Comments on

Coupled Multi-physics Simulations

SIAM CS&E 07: Panel on Research Directions and Enabling Technologies for CS&E

John N. Shadid

Computational Science R&D Group
Sandia National Laboratories
Albuquerque, NM

DOE/SC AMR Program

DOE / NNSA

SIAM CS&E Feb. 19-23, 2007

Sand #: 2007-1360C

Multi-physics systems are characterized by a myriad of complex, interacting, nonlinear multiple time and length scale physical mechanisms. These interactions can be limited to the same domain or can occur across boundaries with heterogeneous physics.

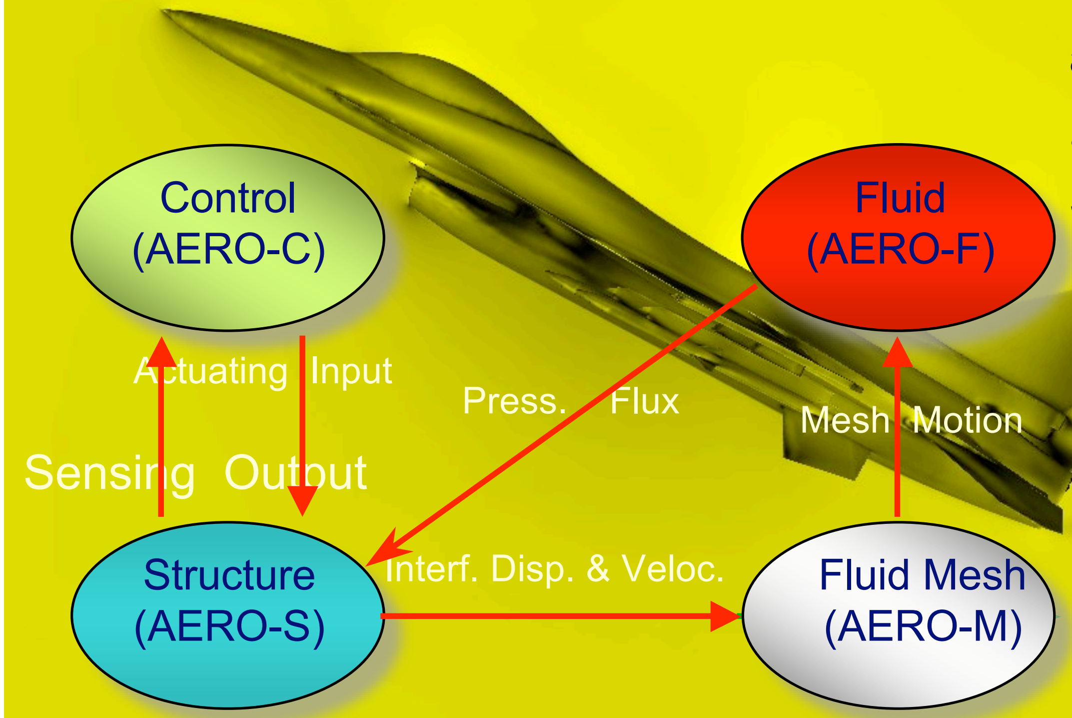
e.g.

- Fusion Reactors (Tokomak -ITER; Pulsed - NIF & Z-pinch)
- Fission Reactors (GNEP)
- Astrophysics
- Combustion, Chemical Processing, Fuel Cells, etc.
- Aircraft Design, Flow & structural response
- Porous media flow, transport, reaction with coupled mechanics
- Particle Accelerator Design
- etc.

A FOUR-FIELD COMPUTATIONAL FRAMEWORK FOR THE AERO-SERVO-ELASTIC ANALYSIS OF MODERN FIGHTERS

Stanford University, Charbel Farhat

- Transient - Error analysis to support use of loosely coupled (operator split) and iterated (implicit) solution
- Next step: Steady & Optimization - Strongly coupling required


Control (AERO-C)

Fluid (AERO-F)

Actuating Input

Sensing Output

Press. Flux

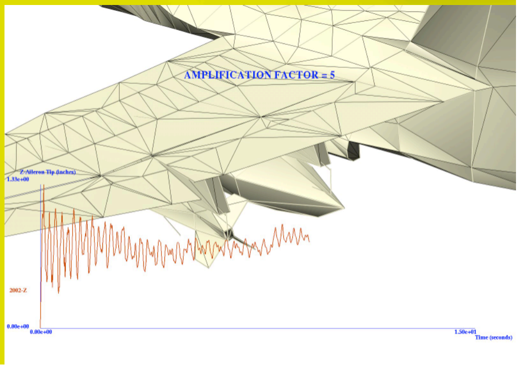
Mesh Motion

Structure (AERO-S)

Interf. Disp. & Veloc.

Fluid Mesh (AERO-M)

- ALE form of Navier-Stokes + Detached Eddy Simulation + Level Sets
- Geometrically Nonlinear Structural Dynamics
- Actuator Dynamics, Flight Control System (ROM - POD)



UT-Austin IPARS (c/o Mary Wheeler)

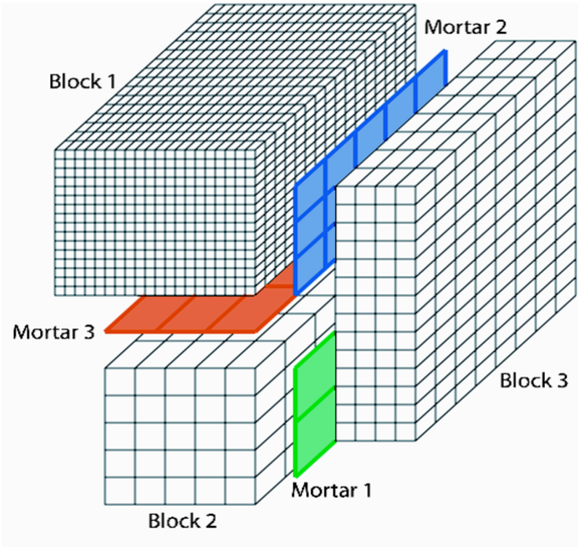
Integrated Parallel Accurate Reservoir Simulation System

State-of-the-art solvers

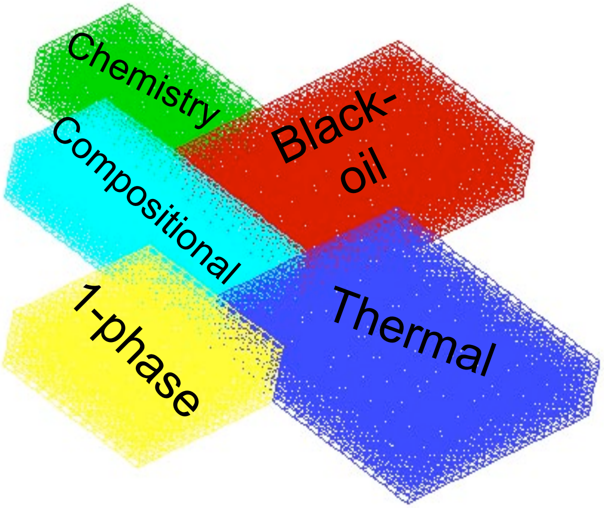
Highly scalable

Couplings with geomechanics and chemistry

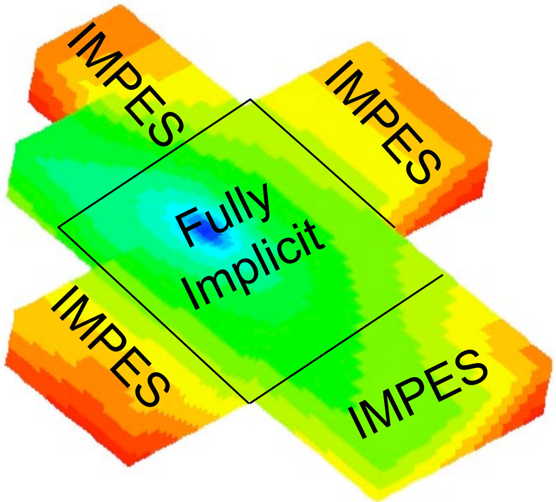
Multiblock approach (subdomain can treat unstructured grids, DG or MPFMFE)



Multiscale



Multiphysics



Multinumerics

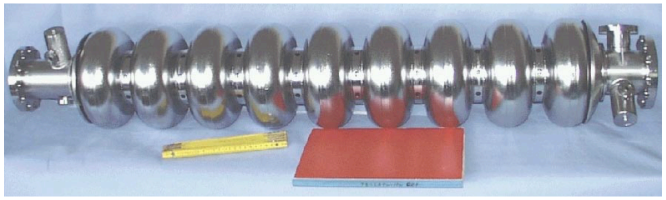
Multiblock Approach

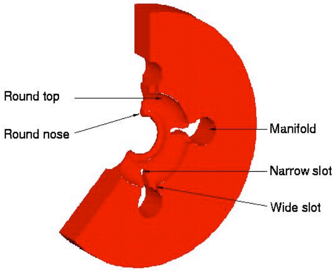
SciDAC ITAPS-TOPS-AST collaboration: optimization for accelerators in Omega3P

- Next generation accelerators have complex cavities that require shape optimization for improved performance and reduced cost

- Numerical modeling in place of cut-and-try approach with Omega3P FE Electromagnetics Code.
- SciDAC adds advances that increase fidelity, speed, and accuracy:
  - Meshing, parallel partitioning and solvers, (h,p) refinement

- AST/TOPS/ITAPS are collaborating to develop an automated capability to accelerate this otherwise manual process:
  - PDE constrained optimization
    Reduced space methods
  - Inner solution by Newton-Krylov
    (Lagrange-Newton-Krylov-Schur)

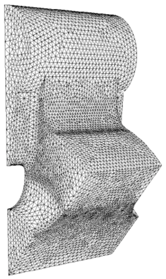




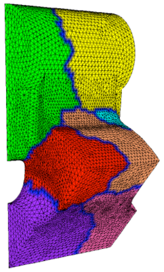
DDS CELL

Omega3P; S3P; T3P; Tau3P

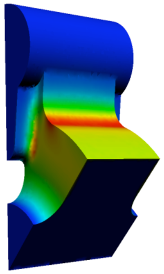
Solvers
(parallel)



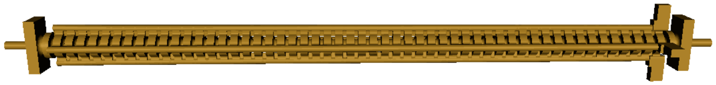
Meshing



Partitioning
(parallel)



Refinement



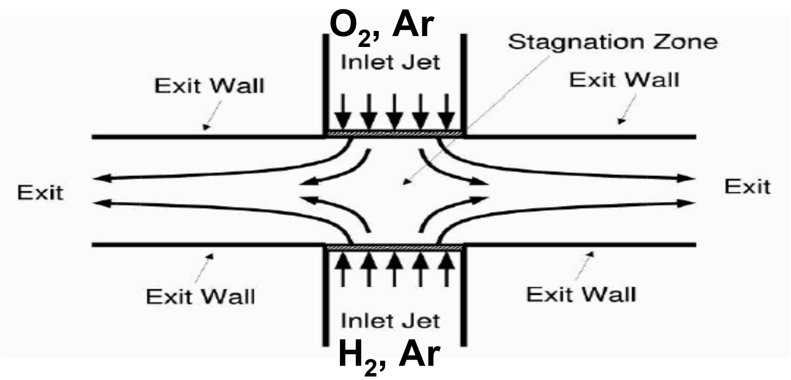
c/o K. Ko (SLAC), D. Keyes (Columbia Univ.), O. Ghattas (U. TX)

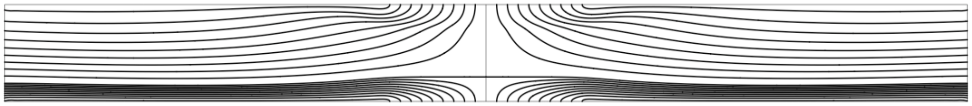
Multiple-time-scale Multi-physics Systems

Multiple-time-scale multi-physics mechanisms can balance to produce:

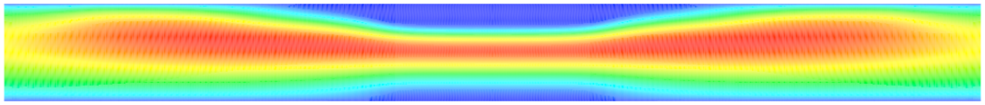
- **steady-state behavior,**
- **nearly balance to evolve a solution on a dynamical time scale that is long relative to the component time scales,**
- **or can be dominated by one, or a few processes, that drive a short dynamical time scale consistent with these dominating modes.**

Bifurcation Analysis of a Steady Reacting H_2, O_2,, Ar, Opposed Flow Jet Reactor

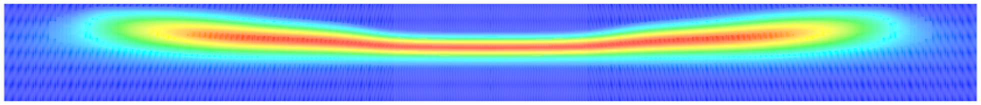




Streamlines

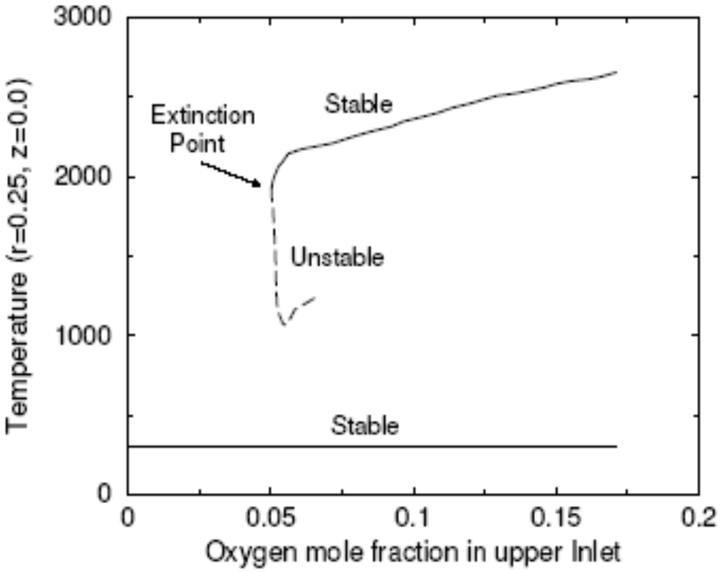


Temperature (Min. 300°K, Max 2727°K)



OH (Min. 0.0, Max 0.177)

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

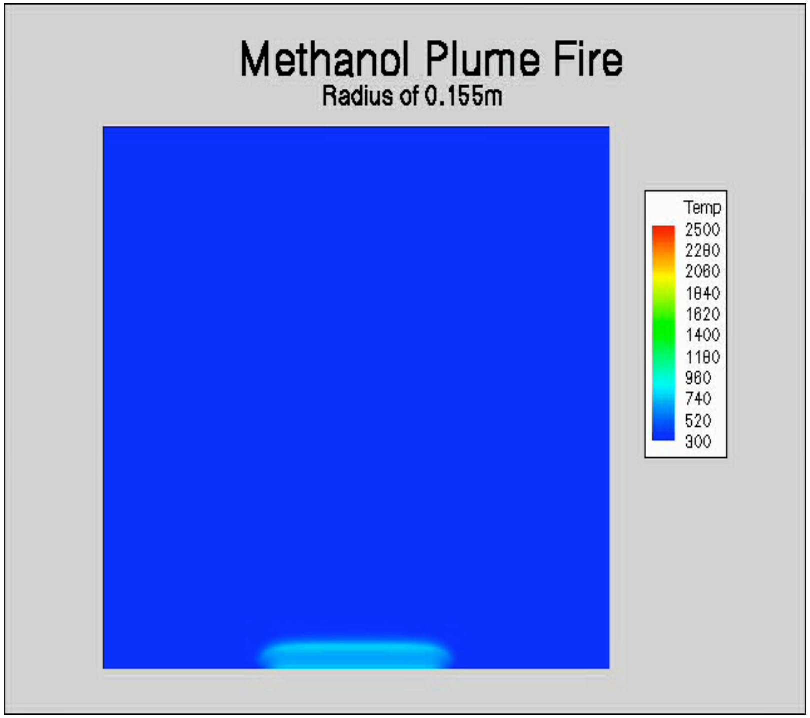


<u>Approx. Time scales (sec.):</u>

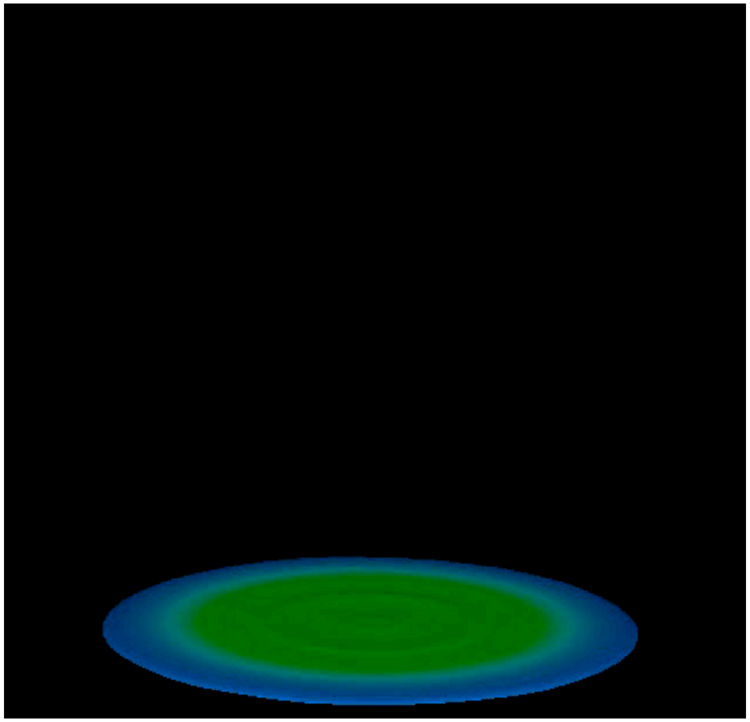
- **Chemical kinetics: 10^{-12} to 10^{-4}**
- **Momentum diffusion: 10^{-6}**
- **Heat conduction: 10^{-6}**
- **Mass diffusion: 10^{-5} to 10^{-4}**
- **Convection: 10^{-5} to 10^{-4}**
- **Diffusion flame dynamics: ∞ (steady)**

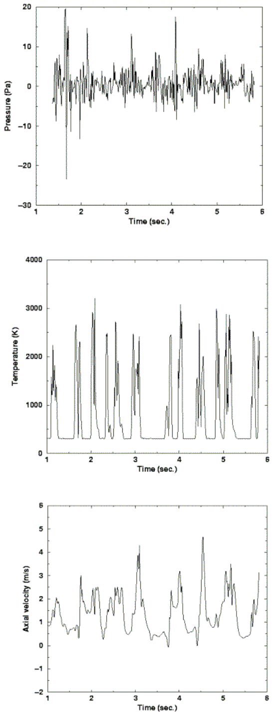
Multiple-time-scale systems: E.g. Methanol Pool Fire
LES-ksgs and Flamelet Combustion Model (w/ T. Smith – MPSalsa)

2D axisymmetric Simulation



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



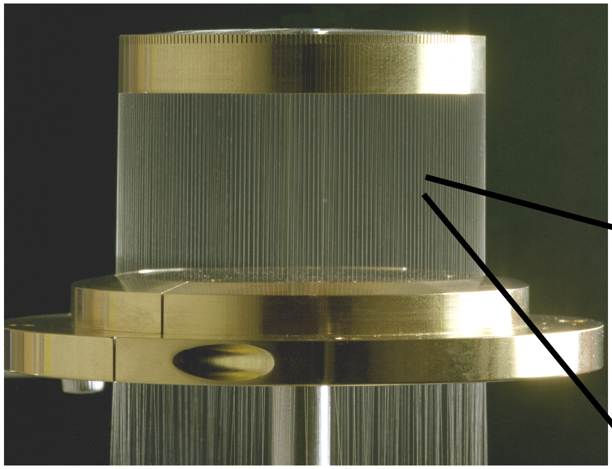


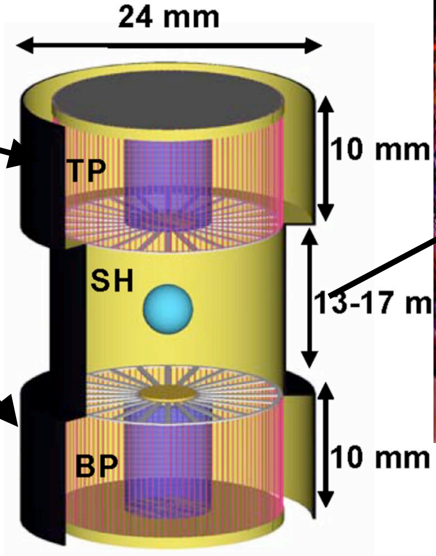
Approx. Time scales (sec.):

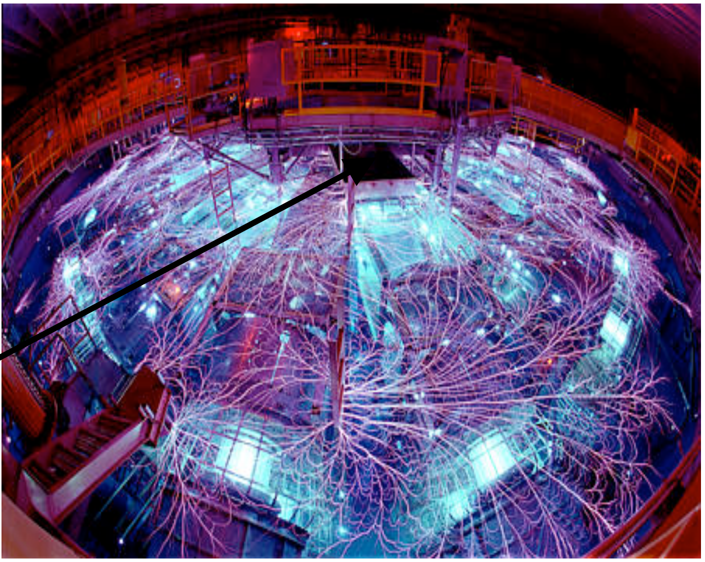
- **Chemical kinetics: 10^{-10} to 10^{-3}**
- **Momentum diffusion: 10^{-6}**
- **Heat conduction: 10^{-6}**
- **Convection: 10^{-3} to 10^{-1}**
- **Buoyancy (puffing freq. = 2.8Hz): 10^{-1} to 10^{0}**
- **Meandering mode: 10^{0}**

Sandia National Laboratories

Z-pinch Double Hohlraum Schematic







Z Machine (Approximate Ranges)

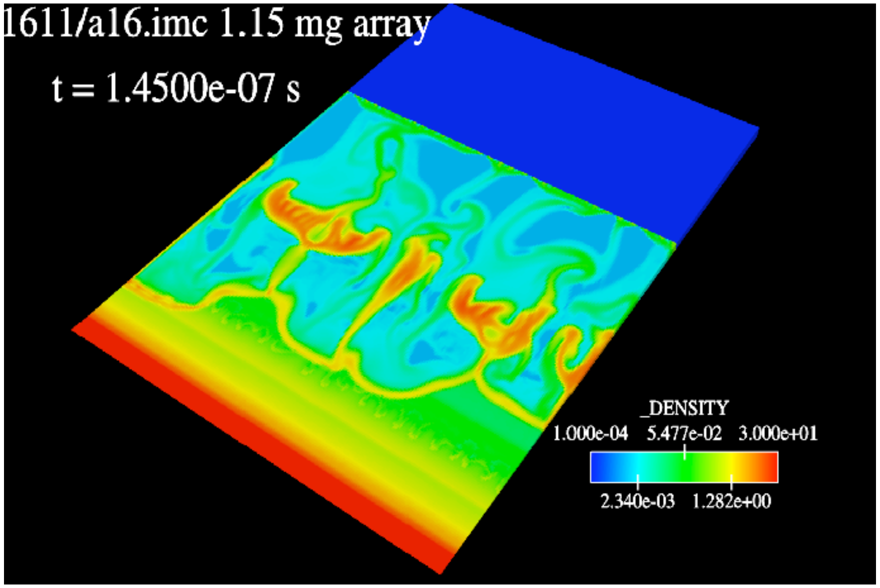
100ns current rise time for 20 MA Electrical Current

250 ns plasma shell collapse and stagnation

10-30 ns X-ray power pulse - 20-50 TW power

Even this system requires some implicit aspect of solution because of small element length scales required for high resolution near ablating wires and the corresponding resistive and diffusion stability constraints $\Delta t \approx (\Delta x)^2$

A Recent Review: K. Matzen, et. al., PHYSICS OF PLASMAS 12, 055503 (2005)



Movie courtesy of R. Lemke: Pulsed Power Sciences; Sandia Nat. Labs

C. J. Garasi, D. E. Bliss, T. A. Mehlhorn, B.V. Oliver, A. C. Robinson and G. S. Sarkisov, ”Multi-dimensional high energy density physics modeling and simulation of wire array Z-pinch physics,” Physics of Plasmas, 11 (5), May 2004, pp. 2729-2737

Numerical Solution of Multiple-time-scale Multiphysics Systems

A Perspective (an attempt to be controversial!):

Historically,

linearization, semi-implicit, lagged, operator split transient solution methods,

and decoupled, loosely coupled and fixed point nonlinear solution strategies

were devised out of necessity in a time when limitations in computer memory and CPU power were acute.

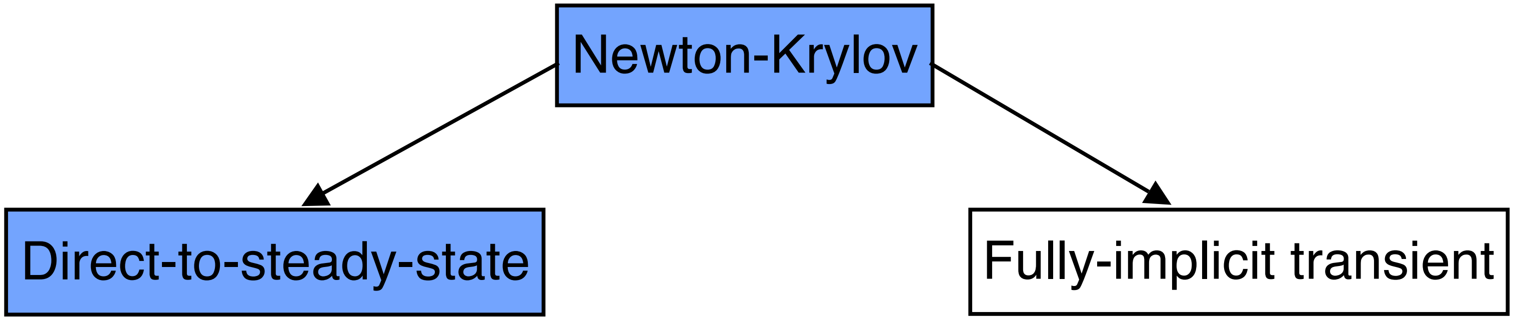
The resulting numerical stability, accuracy, convergence and appropriate time step controls are only heuristically understood, in most cases. Applying these solution methods to complex systems can often be fragile and exhibit non-intuitive instabilities or they can be stable but very inaccurate.

We believe that with the recent significant increase in computing resources and advances in numerical methods, these earlier choices should be critically re-evaluated.

We need to pursue new approaches that include robust, accurate, scalable, efficient and predictive simulation technologies for complex coupled multi-physics systems.

(Based on Shadid/Knoll DOE NNSA: ASC Multi-physics Workshop & Office of Science: SciDAC Multi-physics Session Talks)

Why Newton-Krylov Methods?



Newton-Krylov

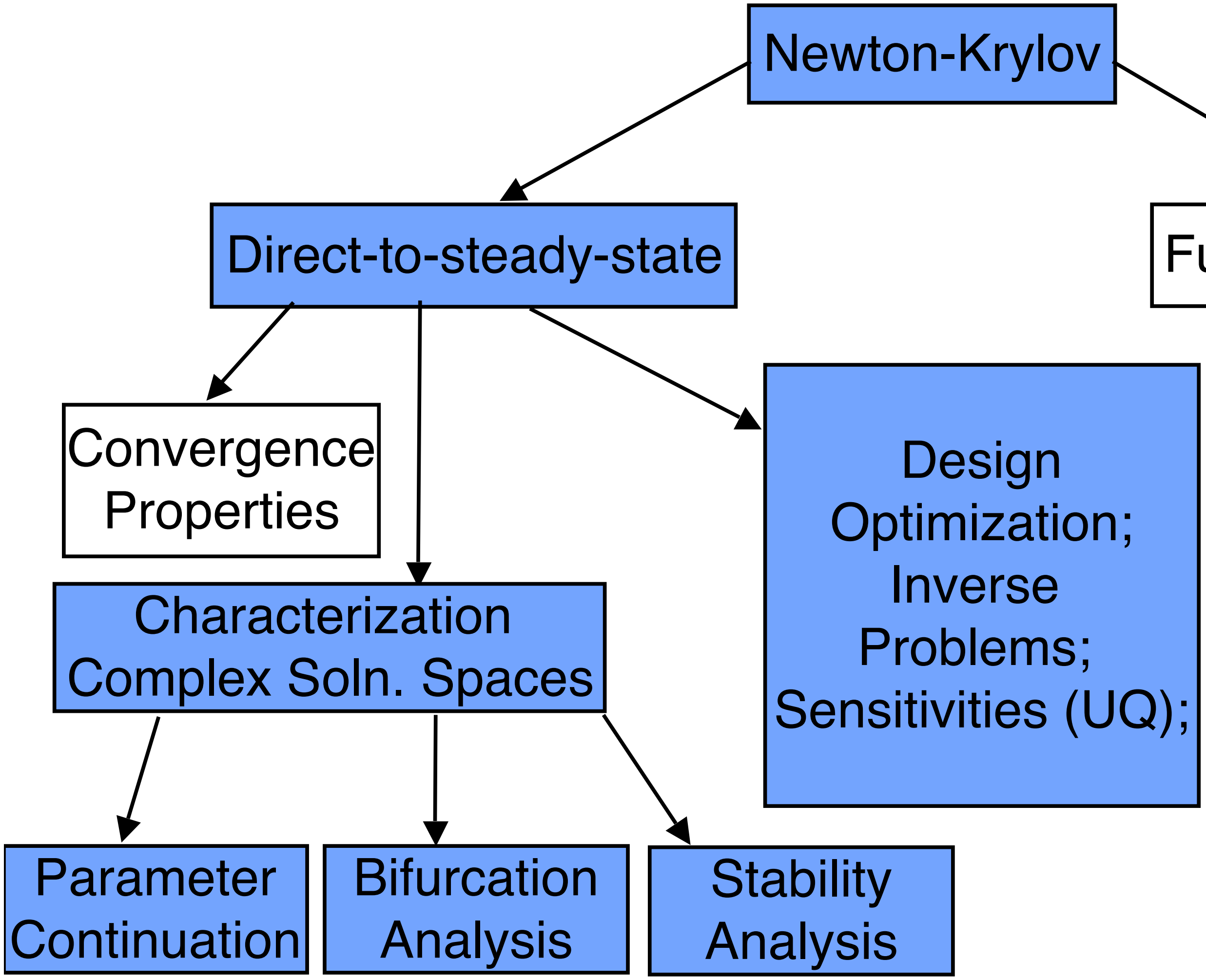
Direct-to-steady-state

Fully-implicit transient

<u>Convergence properties</u>

- Strongly coupled multi-physics often requires a strongly coupled nonlinear solver
- Quadratic convergence near solutions (backtracking, adaptive convergence criteria)
- Often only require a few iterations to converge, if close to solution, independent of problem size

Why Newton-Krylov Methods?



Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

Convergence Properties

Characterization Complex Soln. Spaces

Design Optimization; Inverse Problems; Sensitivities (UQ);

Parameter Continuation

Bifurcation Analysis

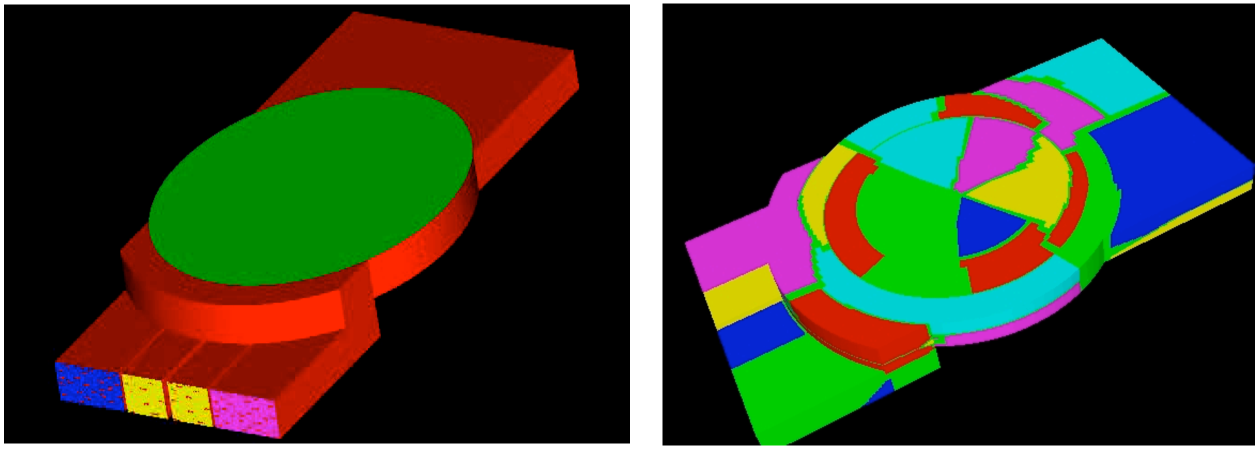
Stability Analysis

Sandia
National
Laboratories

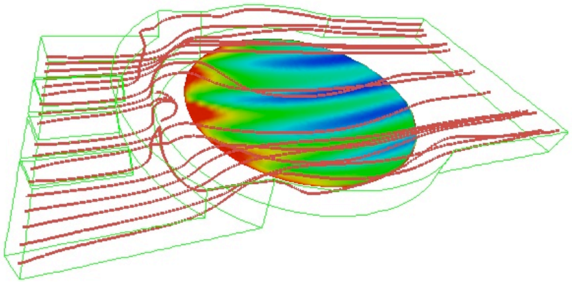
PDE Constrained Optimization of Poly-Silicon CVD Reactor

Poly-Silicon Epitaxy from Trichlorosilane in Hydrogen Carrier;

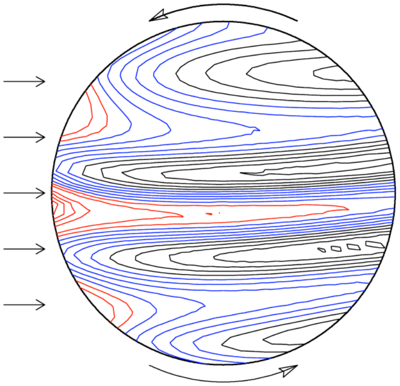
3D (u,v,w,P,T)
3 chemical species
1.2M unknowns

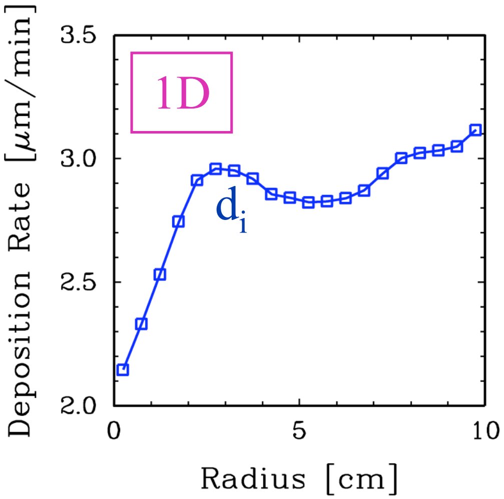


3D



2D

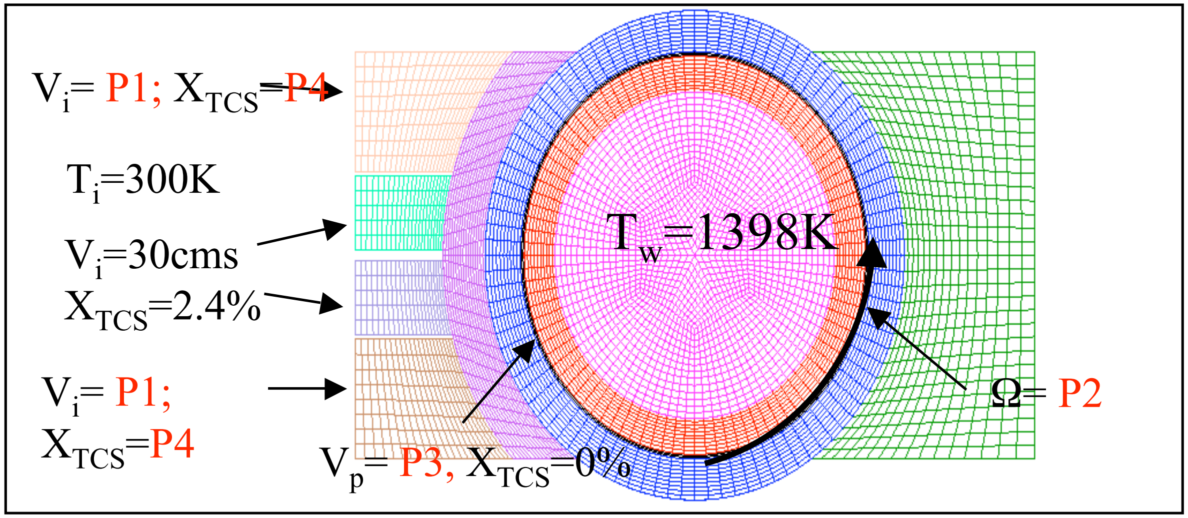




0D Objective Function:

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

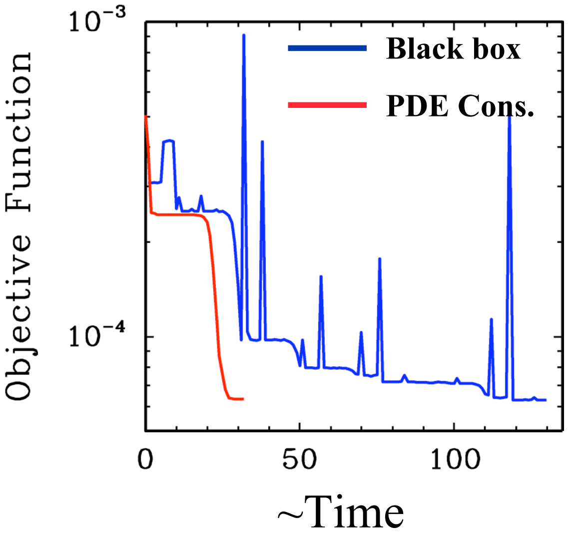
PDE Constrained Optimization of Poly-Silicon CVD Reactor

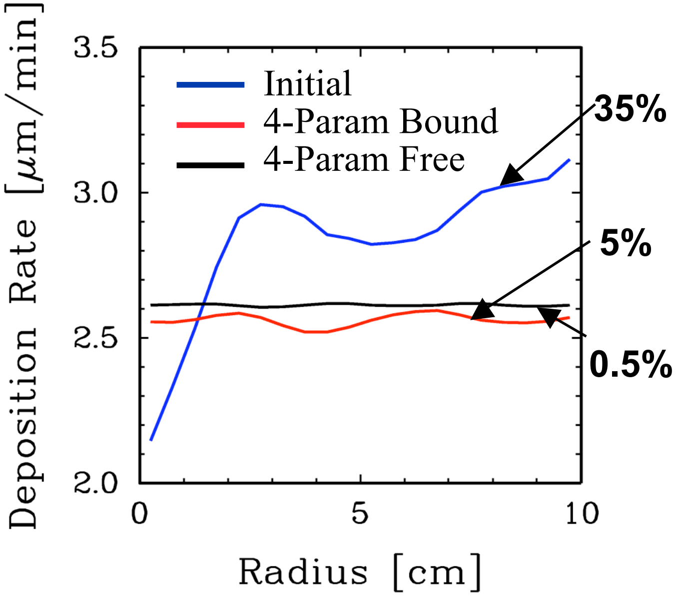


PDE Constrained Optimization:

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

Use Newton’s Method solve KKT system



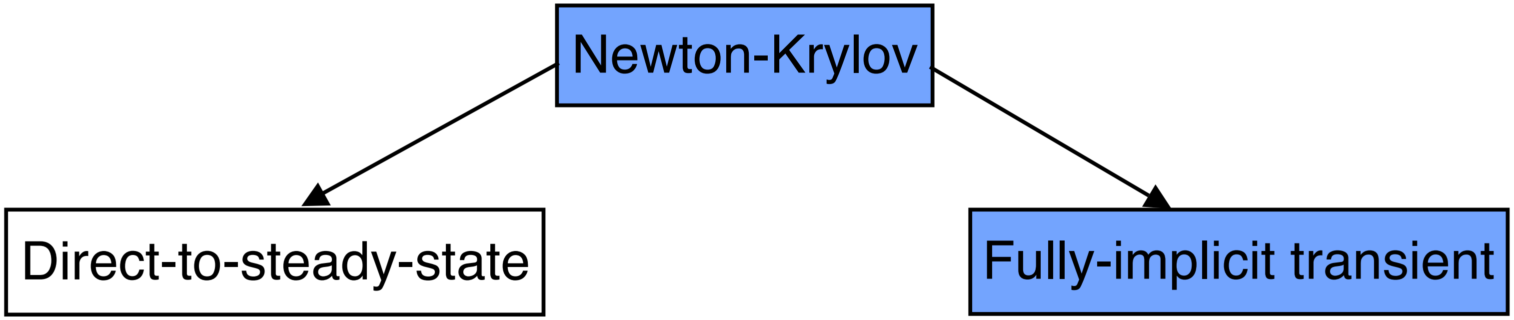


Unks	Procs	Time (hrs.)
1.2	48	6.2 (3GHz Cluster)
4.8M	128	~ 6 (Red Storm: XT3)
38M	1024	~ 8 (Red Storm: XT3)

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

Sandia National Laboratories

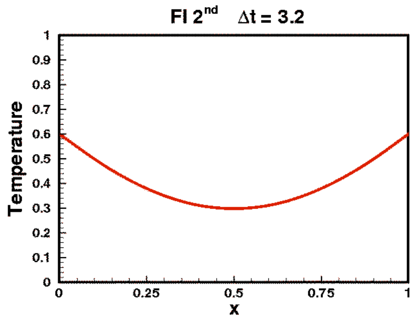
Why Newton-Krylov Methods?



Stability and Accuracy Properties

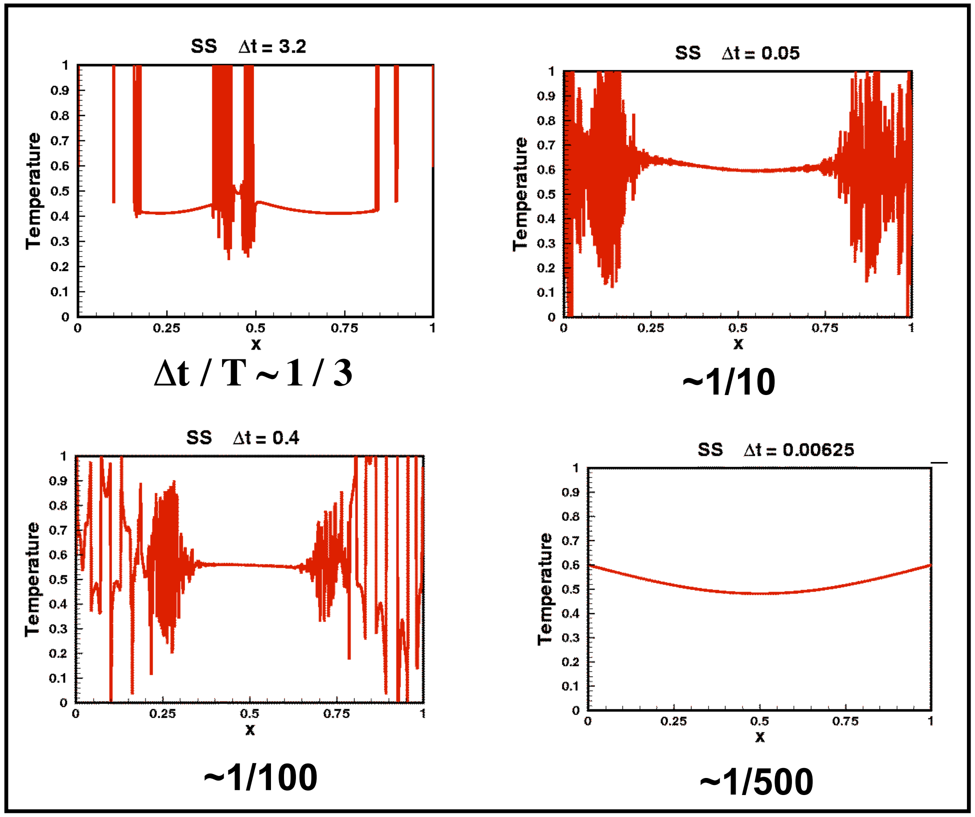
- Stable (stiff systems)
- High order methods
- Variable order techniques
- Local and global error control possible
- Can be stable and accurate run at dynamical time-scale of interest in multiple-time-scale systems

Operator Splitting Methods can Sometimes Destroy a Critical Balance Present in the Coupled Physics. (Brusselator)



FI

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

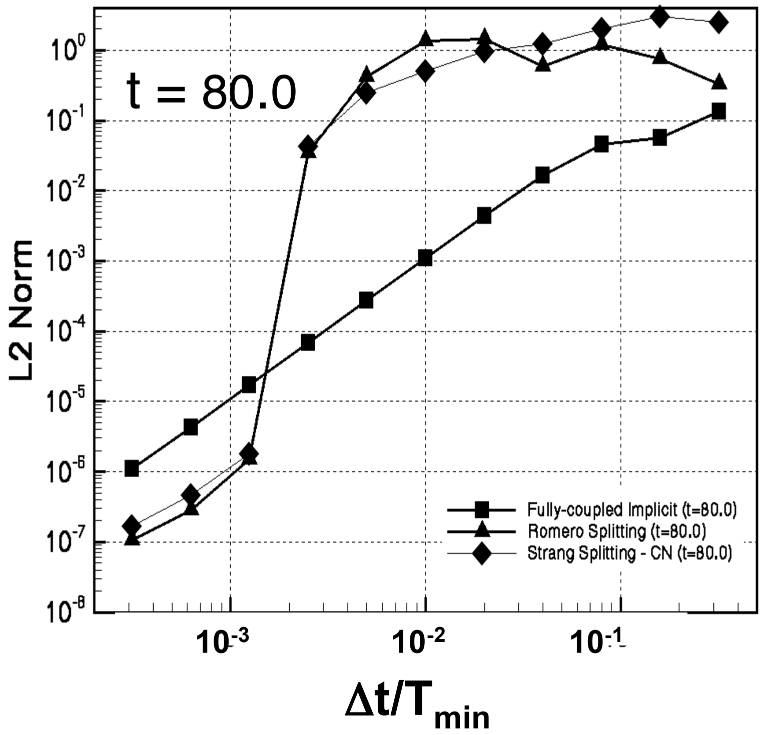


$\Delta t / T \sim 1/3$

~1/10

~1/100

~1/500



Multiple time scales:
Ropp, Shadid, JCP 2004, 2005
Ober, Shadid JCP 2004

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

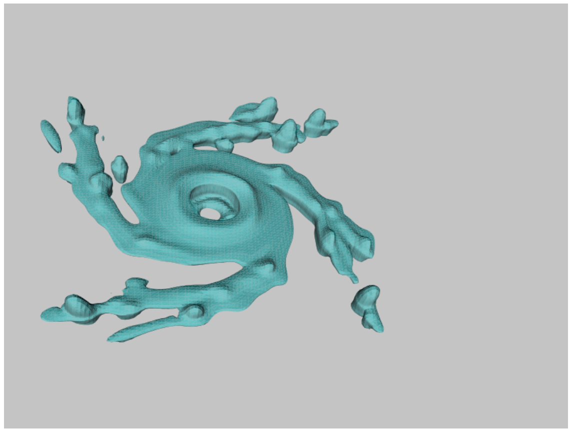
(Riesner, Mousseau, Wyszogrodzki, Knoll, MWR 2004)

- **3D compressible N-S & phase change**
- **Error/CPU time Comparison of**
    - **Semi-implicit (SI)**
    - **JFNK with SI as preconditioner (M)**

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

$$\mathbf{J}\mathbf{p} = \frac{\mathbf{R}(\mathbf{x} + \delta\mathbf{p}) - \mathbf{R}(\mathbf{x})}{\delta}$$

- **Study transient hurricane intensification to ramped increase in sea surface temperature**



(Courtesy of D. Knoll - INL)

Hurricane Equation Set

$$\frac{\partial u\rho}{\partial t} + \frac{\partial uu\rho}{\partial x} + \frac{\partial vu\rho}{\partial y} + \frac{\partial wu\rho}{\partial z} = -\frac{\partial p'}{\partial x} + f\rho(v - v_e) - \tilde{f}w + \frac{\partial \kappa\rho\tau^{11}}{\partial x} + \frac{\partial \kappa\rho\tau^{12}}{\partial y} + \frac{\partial \kappa\rho\tau^{13}}{\partial z}, \tag{1}$$

$$\frac{\partial v\rho}{\partial t} + \frac{\partial uv\rho}{\partial x} + \frac{\partial vv\rho}{\partial y} + \frac{\partial wv\rho}{\partial z} = -\frac{\partial p'}{\partial y} - f\rho(u - u_e) + \frac{\partial \kappa\rho\tau^{21}}{\partial x} + \frac{\partial \kappa\rho\tau^{22}}{\partial y} + \frac{\partial \kappa\rho\tau^{23}}{\partial z}, \tag{2}$$

$$\frac{\partial w\rho}{\partial t} + \frac{\partial uw\rho}{\partial x} + \frac{\partial vw\rho}{\partial y} + \frac{\partial ww\rho}{\partial z} = -\frac{\partial p'}{\partial z} + \tilde{f}\rho(u - u_e) - (\rho + q_c)g + \frac{\partial \kappa\rho\tau^{31}}{\partial x} + \frac{\partial \kappa\rho\tau^{32}}{\partial y} + \frac{\partial \kappa\rho\tau^{33}}{\partial z}, \tag{3}$$

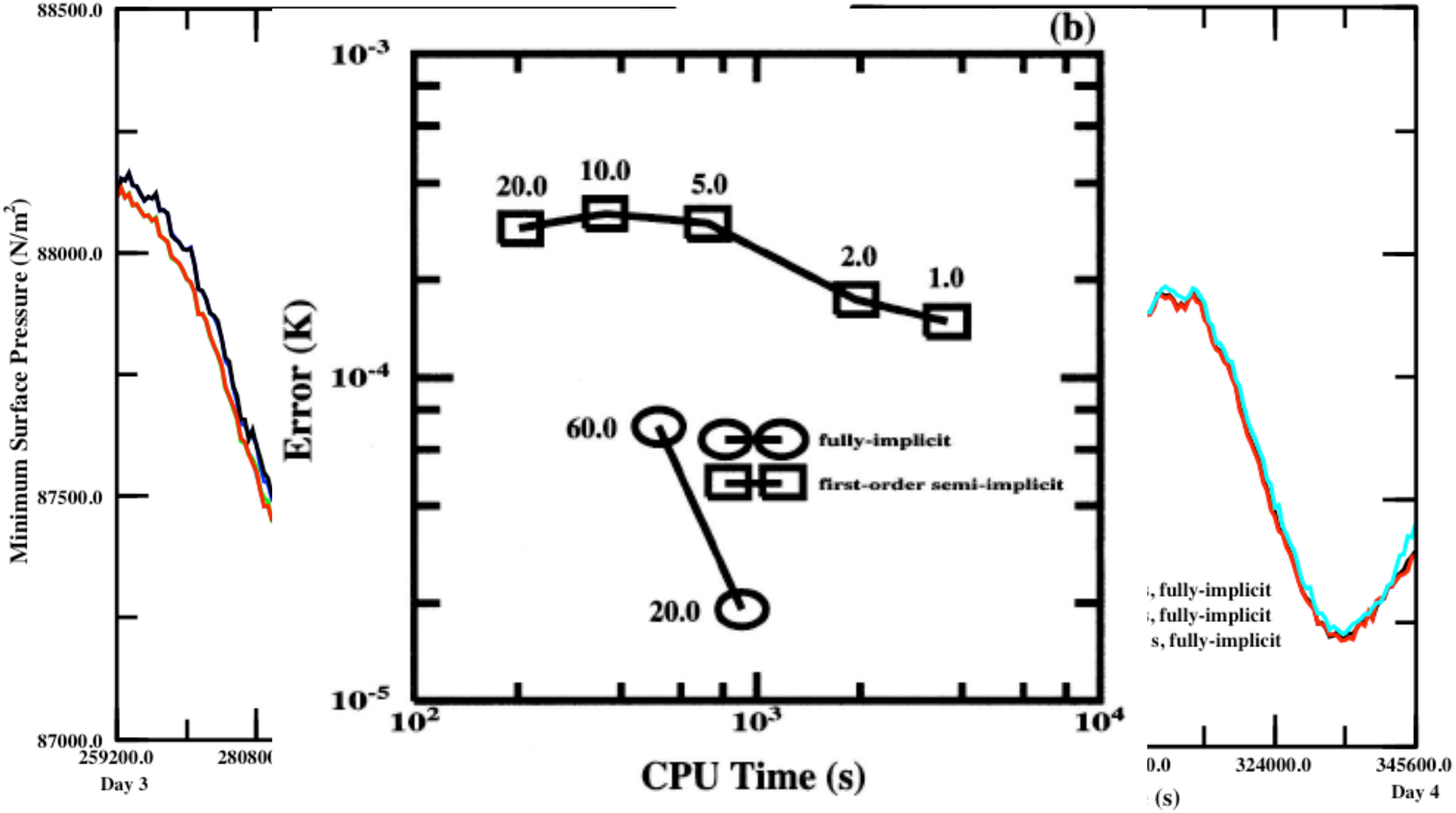
$$\frac{\partial \theta\rho}{\partial t} + \nabla \cdot (\mathbf{V}\theta\rho) = \frac{\theta\rho L}{TC_p} f_{cloud} + f_{surface-energy} + \nabla \cdot (\mathbf{F}_\theta) \tag{4}$$

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

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

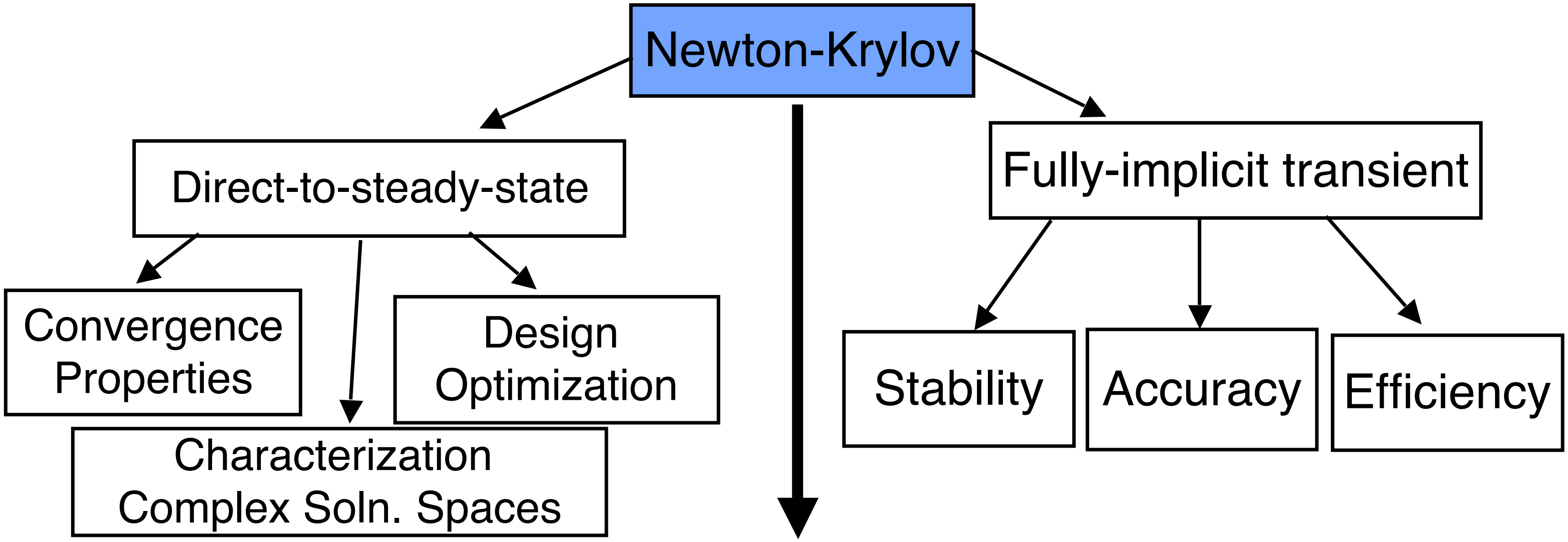
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{V}\rho) = -f_{cloud} + f_{surface-gas} \tag{7}$$

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

Convergence Properties

Characterization Complex Soln. Spaces

Design Optimization

Fully-implicit transient

Stability

Accuracy

Efficiency

Very Large Problems -> Iterative Solution of Sub-problems

Krylov Methods - Robust, Scalable and Efficient Preconditioners

http://software.sandia.gov/trilinos/Trilinos

http://software.sandia.gov/trilinos/packages/ml/ML

http://www-unix.mcs.anl.gov/scidac-tops/Tops

http://www-unix.mcs.anl.gov/petsc/petsc-as

http://www.llnl.gov/CASC/linear_solvers

⇒Achieving Predictive Simulations of Complex Multi-physics Systems

Important Challenges (varying levels of detail):

- **Stable, Higher-Order, Efficient Time Integration with Error Estimation/Control**
  - **Fully-implicit, Implicit-explicit, Predictor-corrector, Adv. Operator-split**
  - **Interaction of deterministic and stochastic sub-component integrators**
- **Stable, Higher-Order Spatial Discretizations with Error Estimation/Adaptivity**
  - **Integration of compatible single physics discretizations (e.g. electromagnetics, compressible CFD) into provably stable multi-physics system discretizations (rad-MHD)**
  - **DG, mortar element and computable optimization based methods for coupling heterogeneous physics**
- **Stable and Efficient Numerical Solution Methods for Strongly Coupled Nonlinear Systems**
  - **Newton-Krylov, Jacobain-Free N-K**

⇒ Achieving Predictive Simulations of Complex Multi-physics Systems

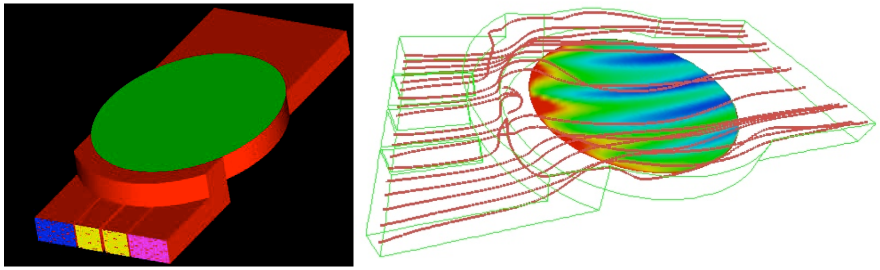
- **Scalable and Efficient Linear Solvers for strongly coupled systems (Petaflop platforms)**
  - **Physics-based Preconditioners, Approximate block factorizations**
  - **Multi-level solvers (multi-grid, AMG) for scalar/vector systems and anisotropic effects**
  - **AMG for compatible discretizations (e.g. node, edge, face, volume unknowns)**
- **Analysis, Design, Optimization and control methods for large-scale complex nonlinear spaces**
  - **PDE constrained optimization**
  - **Efficient ROM methods for complex multi-parameter nonlinear systems**
- **Multi-scale techniques for continuum-to-continuum, continuum-to-molecular and continuum-to-atomistic coupling in multi-physics context**
- **V&V and Uncertainty quantification (UQ) techniques for multi-physics apps**
  - **Analytic solutions to prototype multi-physics problems & MMS**
  - **Techniques to propagate, estimate and control data, discretization, and model error through coupled, decoupled, and operator split solution algorithms**
  - **Estimation/control of error in combined deterministic / stochastic methods**

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

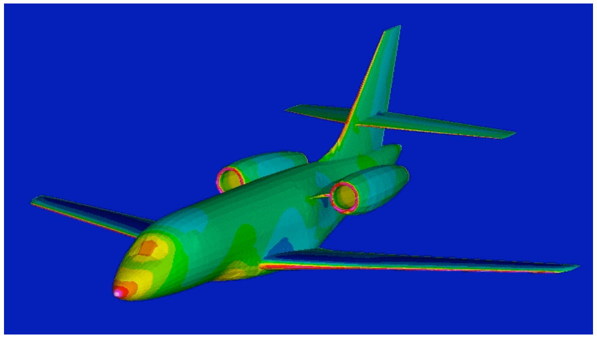
Optimization Unconstrained: Constrained:	Find $u \in \Re^n$ that minimizes $g(u)$ Find $x \in \Re^m$ and $u \in \Re^n$ that minimizes $g(x,u)$ s.t. $f(x,u) = 0$	**MOOCHO**
Bifurcation Analysis	Given nonlinear operator $F(x,u) \in \Re^{n+m} \rightarrow \Re^n$ For $F(x,u) = 0$ find space $u \in U \ni \frac{\partial F}{\partial x}$ singular	**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 $x(t) \in \Re^n, t \in [0,T]$	**Rhythmos**
Nonlinear Problems	Given nonlinear operator $F(x,u) \in \Re^{n+m} \rightarrow \Re^n$ Solve $F(x) = 0$ $x \in \Re^n$	**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) $\nu \in \Re^n$, $\lambda \in \Re$	**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**

Multi-level Methods for Coupled Systems of Equations (ML)

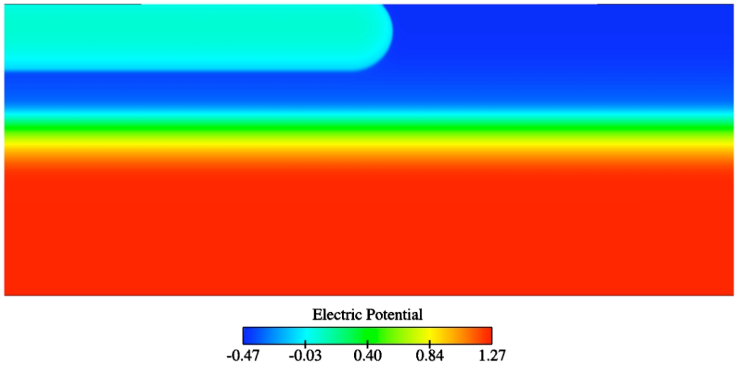
Incompressible and Chemically Reacting Flows - MPSalsa (Nodal FE)



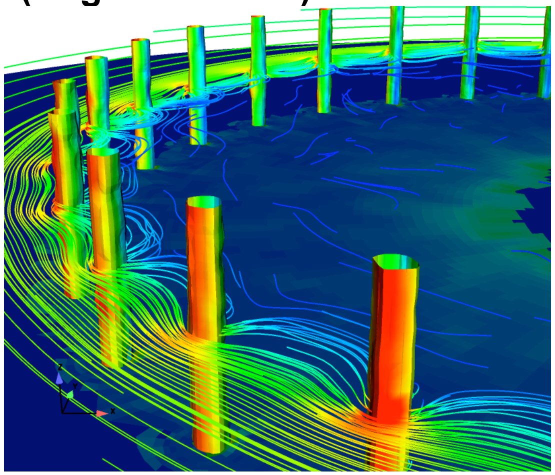
Compressible Euler / Navier-Stokes - Premo (Vertex based FV)



Drift Diffusion Eq. Semiconductor Devices - Charon (Nodal FE)



Magnetic Diffusion Solver - Alegra (Edge based FE)



Sandia National Laboratories

Enabling Technology software

http://www-unix.mcs.anl.gov/scidac-tops/Tops

http://software.sandia.gov/trilinos/Trilinos
http://software.sandia.gov/trilinos/packages/ml/ML

http://www-unix.mcs.anl.gov/petsc/petsc-as

http://www.llnl.gov/CASC/linear_solvers

The End