Linear and Nonlinear Stability Analysis of Incompressible Flows on Parallel Computers

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

The Stability Analysis Project

Mission: To develop linear and nonlinear stability analysis algorithms to enable sophisticated design and analysis of **large-scale** nonlinear models.

Motivation: Nonlinear systems can exhibit:

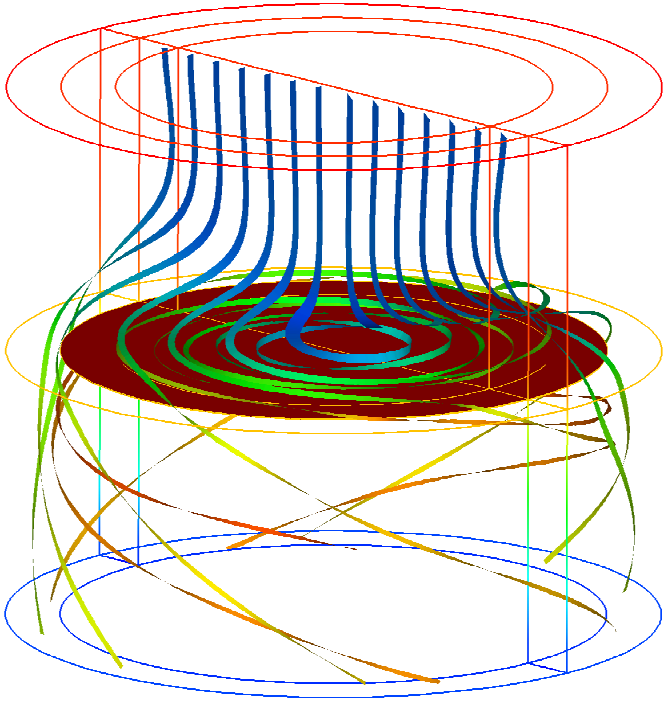
- Multiple Steady States
- Turning Points, including Ignition/Extinction phenomenon
- Pitchfork Bifurcations from symmetry breaking
- Hopf Bifurcations to oscillating states
- Phase Transitions

Methodology:

1. LOCA library for tracking steady-state solutions and bifurcation points.
2. Linear Stability analysis capability to determine the stability of a solution (eigenvalue calculations).

This Work Builds on Massively Parallel Reacting Flows, Linear Solver, and Eigen-Analysis Codes

MPSalsa: An unstructured grid, finite element code for incompressible flows coupled with heat and mass transfer, using fully-coupled Newton solver with analytic Jacobian.



Aztec: An iterative, preconditioned Krylov linear solver library, with domain-decomposition algebraic preconditioners.

ARPACK: Parallel implicitly restarted Arnoldi method for calculating selected Eigenvalues.

LOCA Library Of Continuation Algorithms

Interface Requirements:

• Residual Calculation	• Linear Solve of Jacobian
• Jacobian Calculation	• Matrix Vector Multiply

Capabilities:

• Parameter Continuation	• Arc-length Continuation
• Turning Point Tracking	• Pitchfork Bifurcation Tracking
• Hopf Bifurcation Tracking	• Phase Equilibrium Tracking
+ rSQP Optimization (CMU)	+ Periodic Orbits (Princeton)

Codes:

1. MPSalsa: Reacting Flows (MP, Unstructured grid, Finite Element)
2. Tramonto: Classical DFT (MP, moderate-range integrals, structured grid)
3. GOMA: Free-surface flows, visco-elastic flows, fluid-structure interaction (FE)

Summary of Bifurcation Algorithms in LOCA

Simple Parameter Continuation (N):

$$R(x, p) = 0$$

Arc-Length Continuation (N+1):

$$R = 0$$

$$G(x, p, s) = 0$$

Turning Point (Fold) Tracking (2N+1):

$$R = 0$$

$$\mathbf{J}n = 0$$

$$l \cdot n = 1$$

Phase Transition Tracking (2N+1):

$$R(x_1, p) = 0$$

$$R(x_2, p) = 0$$

$$\Omega(x_1) - \Omega(x_2) = 0$$

Pitchfork Bifurcation Tracking (2N+2):

$$R + \varepsilon\Psi = 0$$

$$\mathbf{J}n = 0$$

$$\langle x, \Psi \rangle = 0$$

$$l \cdot n = 1$$

Hopf Bifurcation Tracking (3N+2):

$$R = 0$$

$$\mathbf{J}y + \omega \mathrm{M} z = 0$$

$$\mathbf{J}z - \omega \mathrm{M} y = 0$$

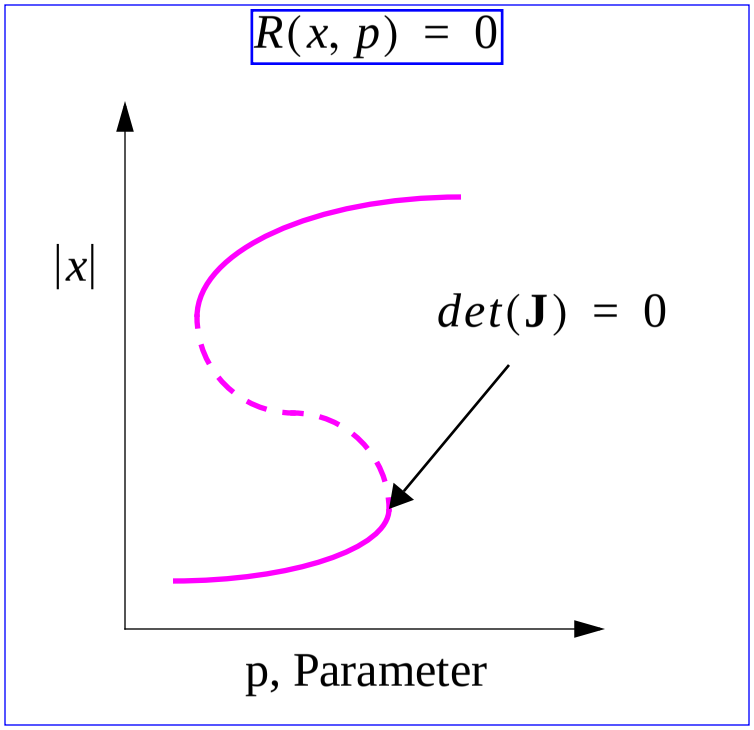
$$l \cdot y = 1$$

$$l \cdot z = 0$$

Bordering Algorithms. Ex: Turning Point Tracking

1. $$R = 0$$
$$\mathbf{J}n = 0$$
$$l \cdot n = 1$$

2. $$\begin{bmatrix} \mathbf{J} & 0 & R_p \\ \mathbf{J}_x n & \mathbf{J} & \mathbf{J}_p n \\ 0 & l^t & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta n \\ \Delta p \end{bmatrix} = \begin{bmatrix} -R \\ -\mathbf{J}n \\ 1 - l \cdot n \end{bmatrix}$$



3. $$\mathbf{J}a = -R$$
$$\mathbf{J}b = -R_p$$
$$\mathbf{J}c = -\mathbf{J}_x n a - \mathbf{J}n$$
$$\mathbf{J}d = -\mathbf{J}_x n b - \mathbf{J}_p n$$

$$\Delta p = (1 - l \cdot n - l \cdot c)/(l \cdot d)$$
$$\Delta x = a + \Delta p\, b$$
$$\Delta n = c + \Delta p\, d$$

Computational Cost of Bordering Algorithms

Parameter Continuation	N	1 Solve of $\mathbf{J}$
Arc-length Continuation	N+1	2 Solves of $\mathbf{J}$
Turning Point Tracking	2N+1	4 Solves of $\mathbf{J}$
Phase Transition Tracking	2N+1	4 Solves of $\mathbf{J}$
Pitchfork Bifurcation Tracking	2N+2	6 Solves of $\mathbf{J}$
Hopf Bifurcation Tracking	3N+2	2 Solves of $\mathbf{J}$ and 3 Solves of $\begin{bmatrix} \mathbf{J} & \omega\mathbf{M} \\ -\omega\mathbf{M} & \mathbf{J} \end{bmatrix}$

Note: For large problems, filling of finite element matrices and residuals is free (<2%) compared to solving them

Linear Stability Analysis Performed using an Arnoldi-Based Eigenvalue Approximation Method

Linearizing around SS gives generalized eigenvalue problem:

$$\boldsymbol{J}x = \lambda \boldsymbol{M}x$$

Goal: To locate rightmost λ_i on complex plane.

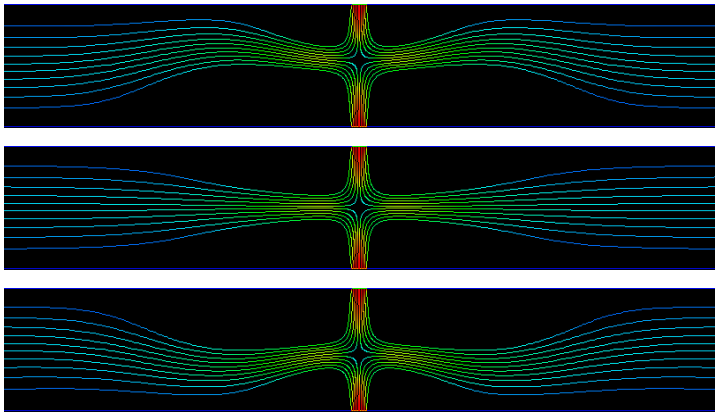
Three spectral transformations have been implemented:

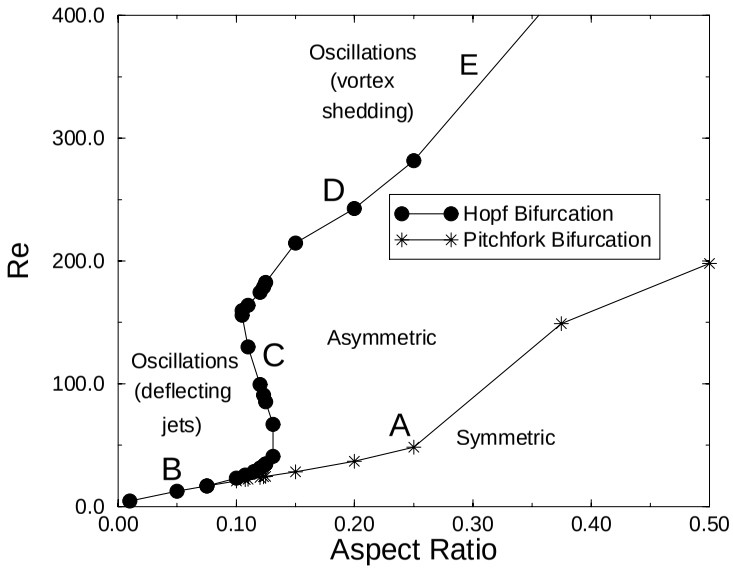
- Cayley Transformation v.1: $(\boldsymbol{J} - \sigma \boldsymbol{M})^{-1}(\boldsymbol{J} - \mu \boldsymbol{M})z = \theta z$ with $\sigma < \mu$
- Cayley Transformation v.2: same with $\mu < \sigma$
- Complex Shift-and-Invert: $(\boldsymbol{J} - (a + b\mathbf{i})\boldsymbol{M})^{-1}\boldsymbol{M}x = \dfrac{1}{\lambda - (a + b\mathbf{i})}x$

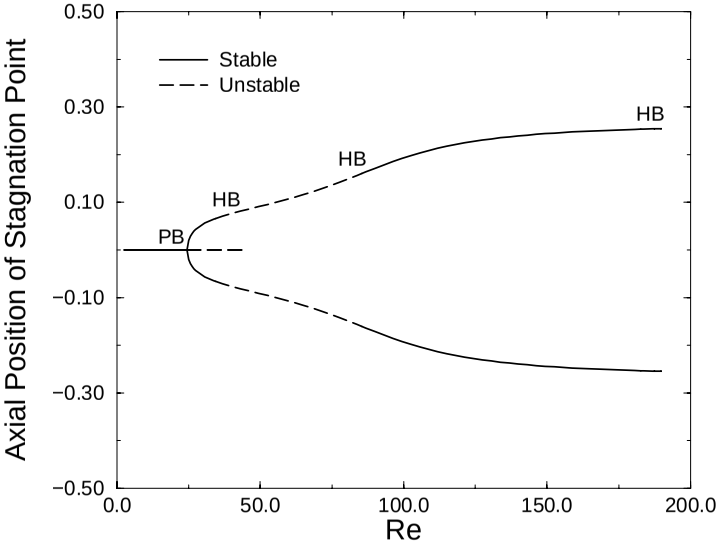
These <u>Ordinary Eigenvalue Problems</u> require 10-50 Arnoldi iterations using ARPACK (each requiring one linear solve).

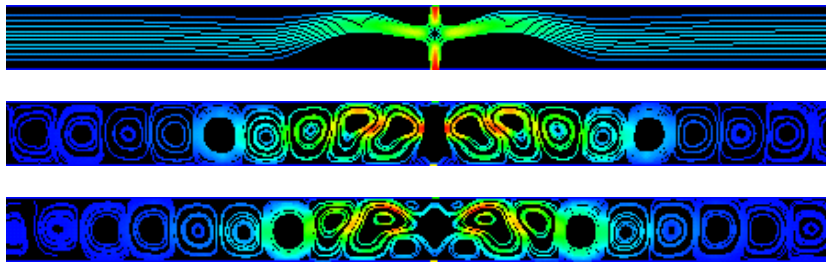
Stability and Bifurcation in Counterflow Jet Reactors

(see Pawlowski *et al.*, CFD Poster Session 74ak, 4:30 today)

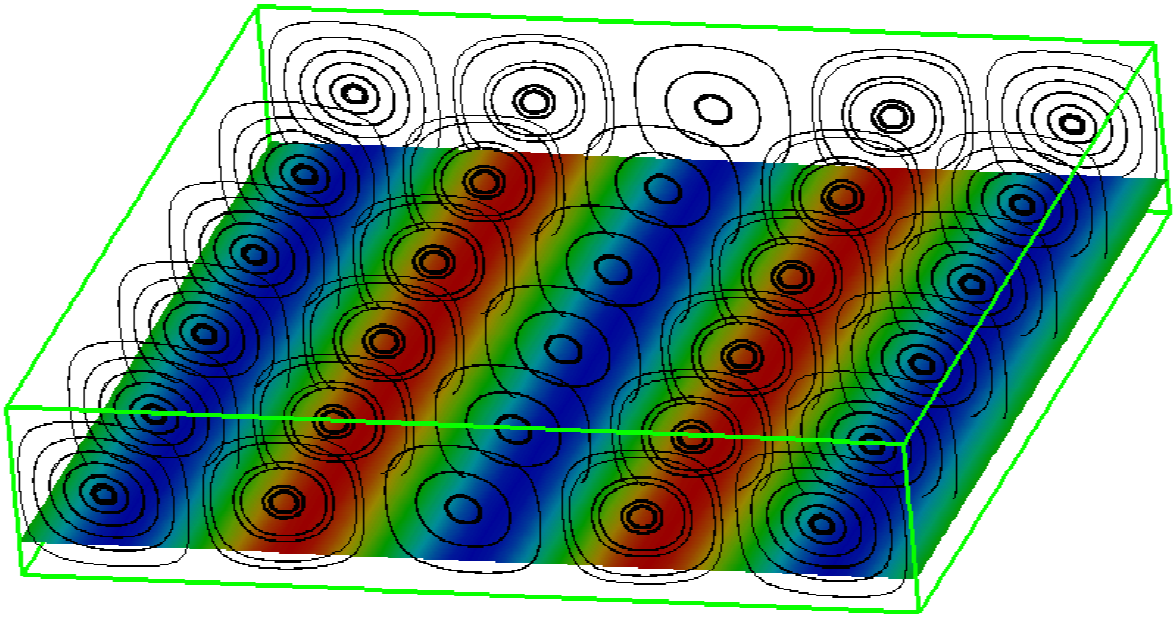


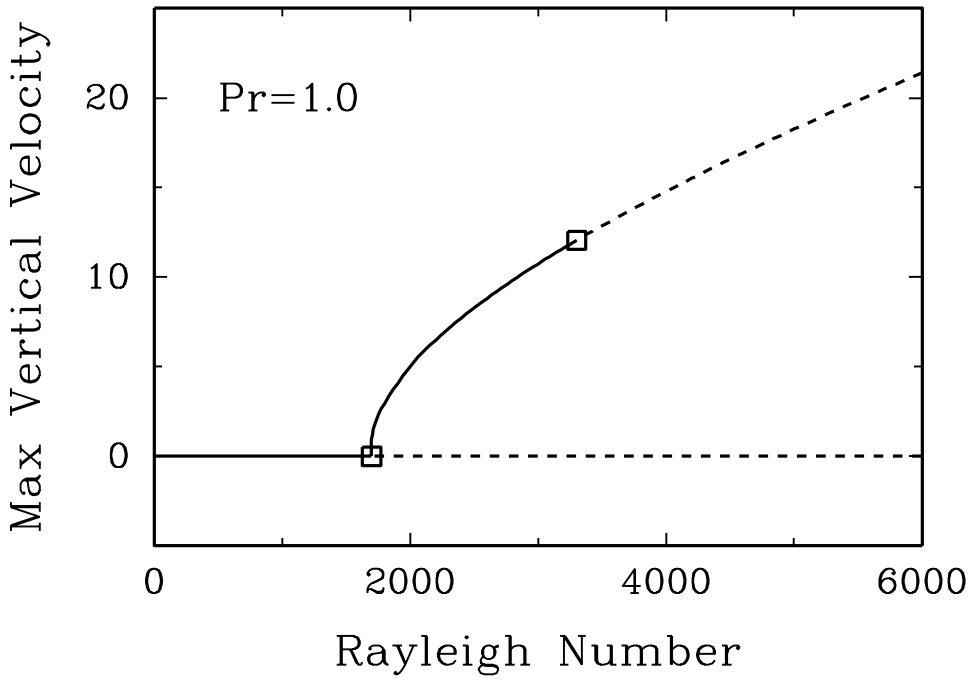






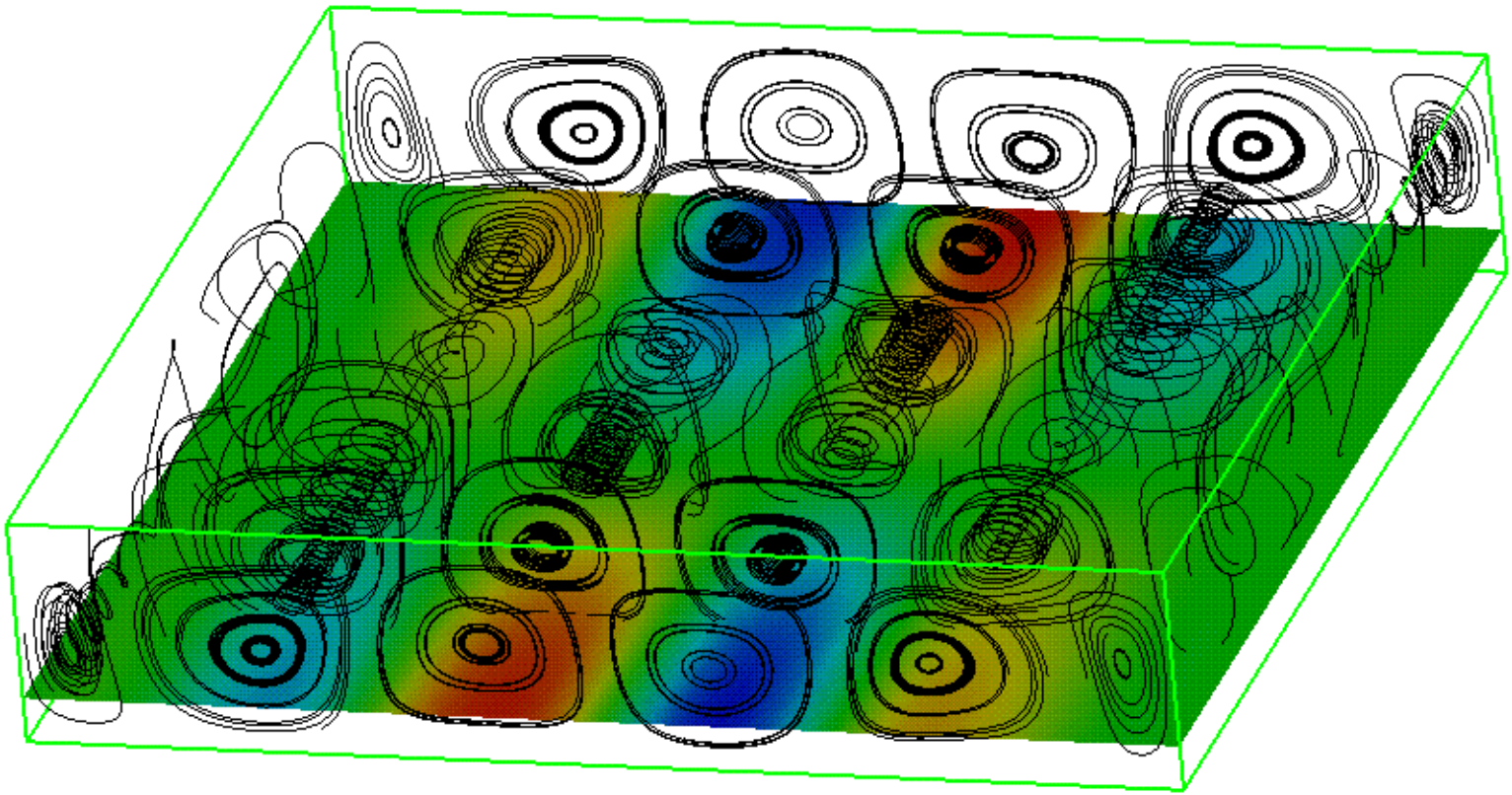
Rayleigh Benard Rolls in a 5x5x1 Box: Eigenvalue calcs find second pitchfork





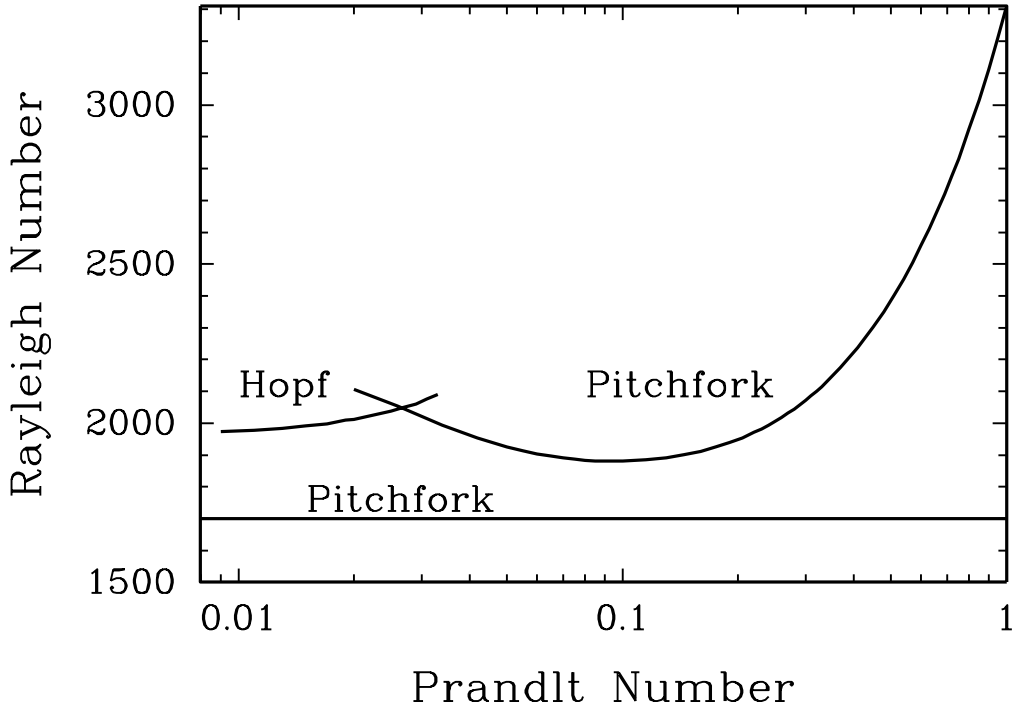
Pitchfork bifurcation algorithm locates bifurcation and Null vector with Newton convergence

Bifurcation at Ra=3304.5 <u>for this mesh</u>



Bifurcation determined to be subcritical.

Bifurcation is directly tracked as a function of a second parameter: Hopf at small Prandlt



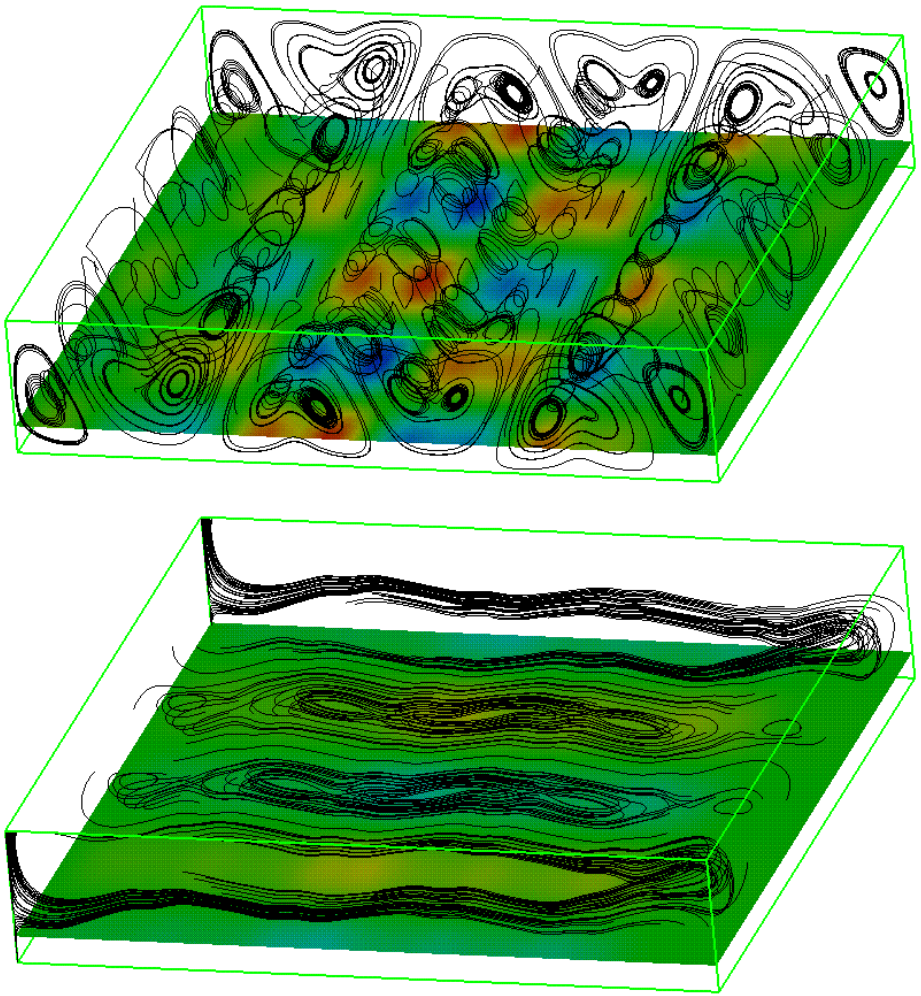
Codimension 2 bifurcation located near (Ra=2050, Pr=0.27)

Real and Imaginary components of Eigenvector at Hopf bifurcation show us that...

Pr=0.015

Ra=1990

ω = 1.24

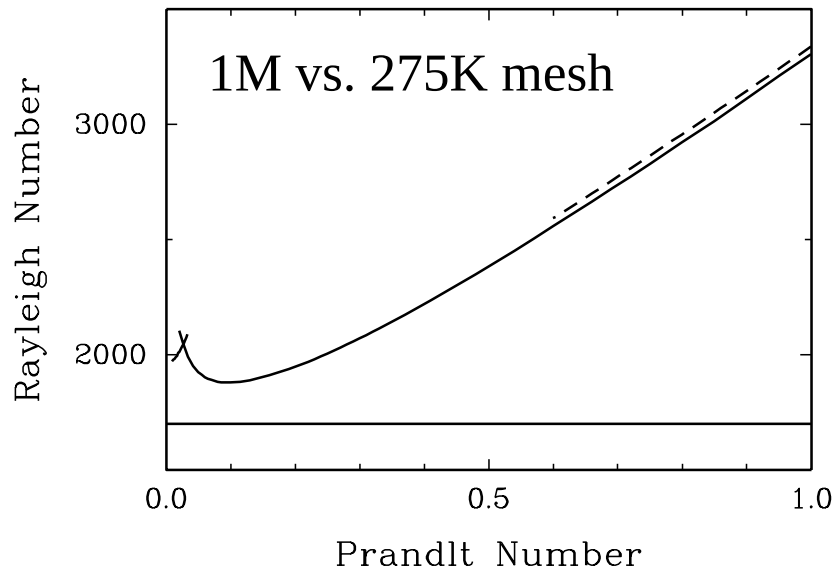


Details of Calculations

50x50x20 element mesh --> 275000 unknowns;

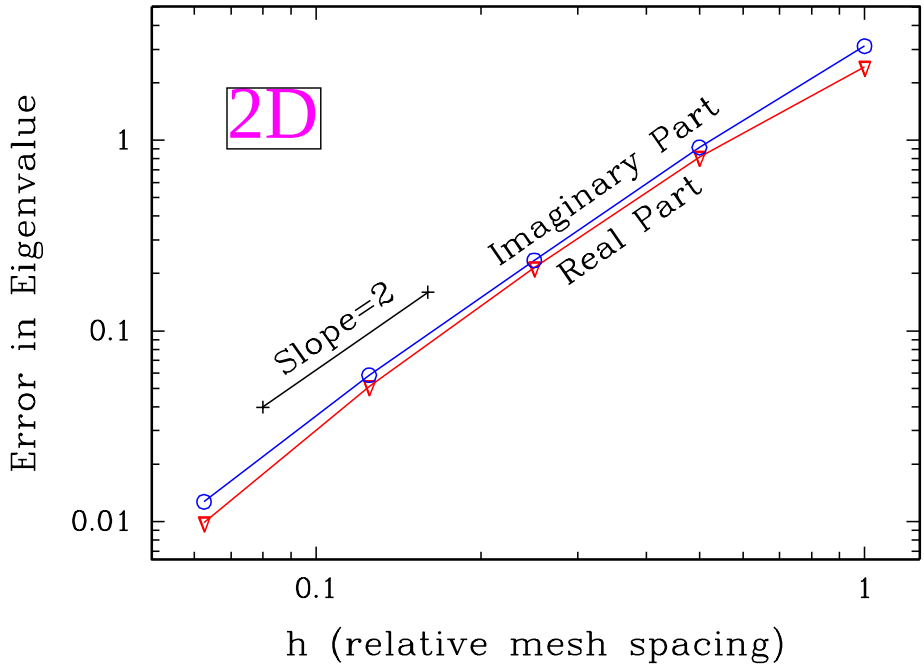
Solved on 128 processors (333MHz PII, ASCI Red)

Steady State Solve	5 Minutes
Eigenvalue Calculation	6-20 Minutes
Pitchfork Bifurcation	25 Minutes
Hopf Bifurcation (p=200)	80 Minutes



Mesh Resolution of Eigenvalue Calculations Up to 4 Million Unknowns. 2D Calc Shows $O(h^2)$ Convergence

# Unknowns	1st Eigen Pair	2nd Eigen Pair	3rd Eigen Pair
0.25 Million	$-0.08 \pm 25.33i$	$-0.49 \pm 9.63i$	$-1.44 \pm 5.96i$
0.5 Million	$0.35 \pm 25.16i$	$-0.05 \pm 9.50i$	$-1.13 \pm 5.91i$
1 Million	$0.57 \pm 25.06i$	$0.21 \pm 9.36i$	$-0.98 \pm 6.01i$
2 Million	$0.73 \pm 25.02i$	$0.39 \pm 9.31i$	$-0.85 \pm 6.03i$
4 Million	$0.84 \pm 24.94i$	$0.50 \pm 9.22i$	$-0.78 \pm 6.08i$
2 Million 2D-Axisym	$1.06 \pm 24.86i$		



Bifurcation and Linear Stability Analysis Tools Can Enable Sophisticated Computational Design

Scalable stability analysis algorithms are being developed, and have been interfaced with a parallel, unstructured grid incompressible reacting flow code.

- Eigenvalue Calculations (16 Million Unknowns)
- Continuation Algorithms (16 Million Unknowns)
- Turning Point Bifurcations (1 Million Unknowns)
- Pitchfork Bifurcations (1.0 Million Unknowns)
- Hopf Bifurcations (710K Unknowns)

Easy implementation leads to solves of singular matrices.

Locus of bifurcations tracked in 3D model flow problem.

Robust preconditioned iterative linear solvers are the key.