From steady solutions to chaotic flows in a Rayleigh-Bénard problem at moderate Rayleigh numbers

## Carles Simó

Dept. Matemàtica Aplicada i Anàlisi, UB, Barcelona, Catalunya carles@maia.ub.es

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Goal: to study the dynamics of a Rayleigh-Bénard convection problem. To understand different dynamical mechanisms.
This is the dynamics in a bounded domain created by differences of temperature between the walls.
One of the most difficult problems is the case of a cubical cavity due to multiplicities because of the symmetries.
For concreteness the cubical domain is assumed to be heated from below with perfectly conducting sidewalls and uniform temperature at the top and bottom walls.
The main physical parameters are Rayleigh and Prandtl numbers. Our goal is to give strong evidence that chaotic dynamics and chaotic attractors exist at moderate Rayleigh numbers.
A realistic motivation is to have enhanced mixing properties in small domains where a chemical reaction is made possible by the presence of some bacterias. Their presence prevents from large temperature changes.

## The equations

We assume the cube to be of side $L$ and normalised to $\Omega=[-1 / 2,1 / 2] \times$ $[-1 / 2,1 / 2] \times[-1 / 2,1 / 2]$ with top and bottom temperatures $T_{c}$ and $T_{h}, T_{c}<T_{h}, \Delta T=T_{h}-T_{c}$.

## Physical parameters:

$\rho=$ density, $\beta=$ thermal expansion, $\alpha=$ thermal conductivity, $\nu=$ kinematic viscosity, $g=$ gravity acceleration. Then the Rayleigh, $R a$, and Prandtl, Pr, numbers are defined as

$$
R a=\beta(\Delta T) g L^{3} / \alpha \nu, \quad \operatorname{Pr}=\nu / \alpha
$$

The main parameter to change is $R a$ for a fixed $\operatorname{Pr}$. Most of the computations will be done with $\operatorname{Pr}=0.71$ (air at 300 K ).
Later on it will be necessary for our purpose to change the value of $\operatorname{Pr}$. The values $\operatorname{Pr}=0.75\left(\mathrm{CO}_{2}\right.$ at 380 K$)$ and $\operatorname{Pr}=0.80$, (butane at 300 K ), will be used.

For the presentation of some results we shall use the Nüsselt number $N u$, that is, the dimensionless convective heat transfer coefficient at the hot bottom wall. $N u_{a}$ is the averaged value of $N u$ for an amount of time, to be taken equal to the period in the case of p.o.
In most of the plots $N u$ is replaced by the modified value $N u-0.012 R a^{1 / 2}$ for plot clarity.

## Variables:

The velocity $\mathbf{V}=(u, v, w)$, temperature departure from the linear motionless conductive state $\theta$ and the pressure $p$. Then we have

$$
\begin{gathered}
\operatorname{Pr}^{-1}\left(\frac{\partial \mathbf{V}}{\partial t}+R a^{1 / 2}(\mathbf{V} \cdot \nabla) \mathbf{V}\right)-\nabla^{2} \mathbf{V}-R a^{1 / 2} \theta \mathbf{e}_{z}+\nabla p=0 \\
\frac{\partial \theta}{\partial t}+R a^{1 / 2}(\mathbf{V} \cdot \nabla) \theta-\nabla^{2} \theta-R a^{1 / 2} w=0, \quad \nabla \cdot \mathbf{V}=0
\end{gathered}
$$

The boundary conditions are

$$
u=v=w=\theta=0 \text { along }|x|=1 / 2,|y|=1 / 2, \text { and }|z|=1 / 2
$$

The equations are adimensionalised taking suitable units and are written using the vorticity, so that instead of $(\mathbf{V} \cdot \nabla) \mathbf{V}$ appears $\omega=\nabla \times \mathbf{V}$ and instead of $\nabla p$ appears $\nabla \Pi$ where $\Pi=p+|\mathbf{V}|^{2} / 2$.

## Symmetries

$$
\begin{array}{lll}
S_{x}:(x, y, z) \rightarrow(-x, y, z), & (u, v, w, \theta) \rightarrow(-u, v, w, \theta), \\
S_{y}:(x, y, z) \rightarrow(x,-y, z), & (u, v, w, \theta) \rightarrow(u,-v, w, \theta), \\
S_{z}:(x, y, z) \rightarrow(x, y,-z), & (u, v, w, \theta) \rightarrow(u, v,-w,-\theta), \\
S_{d_{+}}:(x, y, z) \rightarrow(y, x, z), & (u, v, w, \theta) \rightarrow(v, u, w, \theta) .
\end{array}
$$

These elements generate the symmetry group $D_{4 h}=\mathbb{Z}_{2} \times D_{4}$ where $\mathbb{Z}_{2}$ is generated by the reflection about the horizontal midplane, $S_{z}$, and $D_{4}$ is the dihedral group generated by $S_{y}$ and $S_{d_{+}}$. These symmetries are responsible for the existence of multiple invariant subspaces in the space of solutions of the equations.
There are solutions invariant under some subgroup of $D_{4 h}$. We denote these subgroups as $G_{i}$. They leave invariant a subspace, denoted as $E_{i}$. In particular we shall make strong use of $G_{7}$, generated by $-S_{z}=-I \cdot S_{z}$, i.e., a rotation by $\pi$ around the $z$-axis, and leaving invariant $E_{7}$. The full space is denoted as $E_{0}\left(G_{0}\right.$ generated by $\left.I\right)$.

## What we want to do, why and how

What: We want to obtain, in a moderate range of $R a$ the skeleton of the dynamics, that is, the different invariant objects, like steady state solutions, periodic orbits, their stability properties and some invariant manifolds.

Why: As said at the Introduction we look for the existence of chaotic dynamics and chaotic attractors for moderate values of $R a$. Another motivation is to realise that techniques used typically in low dimensional dynamical systems can be applied systematically to infinite dimensional ones.
An additional motivation is to stress the importance of following unstable solutions. They can become stable and attract the dynamics or be involved in homoclinic/heteroclinic phenomena leading to chaotic dynamics.

How: We use numerical tools guided by the knowledge on dynamical systems. We give an interpretation of the results concerning the dynamics.

A short comment on the numerical methods
The equations are discretised in space by means of a Galerkin spectral method with a complete divergence-free set of basis functions. The velocity and temperature fields are approximated by

$$
\binom{\mathbf{V}}{\theta}(t, x, y, z)=\sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{4} c_{i j k}^{(l)}(t) \mathbf{F}_{i j k}^{(l)}(x, y, z),
$$

where $c_{i j k}^{(l)}(t)$ are the unknown time-dependent coefficients, and $F_{i j k}^{(l)}(x, y, z)$ are the basis functions.
Typically $\mathbf{n}=\mathbf{1 4}$ has been used. Hence the number of unknown coefficients amounts to $N=14^{3} \times 4=10976$. For checks values like $n=12$ ( $N=6912$ ) or $n=16(N=16384)$ have been used. The symmetry of some solutions reduces the number of unknowns in some cases.
The set of ODE obtained can be represented in matrix form as

$$
B d \mathbf{x} / d t=\left(L_{1}+\lambda L_{2}\right) \mathbf{x}+\lambda Q(\mathbf{x}, \mathbf{x}), \quad \lambda=R a^{1 / 2}
$$

where $\mathbf{x}$ are the coefficients, $B, L_{1}$ and $L_{2}$ are linear operators and $Q$ is a quadratic operator.

A list of tools:

- Computation of steady states (fixed points) and its stability,
- Computation of periodic solutions and its stability. As in the previous case Newton-Krylov methods are used,
- Continuation of solutions via arc-length and variants,
- Detection of bifurcations in both cases,
- Computation of invariant unstable manifolds for the flow or suitable Poincaré maps,
- Detection/computation of homoclinic and heteroclinic connections,
- Computation of the relevant Lyapunov exponents,
- Multiple checks using different values of $n$, different time integration steps, different ways to evaluate the quadratic terms, many random initial conditions and several long time integrations.


## A sample of results

Next we shall show some bifurcation diagrams of steady state and periodic solutions. For other diagrams, the symmetries of the different solutions (if any), numerical values of the ranges of stability and illustrations for other kinds of orbits, see the paper.
Notation: Steady solutions bifurcating from the motionless state are labelled as $B_{i}$. In subsequent bifurcations appear the ones labelled $B_{i j}, B_{i j k}, \ldots$ Similar notation for periodic orbits: $p_{j} B_{i}, p o_{j k} B_{i}$, $p o_{k} B_{i j}$, etc. This allows to follow the genealogy of the different families.
The steady solutions not bifurcating from the motionless state are labelled as $A_{i}$. They appear by fold (SN) bifurcation.
Typically stable (unstable) solutions shown with solid (dashed) lines.
For steady state solutions pitchfork (Hopf) bifurcations are marked with filled (hollow) circles,
For periodic solutions
Filled circles, squares, triangles $\Longrightarrow$ pitchfork, homoclinic and Neimark-Sacker.
Hollow circ., squa., triang. $\Longrightarrow$ Hopf, fold and period doubling.


Bifurcation diagram of the steady solutions $B_{1}, B_{3}, B_{4}, A_{2}, B_{11}, B_{14}$, $B_{312}$ and $B_{143}$ for $\operatorname{Pr}=0.71$.
The branches $B_{1}, B_{3}$ and $B_{4}$ are born at the basic conductive state at $R a=6799,11612$ and 8353 respectively.


Bifurcation diagram of periodic orbits related to the $B_{11}$ solution. Note that the $p o_{1} B_{11}$ and $p o_{2} B_{11}$ branches do not intersect near $N S_{2}$. It is due to the projection. $p o_{1} B_{11}$ joints $H_{2}$ to $H_{4}$ and loses stability at $N S_{2}$.
$p o_{2} B_{11}$ starts unstable at $H_{3}$ and becomes stable at $N S_{3}$. It loses stability at $T_{1}$.


An example with several orbits.
Left: $p o_{2} B_{11}$ at $R a=91801.95$ after $4^{t h}$ turning point, close to the last computed point . We show also $S_{y}$-symmetric solutions: $\mathrm{po}_{1} B_{11}, B_{11}$ and two $S_{y}$-symmetrically related $B_{143}$. They are involved in heteroclinic connections.
Right: Evolution with time of the Nüsselt number.


Sketch of the ranges of stability of all the stable identified solutions. Each solution is stable within the Rayleigh range represented by the segment delimited by two bifurcation symbols. Exchange of stability between solutions is represented by adjacent segments in the sketch. For clarity the scale in the horizontal axis is magnified in the interval [60, 100].
Note that in the full range there is always a stable steady or p.o.

## Chaotic dynamics at $\operatorname{Pr}=0.71$

Chaotic dynamics has been found for $R a<10^{5}$ for $\operatorname{Pr}=0.71,0.75,0.80$.
A problem: the dynamics for $\operatorname{Pr}=0.71$ has been found to be chaotic only in $E_{7}$, a non-attracting subspace. A small initial departure from $E_{7}$ takes the points away from it. They are attracted by $B_{11}, p o_{1} B_{11}$, $p_{2} B_{11}$ or $B_{3}$, depending on the value of $R a$ (see previous page).

But even restricted to $E_{7}$ the dynamics is interesting: a potential strange attractor is promoted to a true attractor.

Concretely: There are different unstable objects (steady and p.o.) in $E_{7}$ with heteroclinic connections. This give rise to a strange attractor in $E_{7}$. But the orbit comes close to $p_{1} B_{312}$, attracting (in $E_{7}$ ) in a range ending at $R a_{H C_{1}}$ and it is attracted by it.

When $p o_{1} B_{312}$ ends at that $R a_{H C_{1}}$ the potential attractor becomes a true one (still only in $E_{7}$ ).


Bifurcation diagram of steady solutions and periodic orbits that are related to chaotic dynamics.
$B_{4}$ has been included to clarify the origin of the $p o_{1} B_{4}$.
In contrast, $p o_{1} B_{312}$ plays a crucial role in the generation of chaotic dynamics. The initially stable $p o_{1} B_{312}$ arises at an $H_{3}$ on $B_{312}$. It ends on a homoclinic $H C_{1}\left(R a=R a_{H C_{1}}=74256.8441\right)$ with $\lambda_{1}=$ 18.22, $\lambda_{2}=-42.17$ (in $E_{7}$ ) with $\sigma=\lambda_{1}+\lambda_{2}<0$ (inside $E_{7}$ ) and, hence, limit of stable p.o..


Evolution with time of $c_{I I I}$, the first coefficient belonging to the third symmetry block in the truncated expansion. Left: at $R a=74000<R a_{h}$. Right: at $R a=74260>R a_{h}$. Note that both $R a$ are close to $R a_{h}=$ $R a_{H C_{1}}$.
On the left: After a chaotic transient the orbit is attracted by a stable periodic orbit in the $p o_{1} B_{312}$ branch.
On the right: the p.o. do not longer exists. The chaotic behavior persists.
All these orbits belong to $E_{7}$.


Qualitative sketch of the ranges of existence and stability of solutions relevant to the occurrence of chaotic attractors. Gray rectangles: regions where the solutions attract in the full space $E_{0}$. Black rectangles regions where the solutions attract only in $E_{7}$. Empty rectangles: regions with solutions not attracting neither in $E_{0}$ nor in $E_{7}$. In particular, the dependence of the ranges of existence of chaotic attractors as a function of $\operatorname{Pr}$ is shown.


Projection on $\left(c_{I I}, c_{I I I}\right)$ of the chaotic dynamics (attractor only in $E_{7}$ ) and involved solutions at $R a=8 \times 10^{4}$ (left) and $R a=9 \times 10^{4}$ (right). Attractor in solid gray lines. The two symmetric $B_{3}$ with filled circles. On the left 4 copies (by symmetries) of $p o_{11} B_{4}$ in dashed black lines. On the right several orbits of the family $p o_{1} B_{4}$ in solid, dotted and dot-dashed black lines.


Similar to previous plot for $R a=8.3 \times 10^{4}$ (left) and a magnification (right). Attractor (inside $E_{7}$ ) in solid gray lines. Two symmetrically related $p o_{1} B_{4}$ in solid black lines.
Note that, similar to the previous plots, the orbit in the attractor remains for a long time close to the $p o_{1} B_{4}$ orbits, which are mildly unstable.


Evolution with time of the Nüsselt number for the chaotic attractor (in $E_{7}$ ) at $R a=8.3 \times 10^{4}$. The dashed horizontal line shows the $N u$ value corresponding to the $B_{3}$ solution.
Departure from $E_{7}$ leads the dynamics to be attracted by $B_{3}$.
But we know from previous work that $B_{3}$ becomes stable for increasing values of $R a$ if $\operatorname{Pr}$ increases. See the sketch page. This suggests...

Chaotic attractors at $\operatorname{Pr}=0.75$ and $\operatorname{Pr}=0.80$



Projection and time evolution of the chaotic attractor at $R a=$ $9.5 \times 10^{4}$ and $\operatorname{Pr}=0.75$.
For these values all the steady and periodic solutions that have been found are unstable.
Checked for long time intervals (several thousands of units), for many random initial conditions and different space discretisations (coarser and finer) and by computing Lyapunov exponents.


Projection and time evolution of the chaotic attractor at $R a=$ $10^{5}$ and $\operatorname{Pr}=0.80$.
For these values all the steady and periodic solutions that have been found are unstable.
Checked for long time intervals (several thousands of units), for many random initial conditions and different space discretisations (coarser and finer) and by computing Lyapunov exponents.

## Thanks for your attention!

And sorry for changing from DANCE to DNASC:

Dynamics, Nonlinearity, Attractors, Stability and Chaos

