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Scalable Fully-implicit Fully-coupled Solution Methods for Multiple-time-scale Multiphysics Systems

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DOE / NNSA

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Outline

- **Motivation: Multiple-time-scale Multiphysics Nonlinear Systems**
- **Brief Outline of Stabilized FE Formulation for Transport/Reaction & Resistive MHD**
- **Why Newton-Krylov Methods?**
  - **Comments about Operator Splitting and Semi-implicit in contrast to Fully-implicit**
  - **Benefits of Fully-implicit and Steady-state Solution Methods**
  - **Characterization of Complex Solution Spaces: Hydromagnetic Rayleigh-Bernard**
  - **Brief optimization example – Transport/Reaction simulation for CVD of Poly-silicon**
- **Representative Solution Algorithm Performance**
  - **Additive Schwarz Domain Decomposition**
  - **Fully-coupled Algebraic Multi-level**
  - **Approximate Block Factorization / Physics-based Preconditioners**
- **Conclusions**

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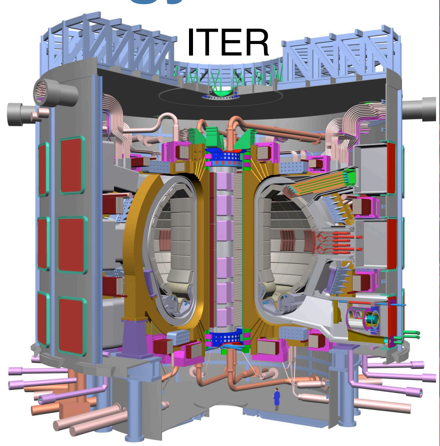
Scientific / Technology Motivation

Resistive and extended MHD systems model a variety of important plasma physics

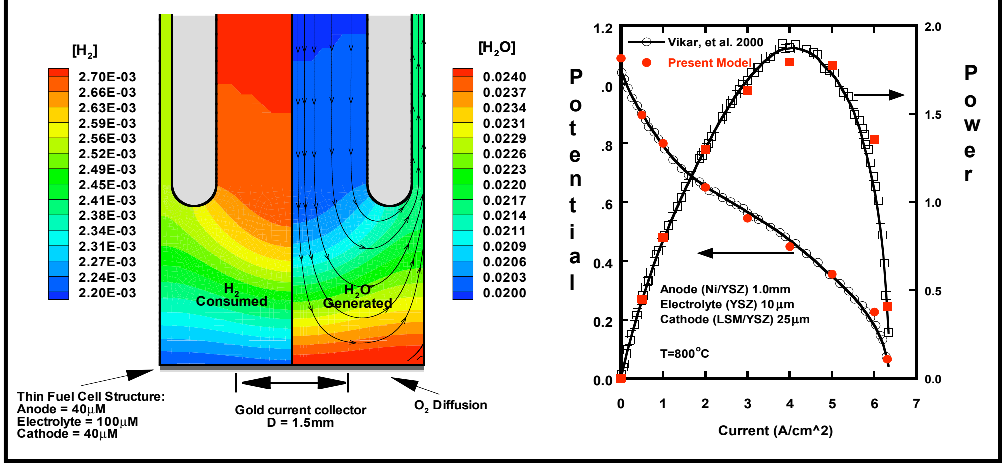
- **Astrophysics: Solar flares, sunspots, magnetic reconnection**
- **Geophysics: Earth's magnetospheric sub-storms, geo-dynamo**
- **Fusion: Magnetic confinement (ITER - Tokamak), Inertial conf. (NIF, Z-pinch)**
- **Technology/Engineering: Plasma Reactors, MHD Pumps, ..**
- **…**

Transport / Reaction Systems model a very broad range of applications

- **Conventional / Alternate Energy: Combustion, Fuel Cells, …**
- **Chemical Processing: CVD for semiconductors, Solar / Photo-voltaic**
- **Partial Catalytic Reactors e.g. methane (g) ⟶ methanol (l), ..**
- **Biological cell modeling**
- **….**



Simulation of Experimental Solid Oxide H_2 Fuel Cell



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<u>Mathematical / Computational Motivation:</u> Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multiphysics Systems to Enable Scientific Discovery and Engineering Design/Optimization

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 be dominated by one, or a few processes, that drive a short dynamical time-scale consistent with these dominating modes,**
- **consist of a set of widely separated time-scales that produce a stiff system response,**
- **nearly balance to evolve a solution on a dynamical time-scale that is long relative to the component time scales,**
- **or balance to produce steady-state behavior.**

Our goal is to develop:

- **Stable and higher-order accurate fully-implicit formulations,**
- **Robust fully-coupled nonlinear/linear iterative solution methods,**
- **Scalable and efficient parallel preconditioners,**
- **Integrated sensitivity and error-estimation to enable UQ capabilities.**

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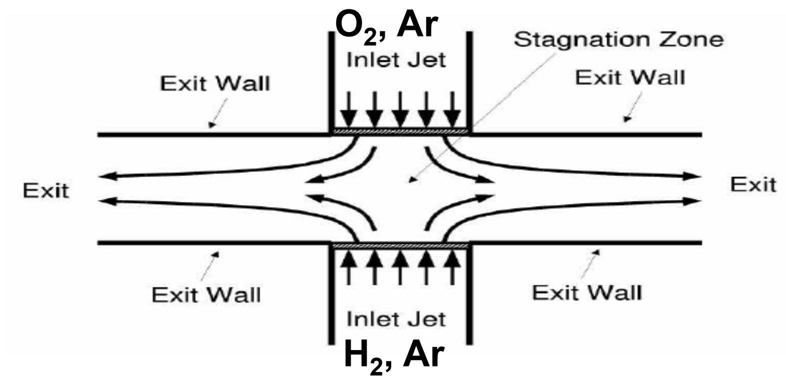
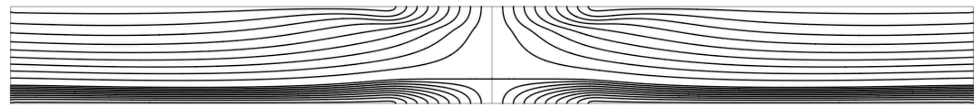
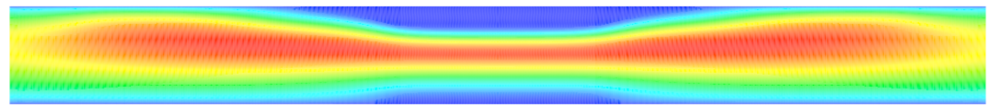
Multiple-time-scale systems: Bifurcation Analysis of a Steady Reacting H_2, O_2,, Ar, Opposed Flow Jet Reactor

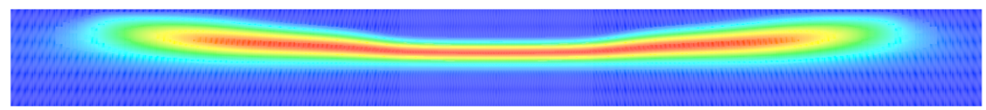




Streamlines

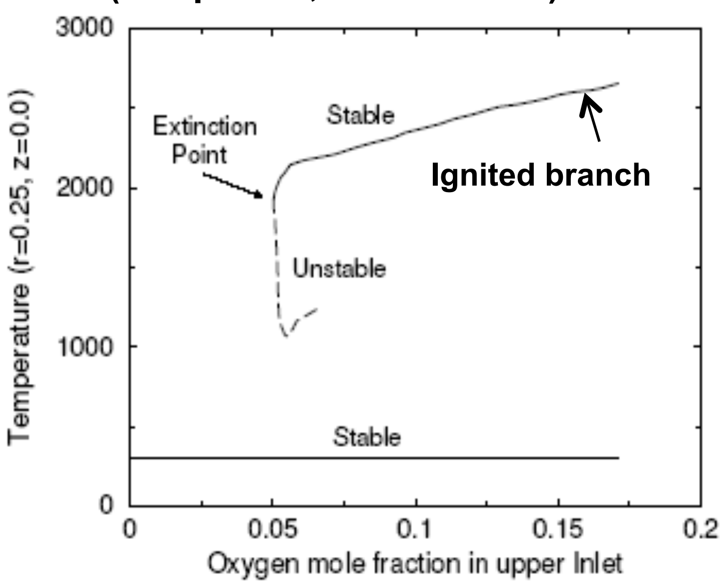


Temperature (Min. 300°K, Max 2727°K)



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)**

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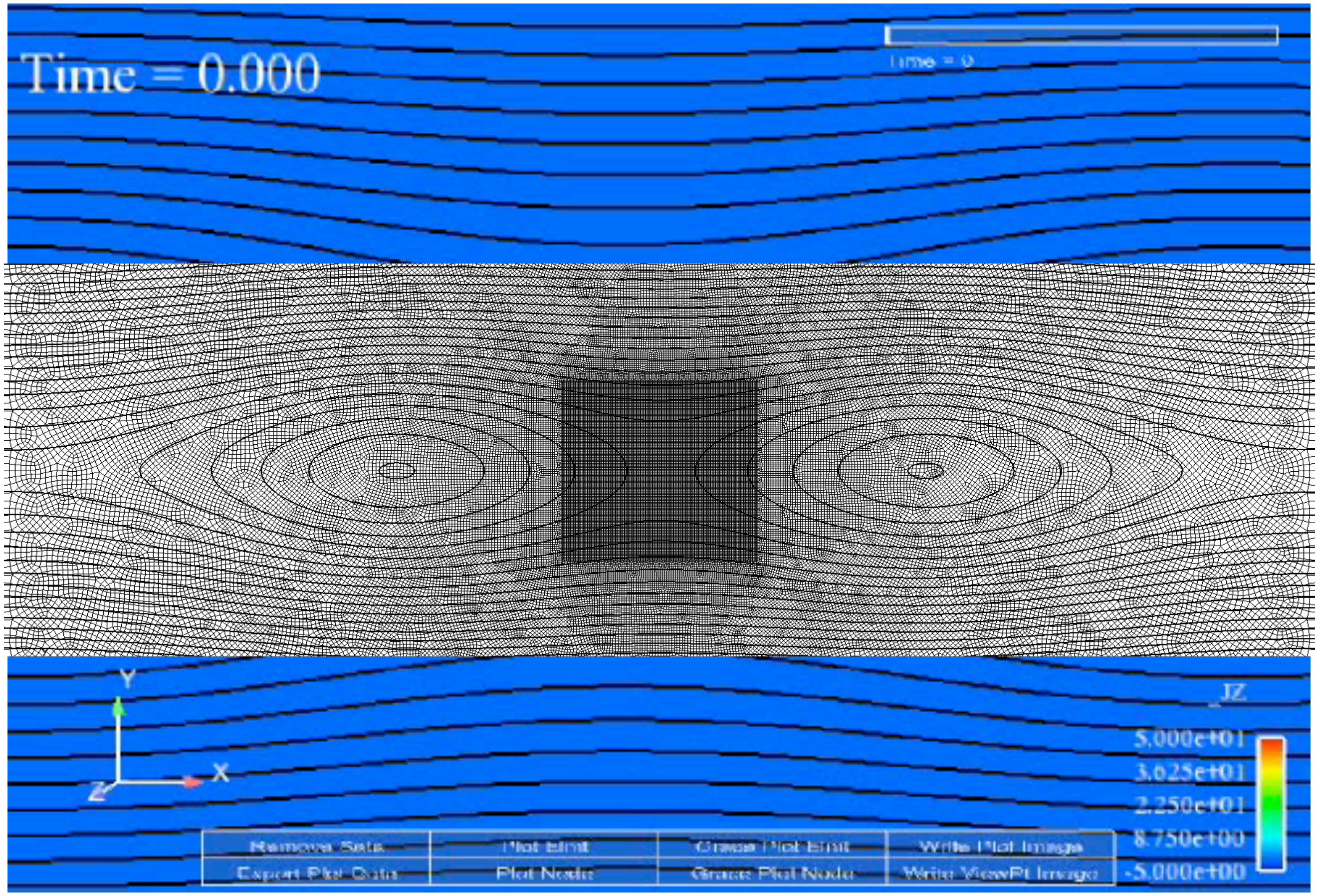
Multiple-time-scale systems: E.g. Driven Magnetic Reconnection with a Magnetic Island Coalescence Problem (Incompressible)

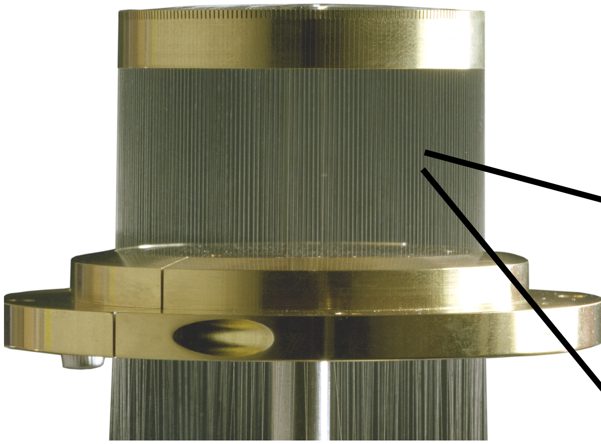


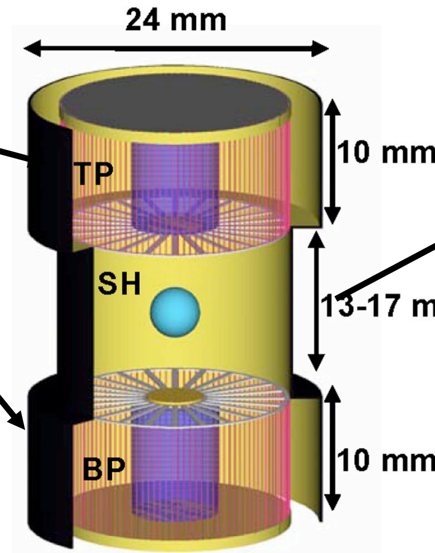
<u>Approx. Computational Time Scales:</u>

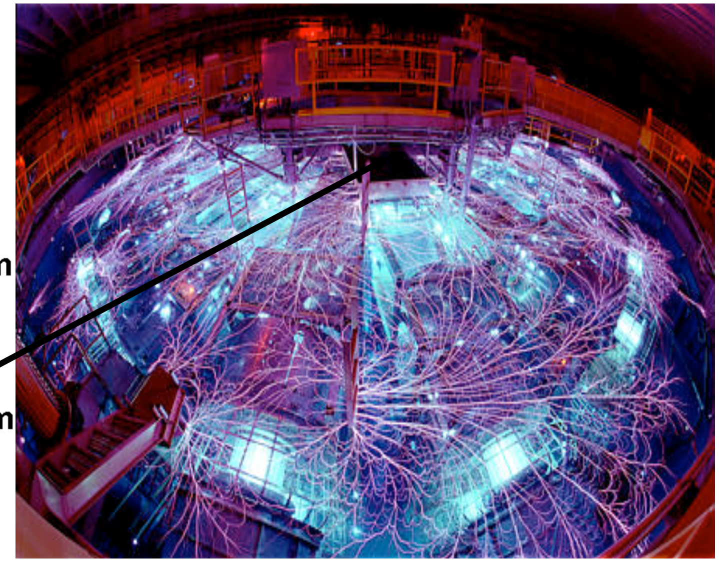
- **Ion Momentum Diffusion: 10^{-7} to 10^{-3}**
- **Magnetic Flux Diffusion: 10^{-7} to 10^{-3}**
- **Ion Momentum Advection: 10^{-4} to 10^{-2}**
- **Alfven Wave** $\left(\tau_A = \frac{h\sqrt{\rho\mu_0}}{B_O}\right)$ **: 10^{-4} to 10^{-2}**
- **Whistler Wave** $\left(\tau_w = \frac{h^2}{V_A d_i}\right)$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

[Finn and Kaw 1977; Chacon and Knoll Phys. 2006]

Z-pinch Double Hohlraum Schematic (ICF concept)







Z Machine (Approximate Ranges)

22 MJ stored energy

100ns current rise time for 26 MA peak electrical current

250 ns plasma shell collapse and stagnation

10-30 ns X-ray power pulse ~350 TW peak power

A Recent Physics Review: K. Matzen, et. al., PoP 12, 055503 (2005)
C. J. Garasi et. al. , Physics of Plasmas, 11 (5), May 2004, pp. 2729-2737
A. C. Robinson et. al. , AIAA, 2008-1235

Computational Stability Constraints:

Hyperbolic Operators: $\Delta t < \Delta x / c$
- **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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Navier-Stokes Equations with Internal Equation

Navier-Stokes and Internal Energy Model in Residual Notation

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

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

$$R_e = \frac{\partial(\rho e)}{\partial t} + \nabla \cdot [\rho\mathbf{v}e + \mathbf{q}] - \mathbf{T} : \nabla\mathbf{v} \qquad = 0$$

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

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Navier-Stokes and Transport/Reaction System

Navier-Stokes and Internal Energy Model in Residual Notation

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

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

$$R_e = \frac{\partial(\rho e)}{\partial t} + \nabla\cdot[\rho\mathbf{v}e + \mathbf{q}] - \mathbf{T} : \nabla\mathbf{v} + \sum_{k=1}^{N}\mathbf{j}_k\cdot\hat{C}_{p,k}\nabla T - \sum_{k=1}^{N}h_k W_k\omega_k = 0$$

Species Transport / Reaction Equation

$$R_{Y_k} = \frac{\partial\left(\rho Y_k\right)}{\partial t} + \nabla\bullet\left(\mathbf{u}Y_k + \mathbf{j}_k\right) - W_k\dot{\omega}_k; \qquad k = 1,2,\ldots,N-1\ ;\ \sum_{k=1}^{N} Y_k = 1$$

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

Visco-resistive MHD System

Resistive MHD Model in Residual Notation

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

$$\mathbf{T_M} = \frac{1}{\mu_0}\mathbf{B}\otimes\mathbf{B} - \frac{1}{2\mu_0}\|\mathbf{B}\|^2\mathbf{I}$$

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

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

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

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

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)	$F_{A_z} = \int_{\Omega} \Phi R_{A_z} d\Omega + \sum_e \int_{\Omega^e} \rho \tau_{A_z} \left(\mathbf{u} \bullet \nabla \Phi \right) R_{A_z} d\Omega + \sum_e \int_{\Omega^e} \nu_{A_z} \nabla \Phi \bullet \mathbf{C}^c \nabla A_z d\Omega$

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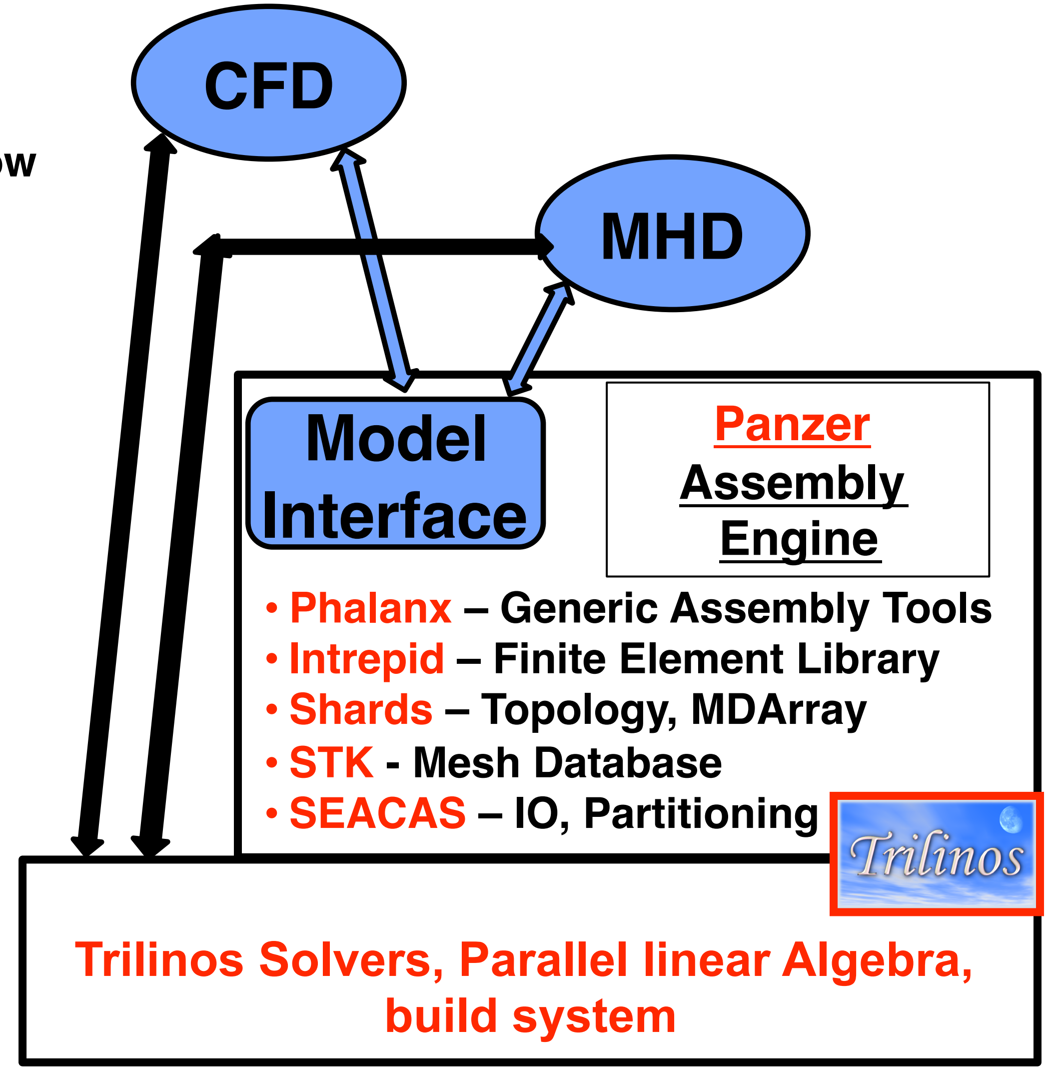
Drekar::CFD/MHD

- Massively Parallel: MPI
- 2D & 3D Unstructured Stabilized FE
- Constant density, variable density, low flow Mach number approx., low flow Mach number compressible
- Fully Coupled Globalized Newton-Krylov solver
  - Sensitivities: Template-based Generic Programminc for Automatic Differentiation (Sacado), UQ, Arb. Prec.
  - GMRES (AztecOO, Belos)
- Fully-implicit: 1st-5th variable order BDF (Rythmos) & TR
- Direct-to-Steady-State (NOX), Continuation, Linear Stability and Bifurcation (LOCA / Anasazi), PDE Constrained Optimization (Moocho)
- Future: Edge/face based elements, high-resolution methods, …



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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

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

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

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.

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

<u>Stability, Accuracy and Efficiency</u>

- **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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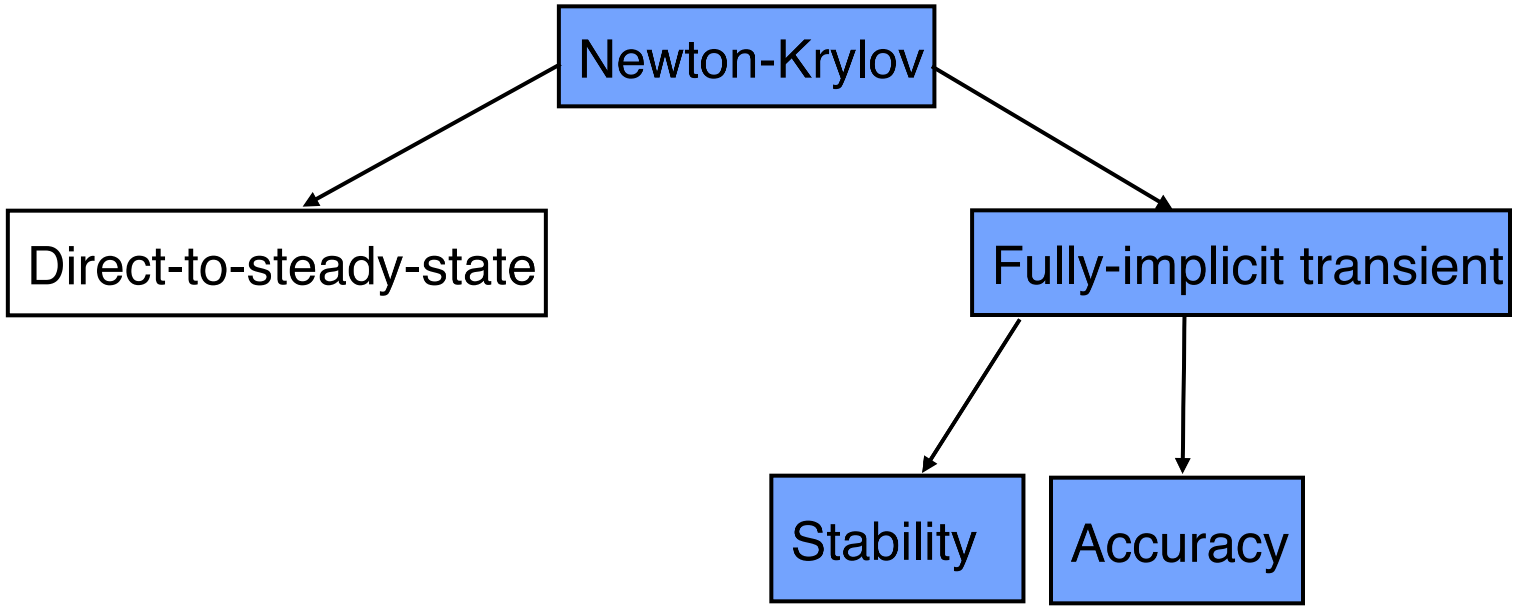
Why Newton-Krylov Methods?



Multiple-time-scale systems: Numerical Experiments
Chemical Dynamics (Brusselator)

$$\frac{\partial T}{\partial t} = D_1 \frac{\partial^2 T}{\partial x^2} + \alpha - (\beta + 1)T + T^2 C$$

$$\frac{\partial C}{\partial t} = D_2 \frac{\partial^2 C}{\partial x^2} + \beta T - T^2 C$$

$D_1 = D_2 = 1/40$
$\alpha = 0.6$
$\beta = 2.0$
$\Delta x = 1/100$
$T_{\min} \approx 10.0$

Fully-implicit Method: **Trapezoidal Rule**

2nd order (FI 2nd):

$$M_k(\dot{\chi}^{n+1}) + D_k^{n+1}(\chi^{n+1}) + S_k^{n+1}(\chi^{n+1}) + F_k = 0$$

$$\dot{\chi}^{n+1} = 2(\frac{\chi^{n+1} - \chi^n}{\Delta t}) - \dot{\chi}^n$$

Strang Splitting (SS):

to advance solution over $\left[t^n, t^n + \Delta t\right]$

$$M_k(\dot{\chi}^*) + D_k^*(\chi^*) + F_k = 0 \quad \text{on } [0, \Delta t/2]$$

$$M_k(\dot{\chi}^{**}) + S_k^{**}(\chi^{**}) = 0 \quad \text{on } [0, \Delta t]$$

$$M_k(\dot{\chi}^{***}) + D_k^{**}(\chi^{***}) + F_k = 0 \quad \text{on } [0, \Delta t/2]$$

$$\chi^{n+1} = \chi^{***}(\Delta t) \longrightarrow \boxed{\chi^{n+1} = \tilde{D}_{\Delta t/2}\tilde{S}_{\Delta t}\tilde{D}_{\Delta t/2}\chi^n}$$

(w/David Ropp, C. Ober)

G. Strang, SIAM J. Numer. Anal. 5,3, 1968

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Diffusion/Reaction System

Operator Split Time Integration (component solvers):

- **Diffusion: 2nd order Crank-Nicholson Galerkin FE (A-stable)**
  2nd order SDIRK Galerkin FE (A & L -stable)

- **Reaction: CVODE Variable order - High accuracy tolerances**

Fully-implicit solution:

- **Trapezoidal rule with fully-coupled Newton-Krylov methods (A-stable)**

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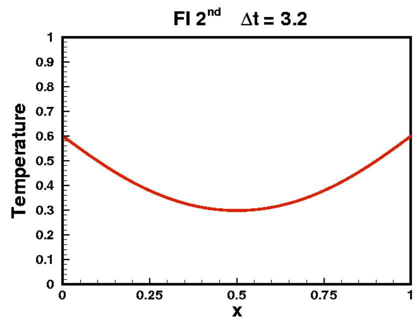
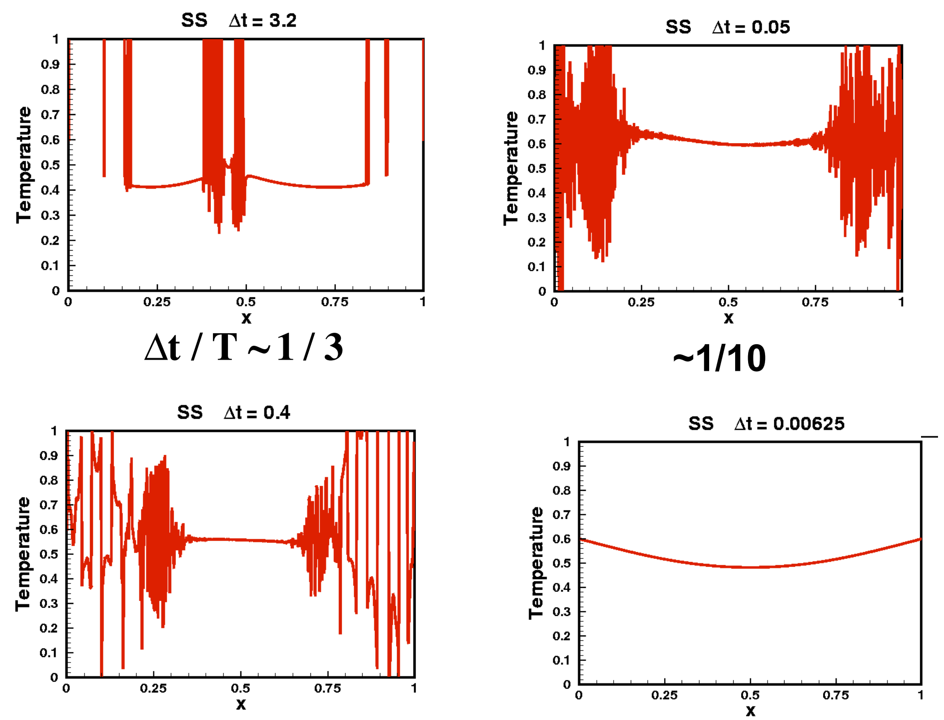
Brusselator: Comparison of Spatial and Temporal Profiles for Strang Split and Fully Implicit Solvers



FI

$\Delta t / T \sim 1/3$

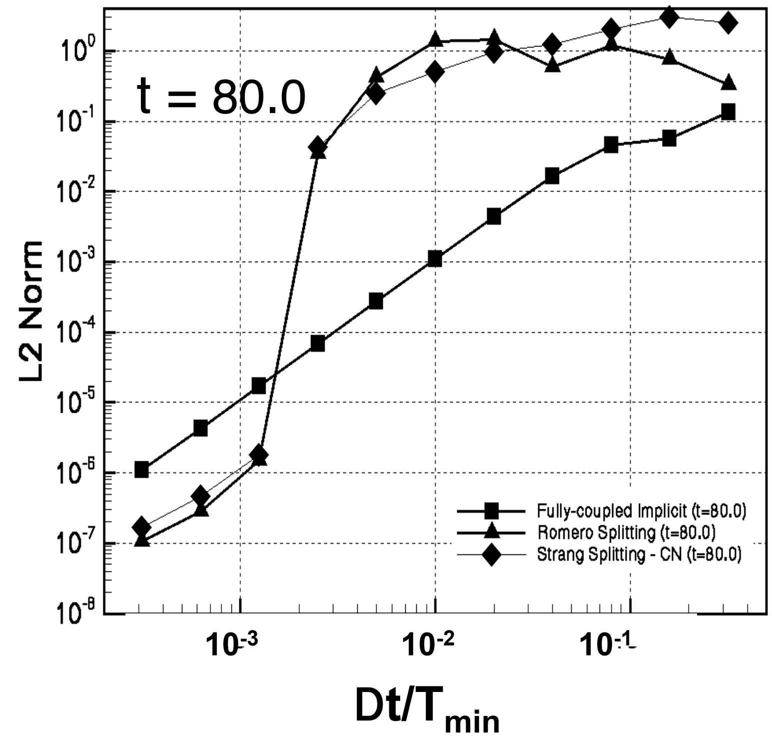


$\Delta t / T \sim 1/3$

~1/10

~1/100

~1/500



Multiple time scales:

Knoll, Chacon, Margolin, Mousseau; JCP 2003
Ropp, S.; JCP 2004, 2005, 2009
Ober, S.; JCP 2004

Brown, Woodward, SISC; 2001
Estep, Ginting, Ropp, S.; Tavener, Sinum 2008

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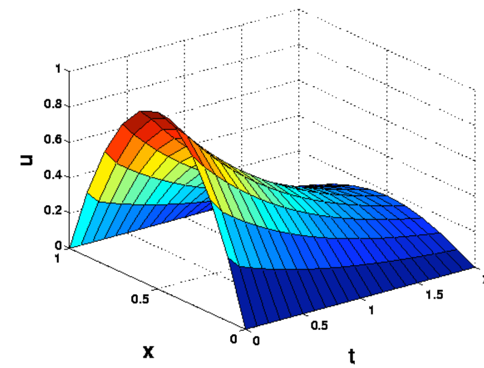
Simplified Diffusion/Reaction PDE: Decay Problem

$$u_t = u_{xx} + 8u,\ x \in [0,1],$$

$$u(t=0) = 4x(1-x).$$



Coupled system negative definite.

Discrete system spatial discretization: finite elements with $\Delta x = 0.1$ has discrete eigenvalues of diffusion operator:

$$\lambda_1 = -9.951,\ \lambda_N = -1116.$$

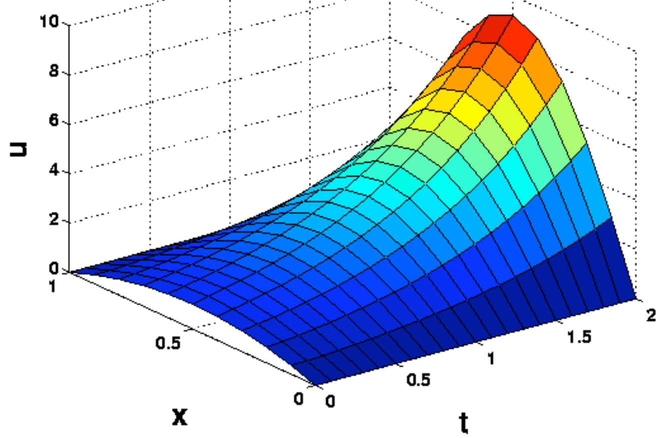
Solve reaction step exactly:

$$v(\Delta t) = \exp(8\Delta t)$$

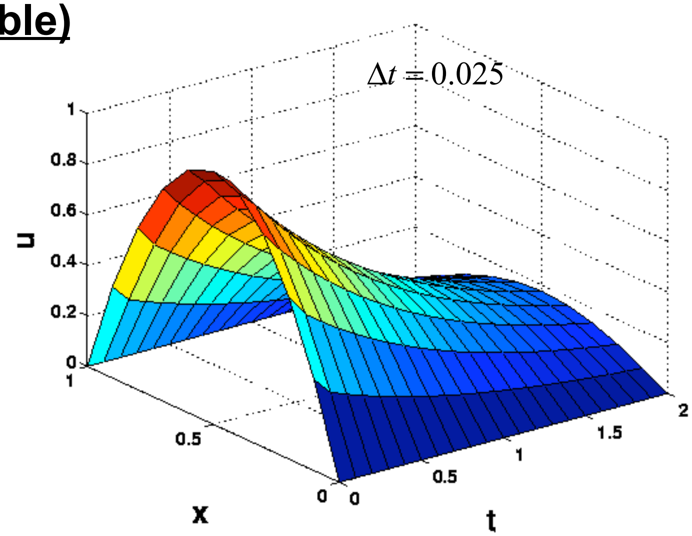
Simple Prototype Operator Splitting Problem: Diffusion-Reaction

1st order splitting : Backward Euler (A & L – stable)

$\Delta t = 0.1$ (low w.n. condition violated)

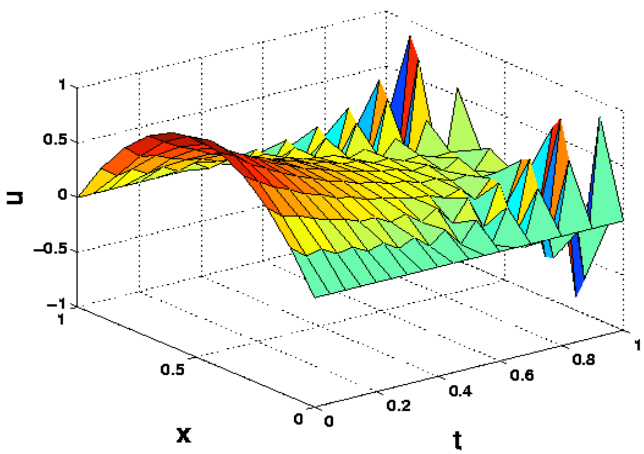


$\Delta t = 0.025$

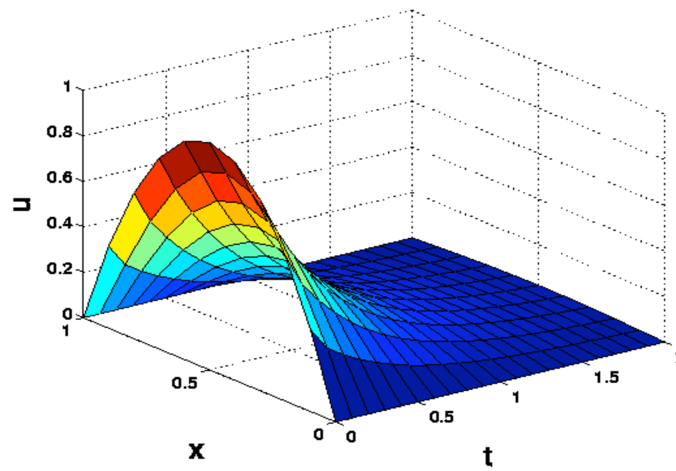


2nd Order Strang Splitting: Diffusion Solve - Trapezoidal Rule (A- stable)

$\Delta t = 0.05$ (high w.n. condition violated)



$\Delta t = 0.0125$



An A-stability theory for operator split integration of diffusion/reaction and convection/diffusion/reaction with indefinite source terms: Ropp, S., JCP 2005, 2009

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Brusselator: L-stability of diffusion solve is critical for stability (SDIRK)

- **SDIRK Parameter γ determines limit of amplification factor "*R*" as $\lambda \Delta t \to -\infty$**

Case 1: A-stable, 2nd order

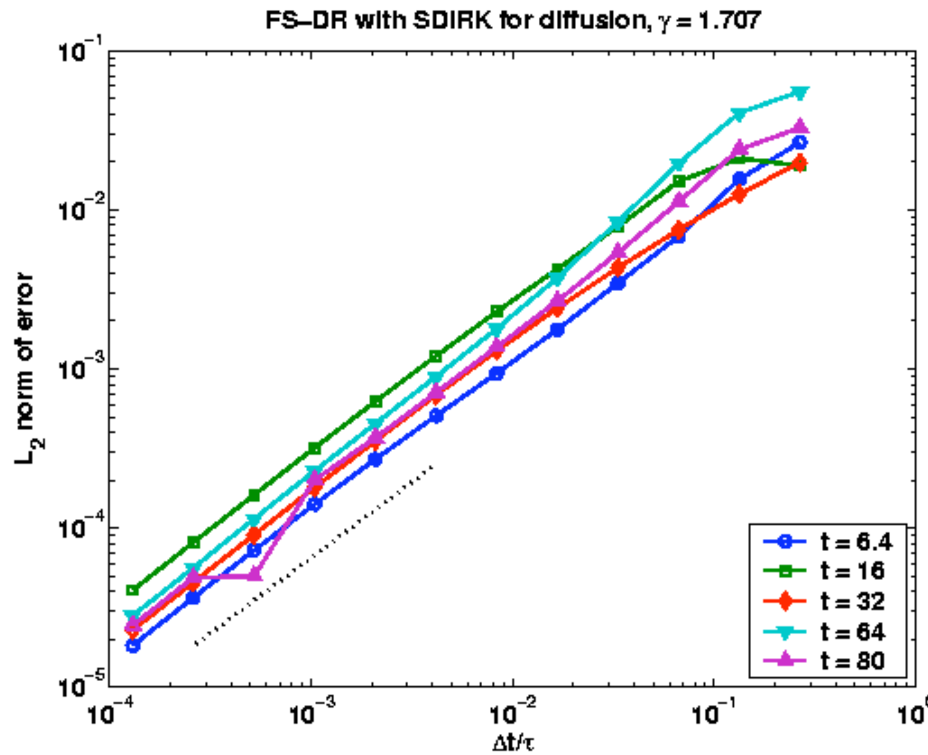
$$\gamma = 0.5, \lim_{z \to -\infty} R(z) = -1$$

Case 2: A-stable, 3rd order

$$\gamma = 0.789, \lim_{z \to -\infty} R(z) = -0.455$$

Case 3: A- and L-stable, 2nd order

$$\gamma = 1.707, \lim_{z \to -\infty} R(z) = 0$$



First order splitting with A- and L-stable diffusion solves demonstrate effect of damping of high wavenumber instability

An A-stability theory for operator split integration of diffusion/reaction and convection/diffusion/reaction with indefinite source terms: Ropp, S., JCP 2005, 2009

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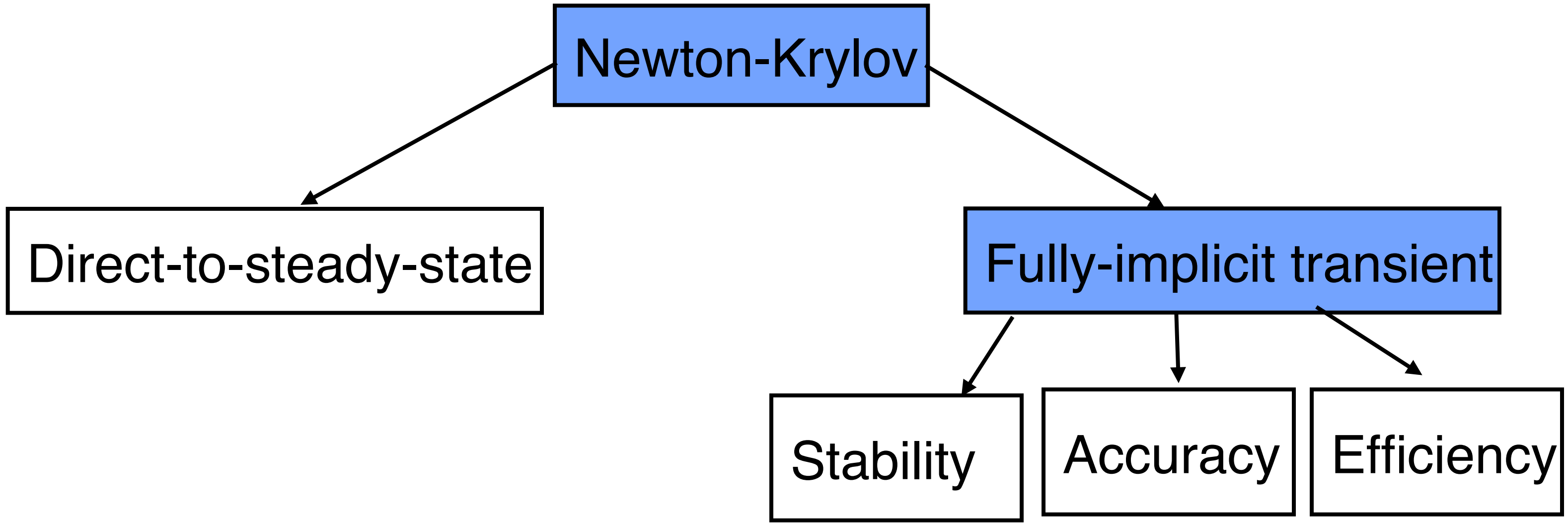
Why Newton-Krylov Methods?



What I am not saying: Fully-implicit is the only way to get these properties

- **Well characterized operator splitting methods in specific application areas: Combustion – P. Colella, J. Bell, …; Composed splitting + predictor-corrector methods (e.g 2nd order Loosely-Coupled FSI - C. Farhat)**

- **Implicit-Explicit (IMEX) methods (Crouzeix, Ascher, Carpenter, Hundsdorfer, ..)**

- **Spectral deferred correction (M. Minion et. al.)**

What I am saying: Fully-implicit is an excellent way to get these properties and this also enables a number of other powerful solution methods when applied to multiple-time-scale multiphysics systems

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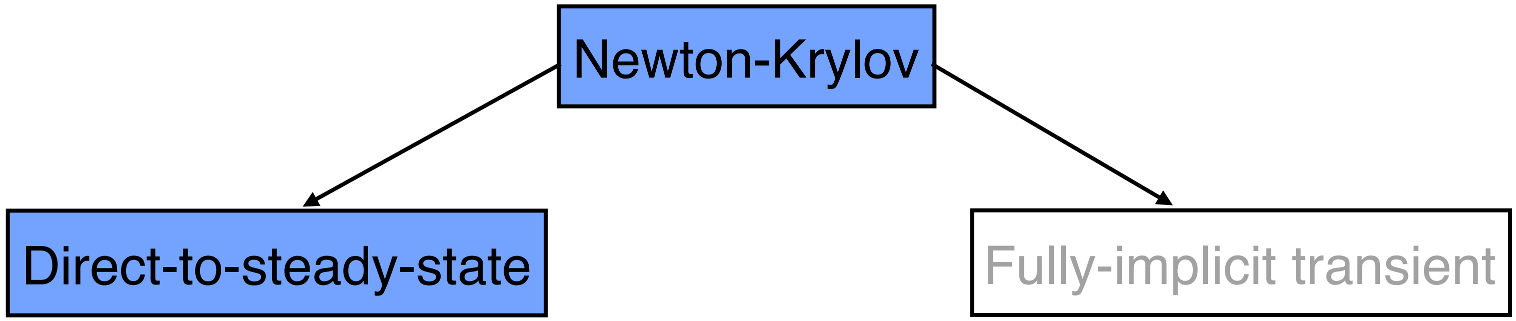
Why Newton-Krylov Methods?



Robustness, Convergence and Flexibility

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

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

Inexact Newton-Krylov

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

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

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

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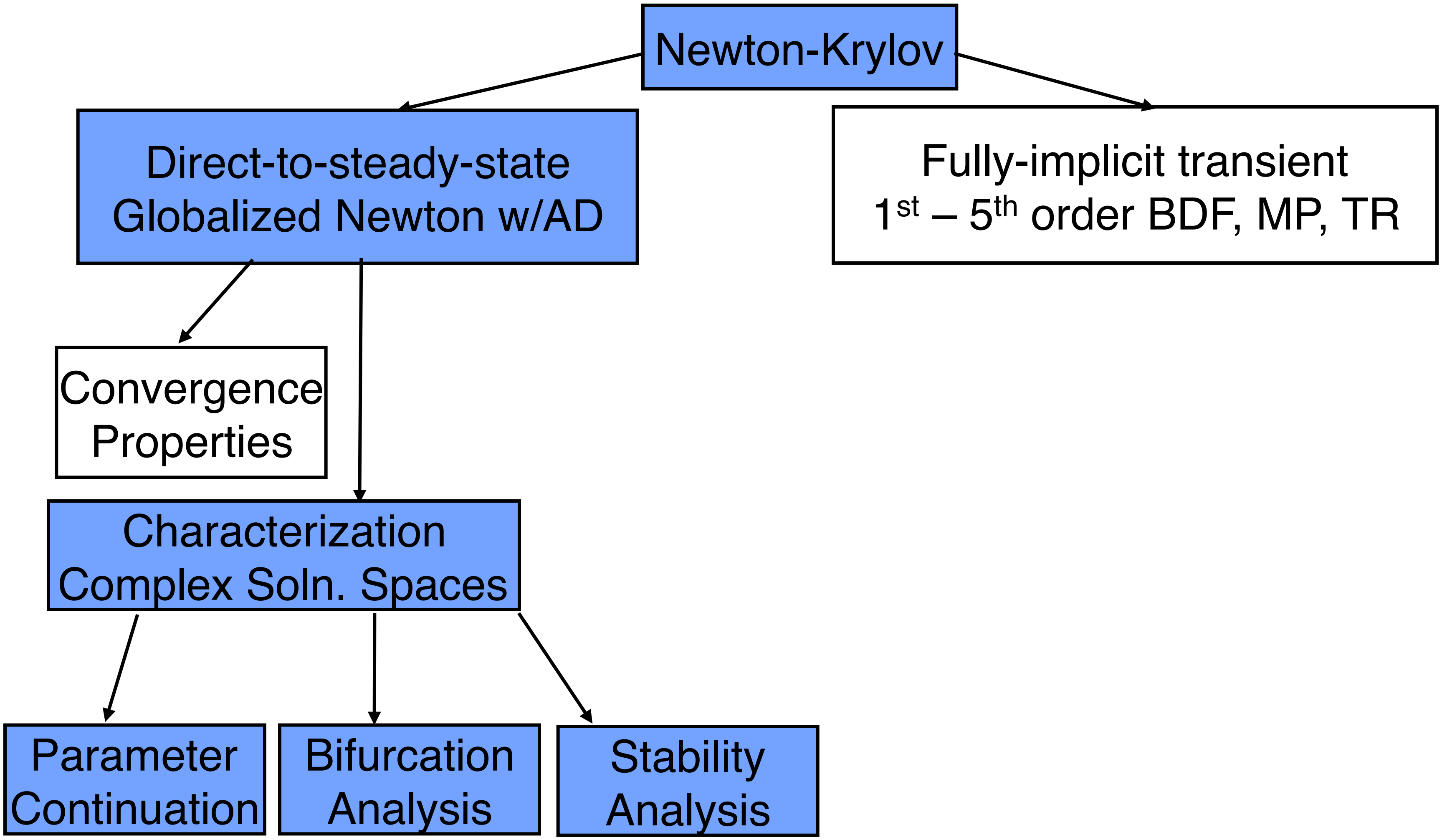
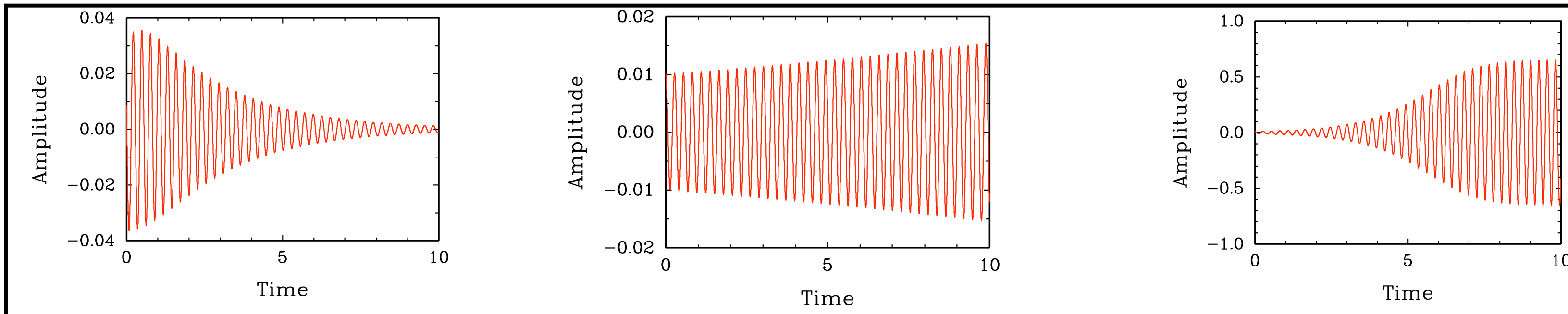
Why Newton-Krylov Methods?



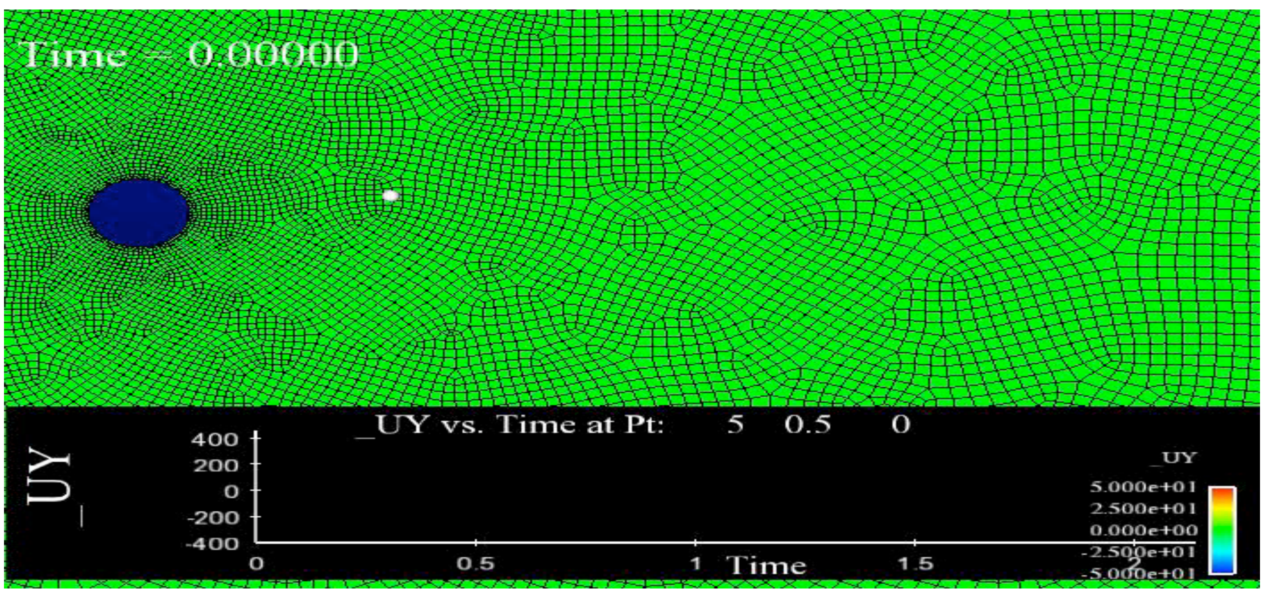
Characterizing Complex Nonlinear Solution Spaces with a Transient Code is Difficult



Re=40 | Re ~ 50 Hopf Bifurcation? | Re=60

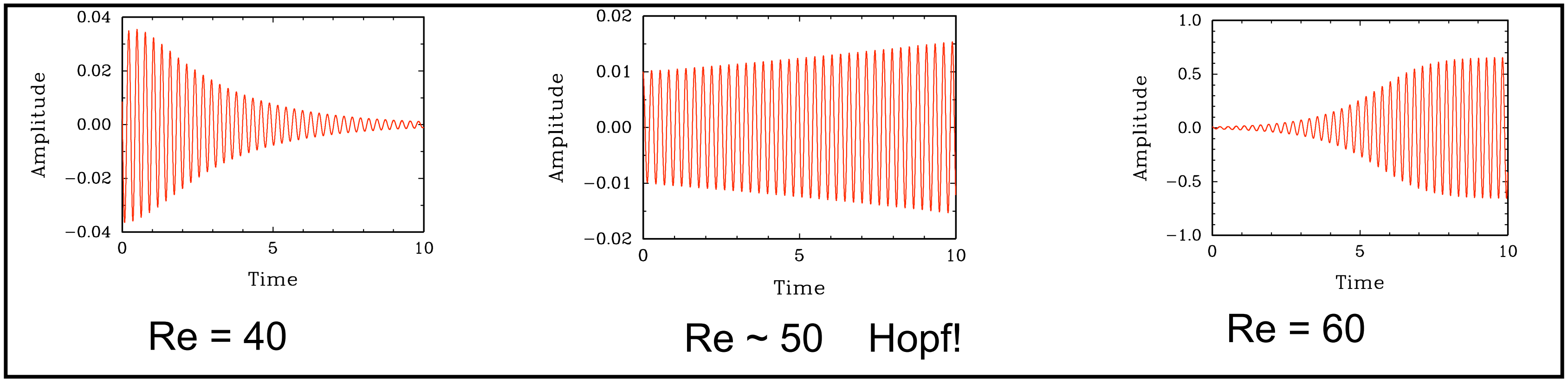
Various discrete time integration methods:

- **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**



e.g. Re = 600

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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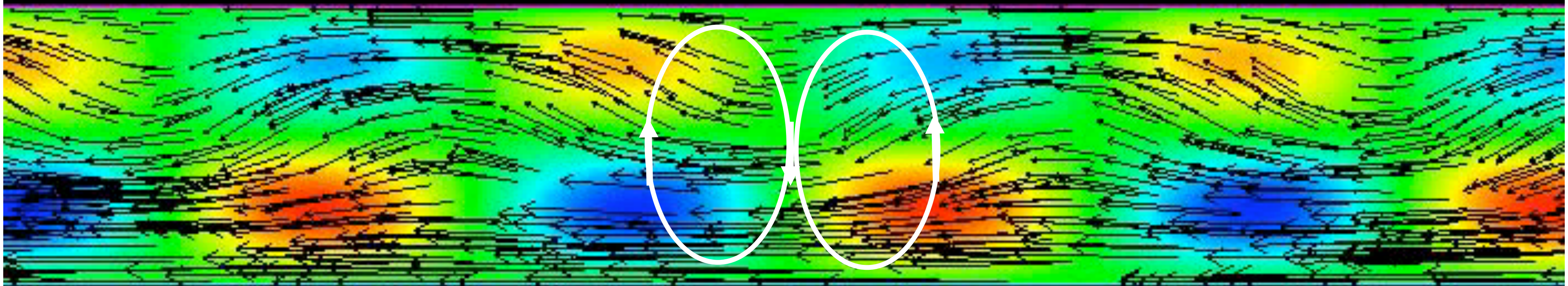
Vx



Hydro-Magnetic Rayleigh-Bernard Stability

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

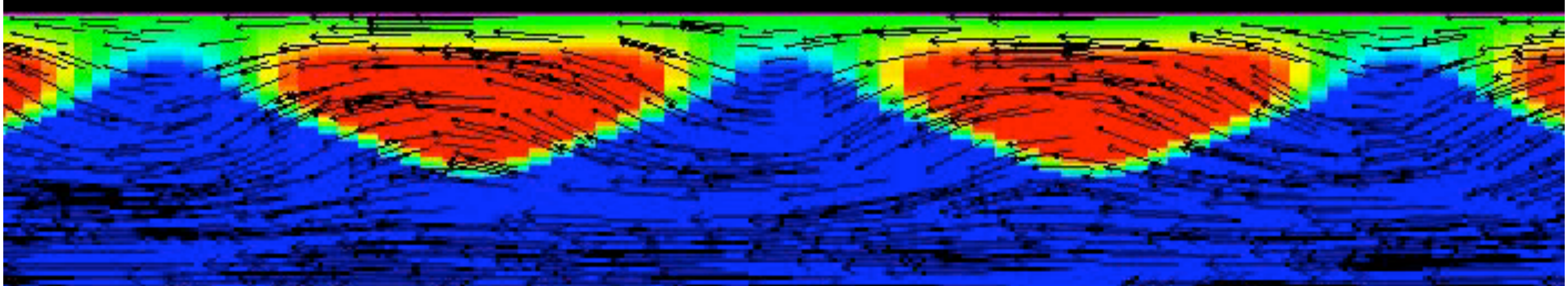
$$Pr = \frac{\nu}{\alpha}$$

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

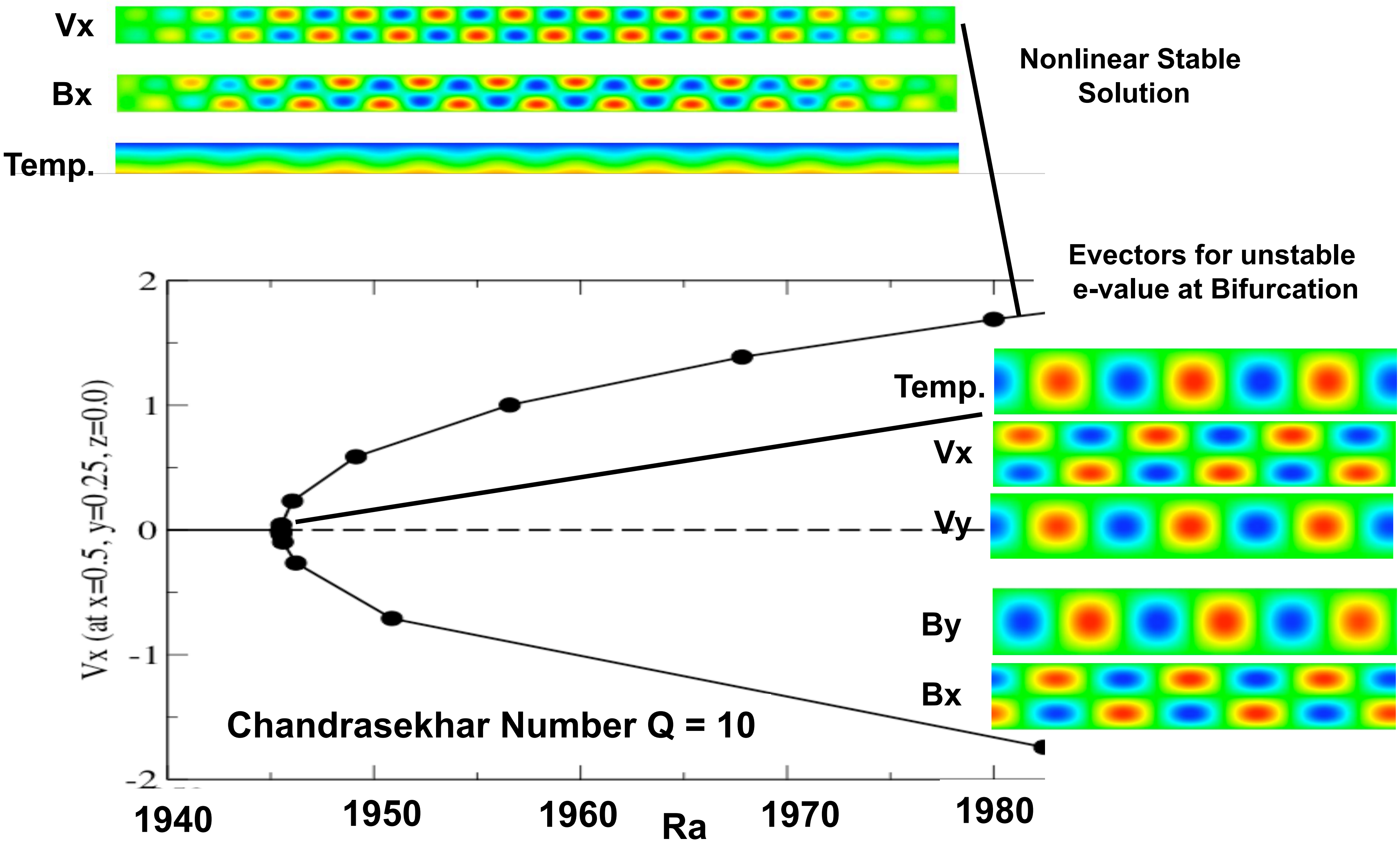
Stable Fields/Flow at Ra = 4000, Q = 81

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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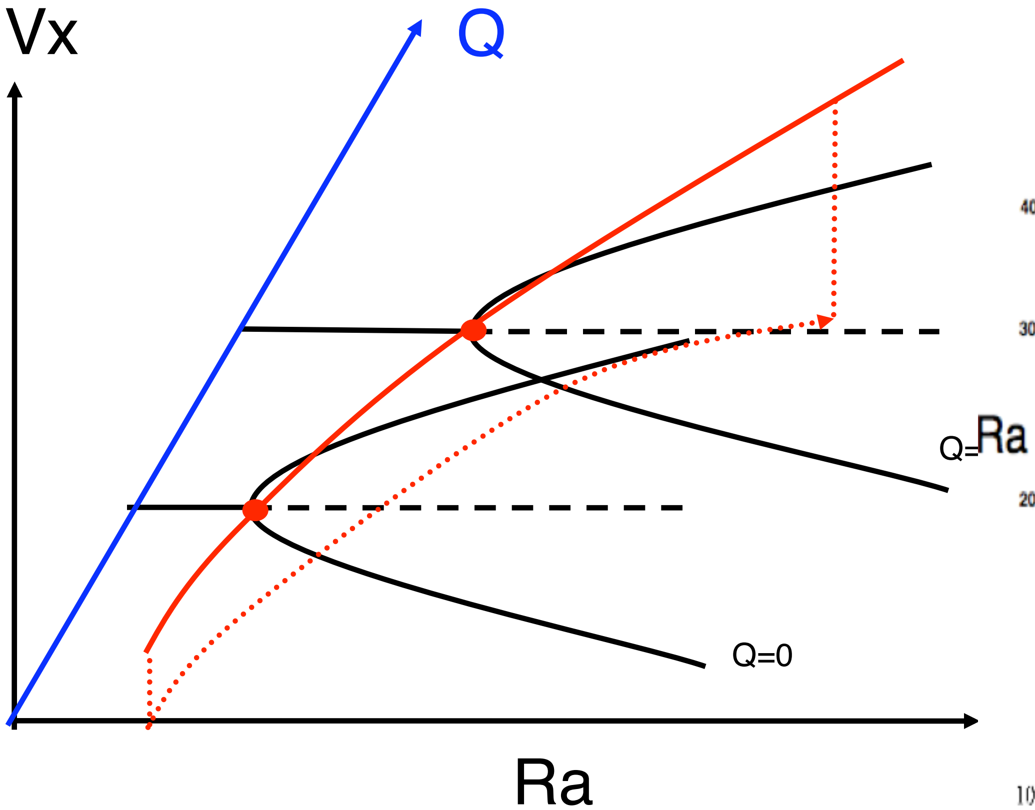
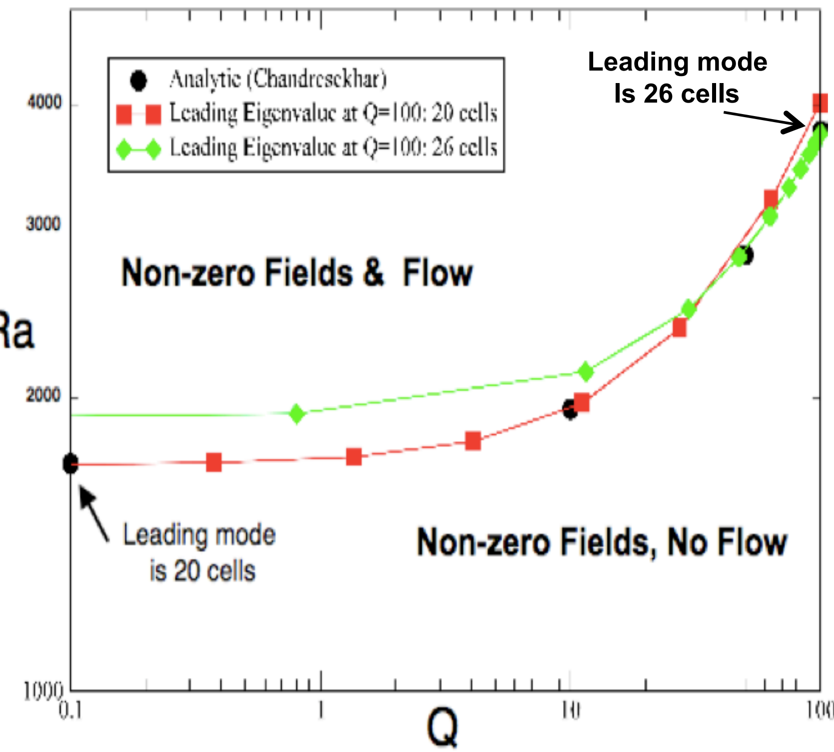
Bifurcation / Stability (Two-Parameter) Diagram

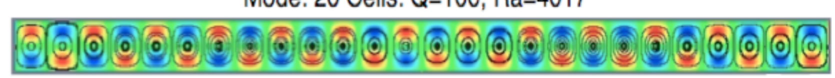


Most unstable mode compresses with increase in magnetic field strength



with Newton's method

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



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

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

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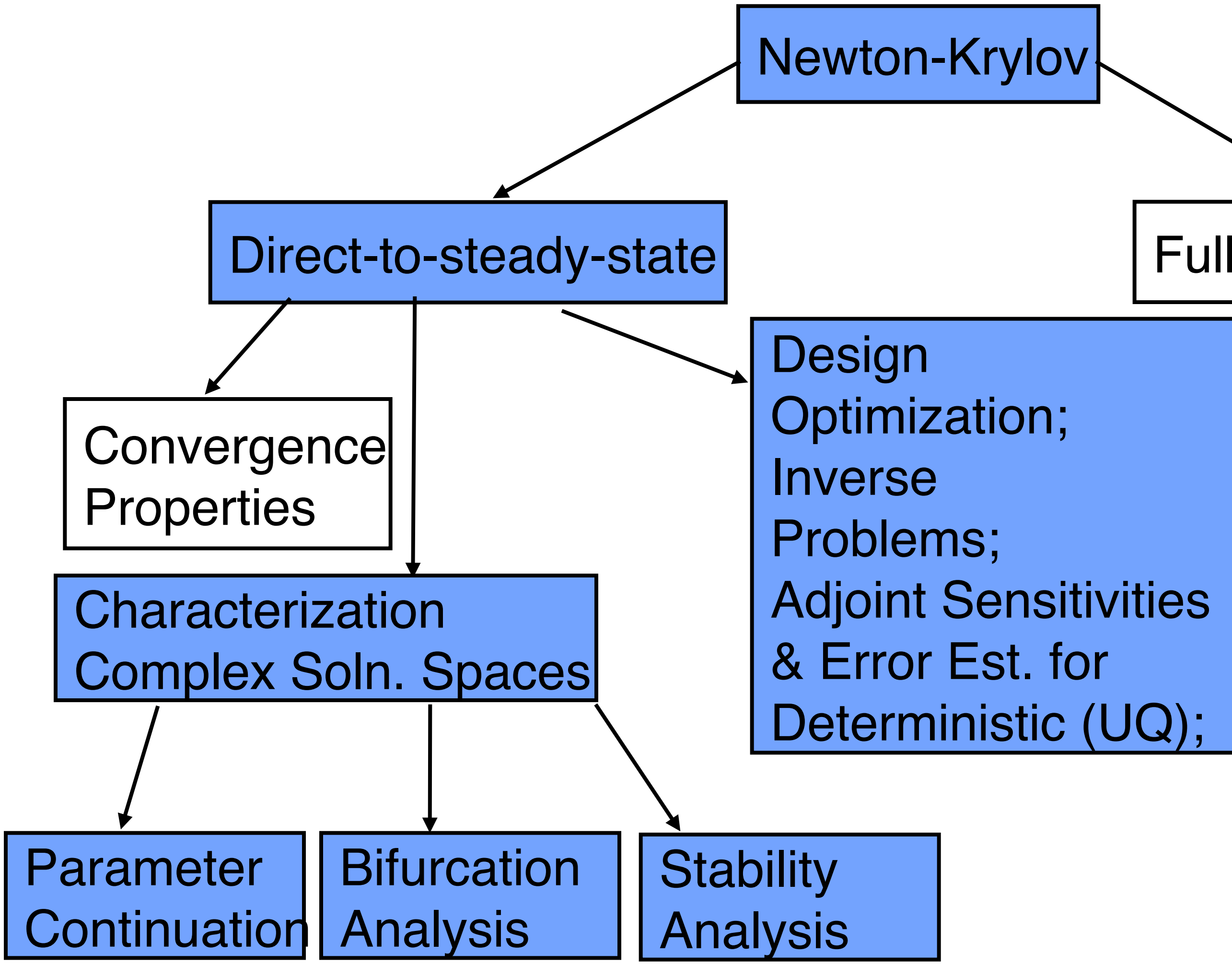
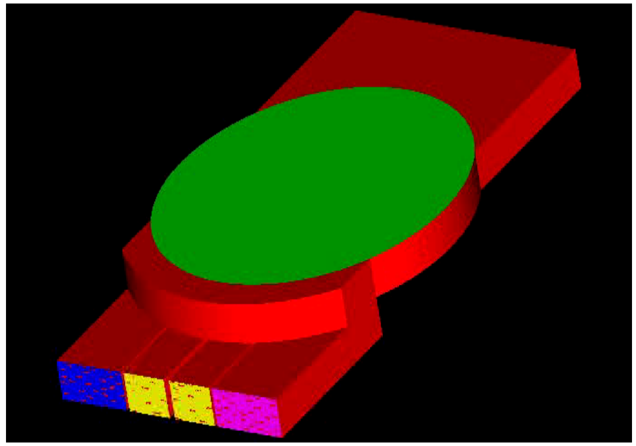
Why Newton-Krylov Methods?

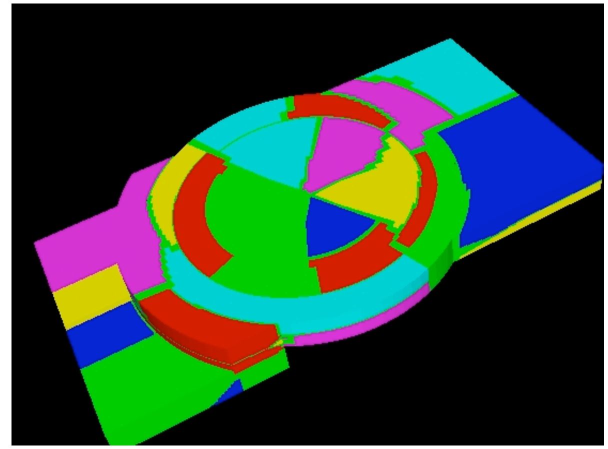


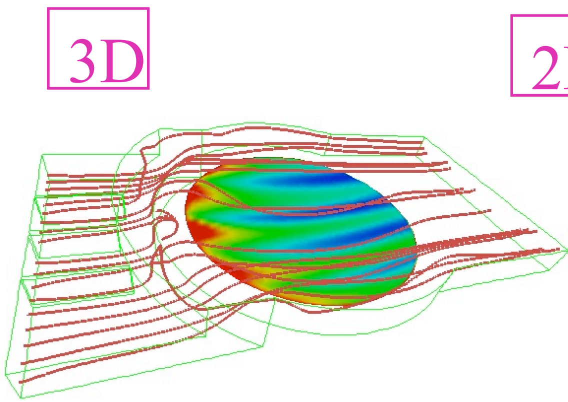
PDE Constrained Optimization of Poly-Silicon CVD Reactor
Parallel Unstructured FE Reacting Flow Simulation Code

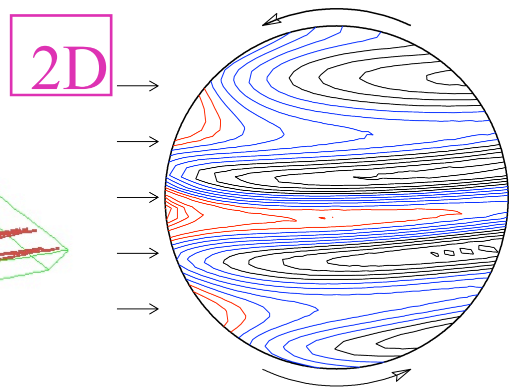
Poly-Silicon Epitaxy from Trichlorosilane in Hydrogen Carrier;

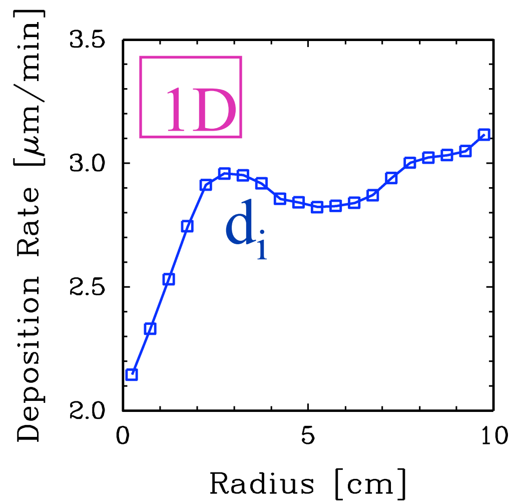
3D (u,v,w,P,T)
3 chemical species
1.2M unknowns











0D Objective Function:

$$f = \frac{1}{2}\sum_{\text{radii}} (d_i/d_{ave} - 1)^2$$

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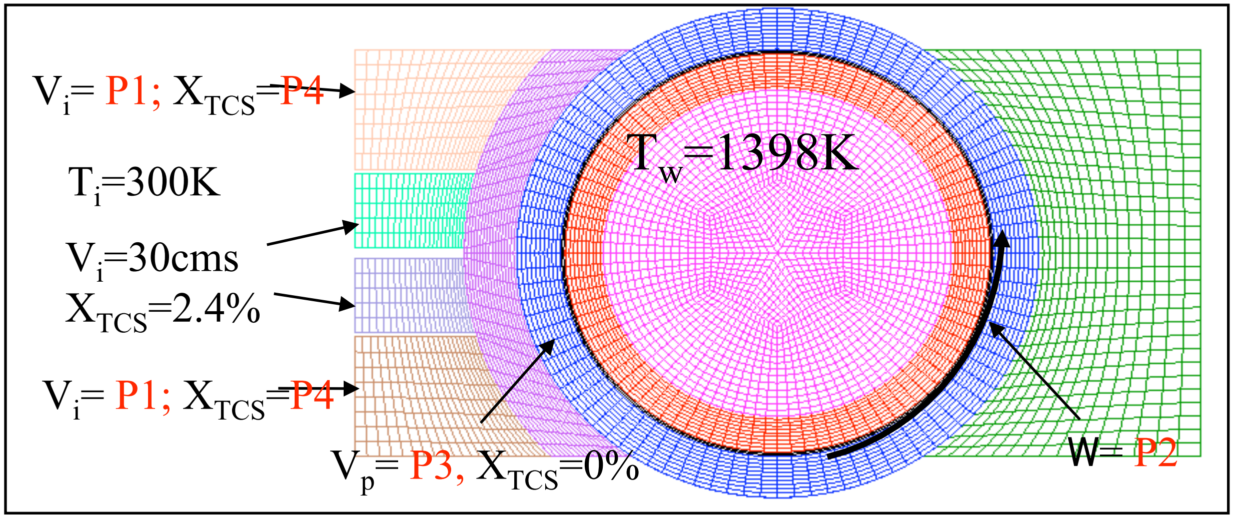
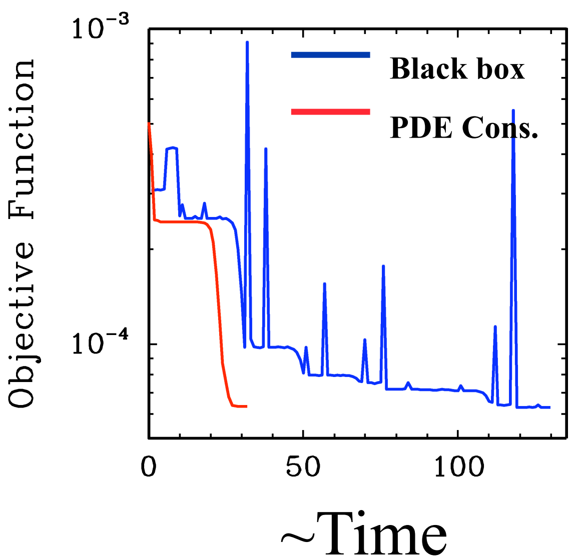
PDE Constrained Optimization of Poly-Silicon CVD Reactor

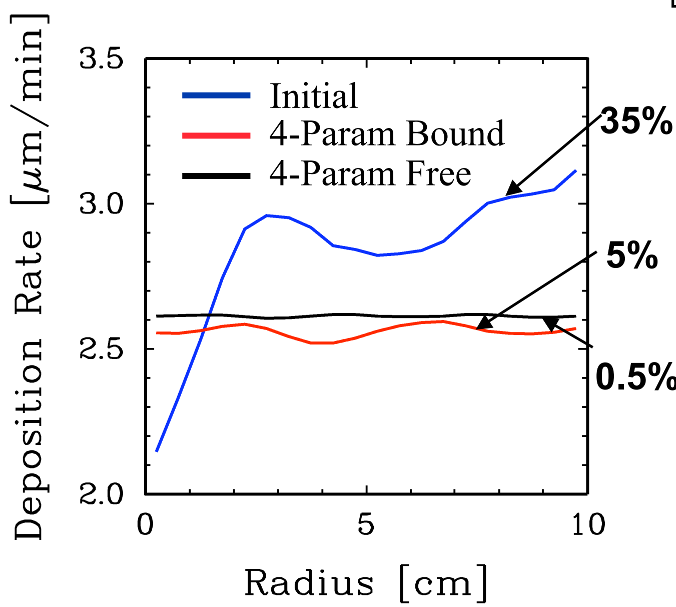


PDE Constrained Optimization:

Minimize: f(**x**,**p**)
such that: **F**(**x**,**p**)=**0**

Use Newton's Method solve KKT system





Unks	Procs	Time (hrs.)
1.2	48	6.2 (3GHz Cluster)
4.8M	128	~ 6 (Red Storm: XT3)
38M	1024	~ 7 (Red Storm: XT3)

W/Pawlowski, Salinger, van Bloemen Waanders, Bartlett, Lin - SNL

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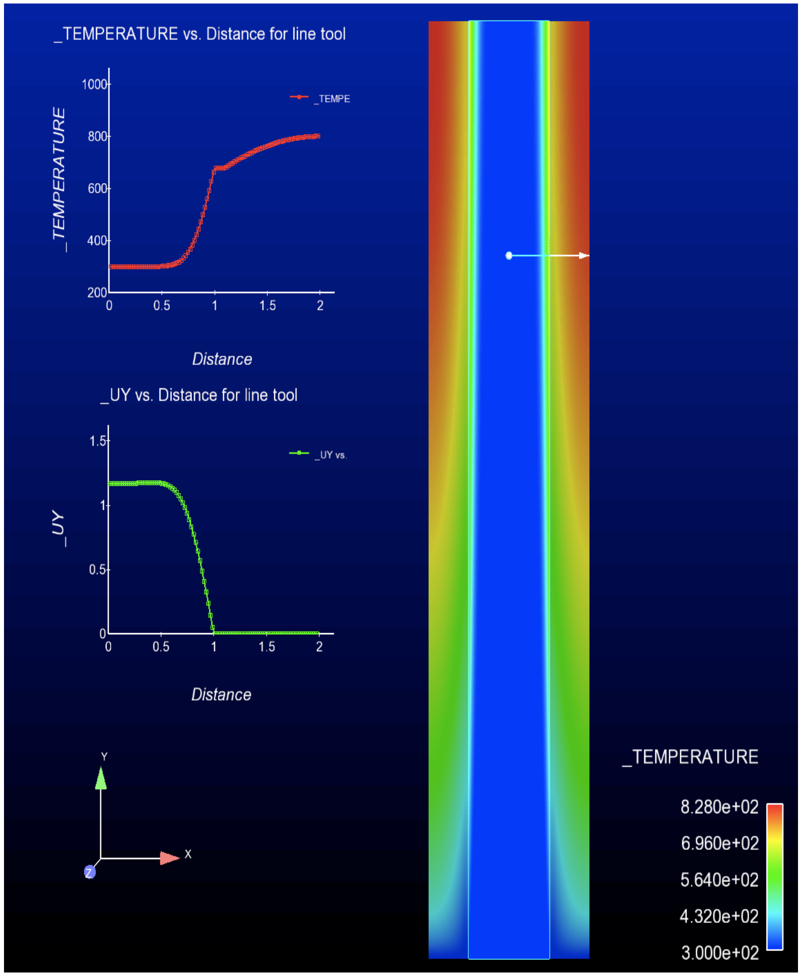
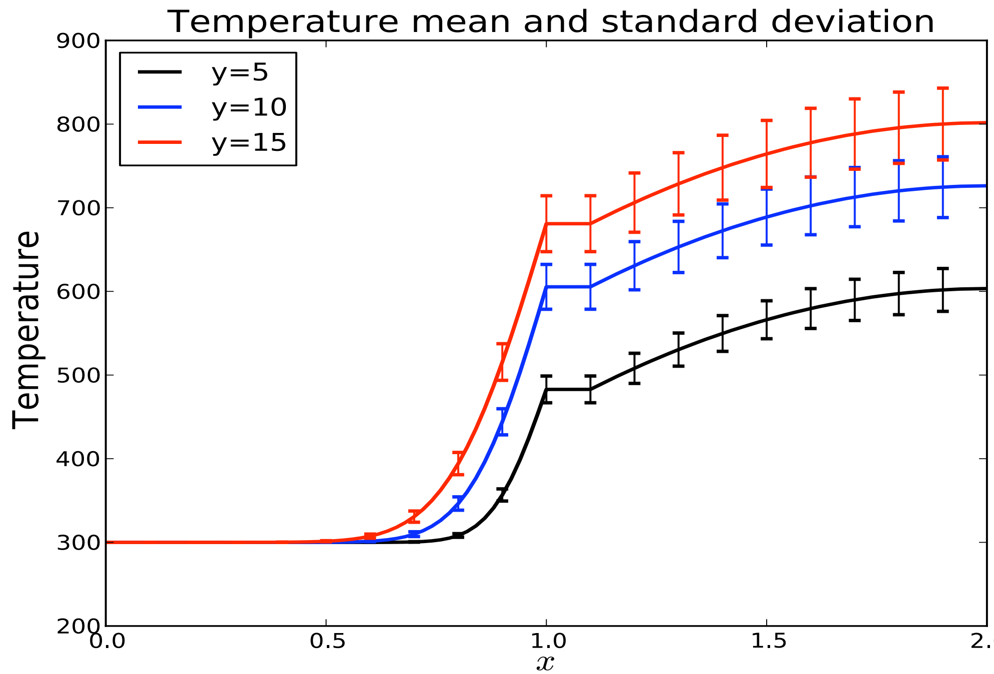
Embedded UQ and Adjoint Analysis for Error Estimation and Sensitivities for QoI



Idealized steady-state flow and heat transfer simulation. Conjugate heat transfer in cooling fluid, clad, and Fuel. Navier-Stokes Re = 1000



Stochastic Galerkin UQ analysis propagating uncertainty in the magnitude of the model fuel source term and the average inflow velocity.

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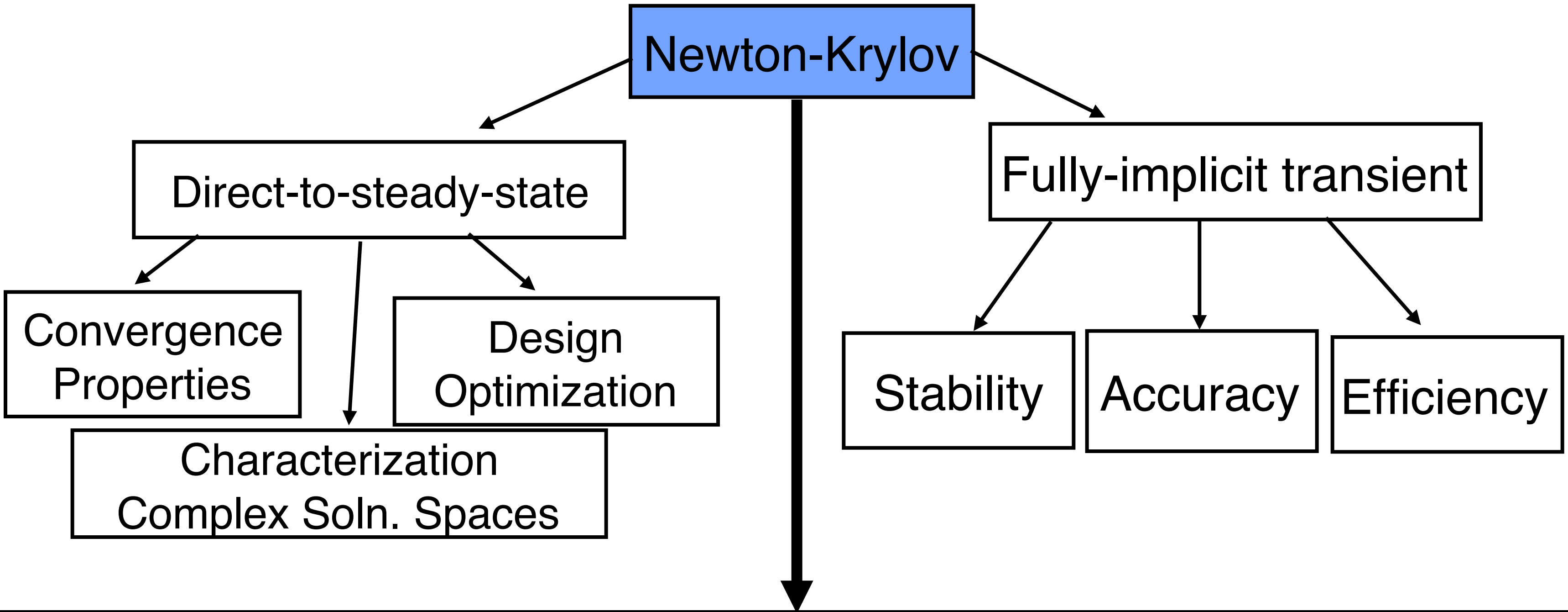
Why Newton-Krylov Methods?

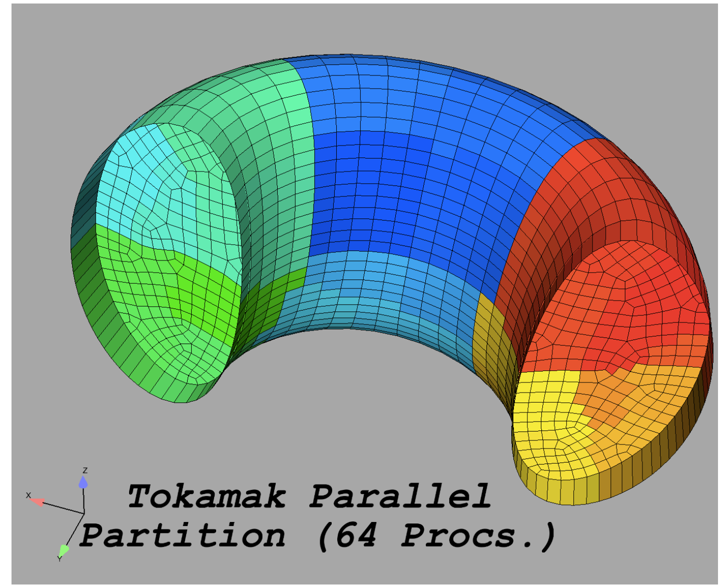


Very Large Problems -> Parallel Iterative Solution of Sub-problems

Krylov Methods - Robust, Scalable and Efficient Parallel Preconditioners

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

Preconditioning



Three variants of preconditioning

1. Domain Decomposition (Trilinos/Aztec & IFPack)

- 1 –level Additive Schwarz DD
- ILU(k) Factorization on each processor (with variable levels of overlap)
- High parallel efficiency, non-optimal algorithmic scalability

2. Multilevel Methods for Systems: ML pkg (Tuminaro, Sala, Hu, Siefert, Gee)

Fully-coupled Algebraic Multilevel methods

- Consistent set of DOF-ordered blocks at each node (e.g. stabilized FE)
- Uses block non-zero structure of Jacobian
- Aggregation techniques and rates can be chosen
- Jacobi, GS, ILU(k) as smoothers
- Can provide optimal algorithmic scalability

3. Approximate Block Factorization / Physics-based (Teko package)

- Applies to mixed interpolation (FE), staggered (FV), physics compatible discretization approaches using segregated unknown blocking
- Applied to systems where coupled AMG is difficult or might fail
- Can provide optimal algorithmic scalability

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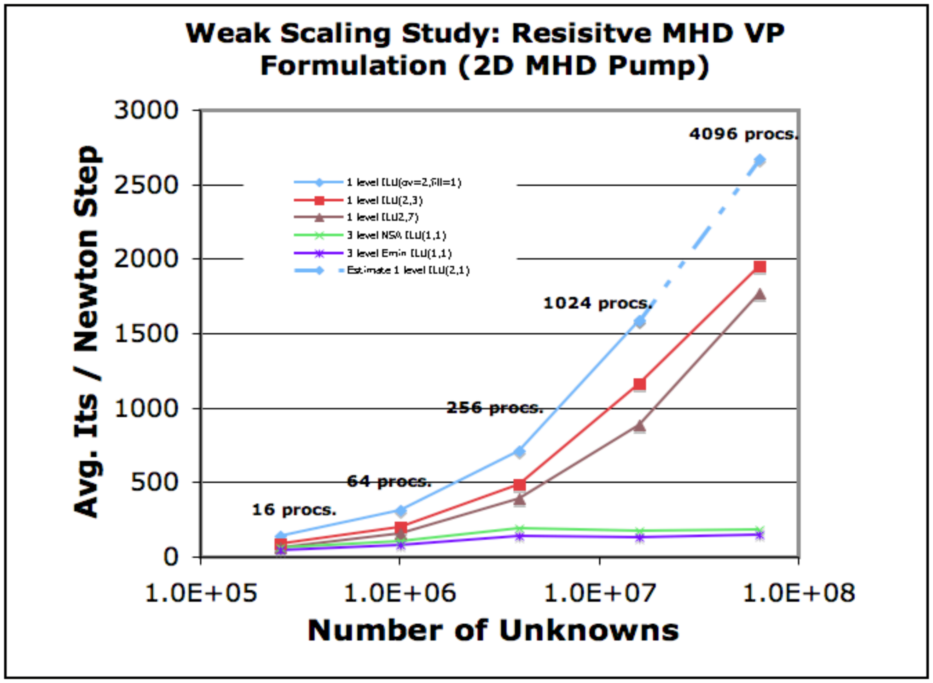
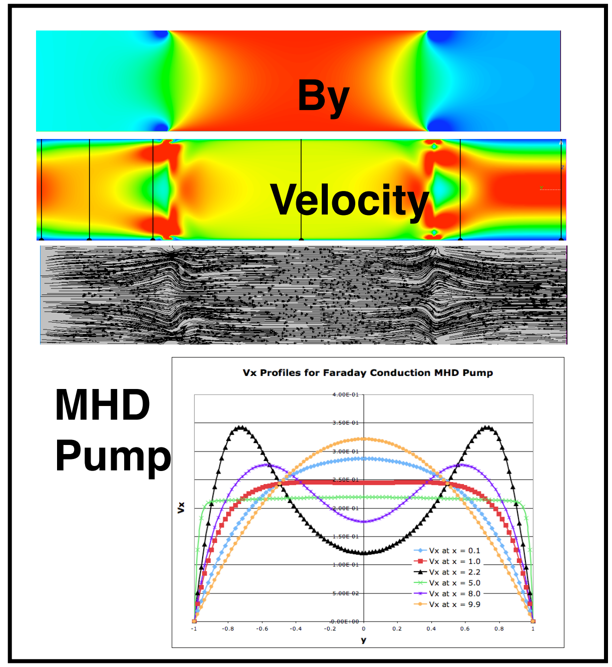
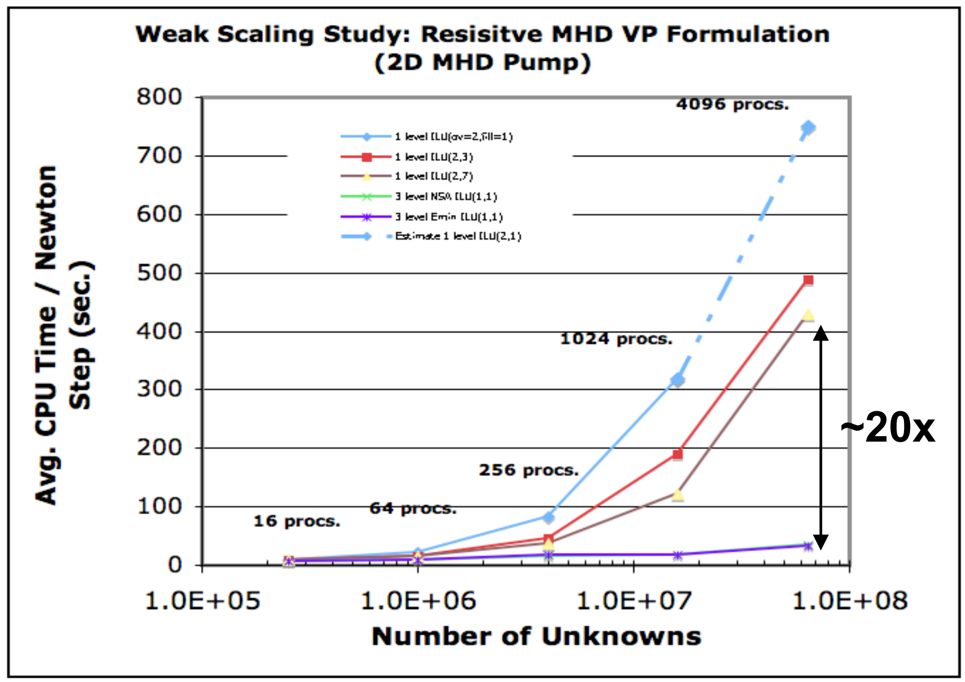
Scaling Performance for Fully-coupled Resistive MHD/ Block AMG - Cray XT3/4







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

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

1+ Billion unknowns; 260 Million Quad elements; 24K cores (4 cores / node)

Cores	Fine Mesh Level 0 Unkns.	Intermed. Level 1 Unkns.	Intermed. Level 2 Unkns.	Coarse Level 3 Unkns.	Newton Iters.	Avg. No. Linear Its. / Newton	Total Sim. Time* (min.)
24,000	1.05 billion	23.3M	.5M	11.2K	18	86	33

Note: The Additive Schwarz DD preconditioner could not be used to obtain solution in reasonable CPU time.

*** Time includes I/O**

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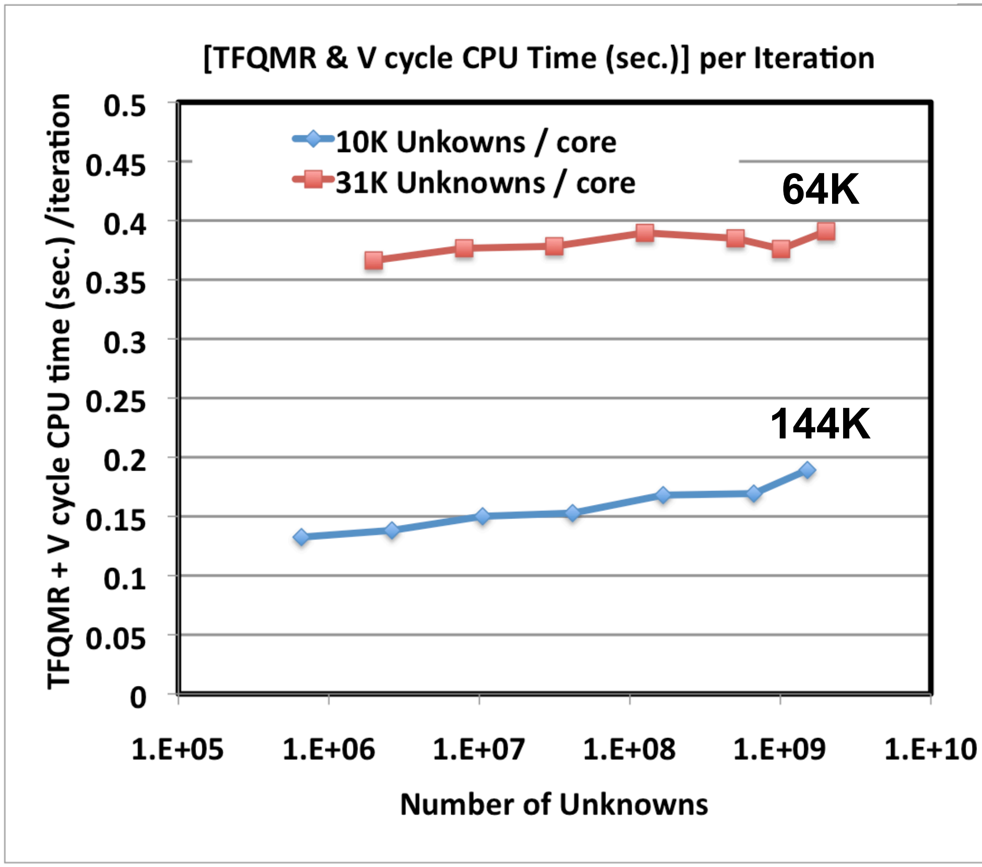
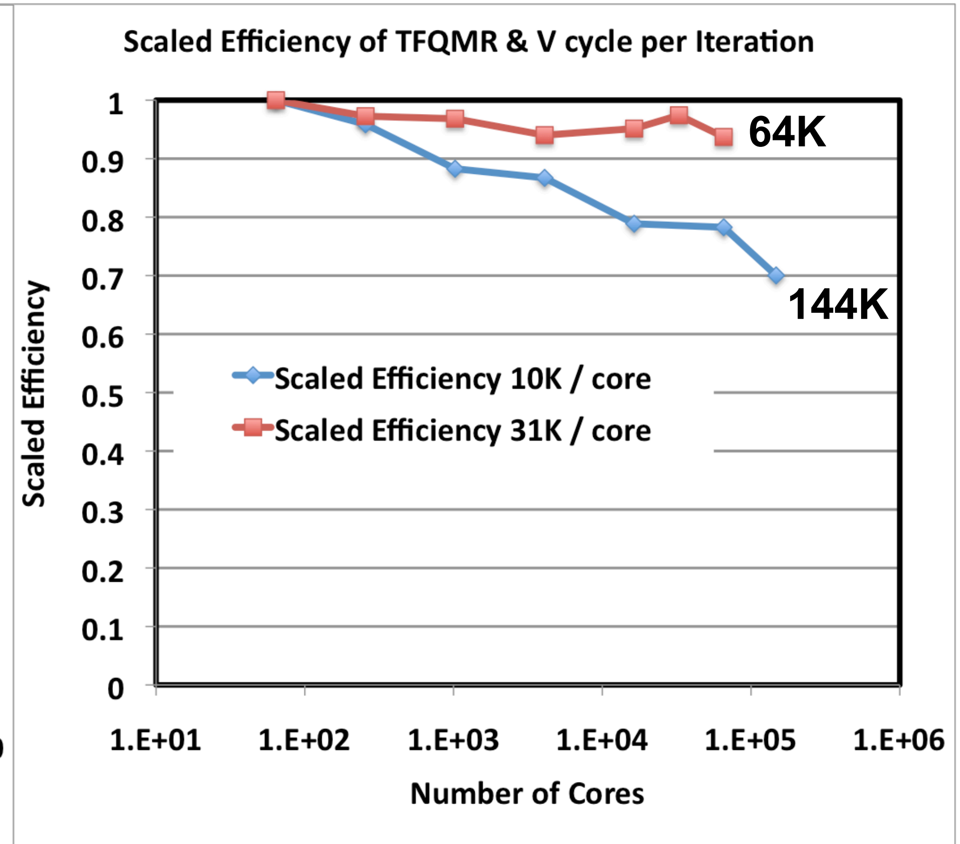
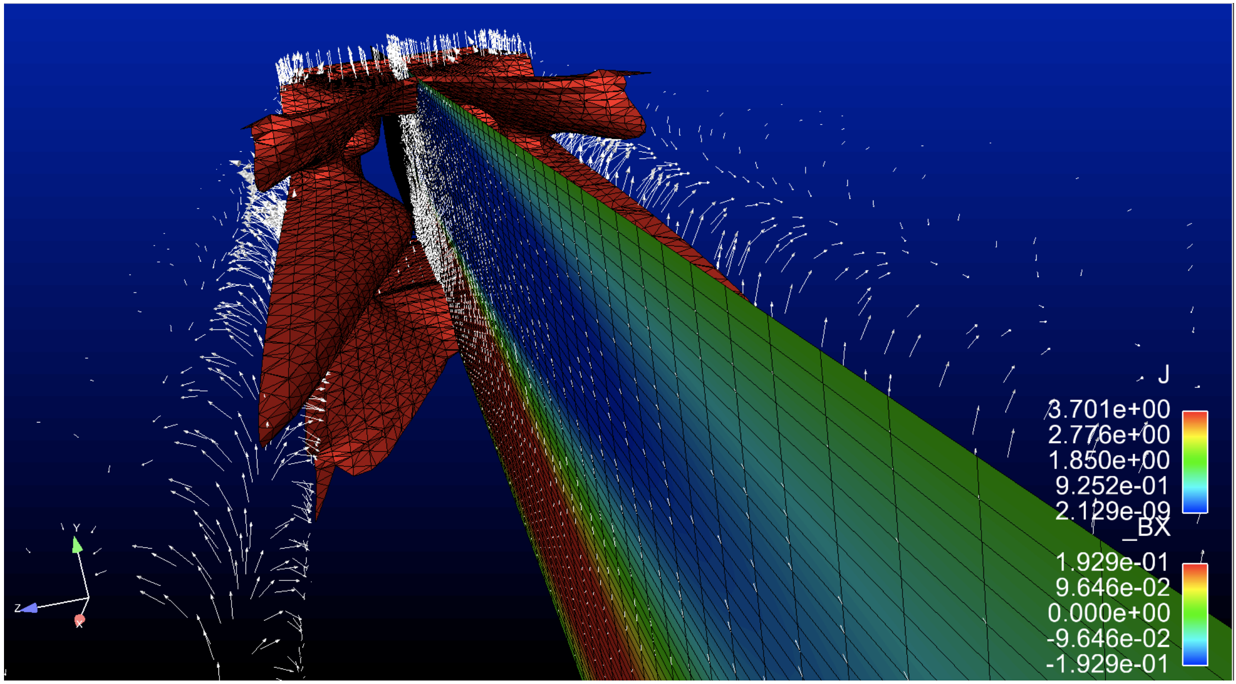
Weak Scaling Uncoupled Aggregation Scheme: Time/iteration on BlueGene/P (Drift – Diffusion BJT: P. Lin)



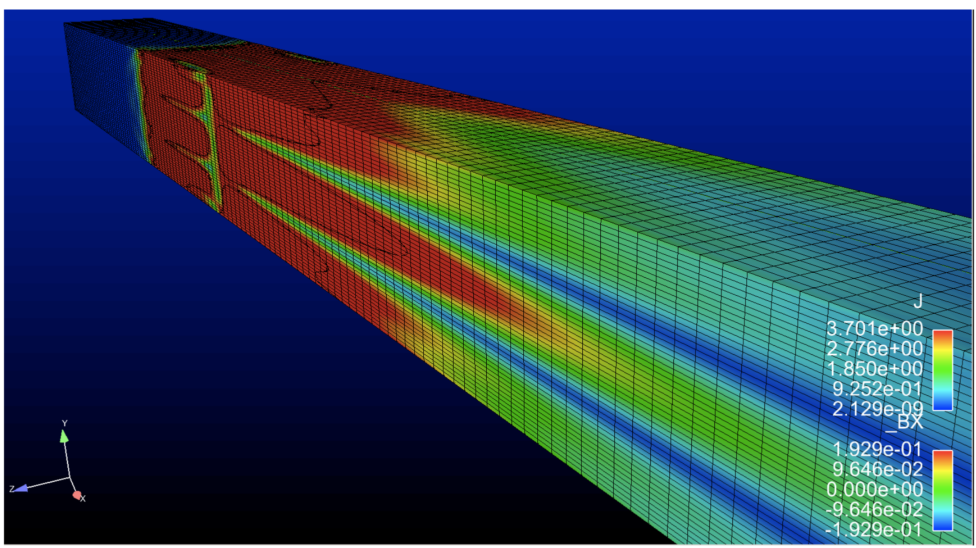


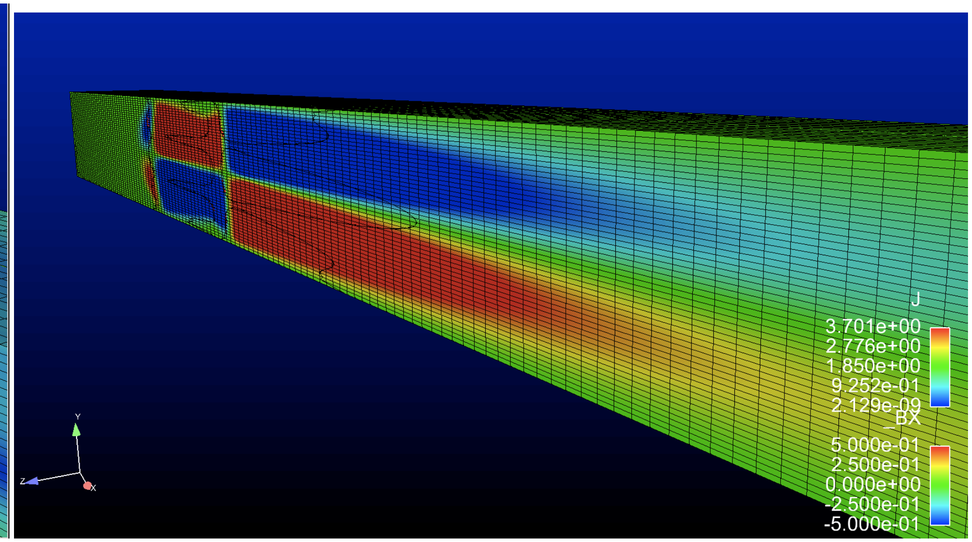
- TFQMR: used to look at time/iteration of multilevel preconditioners.
- W-cyc time/iteration not doing well due to significant increase in work on coarse levels (not shown)
- Good scaled efficiency for large-scale problems on larger core counts for 31K Unknowns / core

3D B-Field Lagrange Multiplier Formulation (Divergence form)



Initial Prototype MHD Generator

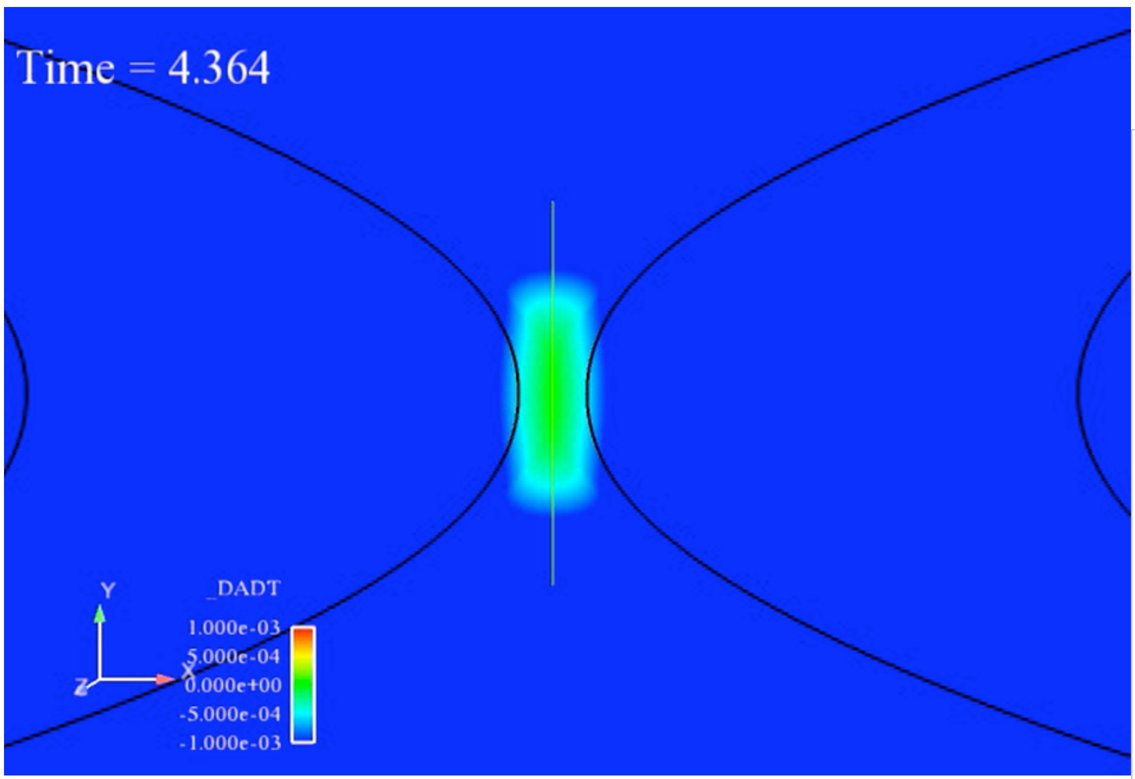


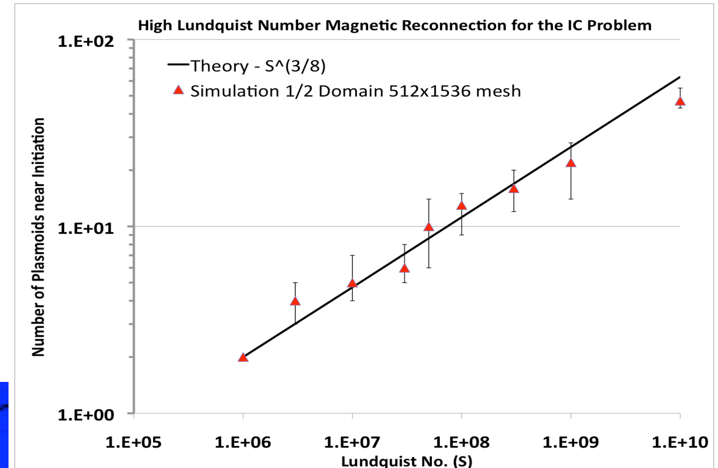


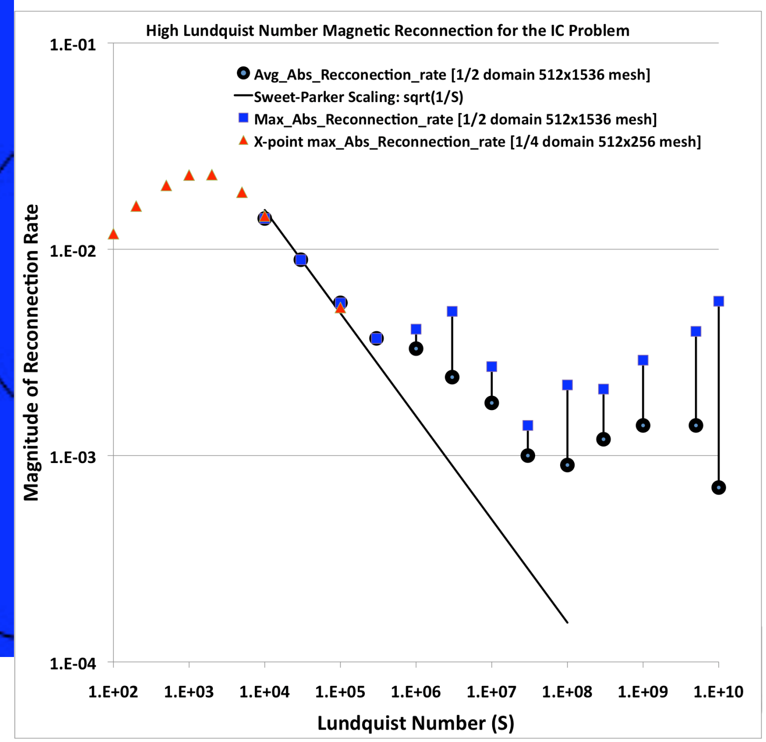
Plasma Physics Studies: Plasmoid formation in magnetic reconnection

Magnetic reconnection: fundamental process whereby magnetic field topology is altered resulting in a rapid conversion of magnetic field energy into plasma energy and significant plasma transport. Mechanisms and time scales have been an open issue for last 50 years.

Critical process in astrophysical and laboratory plasmas.







Step back to CFD for a moment to

Introduce block approximate factorization (physics-based) preconditioners

Brief Overview of Block Preconditioning Methods for Navier-Stokes: (A Taxonomy based on Approximate Block Factorizations, JCP – 2008)

Discrete N-S	Exact LDU Factorization	Approx. LDU
$\begin{pmatrix} F & B^T \\ \hat{B} & -C \end{pmatrix} \begin{pmatrix} \Delta u_k \\ \Delta p_k \end{pmatrix} = \begin{pmatrix} g_u^k \\ g_p^k \end{pmatrix}$	$\begin{pmatrix} I & 0 \\ \hat{B}F^{-1} & I \end{pmatrix} \begin{pmatrix} F & 0 \\ 0 & -S \end{pmatrix} \begin{pmatrix} I & F^{-1}B^T \\ 0 & I \end{pmatrix}$ $S = C + \hat{B}F^{-1}B^T$	$\begin{bmatrix} I & 0 \\ \hat{B}H_1 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & -\hat{S} \end{bmatrix} \begin{bmatrix} I & H_2B^T \\ 0 & I \end{bmatrix}$

Precond. Type	H_1	H_2	$\hat{S}$	References
Pres. Proj; 1st Term Neumann Series	$\mathbf{F}^{-1}$	$(\Delta t\mathbf{I})^{-1}$	$\mathbf{C} + \Delta t\hat{\mathbf{B}}\mathbf{B}^T$	Chorin(1967);Temam (1969); Perot (1993): Quateroni et. al. (2000) as solvers
SIMPLEC	$\mathbf{F}^{-1}$	$(\mathrm{diag}(\sum \lvert\mathbf{F}\rvert))^{-1}$	$\mathbf{C} + \hat{\mathbf{B}}(\mathrm{diag}(\sum \lvert\mathbf{F}\rvert))^{-1}\mathbf{B}^T$	Patankar et. al. (1980) as solvers; Pernice and Tocci (2001) as smothers/MG
Pressure Convection / Diffusion	0	$\mathbf{F}^{-1}$	$\mathbf{A_p}\mathbf{F_p}^{-1}$	Kay, Loghin, Wathan, Silvester, Elman (1999 - 2006); Elman, Howle, S., Shuttleworth, Tuminaro (2003,2008)

Now use AMG type methods on sub-problems.

Momentum transient convection-diffusion: $F\Delta\mathbf{u} = \mathbf{r_u}$

Pressure – Poisson type: $-\hat{S}\Delta p = \mathbf{r}_p$

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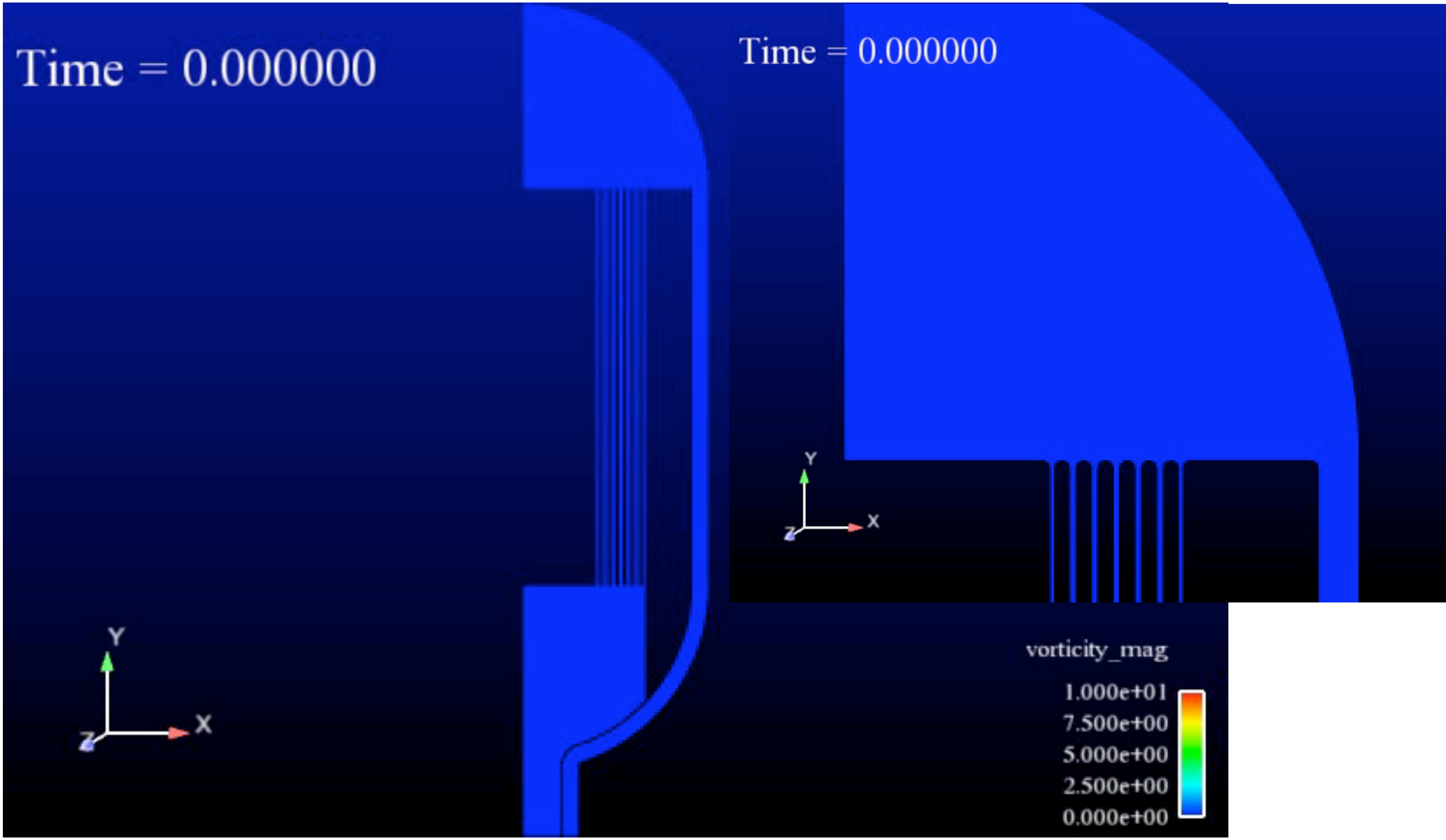
Start-up of Helium fluid flow in NGNP reactor geometry (not actual operating cond.)



NGNP Geometry: Rich Martineau (INL), Unstructured Quad Cubit Mesh SNL

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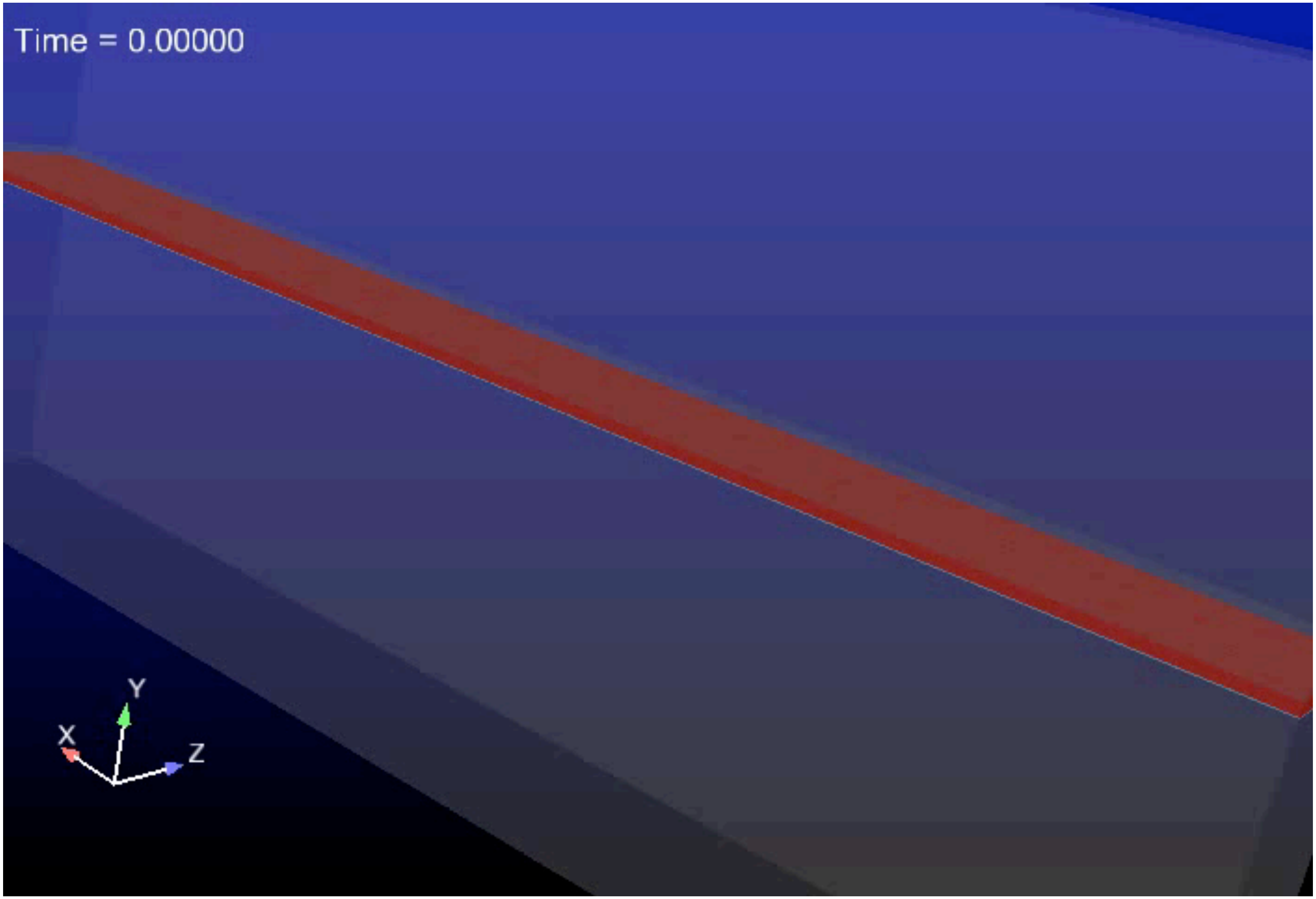
Transient Kelvin-Helmholtz 3D Shear layer Re = 5 x 10^4



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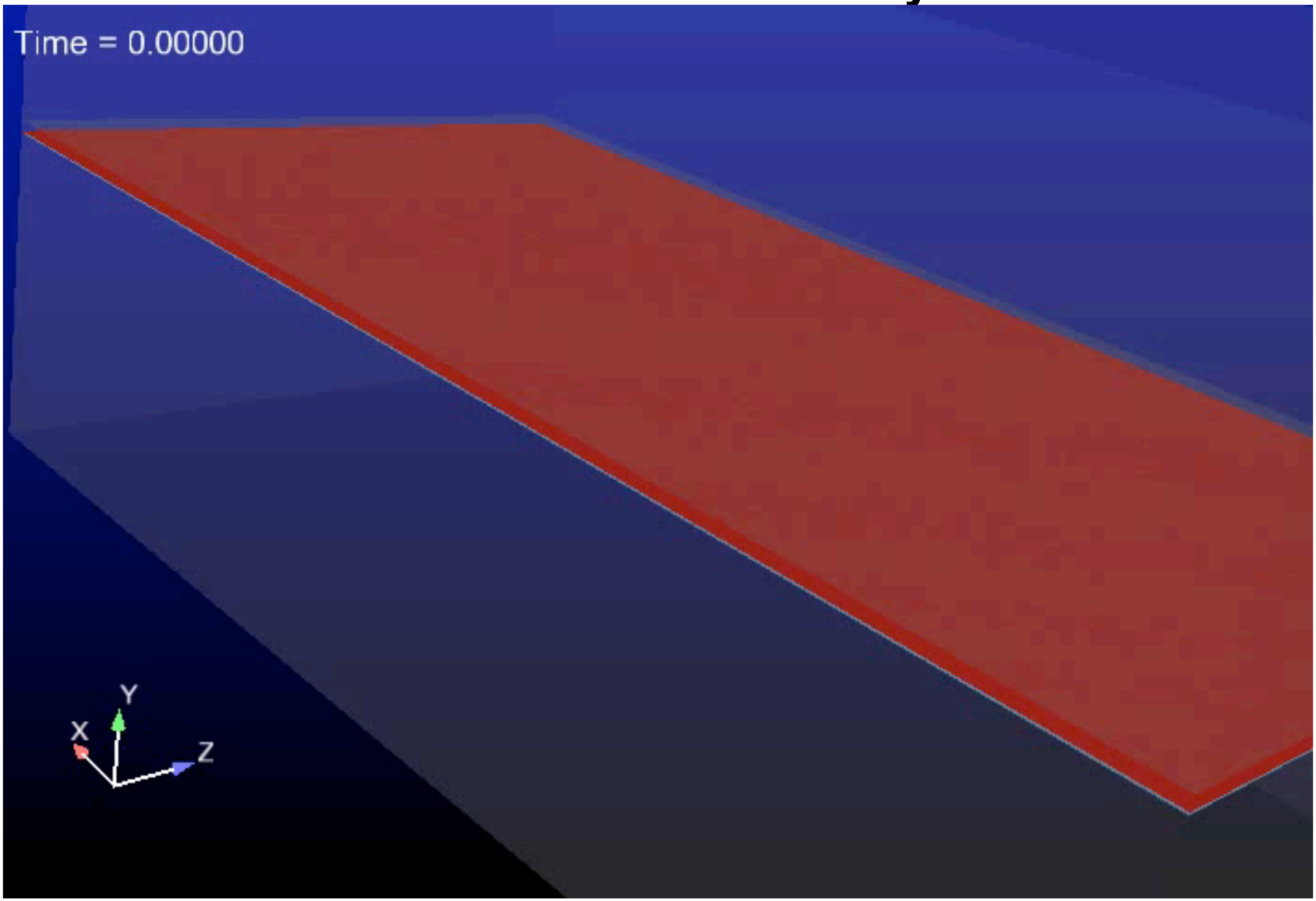
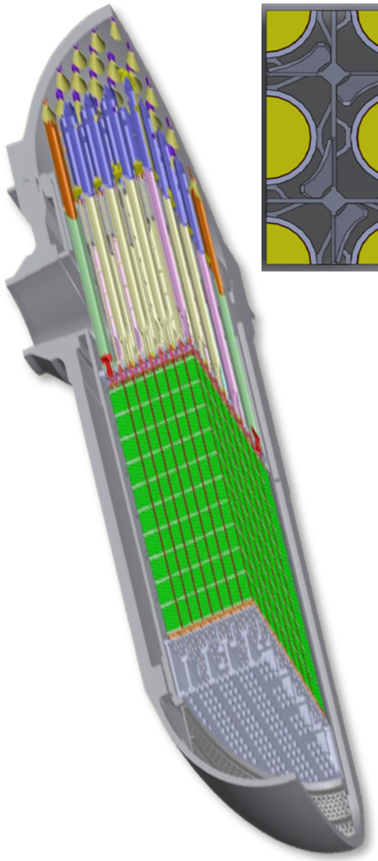
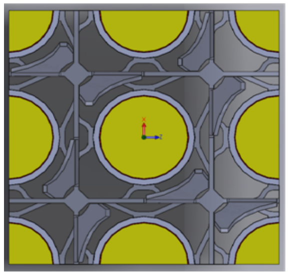
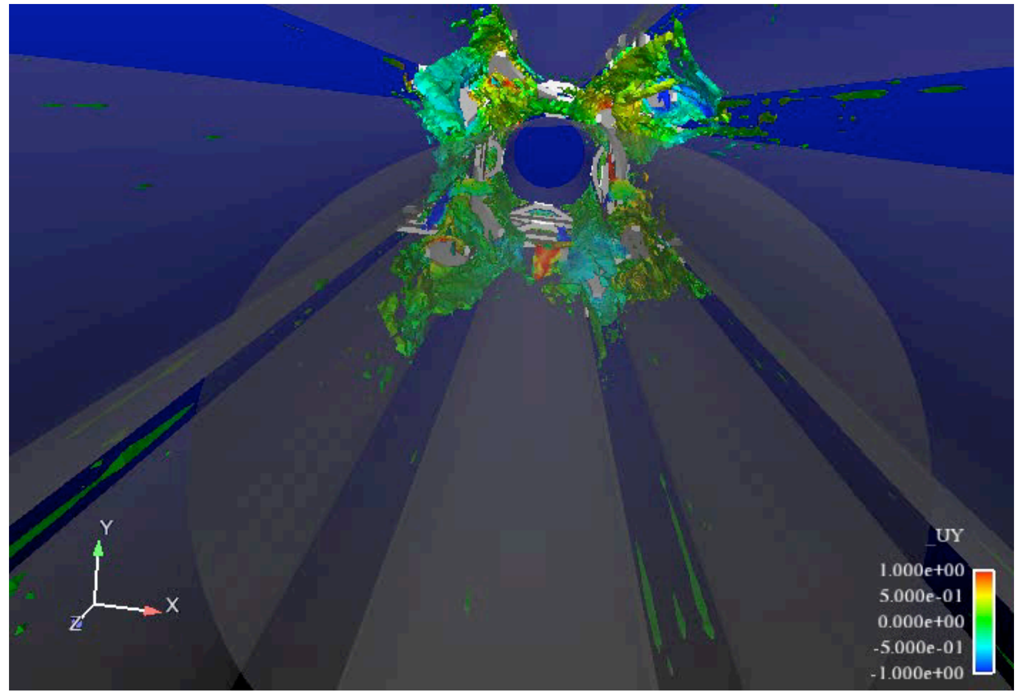
Transient Kelvin-Helmholtz 3D Shear layer Re = 5 x 10^4

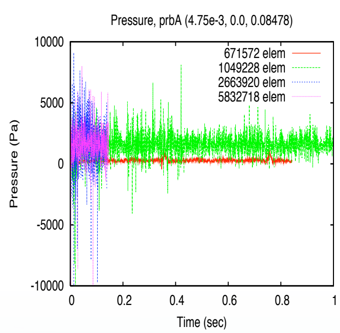


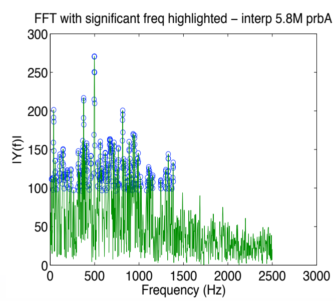
LES CFD + Rod Vibration analysis of Nuclear Reactor Core Flow (Re = 2e+5 simulation of 3x3 pin-geometry with mixing vane)



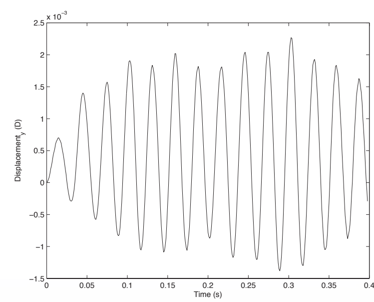


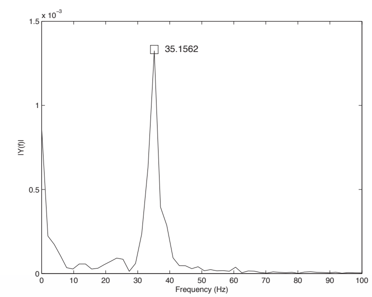






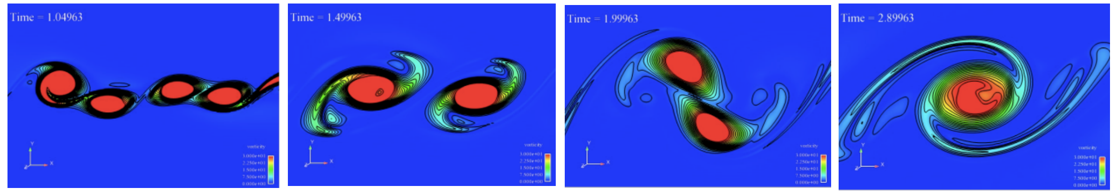
LES Fluid Pressure Load on Fuel Rod

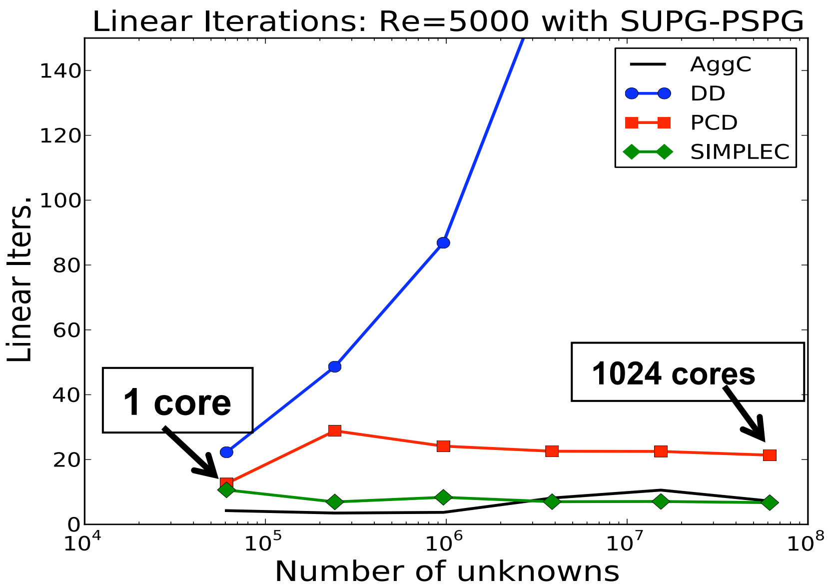


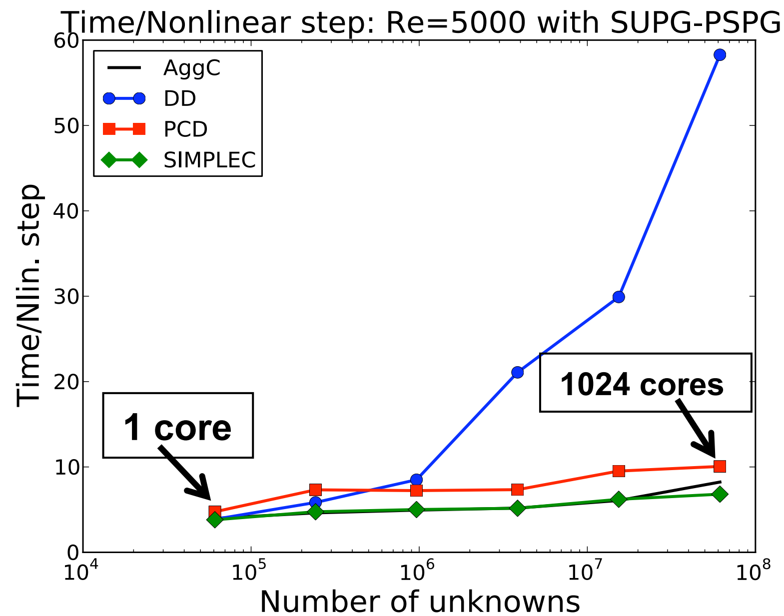


Fuel Rod Vibration Response

Transient Kelvin-Helmholtz







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

- **Run on 1 to 1024 cores**
- **Pressure - PSPG, Velocity - SUPG(residual and Jacobian)**

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Now Return to MHD

Block approximate factorization (physics-based) preconditioners

Incompressible Resistive MHD a New Nested Schur Complement Approach

Block LU factorization gives

$$\begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix} = \begin{bmatrix} I & & \\ BF^{-1} & I & \\ YF^{-1} & -YF^{-1}B^TS^{-1} & I \end{bmatrix} \begin{bmatrix} F & B^T & Z \\ & S & -BF^{-1}Z \\ & & P \end{bmatrix}$$

where

$$S = C - BF^{-1}B^T$$

$$P = D - YF^{-1}(I + B^TS^{-1}BF^{-1})Z$$

- **3x3 system leads to embedded Schur complements**
- **Embedding is independent of ordering (*C*$^{-1}$ doesn't need to exist!)**
- **How is *P* approximated?**
- **Can we simplify this? E.g. Operator split prec.**

$$\begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix} \approx \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix} = \begin{bmatrix} F & B^T & Z \\ B & C & \\ Y & \boxed{YF^{-1}B^T} & D \end{bmatrix}$$

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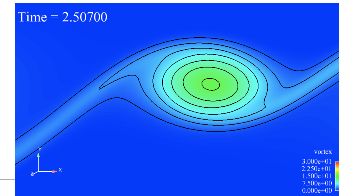
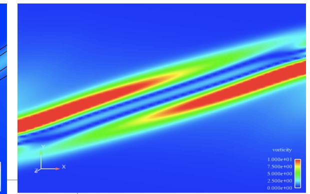
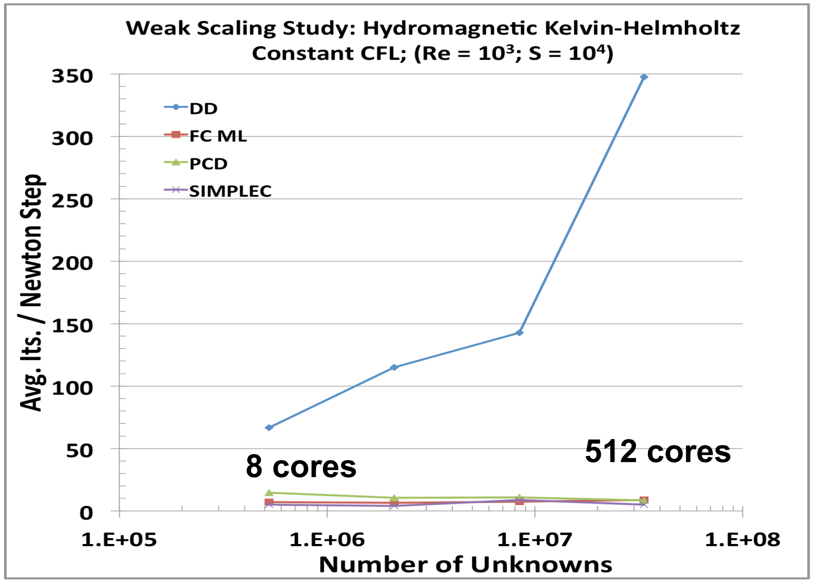
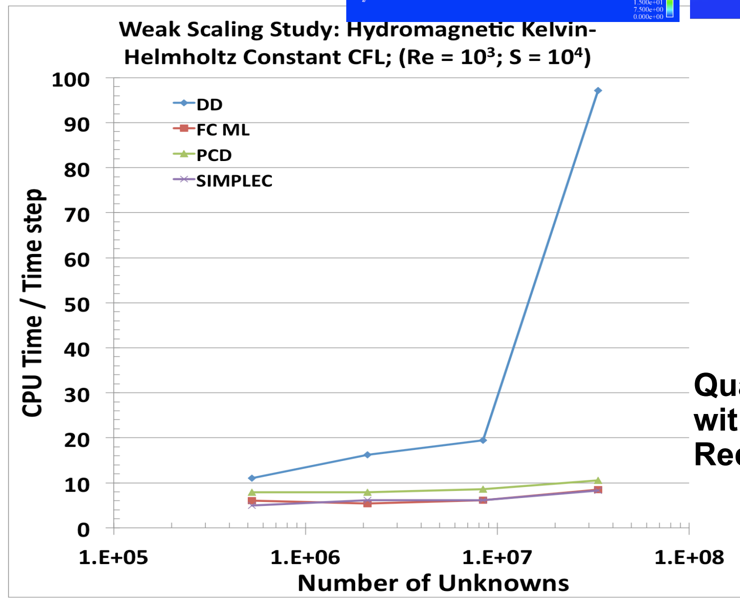
Transient Hydromagnetic Kelvin-Helmholtz Problem Re = 1e+3, S = 1e+4

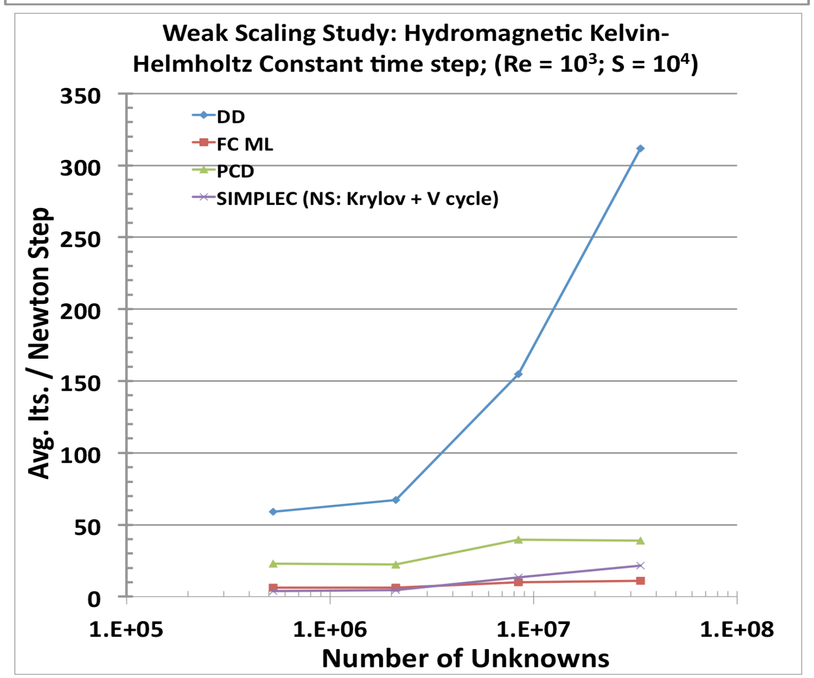


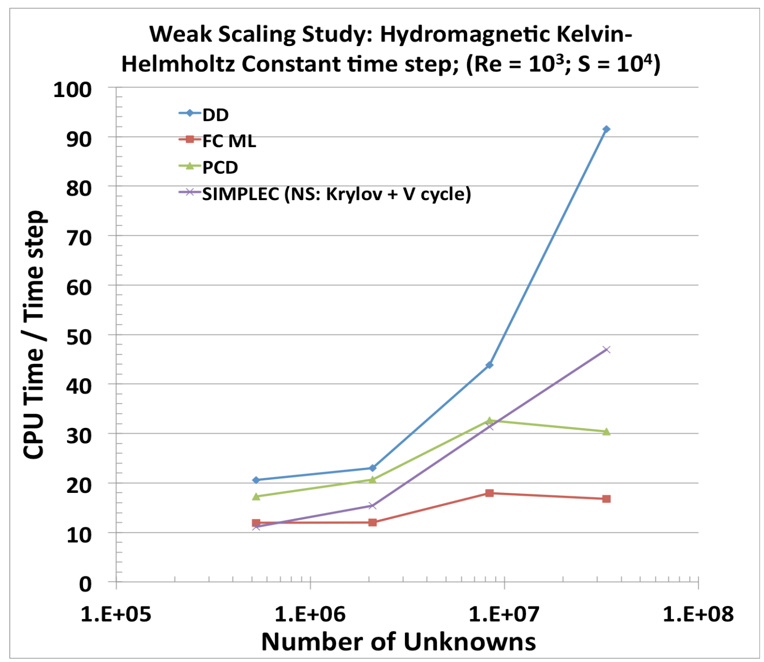






Quad-core Nehalems with Infini-band SNL Red Sky





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Conclusions

- Results for stabilized FE methods for low Mach number Transport/Reaction low flow-Mach number resistive MHD system are encouraging. Can be robust and efficient solvers for direct-to-steady-sate, transient, bifurcation and optimization.

- Parallel Newton-Krylov with fully-coupled block aggressive coarsening AMG preconditioners have shown promising results for algorithmic scalability and CPU time performance for Transport/Reaction and initial MHD solutions.

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

- New approximate block factorization / physics based preconditioners for incompressible / low-flow-Mach number Transport/Reaction and resistive MHD are encouraging. Need more work on efficient/robust Schur complement solvers.

- Future work:
  - Need to verify 3D resistive MHD B-field generalized Lagrange multiplier formulation.
  - Complete development of physics-compatible 3D MHD formulation with face, edge, nodal and volume elements (de Rham complex)
  - Fully Compressible 3D MHD formulation with high-resolution FE methods.

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

Trilinos

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

The End