Newton-Krylov Solution Methods for Multiple-time-scale Multiphysics Systems: Transport/Reaction and Resistive MHD

John N. Shadid

Computational Science R&D Group
Sandia National Laboratories

Collaborators:

Paul T. Lin
Roger P. Pawlowski
Ray S. Tuminaro
Eric Phipps

Sandia National Laboratories

Luis Chacon

Oak Ridge National Laboratory

Jeffery Banks

Lawrence Livermore National Laboratory

DOE / NNSA

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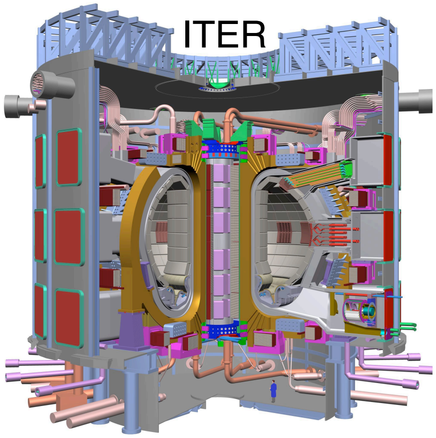
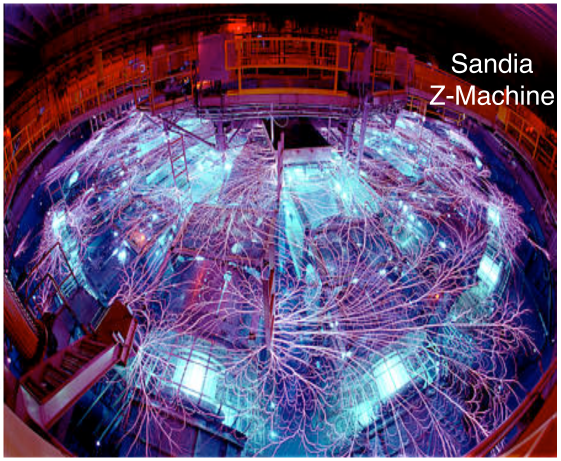
Outline

- **Motivation: Multiple-time-scale Multi-physics Nonlinear Systems**
- **Outline of Example Systems of Coupled Nonlinear PDEs**
- **Why Newton-Krylov Methods?**
  - **Multiple-time-scale Systems (Contrast Operator split, linearized, fully implicit)**
  - **Characterization of Complex Solution Spaces**
  - **Optimization**
- **Representative Solution Algorithm Performance**
  - **N-K and Algebraic Multi-level Preconditioners (unstructured FE)**
  - **JFNK and Physics Based Preconditioners (Mapped Structured FV)**
- **Conclusions**

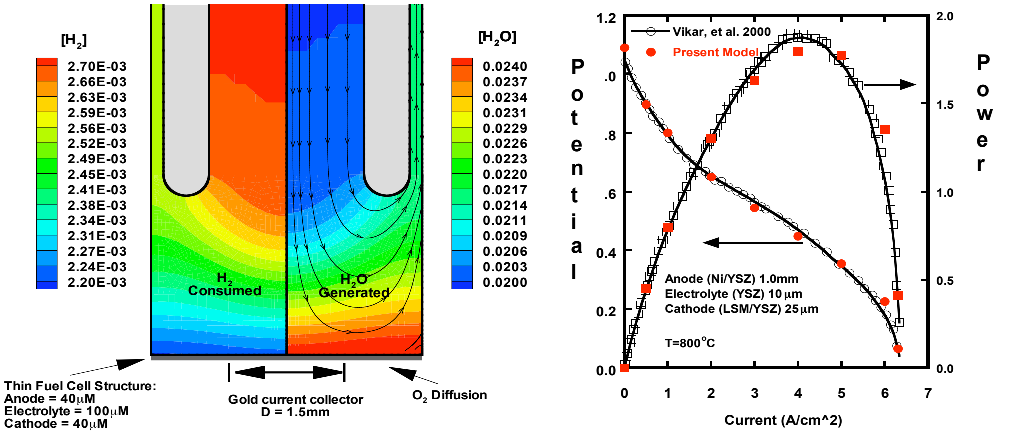
Scientific / Technology Motivation

- **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, ..**
  - **…**
- **Transport / Reaction Systems model a very broad range of systems**
  - **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



Mathematical / Computational Motivation: 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.

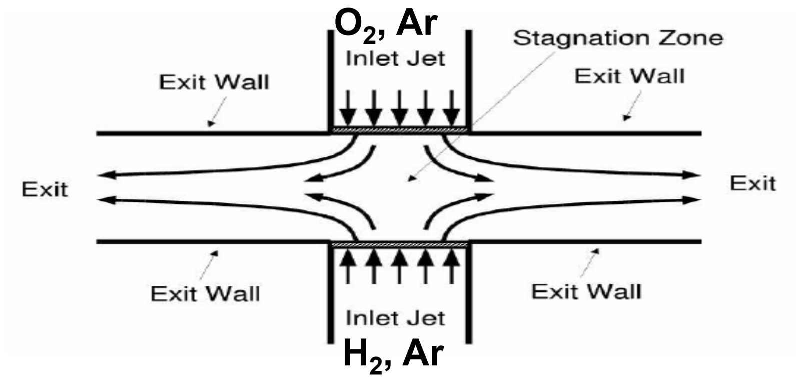
These mechanisms can balance to produce:

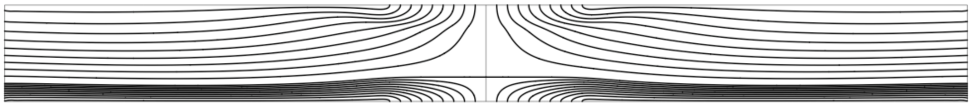
- **steady-state behavior,**
- **nearly balance to evolve a solution on a dynamical time scale that is long relative to the component time scales,**
- **or can be dominated by one, or a few processes, that drive a short dynamical time scale consistent with these dominating modes.**

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

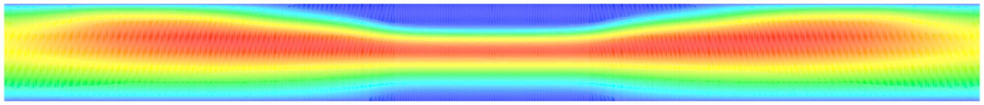
Our approach - pursue new applied math/algorithms to develop robust, accurate, scalable, and efficient implicit formulations and fully-coupled Newton-Krylov methods with integrated optimization/UQ tools for predictive simulation technologies for complex coupled multi-physics systems.

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

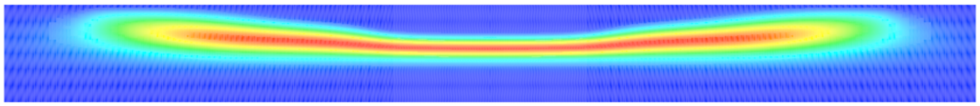




Streamlines

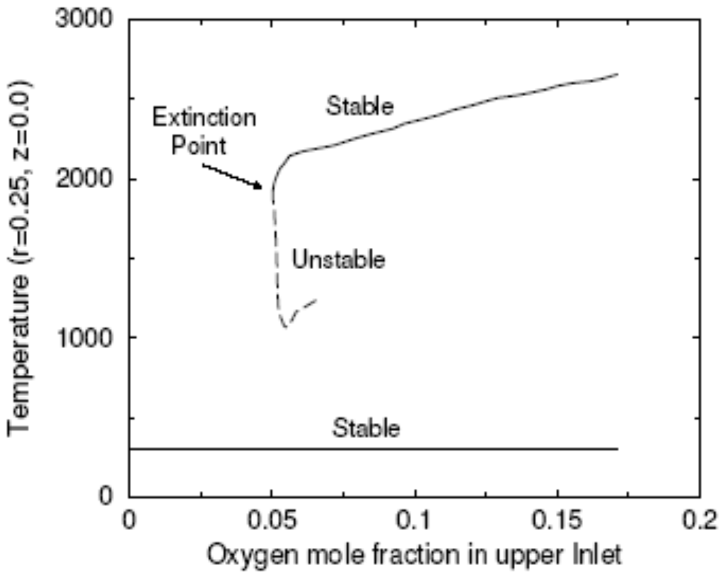


Temperature (Min. 300°K, Max 2727°K)



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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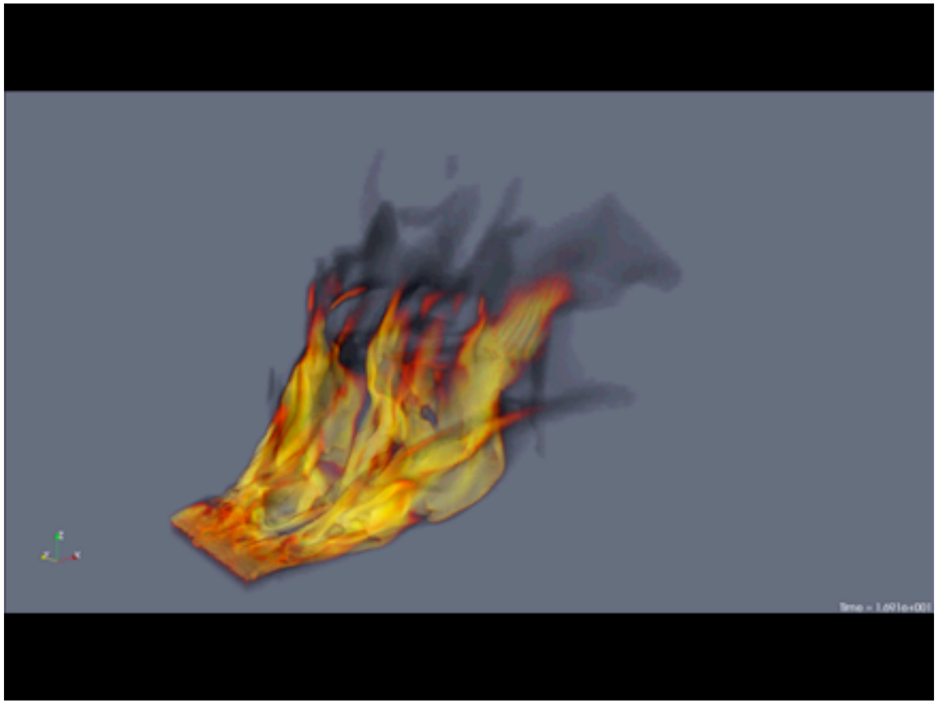
Predicting an Object's Thermal Response Within a Turbulent, Reacting, Participating Media Radiation Environment

Stefan P. Domino et. al.

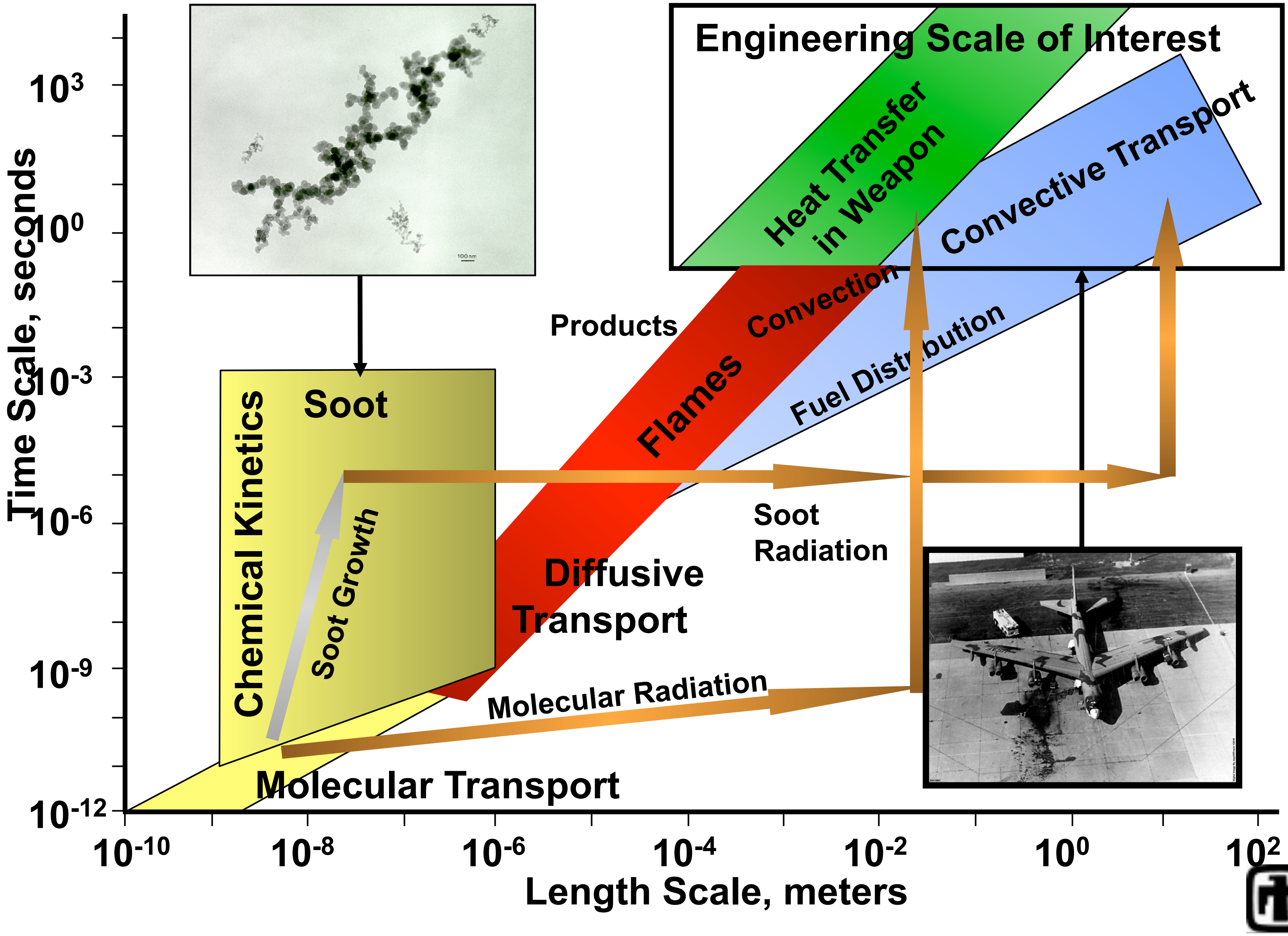
- **DOE NNSA / SNL: Weapon Safety Accident Scenario**
- **Experiment engulfed object within a 10 meter liquid hydrocarbon fuel (Jet fuel: JP-8); moderate cross wind**
- **Turbulent flow, mass species & energy transport w/ chemistry, participating media radiation, soot production**

Lead experimentalist: Jim Nakos

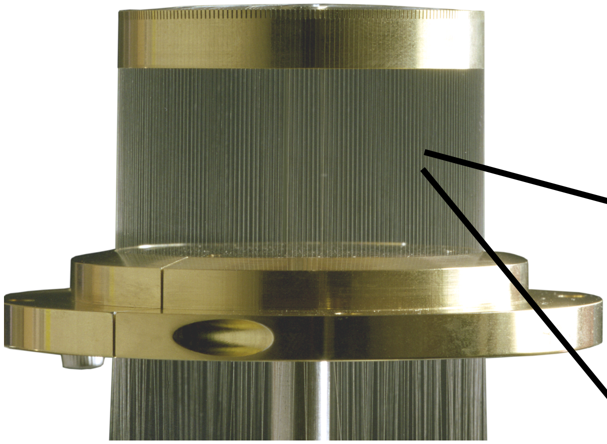


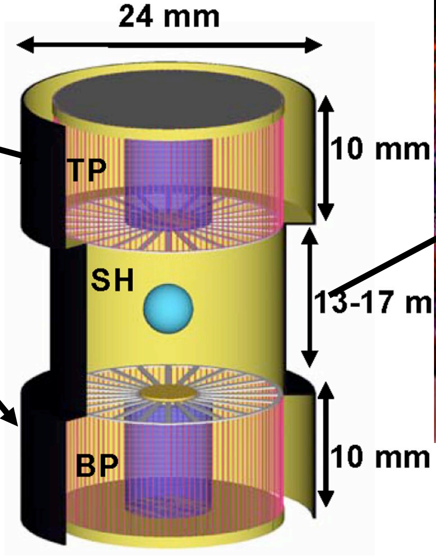
Fuego w/coupled Sierra Mechanics Simulation.

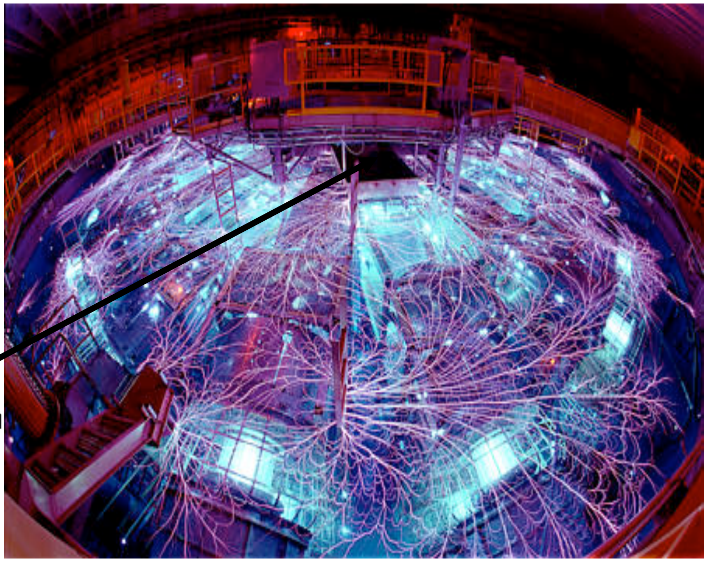
Time and Length Scales



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 ~280 TW power

Computational Stability Constraints:

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
-> $\Delta t < \Delta x^2/(V_A d_i)$

Transport / Reaction and Resistive MHD Models

Navier Stokes

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

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

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

Discretization - Extensions of Stabilized FE Q1/Q1 V-P elements for inf-sup (LBB) stability (Hughes et. al), Convection stabilization SUPG terms and Discontinuity Capturing type operators

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

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

Transport / Reaction and Resistive MHD Models

Navier Stokes + Transport / Reaction Physics

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

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

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

Species Transport / Reaction Equation

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

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

Transport / Reaction and Resistive MHD Models

Navier Stokes + Electro-magnetics

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

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

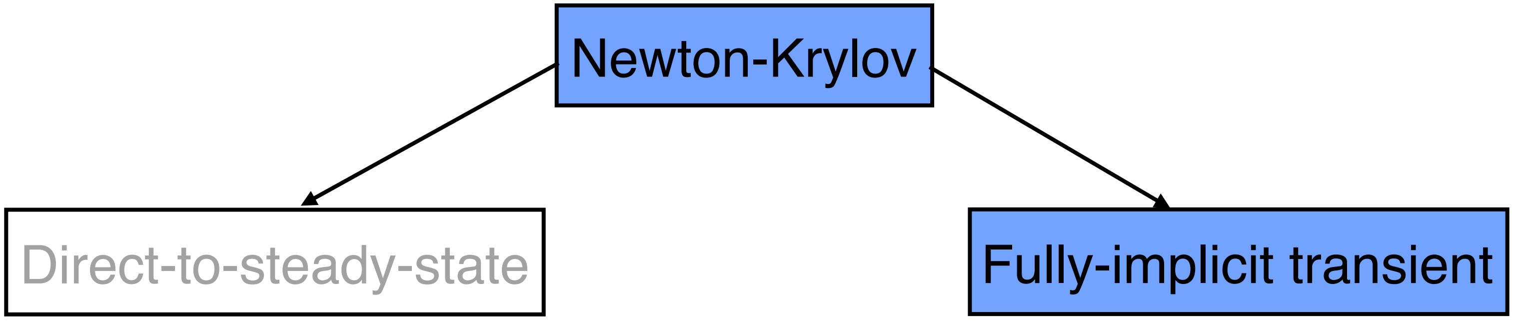
$$\frac{\partial(\rho e)}{\partial t} + \nabla\cdot[\rho\mathbf{v} + \mathbf{q}]\boxed{-\eta\|\mathbf{J}\|^2} = 0$$

Reduced form of Maxwell's Equations

$$\boxed{\frac{\partial\mathbf{B}}{\partial t} - \nabla\times[\mathbf{v}\times\mathbf{B}] + \nabla\times(\eta\mathbf{J}) = 0 \;;\qquad \mathbf{J} = \frac{1}{\mu_0}\nabla\times\mathbf{B}}$$

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

Why Newton-Krylov Methods?



Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

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

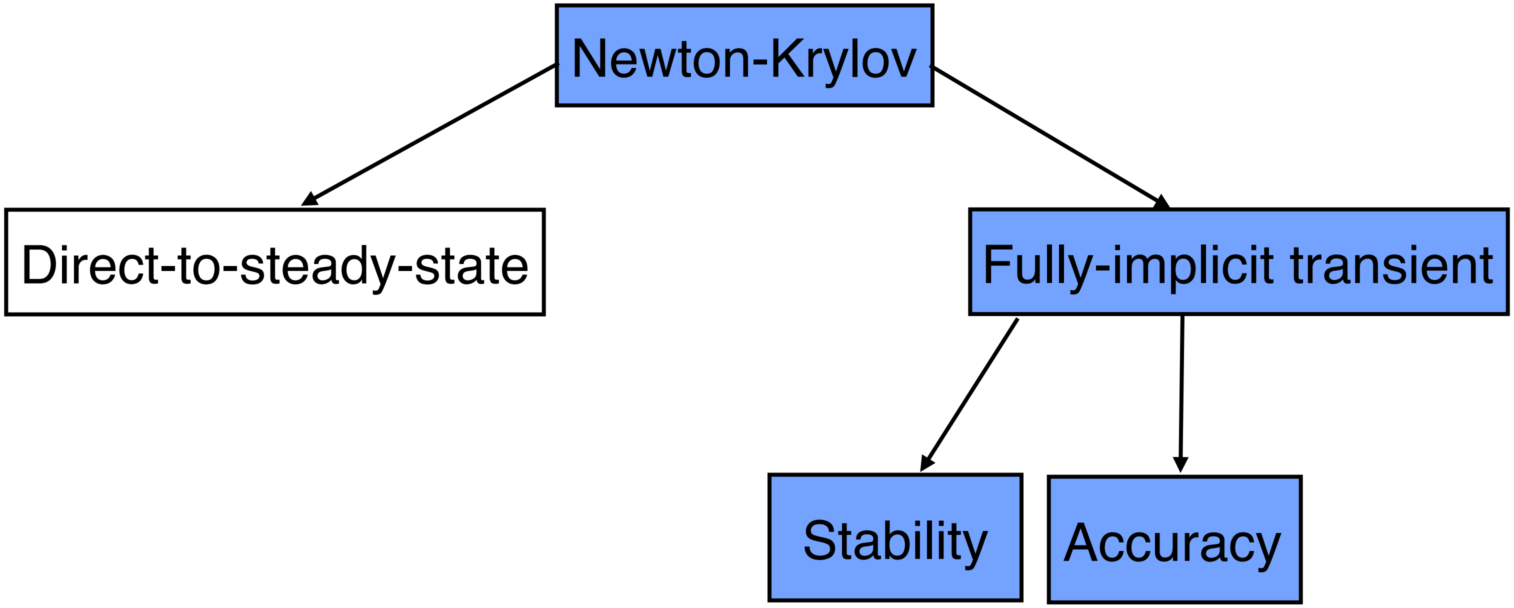
e.g.

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

<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?



Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

Stability

Accuracy

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):

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

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

Strang Splitting (SS):

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

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

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

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

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

(w/David Ropp, C. Ober)

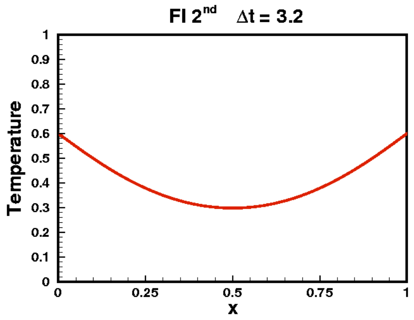
G. Strang, SIAM J. Numer. Anal. 5,3, 1968

Diffusion/Reaction System

Operator Split Component solvers:

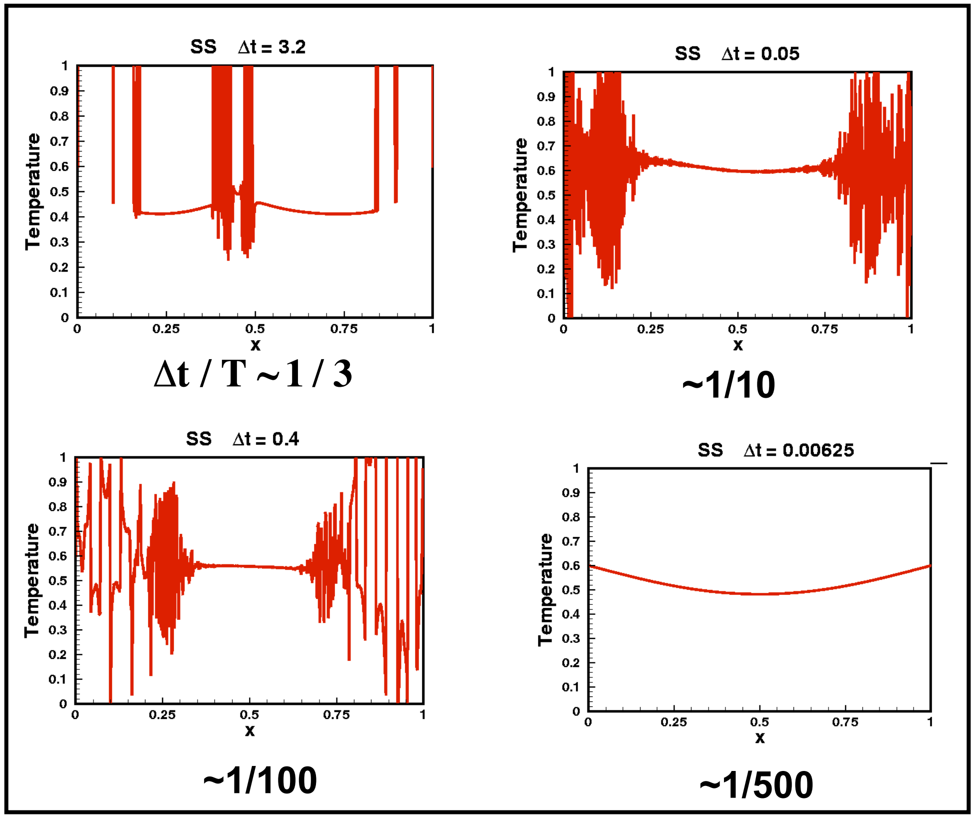
- **Diffusion: 2nd order Crank-Nicholson Galerkin FE (A-stable)**
  2nd order SDIRK Galerkin FE (A & L -stable)
- **Reaction: CVODE Variable order - High accuracy tolerances**

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



FI

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

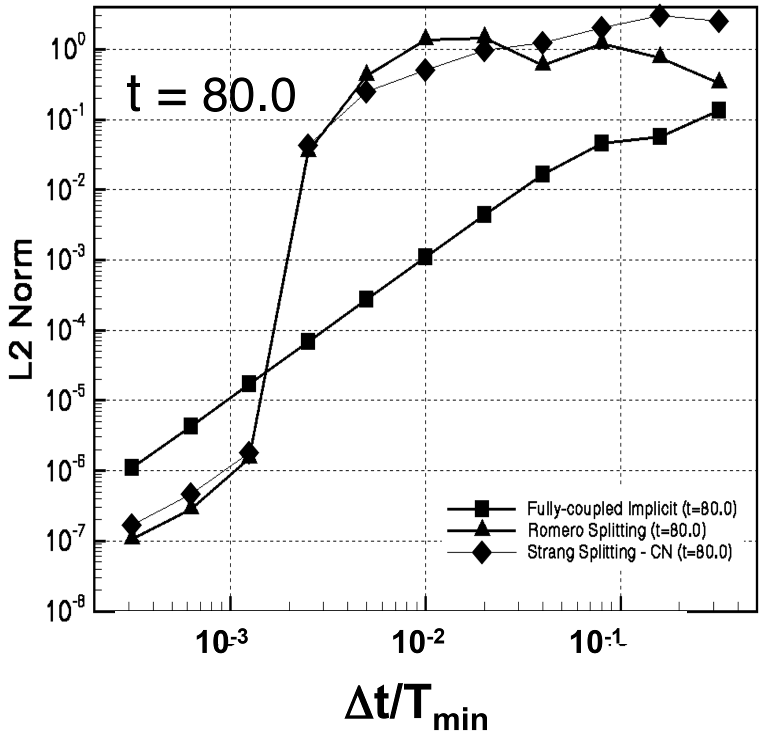


$\Delta t / T \sim 1/3$

~1/10

~1/100

~1/500



Multiple time scales:
Knoll, Chacon, Margolin, Mousseau; JCP 2003
Ropp, S.; JCP 2004, 2005
Ober, S.; JCP 2004

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

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

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

Case 1: A-stable, 2nd order

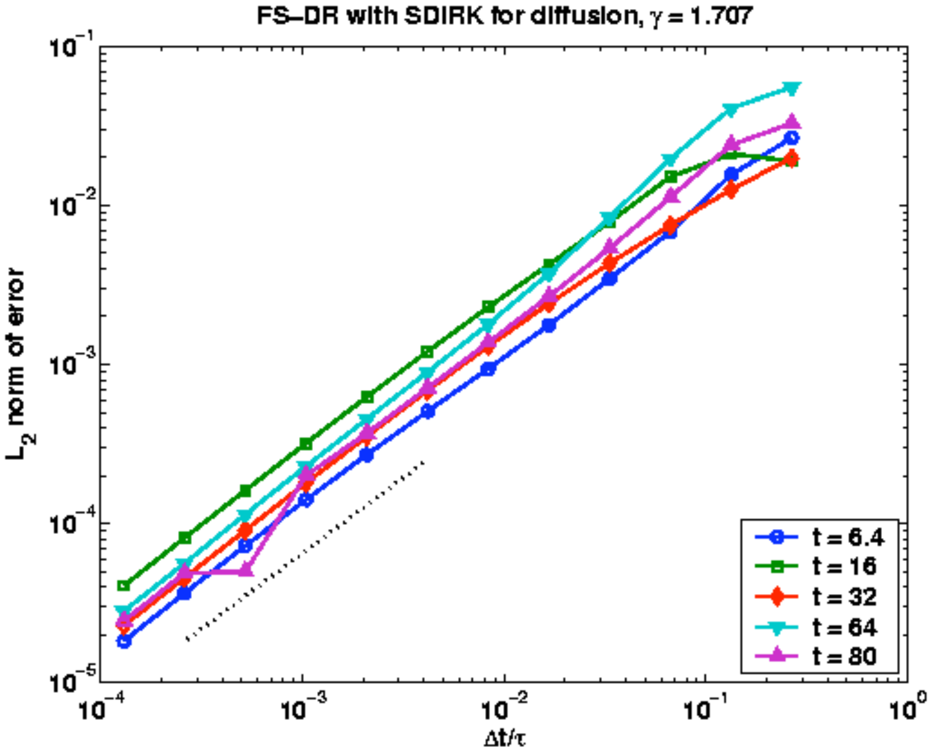
$$\gamma = 0.5, \lim_{z\to-\infty} R(z) = -1$$

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

A-stability theory for Operator split integration for indefinite source terms: Ropp, S., JCP 2005

Convection/Diffusion/Reaction System

Operator Split Component solvers:

- **Advection: 2nd order implicit FE-FCT Kuzmin et. al. (2000)**
- **Diffusion: 2nd order Crank-Nicholson Galerkin FE (A-stable)**
  2nd order SDIRK Galerkin FE (A & L -stable)
- **Reaction: CVODE Variable order - High accuracy tolerances**

A-stability of Operator Split Integration of Convection/Diffusion/Reaction System

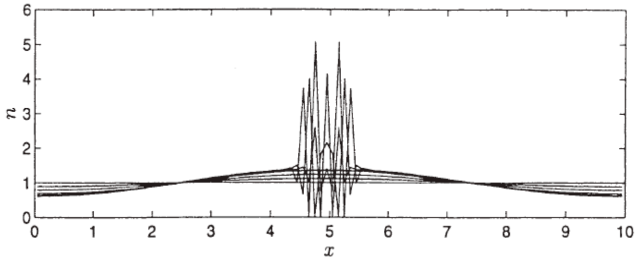
$$\frac{\partial n}{\partial t} + [\alpha \nabla c] \cdot \nabla n - D_n \nabla^2 n + \left(\alpha \nabla^2 c\right) n = 0\,,$$

$$\frac{\partial c}{\partial t} - D_c \nabla^2 c + nc = 0$$

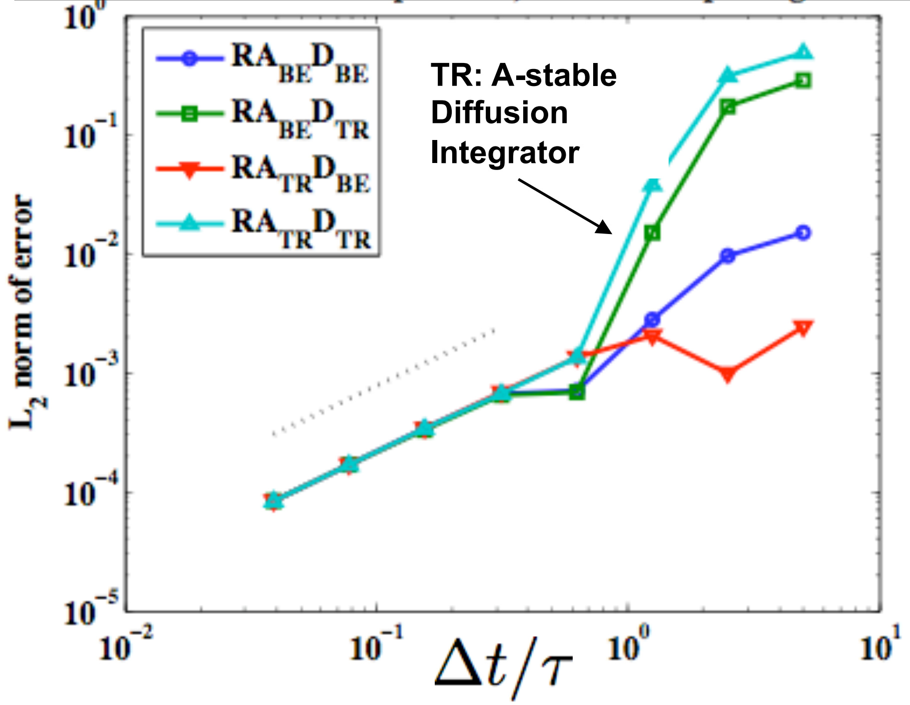
n - cell density;
c - chemo-attractant concentration;

$$D_n = D_c = 0.1 \text{ and } \alpha = 2$$

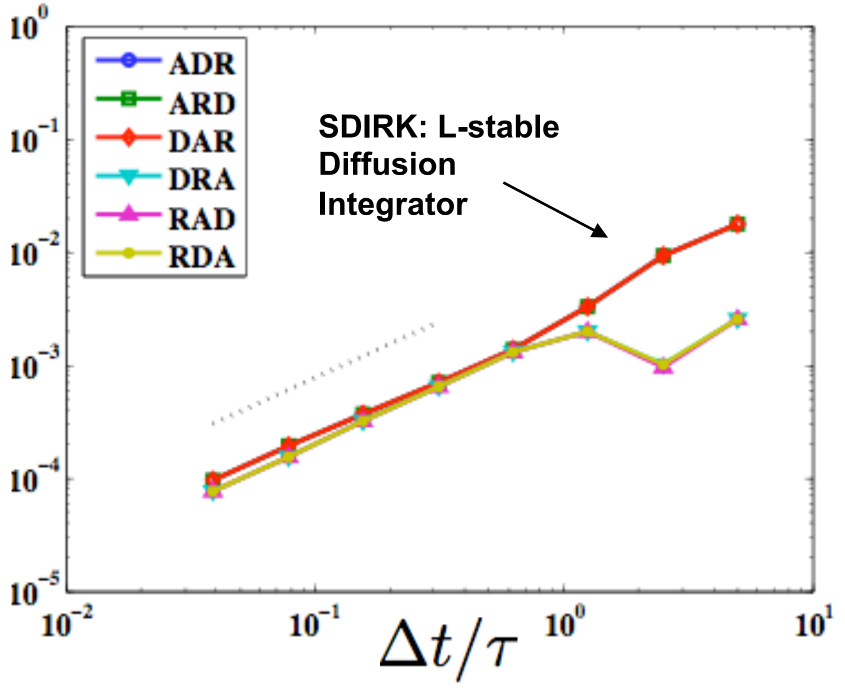
$$n(t=0) = 1\,, \quad c(t=0) = 1 - \frac{\cos(\pi x/5)}{4}\,.$$



Rebecca Tyson · L.G. Stern · Randall J. LeVeque
Fractional step methods applied to a chemotaxis model
J. Math. Biol. 41, 455–475 (2000)



TR: A-stable Diffusion Integrator



SDIRK: L-stable Diffusion Integrator

Ropp, S., JCP in Press

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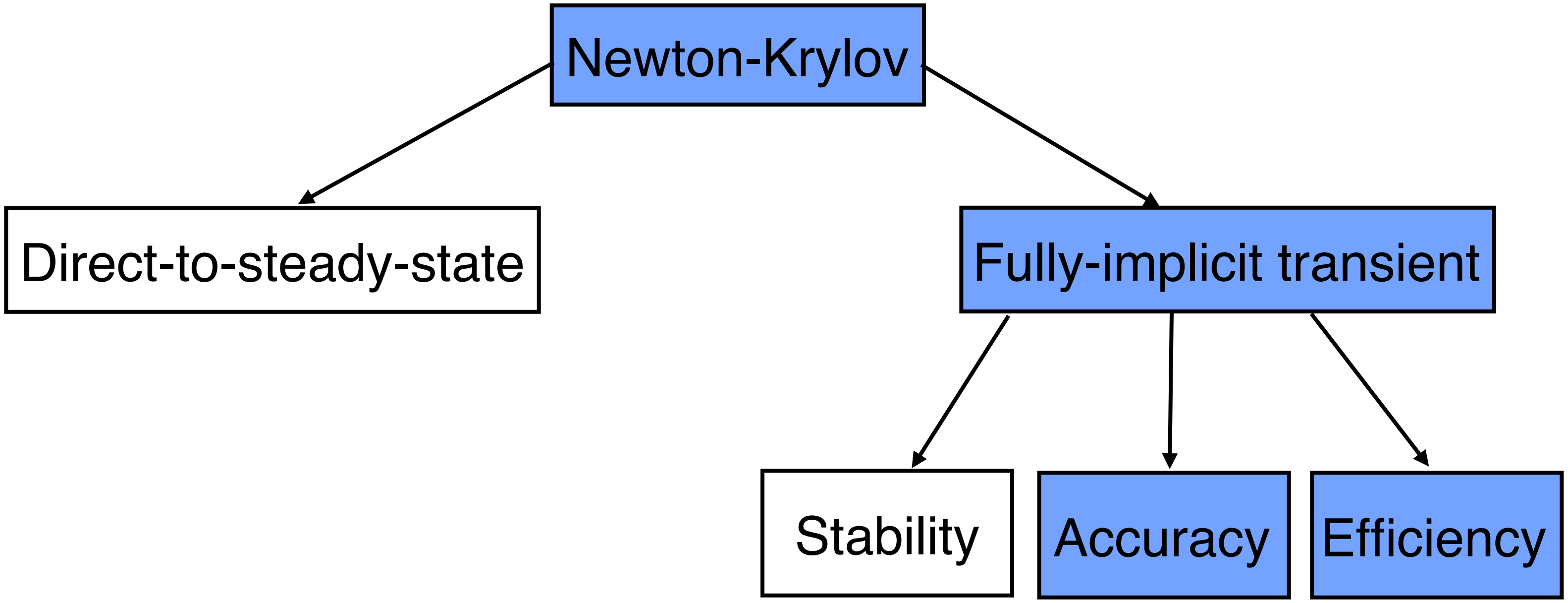
Why Newton-Krylov Methods?



Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

Stability

Accuracy

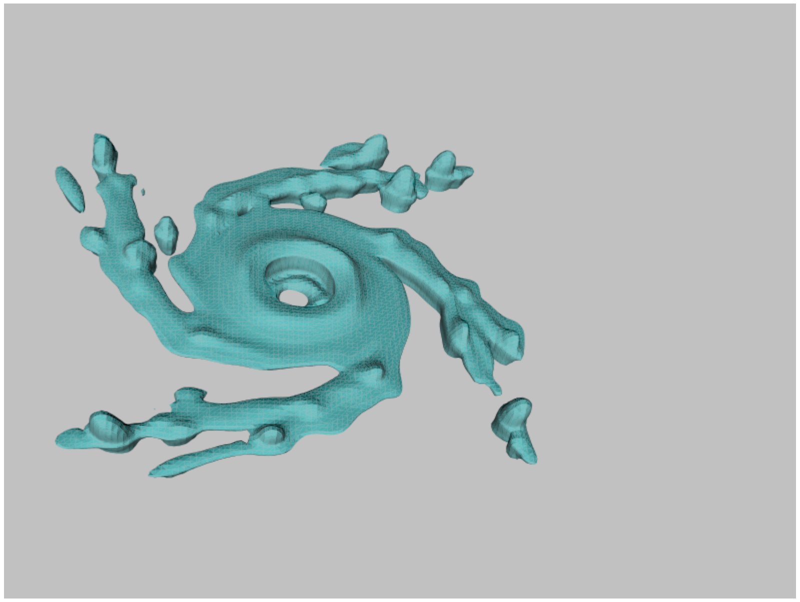
Efficiency

Chacon & Pawlowski Minisymposium
Parallel Implicit MHD - MS81, MS91

Multiple-time-scale Systems: Newton-Krylov Methods for Hurricane Simulations

(Riesner, Mousseau, Wyszogrodzki, Knoll, MWR 2004)

- **3D compressible N-S & phase change**
- **Error/CPU time Comparison of**
  - **Semi-implicit (SI)**
  - **JFNK with SI as preconditioner**
- **Study transient hurricane intensification to ramped increase in sea surface temperature**



(Courtesy of D. Knoll - INL)

Hurricane Equation Set

$$\frac{\partial u\rho}{\partial t} + \frac{\partial uu\rho}{\partial x} + \frac{\partial vu\rho}{\partial y} + \frac{\partial wu\rho}{\partial z} = -\frac{\partial p'}{\partial x}$$

$$+ f\rho(v - v_e) - \tilde{f}w + \frac{\partial \kappa\rho\tau^{11}}{\partial x} + \frac{\partial \kappa\rho\tau^{12}}{\partial y} + \frac{\partial \kappa\rho\tau^{13}}{\partial z}, \qquad (1)$$

$$\frac{\partial v\rho}{\partial t} + \frac{\partial uv\rho}{\partial x} + \frac{\partial vv\rho}{\partial y} + \frac{\partial wv\rho}{\partial z} = -\frac{\partial p'}{\partial y}$$

$$- f\rho(u - u_e) + \frac{\partial \kappa\rho\tau^{21}}{\partial x} + \frac{\partial \kappa\rho\tau^{22}}{\partial y} + \frac{\partial \kappa\rho\tau^{23}}{\partial z}, \qquad (2)$$

$$\frac{\partial w\rho}{\partial t} + \frac{\partial uw\rho}{\partial x} + \frac{\partial vw\rho}{\partial y} + \frac{\partial ww\rho}{\partial z} = -\frac{\partial p'}{\partial z}$$

$$+ \tilde{f}\rho(u - u_e) - (\rho + q_c)g + \frac{\partial \kappa\rho\tau^{31}}{\partial x} + \frac{\partial \kappa\rho\tau^{32}}{\partial y} + \frac{\partial \kappa\rho\tau^{33}}{\partial z}, \qquad (3)$$

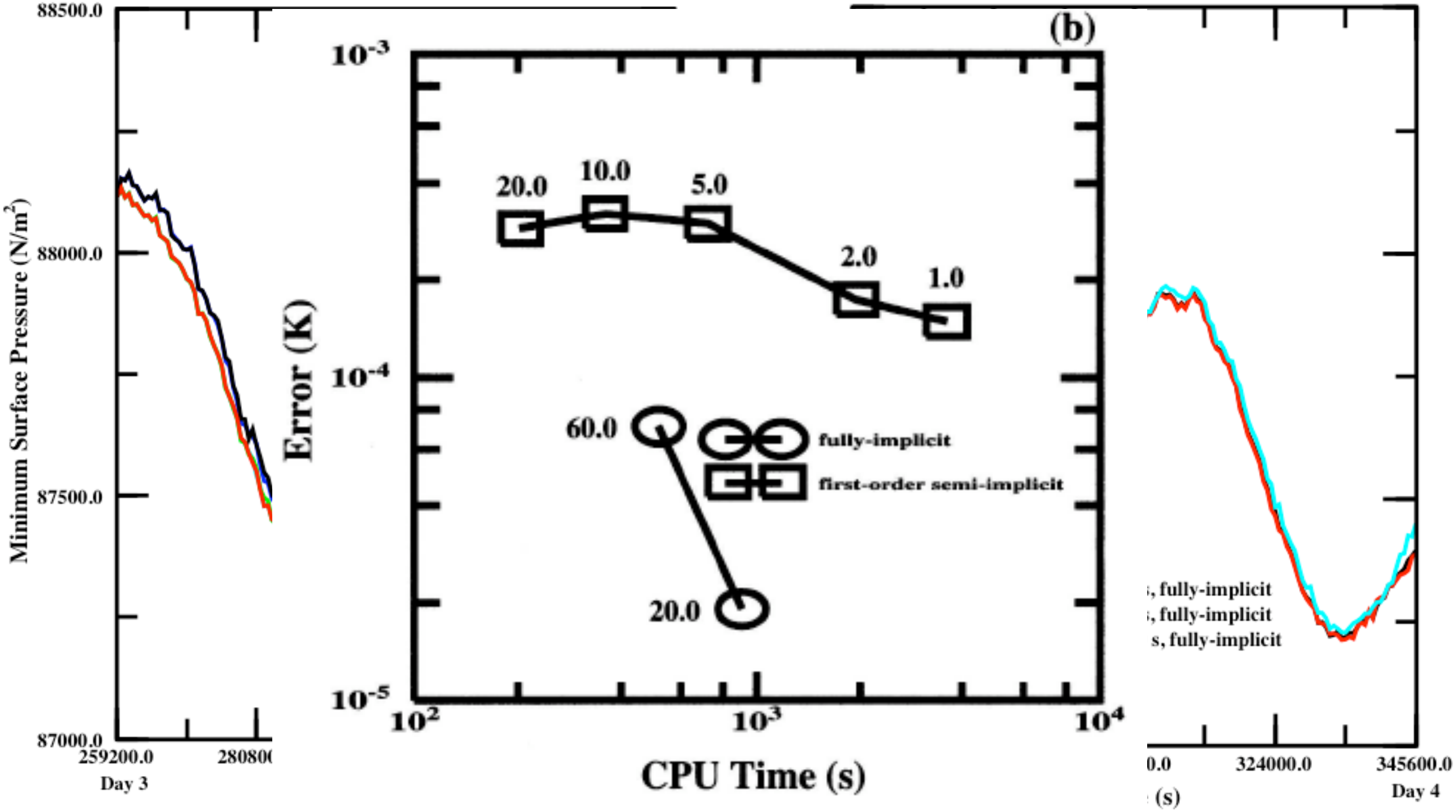
$$\frac{\partial \theta\rho}{\partial t} + \nabla\cdot(\mathbf{V}\theta\rho) = \frac{\theta\rho L}{TC_p} f_{cloud} + f_{surface-energy} + \nabla\cdot(\mathbf{F}_{\theta}) \qquad (4)$$

$$\frac{\partial q_v\rho}{\partial t} + \nabla\cdot(\mathbf{V}q_v\rho) = -f_{cloud} + f_{surface-gas} + \nabla\cdot(\mathbf{F}_{\mathbf{q}_v}) \qquad (5)$$

$$\frac{\partial q_c\rho}{\partial t} + \nabla\cdot(\mathbf{V}q_c\rho) = f_{cloud} - f_{fall} + \nabla\cdot(\mathbf{F}_{\mathbf{q}_c}) \qquad (6)$$

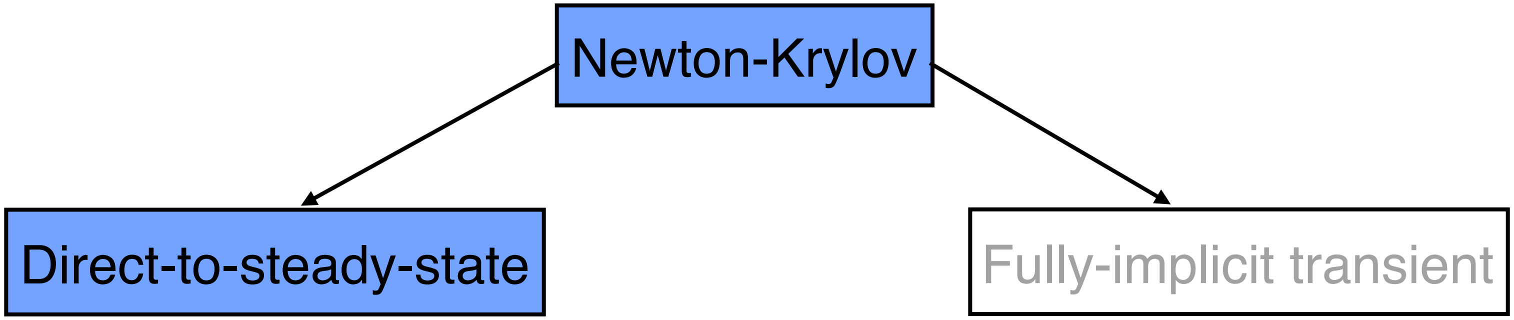
$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\mathbf{V}\rho) = -f_{cloud} + f_{surface-gas} \qquad (7)$$

Multiple-time-scale Systems: Newton-Krylov Methods for Hurricane Simulations (Riesner, Mousseau, Wyszogrodzki, Knoll, MWR 2004)



SI - needs to run at stiff wave CFL; JFNK - dynamical time scale

Why Newton-Krylov Methods?



Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

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

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

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

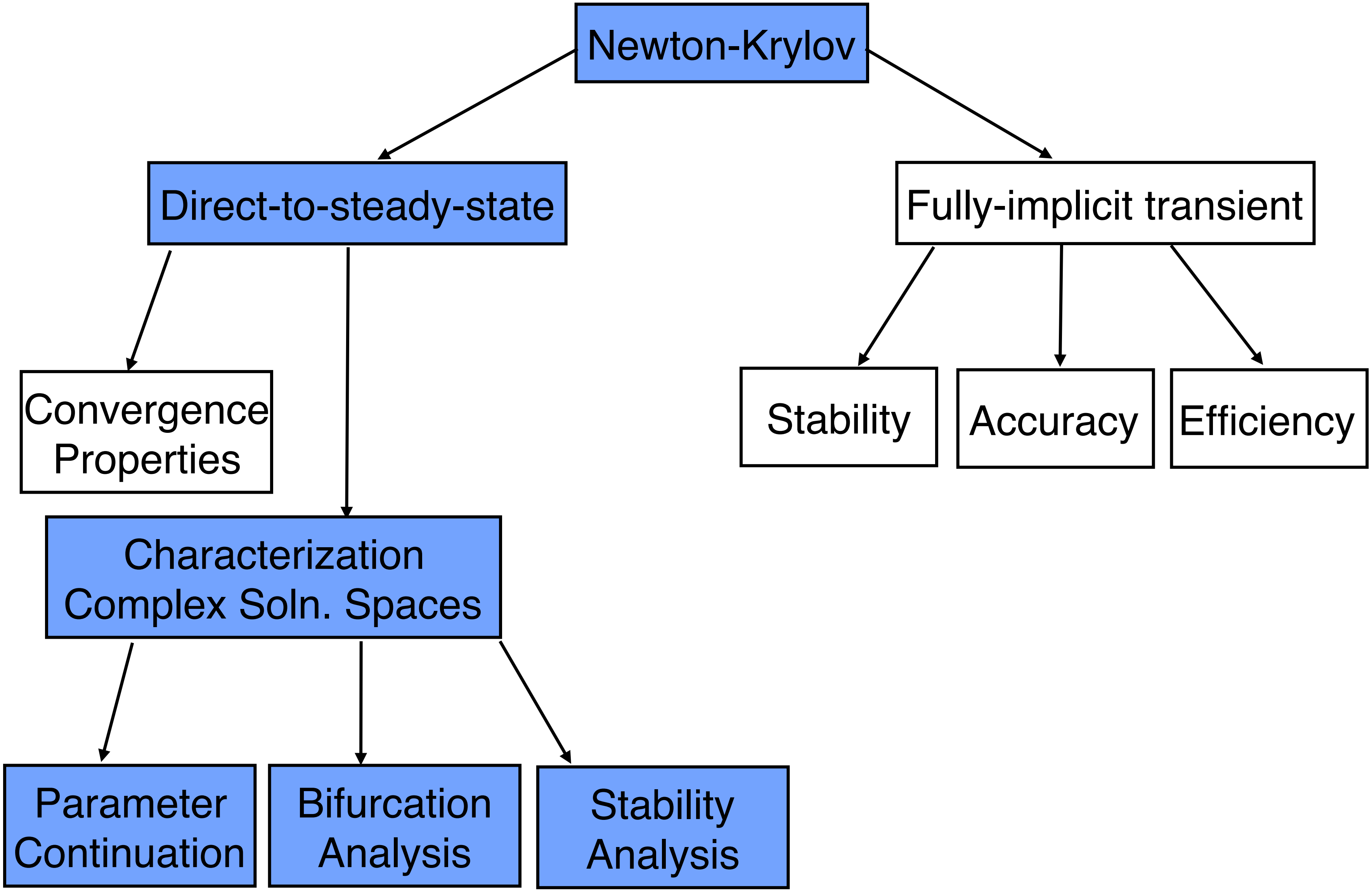
Jacobian Free N-K Variant

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

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

See e.g. Knoll & Keyes, JCP 2004

Why Newton-Krylov Methods?



Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

Convergence Properties

Stability

Accuracy

Efficiency

Characterization Complex Soln. Spaces

Parameter Continuation

Bifurcation Analysis

Stability Analysis

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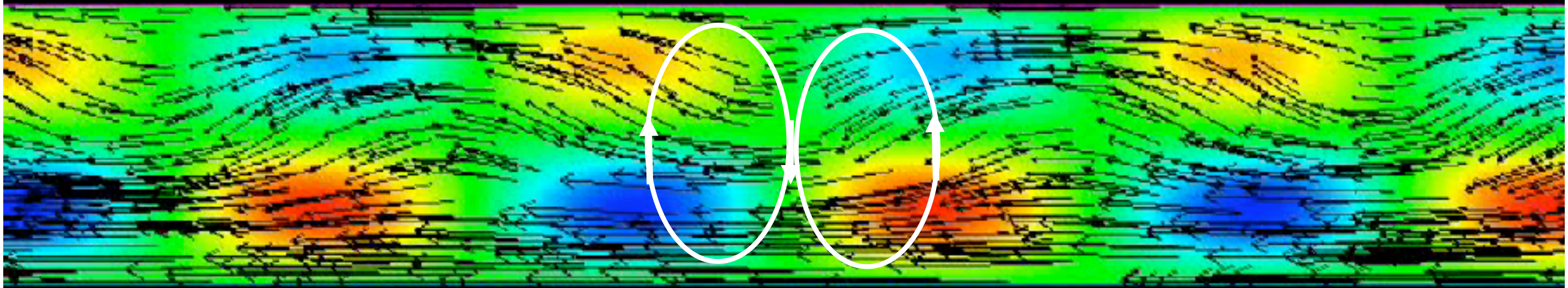
Vx



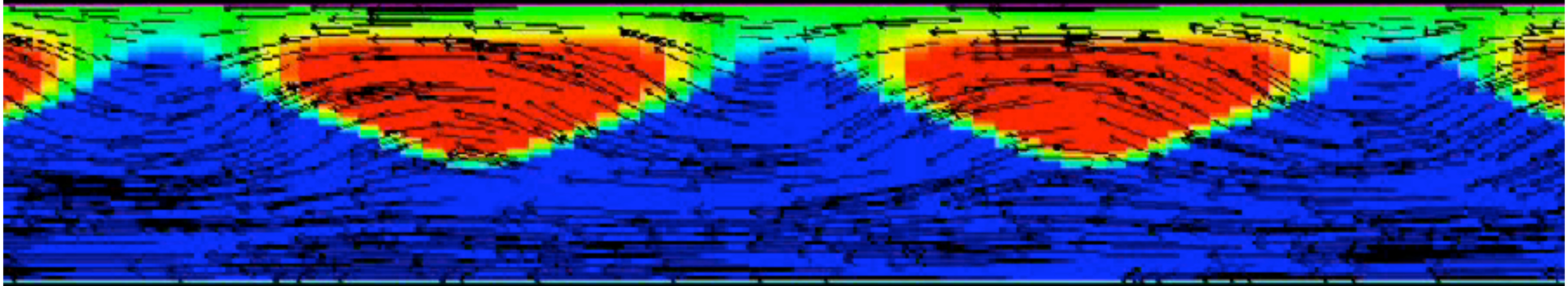
Hydro-Magnetic Rayleigh-Bernard Stability

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

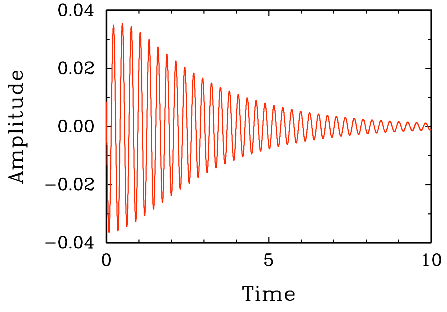
Stable Fields/Flow at
Ra = 4000, Q = 81

Unstable Flow at
Ra = 4000, Q = 144

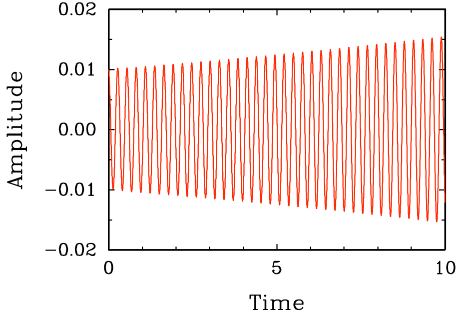
Jz



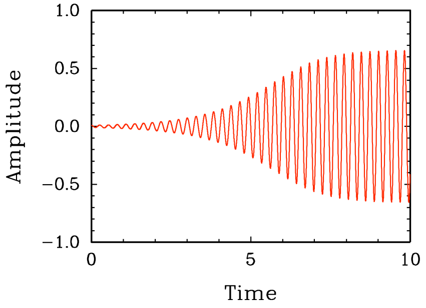
Characterizing Complex Nonlinear Solution Spaces with a Transient Code is Difficult



p=5



p=10   Hopf Bifurcation?

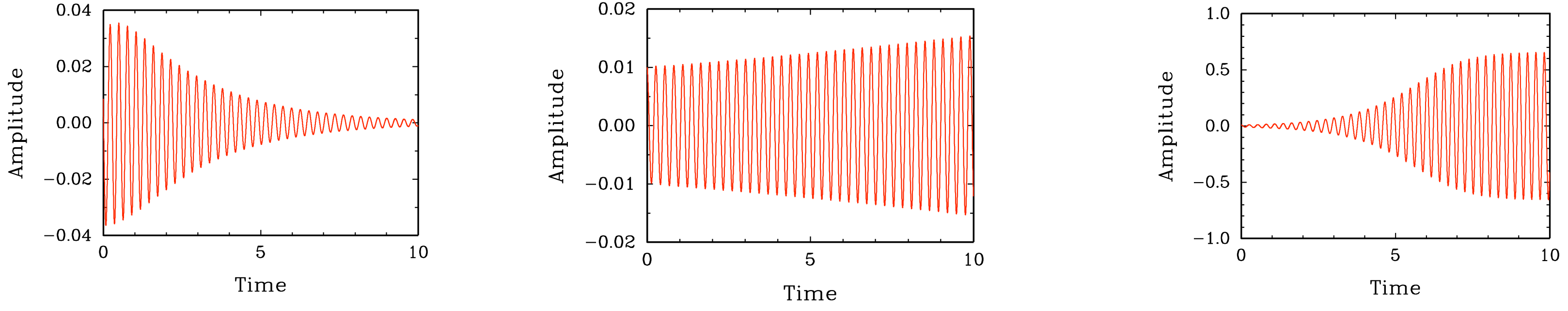


p=15

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



p=5 p=10 Hopf! p=15

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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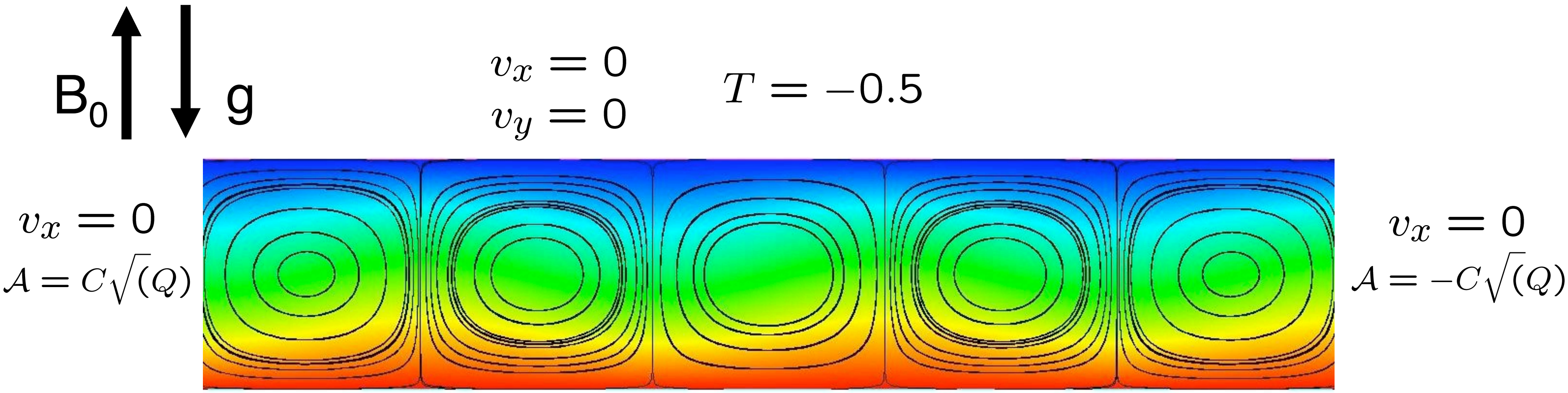
Classical Hydromagnetic Rayleigh-Bernard Stability Problem (mechanisms are important in Geo-dynamo)



$v_x = 0$
$v_y = 0$
$T = -0.5$

$v_x = 0$
$\mathcal{A} = C\sqrt{(Q)}$

$v_x = 0$
$\mathcal{A} = -C\sqrt{(Q)}$

$v_x = 0$
$v_y = 0$
$T = 0.5$

$$Q = \frac{B_0^2 d^2}{\mu_0 \rho \nu \eta}$$

$$Ra = \frac{g\beta\Delta T d^3}{\nu\alpha}$$

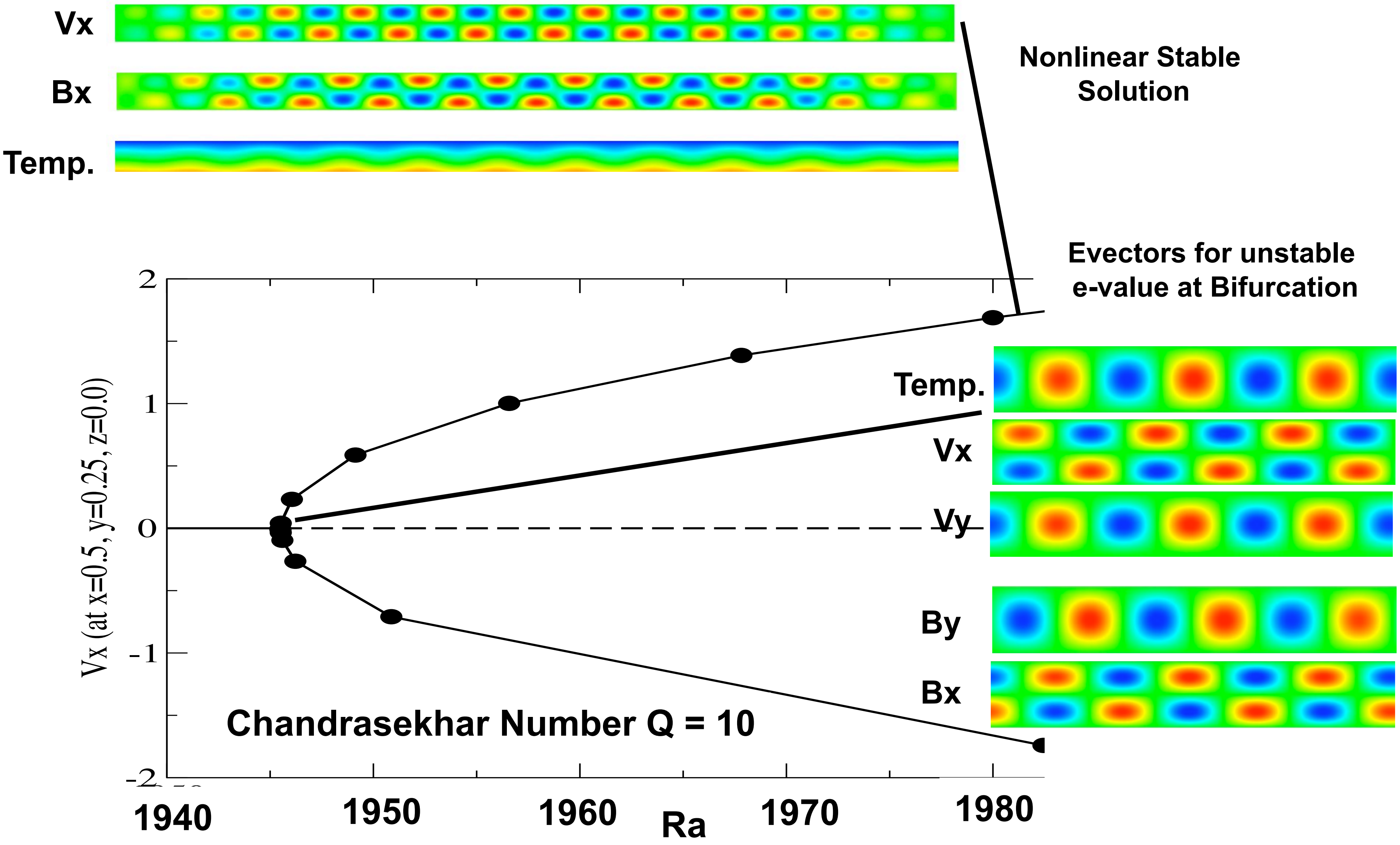
$$Pr = \frac{\nu}{\alpha}$$

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

Parameters:
- Q ~ B_0^2 (Chandrasekhar No. - magnetic field strength)
- Ra ~ ΔT (Rayleigh number)

- Buoyancy driven instability initiates flow at high Ra numbers.
- Maxwell Stress (magnetics) and Buoyancy Competing Mech.
- Domain: 1x20

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



Nonlinear Stable Solution

Evectors for unstable e-value at Bifurcation

Chandrasekhar Number Q = 10

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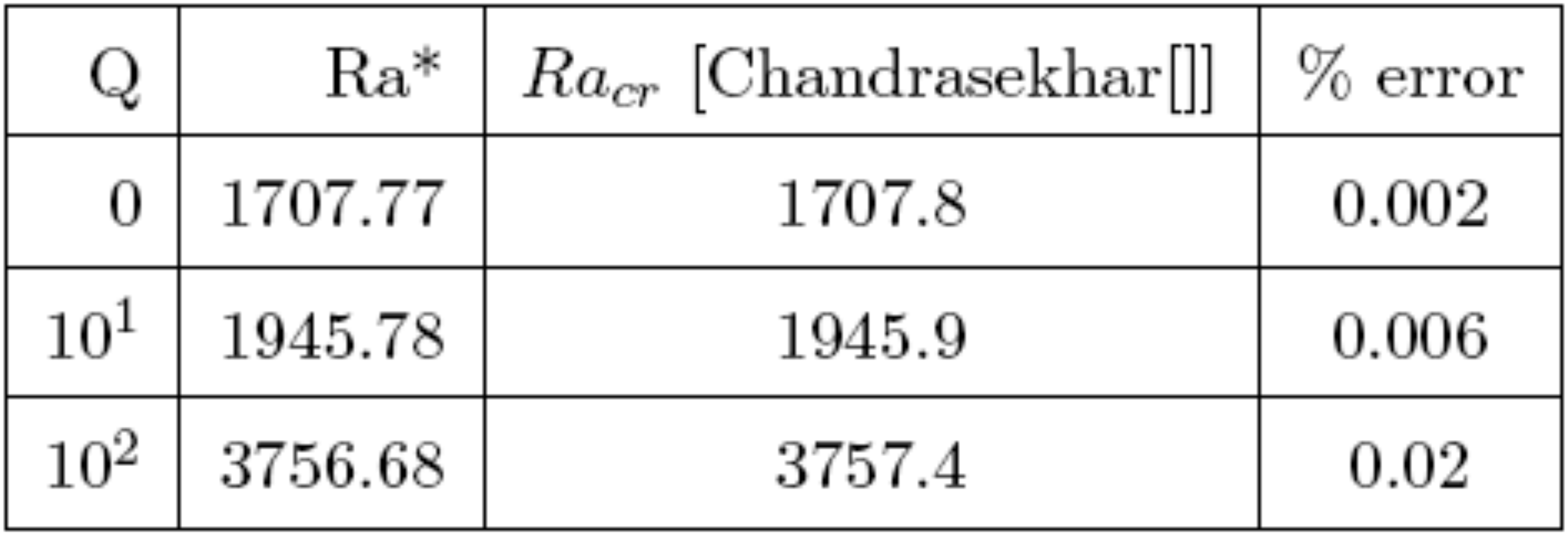
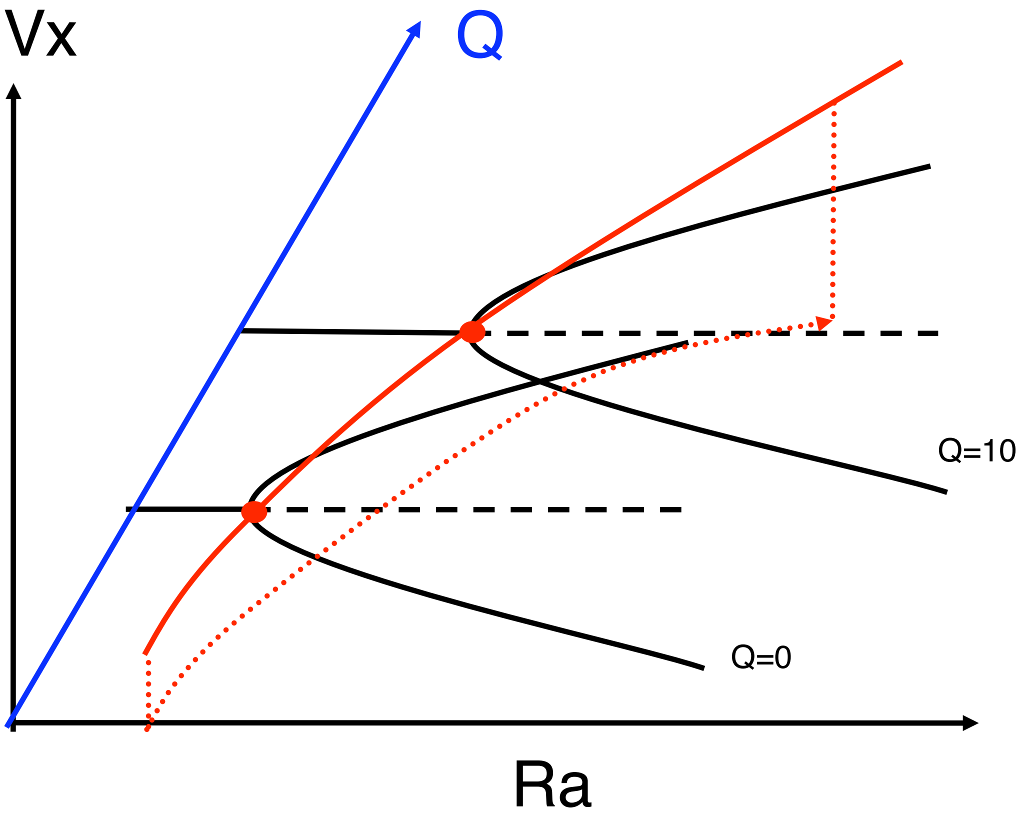
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Linear Stability and Nonlinear Equilibrium Solutions (Steady State Solves)

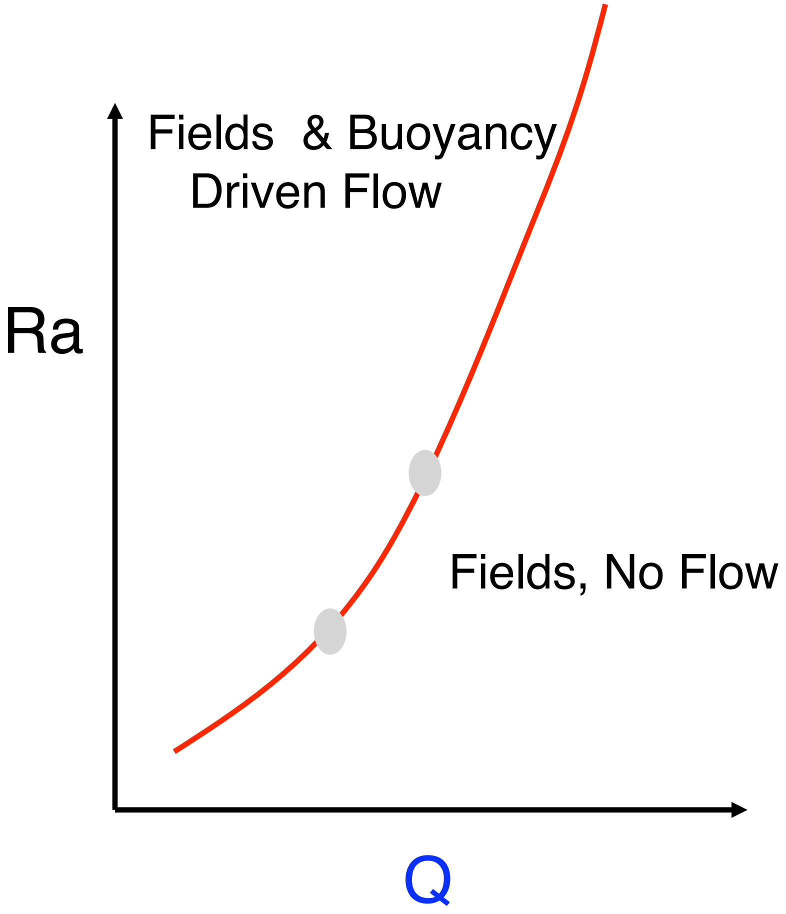


Q	Ra*	Ra_{cr} [Chandrasekhar[]]	% error
0	1707.77	1707.8	0.002
10^1	1945.78	1945.9	0.006
10^2	3756.68	3757.4	0.02

- 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

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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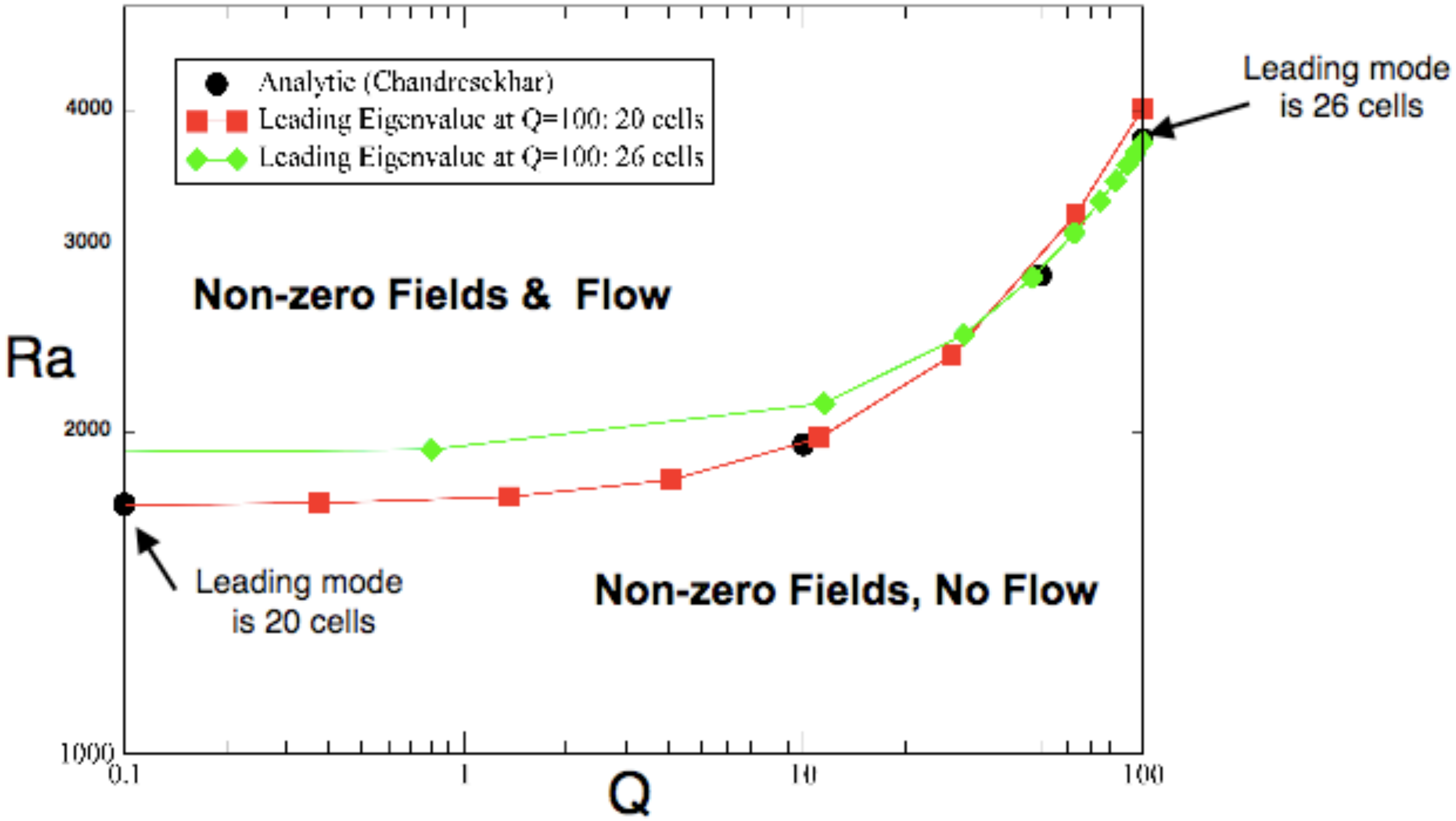
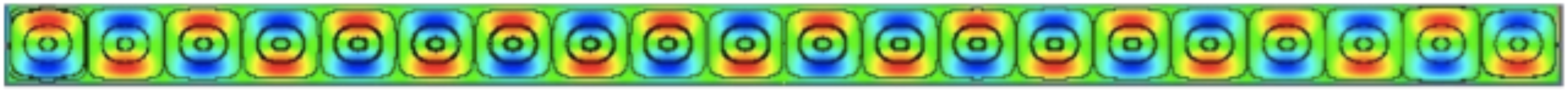
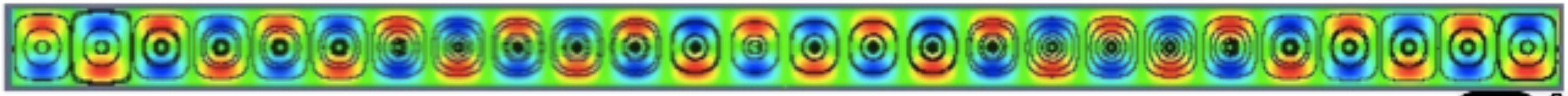
Magnetic Field Compresses Most Unstable Mode as Q Increases





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



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

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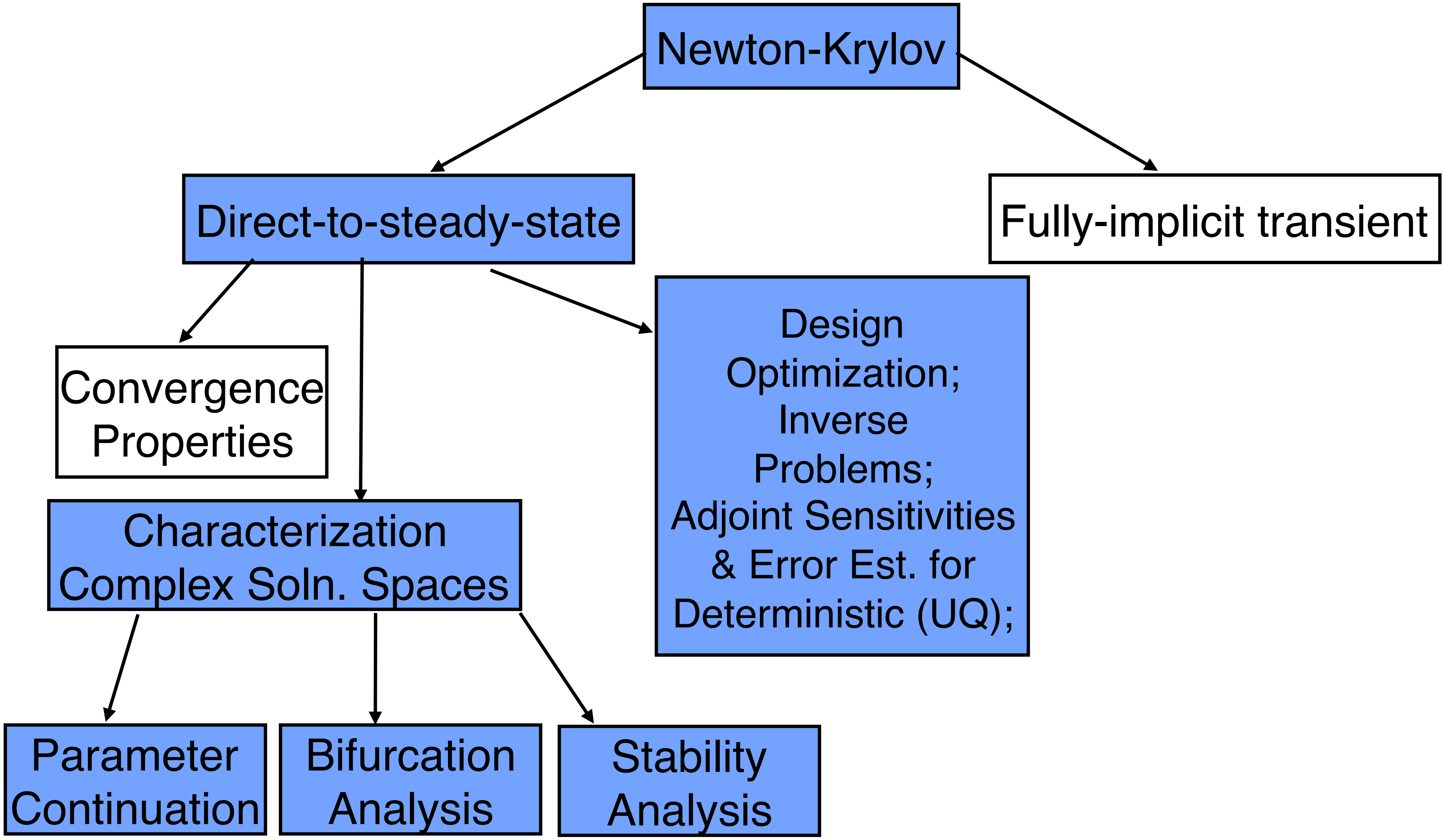
Why Newton-Krylov Methods?



Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

Convergence Properties

Characterization Complex Soln. Spaces

Design Optimization; Inverse Problems; Adjoint Sensitivities & Error Est. for Deterministic (UQ);

Parameter Continuation

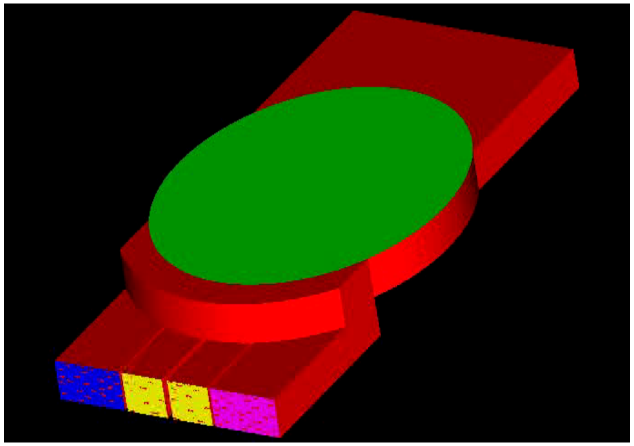
Bifurcation Analysis

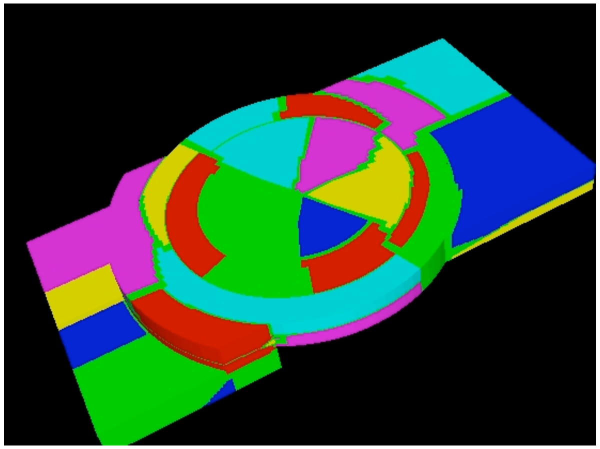
Stability Analysis

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

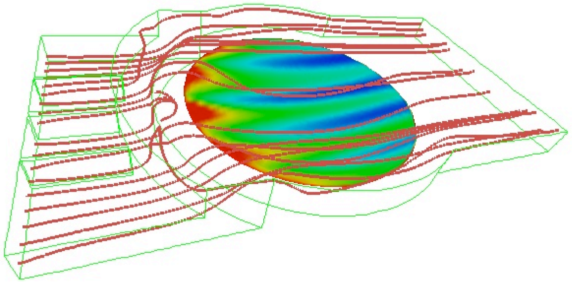
Poly-Silicon Epitaxy from Trichlorosilane in Hydrogen Carrier;

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

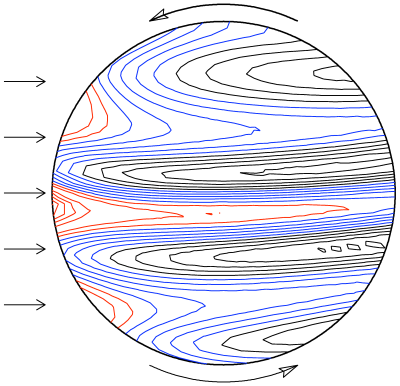


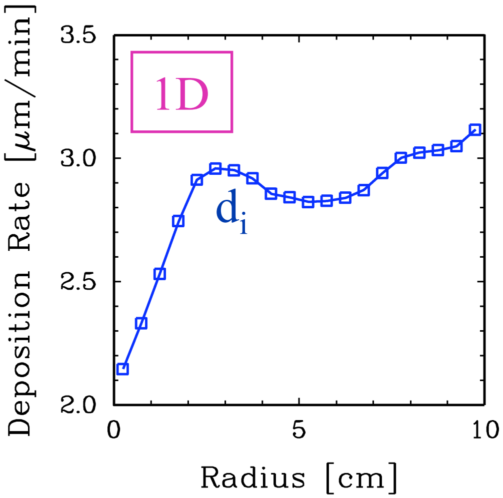


3D



2D





0D Objective Function:

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

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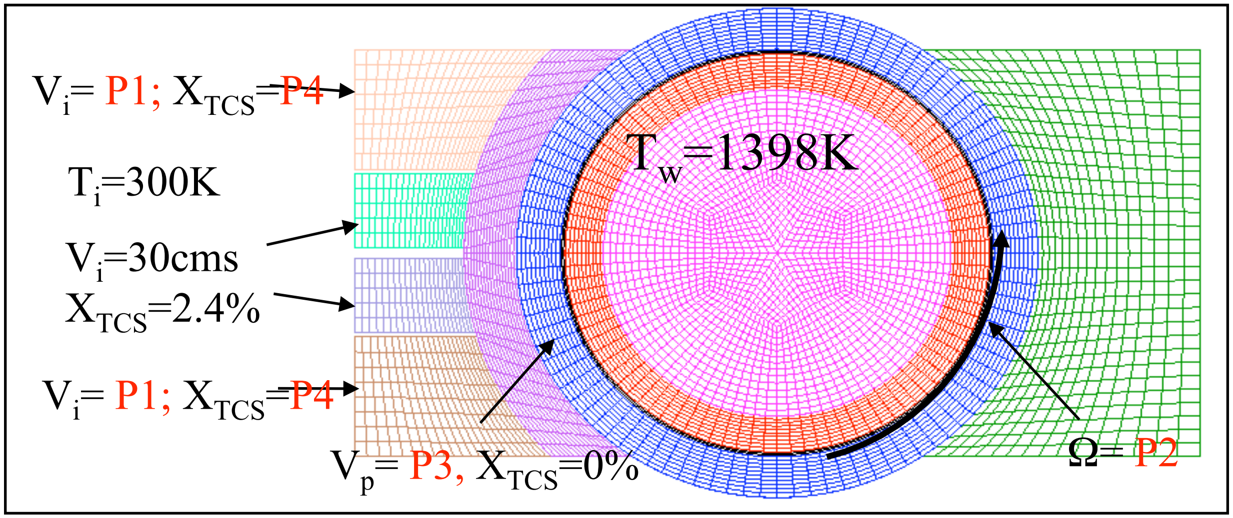
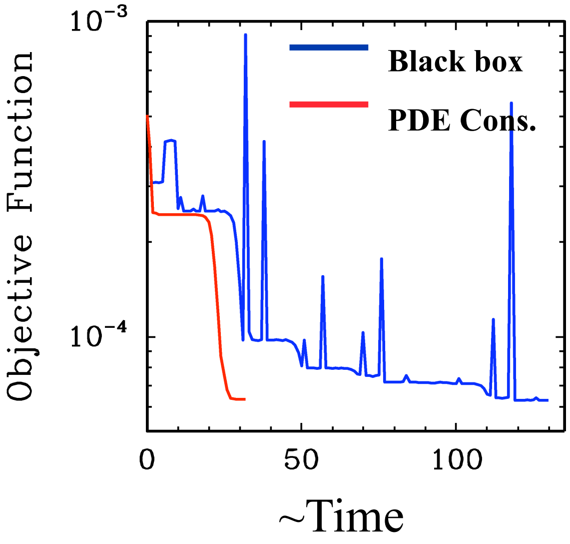
PDE Constrained Optimization of Poly-Silicon CVD Reactor

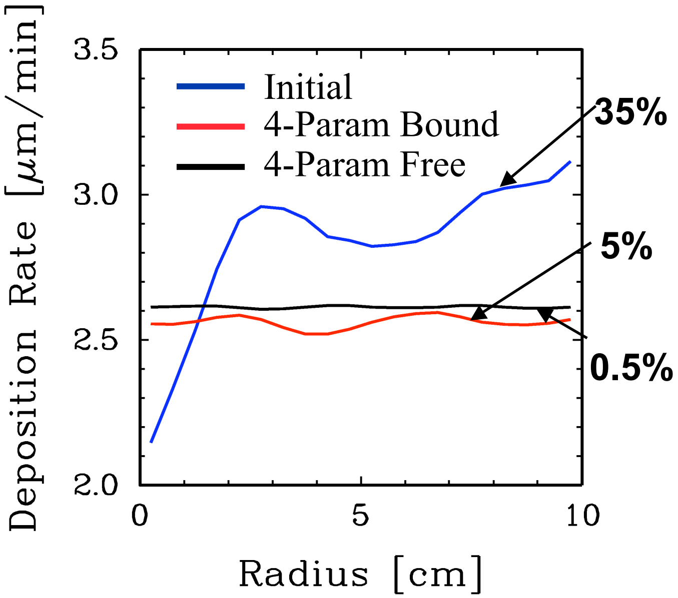


PDE Constrained Optimization:

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

Use Newton's Method solve KKT system

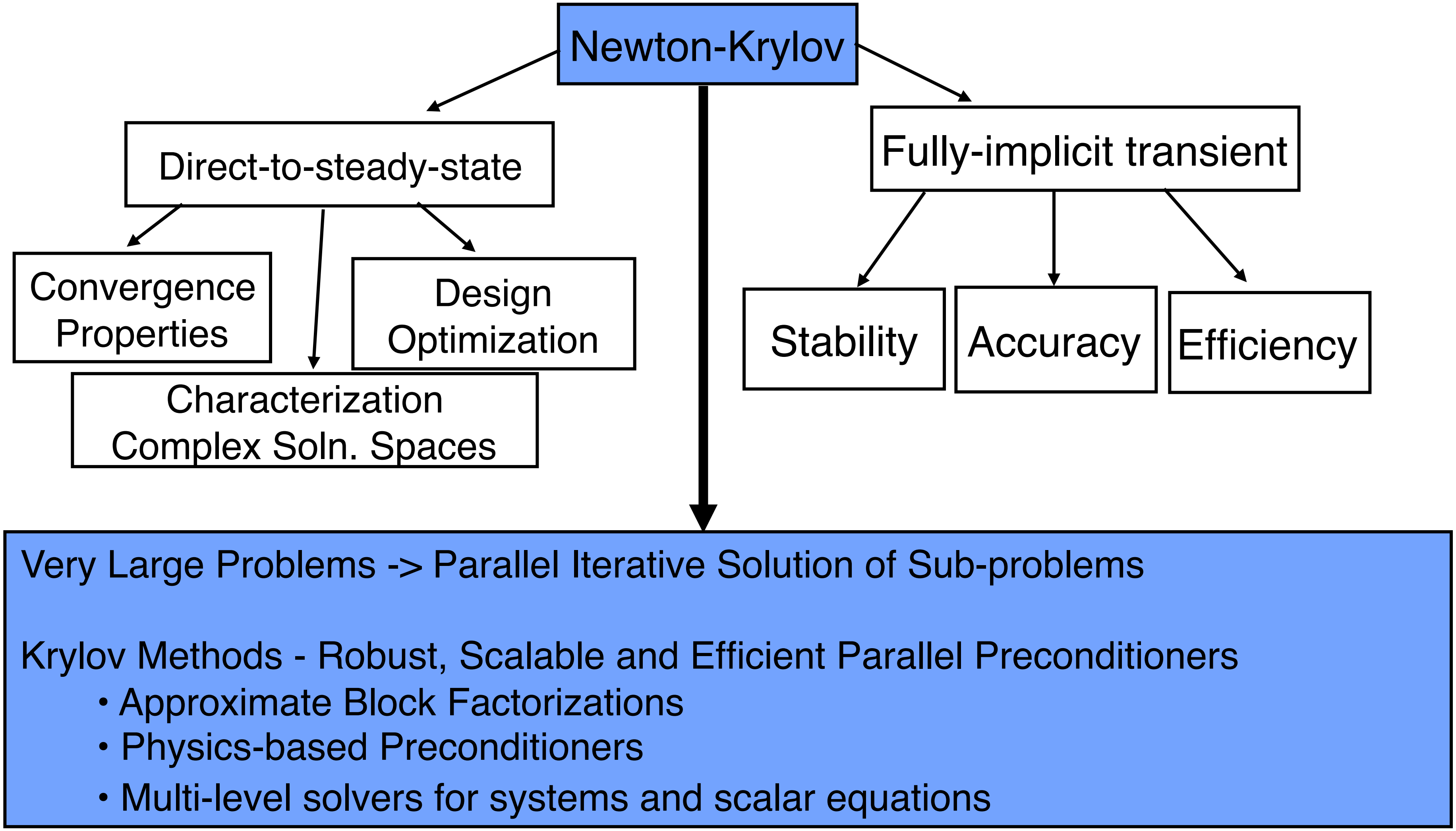




Unks	Procs	Time (hrs.)
1.2	48	6.2 (3GHz Cluster)
4.8M	128	~ 6 (Red Storm: XT3)
38M	1024	~ 7 (Red Storm: XT3)

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

Why Newton-Krylov Methods?



Newton-Krylov

Direct-to-steady-state

Convergence Properties

Characterization Complex Soln. Spaces

Design Optimization

Fully-implicit transient

Stability

Accuracy

Efficiency

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

e.g. Saad, Lanteri, Giraud, Roman: Mini - Parallel Sparse Solvers MS112 (Thur.) , MS136 (Fri.)

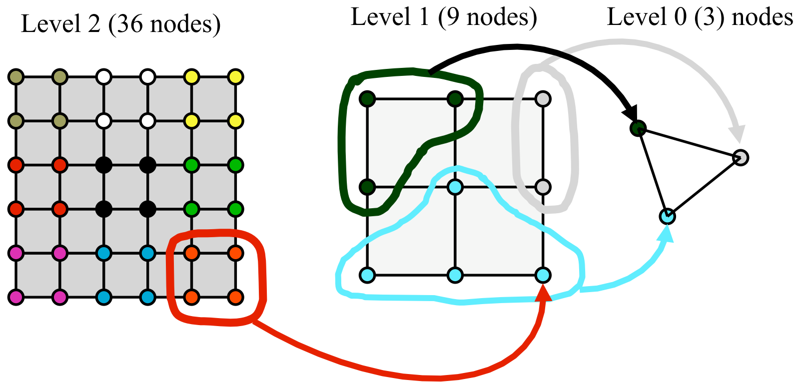
ML library: Multilevel Preconditioners

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

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

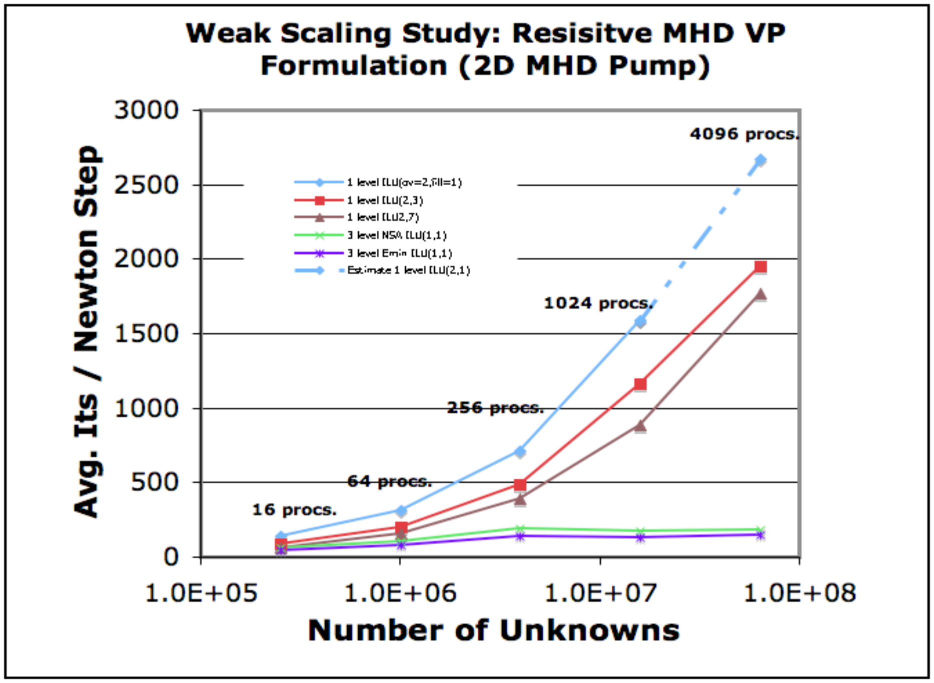


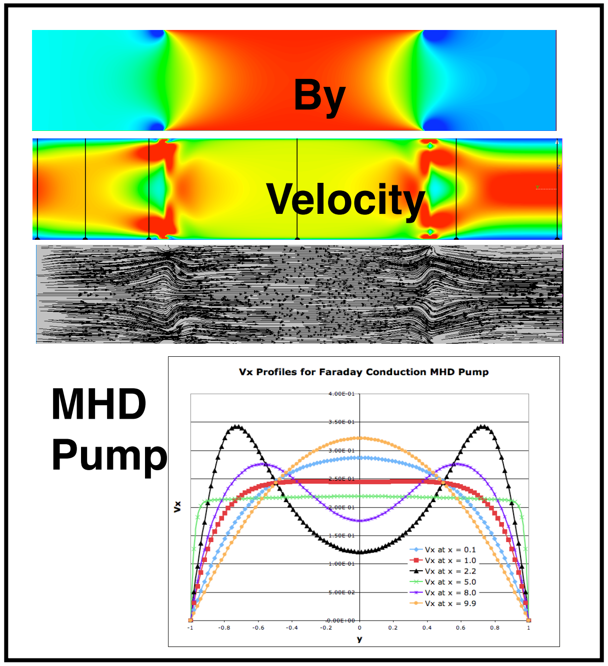
Visualization of effect of partition of matrix graph on mesh

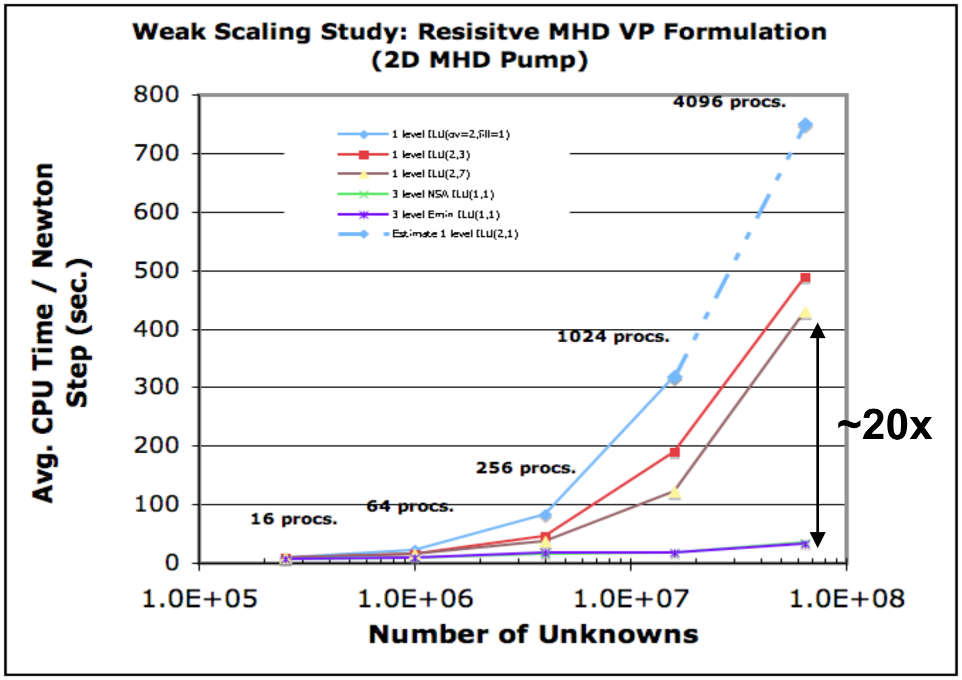
Aggregation based Multigrid:
- **Vanek, Mandel, Brezina, 1996**
- **Vanek, Brezina, Mandel, 2001**

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

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

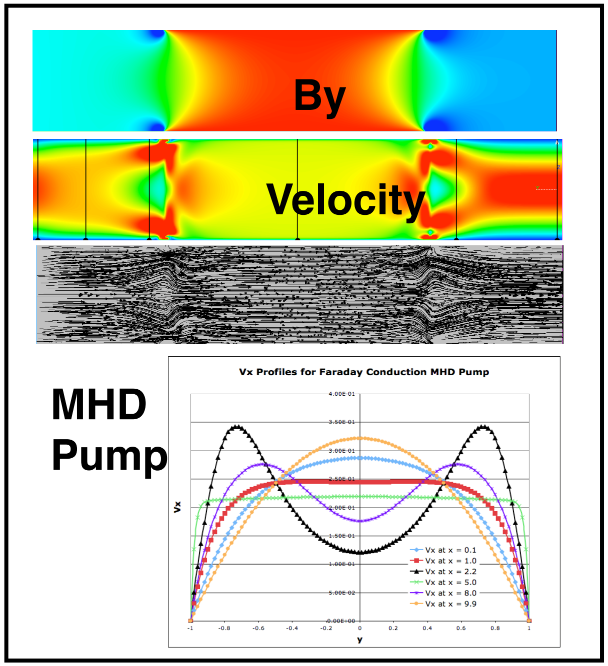






Multicore Performance of Fully-coupled Resistive MHD Simulations - Cray XT3/4

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

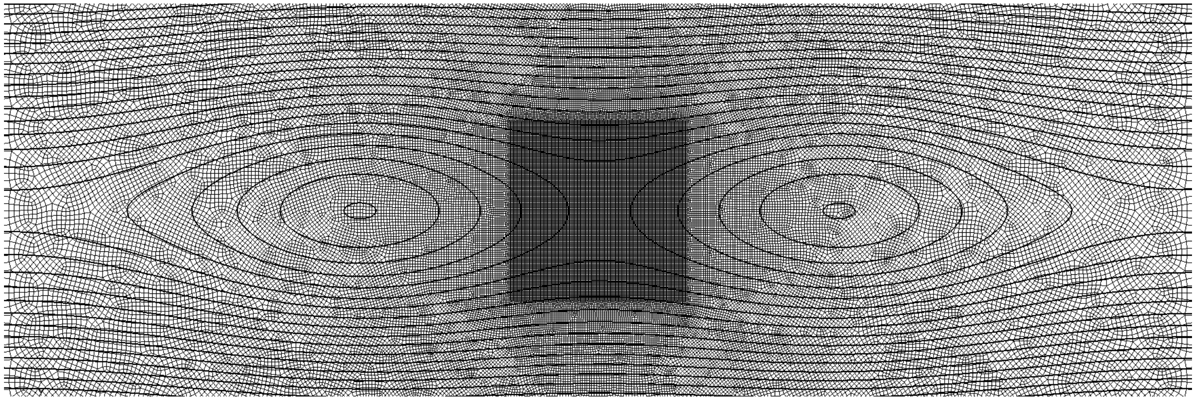


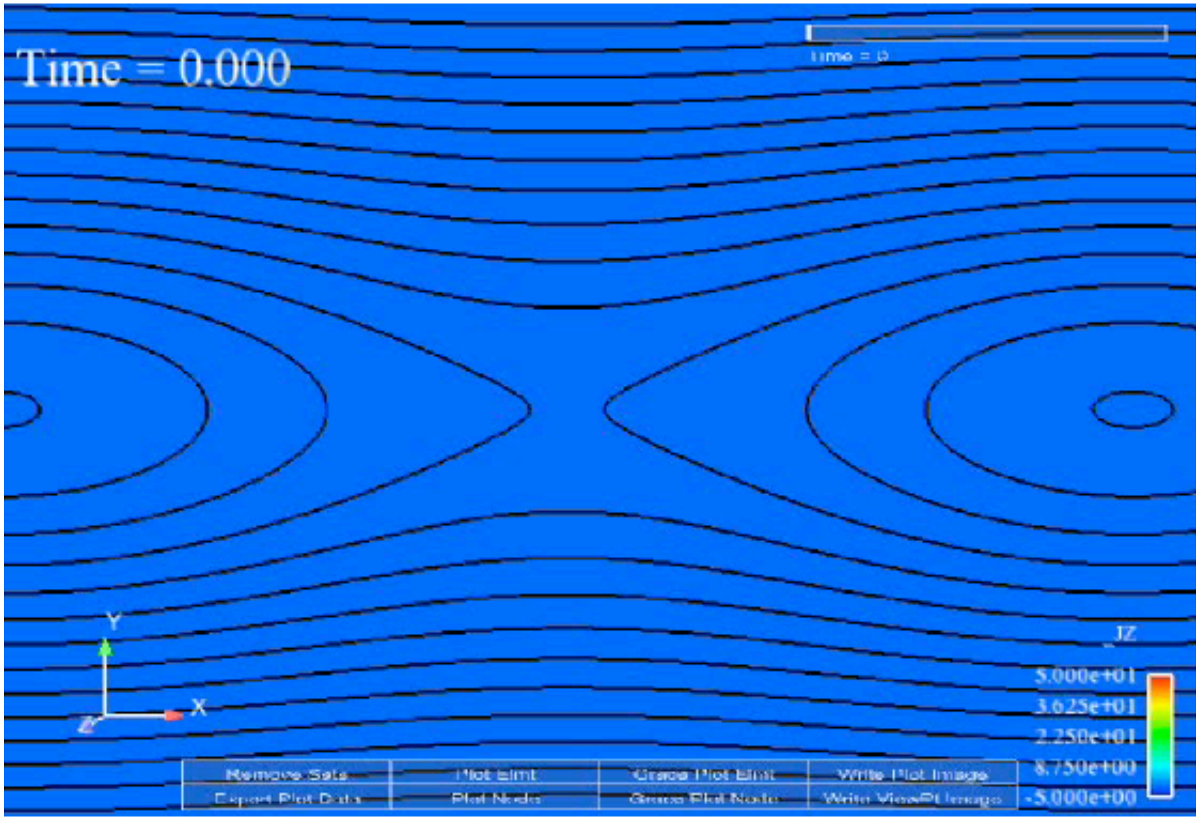
Our Largest Steady-state Simulation to Date:

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

Driven Magnetic Reconnection: Magnetic Island Coalescence
Unstructured Mesh Resistive MHD with Algebraic Multilevel Preconditioners





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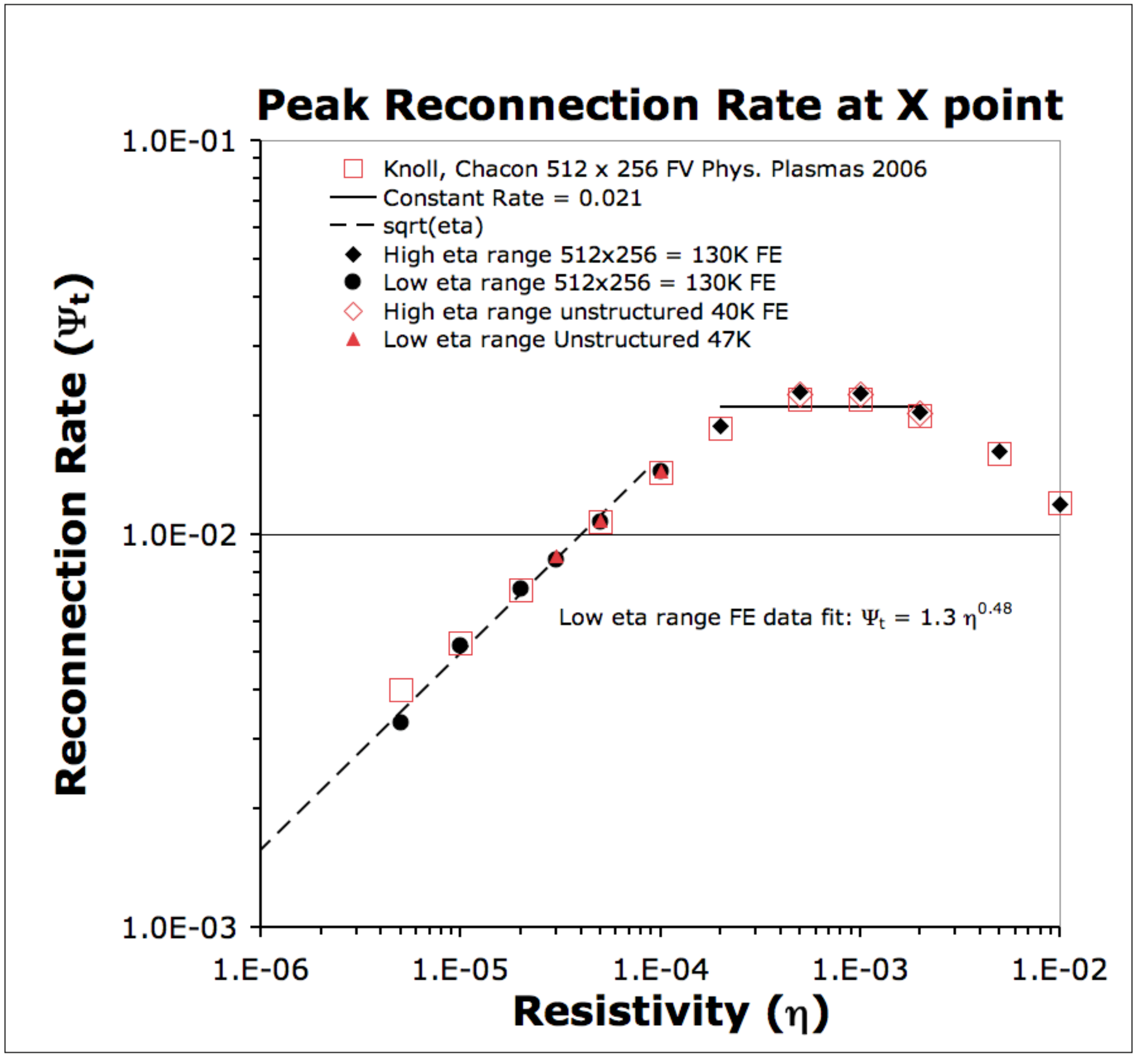
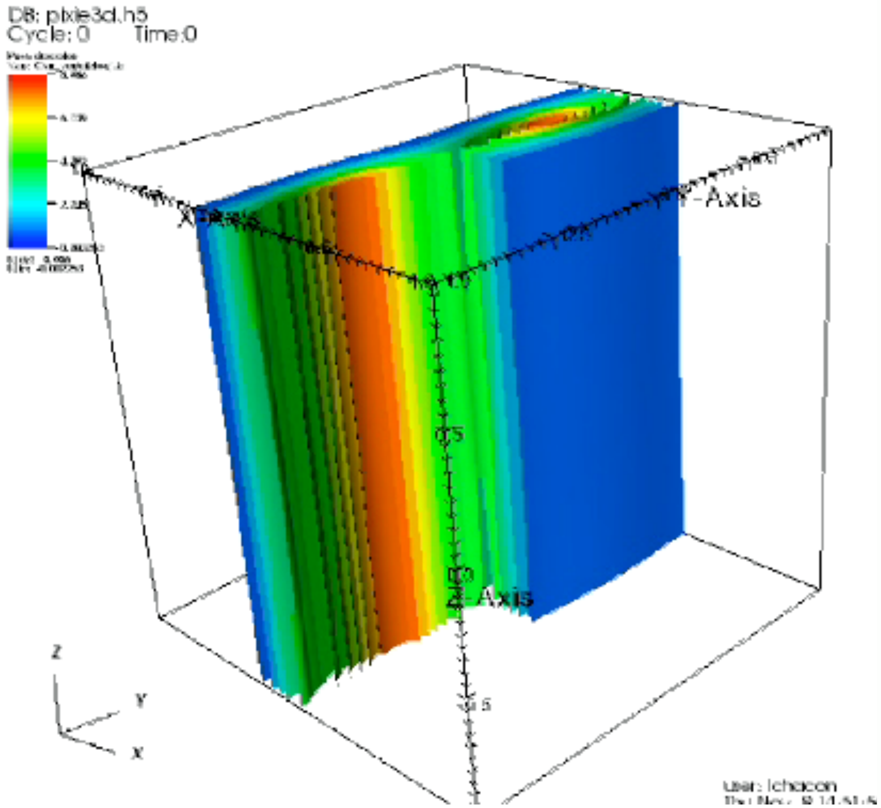
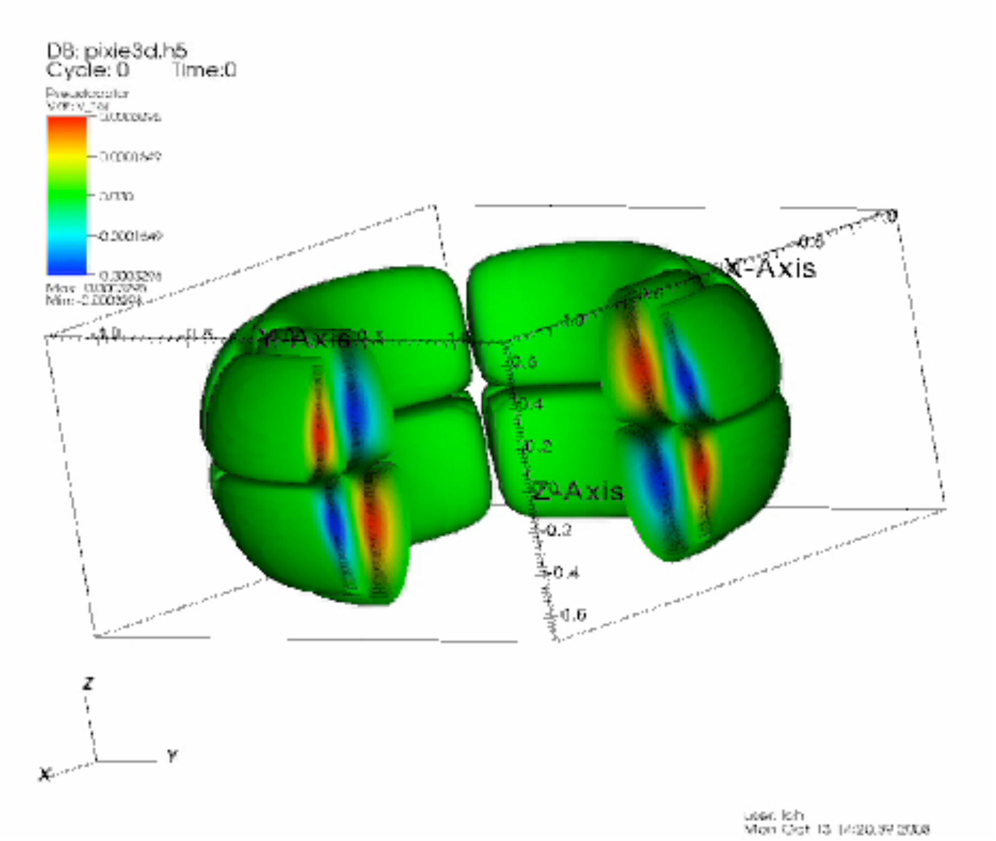
Driven Magnetic Reconnection: Magnetic Island Coalescence
Unstructured Mesh Resistive MHD with Algebraic Multilevel Preconditioners



3D Magnetic Island Reconnection and Ideal Kink Instability in Tokamak Geometry
Mapped Structured FV Discretization with Physics-based preconditioning



3D Island Coalescence



Ideal Kink Instability in Tokamak
Toroidal Velocity Perturbation

Oak Ridge
National Laboratory

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:

$$J\delta\vec{x} = \begin{bmatrix} M & U \\ L & D_v \end{bmatrix} \begin{pmatrix} \delta\vec{y} \\ \delta\vec{v} \end{pmatrix} \; ; \; \delta\vec{y} = \begin{pmatrix} \delta\rho \\ \delta T \\ \delta\vec{B} \end{pmatrix} \; ; \; M = \begin{pmatrix} D_\rho & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_B \end{pmatrix}$$

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

Schur complement analysis of 2x2 block J yields:

$$\begin{bmatrix} M & U \\ L & D_v \end{bmatrix}^{-1} = \begin{bmatrix} I & 0 \\ -LM^{-1} & I \end{bmatrix} \begin{bmatrix} M^{-1} & 0 \\ 0 & P_{Schur}^{-1} \end{bmatrix} \begin{bmatrix} I & -M^{-1}U \\ 0 & I \end{bmatrix},$$

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

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

OAK RIDGE
National Laboratory

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}.
- We consider the small-flow-limit case: $\mathbf{M}^{-1} \approx \Delta t\mathbf{I}$

$$\begin{aligned} \delta\vec{y}^* &= -M^{-1}G_y \\ \delta\vec{v} &\approx P_{SI}^{-1}[-G_v - L\delta\vec{y}^*]\ ;\ P_{SI} = D_v - \Delta tLU \\ \delta\vec{y} &\approx \delta\vec{y}^* - \Delta tU\delta\vec{v} \end{aligned}$$

L. Chacon, Phys. Plasmas, 15, 056103 (2008)

Finite Volume Serial Scaling of resistive and extended MHD Tearing Mode Study

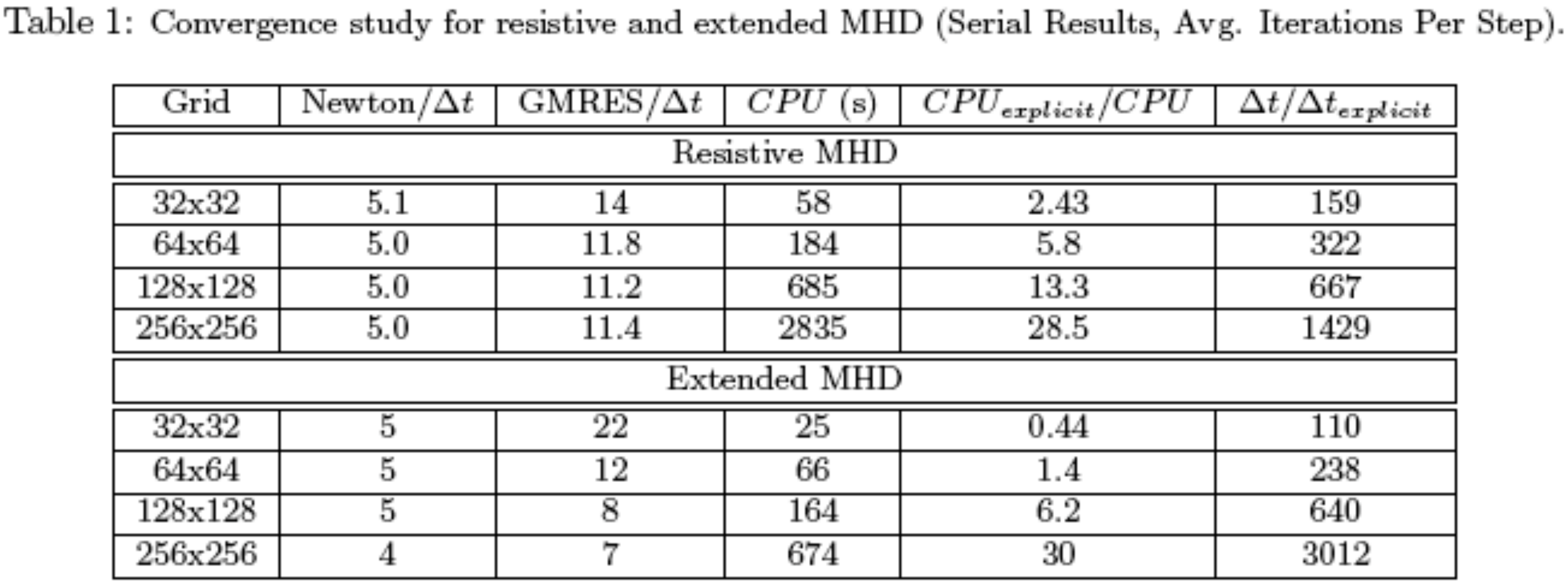


Table 1: Convergence study for resistive and extended MHD (Serial Results, Avg. Iterations Per Step).

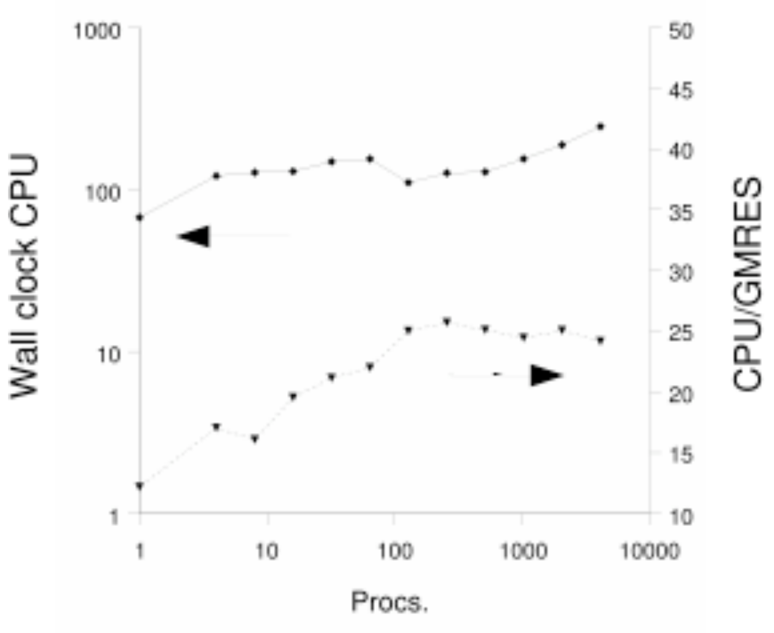
Grid	Newton/Δt	GMRES/Δt	CPU (s)	$CPU_{explicit}/CPU$	$\Delta t/\Delta t_{explicit}$
Resistive MHD					
32x32	5.1	14	58	2.43	159
64x64	5.0	11.8	184	5.8	322
128x128	5.0	11.2	685	13.3	667
256x256	5.0	11.4	2835	28.5	1429
Extended MHD					
32x32	5	22	25	0.44	110
64x64	5	12	66	1.4	238
128x128	5	8	164	6.2	640
256x256	4	7	674	30	3012

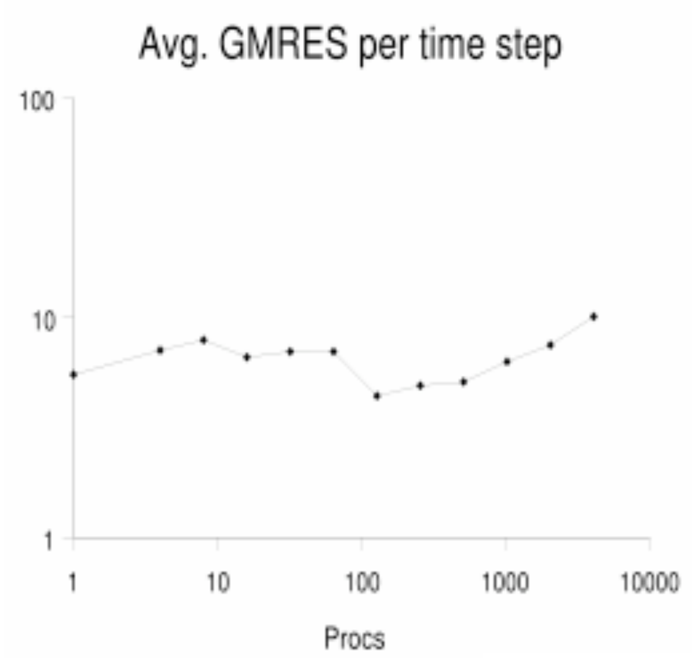
Optimal Serial Results: h - independent

CPU ~ O(N)

JFNK resistive MHD solver: massively parallel performance (3D island coalescence, PETSc, Cray XT4 NERSC)

- Weak scaling with 16^3 unknowns per processor.
- Up to 4096 processors considered.
- Up to 138 million unknowns.





Coarse Grid Solver is now under development for coarse Problems smaller than processor count

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 $u \in U \ni \dfrac{\partial F}{\partial x}$ 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 $F(x) \in \Re^m \to \Re$ 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, etc...** **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**

Conclusions

- Newton-Krylov methods can provide a very effective, robust and flexible solution technology for analysis and characterization of complex nonlinear solution spaces. For steady state, time dependent and optimization type solutions. (e.g. Transport/reaction, resistive MHD)

- Algorithmically scalable and efficient fully-implicit fully coupled Newton-Krylov iterative solvers for a wide range of problems are possible.

- Parallel multilevel aggressive coarsening block AMG preconditioners for systems have shown promising results for algorithmic scalability and CPU time performance of transport solutions.

(Issues: Strong convection, reaction and FE aspect ratios for multilevel methods. -> Physics-based for efficient transient solution)

- Physics-based preconditioners can provide scalable solution and efficient solution methods for challenging transient resistive and extended MHD. Use methods and experience with linearized and operator split solvers as preconditioners.

The End