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Robust, Scalable, Accurate, and Efficient Computational Formulation and Solution Methods for Transport/Reaction and Extended MHD Simulations

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Outline of Overview

- Motivation
- Goals
- Highlights of Previous funding period
  - Overview MHD for Resistive and Extended MHD
  - Some details
    - Scalable Resistive / Hall MHD
    - Scalable Unstructured FE Resistive MHD
  - Selected Impact Highlights

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⇒ **Computational Simulations of Complex Highly Nonlinear Multiphysics**

⇒**<u>Achieving Predictive Simulations of Complex Multi-physics Systems (PDEs)</u>**

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

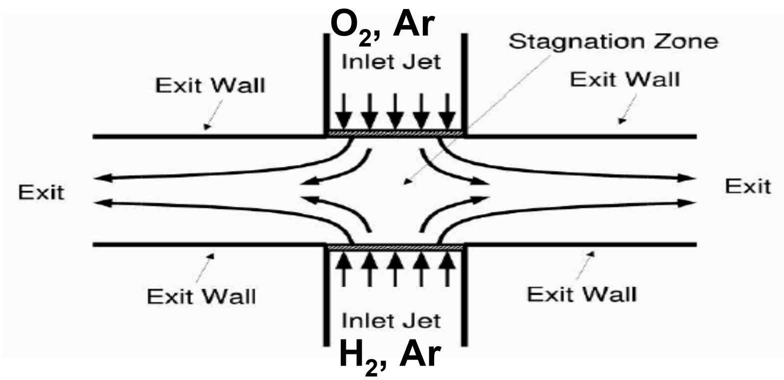
These systems are characterized by a myriad of complex, interacting, nonlinear multiple time and length scale physical mechanisms.

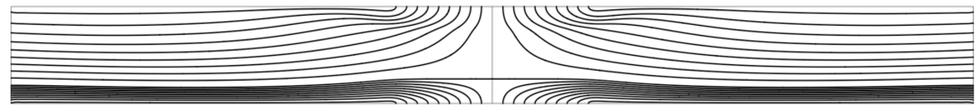
These mechanisms can balance to produce:

- **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.**

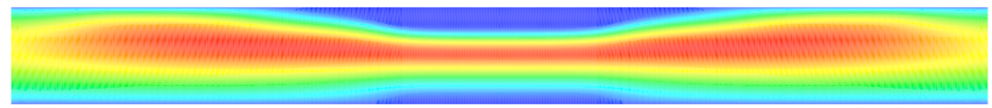
e.g. Fusion Reactors (Tokomak -ITER; Pulsed - NIF & Z-pinch); Fission Reactors (GNEP); Astrophysics; Combustion; Chemical Processing; Fuel Cells; etc.

Multiple-time-scale systems: Bifurcation Analysis of a Steady Reacting H_2, O_2, Ar, Opposed Flow Jet Reactor

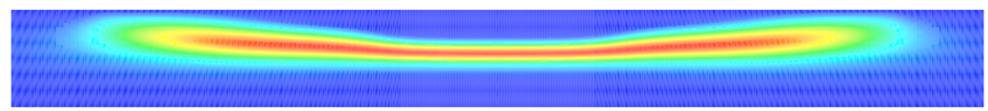




Streamlines

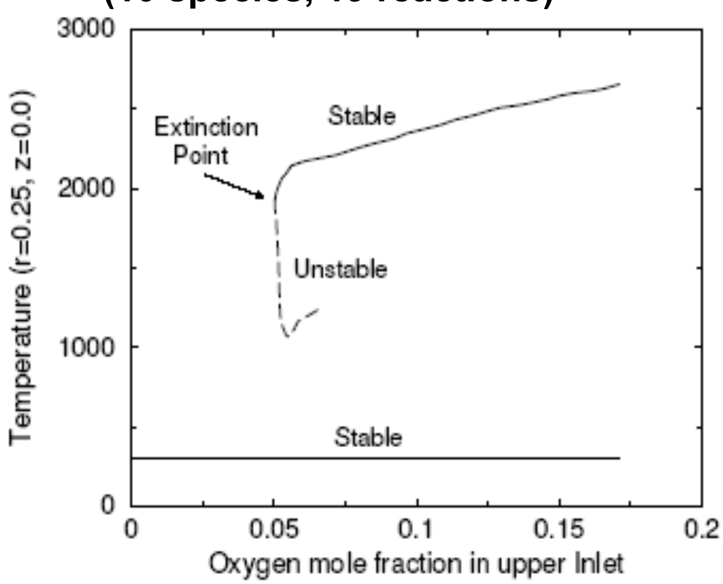


Temperature (Min. 300^{o}K, Max 2727^{o}K)



OH (Min. 0.0, Max 0.177)

70 steady state reacting flow solves (10 species, 19 reactions)



<u>Approx. Physical Time scales (sec.):</u>

- **Chemical kinetics: 10^{-12} to 10^{-4}**
- **Momentum diffusion: 10^{-6}**
- **Heat conduction: 10^{-6}**
- **Mass diffusion: 10^{-5} to 10^{-4}**
- **Convection: 10^{-5} to 10^{-4}**
- **Diffusion flame dynamics: ∞ (steady)**

(w/ Pawlowski, Salinger – MPSalsa)

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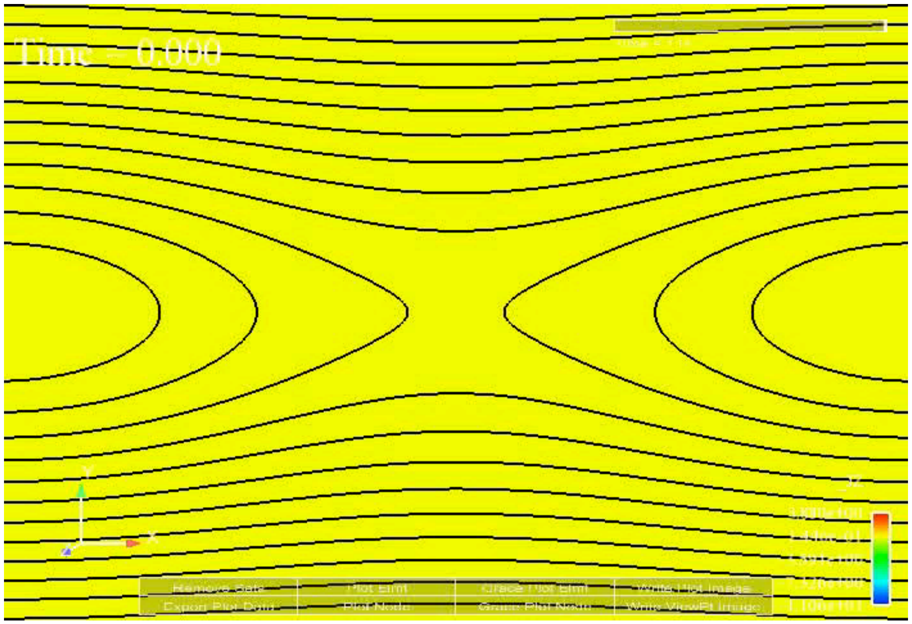
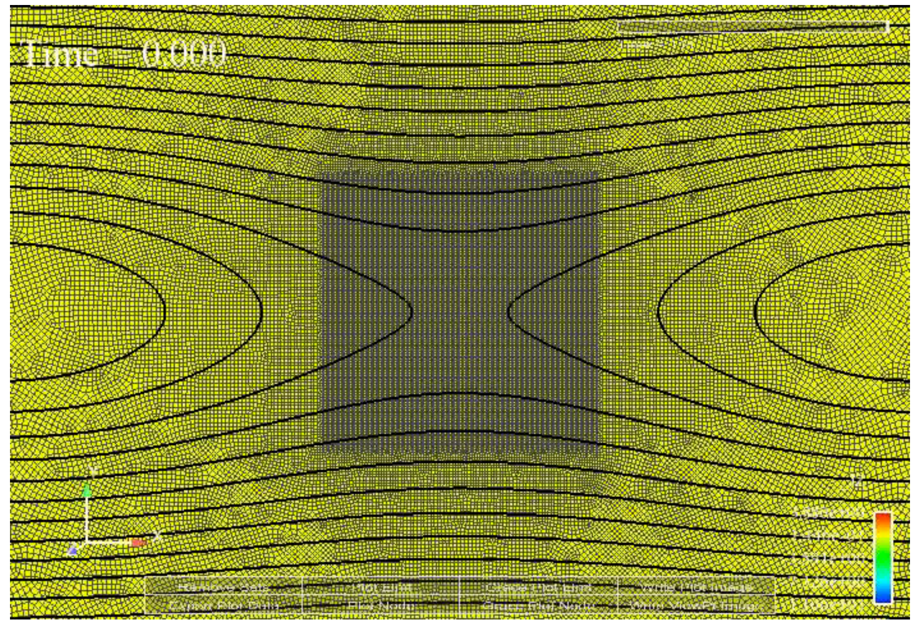
Multiple-time-scale systems: E.g. Driven Magnetic Reconnection with a Magnetic Island Coalescence Problem (Incompressible)

2D axisymmetric Simulation



Full 3D Simulation (note: non-axisymmetric mode)



<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 Merging: 10^0**

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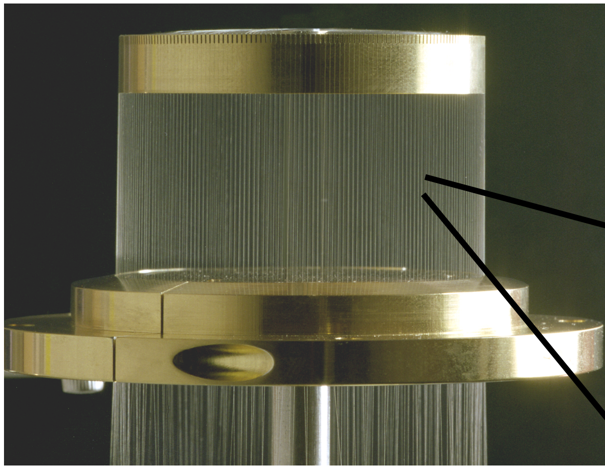
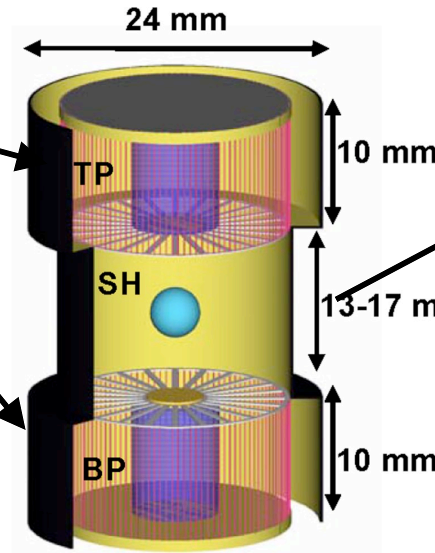
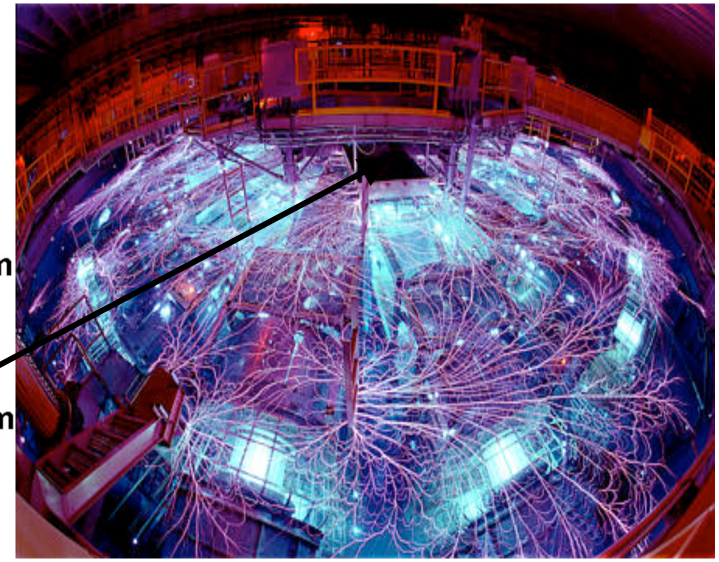
Z-pinch Double Hohlraum Schematic







Z Machine (Approximate Ranges)

100ns current rise time for 20 MA Electrical Current

250 ns plasma shell collapse and stagnation

10-30 ns X-ray power pulse ~200 TW power

A Recent Review: K. Matzen, et. al., POP 12, 055503 (2005)

Computational Stability Constraints:

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

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

Hall Physics -> $\Delta t < \Delta x^2/(V_A\ di)$

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Relevance and Impact of Advanced Resistive and Extended MHD algorithms on DOE Science

Advanced simulation algorithms for MHD are need for a variety of high-profile DOE science areas

- **Fusion:**

  ITER will define whether fusion energy is a viable option as a futre energy source. The Fusion Simulation Project (FSP) is being defined, with the goal of developing a first principles simulation capability for a Tokamak device. Extended MHD (XMHD) will be an essential component of this capability.

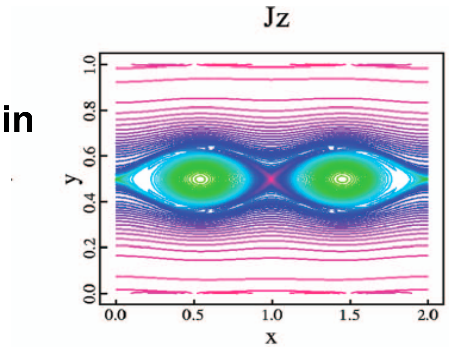
- **Magnetic Reconnection: basic plasma physics**
  - **plasma confinement disruptions in fusion devices. SciDAC center.**
  - **Magnetospheric sub-storms**
  - **Solar flares**
  - **Formation of intergalactic jets**

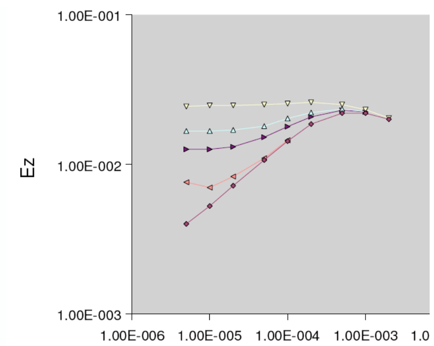
Overall Project Goals:

- **Develop stable, accurate, physics compatible, scalable and efficient fully-implicit computational formulations for xMHD and PTR (e.g. SNL Cray XT3 12.5K nodes, 25K cores)**
- **Develop and evaluate scalable physics-based preconditioners, based on multi-level methods**
- **Produce comprehensive accuracy, convergence, stability and scalability studies employing challenging prototype problems.**
- **Produce large-scale computational demonstrations on selected science / technology problems**

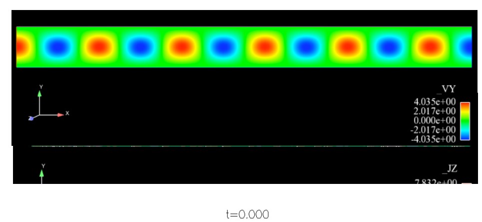
<u>Examples</u>

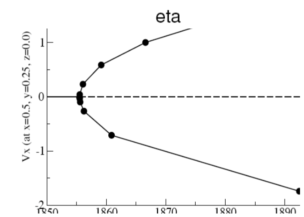
- **Magnetic Reconnection Studies with application in Astrophysics (solar flares, …) and Fusion Energy (instabilities, …)**





- **Hydro-Magnetic Rayleigh Bernard with application to Astrophysics, Geodynamo**

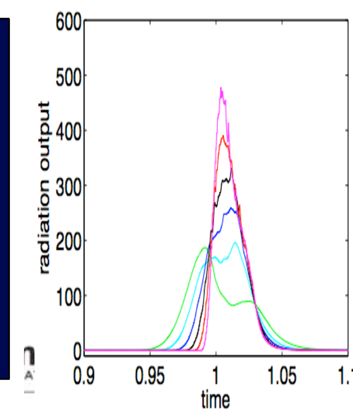




- **Hydro-Magnetic Rayleigh-Taylor**

(e.g. Z-pinch [HEDP])

Driven Euler Simulation



Currently: Low Mach Number MHD Formulation(s)

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla \cdot [\rho\mathbf{u} \otimes \mathbf{u} + P\mathbf{I} + \mathbf{\Pi}] - \mathbf{J} \times \mathbf{B} = \mathbf{0}$$

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

$$\frac{\partial E}{\partial t} + \nabla \cdot [E\mathbf{u}] + \gamma E \ \nabla \cdot \mathbf{u} + \mathbf{\Pi} : \nabla\mathbf{u} + \nabla \cdot \mathbf{q} = \eta\|\mathbf{J}\|^2 \qquad E = e + \frac{1}{2}\|\mathbf{v}\|^2$$

$$\partial_t\mathbf{B} + \nabla \times \mathbf{E} = \mathbf{0} \qquad \mathbf{E} = -\mathbf{v} \times \mathbf{B} + \eta\mathbf{J} + \underbrace{\frac{1}{en}(\mathbf{J} \times \mathbf{B} - \nabla\mathbf{P_e})}_{\text{Hall}} \cdot \qquad \mathbf{J} = \frac{1}{\mu_0}\nabla \times \mathbf{B}$$

Conservation Law System: Magnetic Flux

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

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

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

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

Why Newton-Krylov Methods?

Newton-Krylov

→ Direct-to-steady-state

→ Fully-implicit transient

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

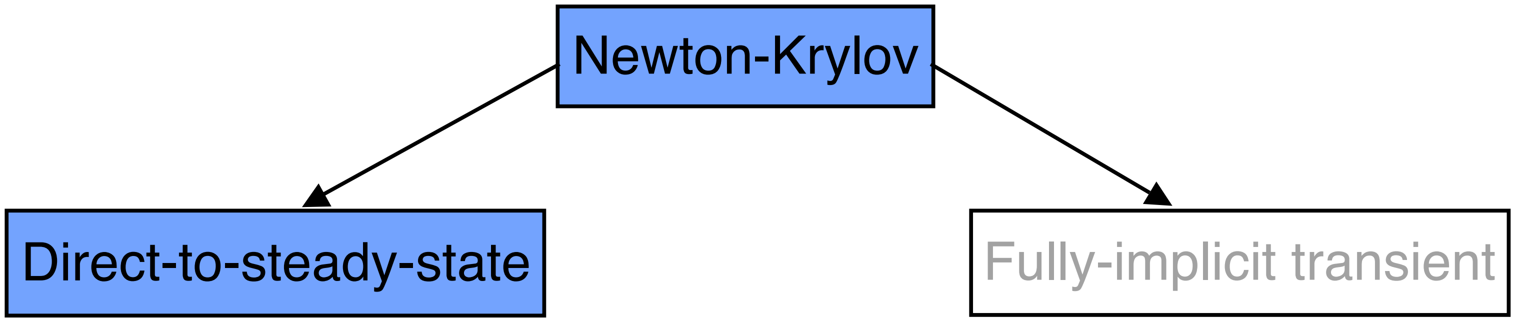
e.g.

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

<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

Why Newton-Krylov Methods?



Convergence properties

• 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

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

Inexact Newton-Krylov

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

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

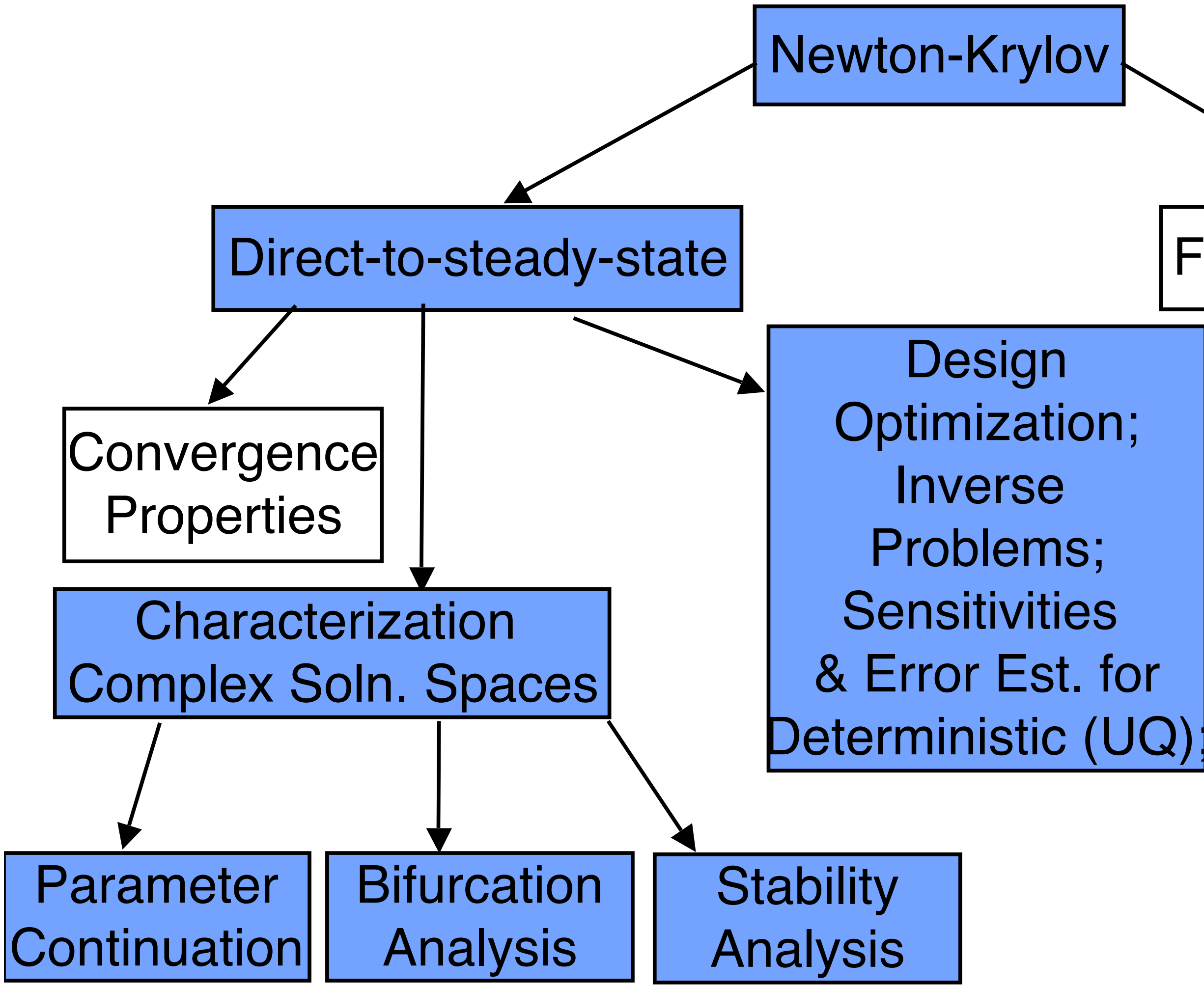
Jacobian Free N-K Variant

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

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

See e.g. Knoll & Keyes, JCP 2004

Why Newton-Krylov Methods?



UQ Probabilistic approaches:

- **Sampling (e.g quadrature, MC, etc.),**
- **Direct (e.g Polynomial Chaos)**

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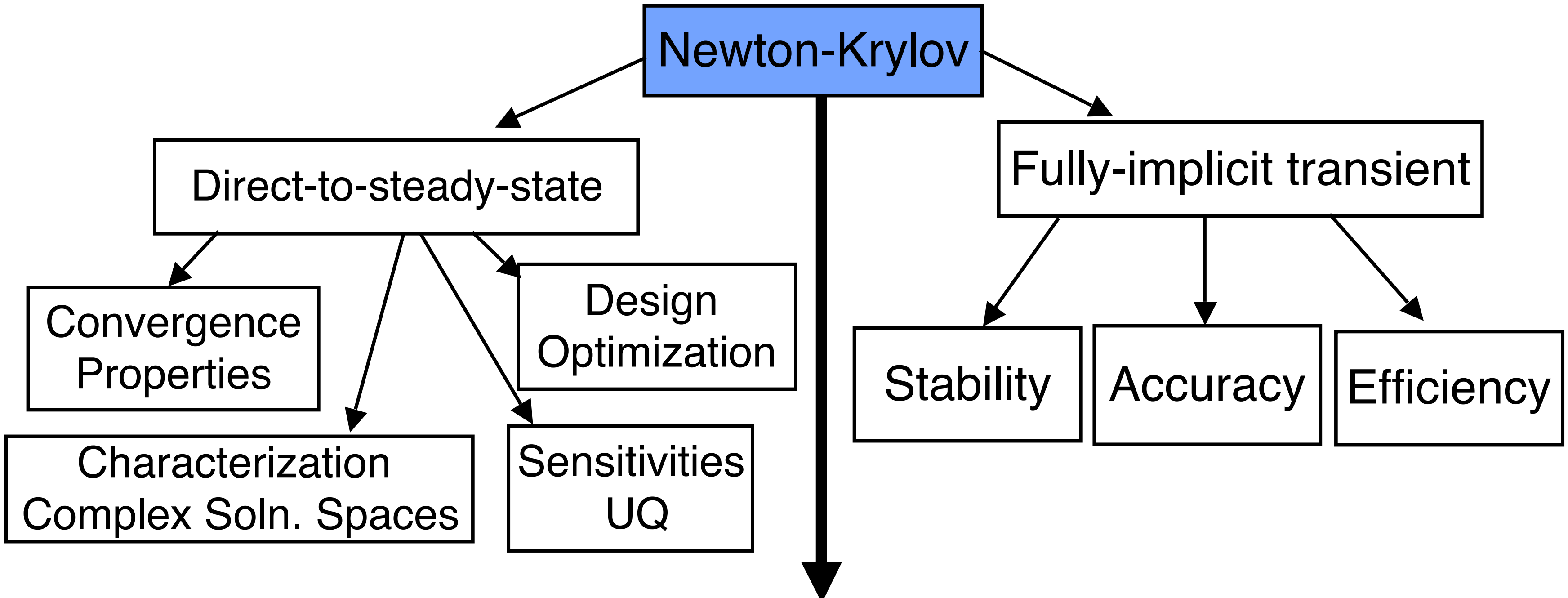
Why Newton-Krylov Methods?



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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Algorithmic challenges in XMHD

- XMHD has mixed character, with strongly hyperbolic and parabolic components.
- Numerically, XMHD is a nonlinear algebraic system of very stiff equations:
  - Elliptic stiffness (diffusion): $\kappa(J) \sim \frac{\Delta t\, D}{\Delta x^2} \gg 1$
  - Hyperbolic stiffness (linear and dispersive waves): $\kappa(J) \sim \Delta t\, \omega_{fast} \sim \frac{\Delta t}{\Delta t_{CFL}} \gg 1$
- Brute-force algorithms will not be able to cover the span between disparate time/length scales, regardless of computer power (SBES report).
- Key algorithmic requirement: SCALABILITY $[CPU \sim \mathcal{O}(N/n_p)]$!
  - Minimize number of degrees of freedom N: spatial adaptivity.
  - Follow slowest time scales (application dependent): implicit time stepping.
- Scalable implicit methods require MULTILEVEL approaches:
  - A fundamental component of iterative ML methods is the SMOOTHER.
  - XMHD is strongly hyperbolic $\Rightarrow$ smoothing is a serious challenge (diagonally submissive for $\Delta t > \Delta t_{CFL}$).
    - Previous attempts to use multilevel methods (two-level NKS, MG-NKS) on XMHD have failed to demonstrate a scalable XMHD solver.

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Parabolization and Schur complement: an example

- PARABOLIZATION EXAMPLE:

$$\partial_t u = \partial_x v \ , \ \partial_t v = \partial_x u.$$

$$u^{n+1} = u^n + \Delta t \partial_x v^{n+1}, v^{n+1} = v^n + \Delta t \partial_x u^{n+1}.$$

$$\boxed{(I - \Delta t^2 \partial_{xx}) u^{n+1} = u^n + \Delta t \partial_x v^n}$$

- PARABOLIZATION via SCHUR COMPLEMENT:

$$\begin{bmatrix} D_1 & U \\ L & D_2 \end{bmatrix} = \begin{bmatrix} I & UD_2^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} D_1 - UD_2^{-1}L & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} I & 0 \\ D_2^{-1}L & I \end{bmatrix}.$$

Stiff off-diagonal blocks L, U now sit in diagonal via Schur complement $D_1 - UD_2^{-1}L$. The system has been "PARABOLIZED."

$$D_1 - UD_2^{-1}L = (I - \Delta t^2 \partial_{xx})$$

Resistive MHD Jacobian block structure

- The linearized resistive MHD model has the following couplings:

$$
\begin{aligned}
\delta\rho &= L_\rho(\delta\rho, \delta\vec{v}) \\
\delta T &= L_T(\delta T, \delta\vec{v}) \\
\delta\vec{B} &= L_B(\delta\vec{B}, \delta\vec{v}) \\
\delta\vec{v} &= L_v(\delta\vec{v}, \delta\vec{B}, \delta\rho, \delta T)
\end{aligned}
$$

- Therefore, the Jacobian of the resistive MHD model has the following coupling structure:

$$
J\delta\vec{x} = \begin{bmatrix} D_\rho & 0 & 0 & U_{v\rho} \\ 0 & D_T & 0 & U_{vT} \\ 0 & 0 & D_B & U_{vB} \\ L_{\rho v} & L_{Tv} & L_{Bv} & D_v \end{bmatrix} \begin{pmatrix} \delta\rho \\ \delta T \\ \delta\vec{B} \\ \delta\vec{v} \end{pmatrix}
$$

- Diagonal blocks contain advection-diffusion contributions, and are "easy" to invert using MG techniques. Off diagonal blocks L and U contain all hyperbolic couplings.

PARABOLIZATION: Schur complement formulation

- We consider the block structure:

$$J\delta\vec{x} = \left[\begin{array}{cc} M & U \\ L & D_v \end{array}\right]\left(\begin{array}{c} \delta\vec{y} \\ \delta\vec{v} \end{array}\right) \; ; \; \delta\vec{y} = \left(\begin{array}{c} \delta\rho \\ \delta T \\ \delta\vec{B} \end{array}\right) \; ; \; M = \left(\begin{array}{ccc} D_\rho & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_B \end{array}\right)$$

- M is "easy" to invert (advection-diffusion, MG-friendly).

Schur complement analysis of 2x2 block J yields:

$$\left[\begin{array}{cc} M & U \\ L & D_v \end{array}\right]^{-1} = \left[\begin{array}{cc} I & 0 \\ -LM^{-1} & I \end{array}\right]\left[\begin{array}{cc} M^{-1} & 0 \\ 0 & P_{Schur}^{-1} \end{array}\right]\left[\begin{array}{cc} I & -M^{-1}U \\ 0 & I \end{array}\right],$$

$$P_{Schur} = D_v - LM^{-1}U .$$

- EXACT Jacobian inverse only requires M^{-1} and P_{Schur}^{-1}.
- Schur complement formulation is fundamentally unchanged in Hall MHD!

Physics-based preconditioner (I): small-flow approximation

- The Schur complement analysis translates into the following 3-step EXACT inversion algorithm:

$$
\begin{aligned}
\text{Predictor} &: \quad \delta\vec{y}^* = -M^{-1}G_y \\
\text{Velocity update} &: \quad \delta\vec{v} = P_{Schur}^{-1}[-G_v - L\delta\vec{y}^*], \;\; P_{Schur} = D_v - LM^{-1}U \\
\text{Corrector} &: \quad \delta\vec{y} = \delta\vec{y}^* - M^{-1}U\delta\vec{v}
\end{aligned}
$$

- MG treatment of P_{Schur} is impractical due to M^{-1}.

Need suitable simplifications (SEMI-IMPLICIT)!

- We consider the small-flow-limit case: $M^{-1} \approx \Delta t$
- This approximation is equivalent to splitting flow in original equations.

Serial performance (2D tearing mode)

Δt convergence study (128x128)

Δt	Newton/Δt	GMRES/Δt	CPU (s)	CPU_{exp}/CPU	$\Delta t/\Delta t_{CFL}$
0.5	5.0	8.0	526	8.0	380
0.75	5.5	9.5	607	10.0	570
1.0	5.0	11.2	684	12.7	760
1.5	5.6	14.6	856	14.6	1140

Grid convergence study ($\Delta t = 1200\Delta t_{CFL}$)

Grid	Δt	Newton/Δt	GMRES/Δt	CPU	$\widehat{CPU}$
32x32	6	6.0	38.1	145	5.3
64x64	3	5.9	24.2	350	20.4
128x128	1.5	5.6	14.6	856	84.2
256x256	0.75	5.4	9.7	2508	22.1

$CPU \sim \mathcal{O}(N)$ OPTIMAL SCALING!

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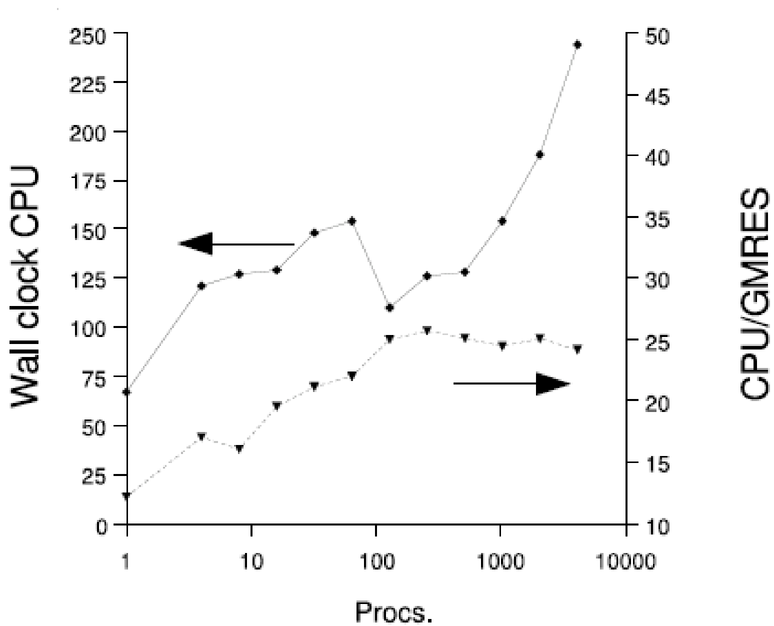
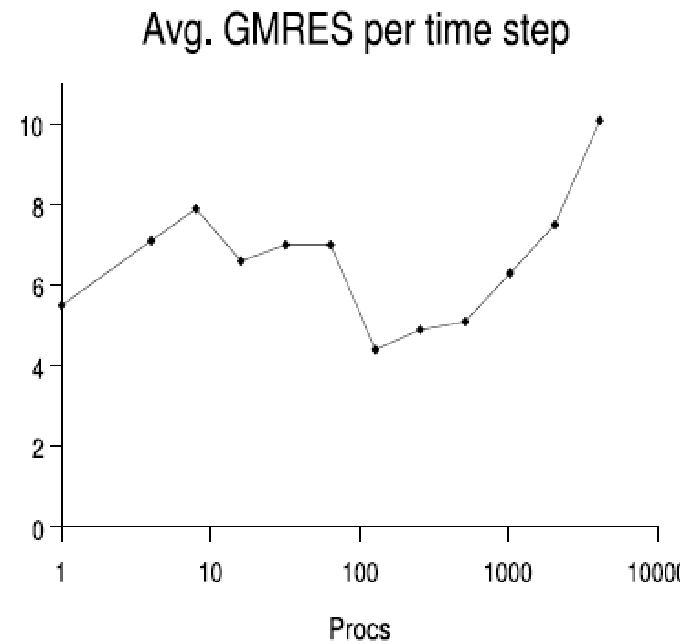
Massively parallel performance with PETSc toolkit (3D island coalescence, 16^3 grid points per processor, on Franklin at NERSC)





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Remarks about Physics based and approximate block factorization For Navier-Stokes

Stable, Accurate, Scalable, and Efficient TR / xMHD Solution Methods

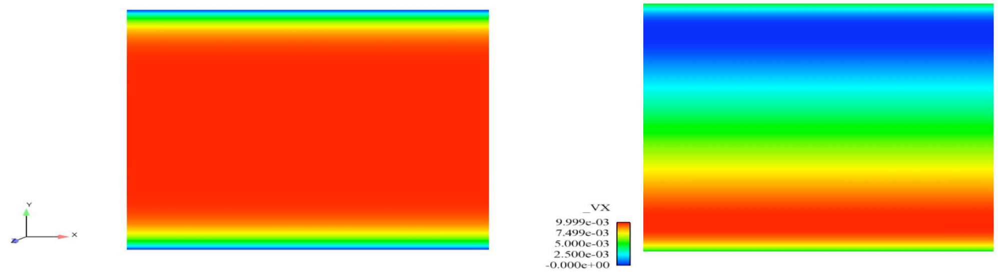
Currently:

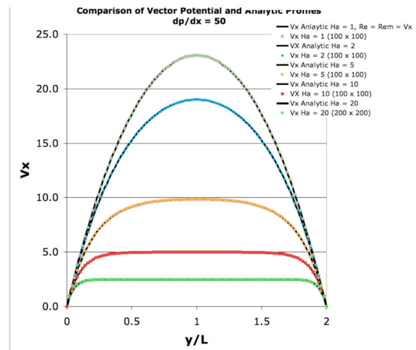
- **2D & 3D Low Mach Number Resistive MHD**
- **Fully-implicit: BE, TR, BDF2 & (Rhythmos);**
- **Unstructured Stabilized Finite Elements**
- **Formulations:**
  - **2D Vector Potential**
  - **2D&3D Projection and Lagrange Multiplier Method;**
- **Direct-to-Steady-State (NOX); Continuation, Linear Stability and Bifurcation (LOCA)**
- **Parallel Newton-Krylov:**
  - **Additive Schwarz DD w/ Var. Overlap; (Aztec)**
  - **Aggressive Coarsening Block AMG for Systems; (ML) [w/ Tuminaro, Lin -SNL];**

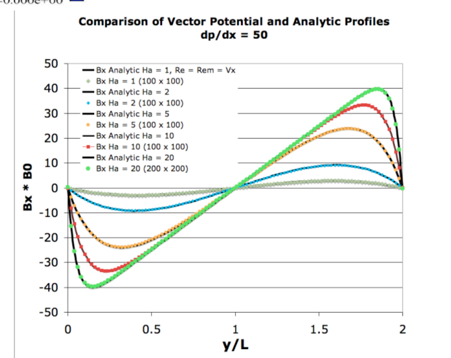
Next:

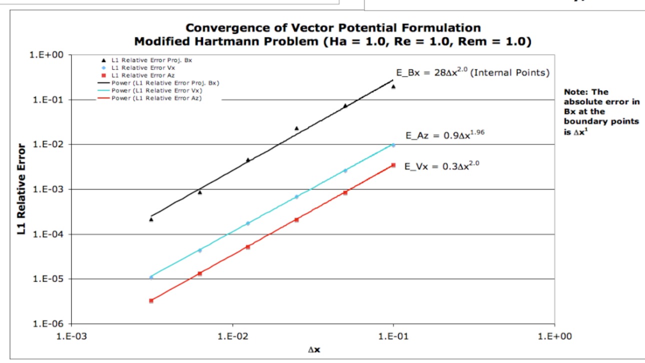
- **Compressible Resistive / Extended MHD**
- **Physics Based Preconditioning [w/ L. Chacon LANL]**
- **High-resolution Hyperbolic Solver (FE-TVD/FCT)**
- **Physics Compatible Discretizations**

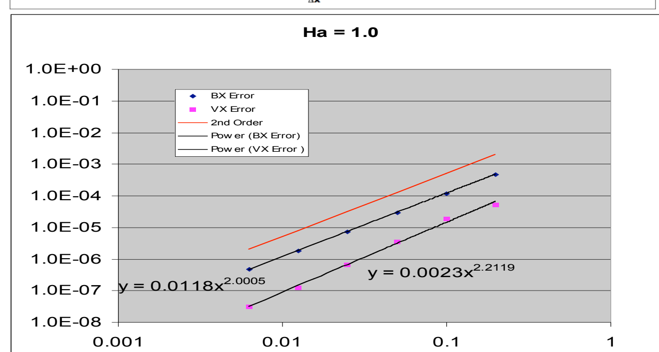
  (e.g De Rham complex - [w/ Bochev, Ridzal SNL])



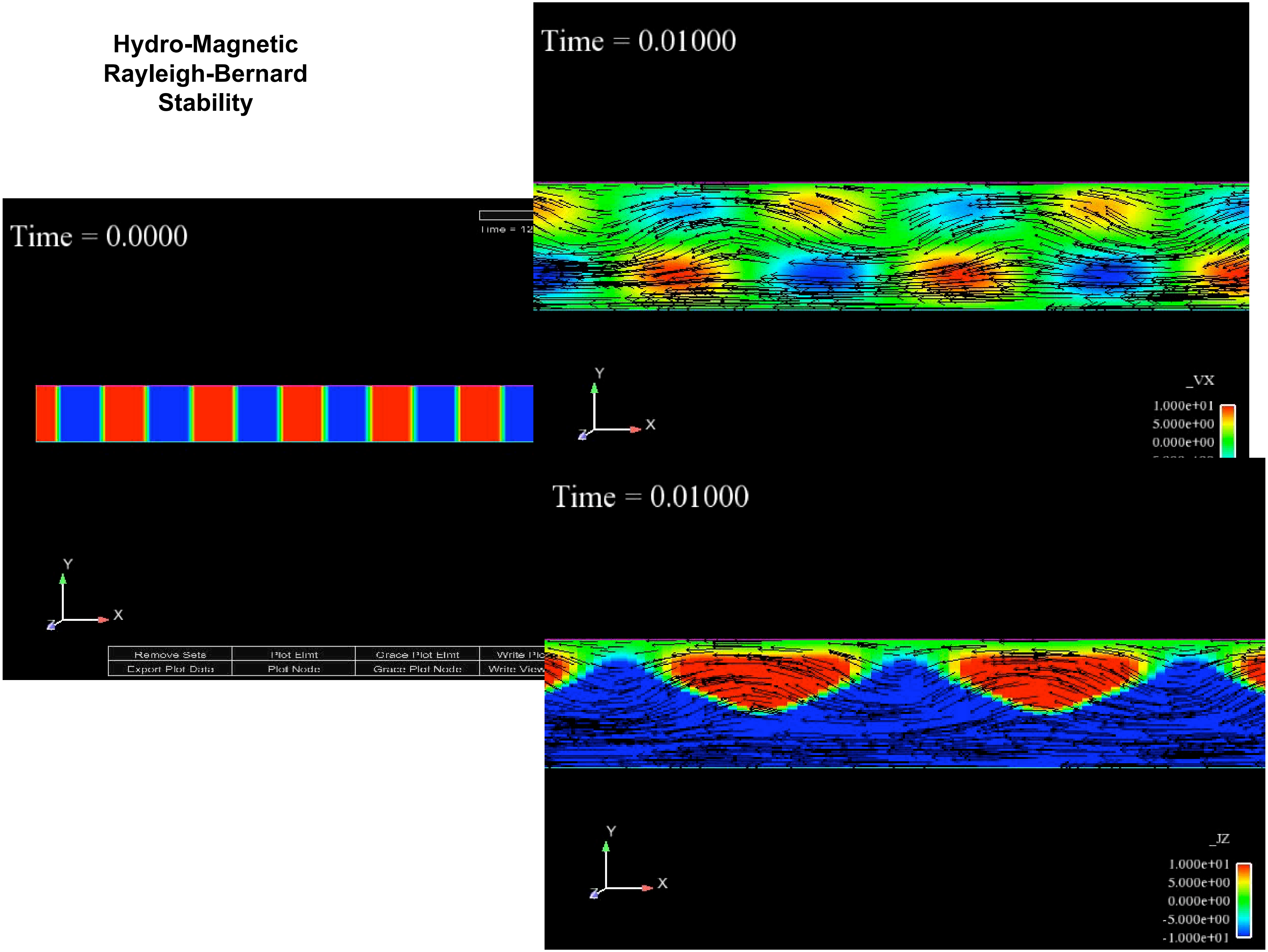




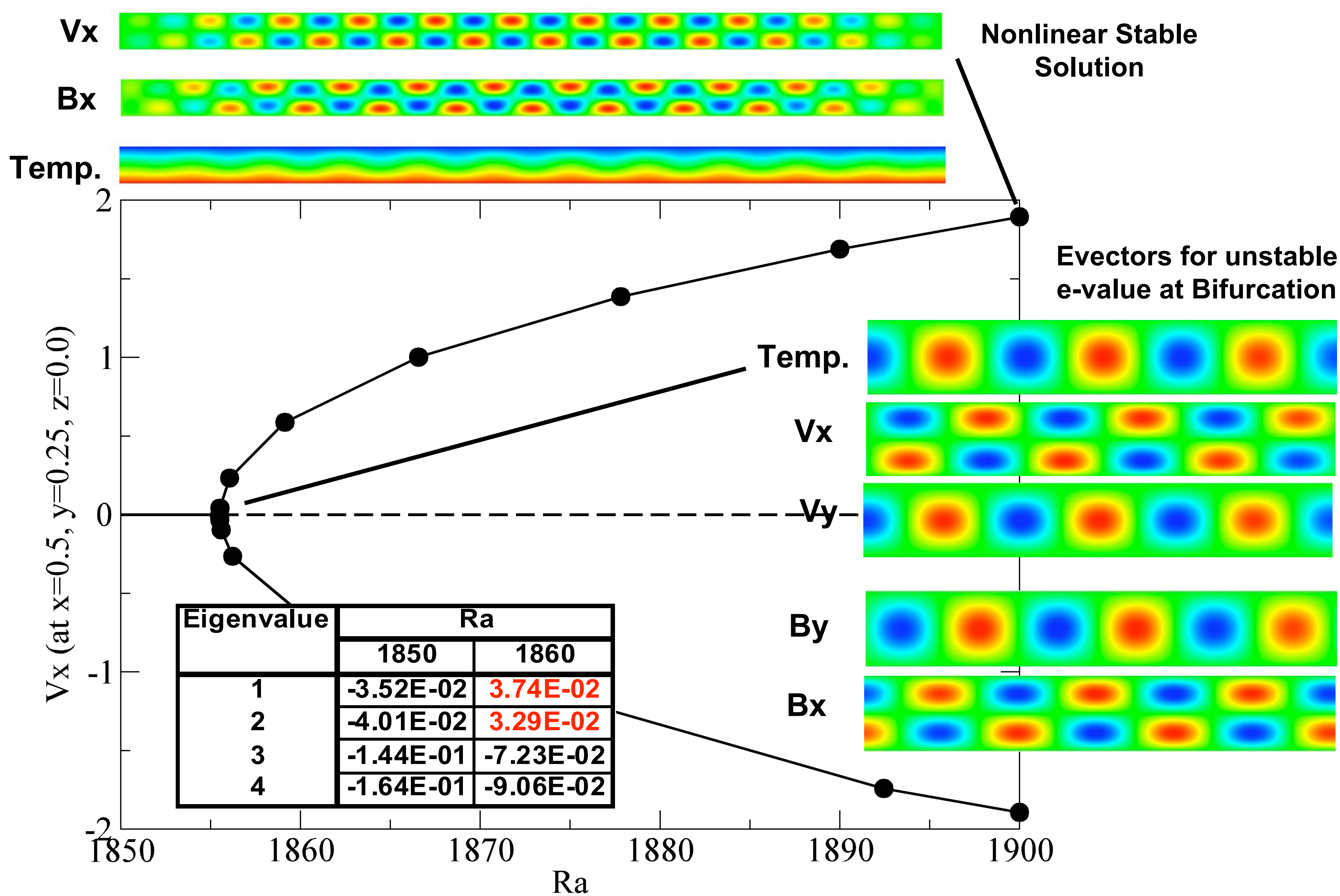




Hydro-Magnetic Rayleigh-Bernard Stability



Hydro-Magnetic Rayleigh-Bernard Stability



Eigenvalue	Ra	
	1850	1860
1	-3.52E-02	3.74E-02
2	-4.01E-02	3.29E-02
3	-1.44E-01	-7.23E-02
4	-1.64E-01	-9.06E-02

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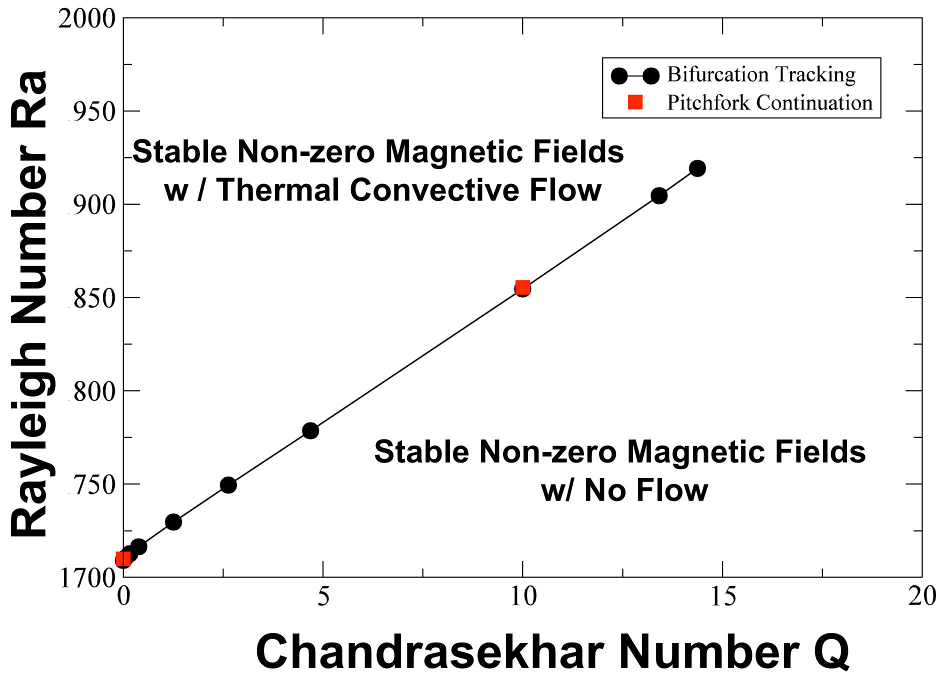
Hydro-Magnetic Rayleigh-Bernard Stability



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

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

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

Solve extended system with Newton's method

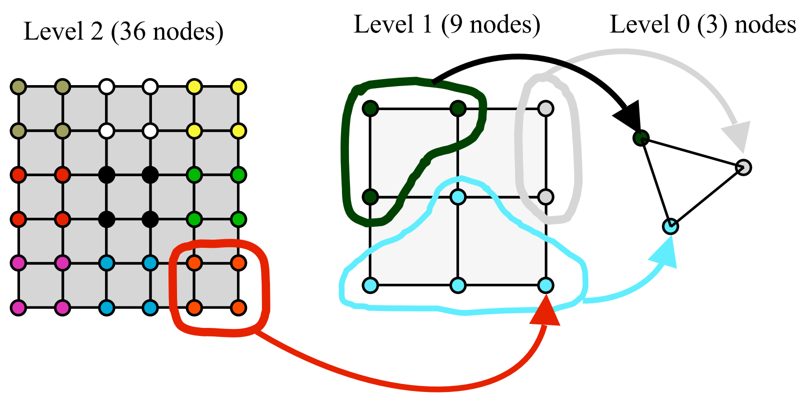
ML library: Multilevel Preconditioners

(R. Tuminaro, M. Sala, J. Hu, 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 $A_{k-1} = R_{k-1} A_k I_{k-1}$

- Nonsmoothed aggregation
- Domain decomposition smoothers (sub-domain GS and ILU)
- 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**

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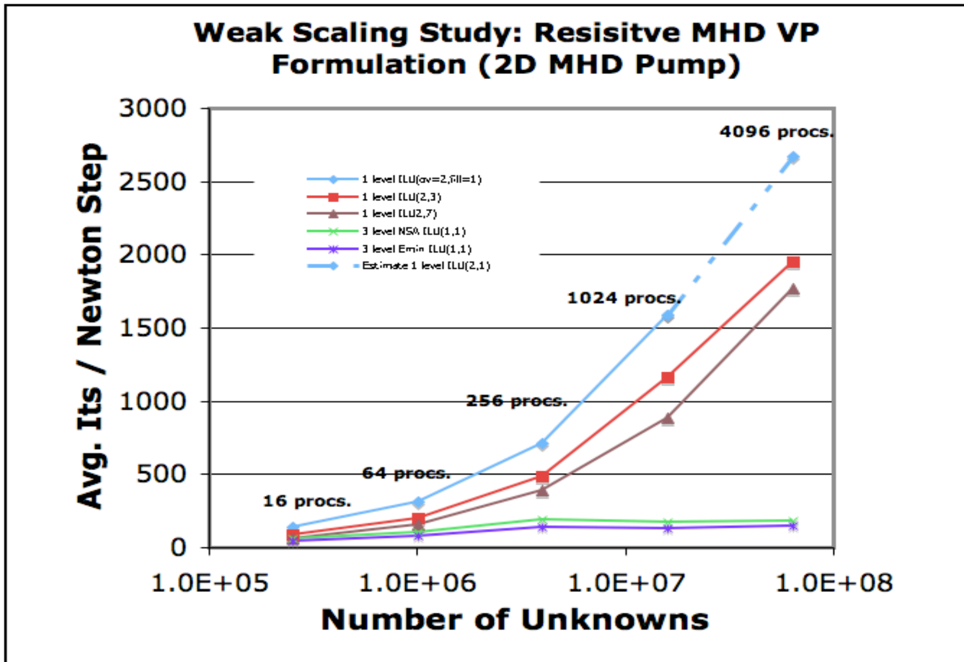
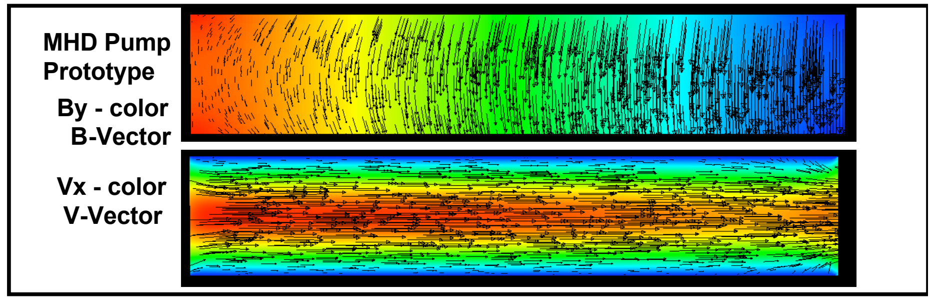
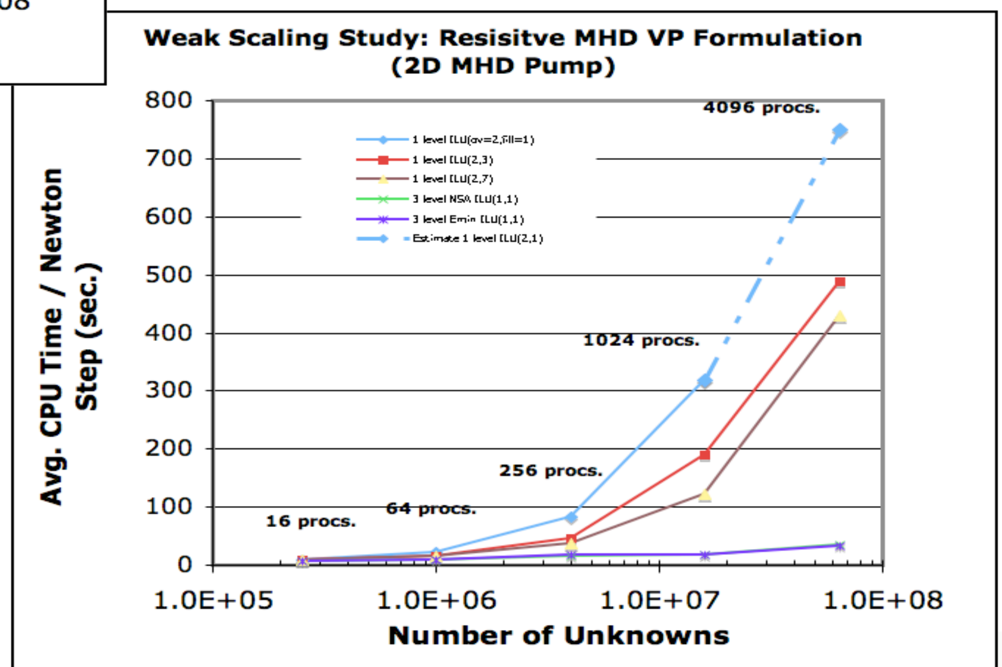
Red Storm - Cray XT3 Results:





Largest Calculation
2D MHD Pump
Vector Potential Formulation

- 4096 processing nodes (single core per node)
- 12.8M FE nodes
- 64M unknowns
- Total Solve time 394 seconds (ML 3 level)



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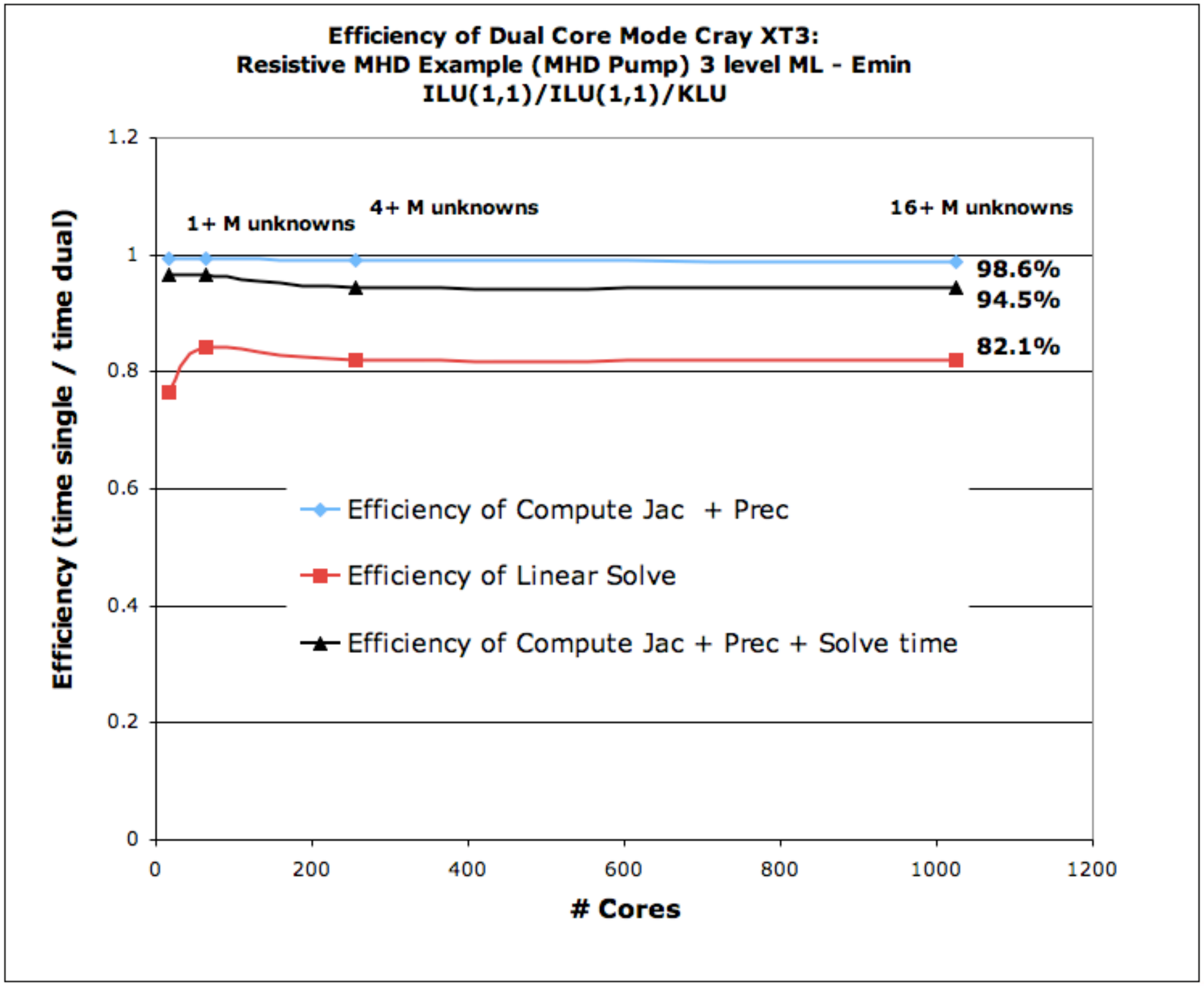
Red Storm - Cray XT3 Results:

Most Processors used
3D Flux Expulsion
Projection formulation

- 20,000 cores (Dual core per node)
- 1.7M FE nodes
- 15.32M unknowns
- Total Solve time 495 seconds (DD 1 level)



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Main Research Topics for Proposed FY09 - FY011 Effort