Newton-Krylov based continuation method to study convection in a tilted parallelepiped cavity.

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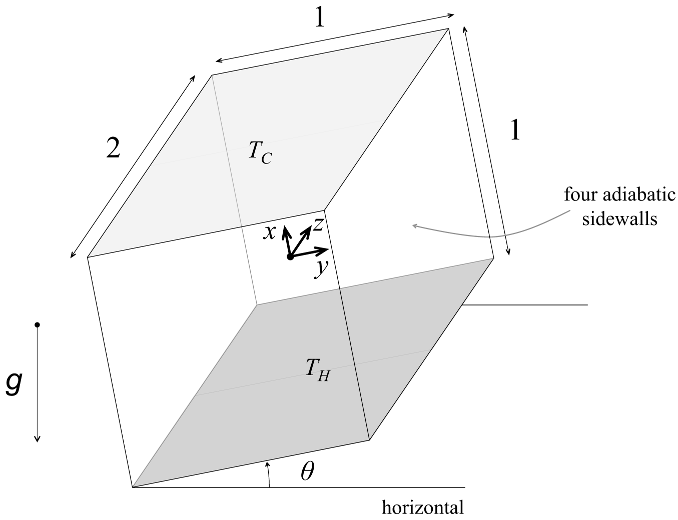
Context

- Studies about convection and its stability:
  - Flow patterns: bifurcation diagram
  - Different influences: magnetic field, acoustic streaming, tilt...
  - Fundamental fluid mechanics and applications (crystal growth,...)
- Development of well-adapted methods:
  - Spectral finite-element method
  - Steady state solver
  - Continuation methods

Geometry of the heated cavity (square cross-section)



Equations

$$\nabla \cdot \mathbf{u} = 0,$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})\mathbf{u} = -\boldsymbol{\nabla} p + Pr\, \boldsymbol{\nabla}^2 \mathbf{u} + Pr\, Ra\, T(\cos(\theta)\, \mathbf{e}_x + \sin(\theta)\, \mathbf{e}_y),$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \boldsymbol{\nabla})T = \boldsymbol{\nabla}^2 T,$$

with boundary conditions given by:

- $T = 1/2$ on $x = -1/2$ and $T = -1/2$ on $x = 1/2$,
- $\partial T/\partial z = 0$ on $z = -A_z/2,\ A_z/2$
- $\partial T/\partial y = 0$ on $y = -A_y/2,\ A_y/2$,
- $\mathbf{u} = 0$ on all the boundaries.

Rayleigh number, $Ra = \dfrac{\beta(T_H^* - T_C^*)gh^3}{\kappa\nu}$

Prandtl number, $Pr = \dfrac{\nu}{\kappa}$

Numerical methods

- Spatial discretization: spectral finite element

  -Spatial discretization obtained through Gauss-Lobatto-Legendre points distributions in each element.

  -In our simple geometry, a single element is used.

- Temporal discretization: splitting method

  -The time discretization is carried out using a semi-implicit splitting scheme (Karniadakis *et al.* (1991))

  -The non-linear terms are first integrated explicitly

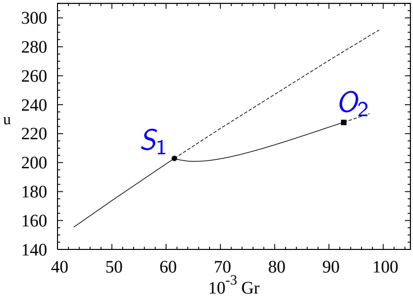
  -The pressure is then solved through a pressure equation enforcing the incompressibility constraint

  -The linear terms are finally integrated implicitly.

At first order: $$\frac{\mathbf{X}^{(n+1)} - \mathbf{X}^{(n)}}{\Delta t} = \mathcal{N}(\mathbf{X}^{(n)}, Ra) + \mathcal{L}\mathbf{X}^{(n+1)}.$$

Numerical methods

- Continuation method: to calculate bifurcation diagrams



Bifurcation diagram

- Steady state calculation
- Solution stability: Arnoldi method or an eigenvalue is followed
- Direct calculation of bifurcation points
- Branching

Steady state solver (Mamun and Tuckerman (1995))

Time iteration: $$\frac{\mathbf{X}^{(n+1)} - \mathbf{X}^{(n)}}{\Delta t} = \mathcal{N}(\mathbf{X}^{(n)}, Ra) + \mathcal{L}\mathbf{X}^{(n+1)}.$$

Slightly modified: $$\frac{0 - 0}{\Delta t} = \mathcal{N}(\mathbf{X}^{(n)}, Ra) + \mathcal{L}\mathbf{X}^{(n+1)}.$$

Derived expressions: $$\mathbf{X}^{(n+1)} = -\mathcal{L}^{-1}\left[\mathcal{N}(\mathbf{X}^{(n)}, Ra)\right].$$

$$\mathbf{X}^{(n+1)} - \mathbf{X}^{(n)} = -\mathcal{L}^{-1}\left[\mathcal{N}(\mathbf{X}^{(n)}, Ra) + \mathcal{L}\mathbf{X}^{(n)}\right].$$

Linearized expressions: $$\delta\mathbf{X}^{(n+1)} - \delta\mathbf{X}^{(n)} = -\mathcal{L}^{-1}\left[\mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L}\right]\delta\mathbf{X}^{(n)}.$$

$$\delta\mathbf{X}^{(n+1)} = -\mathcal{L}^{-1}\left[\mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra)\right]\delta\mathbf{X}^{(n)}.$$

Steady-state problem: $\mathcal{N}(\mathbf{X}, Ra) + \mathcal{L}\mathbf{X} = 0,$

solved with a Newton method, using $-\mathcal{L}^{-1}$ as a preconditioner:

$$\begin{aligned} -\mathcal{L}^{-1}\left[\mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L}\right]\delta\mathbf{X} &= -(-\mathcal{L}^{-1})\left[\mathcal{N}(\mathbf{X}, Ra) + \mathcal{L}\mathbf{X}\right] \\ \mathbf{X} &\leftarrow \mathbf{X} + \delta\mathbf{X}. \end{aligned}$$

Following eigenvalues

- Arnoldi calculation:
  -by time stepping the linearized problem equation
  -10 leading eigenvalues are calculated
  -the process is costly
- An eigenvalue is followed:

For a known steady solution $\mathbf{X}$, calculation of an eigenvalue λ associated with a given eigenvector $\mathbf{h}$:

$$\begin{aligned} \left[\mathcal{N}_{\mathbf{X}}\left(\mathbf{X}, Ra\right) + \mathcal{L}\right]\mathbf{h} - \lambda\mathbf{h} &= 0, \\ \mathbf{h}_l - q &= 0. \end{aligned}$$

One Newton step is:

$$\begin{bmatrix} \mathcal{N}_{\mathbf{X}}\left(\mathbf{X}, Ra\right) + \mathcal{L} - \lambda & -\mathbf{h} \\ e_l^T & 0 \end{bmatrix} \begin{bmatrix} \delta\mathbf{h} \\ \delta\lambda \end{bmatrix} = - \begin{bmatrix} \left[\mathcal{N}_{\mathbf{X}}\left(\mathbf{X}, Ra\right) + \mathcal{L}\right]\mathbf{h} - \lambda\mathbf{h} \\ 0 \end{bmatrix}$$

$$\begin{aligned} \mathbf{h} &\leftarrow \mathbf{h} + \delta\mathbf{h}, \\ \lambda &\leftarrow \lambda + \delta\lambda. \end{aligned}$$

Direct calculation of bifurcation points (Bergeon *et al.* (1998))

At such a point, $\mathbf{X}$ is a solution and the Jacobian is singular, with a null eigenvector $\mathbf{h}$:

$$\begin{aligned} \mathcal{N}(\mathbf{X}, Ra) + \mathcal{L}\mathbf{X} &= 0, \\ [\mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L}]\,\mathbf{h} &= 0, \\ \mathbf{h}_l - q &= 0. \end{aligned}$$

One Newton step is:

$$\begin{bmatrix} \mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L} & 0 & \mathcal{N}_{Ra}(\mathbf{X}, Ra) \\ \mathcal{N}_{\mathbf{X},\mathbf{X}}(\mathbf{X}, Ra)\,\mathbf{h} & \mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L} & \mathcal{N}_{\mathbf{X},Ra}(\mathbf{X}, Ra)\,\mathbf{h} \\ 0 & e_l^T & 0 \end{bmatrix} \begin{bmatrix} \delta\mathbf{X} \\ \delta\mathbf{h} \\ \delta Ra \end{bmatrix} = - \begin{bmatrix} \mathcal{N}(\mathbf{X}, Ra) + \mathcal{L}\mathbf{X} \\ [\mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L}]\,\mathbf{h} \\ 0 \end{bmatrix},$$

$$\begin{aligned} \mathbf{X} &\leftarrow \mathbf{X} + \delta\mathbf{X}, \\ \mathbf{h} &\leftarrow \mathbf{h} + \delta\mathbf{h}, \\ Ra &\leftarrow Ra + \delta Ra. \end{aligned}$$

At a primary bifurcation, $\mathbf{X}$ is the known conductive solution:

$$\begin{bmatrix} \mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L} & \mathcal{N}_{\mathbf{X},Ra}(\mathbf{X}, Ra)\,\mathbf{h} \\ e_l^T & 0 \end{bmatrix} \begin{bmatrix} \delta\mathbf{h} \\ \delta Ra \end{bmatrix} = - \begin{bmatrix} [\mathcal{N}_{\mathbf{X}}(\mathbf{X}, Ra) + \mathcal{L}]\,\mathbf{h} \\ 0 \end{bmatrix},$$

$$\begin{aligned} \mathbf{h} &\leftarrow \mathbf{h} + \delta\mathbf{h}, \\ Ra &\leftarrow Ra + \delta Ra. \end{aligned}$$

Linear solver at each Newton step

-We use the iterative GMRES solver, which was found more robust than the BCGS solvers.

-The Jacobian matrices are not calculated, but we know how to provide the matrix-vector products to GMRES.

-Different time iterations of the linearized problem are needed for that.

At each Newton step:
-One or two normal or linearized iterations to calculate the right-hand side term.
-One to five linearized iterations for the matrix-vector products at each step of GMRES.

Linear systems solved by GMRES with a precision of 10^{-2}
Newton systems solved with a precision of 10^{-6}
(L^2 norm of the right-hand-side of the Newton system).

Simulations of the tilted cavity

-Grid: $27 \times 27 \times 41$, i.e. 29 989 mesh points

-Four variables: three velocities, temperature, i.e.

- -119 556 unknowns for steady state solving, steady eigenvalue calculation and primary bifurcation points
- -239 112 unknowns for secondary bifurcation points and oscillatory eigenvalue calculation
- -358 668 unknowns for Hopf bifurcation points

-Middle-size problem run on

- -Vectorial computer NEC SX8 at IDRIS
- -Sequential computer SGI Altix UV 1000 at Ecole Centrale

Results: horizontal cavity

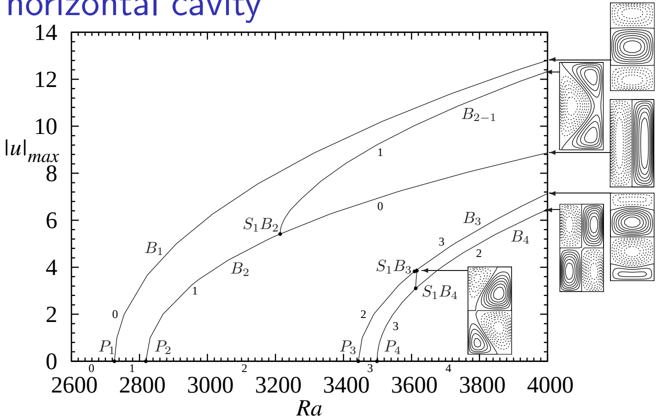
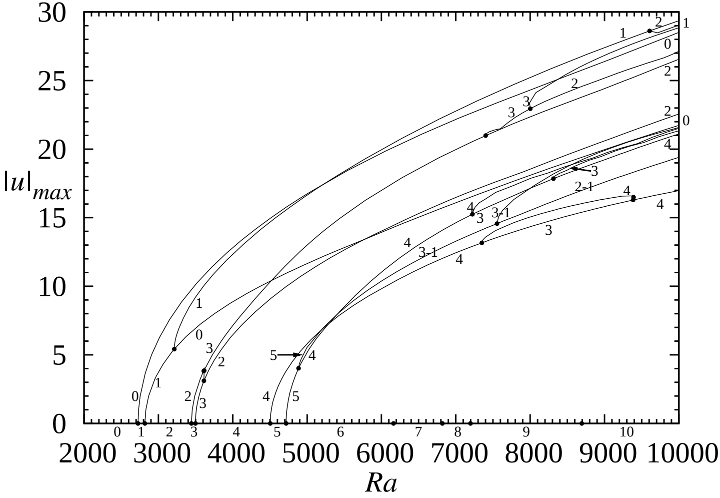
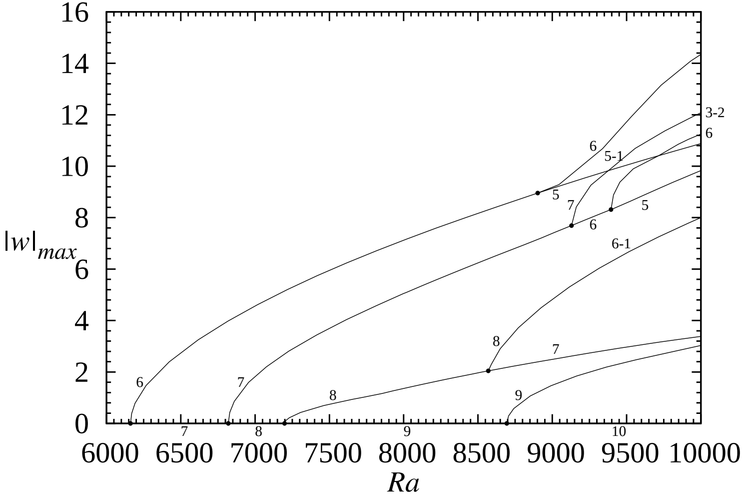


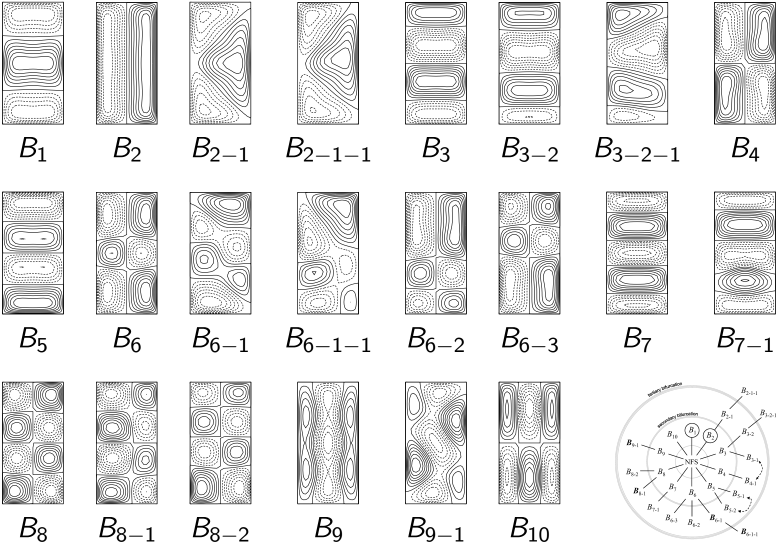
Diagram	Steady state		Stability		Bifurcation point	
Nec SX8 Single run $\approx 1700s$	Trivial 11 0.2 s	Conv. 75 2-10 s	Arnoldi 24 40-60 s	Eigenv. 74 2-5 s	Prim. 4 2-6 s	Sec. 4 10-20 s
Time/Newt. GMRES Unknowns		5.7 s/4 58,72,94,95 $\sim$ 120 000		4.8 s/4 28,44,70,74 $\sim$ 120 000	4.7 s/4 57,58,76,75 $\sim$ 120 000	12.8 s/5 42,38,59,52,68 $\sim$ 240 000



Bifurcation diagram: solution branches obtained in the range $2000 \leq Ra \leq 10000$ and initiated from the first six primary bifurcations.

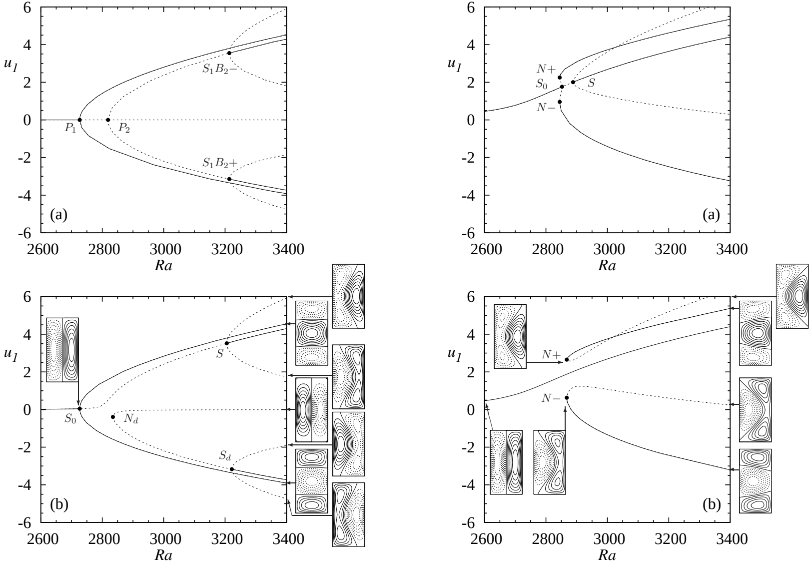


Bifurcation diagram: solution branches obtained in the range $6000 \leq Ra \leq 10000$ and initiated from the four primary bifurcations in this range (P_7 to P_{10}).



Solutions at $Ra = 10000$ on the different branches issued from the ten first primary bifurcation points. Note the different symmetries.

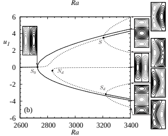
Results: inclined cavity

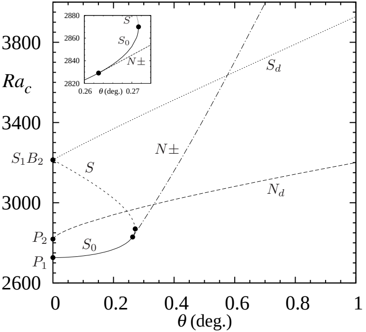


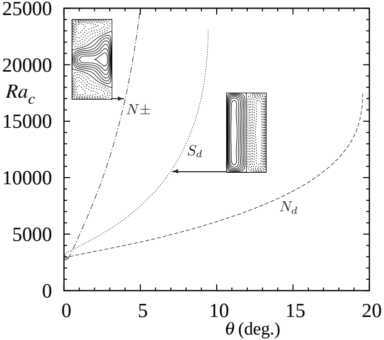
Bifurcation diagrams for inclined cavities:

$\theta = 0^\circ$ (a) and 0.01°(b) (left), $\theta = 0.27^\circ$ (a) and 0.28°(b) (right).

Path of the main bifurcation points





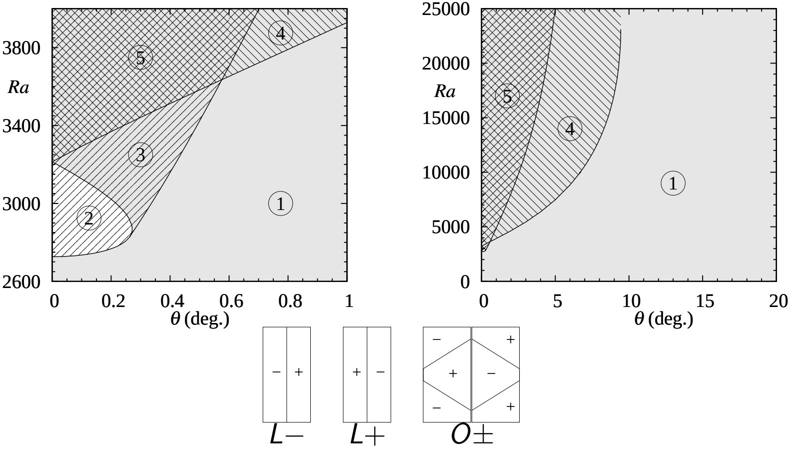


$N\pm$ appear at $\theta = 0.263°$; the collision between S_0 and S at $\theta = 0.2714°$.

Limiting values of θ for $N\pm$, S_d and N_d: $\theta = 9.235°$, $9.445°$and $19.56°$.

SGI Altix UV 1000	S_d bif. point ($\theta = 2° \rightarrow 9°$: step 1°)	
∼ 240 000 Unknowns	Min.	Max.
Time/Newt.	31.4 s/5	83.8 s/7
GMRES	42,44,56,49,55	59,47,87,76,82,106,124

Domains of existence of the stable solutions



Leading longitudinal roll $L-$ solution (grey background),
opposite longitudinal roll $L+$ solution (up-left directed oblique lines),
two oblique roll $O\pm$ solutions (up-right directed oblique lines).

Types of solutions: one in zones 1 and 2, two in 3 and 4, three in 5.

Conclusion

- Very efficient method for bifurcation analysis in middle-size problems
  - Continuation method
  - Steady state solving
  - Calculation of eigenvalues
  - Calculation of bifurcation points
  - Branching
- Interesting results obtained for a tilted cavity
  - Influence of the tilt on the bifurcation diagram
  - Existence range of the different stable solutions
- Tests to be done for the extension to larger-size problems
  - Use of parallel computing
  - Main problem: cost of Arnoldi calculations

Thank you for your attention