Understanding the 8 : 1 cavity problem via scalable stability analysis algorithms

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Abstract

Stability analysis algorithms coupled with a robust steady state solver are used to understand the behavior of the 2D model problem of thermal convection in a 8 : 1 differentially heated cavity. The system is discretized using a Galerkin/Least Squares Finite Element formulation, and solved to steady state on parallel computers using a fully coupled Newton method and iterative linear solvers. An eigenvalue capability is used to probe the stability of the solutions, and the neutral stability curves are tracked directly using a Hopf tracking algorithm.

Keywords: Bifurcations; Convection; Eigenvalues; Parallel computers; Finite element; CFD; Incompressible flow

1. Introduction

This manuscript presents a preliminary computational analysis of a model problem of confined thermal convection flow in an 8 : 1 enclosure. The computational method employs a robust steady state solver for the nonlinear systems, continuation methods for tracking solutions, and linear stability analysis capabilities. The fluid flow equations are discretized using the MPSalsa unstructured grid finite element code, which has been developed for robust steady state solves on distributed memory parallel computers [1–4]. A linear stability analysis capability has been added to MPSalsa by interfacing with the ARPACK eigensolver. The critical value of the Rayleigh *Ra* number is located (for a given mesh) by incrementing the parameter value, calculating a steady state solution, calculating a handful of rightmost eigenvalues, and finding where the rightmost eigenvalues have positive real parts. In this problem, the first modes to cross the imaginary axis with increasing *Ra* are a imaginary conjugate pair indicating a Hopf bifurcation. An algorithm for directly calculating Hopf bifurcations, which has recently been developed and interfaced with the MPSalsa code, is then used to converge directly to the bifurcation point. Continuation of the Hopf point with respect to a second parameter traces neutral stability curves and provides insight into the structures of solution branches and the behavior of the system.

2. Numerical methods overview

2.1. Galerkin/Least-Squares Finite Element formulation

The MPSalsa code developed at Sandia National Labs uses an unstructured grid finite element formulation. The governing transport PDEs describing fluid flow and thermal energy transfer are presented in Table 1 in residual form. The continuous problem, defined by the transport equations, is approximated by a Galerkin Least Squares formulation [5–7]. This formulation allows for equal order interpolation of pressure and velocity (without spurious pressure solutions), for stabilization of highly convected flows and for a discontinuity capturing operator that smooths oscillation in the vicinity of large gradients. The resulting GLS equations are shown in Table 2.

The equations are solved to state using a fully coupled inexact Newton method [8,9] and robust parallel iterative linear solvers. A distributed memory parallel implementation and domain decomposition preconditioners enable solutions of problems of order one million unknowns [10].

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Table 1
Governing transport PDEs

Momentum	$\mathbf{R}_{\mathbf{m}} = \rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla \mathbf{u}) - \nabla \cdot \mathbf{T} - \rho \mathbf{g}$
Total mass	$\mathrm{R}_{\mathrm{P}} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u})$
Thermal energy	$\mathrm{R}_T = \rho \hat{C}_p \left[\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right] + \nabla \cdot \mathbf{q}_c - \phi - \dot{Q} + \sum_{k=1}^{N_s} \mathbf{j}_k \cdot \hat{C}_{p,k} \nabla T - \sum_{k=1}^{N_s} h_k W_k \dot{\omega}_k + \nabla \cdot \mathbf{q}_{\mathrm{r}}$

Table 2
GLS formulation of transport PDEs

Momentum	$\mathcal{F}_{\mathrm{m},i} = \int\limits_{\Omega} \Phi \mathrm{R}_{\mathrm{m},i}\, \mathrm{d}\Omega + \int\limits_{\Omega_e} \rho \tau_m (\mathbf{u} \cdot \nabla \Phi) \mathrm{R}_{\mathrm{m},i}\, \mathrm{d}\Omega + \int\limits_{\Omega_e} \rho \tau_c [\nabla \Phi]_i \mathrm{R}_{\mathrm{P}}\, \mathrm{d}\Omega + \int\limits_{\Omega_e} \nu_{m,i} \nabla \Phi \cdot \mathbf{G}^c \nabla u_i\, \mathrm{d}\Omega$
Total mass	$\mathcal{F}_{\mathrm{P}} = \int\limits_{\Omega} \Phi \mathrm{R}_{\mathrm{P}}\, \mathrm{d}\Omega + \int\limits_{\Omega_e} (\rho \tau_m \nabla \Phi \cdot \mathbf{R}_{\mathbf{m}})\, \mathrm{d}\Omega$
Thermal energy	$\mathcal{F}_T = \int\limits_{\Omega} \Phi \mathrm{R}_T\, \mathrm{d}\Omega + \int\limits_{\Omega_e} \rho \hat{C}_p \tau_T (\mathbf{u} \cdot \nabla \Phi) \mathrm{R}_T\, \mathrm{d}\Omega + \int\limits_{\Omega_e} \nu_T \nabla \Phi \cdot \mathbf{G}_c \nabla T\, \mathrm{d}\Omega$

2.2. Linear stability analysis algorithms

Having a fully assembled Jacobian matrix and robust linear solvers enables the use of stability analysis tools. Details relating to the methods and parallel implementation of the linear stability analysis algorithms can be found in [11–13]. The analysis begins at a given steady state solution point. A normal mode linear stability analysis produces a linearization of the evolution equations around this steady state solution and produces a generalized eigenvalue problem of the form

$$\mathbf{J}z = \lambda \mathbf{M}z, \tag{1}$$

where **J** is the Jacobian matrix, **M** is the mass matrix (i.e. coefficient matrix of time derivative terms), z is an eigenvector (generally complex), and λ its associated eigenvalue (also complex). A Cayley transformation, which includes two adjustable real parameters, σ and μ, is used to reformulate the generalized eigenvalue problem into an ordinary eigenvalue problem for the transformed eigenvalues γ:

$$(\mathbf{J} - \sigma \mathbf{M})^{-1}(\mathbf{J} - \mu \mathbf{M})z = \gamma z. \tag{2}$$

A simple relationship exists between the transformed and original eigenvalues, $\gamma = (\lambda - \mu)/(\lambda - \sigma)$. Appropriate choices of σ and μ are made so that the eigenvalues of interest (those λ with largest real part) are mapped to large γ.

The eigenvalue problem defined in Eq. (2) is solved using Arnoldi's method with a version of the P_ARPACK software [14,15] modified to perform the Cayley transformation.

2.3. Bifurcation analysis algorithm

An Newton algorithm for directly locating and tracking a Hopf bifurcation has been implemented as part of the LOCA library at Sandia National Labs. A thorough treatment of bifurcation tracking algorithms has recently been published [16]. At a Hopf bifurcation, one complex conjugate pair of eigenvalues of Eq. (1) is pure imaginary (i.e. $\lambda = \pm \omega \iota$), and we use this fact to directly calculate the bifurcation. In real arithmetic, this leads to a system of system of $3N_x + 2$ unknowns (x, y, z, ω and p). Here N_x is the length of x (and the order of **J**), while y and z are vectors (of length N_x) containing the real and imaginary parts of the eigenvector. The $3N_x + 2$ equations specifying the Hopf bifurcation are then,

$$\begin{aligned} &R = 0 \\ &\mathbf{J}y + \omega \mathbf{M}z = 0 \\ &\mathbf{J}z - \omega \mathbf{M}y = 0\ . \\ &l^t y = 1 \\ &l^t z = 0 \end{aligned} \tag{3}$$

The first vector equation requires a steady state solution (where $R(x, p)$ is the vector of residuals), the next two vector equations specify that a purely imaginary eigenvalue exists, and the last two scalar equations are used to set the length and phase of the eigenvector $y + \iota z$.

These equations are solved using a Newton method. A block elimination (or bordering) algorithm is used at each Newton step, this requires two linear solves of the matrix **J** and three solves of the matrix $\begin{bmatrix} \mathbf{J} & \omega \mathbf{M} \\ -\omega \mathbf{M} & \mathbf{J} \end{bmatrix}$. This matrix is solved using a novel implementation for solving complex matrices with an existing real-valued linear solver [17]. The numerical difficulty in solving for the Hopf bifurcation is in using an iterative solver, which is singular at the Hopf point. However, our initial experiences indicate that the iterative solvers work well unless more than four digits of accuracy is requested.

3. Application of scalable stability analysis

Preliminary results are shown for studying bifurcations in the thermal cavity problem. A highly graded mesh of 80 × 180 bilinear finite elements was used for these calculations. The problem of 58 644 unknowns was solved in parallel on 24 333 Mhz Pentium processors of the Sandia-Intel Tflop machine (ASCI Red). A typical matrix fill requires 0.35 s and an iterative matrix solve (using a domain decomposition preconditioner with overlap and a GMRES solver) about 15 s, and 3–6 Newton iterations (1–2 min) were sufficient to converge to a steady state using a guess from a nearby parameter value. Fig. 1 shows the evolution of the three rightmost eigenvalues as a function of the Rayleigh number. Two Hopf bifurcations are detected, the first is a symmetric mode near $Ra = 3.61 \times 10^5$ and a second skew symmetric mode near $Ra = 3.86 \times 10^5$. Because of the large imaginary parts, an Arnoldi space of 180 was needed to converge the first several eigenvalues using Cayley parameters of $\sigma = 2000$ and $\mu = 5000$. An eigensolve required about 30 min. While we believe the nonlinear solver and the eigensolver are converged to 3 or more digits, the calculation is not converged with mesh spacing. Mesh resolution studies will soon be undertaken to investigate the apparent discrepancy between our bifurcation point at $Ra = 3.61 \times 10^5$ and the value of $Ra = 3.1 \times 10^5$ found in previous work.

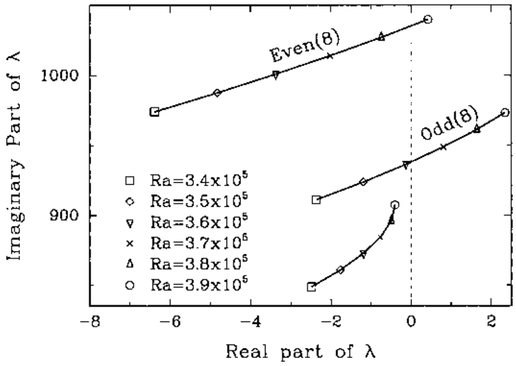

Fig. 1. A plot showing the movement of the three leading eigenvalues as a function of the Rayleigh number shows two Hopf bifurcations, the first occurring near $Ra = 3.61 \times 10^5$. The mesh of 58 644 unknowns requires 1–2 min for a steady state solve and about 30 min for an eigenvalue calculation on 24 processors of the Sandia-Intel Tflop (ASCI Red) machine. The curve labeled Odd has symmetric (odd) eigenfunctions, and the curve labeled Even has skew symmetric eigenfunctions.

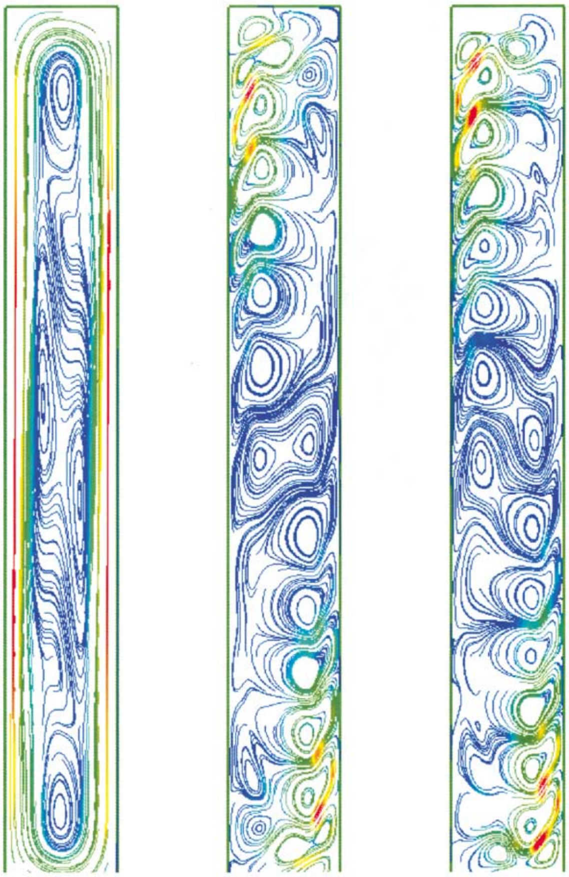

Fig. 2. Three streamline plots are shown: the first is the solution at the first Hopf bifurcation at $Ra = 3.61 \times 10^5$, the second is the symmetric eigenfunction at that point, and the third is the skew symmetric eigenfunction at the second Hopf bifurcation at $Ra = 3.86 \times 10^5$.

Three streamline plots are shown in Fig. 2: the solution at the bifurcation point, the symmetric instability at this point, and the skew symmetric instability at the second Hopf bifurcation.

The Hopf bifurcation tracking algorithm was run using results from the eigenvalue calculation as initial guesses, the results of which are shown in Fig. 3. To calculate a Hopf bifurcation after taking a step in *Ra* from another converged solution required about 30 min. Once started, the curves were traced automatically. The two bifurcations seen in Fig. 1 were initially tracked, and it was found that the symmetric bifurcation (labeled Odd(8)) always occurs at lower parameter values than the skew symmetric (Even(8)). Eigenvalue calculations at aspect ratios of 7.0 and 9.0 revealed that other modes had overtaken these modes.

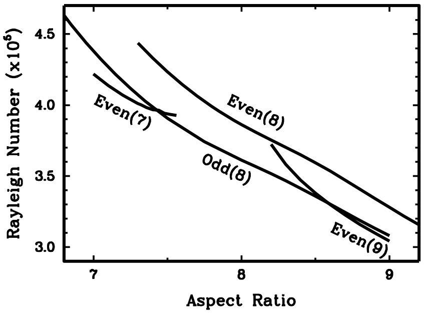

Fig. 3. Neutral stability curves showing the locus of Hopf bifurcations for a range of aspect ratios, calculated directly using the Hopf tracking algorithm. The destabilizing mode at an aspect ratio of 8 is no longer the destabilizing mode at aspect ratios below 7.4 or above 9.6.

Tracking the locus of neutral stability points of these two symmetric modes (labeled Even(7) and (Even(9)) show how the destabilizing mode transitions from the Even(7) to the Odd(8) to the Even(9) mode. The two transition points (near aspect ratios of 7.4 and 8.6) are points where two Hopf bifurcations occur simultaneously. Chaotic behavior exists in the neighborhood of such a point.

4. Conclusions

Stability analysis algorithms have been used to locate the Hopf bifurcations where 2D Boussinesq flow in a thermal cavity goes unstable. Steady state solutions are solved for directly using a fully-coupled Newton method on a parallel computer. An eigenvalue capability is used to initially locate the bifurcations, and a Hopf tracking algorithm is used to track out the neutral stability curves as a function of the aspect ratio. Two double Hopf bifurcations are found to exist nearby in parameter space. Future work will include mesh resolution studies, and may include periodic orbit tracking or 3D calculations.

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