Dynamics of particle trajectories in a Rayleigh–Bénard problem

Dolors Puigjaner[(1)] Joan Herrero[(2)]
Carles Simó[(3)] Francesc Giralt[(2)]

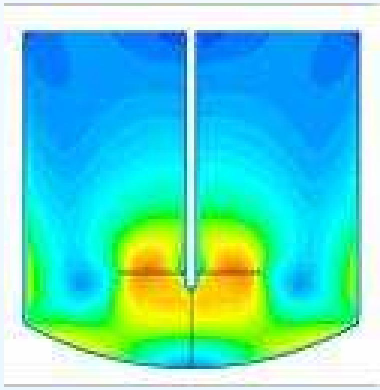
(1) Dept. Enginyeria Informàtica i Matemàtiques. Universitat Rovira i Virgili.

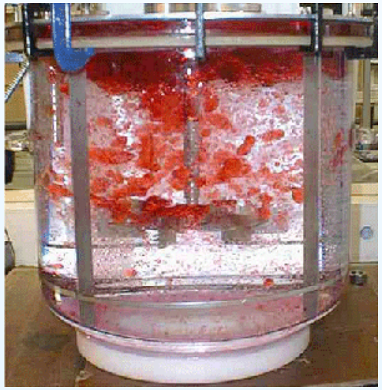
(2) Dept. Enginyeria Química. Universitat Rovira i Virgili.

(3) Dept. Matemàtica Aplicada i Anàlisi. Universitat de Barcelona.

Motivation

- Fluid mixing efficiency is a crucial issue in many engineering applications
- Efficient mixing is usually related to turbulent regimes and to mechanical devices





- Some industrial applications require an efficient mixing in the absence of turbulence or high shear stresses
- Rayleigh–Bénard convection can offer an alternative to the use of mechanical devices

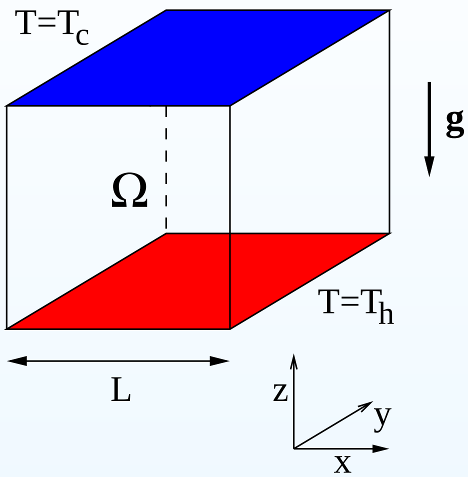
Objectives

The design of reactors in which **efficient mixing** is achieved without moving parts

The application of **dynamical systems theory** to the analysis of dynamics and mixing properties in flows induced by Rayleigh–Bénard convection inside a cube

- Analyze the rich dynamics of fluid particle trajectories
- Characterize well-mixed regions inside the cube
- Investigate the dependence of mixing properties on the Rayleigh number

Flow system and equations



$\mathbf{Ra} = g\beta L^3 \Delta T / \alpha\nu$

$\mathbf{Pr} = \nu / \alpha$

β thermal expansion

ν kinematic viscosity

α thermal diffusivity

$\Delta T = T_h - T_c$

$$\theta = [T - (T_h + T_c)/2]/\Delta T - z$$

Continuity

$$\nabla \cdot \vec{V} = 0$$

Momentum

$$\frac{1}{Pr}\left(\frac{\partial \vec{V}}{\partial t} + Ra^{\frac{1}{2}}(\vec{V} \cdot \nabla)\vec{V}\right) =$$
$$\nabla^2 \vec{V} + Ra^{\frac{1}{2}} \theta \vec{e_z} - \nabla p$$

Energy

$$\frac{\partial \theta}{\partial t} + Ra^{\frac{1}{2}}(\vec{V} \cdot \nabla)\theta =$$
$$\nabla^2 \theta + Ra^{\frac{1}{2}} \vec{V} \cdot \vec{e_z}$$

Boundary conditions

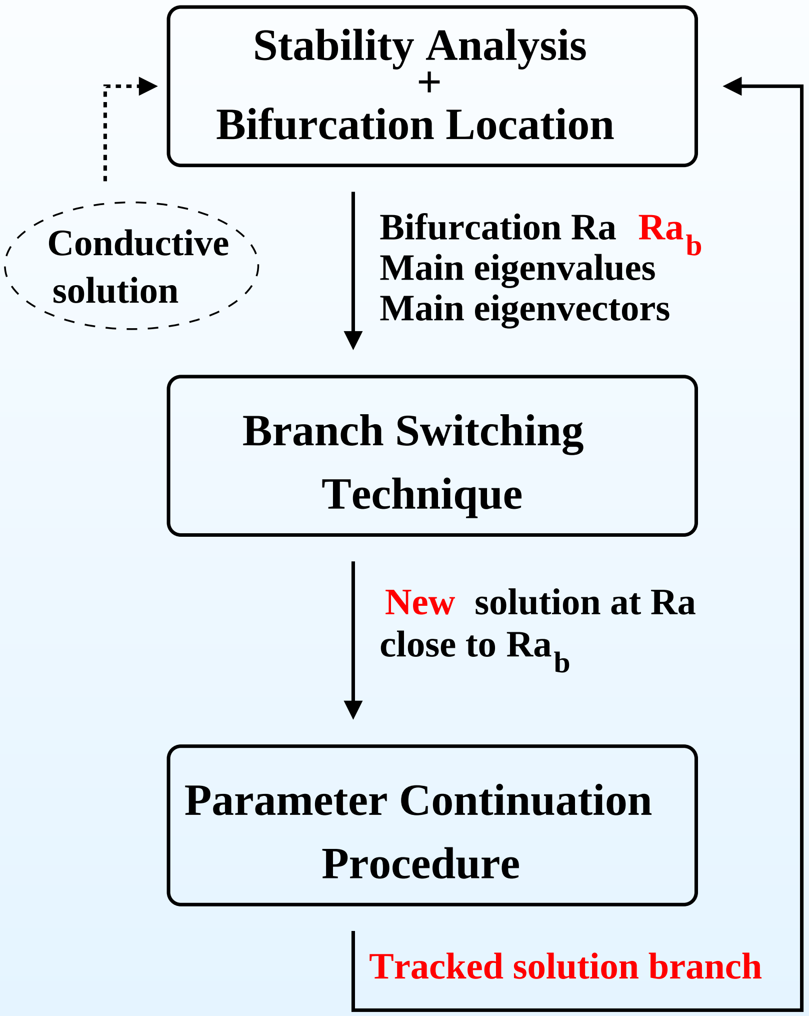
$\vec{V} = \theta = 0$ en $\partial\Omega$

Continuation method

Galerkin spectral method with basis functions $\{\vec{F}_i(x, y, z)\}$ satisfying the boundary conditions and the continuity equation

Solution

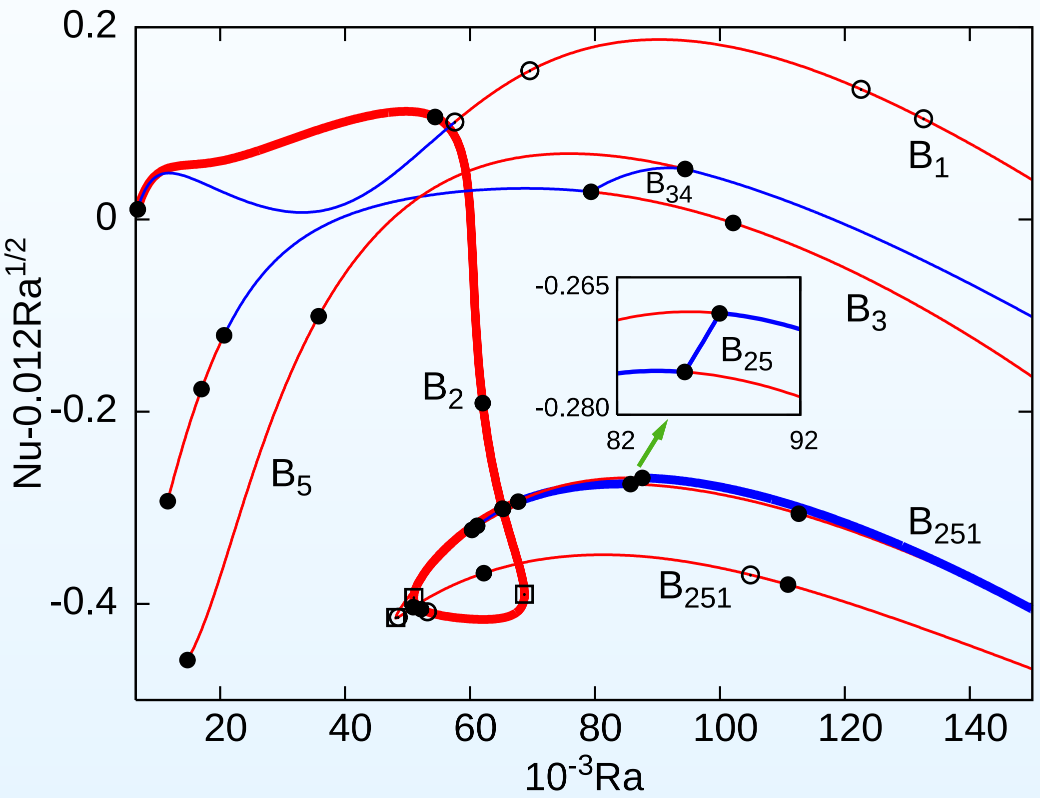
$$\begin{pmatrix} \vec{V} \\ \theta \end{pmatrix} = \sum_i c_i(t) \vec{F}_i$$



D. Puigjaner, J. Herrero, C. Simó, F. Giralt, J. Fluid Mechanics, 598, 393–427, (2008)

Bifurcation diagram ($Pr = 130$)

Steady solutions that are stable over some Ra range



— stable
— unstable

● steady bifurcation
○ Hopf bifurcation
□ turning point

Flow patterns: $\lambda_2 = 0$ surfaces

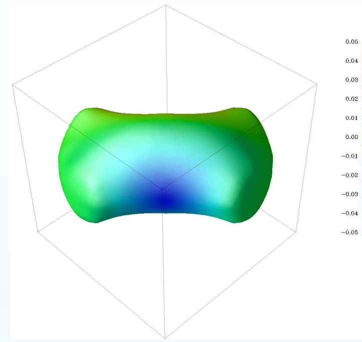
B_2

Initial Ra

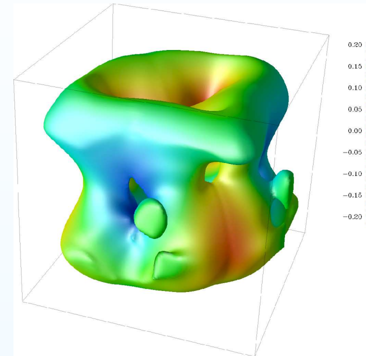
6 798

Stability Range

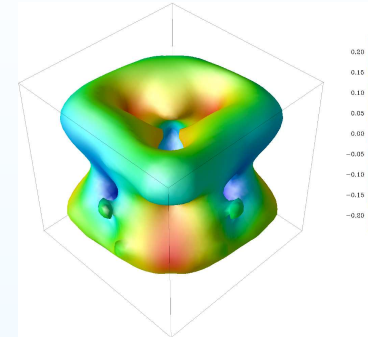
67 730–85 694



Ra=7 000



Ra=51 000



Ra=80 000

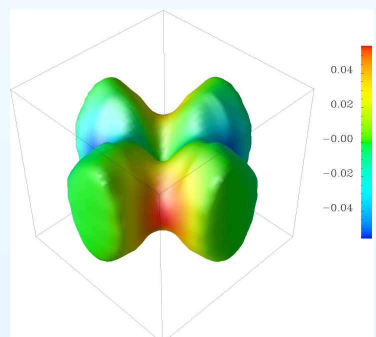
B_3

Initial Ra

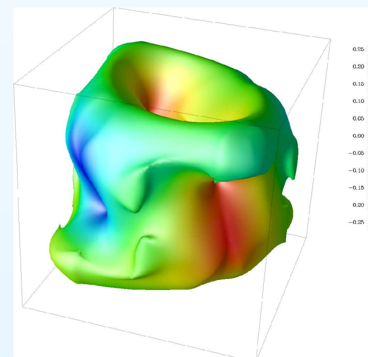
11 612

Stability Range

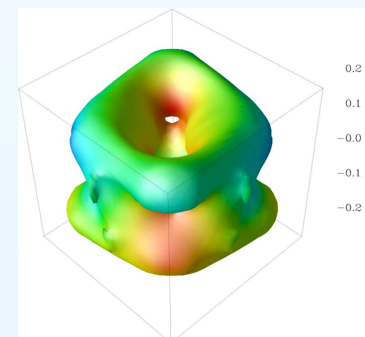
20 637–79 362



Ra=12 000



Ra=51 000



Ra=80 000

λ_2 is the second largest eigenvalue of the tensor $S^2 + \Omega^2$

Symmetries and invariant planes

Solution	Symmetry Group (generators)	Invariant Planes
B_2	$S_{d_-}, -I$	$x+y=0$
B_{25}	$-I$	–
B_{251}	$S_y, -I$	$y=0$
B_3	$S_{d_+}, -S_y$	$\begin{cases} x+y=0 \\ x-y=0 \end{cases}$

S_y	reflection about the plane $y=0$
S_{d_+}	reflection about the plane $x-y=0$
S_{d_-}	reflection about the plane $x+y=0$
$-I$	simmetry with respect the origin
$-S_y$	rotation of angle π around the y–axis

Numerical methods

Particle trajectories (Negligible diffusivities)

$$\begin{cases} \dot{x} = u(x, y, z) \\ \dot{y} = v(x, y, z) \\ \dot{z} = w(x, y, z) \end{cases}$$

Advection equations

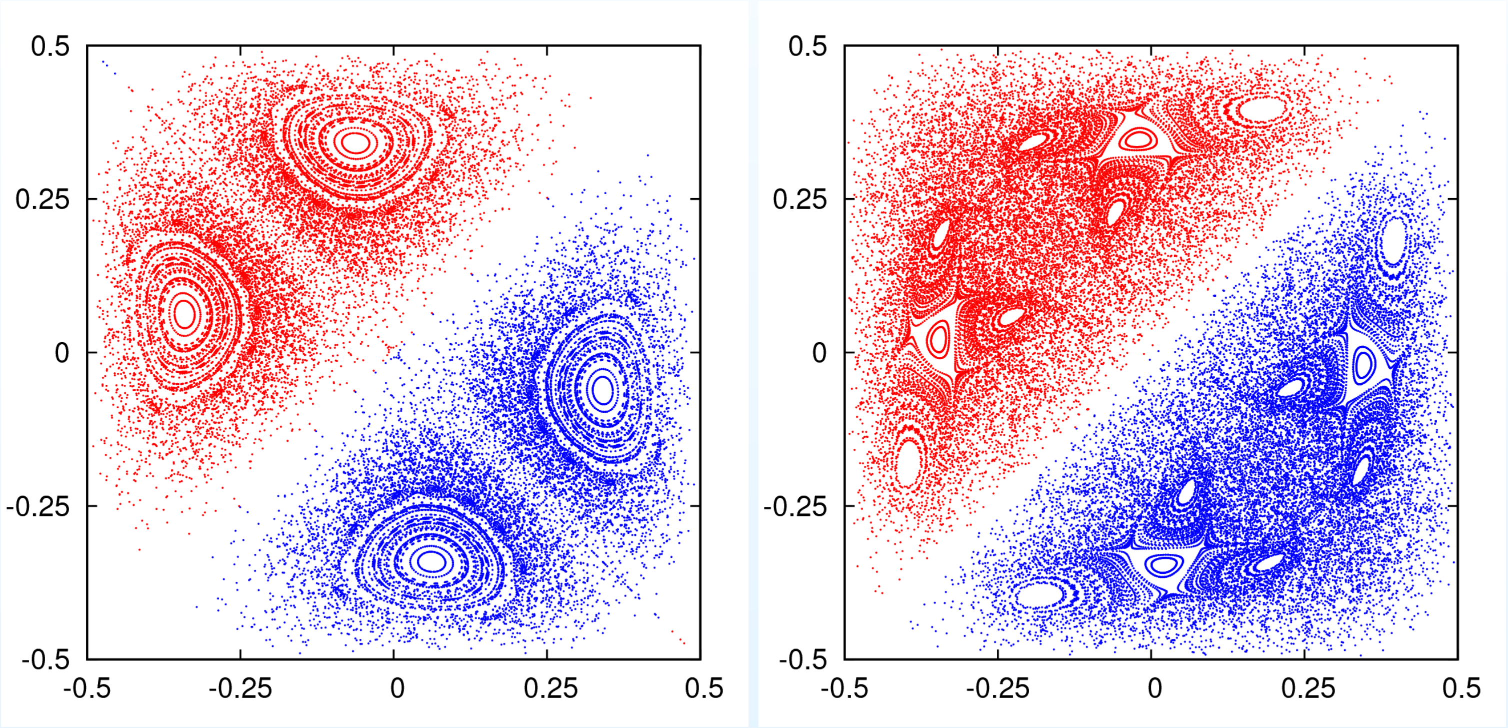
- Symmetries and invariant planes
- Poincaré sections
- Periodic orbits and their stability
- Size and shape of regular regions
- Maximal Lyapunov exponents and metric entropy
- Critical points in the interior and on the boundary
  - Stability analysis
  - Poincaré–Hopf index theorem

C. Simó, D. Puigjaner, J. Herrero, F. Giralt, Communications in Nonlinear Science and Numerical Simulation, doi:10.1016/j.cnsns.2008.07.012. In Press

Poincaré Maps I

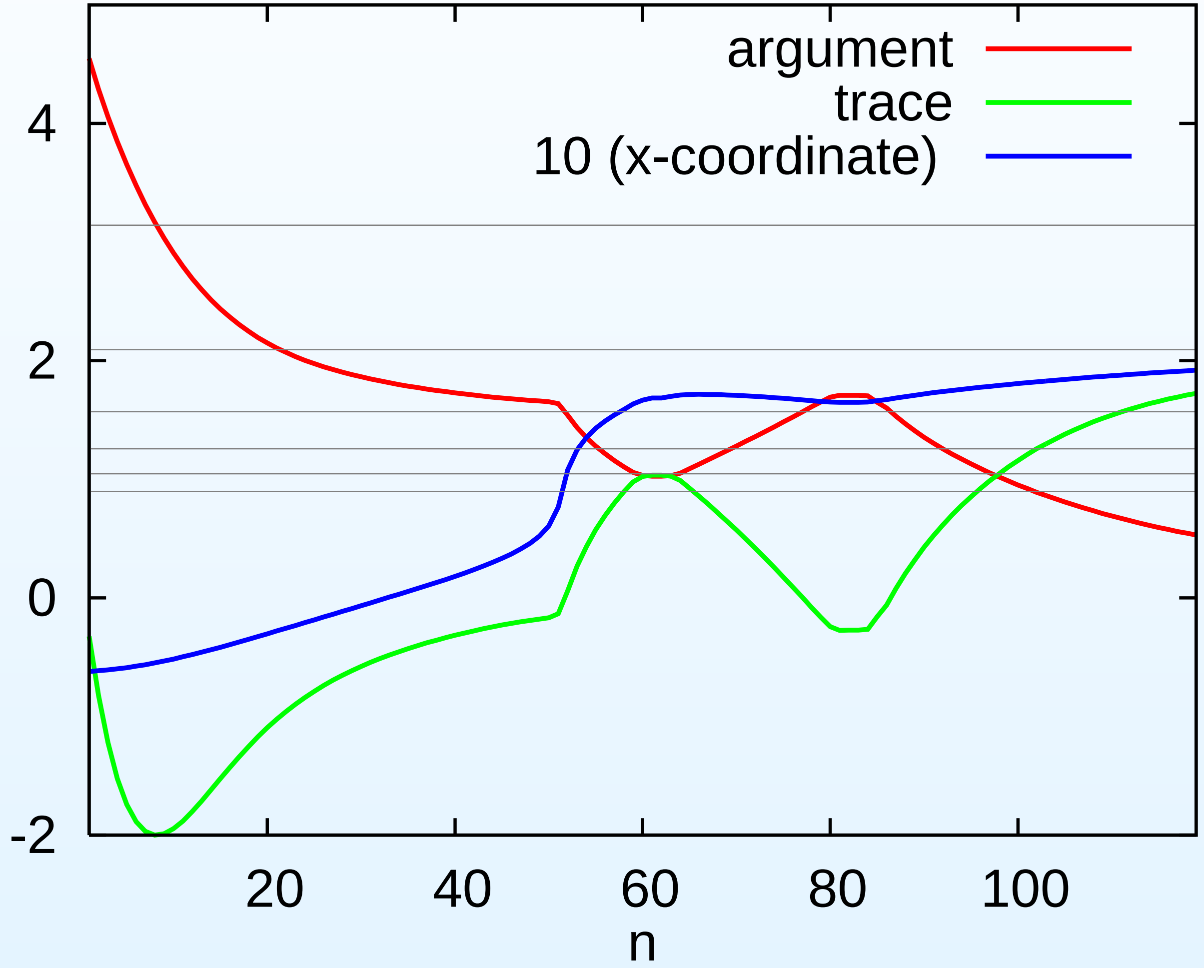
512 equidistributed initial conditions integrated up to $t = 10^3$

B_2, $z = 0$



$Ra = 10^4$ $\qquad$ $Ra = 3.3 \times 10^4$

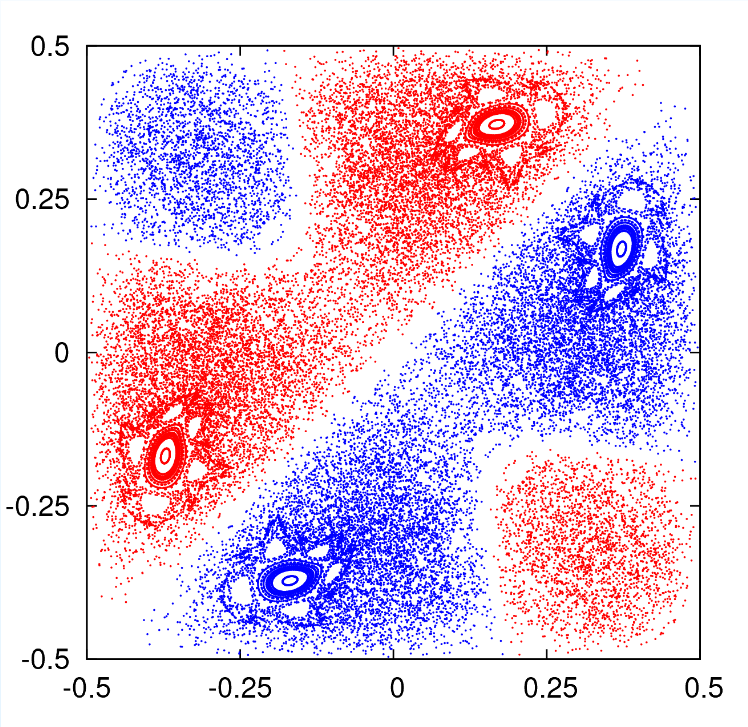
Main stable periodic orbit (fixed elliptic point)



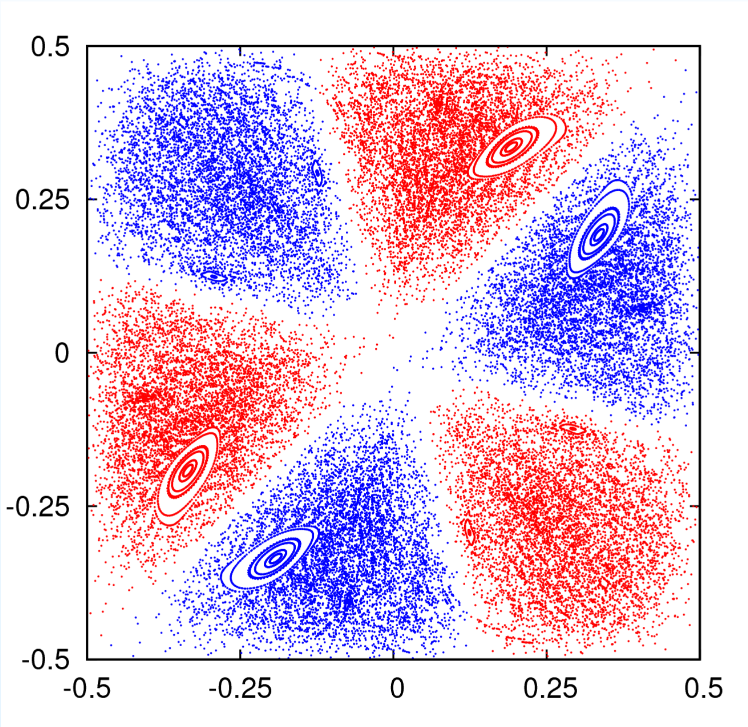
—— $y = 2\pi/k,\ k = 2, \cdots, 7$

Poincaré Maps II

$$B_2,\, z = 0$$



$$Ra = 6.87099 \times 10^4$$



$$Ra = 8.5 \times 10^4$$

Regular regions

V_c= volume occupied by the chaotic zone (points outside invariant tori)

Computation Procedure

- Divide the cavity into $n \times n \times n$ cubic cells ($n = 200$)
- Compute trajectories of fluid particles initially located at x_0, for any x_0 in the set C_I (final time $t_M = 10^6$)
  $$C_I = \left\{ \left(-0.375 + \frac{i}{8}, 0.48, -0.375 + \frac{j}{8} \right), i, j = 0, \cdots, 6 \right\}$$
- Store the cells visited by one or more trajectories
- $N_r(t) =$ number of cells that at time t have not yet been visited by any particle trajectory (every $\Delta t = 200$)
- Check that $N_r(t)$ is almost constant in $t \in [\frac{3}{4}t_M, t_M]$
- Points at a distance less than 0.01 from the boundaries are considered as non-regular

Maximal Lyapunov exponents I

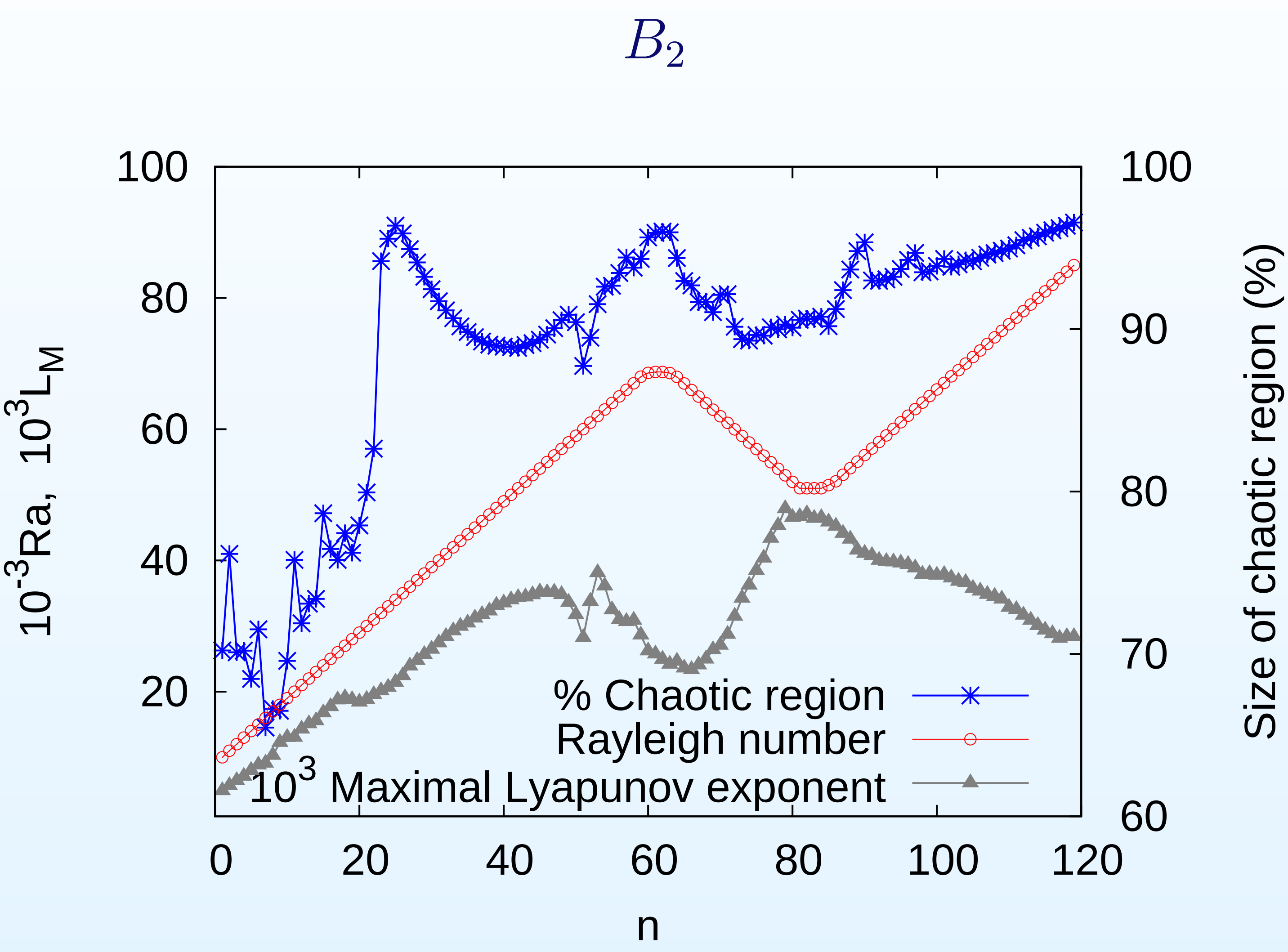
$$L_M(x_0) = \lim_{t\to\infty} \frac{1}{t} \log\left(\frac{\| l_t \|}{\| l_0 \|}\right)$$

$l_t = D_x\phi(t, x_0)l_0$ where l_0 is an arbitrary vector and $\phi(t, x_0)$ is a solution of the differential equation with $\phi(0, x_0) = x_0$

Computation Procedure

- 49 equidistributed initial conditions on the plane $y = 0.48$
- finite time approximations of L_M (final time=10^5)
- transient values ($t \leq 10^4$)
- calculate $\log\left(\| l_t \| \,/\, \| l_0 \|\right)/t$ every 10^3 units of time after the transient ($t > 10^4$)
- average with respect to time and initial conditions

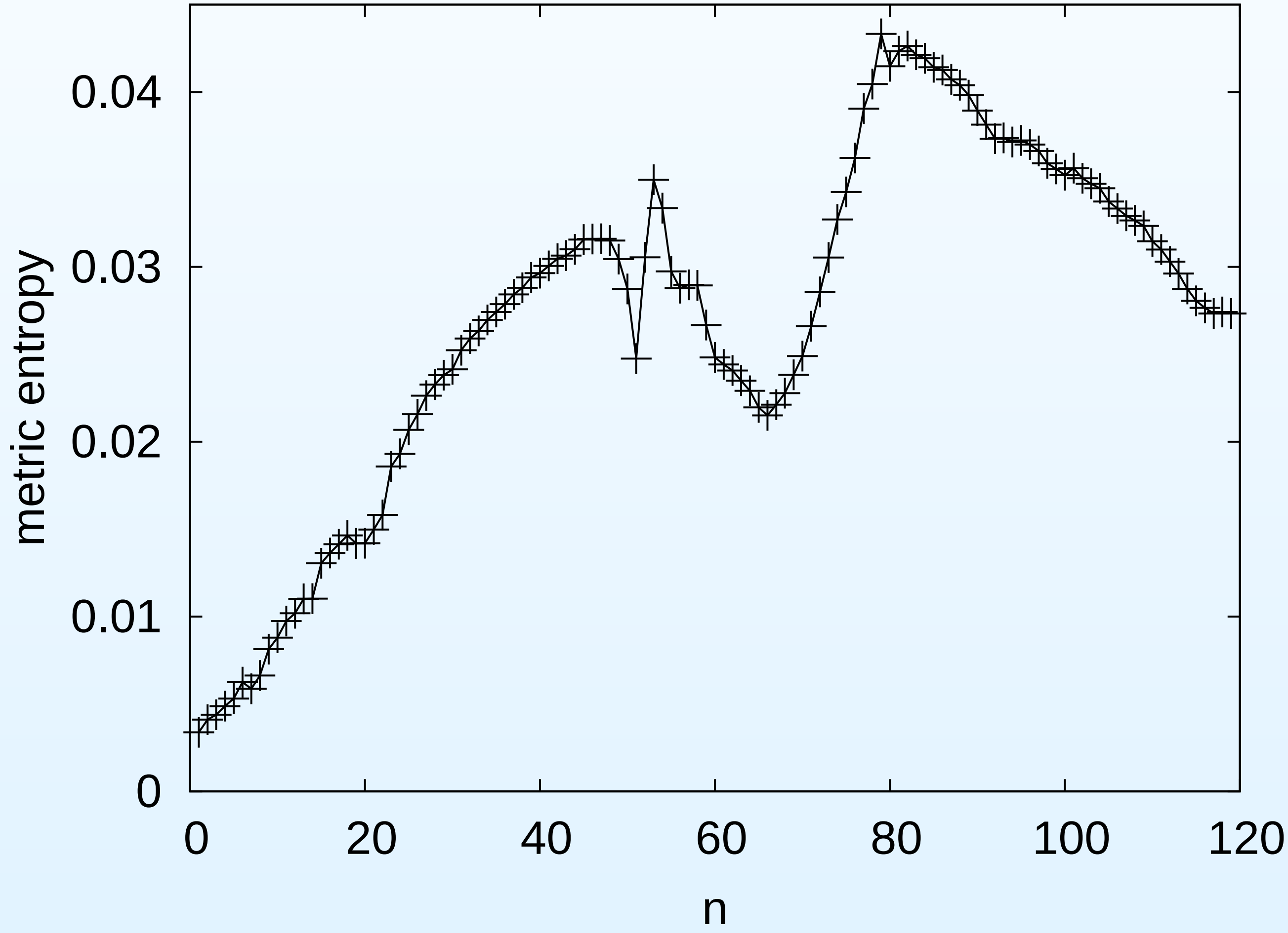
L_M and V_c evolution



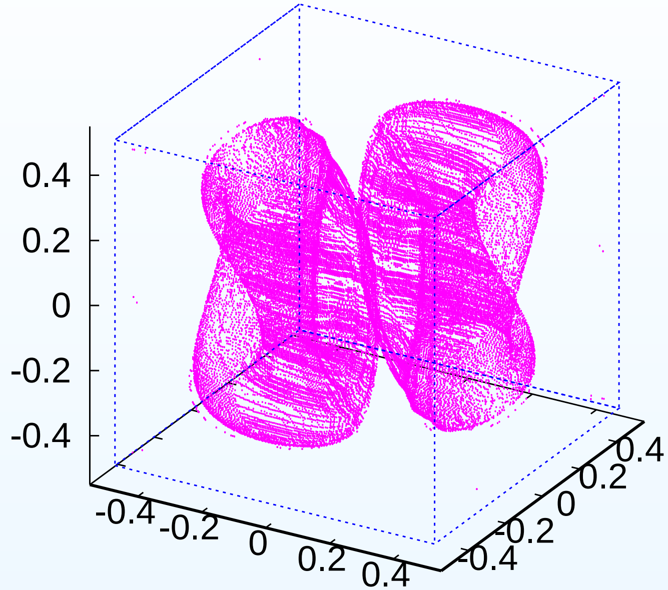
Metric entropy, h_m

$$h_m = L_M \times V_c$$

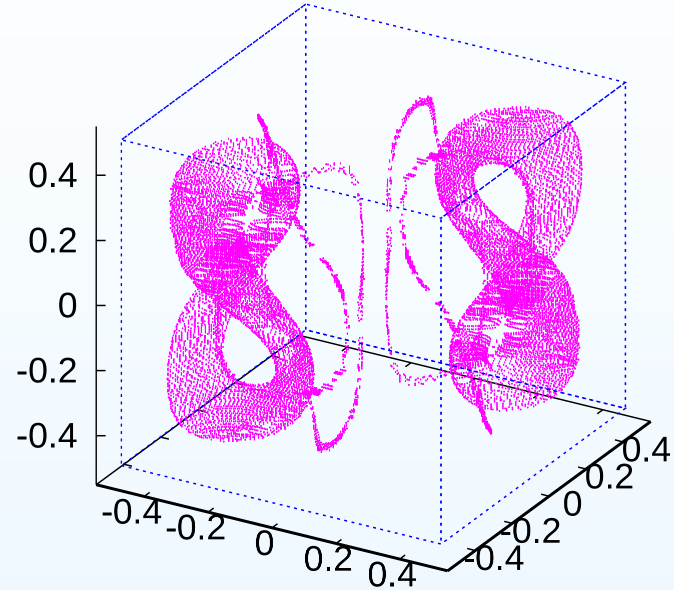
B_2



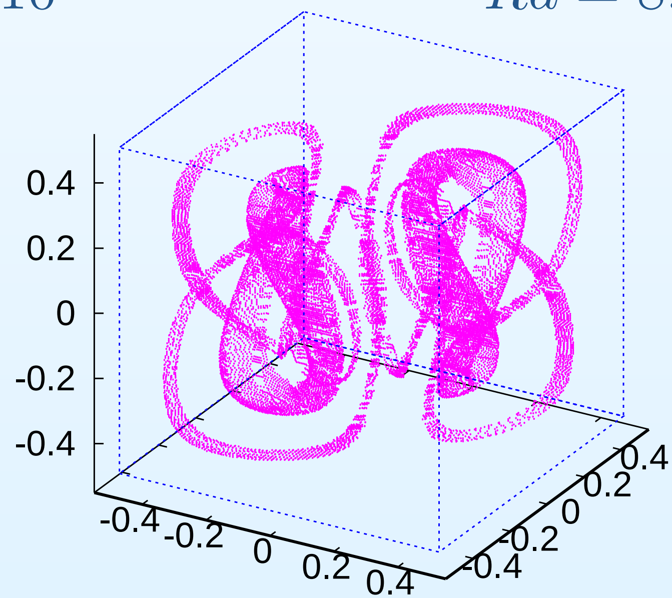
Shape of regular regions



$Ra = 10^4$



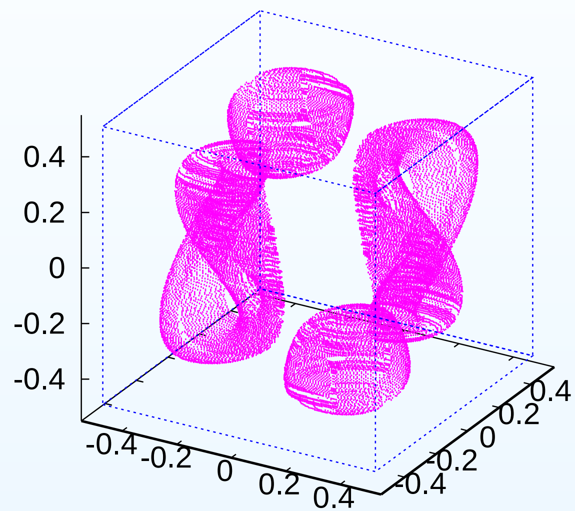
$Ra = 8.5 \times 10^4$

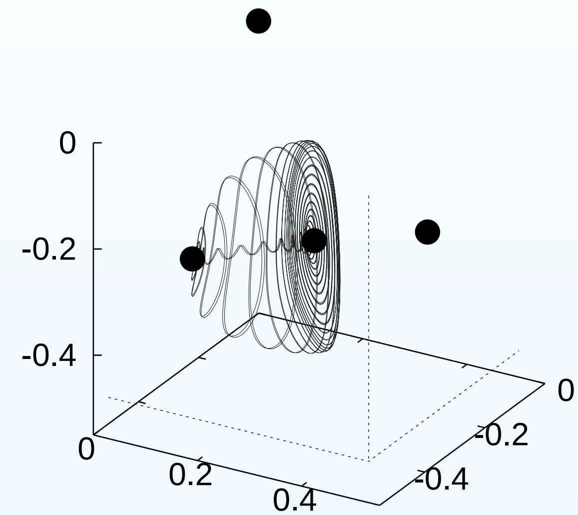


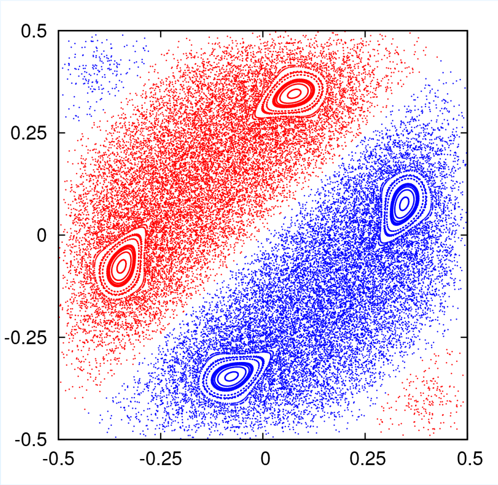
$Ra = 3.4 \times 10^4$

Spherical–like regular regions

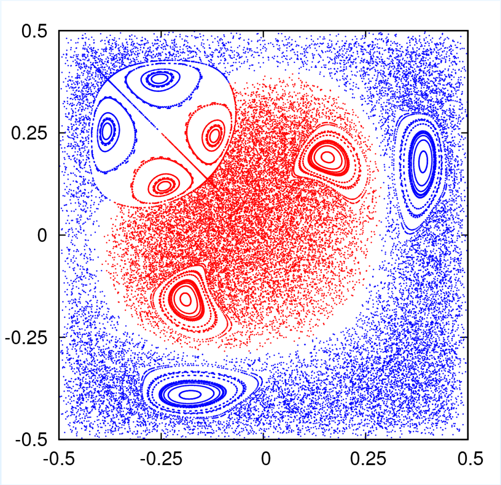
B_2, $Ra = 6 \times 10^4$



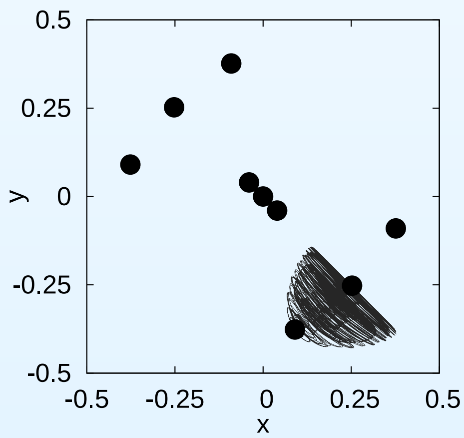




$z = 0$



$z = 0.4$



Critical points: interior and boundaries

Interior: fixed points of the advection equations ($\vec{V} = 0$)

Boundary: wall $x_3 = 0$

$$\frac{dx_i}{d\tau} = \frac{\partial u_i}{\partial x_3} + \frac{\partial^2 u_i}{\partial x_3 \partial x_1}(x_1 - b_1) + \frac{\partial^2 u_i}{\partial x_3 \partial x_2}(x_2 - b_2) + \frac{1}{2}\frac{\partial^2 u_i}{\partial x_3^2} x_3$$

$$\frac{dx_3}{d\tau} = -\frac{1}{2}\left(\frac{\partial^2 u_1}{\partial x_1 \partial x_3} + \frac{\partial^2 u_2}{\partial x_2 \partial x_3}\right) x_3$$

$\tau = x_3 t$ rescaled time

$b = (b_1, b_2, 0)$ point on the wall $x_3 = 0$

Trajectories of particles passing very close to the wall are obtained by taking the limit $(x_1, x_2, x_3) \to (b_1, b_2, 0)$

$$\boxed{\frac{dx_i}{d\tau} = \frac{\partial u_i}{\partial x_3} \quad i = 1, 2}$$

Critical points: stability

λ_1, λ_2, λ_3 eigenvalues associated to the linearization of the vector velocity field about a critical point x_c.

Divergence–free flow (volume–preserving flow)

$$\lambda_1 + \lambda_2 + \lambda_3 = 0 \qquad \textit{if } x_c \textit{ is in the interior of the cube};$$

$$\frac{1}{2}(\lambda_1 + \lambda_2) + \lambda_3 = 0 \qquad \textit{if } x_c \textit{ is on a wall of the cube };$$

$$2(\lambda_1 + \lambda_2) + \lambda_3 = 0 \qquad \textit{if } x_c \textit{ is on an edge of the cube;}$$

Classification of critical points

- **SF**: stable focus with a 1D unstable manifold
- **UF**: unstable focus with a 1D stable manifold
- **2S**: saddle with a 2D stable manifold
- **1S**: saddle with a 1D stable manifold

Poincaré–Hopf index

Poincaré–Hopf index theorem

The sum of the Poincaré indexes over all the isolated critical points of a vector field on a compact orientable differentiable manifold is equal to the Euler characteristic of the manifold

Change from the cubical domain to the 3D sphere $\mathbb{S}^3$

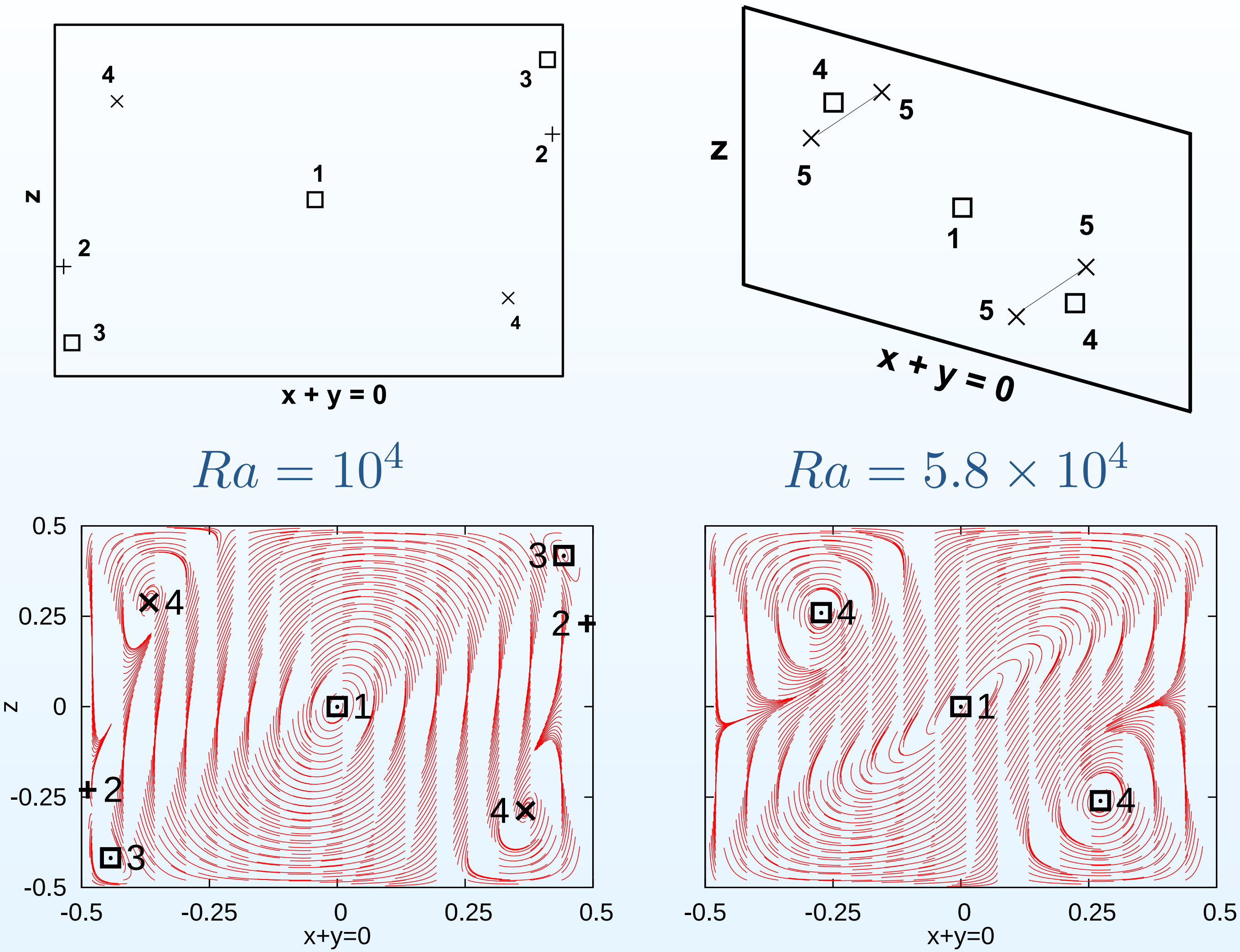
- the interior of the cubical domain is topologically equivalent to a 3D open ball B^3 and its boundary is equivalent to a 2D sphere $\mathbb{S}^2$
- deform B^3 to get a 3D hemisphere whose equator is $\mathbb{S}^2$
- take a symmetric copy of the 3D hemisphere and glue both hemispheres after identifying the $\mathbb{S}^2$ boundaries

The Poincaré index of a critical point x_c satisfying $Re\lambda_i \neq 0$, is $(-1)^{n_p}$, where $n_p = \#\{\lambda_i \mid Re\lambda_i < 0,\ i = 1, 2, 3\}$. Interior critical points must be counted twice.

Critical points: bifurcations and Poincaré indexes

	Interior				Walls			Edges	
$10^{-3}Ra$	SF (2)	UF (-2)	2S (2)	1S (-2)	SF (1)	2S (1)	1S (-1)	2S (1)	1S (-1)
10	2	3	2	0	4	2	6	0	2
11	2	3	0	0	4	2	2	2	4
28	2	1	0	0	4	0	2	0	4
41	2	1	0	0	0	4	2	0	4
58	4	3	0	0	0	4	2	0	4
60	4	2	1	2	0	4	2	0	4
61	4	4	1	0	4	0	2	0	4
63	6	6	1	0	4	0	2	0	4
65	6	6	1	0	4	2	4	0	4
68.58	6	6	2	1	4	2	4	0	4
68.71	6	6	2	1	4	6	8	0	4
68	6	6	1	0	8	2	8	0	4
58	6	6	1	0	8	0	6	0	4
57	6	6	1	0	4	4	6	0	4
52	6	6	1	0	4	0	2	0	4

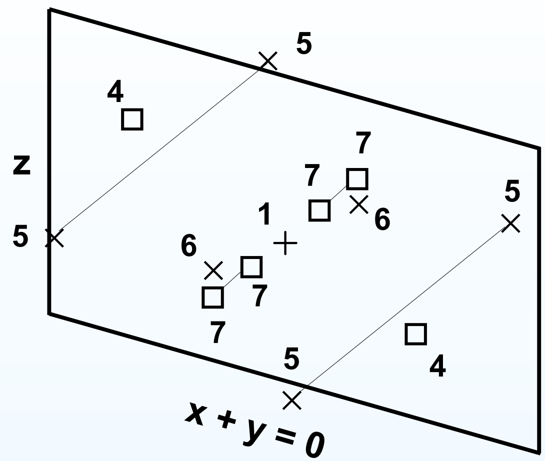
Critical points:bifurcations and invariant planes I



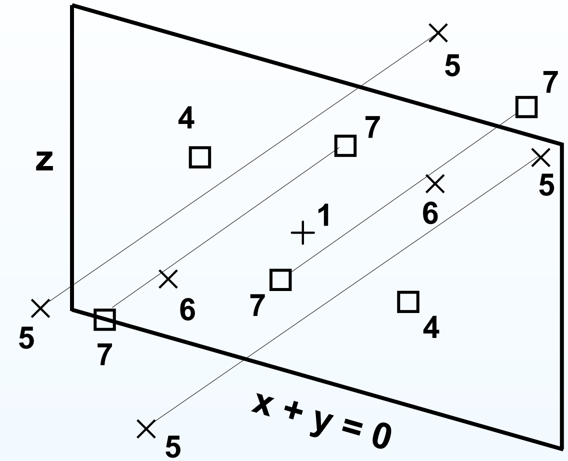
× SF: stable focus + 2S: saddle with two stable directions

□ UF: unstable focus

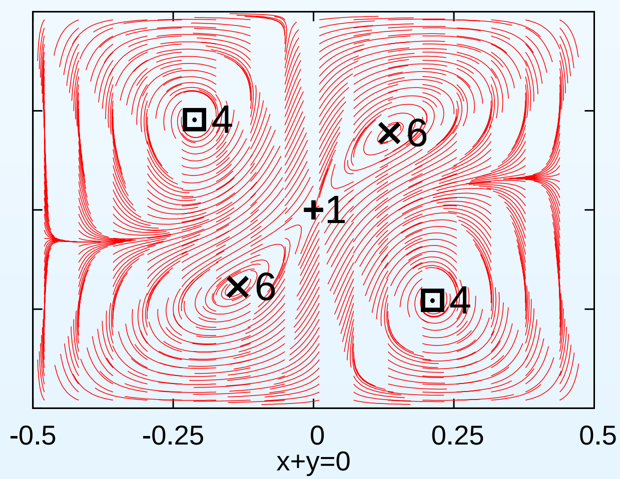
Critical points:bifurcations and invariant planes II

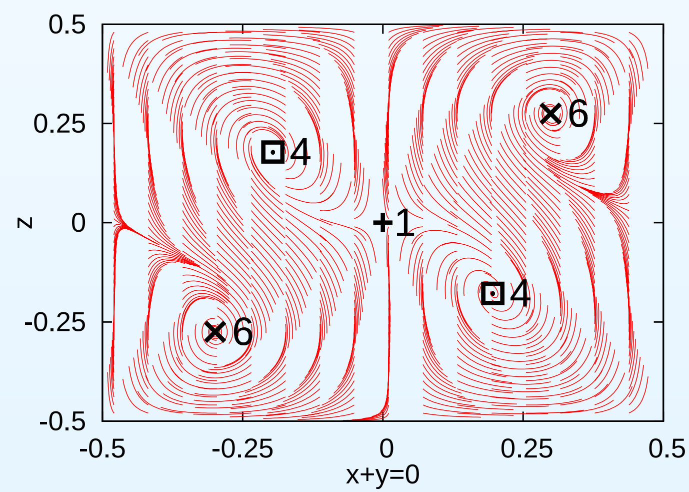


$Ra = 6.3 \times 10^4$



$Ra = 8.5 \times 10^4$





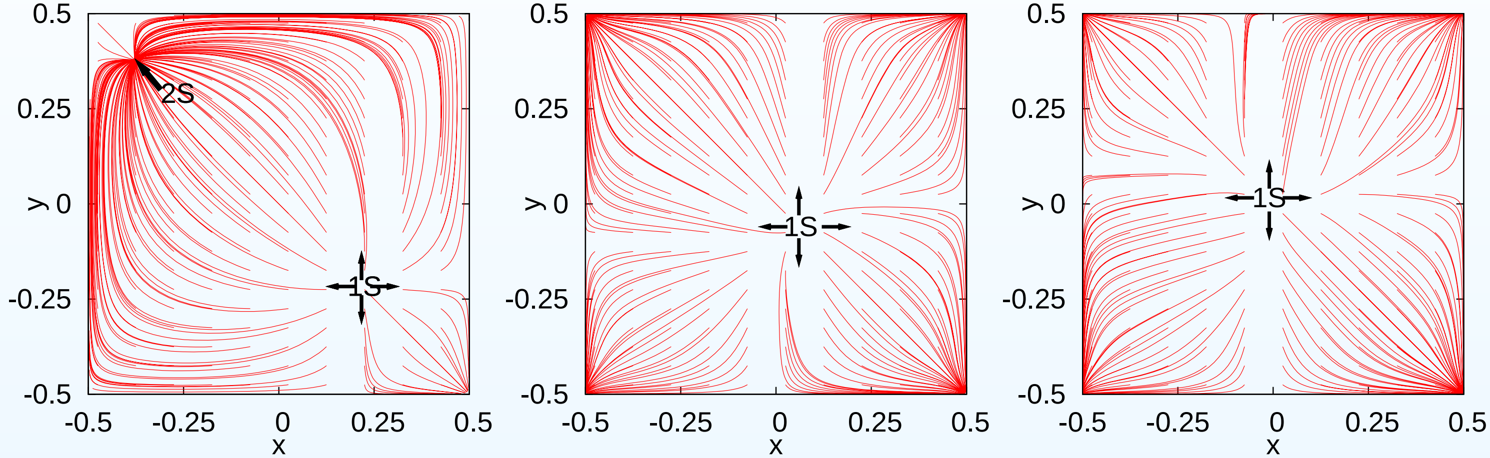
× SF: stable focus

+ 2S: saddle with two stable directions

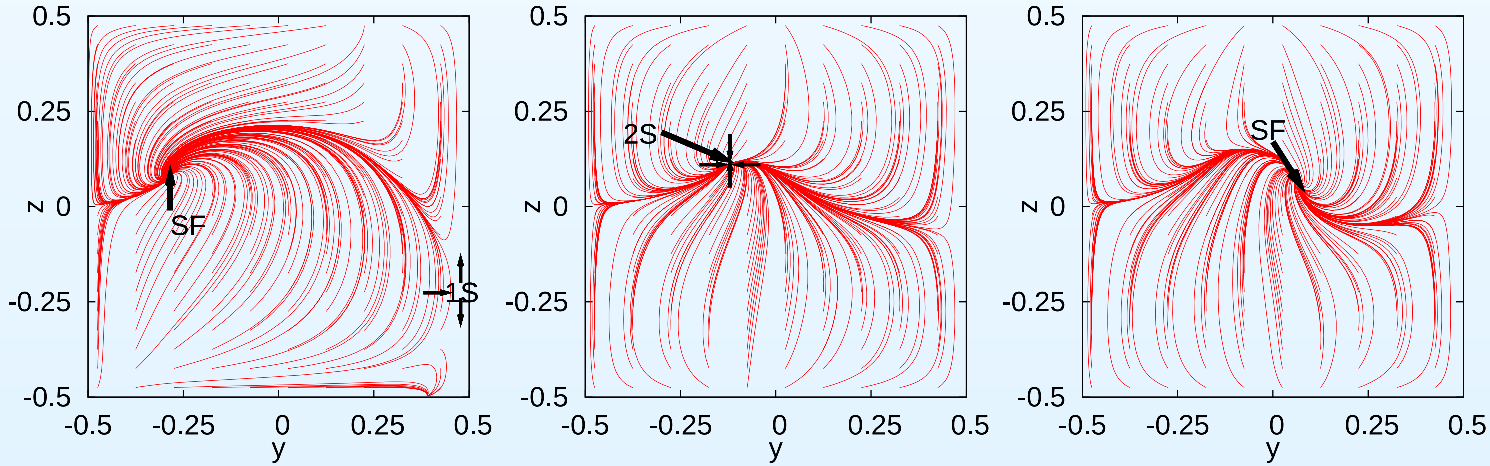
□ UF: unstable focus

Limiting Streamlines (B_2)

$z = -0.5$

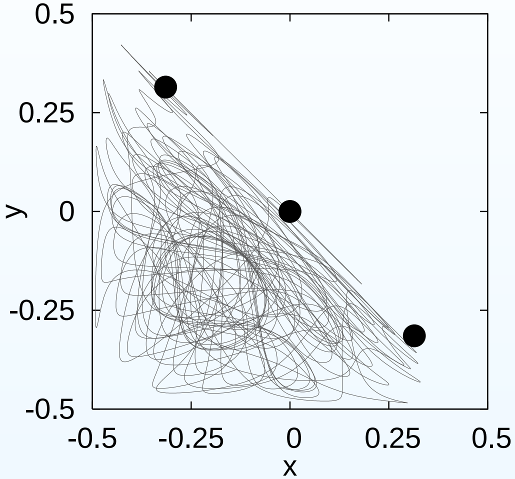


$x = -0.5$

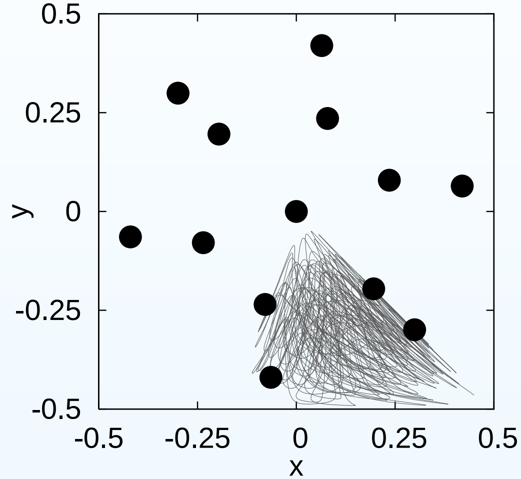


10^4 $\quad$ 6×10^4 $\quad$ 8.5×10^4

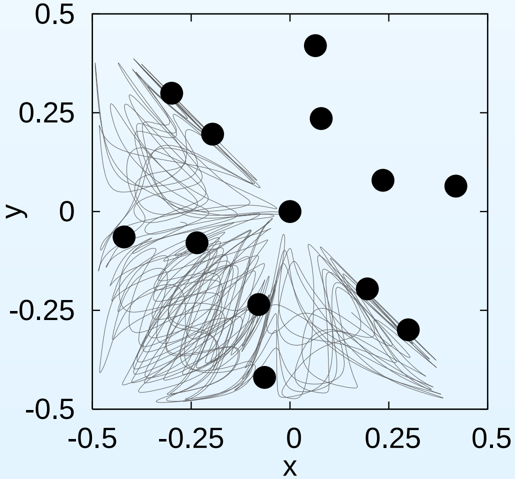
Projected trajectories (B_2)



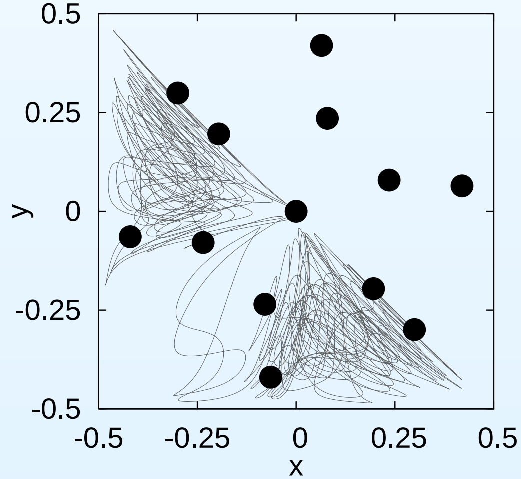
4×10^4



8.5×10^4

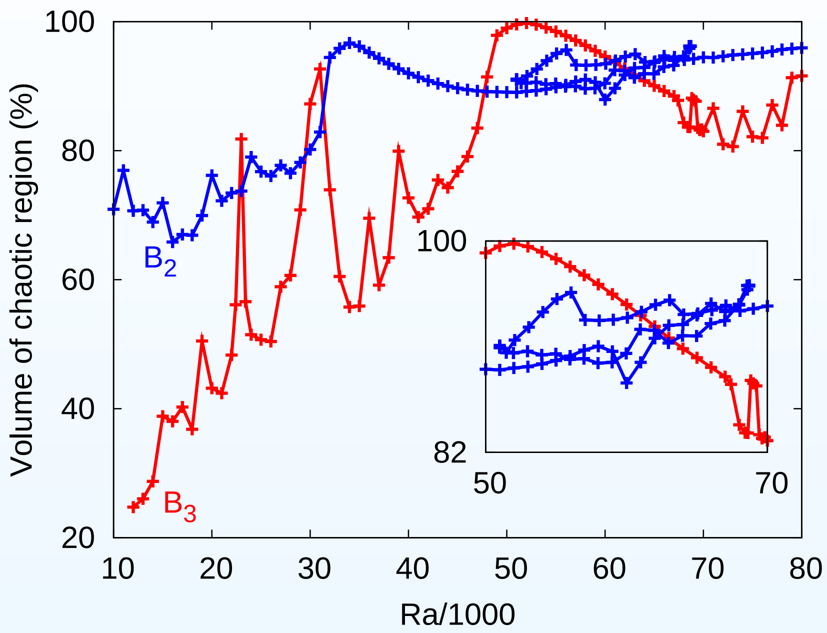


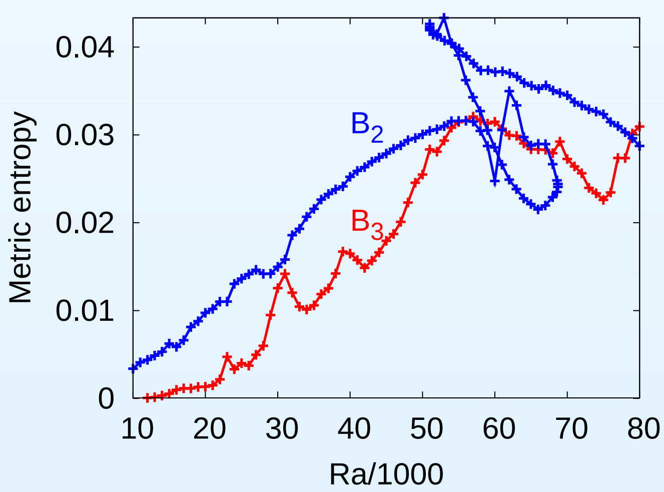
8.5×10^4

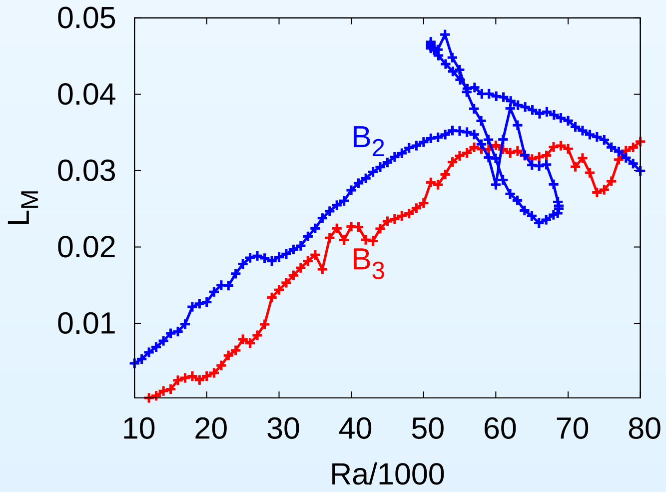


8.5×10^4

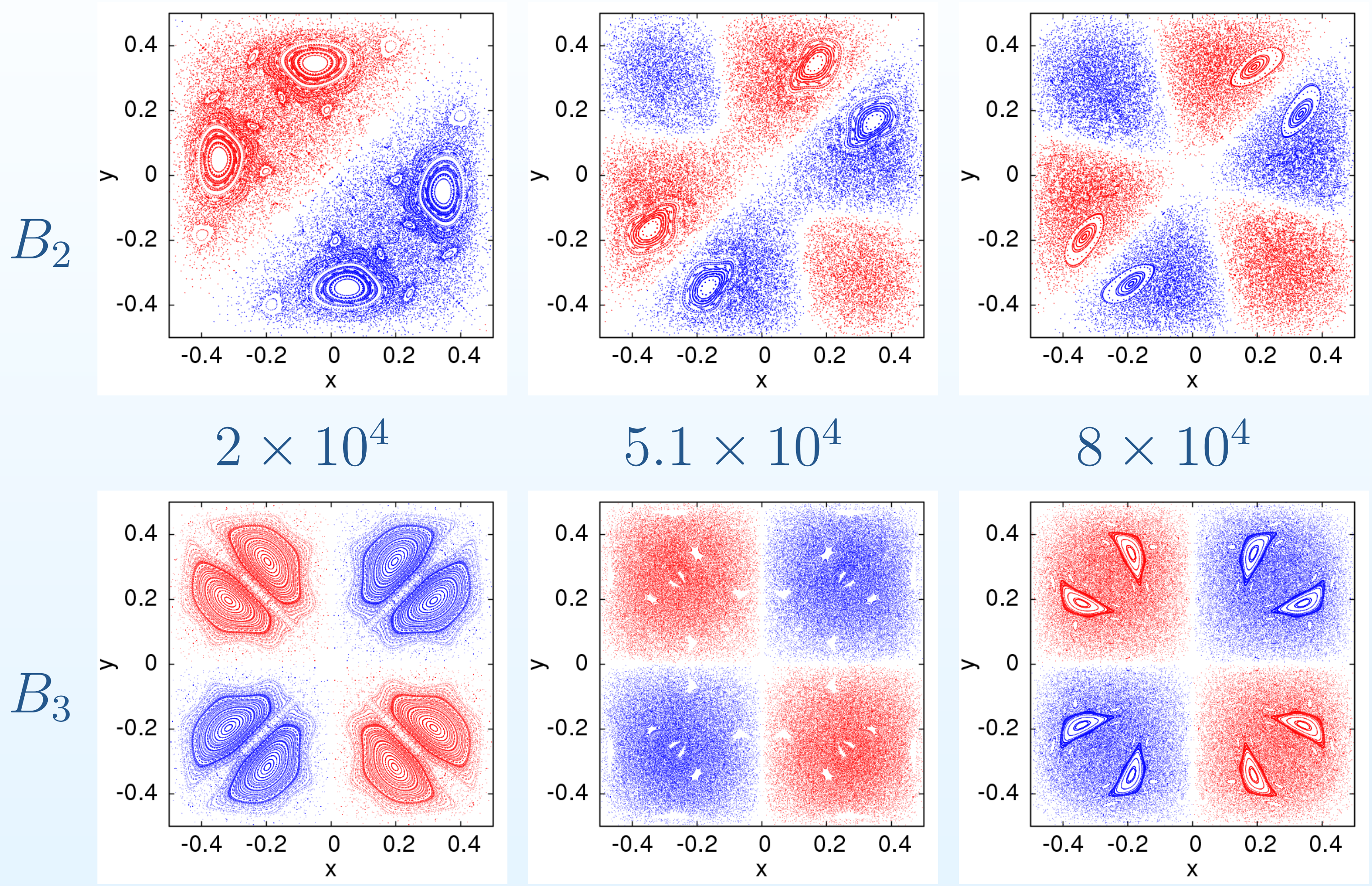
V_c, L_M and h_m


Volume of chaotic region (%)
100
80
60
40
20
10
20
30
40
50
60
70
80
Ra/1000
B2
B3
100
82
50
70


Metric entropy
0.04
0.03
0.02
0.01
0
10
20
30
40
50
60
70
80
Ra/1000
B2
B3


LM
0.05
0.04
0.03
0.02
0.01
10
20
30
40
50
60
70
80
Ra/1000
B2
B3

Poincaré sections



Conclusions

- The dynamics are characterized by regions with regular motion surrounded by regions of chaotic motion
- Changes on the topology and on the chaotic level of the flows are related to bifurcations of critical points
- The detailed knowledge of the flow provided by the dynamical systems approach can be relevant in selecting the parameter ranges and flow patterns at which more efficient mixing is achieved

Future work

- Study the relative position of the most relevant invariant manifolds of the fixed points and hyperbolic periodic orbits
- Study the effect of a non–negligible molecular diffusion on the dynamics of particle trajectories
- Extend the study to non-stationary flows

Basis Functions I

$$\begin{pmatrix}\mathbf{V}\\ \theta\end{pmatrix}=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}\left[a_{ijk}^{(1)}\mathbf{G}_{ijk}^{(1)}+a_{ijk}^{(2)}\mathbf{G}_{ijk}^{(2)}+a_{ijk}^{(3)}\mathbf{G}_{ijk}^{(3)}+a_{ijk}^{(4)}\mathbf{G}_{ijk}^{(4)}\right]$$

$$\mathbf{G}_{ijk}^{(1)}=\begin{pmatrix}0\\ -g_i f_j f_k'\\ \frac{1}{h_2}g_i f_j' f_k\\ 0\end{pmatrix},\qquad \mathbf{G}_{ijk}^{(2)}=\begin{pmatrix}-f_i g_j f_k'\\ 0\\ \frac{1}{h_1}f_i' g_j f_k\\ 0\end{pmatrix},$$

$$\mathbf{G}_{ijk}^{(3)}=\begin{pmatrix}-\frac{1}{h_2}f_i f_j' h_k'\\ \frac{1}{h_1}f_i' f_j h_k'\\ 0\\ 0\end{pmatrix},\quad \mathbf{G}_{ijk}^{(4)}=\begin{pmatrix}0\\ 0\\ 0\\ g_i g_j g_k\end{pmatrix}$$

$N = 4 \times 8 \times N_x \times N_y \times N_z$ terms

Basis Functions II

$$f_k(x):\quad C_k(x) = \frac{\cosh(\lambda_k x)}{\cosh(\lambda_k/2)} - \frac{\cos(\lambda_k x)}{\cos(\lambda_k/2)};$$

$$S_k(x) = \frac{\sinh(\mu_k x)}{\sinh(\mu_k/2)} - \frac{\sin(\mu_k x)}{\sin(\mu_k/2)}$$

$$g_k(x):\quad \cos((2k-1)\,\pi\, x)\,;$$

$$\sin(2k\,\pi\,x)$$

λ_k y μ_k are the positive solutions of

$$\begin{aligned} \tanh(\lambda_k/2) + \tan(\lambda_k/2) &= 0 \\ \coth(\mu_k/2) - \cot(\mu_k/2) &= 0 \end{aligned}$$