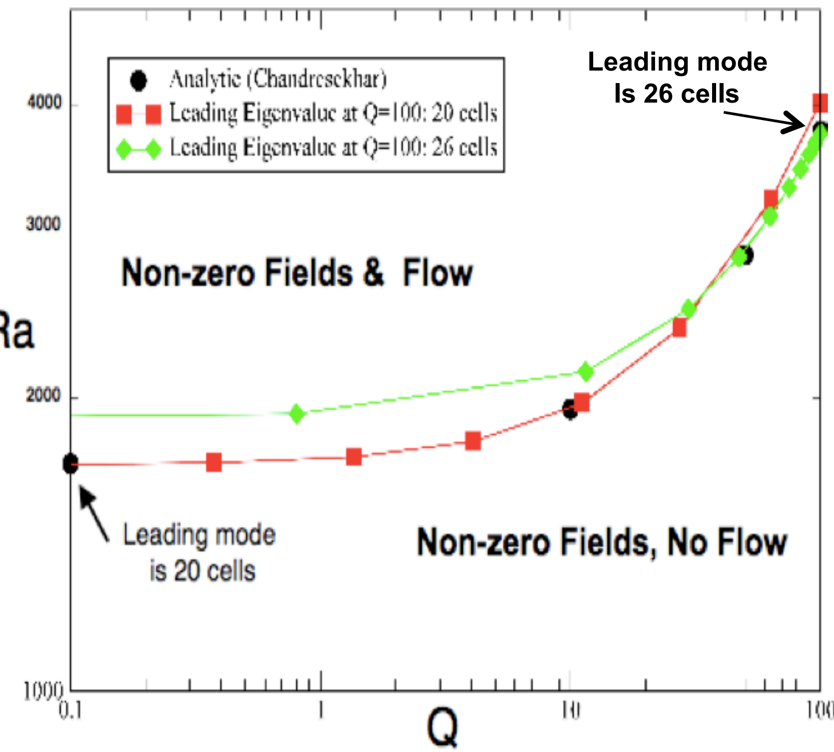
Bifurcation / Stability (Two-Parameter) Diagram

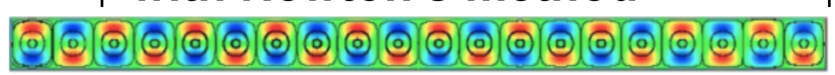


Multi-parameter continuation can track critical points (pitchfork bifurcation, Hopf bifurcation, turning points, etc.) with NK solvers [LOCA - Salinger, Pawlowski, Phipps]

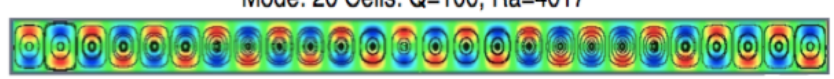
Most unstable mode compresses with increase in magnetic field strength



with Newton's method



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



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

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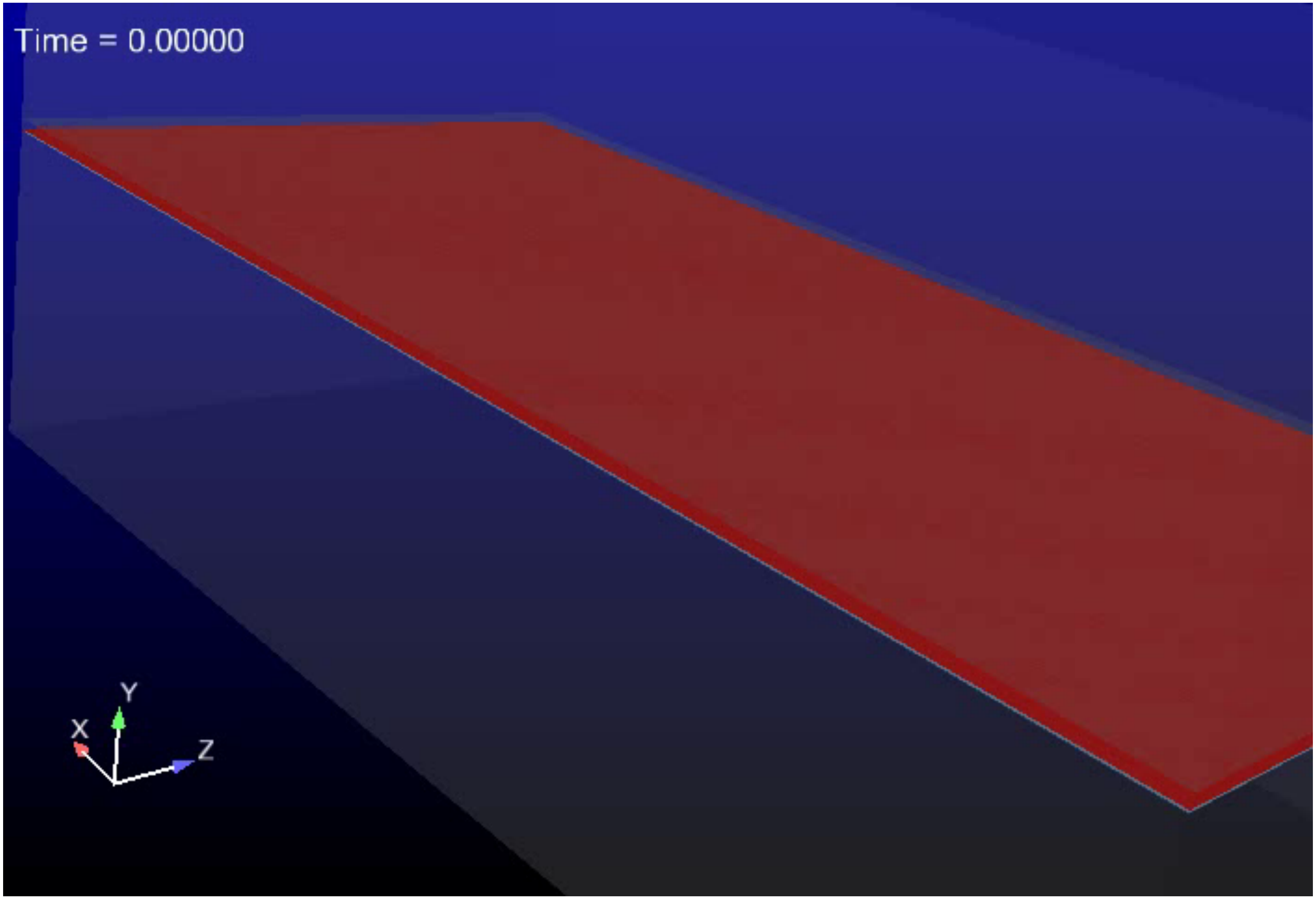
Kelvin-Helmholtz Unstable Shear Layer: Re = 50,000



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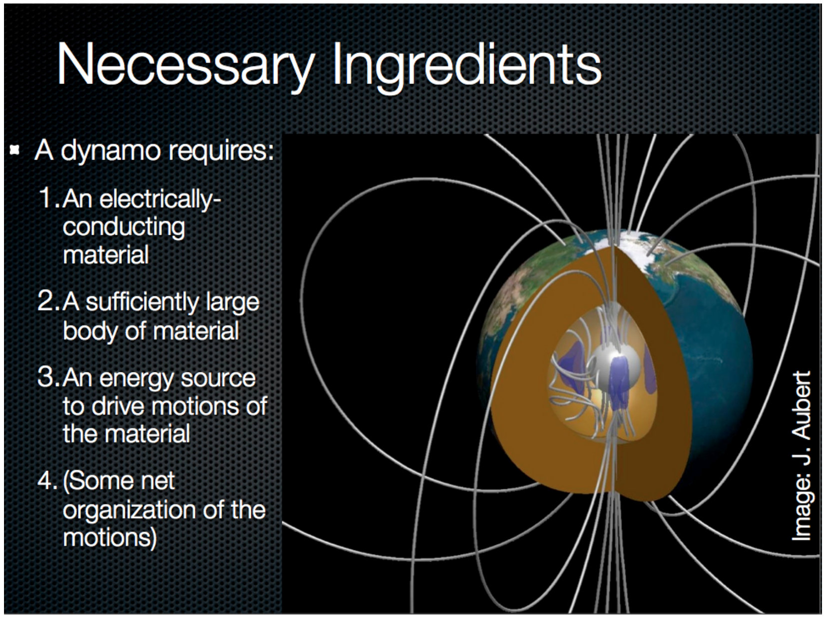
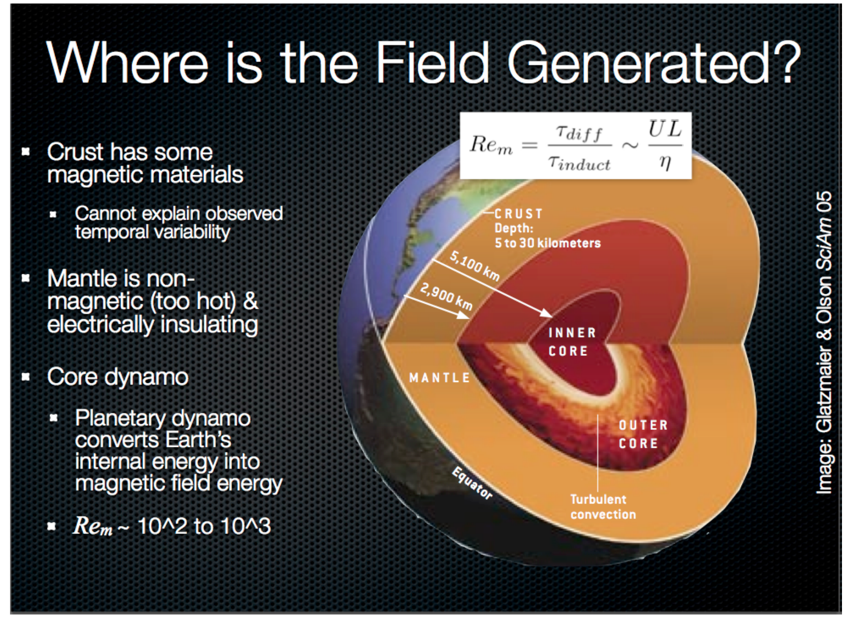
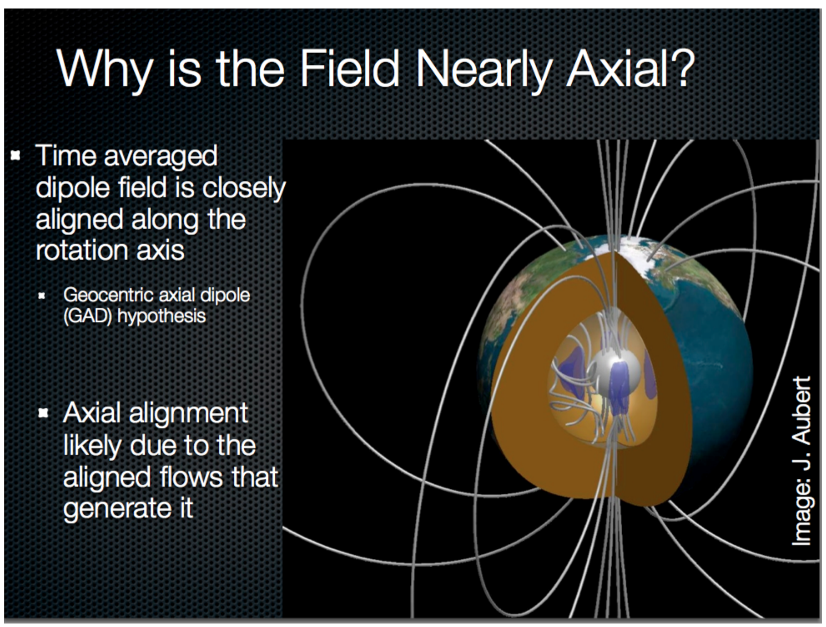
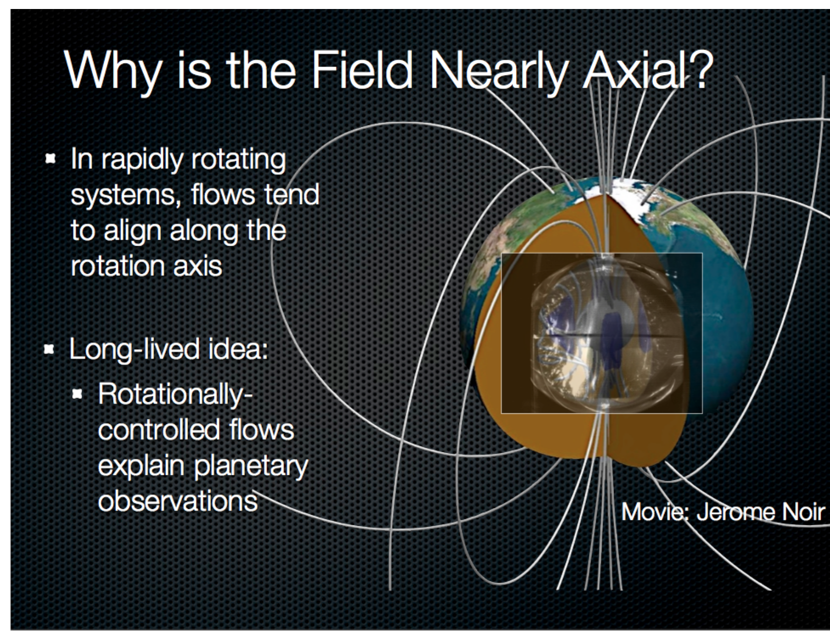
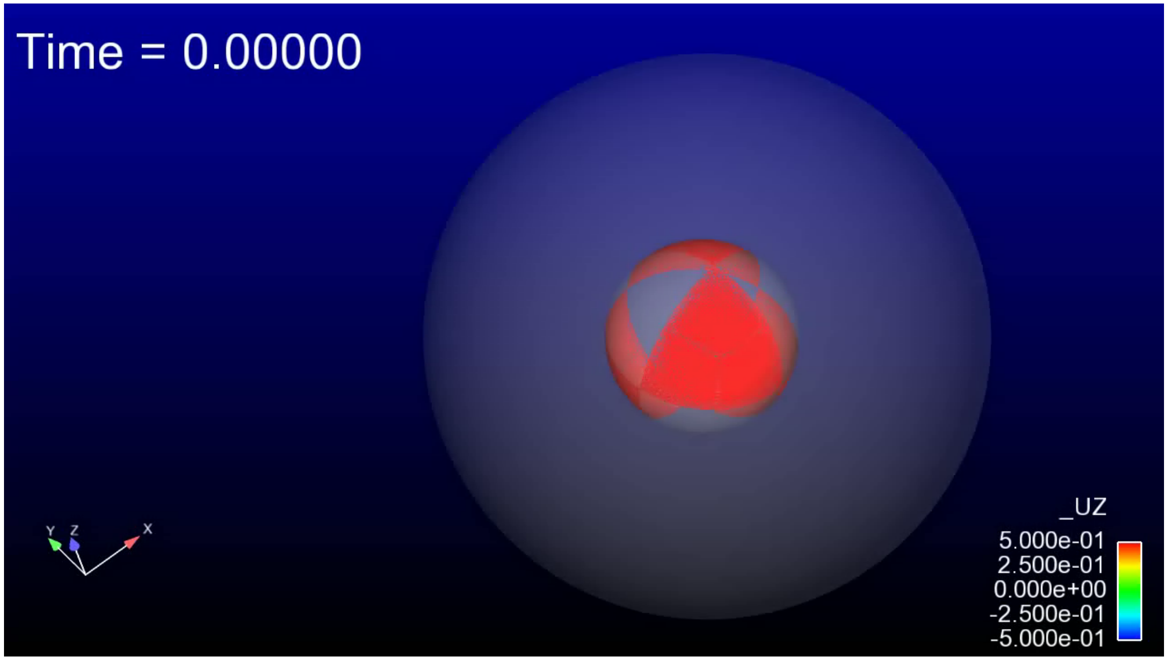
E.g. Geodynamo Mechanisms and Simulations
Geodynamo Slides from J. Aurnou Talk (UCLA – Earth and Space Sciences Dep









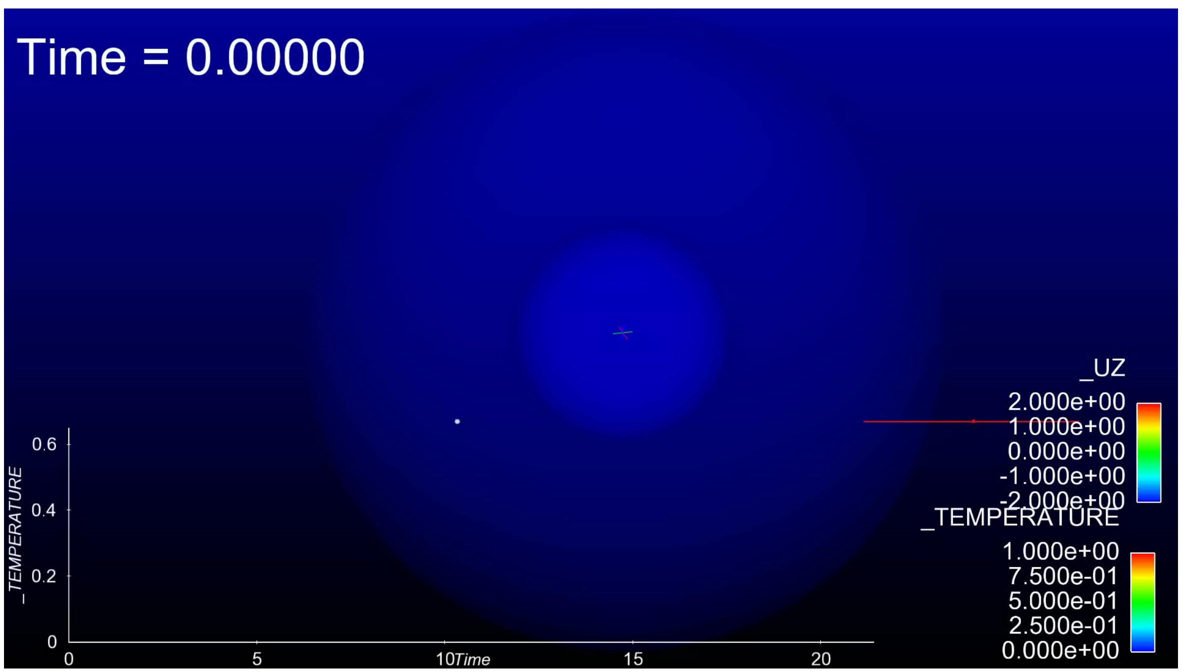


Christensen et. al.
Rotating Thermal Conv. Benchmark
Ra = 1e5, E = 1e-3;

E_kin = 58.348 +- 0.050

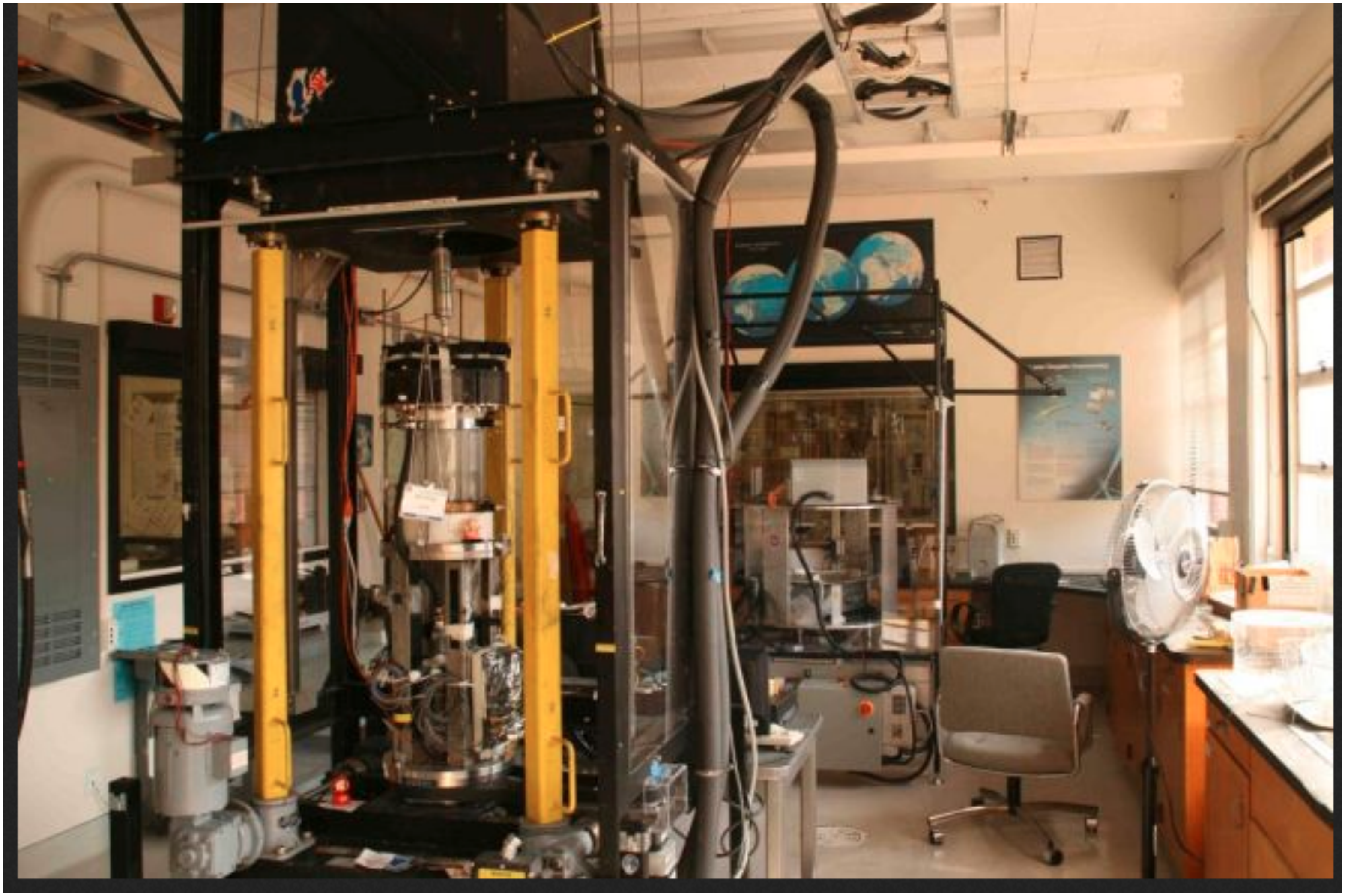
Preliminary
Drekar 1.3M elem. Soln.

E_kin = 58.86462
This is within .9%



Ra = 1.54e5, E = 1e-3;

E.g. Geodynamo Mechanisms and Experiments
J. Aurnou - Spin Laboratory (UCLA – Earth and Space Sciences Dept.)



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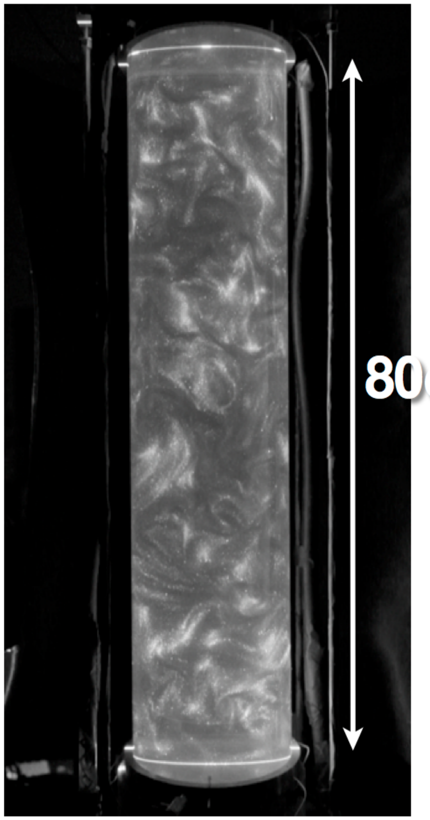
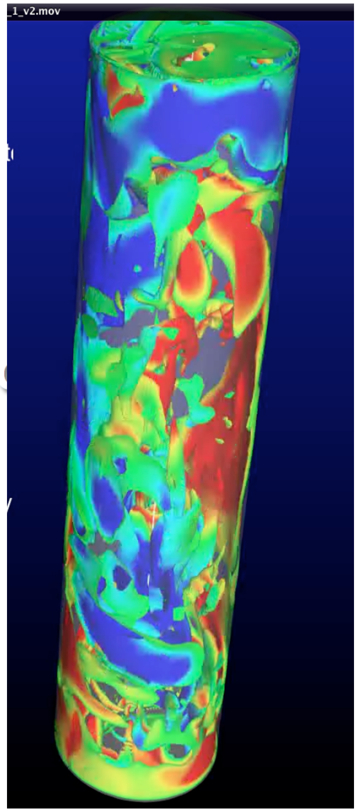


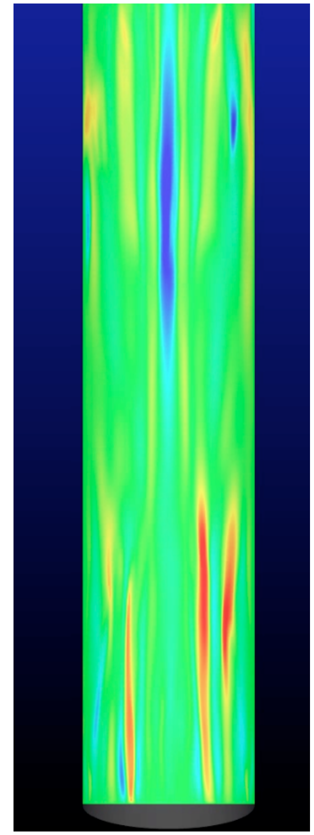


Ra~ 3e10

Ra = 1e10

Aurnou
Lab Exp.

Preliminary Drekar Simulation



Ra~ 6e10; E ~1e-7

Ra = 1e11; E = 1e-7

Preliminary Drekar Simulation

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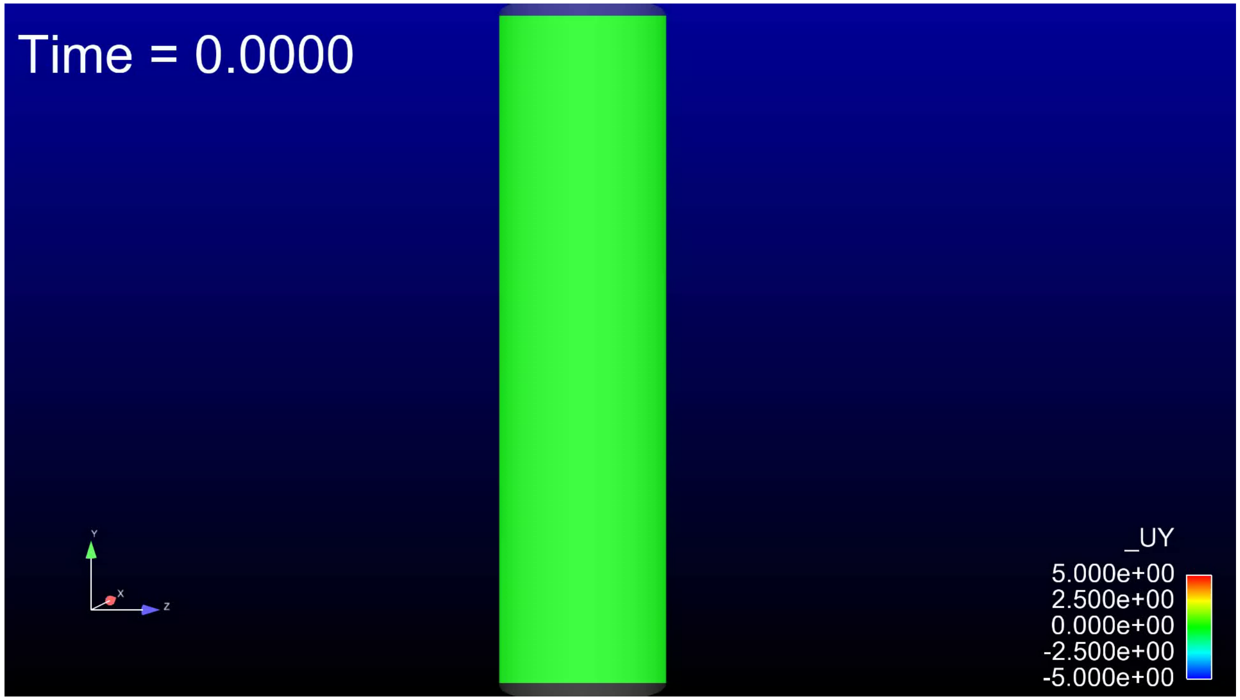
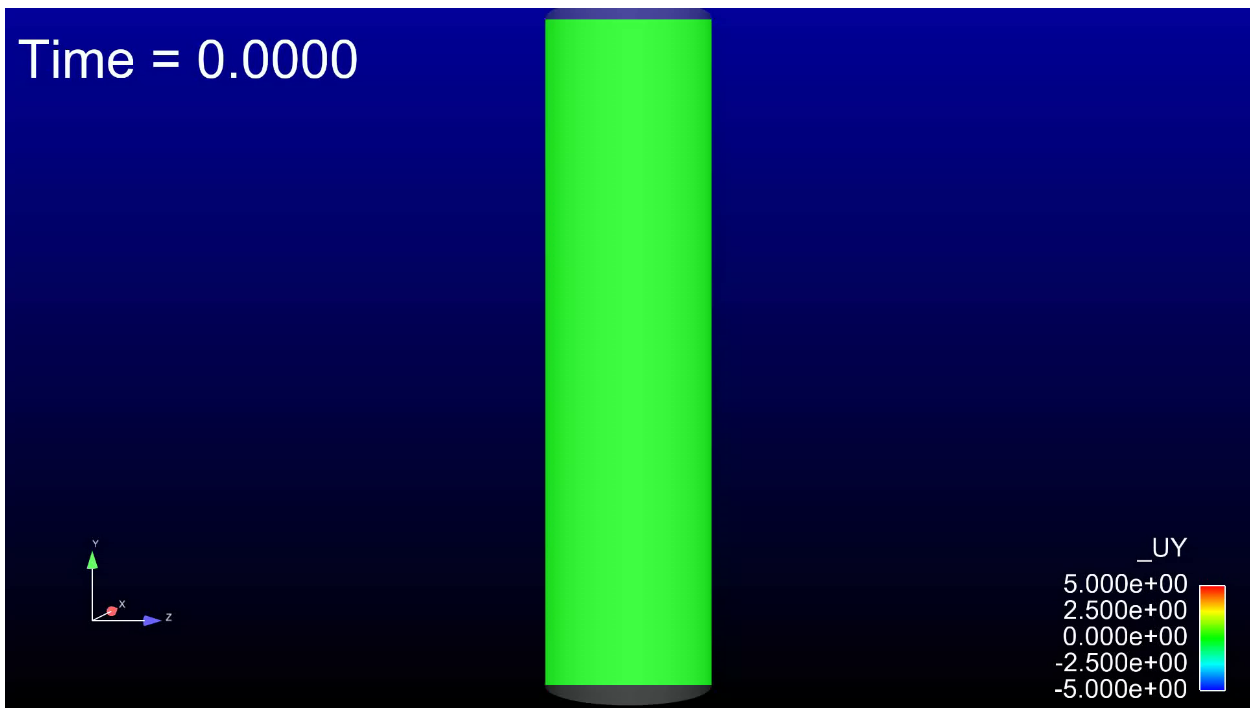
Ra = 1e11;
E = 0



Ra = 1e11;
E = 1e-7



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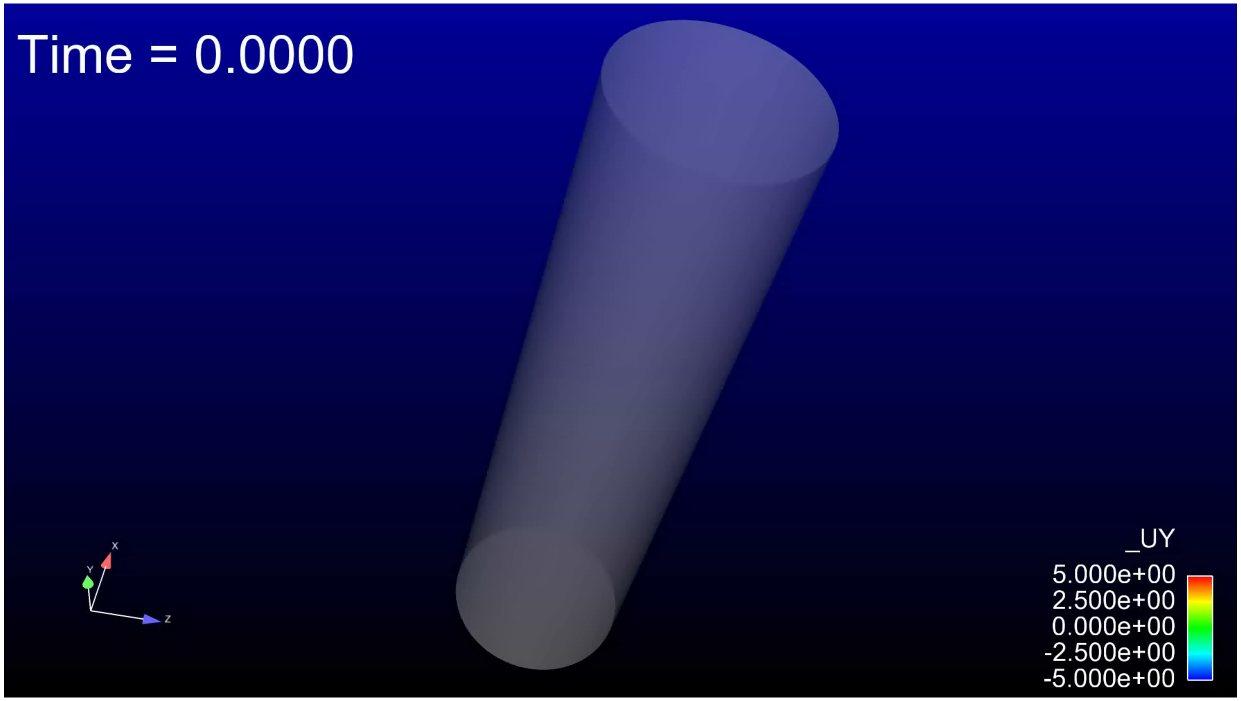
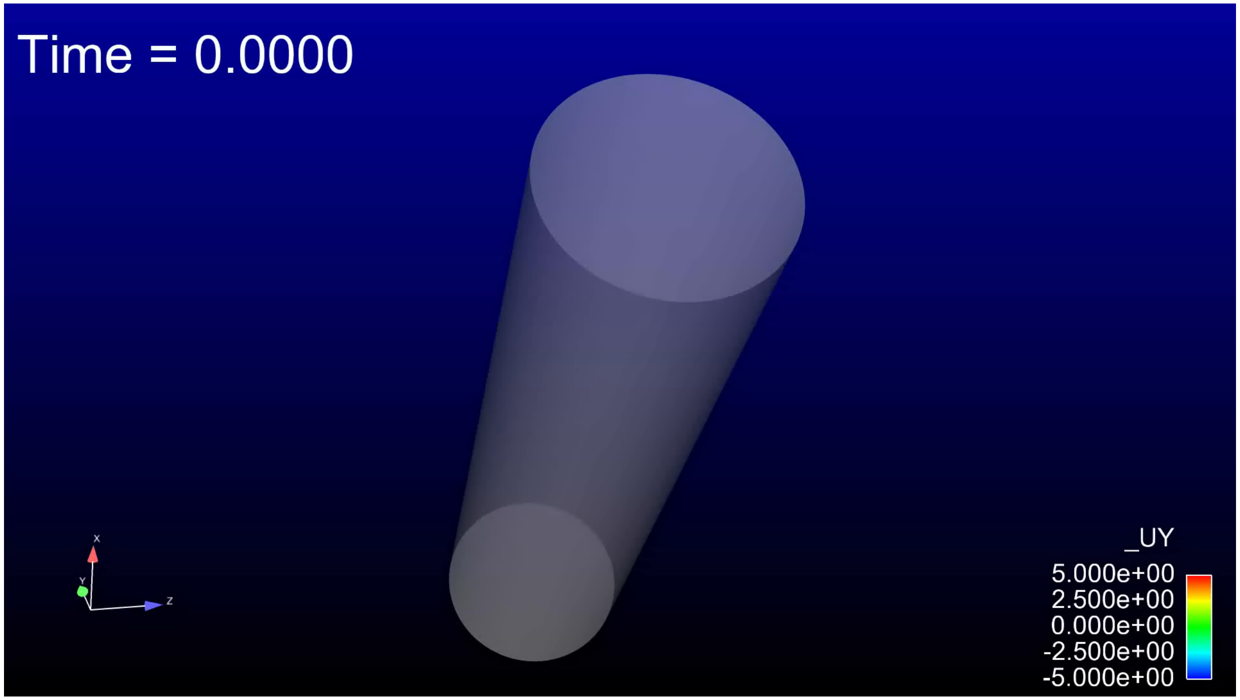
Ra = 1e11;
E = 0



Ra = 1e11;
E = 1e-7



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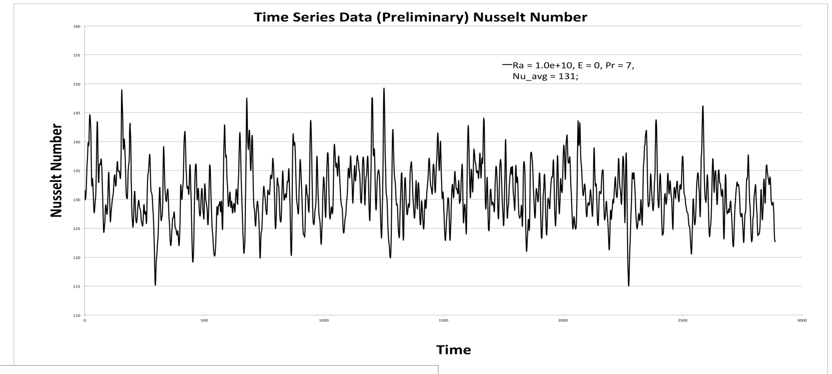
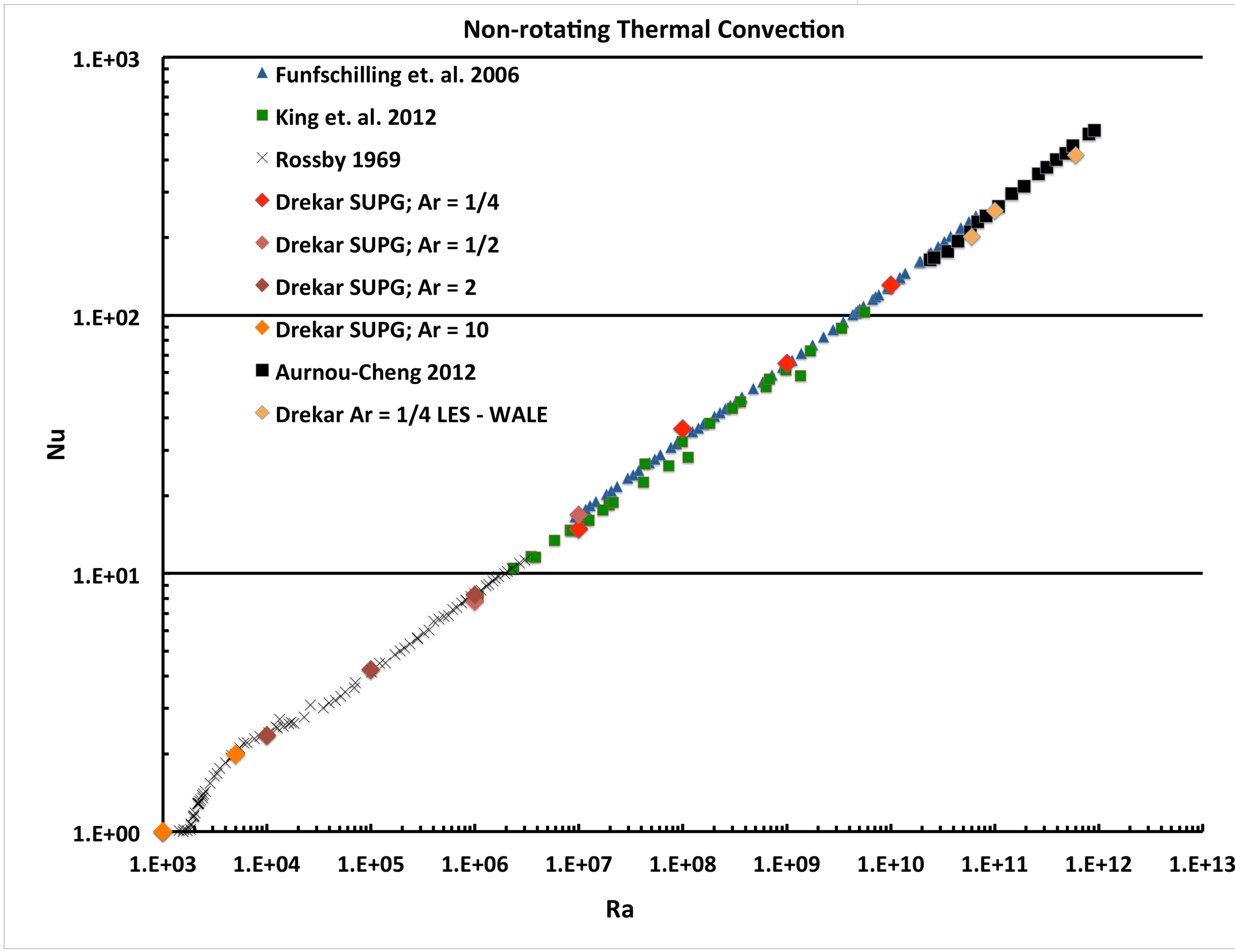
Preliminary Comparison Non-rotating Thermal Convection Experiments and Drekar





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Initial Exploration of Variational Multi-Scale LES for Resistive MHD

(with D. Sondak and A. Oberai)

VMS MHD Spectral Method

- Momentum and induction cross-correlation terms
- Periodic BCs -> only nonlinear terms
- VMS provides high wavenumber stability (cross-correlation and self-correlation terms, Hughes et. al.)
- Residual based models

(D. Sondak and A. Oberai to appear in Phy. of Plasmas)

VMS FE MHD Method

- VMS for FE implementation
- Fully-implicit Newton-Krylov w/AMG prec.
- Residual based cross-terms, self-corr.
- $(\Delta x)^2$, $(\Delta x)^3$, ... high order possible
- MHD Studies Underway
  - Isotropic decay: Taylor – Green
  - Turbulent MHD channel flow

Taylor-Green MHD Isotropic Decay

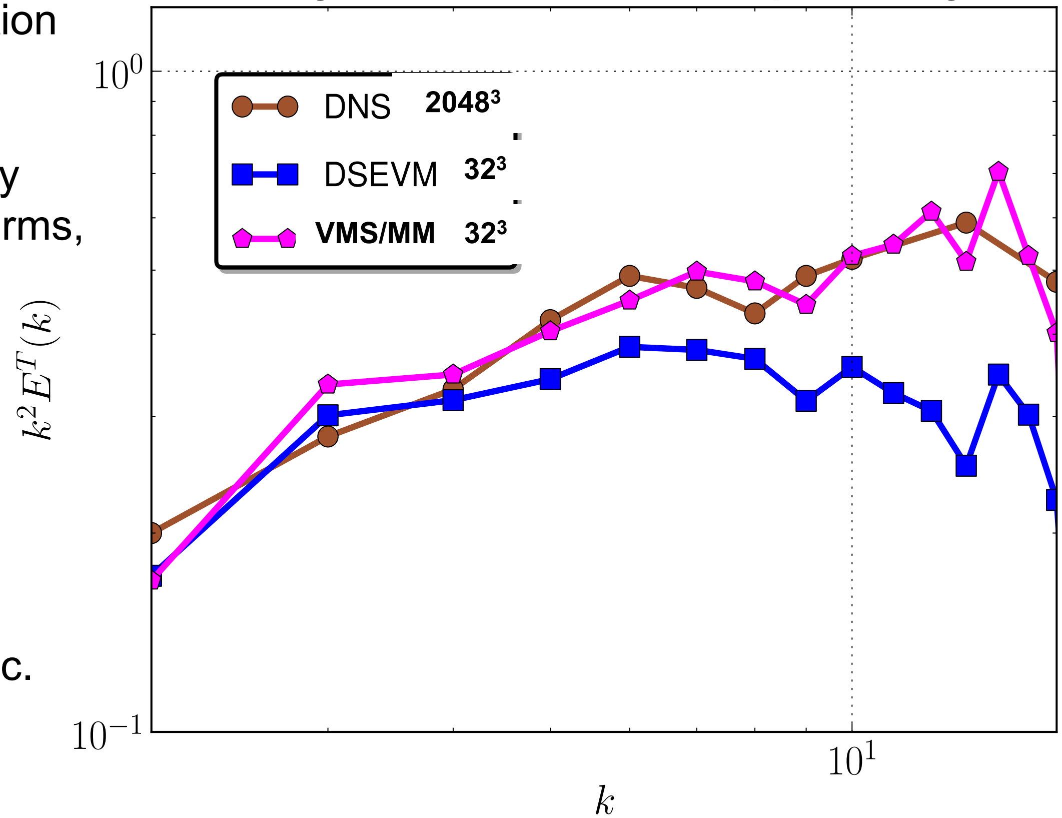

Figure: DNS: A. Pouquet et. al. Geo. Astro. Fluid Dyn. (2010); DSEVM after Germano (1991) & Theobald et. al. (1994);

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The End