Newton-Krylov methods beyond the computation of steady solutions: two applications to Fluid Dynamics problems

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Continuation of fixed points of maps by N-K methods

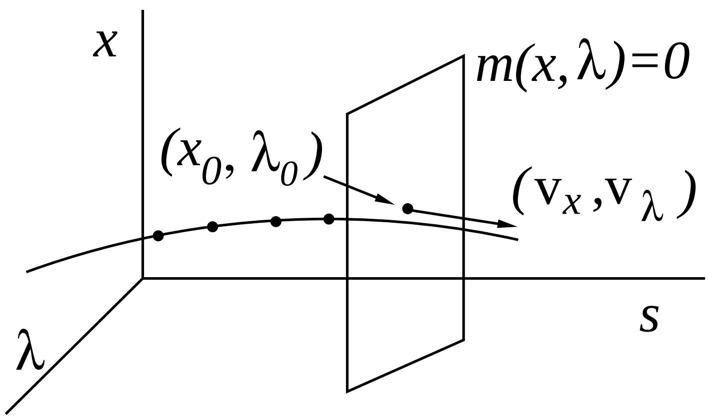
Consider a dissipative map

$$x \to G(x, \lambda), \quad (x, \lambda) \in \mathcal{U} \subset \mathbb{R}^n \times \mathbb{R}$$

with $n >> 1$. We are interested in the fixed points of the map and their dependence on λ. Parameter and pseudo-arclength-like continuation methods are used to obtain the curves $(x(s), \lambda(s))$ of fixed points. They admit an unified formulation by adding an equation

$$m(x, \lambda) \equiv \theta < v_x, x - x_0 > + (1-\theta) v_\lambda (\lambda - \lambda_0) = 0,$$

(x_0, λ_0) and (v_x, v_λ) being the predicted point and the tangent to the curve of solutions, and $\theta \in [0, 1]$.



The system that determines a unique solution, $x \in \mathbb{R}^n$, is then

$$F(x, \lambda) = \begin{pmatrix} x - G(x, \lambda) \\ m(x, \lambda) \end{pmatrix} = 0 \in \mathbb{R}^n \times \mathbb{R}\,.$$

The system $F(x, \lambda) = 0$ is solved by Newton's method,

$$(x^{i+1}, \lambda^{i+1}) = (x^i, \lambda^i) + (\Delta x^i, \Delta \lambda^i),$$

and, at each iteration, the linear system

$$\begin{pmatrix} I - D_x G(x^i, \lambda^i) & -D_\lambda G(x^i, \lambda^i) \\ \theta v_x^\top & (1-\theta) v_\lambda \end{pmatrix} \begin{pmatrix} \Delta x^i \\ \Delta \lambda^i \end{pmatrix} = \begin{pmatrix} -x^i + G(x^i, \lambda^i) \\ -m(x^i, \lambda^i) \end{pmatrix}$$

is solved iteratively by matrix-free methods (using GMRES(M), BICGSTAB, etc.) which only require the computation of matrix products, i.e., products of the form

$$D_x G(x^i, \lambda^i) \delta x + D_\lambda G(x^i, \lambda^i) \delta \lambda.$$

The key point is that these systems need no preconditioning if the Jacobian $D_x G(x^i, \lambda^i)$ has most of its spectrum clustered around the origin. This is what happens for the fixed points of dissipative problems we want to compute.

Iterative linear algebra

Linear systems are solved by iterative Krylov methods. The class of projection methods produce, from an initial guess y_0, sequences of approximations, y_m, to the solution of a linear system $Ay = b$, which satisfy the conditions

$$y_m \in y_0 + \mathcal{K}_m \quad \text{and} \quad b - Ay_m \perp \mathcal{L}_m,$$

where $\mathcal{K}_m$ and $\mathcal{L}_m$ are two m-dimensional linear subspaces. If $\mathcal{L}_m = A\mathcal{K}_m$, y_m minimizes $||b - Ay||_2$ over $y \in y_0 + \mathcal{K}_m$.
In the particular case of GMRES, $\mathcal{L}_m = A\mathcal{K}_m$, and $\mathcal{K}_m$ is the Krylov subspace

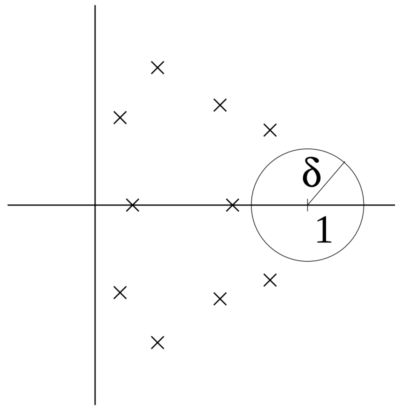
$$\mathcal{K}_m = \{r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0\},$$

with $r_0 = b - Ay_0$. It follows that $r_m = b - Ay_m = b - A(y_o + z_m) = r_0 + Az_m =$ $= p_m(A)r_0$, p_m being a polynomial of degree m, with $p_m(0) = 1$.

Proposition 1 *(Saad and Schultz 1986) Assume that A is diagonalizable with $A = V\Lambda V^{-1}$, where $\Lambda = diag\{\lambda_1, \cdots, \lambda_n\}$ is the diagonal matrix of eigenvalues, P_m is the set of polynomials of degree at most m, and $\kappa_2(V) = ||V^{-1}||_2 ||V||_2$ is the norm-2 condition number of V. Then at the m-th step of GMRES*

$$||b - Ay_m||_2 / ||b - Ay_0||_2 \leq \kappa_2(V) \inf_{\substack{p \in P_m \\ p(0)=1}} \sup_{i=1,\cdots,n} |p(\lambda_i)|.$$

Consider now a linear systems of the form



$$(I - D_x G(x,\lambda))\,\Delta x = -x + G(x,\lambda).$$

Proposition 2 *Let $\mu_1, \cdots, \mu_k$ be the eigenvalues of $D_x G(x,\lambda)$ verifying $|\mu_i| > \delta$ with a fixed $\delta < 1$, $D = \max_{i=1,\cdots,n} |\mu_i|$ and $d = \min_{i=1,\cdots,k} |1-\mu_i|$. Then the polynomial of degree $k+p$,*

$$q(z) = (1-z)^p \prod_{i=1,\cdots,k} \frac{(1-\mu_i) - z}{1-\mu_i},$$

verifies $q(0) = 1$, and

$$\sup_{i=1,\cdots,n} |q(1-\mu_i)| < \delta^p S \quad \text{with} \quad S = \sup_{|z-1|=\delta} \prod_{i=1,\cdots,k} \frac{|(1-\mu_i) - z|}{|1-\mu_i|}.$$

Moreover, $S < (\delta + D)^k / d^k$.

Continuation of fixed points of ODEs

Given a system of ODEs obtained by discretizing a system of parabolic PDE

$$\dot{x} = f(x, \lambda), \quad (x, \lambda) \in \mathcal{U} \subset \mathbb{R}^n \times \mathbb{R},$$

its fixed points can be obtained from the vector field $f(x, \lambda)$, or from the map $\varphi(T, x, \lambda) \in \mathcal{U} \subset \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$, with $\varphi(t, x, \lambda)$ the solution of the ODEs with initial condition x, because

$$f(x, \lambda) = 0 \Rightarrow x - \varphi(T, x, \lambda) = 0.$$

The time T must be large enough to have most of the spectrum of $D_x\varphi(T, x, \lambda)$ clustered at the origin, but as short as possible to save computing time.
The matrix products required can be computed by integrating the first variational equation

$$\begin{aligned} \dot{x} &= f(x, \lambda) \\ \dot{y} &= D_x f(x, \lambda) y + D_\lambda f(x, \lambda)\Delta\lambda \end{aligned} \qquad \text{with initial conditions} \qquad \begin{aligned} x(0) &= x \\ y(0) &= \Delta x. \end{aligned}$$

Then

$$D_x\varphi(T, x, \lambda)\Delta x + D_\lambda\varphi(T, x, \lambda)\Delta\lambda = y(T).$$

Each matrix product requires the time integration of a system of $2n$ equations.

Continuation of periodic orbits of ODEs

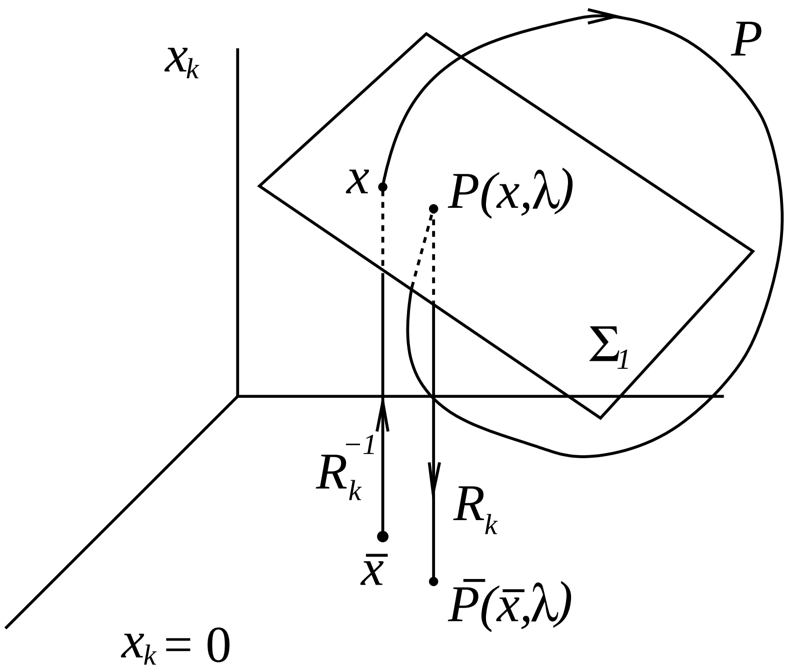
Given the system of ODEs

$$\dot{x} = f(x, \lambda), \quad (x, \lambda) \in \mathcal{U} \subset \mathbb{R}^n \times \mathbb{R},$$

its periodic orbits are obtained as fixed points of a Poincaré map $P : \mathcal{V} \subset \Sigma \to \Sigma$ defined on a hyperplane given by

$$\Sigma_1 = \left\{ x \in \mathbb{R}^n \,/\, < v_1, x - x_1^\Sigma >= 0 \right\}.$$

If v_{1_k} is the largest component of v_1, let us define R_k as the orthogonal projection from Σ_1 onto the hyperplane $x_k = 0$.



If we now define

$$\bar{P}(\bar{x}, \lambda) = R_k(P(R_k^{-1}(\bar{x}), \lambda)),$$

the fixed points of $\bar{P}$ verifying

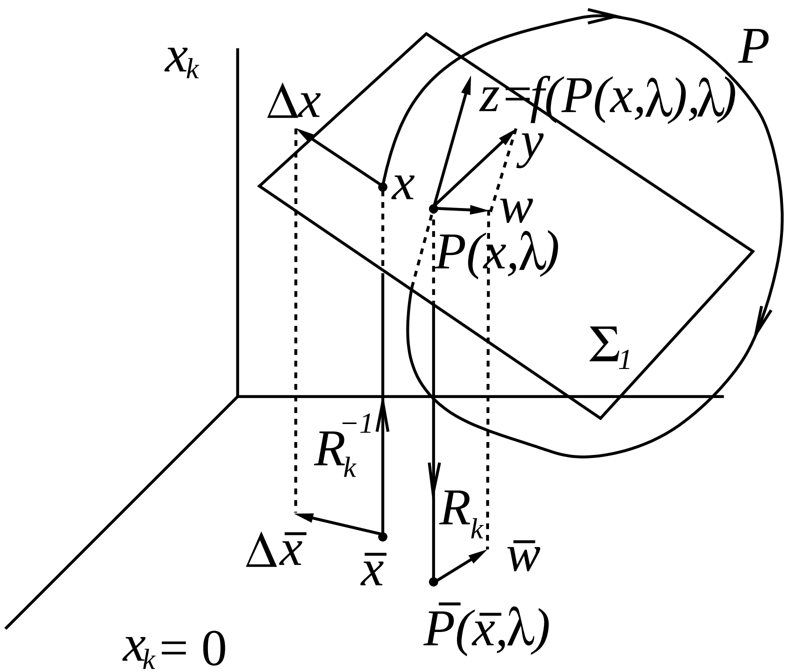
$$\bar{x} - \bar{P}(\bar{x}, \lambda) = 0, \quad \bar{x} \in \mathbb{R}^{n-1},$$

are in one-to-one correspondence with those of P by the map $x = R_k^{-1}(\bar{x})$.

By applying the chain rule to $\bar{P}(\bar{x}, \lambda)$, each matrix product requires the computation of

$$w = D_x P(x, \lambda)\Delta x + D_\lambda P(x, \lambda)\Delta\lambda = y - \frac{< v_1, y >}{< v_1, z >} z,$$

where $\Delta x = DR_k^{-1}(\bar{x})\Delta\bar{x}$ with $< v_1, \Delta x >= 0$, $z = f(P(x, \lambda), \lambda)$, $< v_1, w >= 0$, and y is the solution of the first variational equation



$$\dot{x} = f(x, \lambda)$$

$$\dot{y} = D_x f(x, \lambda)y + D_\lambda f(x, \lambda)\Delta\lambda$$

with initial conditions

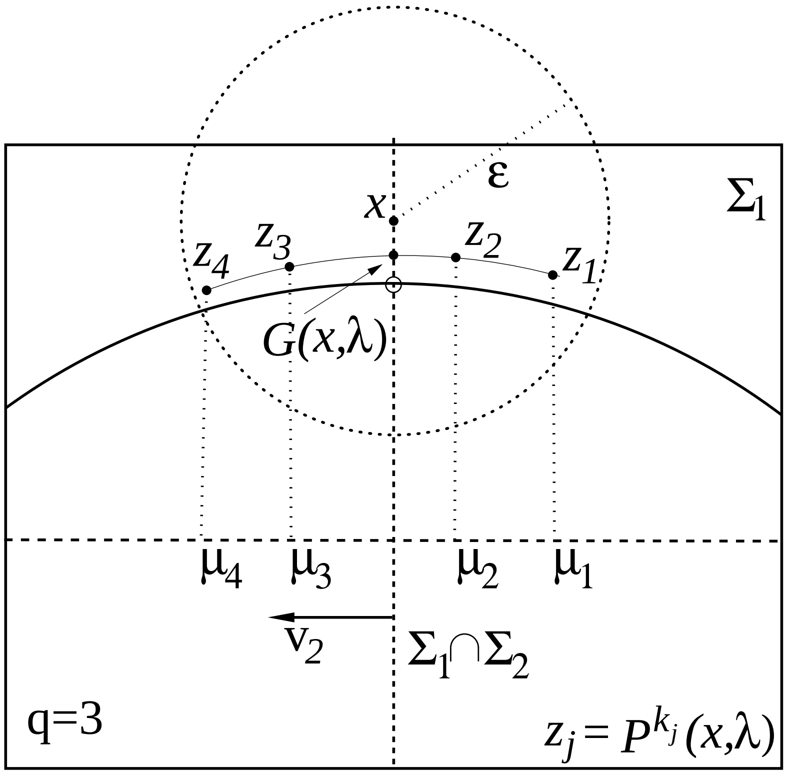
$$x(0) = x = R_k^{-1}(\bar{x})$$

$$y(0) = \Delta x = DR_k^{-1}(\bar{x})\Delta\bar{x}.$$

Each matrix product requires, the time integration of a system of $2n$ equations.

’Continuation’ of invariant 2-tori of ODEs (first method)

Let $P : \mathcal{V} \subset \Sigma_1 \to \Sigma_1$ be the Poincaré map defined on a hyperplane Σ_1, and Σ_2 another hyperplane, given by $< v_2, x - x_2^{\Sigma} >= 0$, transversal to both Σ_1 and the invariant 2-tori. Then we define the map $G(x, \lambda) : \mathcal{U} \subset \mathbb{R}^{n-2} \times \mathbb{R} \to \mathbb{R}^{n-2}$ as follows.



If $R : \Sigma_1 \cap \Sigma_2 \to \mathbb{R}^{n-2}$ is a parameterization of $\Sigma_1 \cap \Sigma_2$ then

$$G(\bar{x}, \lambda) = R(\sum_{j=1}^{q+1} l_j(0) P^{k_j}(R^{-1}(\bar{x}), \lambda)),$$

where the l_j are the Lagrange interpolation polynomials of degree q at the points

$$\mu_j =< v_2, P^{k_j}(x, \lambda) - x_2^{\Sigma} >, \quad j = 1, \cdots, q+1.$$

The fixed points of the map $G(\bar{x}, \lambda)$ are in one-to-one correspondence, by the map $x = R^{-1}(\bar{x})$, with approximations of the points of the invariant 2-tori in $\Sigma_1 \cap \Sigma_2$.

The action of the Jacobian of G on a vector reduces to the case of the differential of the Poincaré map

$$DG(\bar{x},\lambda) = R\sum_{i=1}^{q+1}\Bigg[l_i(0)DP^{k_i}(x,\lambda) + P^{k_i}(x,\lambda)\sum_{j=1}^{q+1}\partial_{\mu_{k_j}} l_i(0) v_2^T DP^{k_j}(x,\lambda)\Bigg] D_{\bar{x}}R^{-1}(\bar{x}),$$

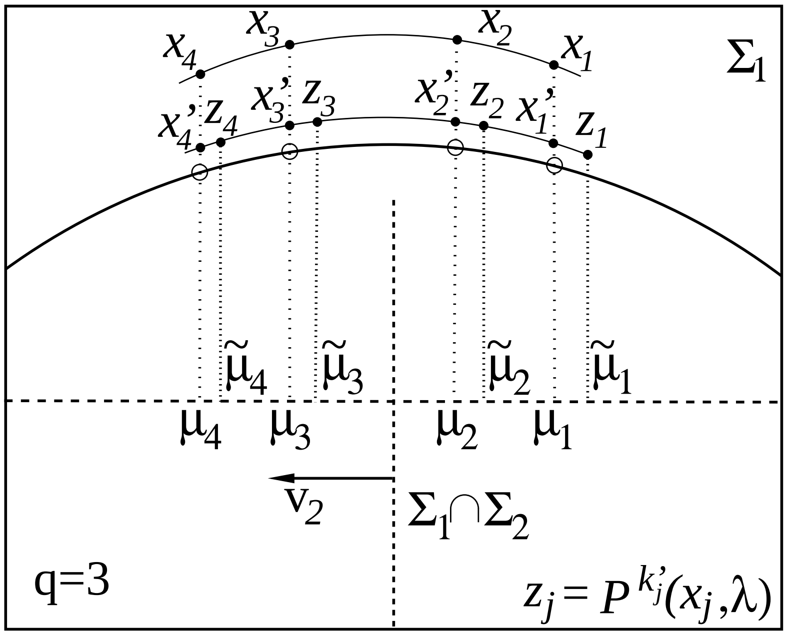
with $x = R^{-1}(\bar{x})$.

The radius ε defining G must be varied adaptively during the continuation process.

'Continuation' of invariant 2-tori of ODEs (second method)

Let $P : \mathcal{V} \subset \Sigma_1 \to \Sigma_1$ be the Poincaré map defined on a hyperplane Σ_1, and Σ_2 another hyperplane, given by $< v_2, x - x_2^{\Sigma} >= 0$, transversal to both Σ_1 and the invariant 2-tori. Let $\mu_1, \cdots, \mu_{q+1}$ be $q+1$ fixed coordinates along the line $x = x_2^{\Sigma} + \mu v_2$. Then we define the map G as follows. If $X = (x_1, \cdots, x_{q+1}) \in \mathcal{U} \subset \mathbb{R}^{(n-1)(q+1)}$

$$G(X, \lambda) : \mathcal{U} \subset \mathbb{R}^{(n-1)(q+1)} \times \mathbb{R} \to \mathbb{R}^{(n-1)(q+1)}.$$



$$G(X, \lambda) = X' = Z(X, \lambda)\tilde{V}(X, \lambda)^{-1}V, \quad \text{with}$$

$$X' = (x_1', \cdots, x_{q+1}'),\ Z(X, \lambda) = (z_1, \cdots, z_{q+1}),$$

and V and $\tilde{V}$ the Vandermonde matrices

$$V = \begin{pmatrix} 1 & \cdots & 1 \\ \mu_1 & \cdots & \mu_{q+1} \\ \cdots & \cdots & \cdots \\ \mu_1^q & \cdots & \mu_{q+1}^q \end{pmatrix}$$

associated with the μ_j and the $\tilde{\mu}_j =< v_2, P^{k_j'}(x_j, \lambda) - x_2^{\Sigma} >, \quad j = 1, \cdots, q+1$ respectively.

The fixed points of the map $G(X, \lambda)$ approximate an arch of the invariant curve in Σ_1.

The action by the Jacobian of $G = Z\tilde{V}^{-1}V$ also reduces to that of the Poincaré map. If $\Delta X = (\Delta x_1, \cdots, \Delta x_{q+1})$ then

$$DG(X,\lambda)(\Delta X, \Delta\lambda) =$$

$$\left[DZ(X,\lambda)(\Delta X,\Delta\lambda) - Z(X,\lambda)\tilde{V}(X,\lambda)^{-1}D\tilde{V}(X,\lambda)(\Delta X,\Delta\lambda)\right]\tilde{V}(X,\lambda)^{-1}V$$

where

$$DZ(X,\lambda)(\Delta X,\Delta\lambda) = (DP^{k'_1}(x_1,\lambda)(\Delta x_1,\Delta\lambda), \cdots, DP^{k'_{q+1}}(x_{q+1},\lambda)(\Delta x_{q+1},\Delta\lambda)),$$

$$D\tilde{V}(X,\lambda)(\Delta X,\Delta\lambda) = \begin{pmatrix} 0 & \cdots & 0 \\ 1 & \cdots & 1 \\ 2\tilde{\mu}_1 & \cdots & 2\tilde{\mu}_{q+1} \\ \cdots & \cdots & \cdots \\ q\tilde{\mu}_1^{q-1} & \cdots & q\tilde{\mu}_{q+1}^{q-1} \end{pmatrix} \begin{pmatrix} \eta_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \eta_{q+1} \end{pmatrix},$$

and $\eta_j =< v_2, DP^{k'_j}(x_j,\lambda)(\Delta x_j,\Delta\lambda) >$. In short, $DG = \left[DZ - Z\tilde{V}^{-1}D\tilde{V}\right]\tilde{V}^{-1}V$.

The radius ε and the position of the μ_j defining G must be varied adaptively during the continuation process.

Thermal convection in binary fluid mixtures

The equations in $\Omega = [0, \Gamma] \times [0, 1]$ for the perturbation of the basic state ($\mathbf{v}_c = 0$, $T_c = T_c(0) - z$, and $C_c = C_c(0) - z$) in non-dimensional form are

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \sigma \nabla^2 \mathbf{v} - \nabla p + \sigma Ra(\Theta + SC)\hat{e}_z,$$

$$\partial_t \Theta + (\mathbf{v} \cdot \nabla)\Theta = \nabla^2 \Theta + v_z,$$

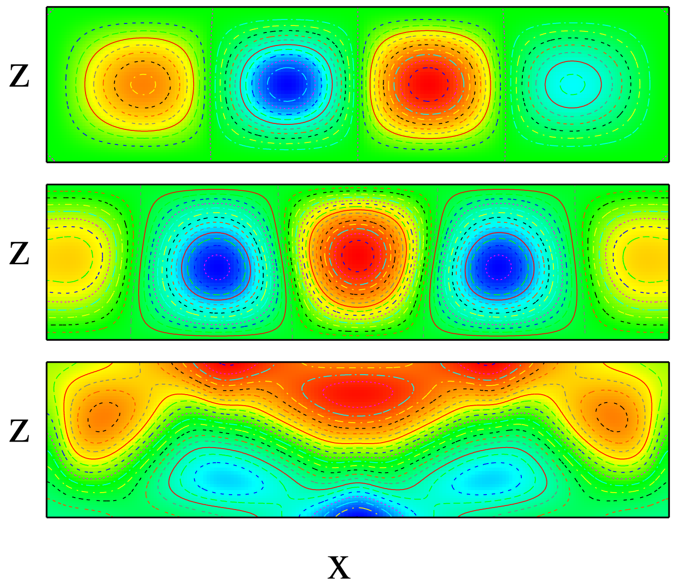
$$\partial_t C + (\mathbf{v} \cdot \nabla)C = L(\nabla^2 C - \nabla^2 \Theta) + v_z,$$

$$\nabla \cdot \mathbf{v} = 0.$$

The boundary conditions are non-slip for $\mathbf{v}$, constant temperatures at top and bottom and insulating lateral walls for Θ, and impermeable boundaries for C.

The parameters are

Γ	Aspect ratio (4)
σ	Prandtl number (0.6)
S	Separation ratio (-0.1)
L	Lewis number (0.03)
Ra	Rayleigh number (control)



To simplify the system, a streamfunction $\mathbf{v} = (-\partial_z\psi, \partial_x\psi)$, and an auxiliary function $\eta = C - \Theta$ are used. Then

$$\begin{aligned}
&\partial_t\nabla^2\psi + J(\psi, \nabla^2\psi) = \sigma\nabla^4\psi + \sigma Ra\left[(S+1)\partial_x\Theta + S\partial_x\eta\right],\\
&\partial_t\Theta + J(\psi, \Theta) = \nabla^2\Theta + \partial_x\psi,\\
&\partial_t\eta + J(\psi, \eta) = L\nabla^2\eta - \nabla^2\Theta,
\end{aligned}$$

with $J(f, g) = \partial_x f\partial_z g - \partial_z f\partial_x g$. The boundary conditions are now

$$\begin{aligned}
\psi = \partial_n\psi = \partial_n\eta = 0 \quad &\text{at} \quad \partial\Omega,\\
\Theta = 0 \quad &\text{at} \quad z = 0, 1,\\
\partial_x\Theta = 0 \quad &\text{at} \quad x = 0, \Gamma.
\end{aligned}$$

The symmetry group of the equations is $\mathbb{Z}_2 \times \mathbb{Z}_2$ generated by the two reflections:

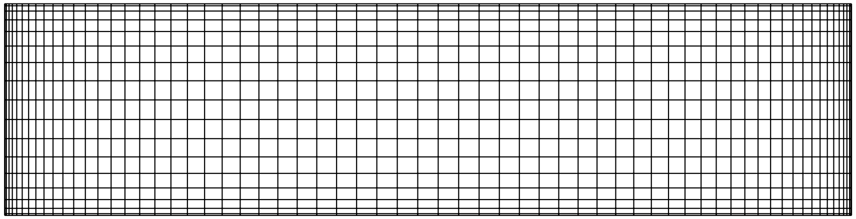
$$\begin{aligned}
R_x &: (t, x, z, \psi, \Theta, \eta) \to (t, \Gamma - x, z, -\psi, \Theta, \eta),\\
R_z &: (t, x, z, \psi, \Theta, \eta) \to (t, x, 1 - z, -\psi, -\Theta, -\eta).
\end{aligned}$$

Spatial discretization

The functions ψ, Θ, and η are approximated by a collocation method on a mesh of $n_x \times n_y = 64 \times 16$ Gauss-Lobatto points (the number of unknowns is $3n_x n_y = 3072$)

$$(x_i, y_j) = \left(\frac{\Gamma}{2}\left(1 - \cos\left(\frac{\pi i}{n_x + 1}\right)\right), \frac{1}{2}\left(1 - \cos\left(\frac{\pi j}{n_y + 1}\right)\right)\right)$$

with $i = 0, \cdots, n_x + 1$, and $j = 0, \cdots, n_y + 1$ is used. A function f is approximated by



$$f(x, y) \approx \sum_{i=0}^{n_x+1} \sum_{j=0}^{n_y+1} f(x_i, y_j) L_{x_i}(x) L_{y_j}(y)$$

where $L_{x_i}(x)$ and $L_{y_j}(y)$ are the Lagrange polynomials verifying $L_{x_i}(x_k) = \delta_{ik}$ and $L_{y_j}(y_l) = \delta_{jl}$, and the spatial derivatives are approximated as

$$\partial_x^p \partial_y^q f(x, y) \approx \sum_{i=0}^{n_x+1} \sum_{j=0}^{n_y+1} f(x_i, y_j) L_{x_i}^{(p)}(x) L_{y_j}^{(q)}(y).$$

Time integration

The system of ODEs obtained after spatial discretization,

$$L_0 \dot{u} = Lu + B(u,u),$$

can be integrated with fixed or variable stepsize and order.
The most sophisticated method employed is a semi-implicit variable-stepsize variable-order (VSVO) implementation of the BDF-extrapolation formulas (IMEX-BDF) which, for a fixed time step, are

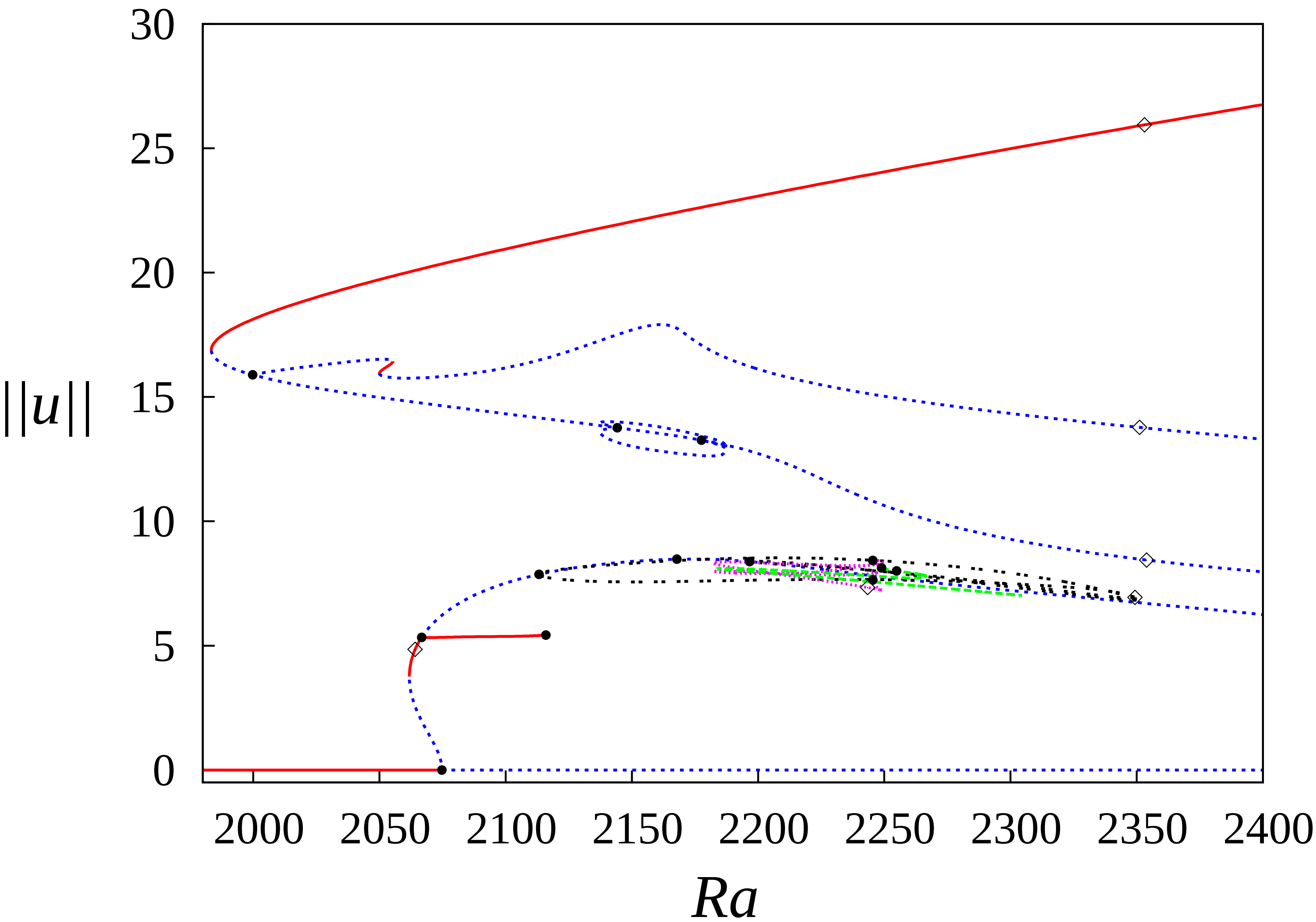
$$\frac{1}{\Delta t} L_0 \left(\gamma_0 u^{n+1} - \sum_{i=0}^{k-1} \alpha_i u^{n-i} \right) = L u^{n+1} + \sum_{i=0}^{k-1} \beta_i B(u^{n-i}, u^{n-i}).$$

A linear system

$$\left(I - \frac{\Delta t}{\gamma_0} L_0^{-1} L \right) u^{n+1} = \sum_{i=0}^{k-1} \frac{\alpha_i}{\gamma_0} u^{n-i} + \Delta t \sum_{i=0}^{k-1} \frac{\beta_i}{\gamma_0} L_o^{-1} B(u^{n-i}, u^{n-i})$$

has to be solved at each time step. This done by direct methods or by using GMRES again with a suitable preconditioner which is only updated when it is required.

Results



30
25
20
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10
5
0
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2100
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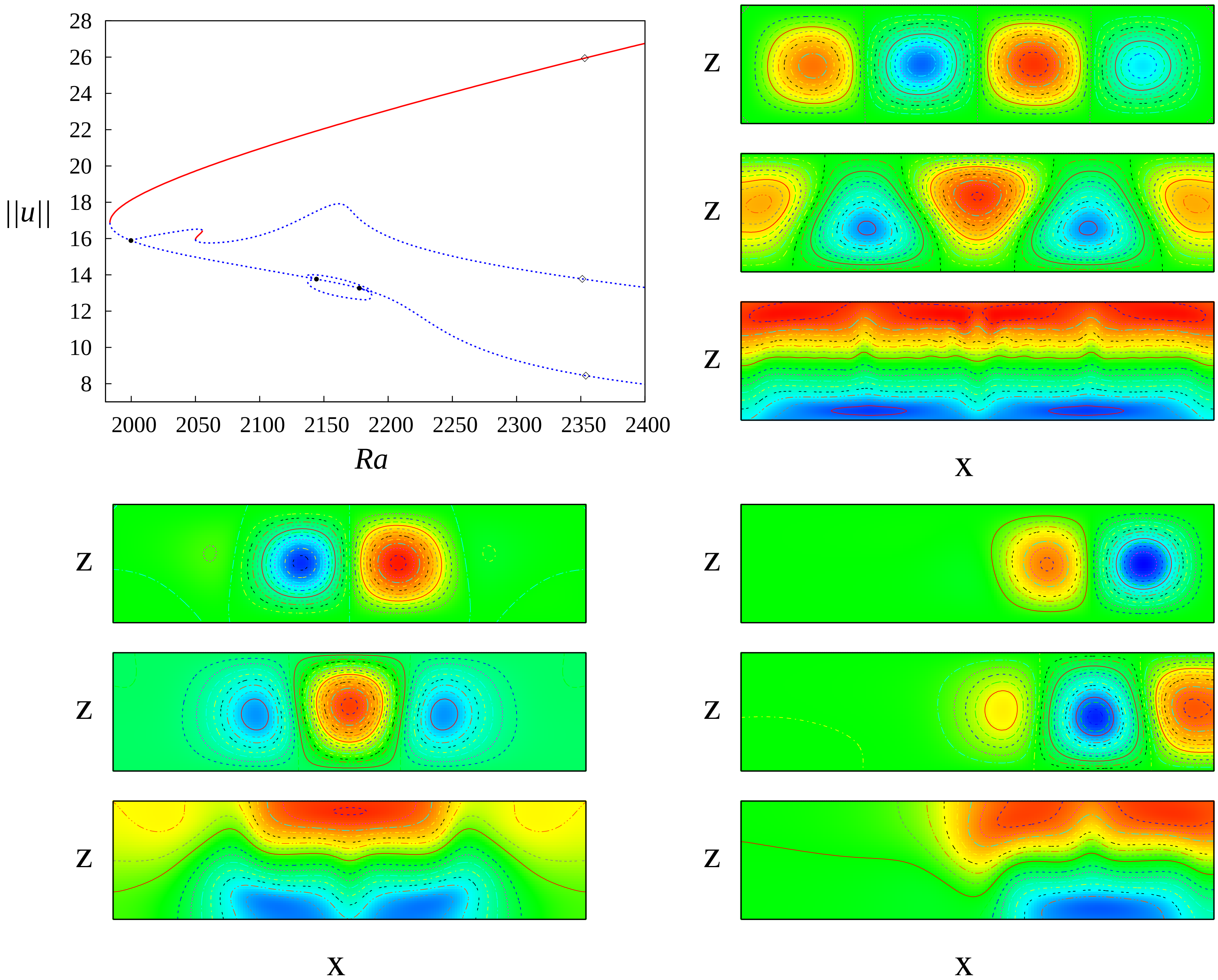
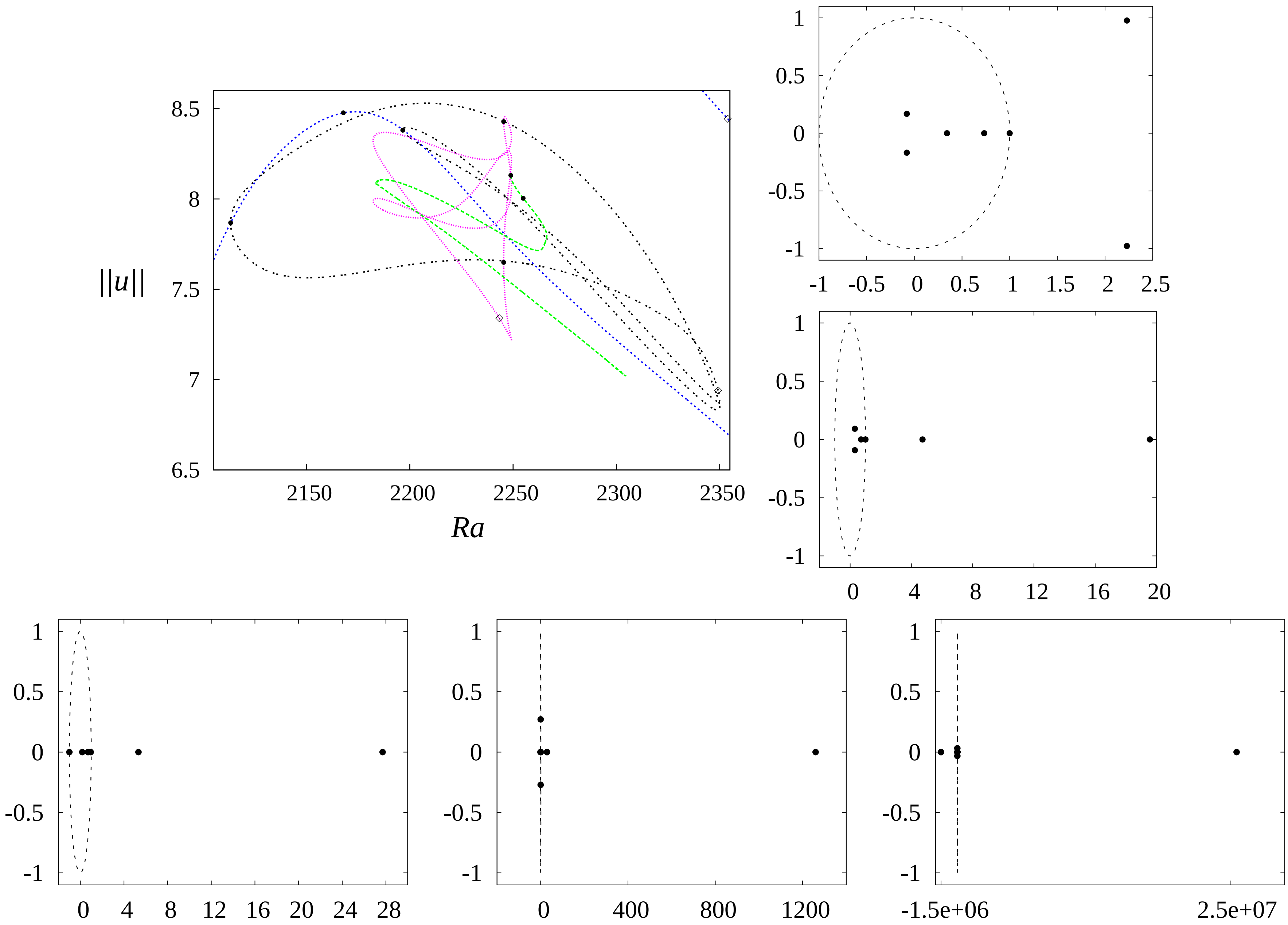
Ra

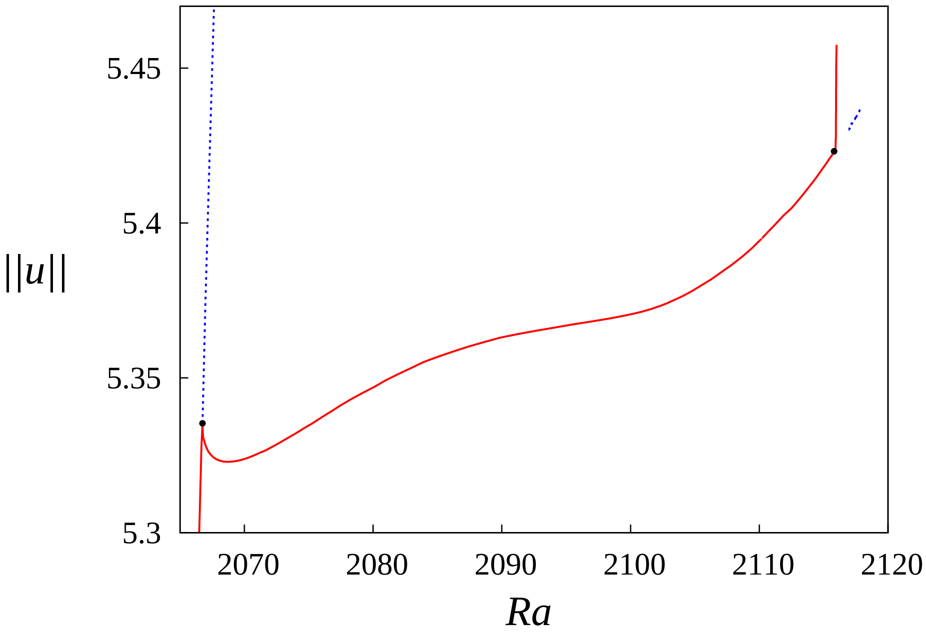
Fixed points

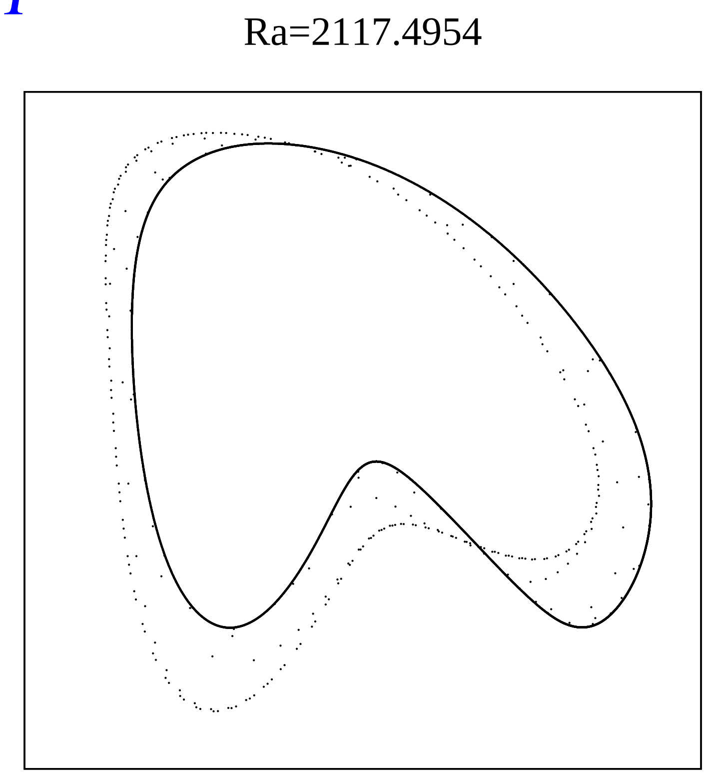


Periodic orbits



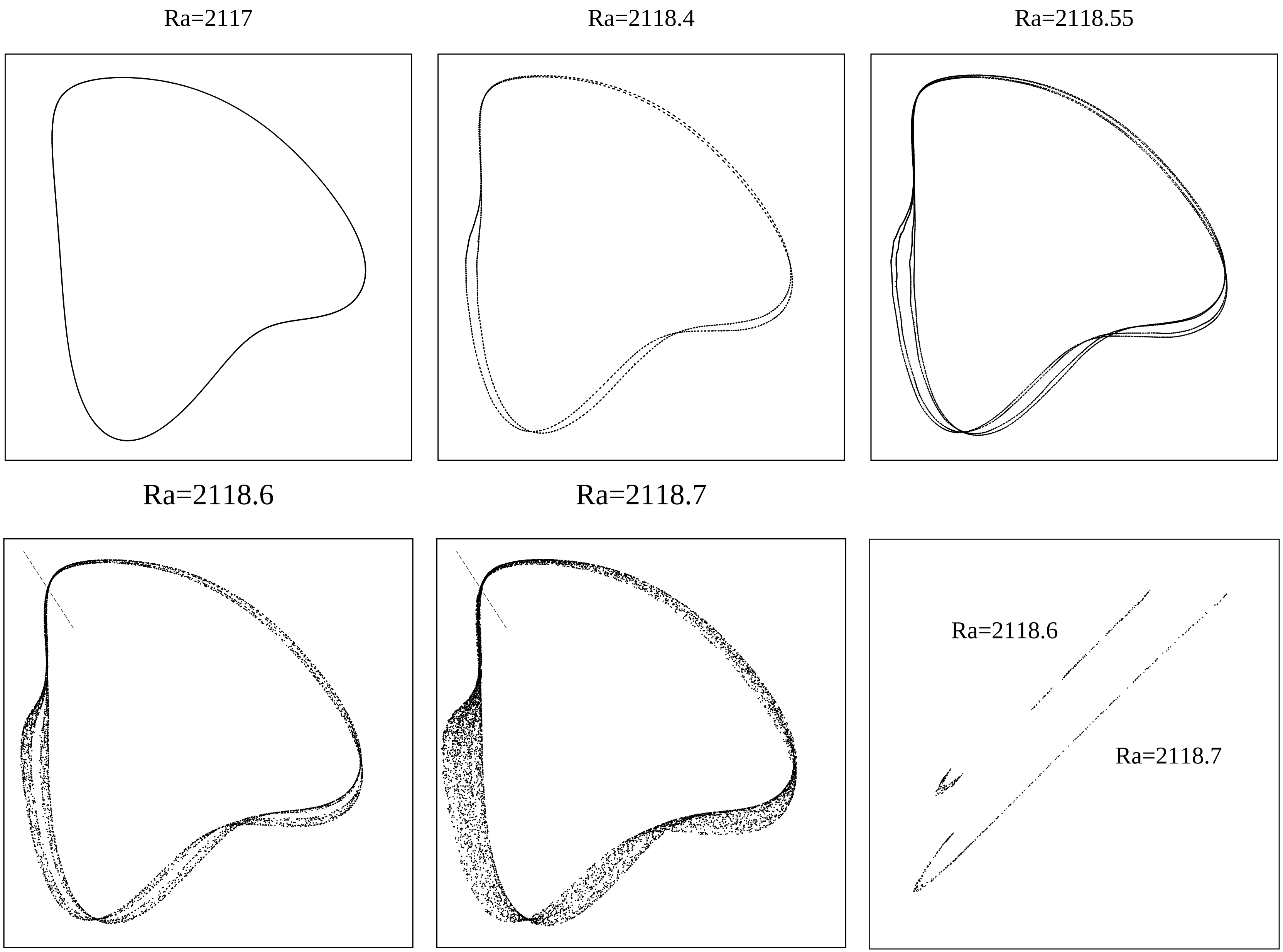
Invariant tori



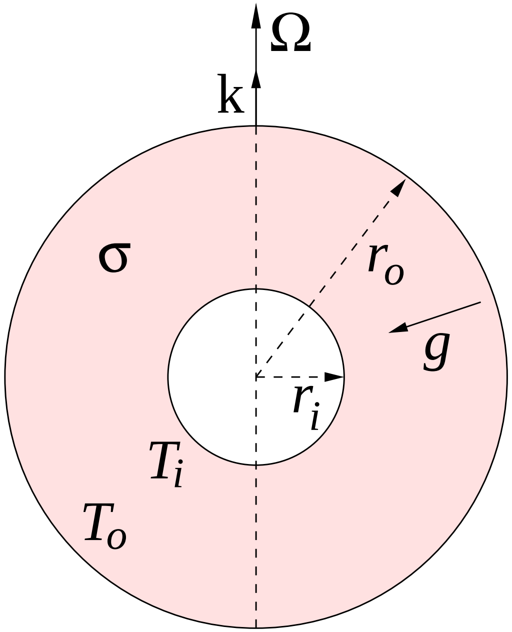


- Beginning of the branch: $Ra = 2066.74$
- $1/7$–resonance interval $2102.79 < Ra < 2102.80$
- Pitchfork bifurcation $Ra \approx 2115.92$
- $1/8$–resonance interval $2116.18 \leq Ra \leq 2116.20.$
- First period doubling $Ra \approx 2118.40$
- Second period doubling $Ra \approx 2118.55$
- Breakdown of the torus $Ra \approx 2118.60$

Breakdown of the invariant tori



Thermal convection in rotating spherical shells



We consider $\mathbf{g} = -\gamma\mathbf{r}$, with $\gamma > 0$ and $\mathbf{r} = (x, y, z)$, a difference of temperature between the two bounding spheres $\Delta T = T_i - T_o > 0$, and $\Omega^2/\gamma \ll 1$.
In the Boussinesq approximation all physical parameters are considered constant, except the density which is assumed to vary linearly with the temperature, $\rho = \rho_0(1 - \alpha(T - T_0))$, just in the gravity force term of the momentum equation.

The non-dimensional equations governing the dynamics of the fluid are written in spherical coordinates (r, θ, φ), in the rotating frame of reference of the spheres:

$$\partial_t \mathbf{v} + (\mathbf{v}\cdot\nabla)\,\mathbf{v} + 2E^{-1}\mathbf{k}\times\mathbf{v} = -\nabla p + \nabla^2\mathbf{v} + \Theta\mathbf{r},$$

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

$$\sigma\left(\partial_t\Theta + \mathbf{v}\cdot\nabla\Theta\right) = \nabla^2\Theta + R\eta(1-\eta)^{-2}r^{-3}\mathbf{r}\cdot\mathbf{v}.$$

where $\Theta = T - T_c$, is the temperature perturbation from the conduction state $\mathbf{v} = 0$ and $T_c(r) = T_0 + R\eta/\sigma(1-\eta)^2 r$.

Parameters and scalar potentials for the velocity

The non-dimensional parameters are

$\eta = r_i/r_o$	Radius ratio (0.32–0.35)
$\sigma = \nu/\kappa$	Prandtl number (0.1)
$E = \nu/\Omega d^2$	Ekman number (10^{-4})
$R = \sigma Gr = \gamma\alpha\Delta T d^4/\kappa\nu$	Rayleigh number (control and $O(10^5)$),

with $\Omega = |\mathbf{\Omega}|$, $d = r_o - r_i$, and κ, α, ν, the thermal diffusivity, the thermal expansion coefficient and the kinematic viscosity, respectively.

The symmetry group of the system is $SO(2) \times \mathbb{Z}_2$. Then when the conduction state becomes unstable at a Hopf bifurcation, it gives rise to azimuthal waves.

To reduce the number of equations they are written in terms of two scalar potentials (toroidal and poloidal) for the velocity field, i.e.,

$$\mathbf{v} = \nabla \times (\Psi \mathbf{r}) + \nabla \times \nabla \times (\Phi \mathbf{r}) \,.$$

The equations for the potentials are obtained by applying the operators $\mathbf{r} \cdot \nabla\times$ and $\mathbf{r} \cdot \nabla \times \nabla\times$ to the momentum equation.

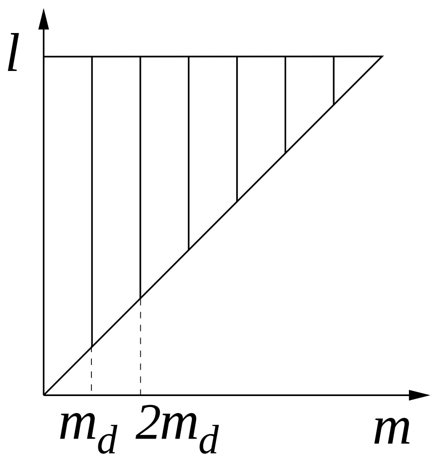
Expansion in spherical harmonics

The velocity potentials and the perturbation of the temperature from the conduction state are expanded in spherical harmonics series up to degree (l) and order (m) L as

$$(\Psi,\Phi,\Theta)(t,r,\theta,\varphi)=\sum_{l=0}^{L}\sum_{\substack{m=-l\\ m=\dot{m}_d}}^{l}(\Psi_l^m,\Phi_l^m,\Theta_l^m)(t,r)Y_l^m(\theta,\varphi),\quad \text{where}$$

$$Y_l^m(\theta,\varphi)=\sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi},\ l\geq 0,\ -l\leq m\leq l,$$

and $\Psi_l^{-m}=\overline{\Psi_l^m}$, $\Phi_l^{-m}=\overline{\Phi_l^m}$, and $\Theta_l^{-m}=\overline{\Theta_l^m}$. Moreover, to have the two potentials completely determined we can choose $\Psi_0^0=\Phi_0^0=0$.



The unknowns are the values of Ψ_l^m, Φ_l^m, and Θ_l^m for $0\leq l\leq L$ and $0\leq m=\dot{m}_d\leq l$, at a mesh of n_r Gauss-Lobatto points in the radius interval $[r_i,r_o]$. In the calculations shown $n_r=32$, and $60\leq L\leq 80$ depending on the selected m_d. This gives a total dimension $57691\leq n\leq 345991$ depending on L and m_d.

The equations for the amplitudes are

$$\partial_t \Psi_l^m = \mathcal{D}_l \Psi_l^m + \frac{1}{l(l+1)} \left[2E^{-1}\left(im\Psi_l^m - [Q\Phi]_l^m\right) - [\mathbf{r}\cdot\nabla\times(\boldsymbol{\omega}\times\mathbf{v})]_l^m\right],$$

$$\partial_t \mathcal{D}_l \Phi_l^m = \mathcal{D}_l^2 \Phi_l^m - \Theta_l^m + \frac{1}{l(l+1)} \left[2E^{-1}\left(im\mathcal{D}_l\Phi_l^m + [Q\Psi]_l^m\right)\right.$$

$$\left. + [\mathbf{r}\cdot\nabla\times\nabla\times(\boldsymbol{\omega}\times\mathbf{v})]_l^m\right],$$

$$\partial_t \Theta_l^m = \sigma^{-1}\mathcal{D}_l \Theta_l^m + \sigma^{-1} l(l+1) R\eta(1-\eta)^{-2} r^{-3} \Phi_l^m - [\mathbf{v}\cdot\nabla\Theta]_l^m.$$

for $0 \le l \le L$ and $0 \le m = \dot{m}_d \le l$, and where $\boldsymbol{\omega} = \nabla\times\mathbf{v}$ is the vorticity, $\mathcal{D}_l = \partial_{rr}^2 + (2/r)\partial_r - l(l+1)/r^2$, and the operator Q is defined by its action on a function f expanded in spherical harmonics as

$$[Qf]_l^m = -l(l+2)c_{l+1}^m D_{l+2}^+ f_{l+1}^m - (l-1)(l+1)c_l^m D_{1-l}^+ f_{l-1}^m,$$

with $c_l^m = ((l^2-m^2)/(4l^2-1))^{1/2}$ and $D_l^+ f = \partial_r f + lf/r$.
On the boundaries $r_i = \eta/(1-\eta)$ and $r_o = 1/(1-\eta)$, stress-free ($\Phi_l^m = \partial_{rr}^2\Phi_l^m = \partial_r(\Psi_l^m/r) = 0$) or non-slip ($\Phi_l^m = \partial_r\Phi_l^m = \Psi_l^m = 0$) boundary conditions may be selected for the velocity field (the second are used in this study).
Perfectly conducting ($\Theta_l^m = 0$) boundaries are used for the temperature.

Waves

The above system will be written as

$$L_0 \partial_t u = Lu + B(u, u),$$

where u is a vector containing the values of the amplitudes at the mesh of collocation points in the radius, L and B are, respectively, linear and bilinear operators, and L depends on all the parameters of the problem. In particular on $p = R$, and we will write $L = L(p)$.
At critical values of $p = p_c$, the conduction state $u = 0$ becomes unstable, and branches of azimuthal waves starts there. Then, at these values of p, there are vectors v_c and frequencies ω_c such that $i\omega_c L_0 v_c = L v_c$.
The waves $u(t, r, \theta, \varphi) = \tilde{u}(r, \theta, \varphi - \omega t)$, satisfy $\omega L_0 \partial_{\tilde{\varphi}} \tilde{u} + L\tilde{u} + B(\tilde{u}, \tilde{u}) = 0$, with $\tilde{\varphi} = \varphi - \omega t$, or, by deleting the tildes,

$$F(u, \omega, p) = \omega L_0 \partial_\varphi u + L(p)u + B(u, u) = 0.$$

This equation must be supplemented by adding a phase condition. We use the condition $G(u) =< u, \partial_\varphi u_c >= 0$, and u_c is a reference solution (the eigenvector, $u_c = v_c$, at $p = p_c$, or a previously computed solution). It is a necessary condition for $||u - u_c||_2^2$ to be minimal with respect to the phase.

Continuation of the waves

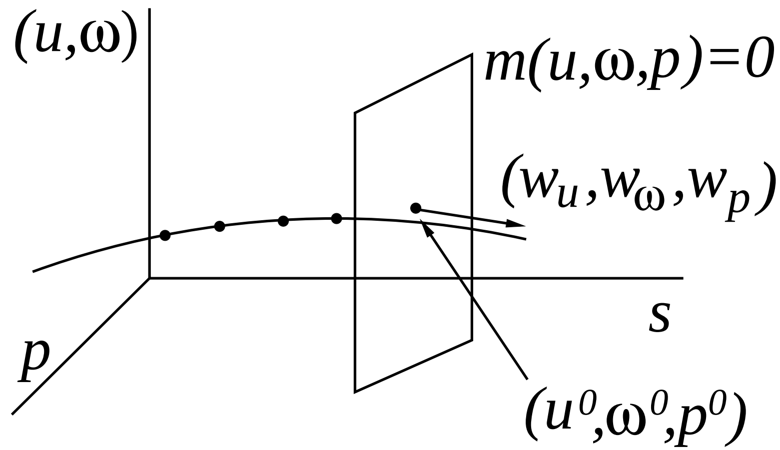
To study the dependence of the waves on p, we use parameter and pseudo-arclength-like continuation methods which allow to obtain the curves $(u(s), \omega(s), p(s))$. They admit an unified formulation by adding an equation

$$m(u, \omega, p) \equiv w_u^\top (u - u^0) + w_\omega(\omega - \omega^0) + w_p(p - p^0) = 0,$$

(u^0, ω^0, p^0) and (w_x, w_ω, w_p) being the predicted point and tangent to the curve of solutions, respectively.

The system which determines a unique solution, $(u, \omega, p) \in \mathbb{R}^{n+2}$ is

$$F(u, \omega, p) = 0,$$
$$G(u) = 0,$$
$$m(u, \omega, p) = 0.$$



Newton-Krylov methods are used to solve it. For the linear systems we use GMRES which requires the action by the matrix and a suitable preconditioner.

The action of the Jacobian $(\partial_u F, \partial_\omega F, \partial_p F)(u, \omega, p)$ on (v, ζ, μ) is

$$\omega L_0 \partial_\varphi v + L(p)v + \zeta L_0 \partial_\varphi u + \mu L^{(2)} u + B(u, v) + B(v, u),$$

due to the dependence of L on p, which has the form $L(p) = L^{(1)} + pL^{(2)}$. The action of the Jacobian $\partial_u G(u)$ on (v, ζ, μ) is $\partial_u G(u)v =< v, \partial_\varphi u_c >$. During the continuation process to study the dependence of the waves with p, linear systems of equations with matrices

$$\begin{pmatrix} \partial_u F & \partial_\omega F & \partial_p F \\ \partial_u G & 0 & 0 \\ w_u^\top & w_\omega & w_p \end{pmatrix}$$

must be solved. They are preconditioned by matrices of the form

$$\begin{pmatrix} \omega_{prec} L_0 \partial_\varphi + L_{prec} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

with $L_{prec} = L(p_{prec})$ and ω_{prec} being the operator L and the frequency of the wave at a previous step. Since L is block-tridiagonal, due to the operator Q, it is possible to solve this latter system efficiently.

Stability of the waves

Suppose a wave of the form $u(t, r, \theta, \varphi) = \tilde{u}(r, \theta, \varphi - \omega t)$ has been found. To study the stability of his solution, the first option is to apply Floquet theory which implies integrating the variational equation

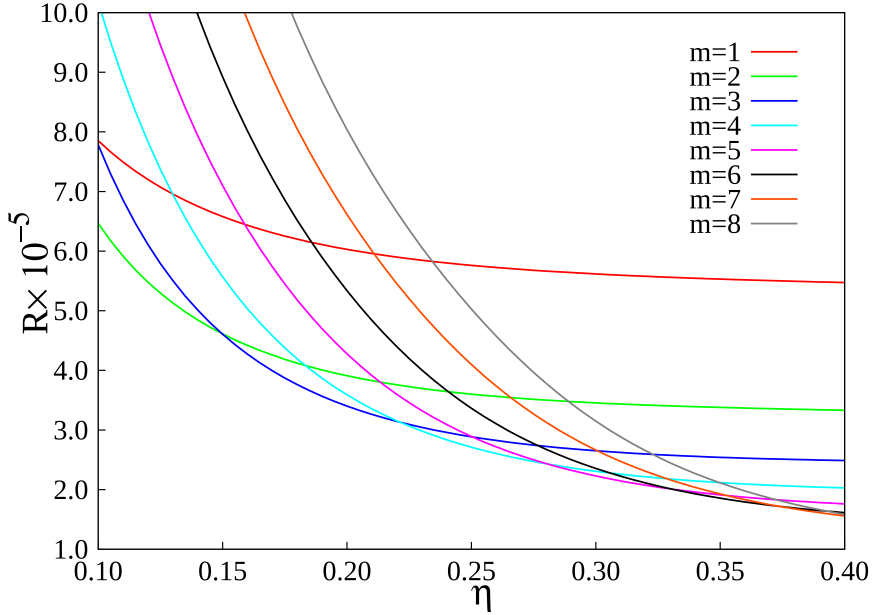
$$L_0 \partial_t v = Lv + B(u(t), v) + B(v, u(t)),$$

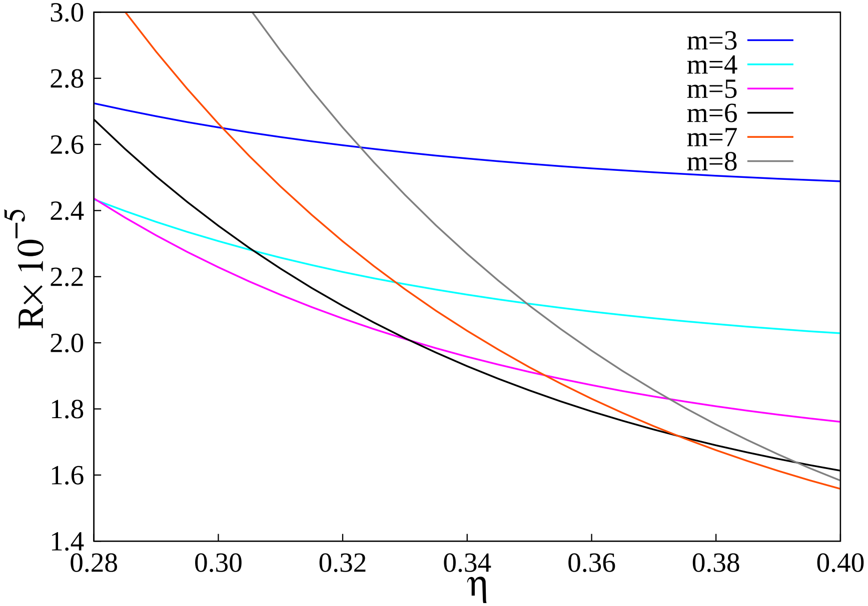
where we have written $u(t) = \tilde{u}(r, \theta, \varphi - \omega t)$. If $\chi(t, v)$ is its solution with initial condition v at $t = 0$, the leading eigenvalues of the map $v \longrightarrow \chi(T, v)$ must be computed, T being the period of the wave. This method is robust but expensive.
Another possibility consists on studying the stability of u as fixed point as it is found. We consider a perturbation $\tilde{u}(r, \theta, \varphi - \omega t) + v(t, r, \theta, \varphi - \omega t)$. Then the eigenvalue problem

$$\lambda v = \mathcal{L} v \quad \text{with} \quad \mathcal{L} v = L_0^{-1} \left(Lv + \omega L_0 \partial_\varphi v + B(\tilde{u}, v) + B(v, \tilde{u}) \right),$$

must be solved. The problem of this second option is that a transformation must be used (shift-invert, Cayley, double complex shift, etc.), and the corresponding linear systems to be solved must be preconditioned. This method is computationally cheap but some of the relevant eigenvalues can be missed.

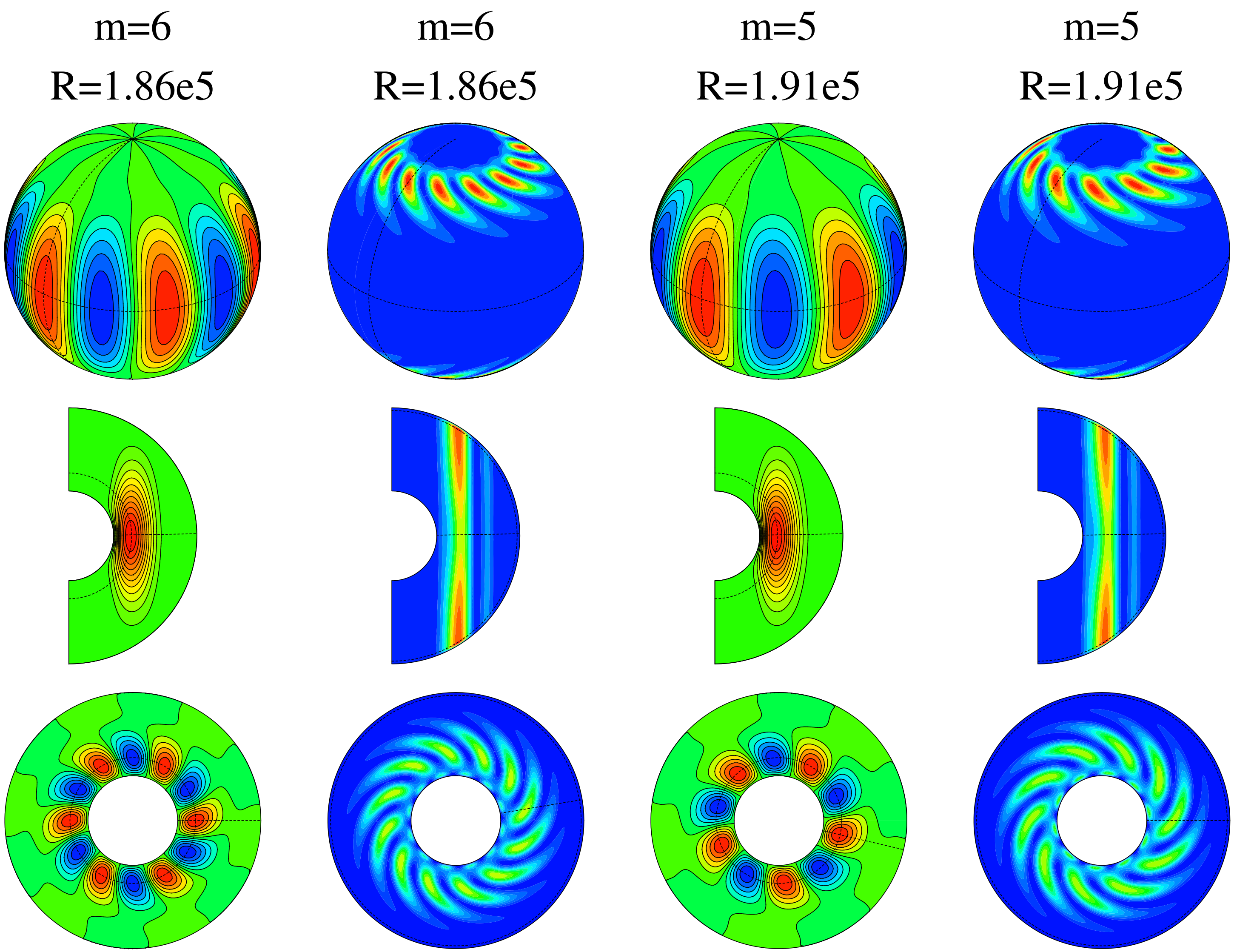
Stability of the conduction state





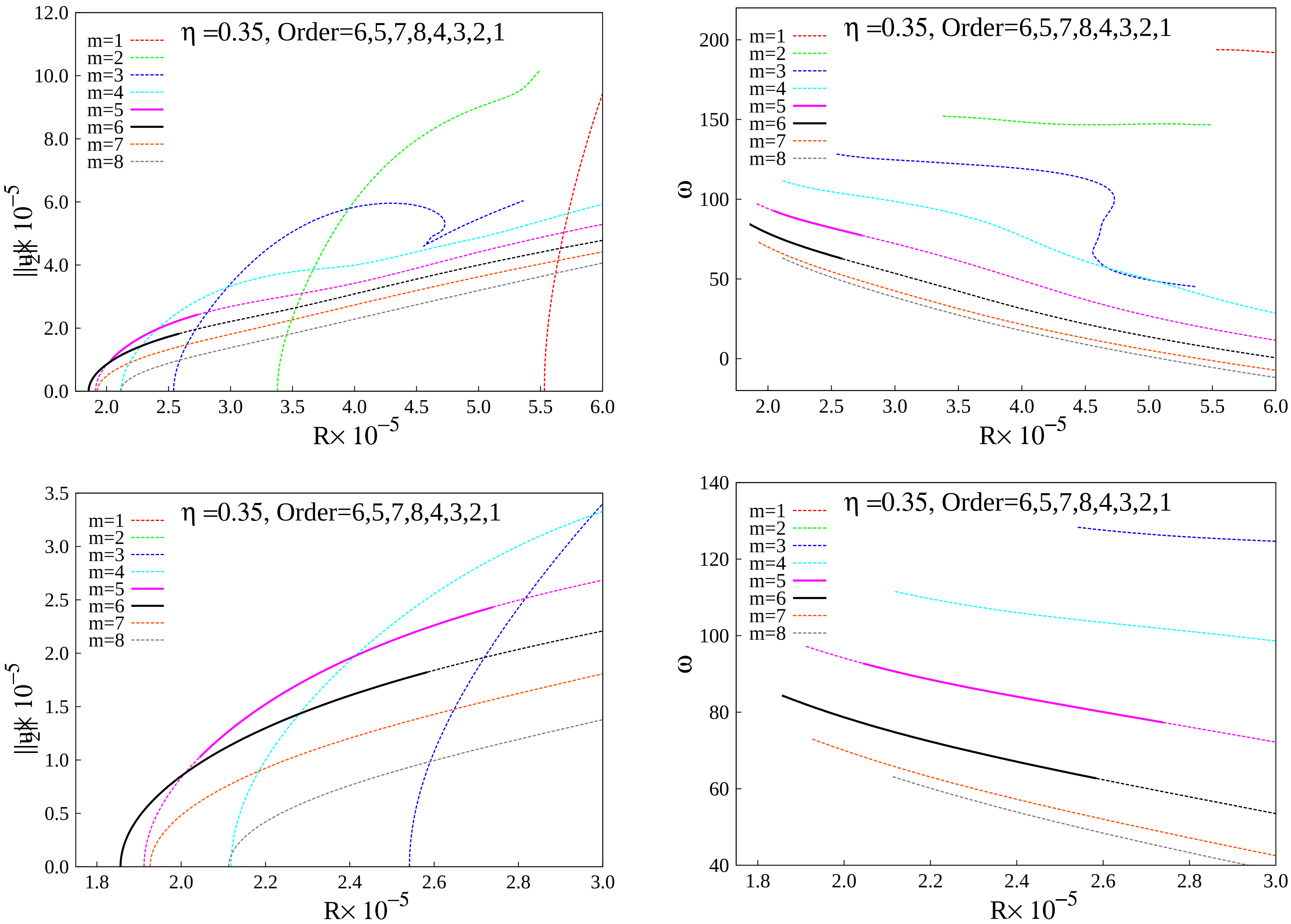
Critical Rayleigh number versus η for $m = 1, \cdots, 8$, $\sigma = 0.1$, and $E = 10^{-4}$.

Eigenfunctions at the bifurcations from the conduction state



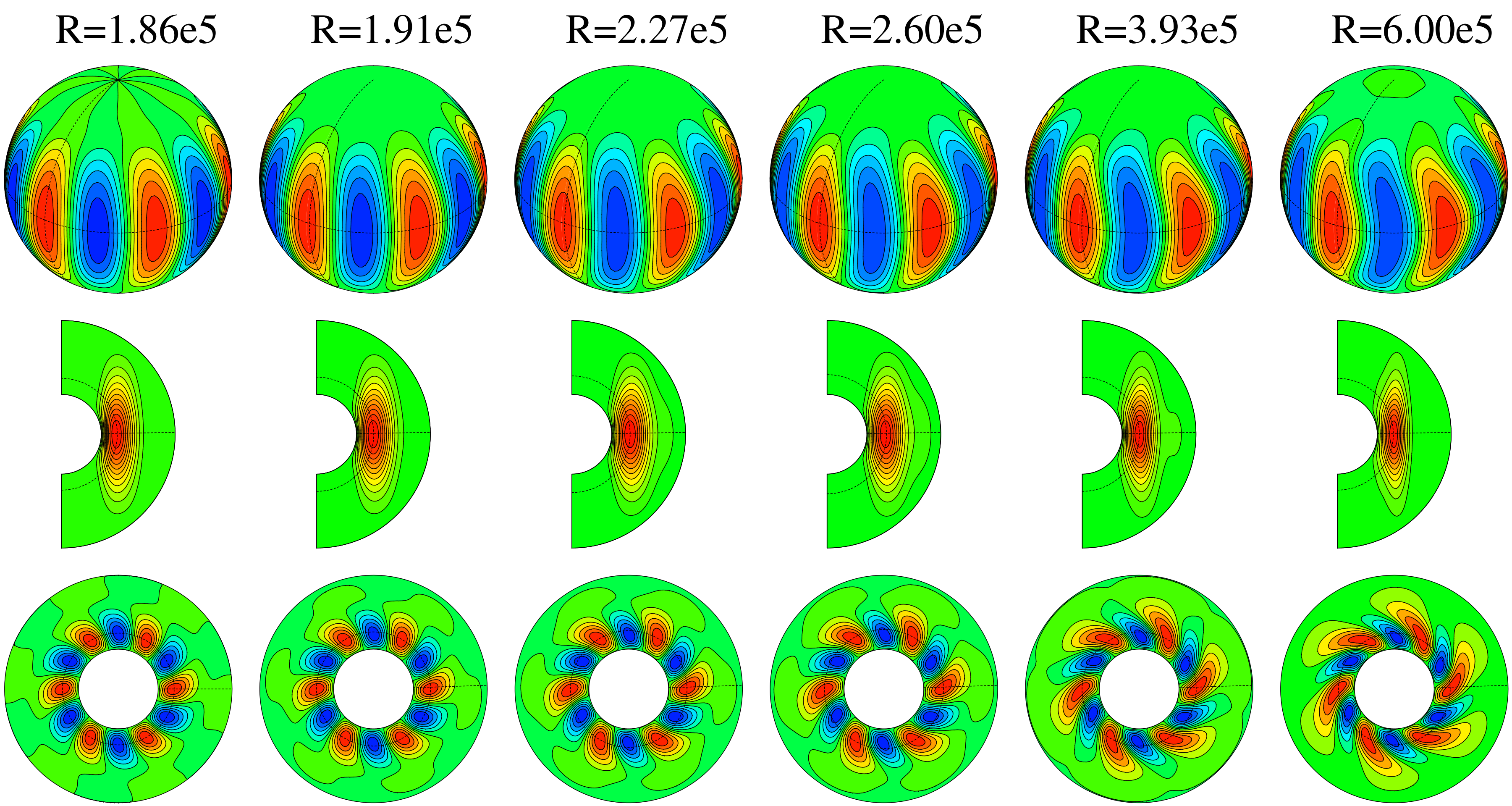
$\eta = 0.35.$

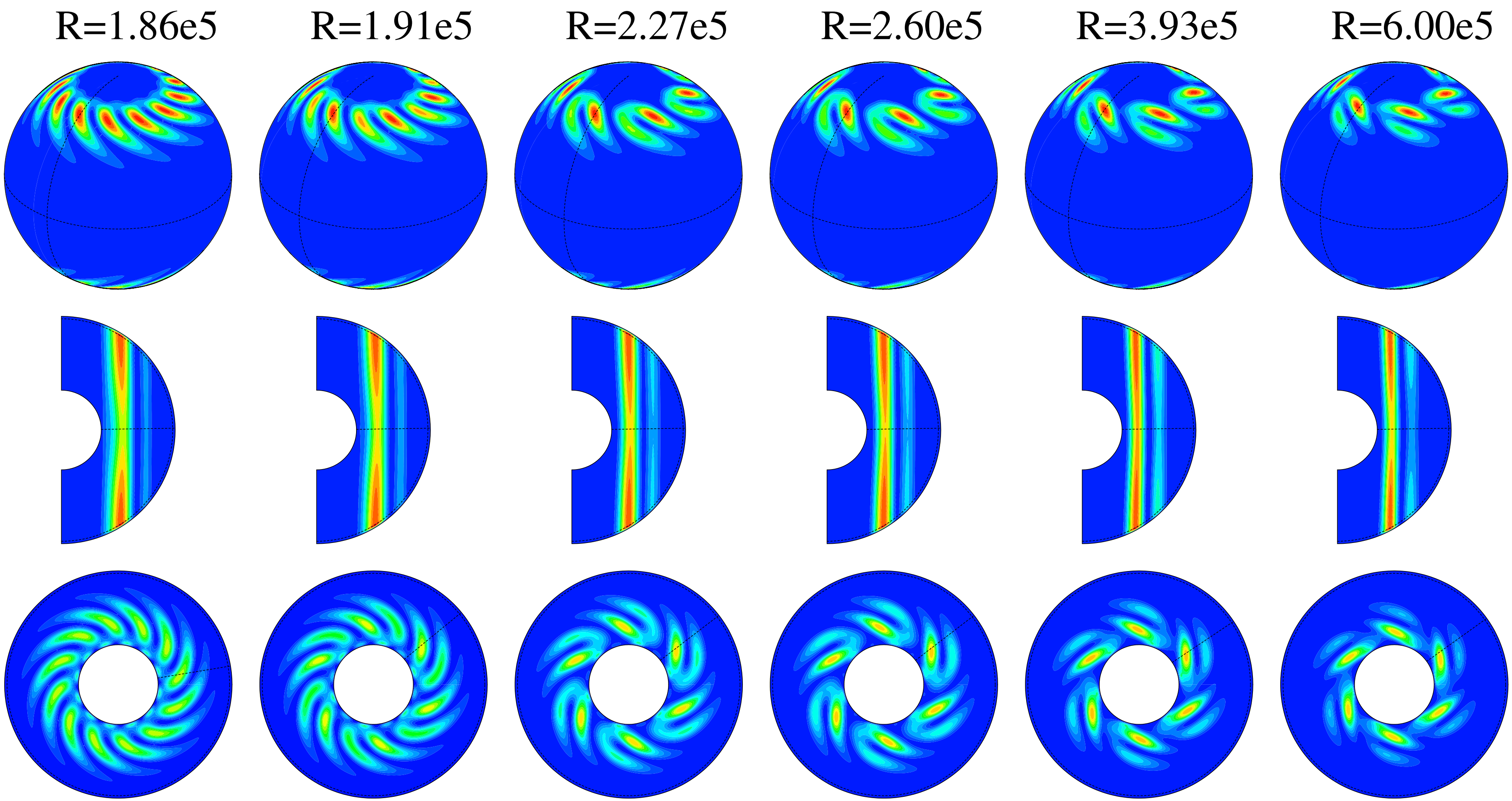
Bifurcation diagram for $\eta = 0.35$



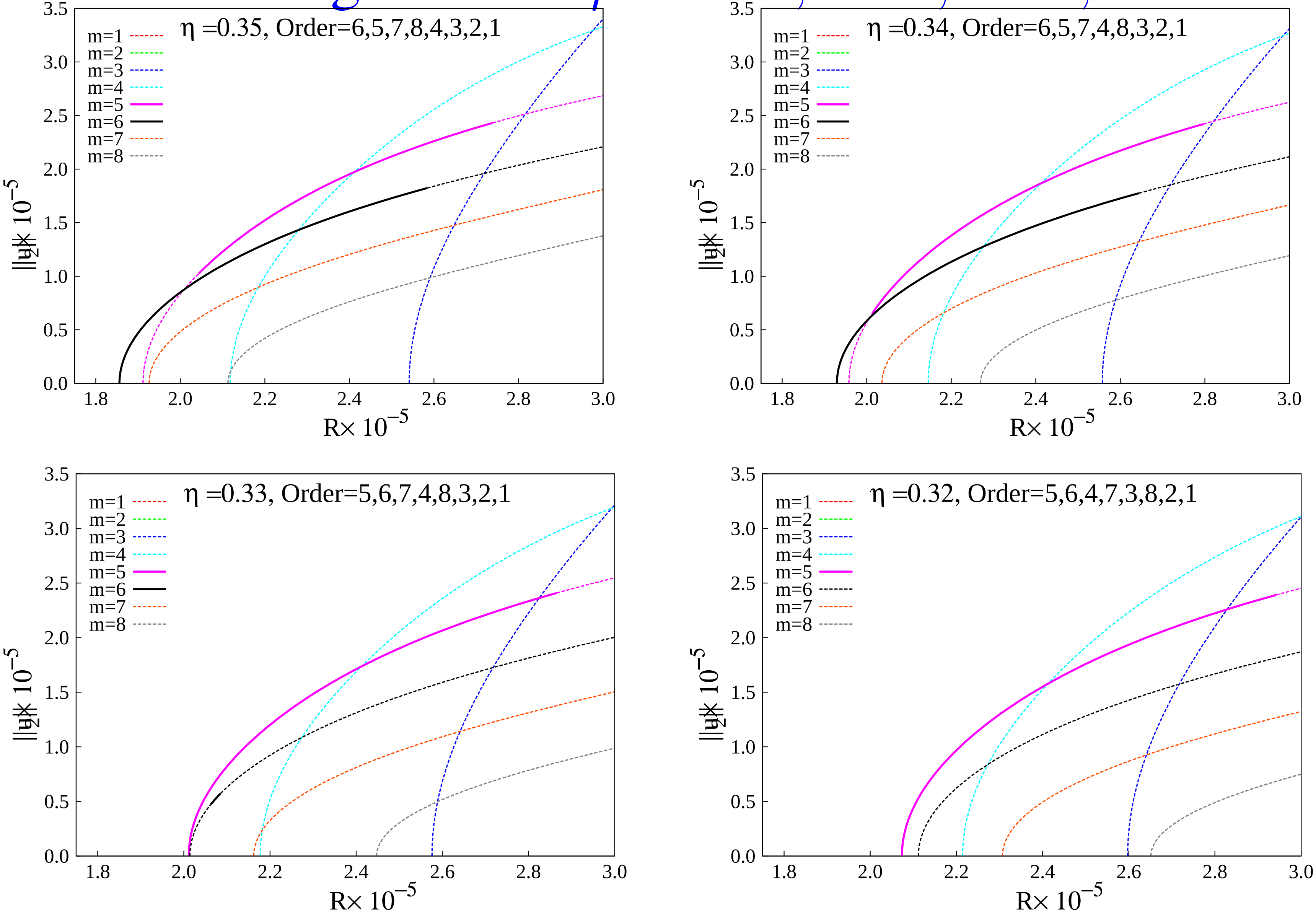
Norm and frequency versus R for $\eta = 0.35$, $\sigma = 0.1$, and $E = 10^{-4}$.

Solutions along the m=6 branch



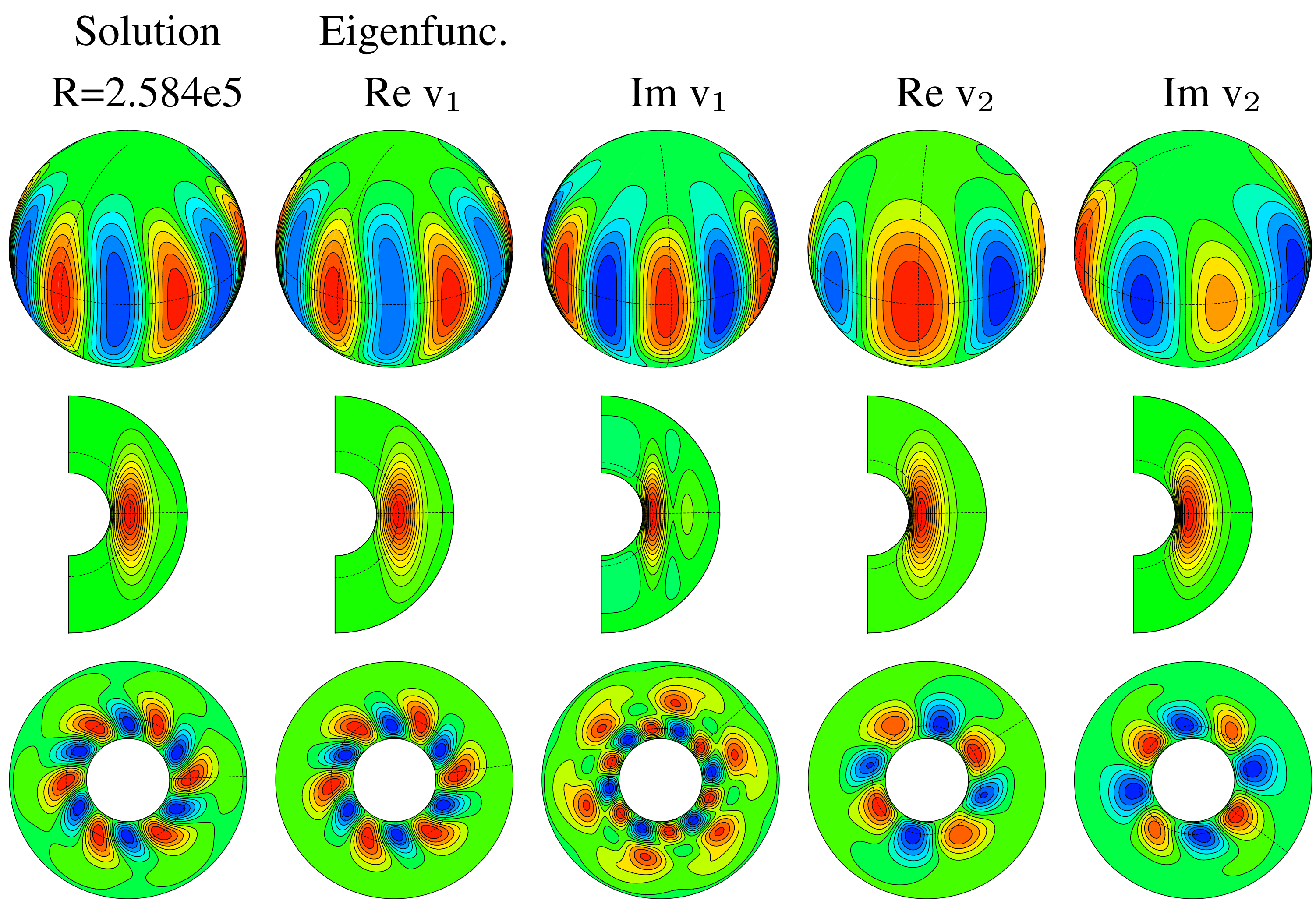

R=1.86e5
R=1.91e5
R=2.27e5
R=2.60e5
R=3.93e5
R=6.00e5

Bifurcation diagrams for $\eta = 0.35,\ 0.34,\ 0.33,$ *and* 0.32

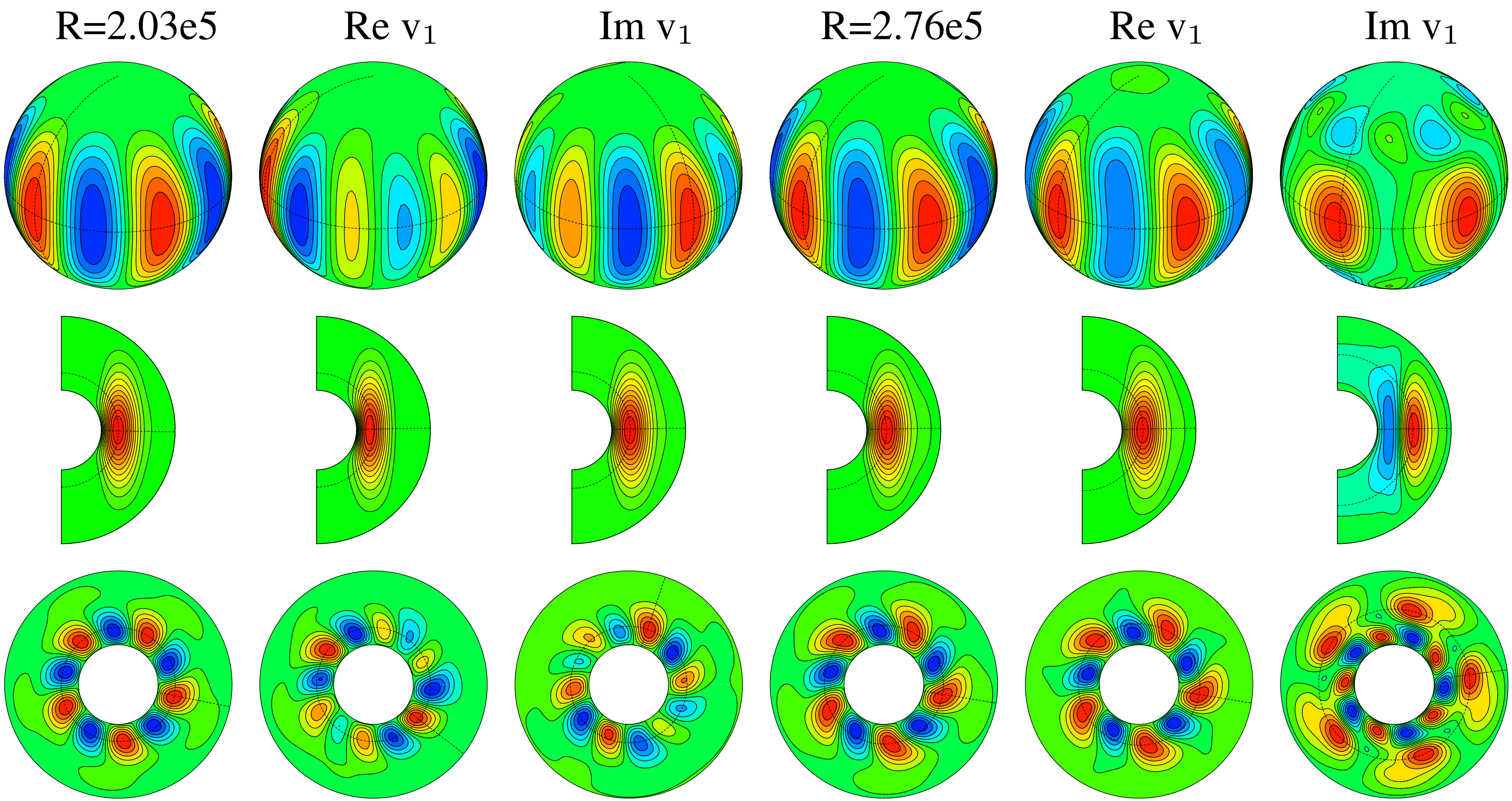


Norm versus R for $\eta = 0.35, 0.34, 0.33, 0.32$, $\sigma = 0.1$, and $E = 10^{-4}$.

Eigenfunctions at the bifurcation from the m=6 wave



Eigenfunctions at the bifurcation from the m=5 wave



Future work

- Computation of curves of bifurcation in two parameters, which require second order derivatives (loci of saddle-node of fixed points and periodic orbits, Neimark-Sacker, and pitchfork bifurcations, boundaries of Arnold's tongues, etc.).

References (http://zowie.upc.es/Joan/Sanchez)

- Sánchez J., Net M., García-Archilla B., Simó C. *Newton-Krylov continuation of periodic orbits for Navier-Stokes flows*, J. Comp. Phys. **201**, 13–33, 2004.
- Sánchez J., Net M. *On the multiple shooting continuation of periodic orbits by Newton-Krylov methods*, Int. J. Bif. Chaos **20** (1), 43–61, 2010.
- Sánchez J., Net M., Simó C. *Computation of invariant tori by Newton-Krylov methods in large scale dissipative systems*, Phys. D **239**, 123–133, 2010.
- Sánchez J., Net M. *A parallel algorithm for the computation of invariant tori in large-scale dissipative systems*, Phys. D **252** , 22–33. 2013.
- Garcia F., Net M., García-Archilla B., Sánchez J. *A comparison of high-order time integrators for the Boussinesq Navier-Stokes equations in rotating spherical shells,* J. Comp. Phys. **229**, 7997–8010, 2010.
- Sánchez J., Garcia F., Net M. *Computation of azimuthal waves and their stability for thermal convection in rotating spherical shells with aplication to the study of a double-Hopf bifurcation,* Physical Review E **87** 033014(11), 2013.