Tècniques de sistemes dinàmics per a equacions en derivades parcials discretitzades

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Overview

- Equilibria and periodic orbits of PDEs.
- Newton-Krylov continuation methods. Iterative matrix-free linear solvers.
- Stability. Subspace iteration and Arnoldi methods.
- Continuation of codimension-one bifurcation points periodic orbits. An example.
- Convection is spherical shells. Waves and modulated waves.
- Other invariant objects.

Equilibria and periodic orbits of ODEs

Assume

$$\dot{y} = f(y,p) \quad (\text{or} \quad B\dot{y} = f(y,p)), \quad (y,p) \in \mathcal{U} \subset \mathbb{R}^n \times \mathbb{R}$$

is a large-scale ($n \gg 1$) autonomous system of ODEs obtained after the spatial discretization of a system of parabolic PDEs and that

$$\varphi(t,x,p)$$

is its solution with initial condition x at $t = 0$ for a fixed value of p, that is, $\varphi(0,x,p) = x$.

We will assume that this system has been obtained as the discretization of a systems of evolutionary parabolic PDEs (reaction-diffusion or Navier-Stokes equations, for instance).

We are interested in the computation of its equilibria x satisfying

$$f(x,p) = 0,$$

their dependence on the parameter p and their stability.

We are also interested in the periodic regimes of the system given by the equations

$$\begin{aligned} x - \varphi(T,x,p) &= 0, \\ g(x) &= 0, \end{aligned}$$

x being a point of the periodic orbit selected by the phase condition $g(x) = 0$ and $T > 0$ its period.

In both cases one has to solve large-scale nonlinear systems of equations and to study the stability of the resulting equilibria or periodic orbits.

Continuation of zeros of a nonlinear system of equations

Consider a system of nonlinear equations depending on a parameter p

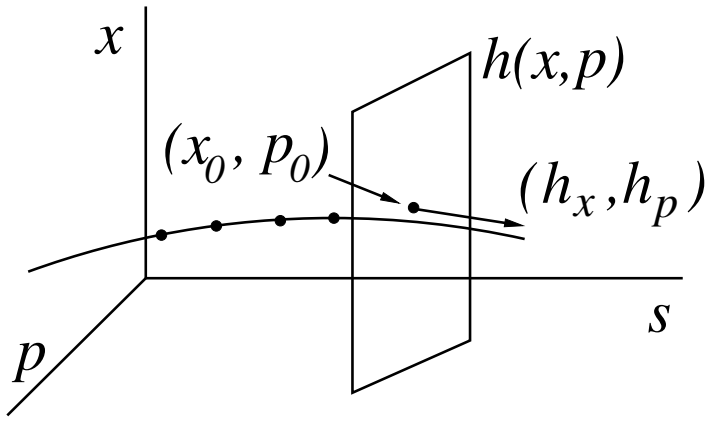
$$H(x,p)=0, \quad (x,p)\in\mathcal{U}\subset\mathbb{R}^m\times\mathbb{R}$$

with $m\gg 1$. We are interested in its solutions and their dependence on p.

Parameter and pseudo-arclength-like continuation methods are used to obtain the curves $(x(s),p(s))$ of fixed points. They admit an unified formulation by adding an equation

$$h(x,p)=0.$$

If $h(x,p)=p-p_0$ the equation fixes the parameter p.
If $h(x,p)=h_x^T(x-x_0)+h_p(p-p_0)$, with (x_0,p_0) and (h_x,h_p) being the predicted point and the tangent to the curve of solutions, the hyperplane is transverse to the curve of solutions if the prediction is not far away from the previous point, and the algorithm allows passing turning poits.



The system that determines a unique solution, $(x,p)\in\mathbb{R}^{m+1}$, is then

$$\widetilde{H}(x,p)=\begin{pmatrix} H(x,p)\\ h(x,p)\end{pmatrix}=0\in\mathbb{R}^{m+1}\,.$$

The system $\widetilde{H}(x,p)=0$ is solved by an inexact Newton's method:
starting from the initial (x_0,p_0),

$$(x_{i+1},p_{i+1})=(x_i,p_i)+(\Delta x_i,\Delta p_i),$$

where $(\Delta x_i,\Delta p_i)$ satisfies the linear system

$$\begin{pmatrix} D_xH(x_i,p_i) & D_pH(x_i,p_i) \\ h_x^\top & h_p \end{pmatrix}\begin{pmatrix}\Delta x_i\\ \Delta p_i\end{pmatrix}=\begin{pmatrix}-H(x_i,p_i)\\ -h(x_i,p_i)\end{pmatrix}$$

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

$$\begin{pmatrix} D_xH(x_i,p_i) & D_pH(x_i,p_i) \\ h_x^\top & h_p \end{pmatrix}\begin{pmatrix}\delta x\\ \delta p\end{pmatrix}$$

and, eventually, the use of preconditioners.

GMRES(M)	=	Generalized Minimal Residual (with restarting dimension M)
BiCGStab	=	Biconjugate Gradient Stabilized
TFQRM	=	Transpose-Free Quasi-Minimal Residual

Krylov methods for linear systems

Large-scale linear systems $Ax = b$ of dimension $n \gg 1$ are usually solved by iterative Krylov methods. The class of projection methods produce, from an initial guess x_0, a sequence of approximations, x_k, to the solution $x^* = A^{-1}b$, in the affine subspace $x_k \in x_0 + \mathcal{K}_k$, which satisfy the Petrov-Galerkin condition

$$b - Ax_k \perp \mathcal{L}_k,$$

where $\mathcal{K}_k$ and $\mathcal{L}_k$ are two k-dimensional linear subspaces. If $\mathcal{L}_k = A\mathcal{K}_k$, then x_k minimizes $||b - Ax||_2$ over $x \in x_0 + \mathcal{K}_k$.

In the particular case of GMRES, $\mathcal{L}_k = A\mathcal{K}_k$, and $\mathcal{K}_k$ is the Krylov subspace

$$\mathcal{K}_k = \{r_0, Ar_0, A^2r_0, \ldots, A^{k-1}r_0\}, \quad \text{with} \quad r_0 = b - Ax_0.$$

It follows that $r_k = p_k(A)r_0$, p_k being a polynomial of degree k, with $p_k(0) = 1$.

Theorem. *(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_k is the set of polynomials of degree at most k, and $\kappa_2(V) = \|V^{-1}\|_2\|V\|_2$ is the norm-2 condition number of V. Then at the k-th step of GMRES*

$$\frac{\|b - Ax_k\|_2}{\|b - Ax_0\|_2} \leq \kappa_2(V) \inf_{\substack{p \in P_k \\ p(0)=1}} \max_{i=1,\ldots,n} |p(\lambda_i)|.$$

Preconditioning

If the spectrum of A is not clustered it is necessary to use preconditioners to accelerate the convergence of the iterative solvers for the linear system $Ax = b$.

Suppose M is a matrix which approximates A ($M \approx A$) and is easy to invert (easy to solve systems with matrix M).

- Left preconditioning. Solve the system

$$M^{-1}Ax = M^{-1}b.$$

  Its solution is that of $Ax = b$.

- Right preconditioning. Solve system

$$AM^{-1}y = b.$$

  Then the solution of $Ax = b$ is $x = M^{-1}y$.

This means that when applying a matrix-free method (GMRES, for instance) each matrix product by A is substituted by a matrix product by A followed by a matrix solve with matrix M in the case of left preconditioning, or by a matrix solve with matrix M followed by a matrix product by A for right preconditioning.

Continuation of equilibria

Summarizing, it is possible to find the equilibria of the system of ODEs

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

by Newton-Krylov methods by a generic continuation code if one can provide three subroutines:

- `fun(X,H)` computing the function $H = f(x,p)$ from $X = (x,p)$,
- `dfun(X,δX,δH)` which computes the action by the Jacobian $\delta H = D_y f(x,p)\delta x + D_p f(x,p)\delta p$ from $X = (x,p)$ and $\delta X = (\delta x, \delta p)$, and
- `prec(X,h,δX,δZ)` which solves $\mathcal{M}\delta Z = \delta X$ from $X = (x,p)$, $h = (h_x, h_p)$, and $\delta X = (\delta x, \delta p)$, $\mathcal{M}$ being an approximation of

$$\begin{pmatrix} D_x f(x_i,p_i) & D_p f(x_i,p_i) \\ h_x^\top & h_p \end{pmatrix}.$$

Approximation of the forms

$$\mathcal{M} = \begin{pmatrix} M & 0 \\ 0 & 1 \end{pmatrix} \quad \text{or} \quad \mathcal{M} = \begin{pmatrix} M & 0 \\ h_x^\top & h_p \end{pmatrix}$$

can be used, with $M \approx D_x f(x_i,p_i)$.

Continuation of periodic orbits of ODEs

To compute periodic orbits of

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

by Newton-Krylov methods two subroutines are needed:

- `fun(X,H)` computing the function

$$H(x,T,p) = \begin{pmatrix} x - \varphi(T,x,p) \\ g(x) \end{pmatrix}$$

  from $X = (x,T,p)$, $g(x)$ being a phase condition. This involves integrating

$$\dot{y} = f(y,p) \quad \text{with initial conditions} \quad y(0) = x \quad \text{during a time} \quad T.$$

- `dfun(X,δX,δH)` which computes the action by the Jacobian of the system

$$\delta H = DH(x,T,p)(\delta x, \delta T, \delta p) = \begin{pmatrix} \delta x - D_x\varphi(T,x,p)\delta x - D_p\varphi(T,x,p)\delta p - D_t\varphi(T,x,p)\delta T \\ D_x g(x)\delta x \end{pmatrix}$$

  from $X = (x,T,p)$ and $\delta X = (\delta x, \delta T, \delta p)$.

If the equation is $\dot{y} = f(y,p)$ then $D_t\varphi(T,x,p) = f(\varphi(T,x,p),p)$.

If it is $B\dot{y} = f(y,p)$ and B is not invertible then $D_t\varphi(T,x,p)$ can be approximated at the end of the time integration by finite differences.

The matrix product

$$D_x\varphi(T,x,p)\delta x + D_p\varphi(T,x,p)\delta p$$

can be computed by integrating a first variational equation. If

$$\begin{aligned} y(t) =& \varphi(t,x,p) \\ y_1(t) =& D_x\varphi(t,x,p)\delta x + D_p\varphi(t,x,p)\delta p \end{aligned}$$

then y_1 satisfies

$$\dot{y}_1 = D_y f(y,p)y_1 + D_p f(y,p)\delta p \quad \text{and} \quad y_1(0) = \delta x,$$

because $\varphi(0,x,p) = x$.

This equation must be solved coupled with that for y,

$$\begin{aligned} \dot{y} &= f(y,p) \\ \dot{y}_1 &= D_y f(y,p)y_1 + D_p f(x,p)\delta p \end{aligned} \qquad \text{with initial conditions} \qquad \begin{aligned} y(0) &= x \\ y_1(0) &= \delta x. \end{aligned}$$

Finally

$$D_x\varphi(T,x,p)\delta x + D_p\varphi(T,x,p)\delta p = y_1(T).$$

Stability

- The stability of equilibria and the detection of their bifurcation needs the computation of the eigenvalues of largest real part of

$$D_x f(x,p)v = \lambda v \quad \text{(or} \quad D_x f(x,p)v = \lambda B v \quad \text{if the equation is} \quad B\dot{y} = f(x,p)).$$

- The stability of periodic orbits and the detection of their bifurcation needs the computation of the eigenvalues (Floquet multipliers) of largest modulus of

$$D_x \varphi(T,x,p)v = \lambda u.$$

Two main methods are available to obtain the eigenvalues the largest modulus of a $n \times n$ large-scale $(n \gg 1)$ matrix A:

- Subspace iteration. Implemented, for instance, in the packages LOPSI(1981) and SRRIT(1997). Generalization of the power method.
- Arnoldi methods. Implemented in ARPACK(1997). Based on Krylov subspaces

$$\mathcal{K}_k = \{v, Av, A^2 v, \ldots, A^{k-1} v\}.$$

Both require the computation of matrix actions $u \to Au$.

- The case of periodic orbits is, in principle, straightforward.
- The case of equilibria needs transformations of eigenvalues.

Eigenvalue Transformations

To find the leading (maximal real part) eigenvalues of $Av = \lambda Bv$, with $A = D_x f(x,p)$, the following transformations can be used:

- Shift-invert with real or complex shift:

$$Av = \lambda Bv \implies (A - \sigma B)^{-1} Bv = \mu v \quad \text{with} \quad \mu = 1/(\lambda - \sigma).$$

  The circle $C(\sigma, |\lambda - \sigma|)$ in the λ-plane is mapped to the circle $C(0, |\lambda - \sigma|^{-1})$ in the μ-plane.

- Generalized Cayley transformation:

$$Av = \lambda Bv \implies (A - \sigma B)^{-1}(A - \tau B)v = \mu v \quad \text{with} \quad \mu = (\lambda - \tau)/(\lambda - \sigma).$$

  The line $\mathrm{Re}(\lambda) = (\sigma + \tau)/2$ is mapped to the unit circle and $\mathrm{Re}(\lambda) < (\sigma + \tau)/2$ ($\mathrm{Re}(\lambda) > (\sigma + \tau)/2$) is mapped to the interior (exterior) of the unit circle.

- Exponential:

$$Av = \lambda v \implies \exp(TA)v = \mu v \quad \text{with} \quad \mu = \exp(\lambda T).$$

  The line $\mathrm{Re}(\lambda) = 0$ is mapped to the unit circle and $\mathrm{Re}(\lambda) < 0$ ($\mathrm{Re}(\lambda) > 0$) is mapped to the interior (exterior) of the unit circle.

The previous methods (subspace or Arnoldi iterations) can be used to find the eigenvalues μ with maximal modulus of the transformed problems.

Continuation of codimension-one bifurcations of periodic orbits

Consider an autonomous system of ODEs

$$\dot{y} = f(y, p), \quad (y, p) \in \mathcal{U} \subset \mathbb{R}^n \times \mathbb{R}^2,$$

depending on two parameters $p = (p_1, p_2)$ obtained after spatial discretization of a system of parabolic PDEs ($n >> 1$).

Let $y(t) = \varphi(t, x, p)$ be its solution with initial condition $y(0) = x$ at $t = 0$ and for a fixed p.

We are interested in tracking curves of codimension-one bifurcations of periodic orbits in system with or without symmetries.

Let assume a matrix-free continuation code based on Newton-Krylov methods is available to follow the curves of solutions of

$$H(X) = 0$$

with $X \in \mathcal{U} \subset \mathbb{R}^{m+1}$ and $H(X) \in \mathbb{R}^m$, which requires the user to provide an initial solution X_0, and two subroutines:

- $\texttt{fun}(\texttt{X}, \texttt{h})$ which computes $h = H(X)$ from X, and
- $\texttt{dfun}(\texttt{X}, \delta\texttt{X}, \delta\texttt{h})$ which computes $\delta h = D_X H(X)\delta X$ from X, and δX.

Saddle–node and period doubling bifurcations

The saddle-node ($\lambda = 1$) and period doubling ($\lambda = -1$) bifurcations of periodic orbits are solutions of the system $H(x, u, T, p) = 0$ given by

$$\begin{aligned} x - \varphi(T, x, p) &= 0, \\ g(x) &= 0, \\ \lambda u - \left(D_x \varphi(T, x, p) u - \frac{1}{2}(1+\lambda) \frac{\langle w, u \rangle}{\langle w, w \rangle} w \right) &= 0, \\ \langle u_r, u \rangle &= 1. \end{aligned}$$

- $g(x) = 0$ is a phase condition to select a single point on the periodic orbit. We use $g(x) = \langle v_\pi, x - x^{(\pi)} \rangle = 0$.
- $w = f(x, p)$ is the vector field evaluated at (x, p).
- $\langle u_r, u \rangle = 1$ fixes the indetermined constant of the eigenvalue problem, u_r being a reference vector. We use $u_r = u$.
- The last term of the third equation is Wieland's deflation, which guarantees the regularity of the system by shifting the $+1$ multiplier associated with $f(x, p)$ to zero.

$X = (x, u, T, p)$ has dimension $2n + 3$, and the $2n + 2$ equations define the curve of solutions.

In order to compute $H(x, u, T, p)$, we define

$$y(t) = \varphi(t, x, p)$$
$$y_1(t) = D_x\varphi(t, x, p)u$$

and, taking into account that

$$D_t D_x\varphi(t, x, p) = D_y f(\varphi(t, x, p), p) D_x\varphi(t, x, p), \text{ and } D_x\varphi(0, x, p) = I$$

the following system has to be integrated during a time T

$$\dot{y} = f(y, p), \qquad y(0) = x$$
$$\dot{y}_1 = D_y f(y, p) y_1, \qquad y_1(0) = u.$$

Then

$$\varphi(T, x, p) = y(T)$$
$$D_x\varphi(T, x, p)u = y_1(T).$$

The action of $D_X H(x,u,T,p)$ on $(\delta x, \delta u, \delta T, \delta p)$ is

$$\begin{aligned}
&\delta x - D_x\varphi(T,x,p)\delta x - D_p\varphi(T,x,p)\delta p - D_t\varphi(T,x,p)\delta T,\\
&Dg(x)\delta x,\\
&\lambda\delta u - D^2_{tx}\varphi(T,x,p)(u,\delta T) - D^2_{xx}\varphi(T,x,p)(u,\delta x) - D^2_{xp}\varphi(T,x,p)(u,\delta p)\\
&- D_x\varphi(T,x,p)\delta u\\
&+ \frac{1+\lambda}{2\langle w,w\rangle}\left(\langle w,u\rangle z + \left(\langle z,u\rangle + \langle w,\delta u\rangle - \frac{2\langle w,z\rangle}{\langle w,w\rangle}\langle w,u\rangle\right) w\right),\\
&\langle u_r,\delta u\rangle,
\end{aligned}$$

where $w = f(x,p)$ and $z = D_y f(x,p)\delta x + D_p f(x,p)\delta p$. Lets define

$$\begin{aligned}
y(t) &= \varphi(t,x,p),\\
y_1(t) &= D_x\varphi(t,x,p)u,\\
y_2(t) &= D_x\varphi(t,x,p)\delta x + D_p\varphi(t,x,p)\delta p,\\
y_3(t) &= D^2_{xx}\varphi(t,x,p)(u,\delta x) + D^2_{xp}\varphi(t,x,p)(u,\delta p),\\
y_4(t) &= D_x\varphi(t,x,p)\delta u.
\end{aligned}$$

$$D_t\varphi(T,x,p)\delta T = f(y(T),p)\delta T,$$

$$D^2_{tx}\varphi(T,x,p)(u,\delta T) = \delta T\, D_y f(\varphi(T,x,p),p) D_x\varphi(T,x,p)u = \delta T\, D_y f(y(T),p) y_1(T).$$

If

$$
\begin{aligned}
y(t) &= \varphi(t,x,p),\\
y_1(t) &= D_x\varphi(t,x,p)u,\\
y_2(t) &= D_x\varphi(t,x,p)\delta x + D_p\varphi(t,x,p)\delta p,\\
y_3(t) &= D^2_{xx}\varphi(t,x,p)(u,\delta x) + D^2_{xp}\varphi(t,x,p)(u,\delta p),\\
y_4(t) &= D_x\varphi(t,x,p)\delta u,
\end{aligned}
$$

the system which must be integrated to obtain $y(T)$, $y_i(T)$, $i=1,\dots,4$ is

$$
\begin{aligned}
\dot y &= f(y,p), & y(0) &= x\\
\dot y_1 &= D_y f(y,p)y_1, & y_1(0) &= u\\
\dot y_2 &= D_y f(y,p)y_2 + D_p f(y,p)\delta p, & y_2(0) &= \delta x\\
\dot y_3 &= D_y f(y,p)y_3 + D^2_{yy} f(y,p)(y_1,y_2) + D^2_{yp} f(y,p)(y_1,\delta p), & y_3(0) &= 0\\
\dot y_4 &= D_y f(y,p)y_4, & y_4(0) &= \delta u.
\end{aligned}
$$

Thermal convection in binary fluid mixtures

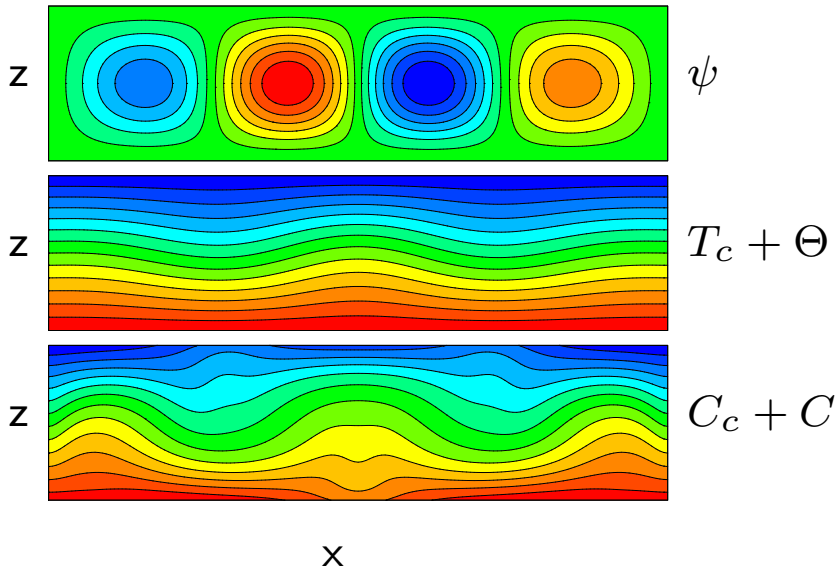
The equations in $\Omega = [0, \Gamma] \times [0, 1]$ for the perturbation of the basic state ($\mathbf{v}_c = 0$, $T_c = T_c(0) - z$, and $C_c = C_c(0) - z$) in non-dimensional form are

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \sigma \Delta \mathbf{v} - \nabla p + \sigma Ra(\Theta + SC)\hat{e}_z,$$
$$\partial_t \Theta + (\mathbf{v} \cdot \nabla)\Theta = \Delta \Theta + v_z,$$
$$\partial_t C + (\mathbf{v} \cdot \nabla)C = L(\Delta C - \Delta \Theta) + v_z,$$
$$\nabla \cdot \mathbf{v} = 0.$$

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

The parameters are

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

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

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:

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

Variational equations

$$
\begin{aligned}
\partial_t \Delta\psi_1 + J(\psi, \Delta\psi_1) + J(\psi_1, \Delta\psi) &= \sigma\Delta^2\psi_1 + \sigma Ra\left[(S+1)\partial_x\Theta_1 + S\partial_x\eta_1\right], \\
\partial_t \Theta_1 + J(\psi, \Theta_1) + J(\psi_1, \Theta) &= \Delta\Theta_1 + \partial_x\psi_1, \\
\partial_t \eta_1 + J(\psi, \eta_1) + J(\psi_1, \eta) &= L\Delta\eta_1 - \Delta\Theta_1,
\end{aligned}
$$

$$
\begin{aligned}
\partial_t \Delta\psi_2 + J(\psi, \Delta\psi_2) + J(\psi_2, \Delta\psi) &= \sigma\Delta^2\psi_2 + \sigma Ra\left[(S+1)\partial_x\Theta_2 + S\partial_x\eta_2\right] + \delta\sigma\Delta^2\psi \\
&\quad + (\sigma\delta Ra + \delta\sigma Ra)\left[(S+1)\partial_x\Theta + S\partial_x\eta\right], \\
\partial_t \Theta_2 + J(\psi, \Theta_2) + J(\psi_2, \Theta) &= \Delta\Theta_2 + \partial_x\psi_2, \\
\partial_t \eta_2 + J(\psi, \eta_2) + J(\psi_2, \eta) &= L\Delta\eta_2 - \Delta\Theta_2,
\end{aligned}
$$

$$
\begin{aligned}
\partial_t \Delta\psi_3 + J(\psi, \Delta\psi_3) + J(\psi_3, \Delta\psi) &= \sigma\Delta^2\psi_3 + \sigma Ra\left[(S+1)\partial_x\Theta_3 + S\partial_x\eta_3\right] + \delta\sigma\Delta^2\psi_1 \\
&\quad + (\sigma\delta Ra + \delta\sigma Ra)\left[(S+1)\partial_x\Theta_1 + S\partial_x\eta_1\right] \\
&\quad - J(\psi_1, \Delta\psi_2) - J(\psi_2, \Delta\psi_1), \\
\partial_t \Theta_3 + J(\psi, \Theta_3) + J(\psi_3, \Theta) &= \Delta\Theta_3 + \partial_x\psi_3 - J(\psi_1, \Theta_2) - J(\psi_2, \Theta_1), \\
\partial_t \eta_3 + J(\psi, \eta_3) + J(\psi_3, \eta) &= L\Delta\eta_3 - \Delta\Theta_3 - J(\psi_1, \eta_2) - J(\psi_2, \eta_1).
\end{aligned}
$$

Discretization

The functions ψ, Θ, and η are approximated by a pseudo-spectral method. Collocation on a mesh of $n_x \times n_z = 64 \times 16$ ($n = 3072$) Gauss-Lobatto points is used.

Higher resolutions have been used to check the results.

The stiff system of ODEs obtained can be written as

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

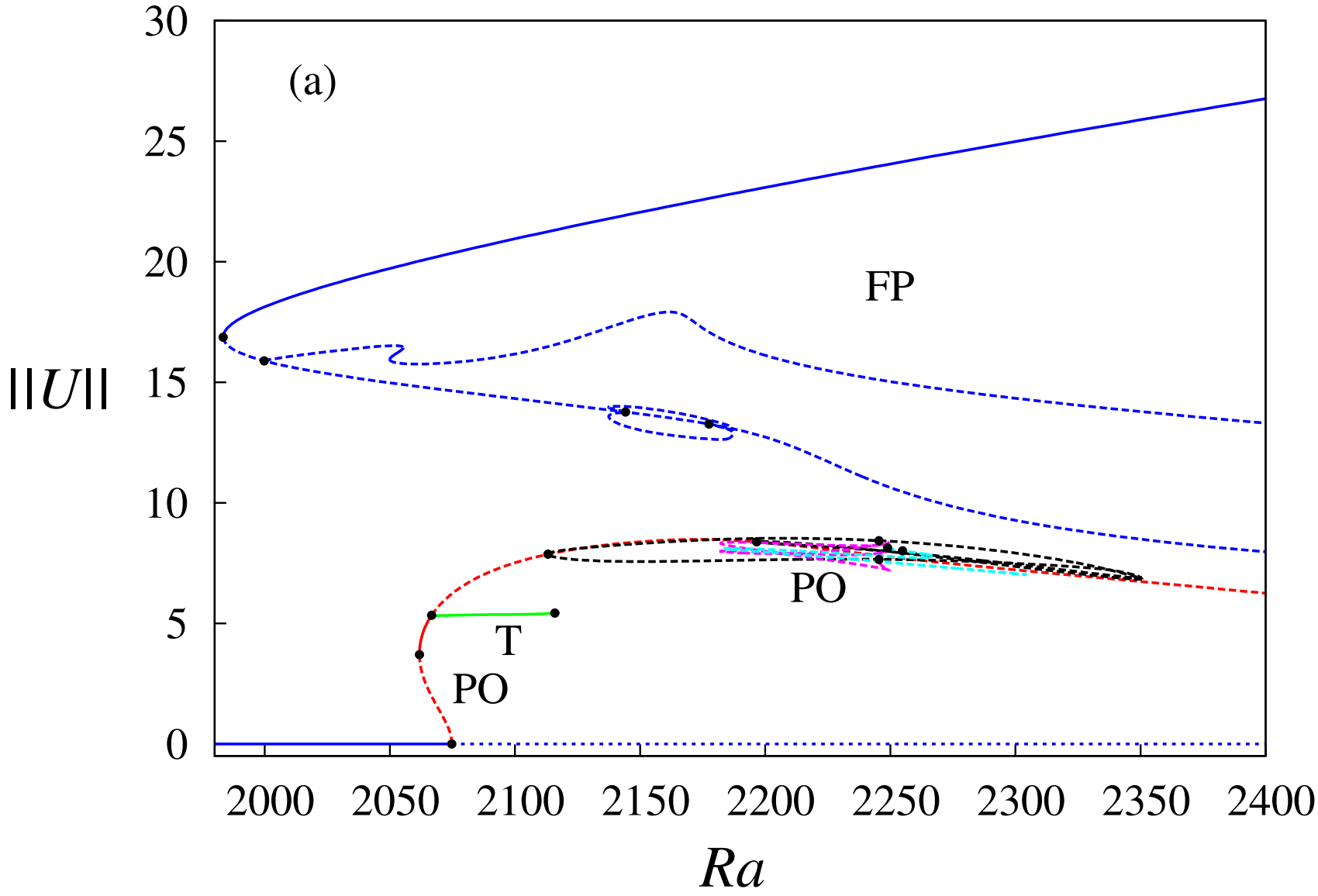
with $u = (\psi_{ij}, \Theta_{ij}, \eta_{ij})$.

It is integrated by using fifth-order BDF-extrapolation formulas:

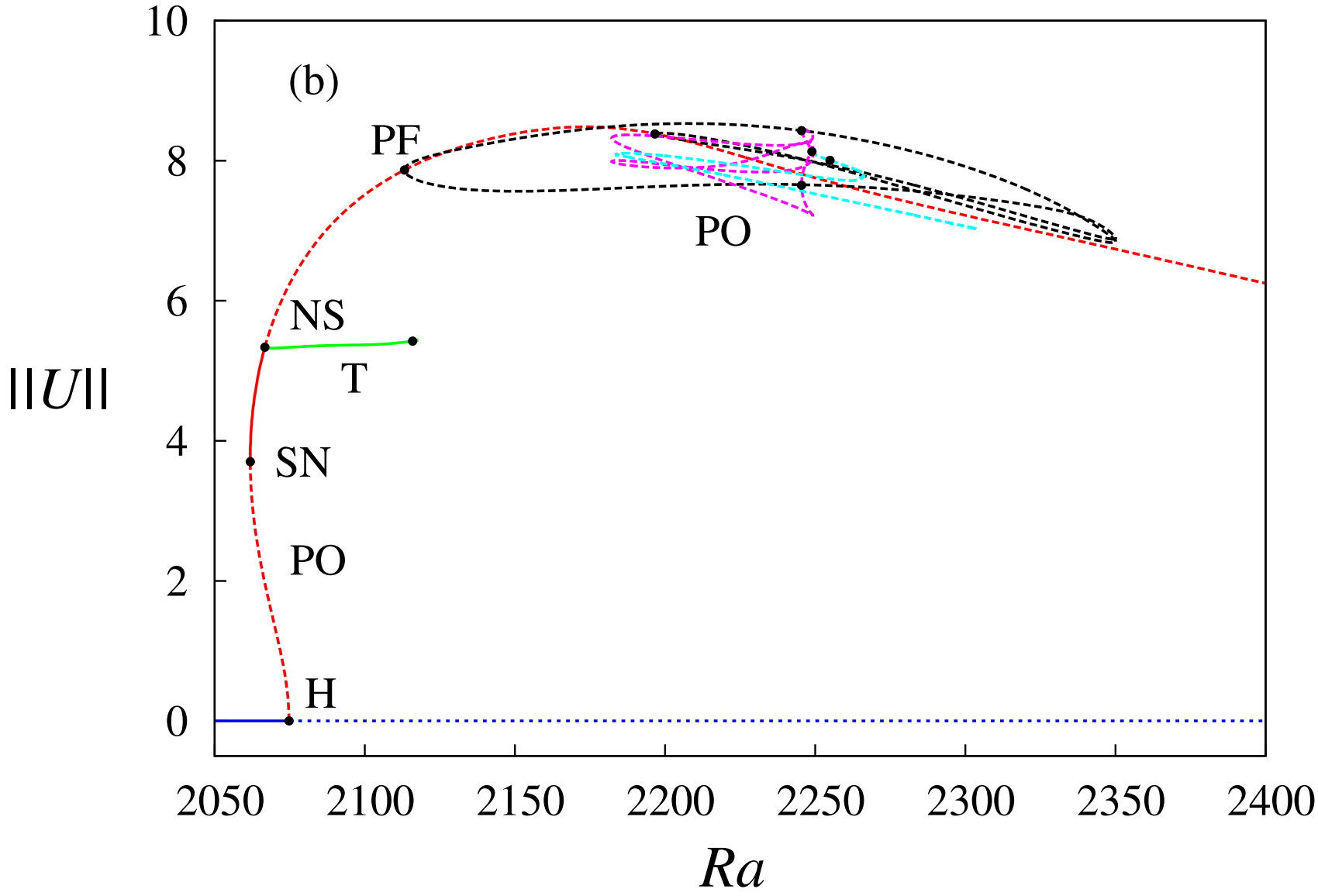
$$\frac{1}{\Delta t} B \left(\gamma_0 u^{n+1} - \sum_{i=0}^{k-1} \alpha_i u^{n-i} \right) = L u^{n+1} + \sum_{i=0}^{k-1} \beta_i N(u^{n-i}).$$

The initial points are obtained by a fully implicit BDF method.

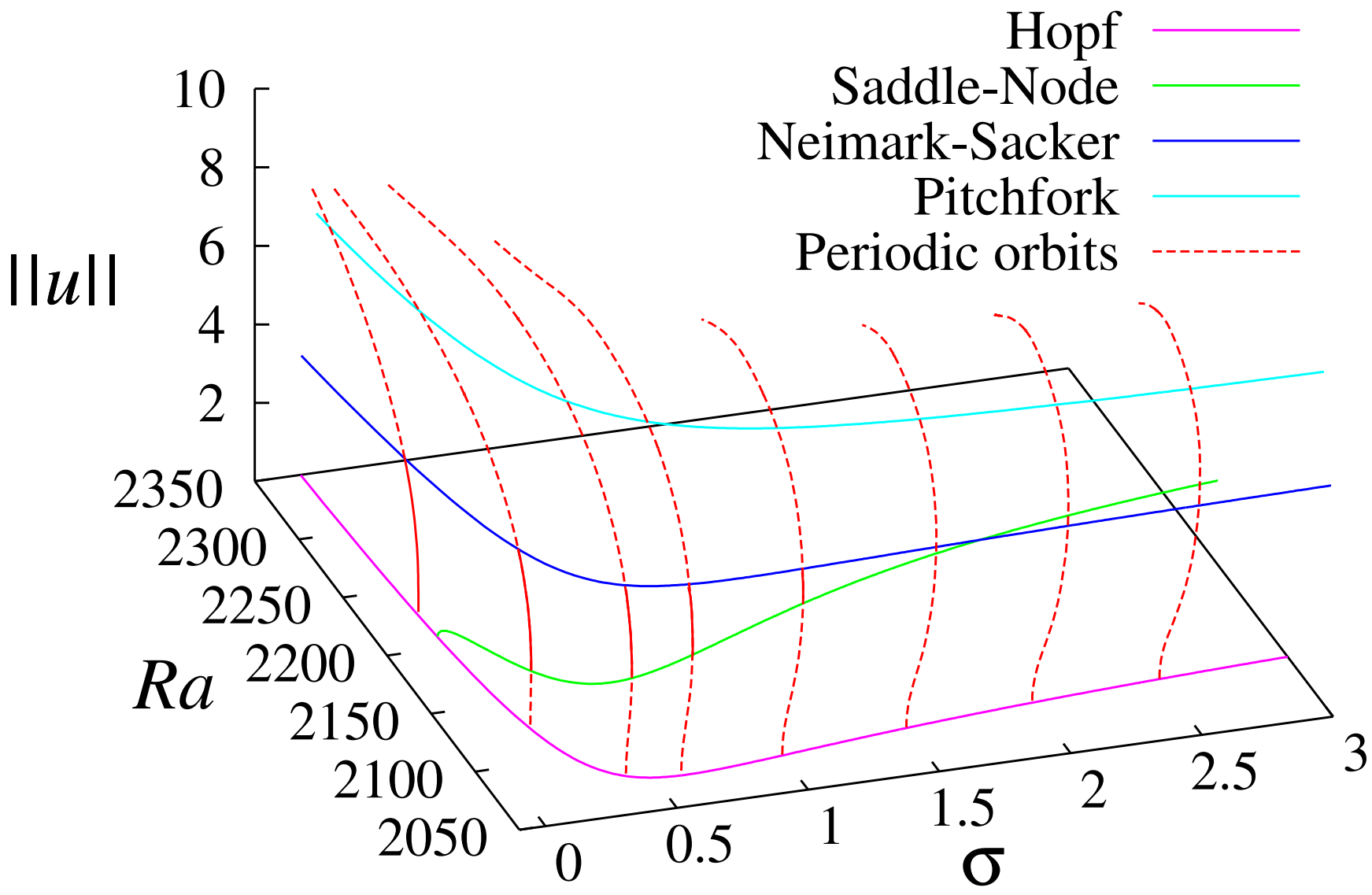
Some results for $\sigma = 0.6$



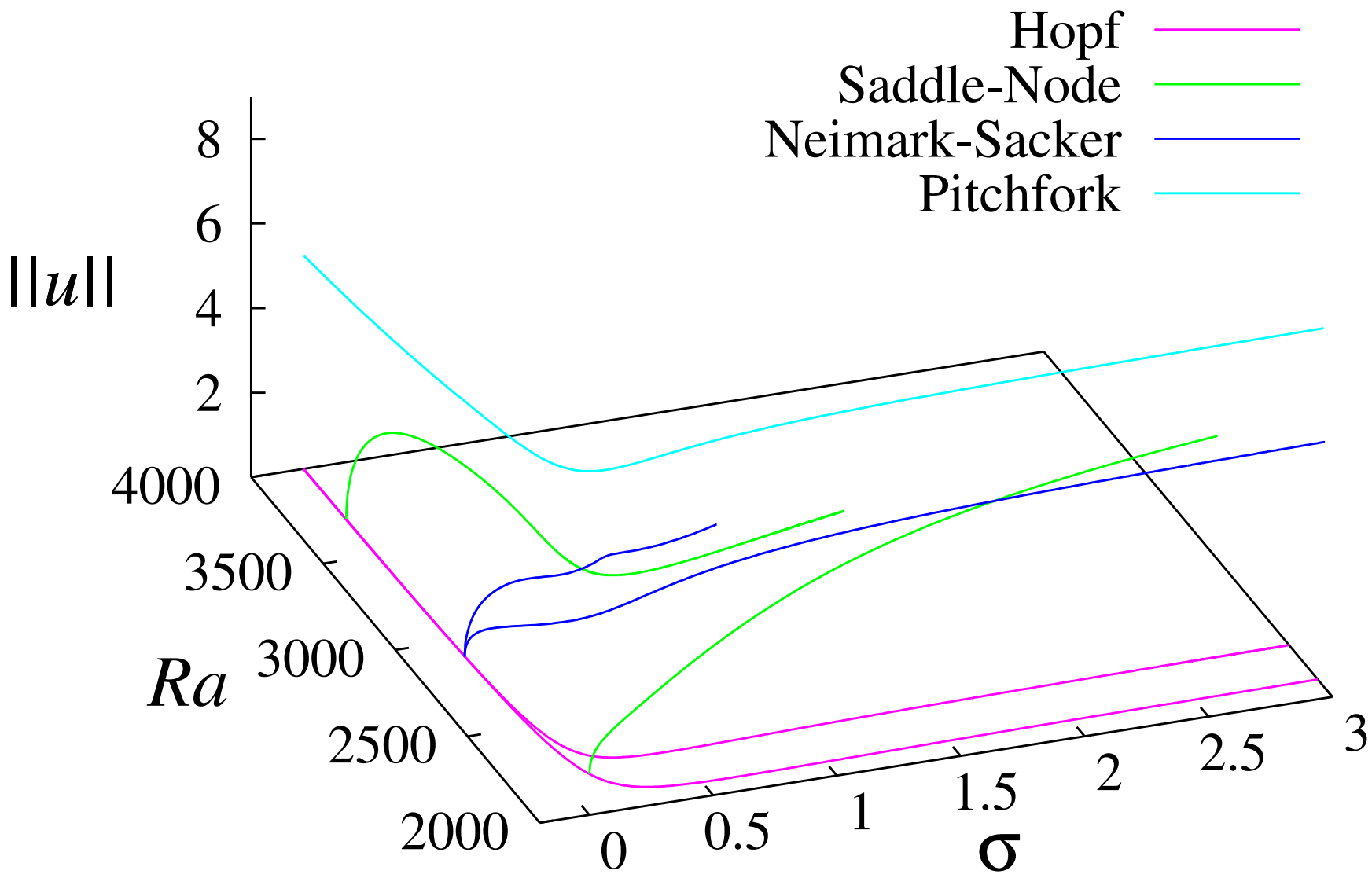
Some results for $\sigma = 0.6$



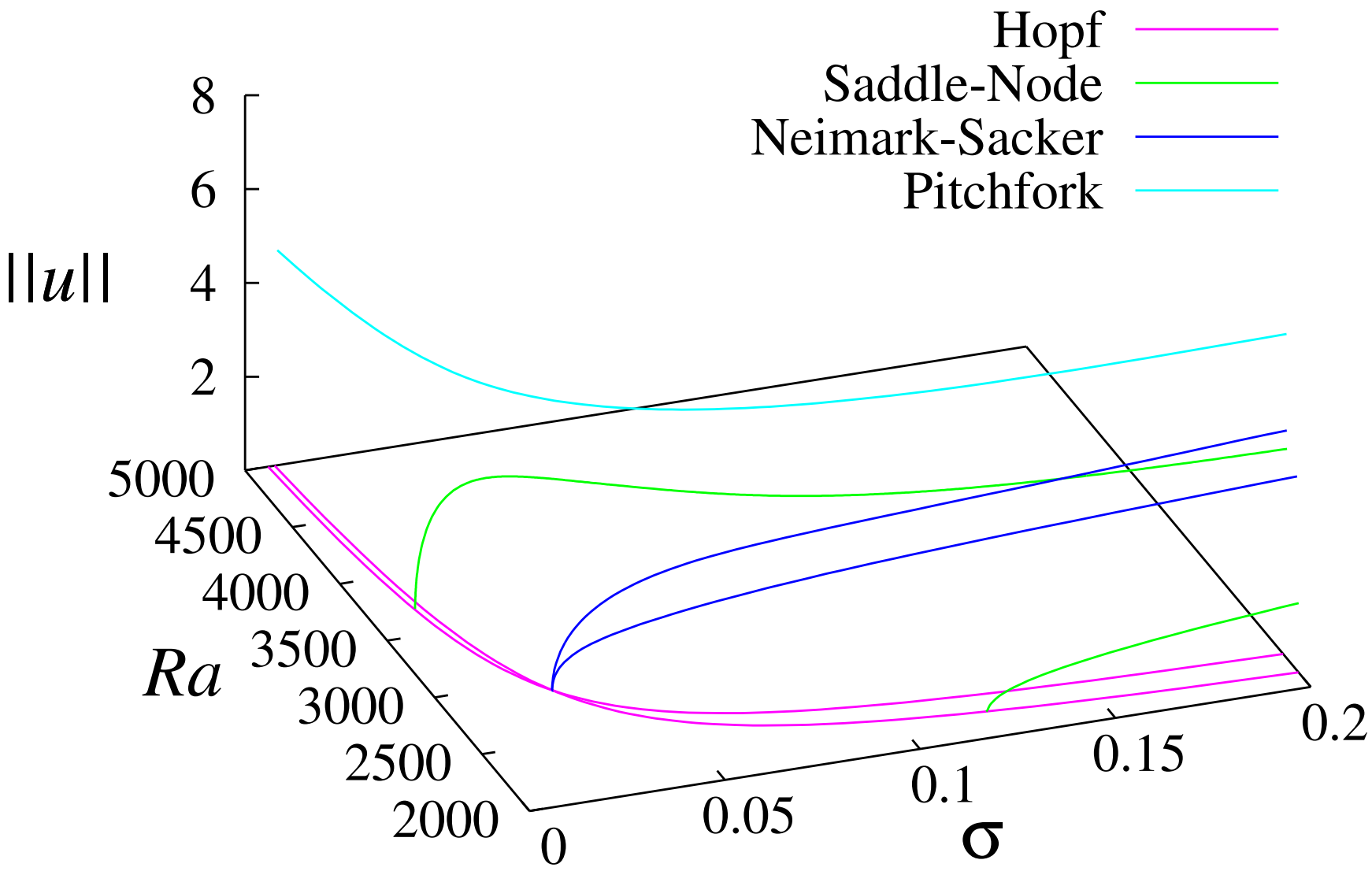
Curves of bifurcations



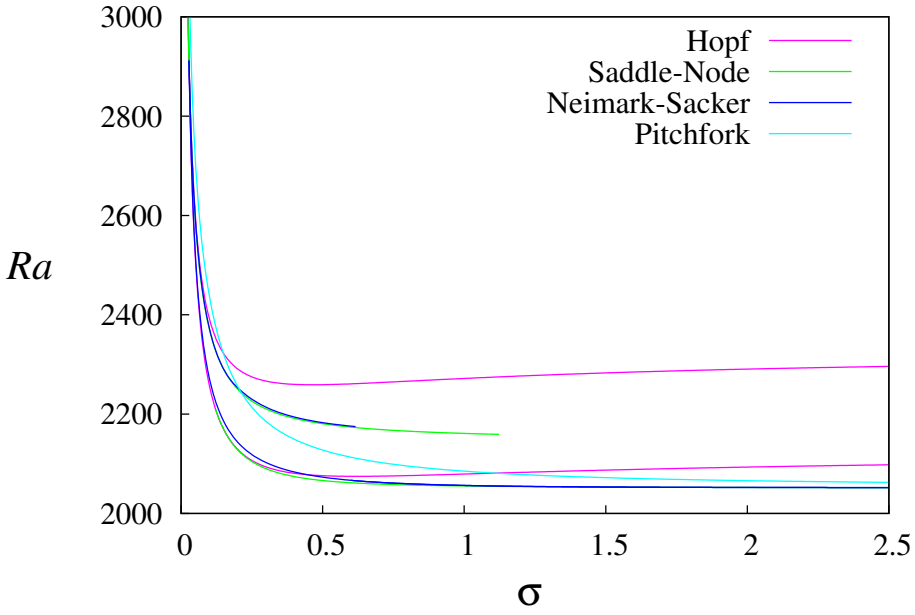
Curves of bifurcations

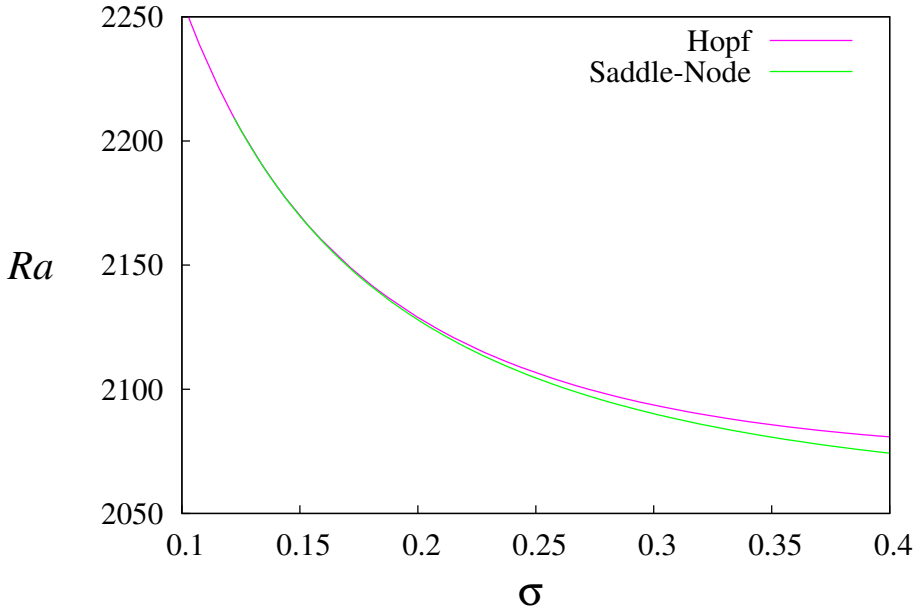


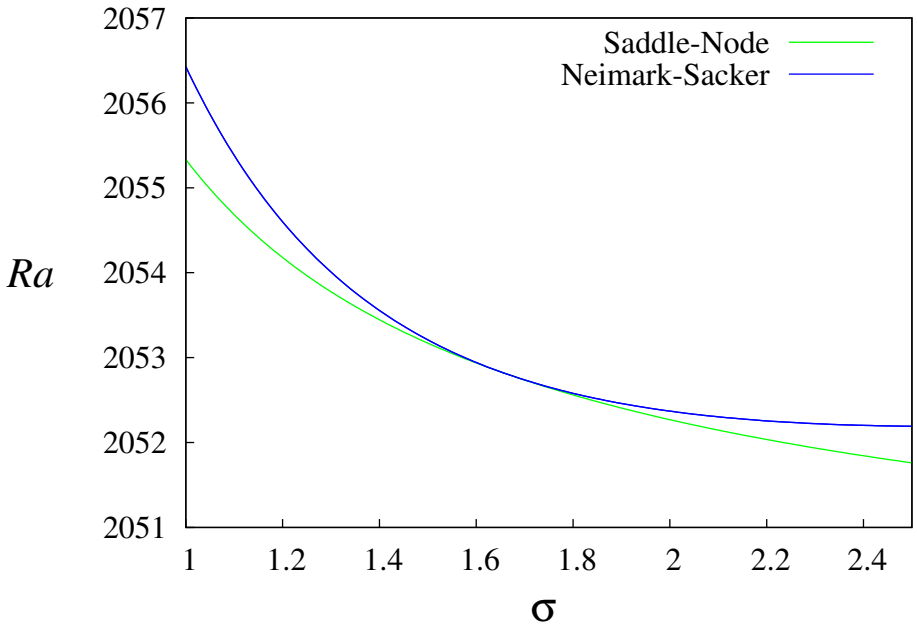
Curves of bifurcations

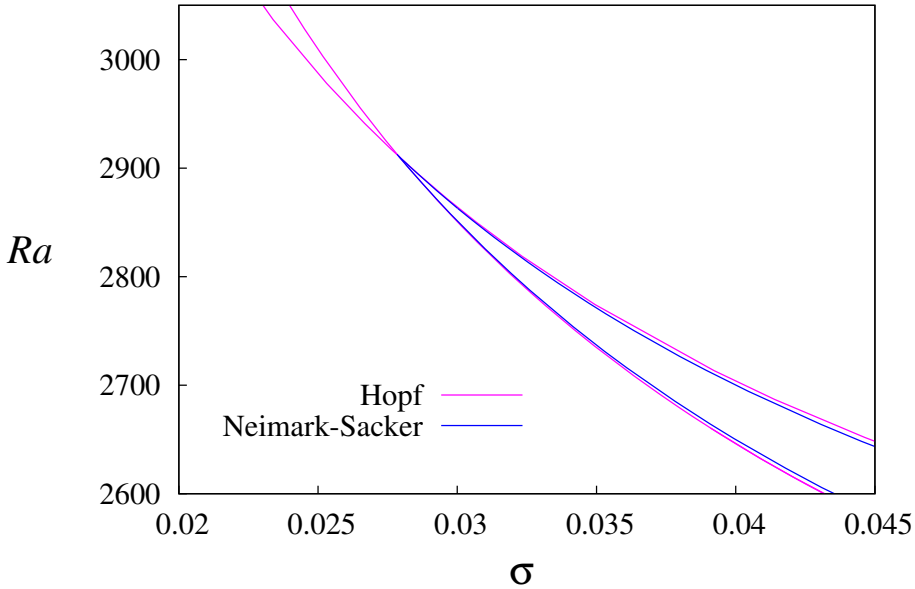


Codimension-two points

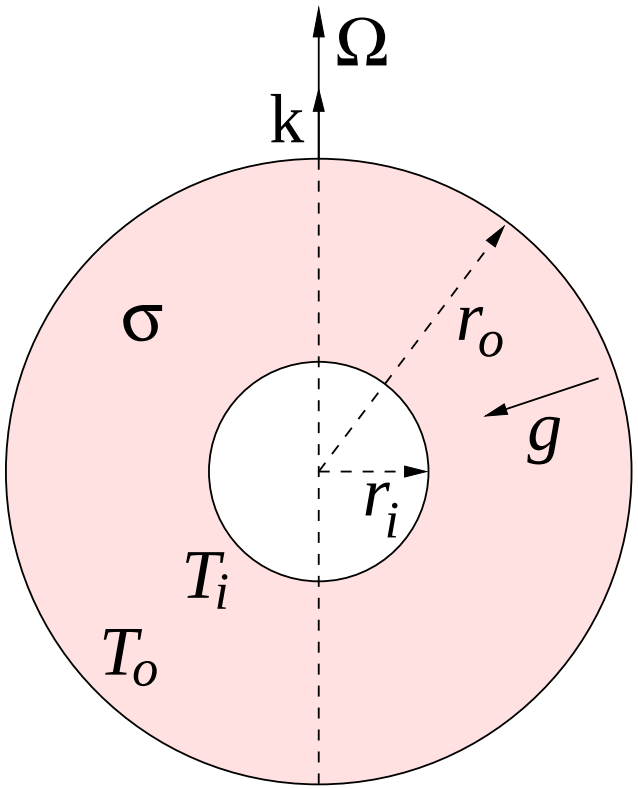








Thermal convection in rotating spherical shells



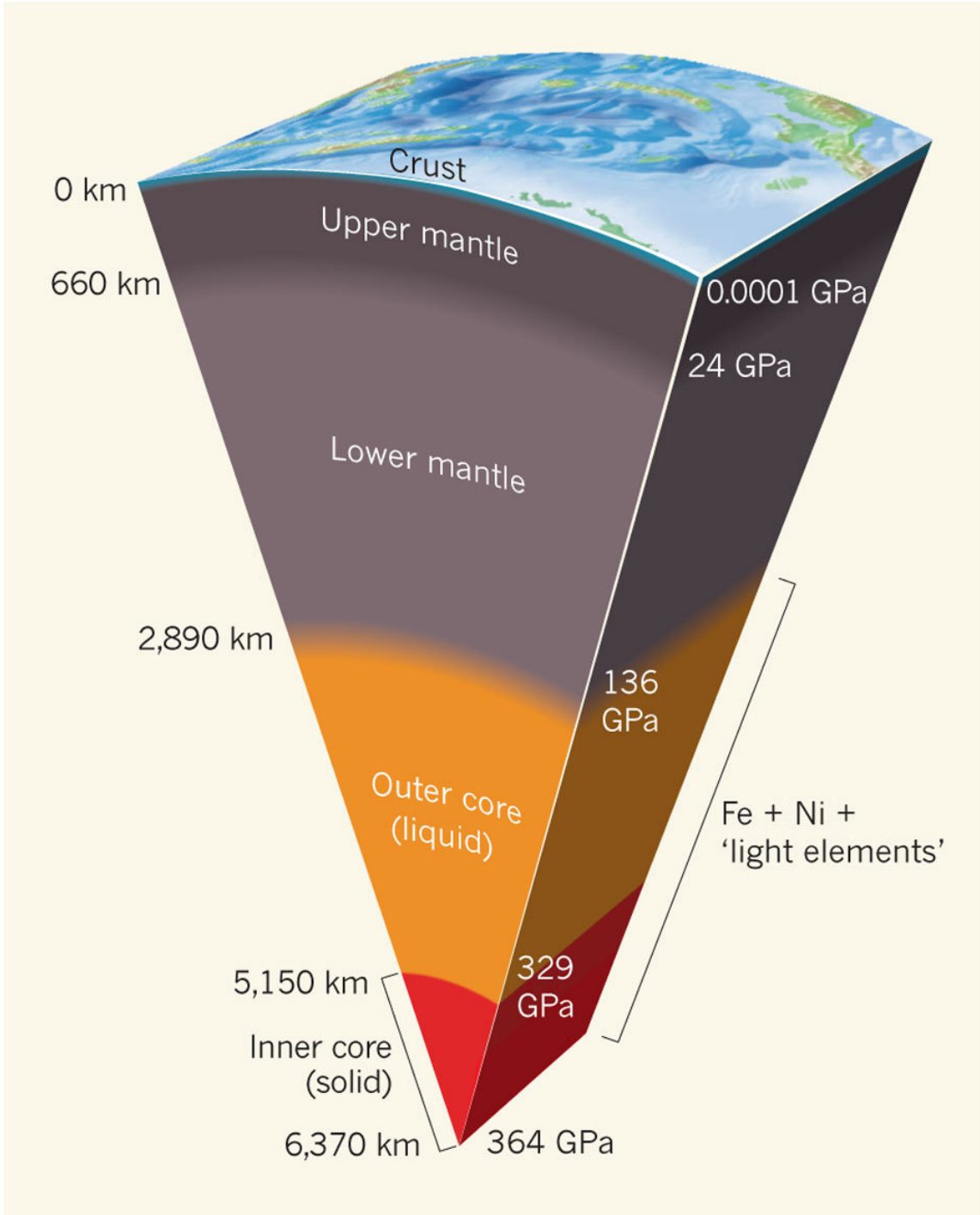
We consider:

- Newtonian fluid
- $\mathbf{g} = -\gamma \mathbf{r}$, with $\gamma > 0$ and $\mathbf{r} = (x, y, z)$
- A difference of temperature between the two boundaries, with $\Delta T = T_i - T_o > 0$
- Non-slip boundary conditions $\mathbf{v} = 0$ at r_i and r_o
- Perfectly conducting boundaries (T_i and T_o constant).

In the absence of movement the heat is transported by conduction.

Physical interest

- Astrophysics. Thermal convection in some stars and the atmospheres of the major planets.
- Geophysics. Thermal convection in the Earth's outer core.


Crust
0 km
Upper mantle
660 km
0.0001 GPa
24 GPa
Lower mantle
2,890 km
136
GPa
Outer core
(liquid)
Fe + Ni +
'light elements'
329
GPa
5,150 km
Inner core
(solid)
6,370 km
364 GPa

Approximations

The mass (ρ), momentum ($\mathbf{v}$) and energy (T) equations, governing the dynamics of the fluid, are written in the rotating frame of reference of the spheres, and we

- apply the Boussinesq approximation, therefore

$$\rho = \overline{\rho}(1 - \alpha(T - \overline{T}))$$

  just in the gravity term, and all the physical quantities are taken constant. In addition we suppose constant density in the Coriolis term and that $\Omega^2/\gamma \ll 1$.

- Write the equations in terms of the perturbation of the temperature, Θ, with respect to the conduction state

$$T_c(r) = T_0 + \frac{\eta d \Delta T}{(1-\eta)^2 r},$$

  with $\eta = r_i/r_o$. Then $\Theta = T - T_c$.

- Nondimensionalize the equations with $d = r_o - r_i$ as length, $\nu^2/\gamma\alpha d^4$ as temperature, and d^2/ν as time scales.

- ν – Kinematic viscosity

- α – Thermal expansion coefficient

The equations

The equations for the perturbation of the conduction state, $\mathbf{v}_c = 0$ and $T_c(r) = T_0 + \eta d \Delta T/(1-\eta)^2 r$, are

$$(\partial_t + \mathbf{v}\cdot\boldsymbol{\nabla})\,\mathbf{v} = \underbrace{-\boldsymbol{\nabla}\pi}_{\text{pressure gradient}} + \underbrace{\nabla^2\mathbf{v}}_{\text{dissipative term}} \underbrace{-2E^{-1}\mathbf{k}\times\mathbf{v}}_{\text{Coriolis term}} + \underbrace{\Theta\mathbf{r}}_{\text{Buoyancy term}},$$

$$\sigma\,(\partial_t + \mathbf{v}\cdot\boldsymbol{\nabla})\,\Theta = \underbrace{\nabla^2\Theta}_{\text{dissipative term}} \underbrace{+Ra\,\eta(1-\eta)^{-2}r^{-3}\mathbf{r}\cdot\mathbf{v}}_{\text{advective term}},$$

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

with $\Theta = T - T_c$.

The non-dimensional parameters are

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

- κ – Thermal diffusivity
- $\Omega = |\boldsymbol{\Omega}|$

The symmetry group of the system (including b.c.) is $SO(2)\times\mathbb{Z}_2$. Then when the conduction state becomes unstable at a Hopf bifurcation, breaking the invariance by arbitrary azimuthal rotations, it gives rise to waves rotating in the azimuthal direction, which are invariant under rotations of $2\pi/m_d$.

Equations for the scalar potentials of the velocity field

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

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

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

$$\begin{aligned}
(\partial_t - \nabla^2) L_2 \Psi &= 2E^{-1} \left(\partial_\varphi \Psi - \mathcal{Q}\Phi\right) - \mathbf{r} \cdot \boldsymbol{\nabla} \times (\boldsymbol{\omega} \times \mathbf{v}), \\
(\partial_t - \nabla^2) L_2 \nabla^2 \Phi &= 2E^{-1} \left(\partial_\varphi \nabla^2 \Phi + \mathcal{Q}\Psi\right) - L_2 \Theta + \mathbf{r} \cdot \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times (\boldsymbol{\omega} \times \mathbf{v}), \\
\left(\sigma \partial_t - \nabla^2\right) \Theta &= Ra \frac{\eta}{(1-\eta)^2} \frac{1}{r^3} L_2 \Phi - \sigma (\mathbf{v} \cdot \boldsymbol{\nabla}) \Theta,
\end{aligned}$$

where $\boldsymbol{\omega} = \nabla \times \mathbf{v}$ is the vorticity. The operators L_2 and $\mathcal{Q}$ are defined as $L_2 \equiv -r^2 \nabla^2 + \partial_r (r^2 \partial_r)$, $Q \equiv r \cos\theta \nabla^2 - (L_2 + r\partial_r)(\cos\theta \partial_r - r^{-1} \sin\theta \partial_\theta)$, (r, θ, φ) being the spherical coordinates, with θ measuring the colatitude.

The boundary conditions at r_i and r_o become

- Non-slip boundaries, $\mathbf{v} = \mathbf{0} \qquad \Rightarrow \qquad \Phi = \partial_r \Phi = \Psi = 0$
- Perfectly conducting boundaries, $\Theta = 0$

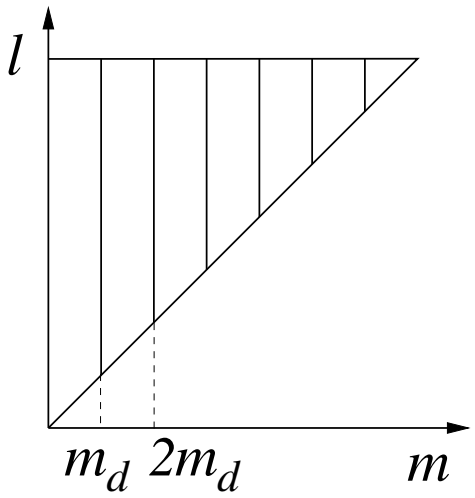
Expansion in spherical harmonics

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

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

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

$P_l^m(\cos\theta)$ is the associate Legendre polinomial, 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-1 Gauss-Lobatto points in the radius interval $[r_i,r_o]$. For some of the solutions without any symmetry shown later, the dimension of the system is larger than 2×10^6.

The equations for the amplitudes of the expansions are

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

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

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

for $0 \leq l \leq L$ and $0 \leq m = \dot{m}_d \leq l$, and where $\mathcal{D}_l = \partial_{rr}^2 + (2/r)\partial_r - l(l+1)/r^2$ and the action of the operator Q on a function f expanded in spherical harmonics is

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

with $c_l^m = ((l^2 - m^2)/(4l^2 - 1))^{1/2}$ and $D_l^+ f = \partial_r f + lf/r$.

The non-slip boundary conditions and the perfectly conducting boundaries are $\Phi_l^m = \partial_r \Phi_l^m = \Psi_l^m = 0$ and $\Theta_l^m = 0$ at $r_i = \eta/(1-\eta)$ and $r_o = 1/(1-\eta)$.

Stability of the conduction state

The above system will be written as

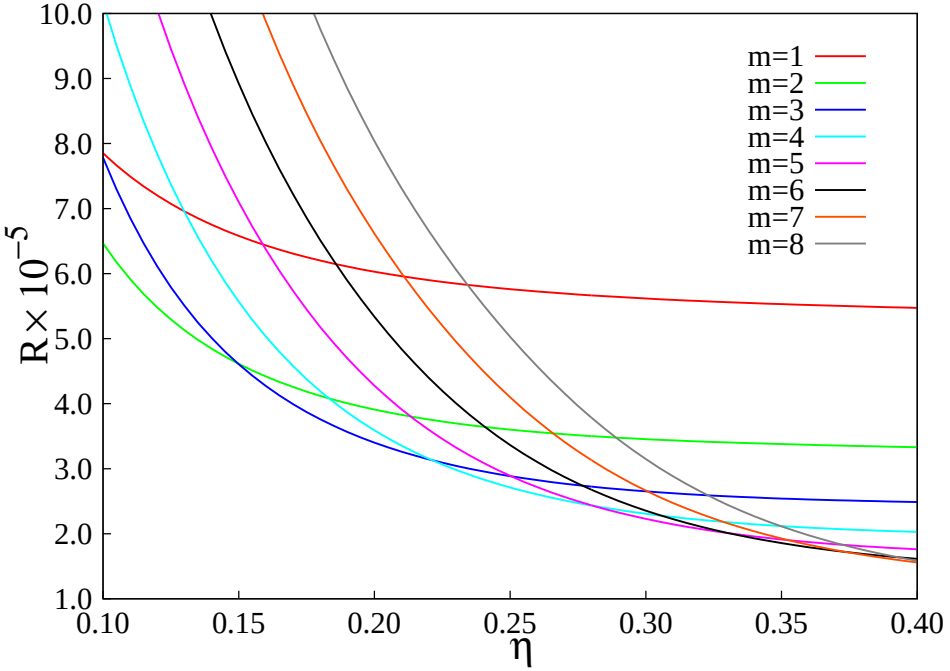
$$L_0 \partial_t u = Lu + B(u, u),$$

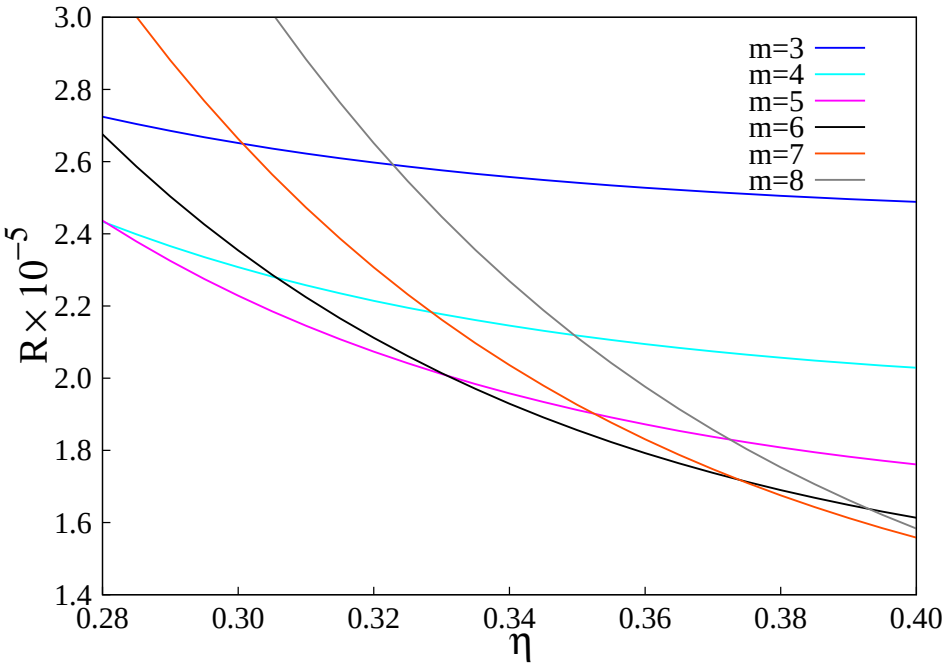
where u is a vector containing the values of the amplitudes at the mesh of collocation points in the radius, L and B are, respectively, linear and bilinear operators, and L depends on all the parameters of the problem, in particular on $Ra = p$, so we will write $L = L(p)$.

At critical values of $p = p_c$, the conduction state $u = 0$ becomes unstable. At the Hopf bifurcation its azimuthal invariance is broken and branches of rotating waves start there. Then, at p_c, there are vectors v_c and frequencies ω_c such that

$$i\omega_c L_0 v_c = L v_c.$$

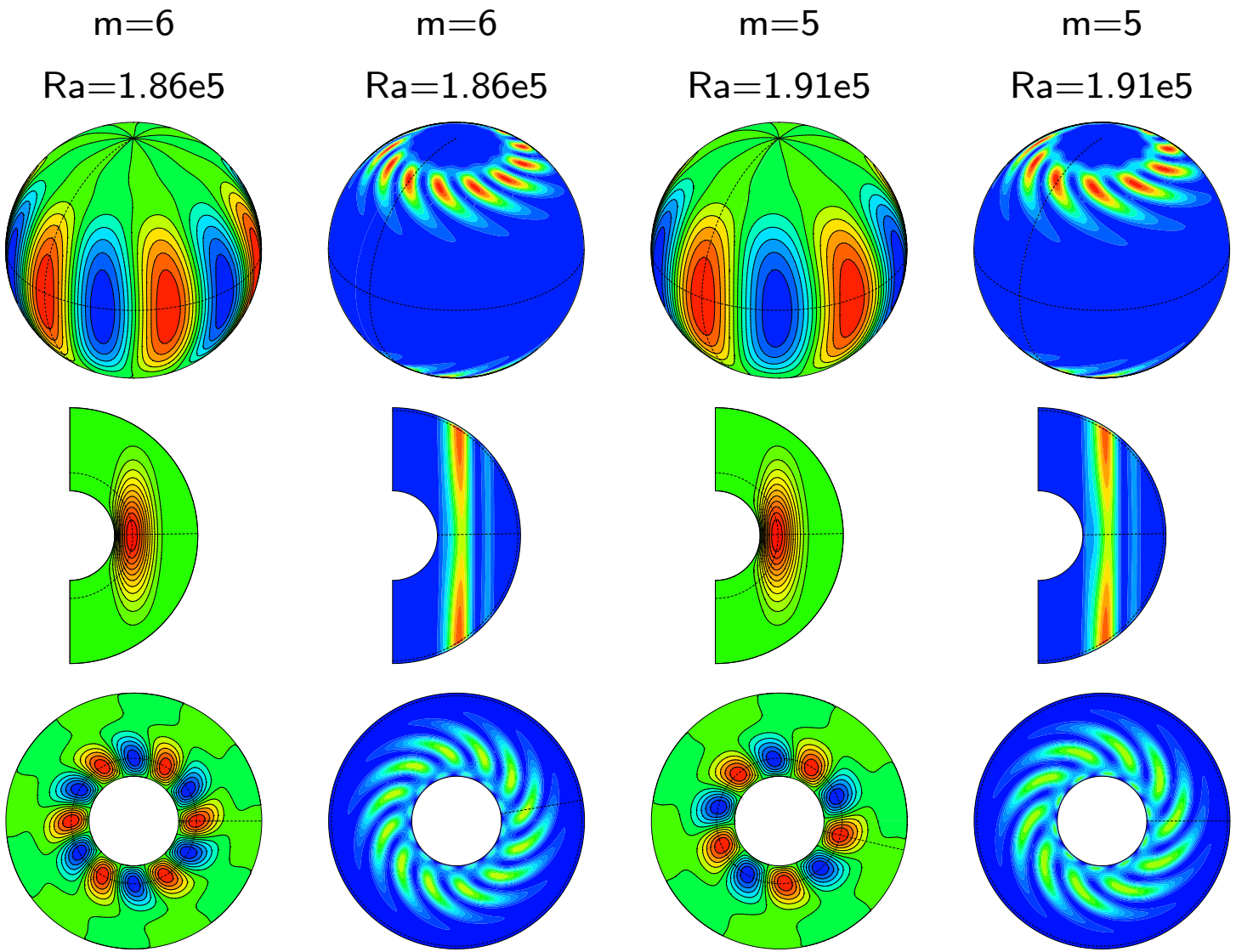
Radius ratio dependence





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



Azimuthal rotating waves

The rotating waves of

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

have a temporal dependence of the form

$$u(t,r,\theta,\varphi) = \tilde{u}(r,\theta,\varphi - \omega t).$$

By defining $\tilde{\varphi} = \varphi - \omega t$, deriving with respect to time, by applying the chain rule, and deleting the tildes, it is inmediate to check that $\tilde{u}$ satisfies

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

To define a curve of solutions this equation must be supplemented by adding a phase condition. We use $g_1(u) =< u, \partial_\varphi u_c >= 0$, where 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.

To study the dependence of the azimuthal waves with the parameter p we use continuation methods applied to the system

$$H(u,\omega,p) = \begin{pmatrix} F(u,\omega,p) \\ < u, \partial_\varphi u_c > \end{pmatrix} = 0,$$

for $X = (u,\omega,p)$.

For the linear systems we use GMRES, which requires the action of the Jacobian matrix $D_X H(u, \omega, p)$ on vectors and a suitable preconditioner for

$$\begin{pmatrix} D_X H(u,\omega,p) \\ \partial_X h(u,\omega,p) \end{pmatrix} = \begin{pmatrix} \partial_u F & \partial_\omega F & \partial_p F \\ \partial_u g_1 & 0 & 0 \\ (\partial_u h)^\top & \partial_\omega h & \partial_p h \end{pmatrix},$$

where $h(u, \omega, p) = 0$ is the pseudo-arclength condition.

We use

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

$L_{prec} = L(p_{prec})$ and ω_{prec} being, respectively, 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 by means of an adapted LU decomposition.

Stability of the waves

Suppose a wave of the form $u(r,\theta,\varphi-\omega t)=u(r,\theta,\tilde{\varphi})$ has been found.

To study its stability we consider a perturbation $v(t,r,\theta,\tilde{\varphi})$ of $u(r,\theta,\tilde{\varphi})$. Then, the linearization of the equation gives the eigenvalue problem

$$\lambda L_0 v = \left(L+\omega L_0\partial_{\tilde{\varphi}}+B(u,\cdot)+B(\cdot,u)\right)v.$$

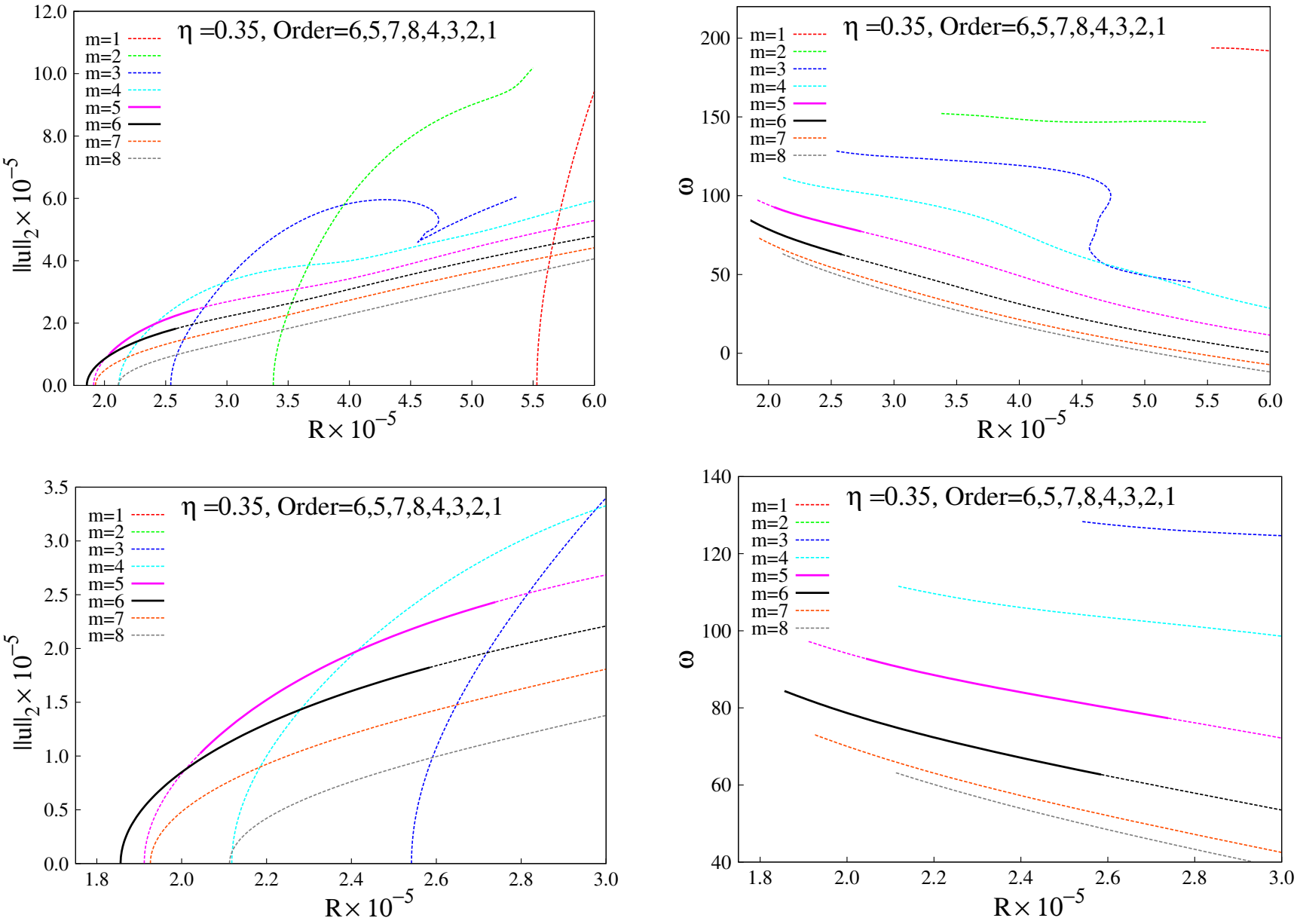
To find the leading spectra, the ARPACK package based on Arnoldi algorithms (Lehoucq & Sorensen(1998)) is employed. The subroutine only needs the action of the operator $L_0^{-1}D_uF(u)$ on vectors, and it provides the eigenvalues of maximal modulus, so to get those of maximal real part some transformation must be used. We use a real shift-invert transformation, with shift β, and compute the eigenvalues of

$$(L_0^{-1}D_uF(u)-\beta I)^{-1}.$$

Then if ζ is eigenvalue of this matrix, $\lambda=\beta+1/\zeta$ is eigenvalue of $L_0^{-1}D_uF(u)$.

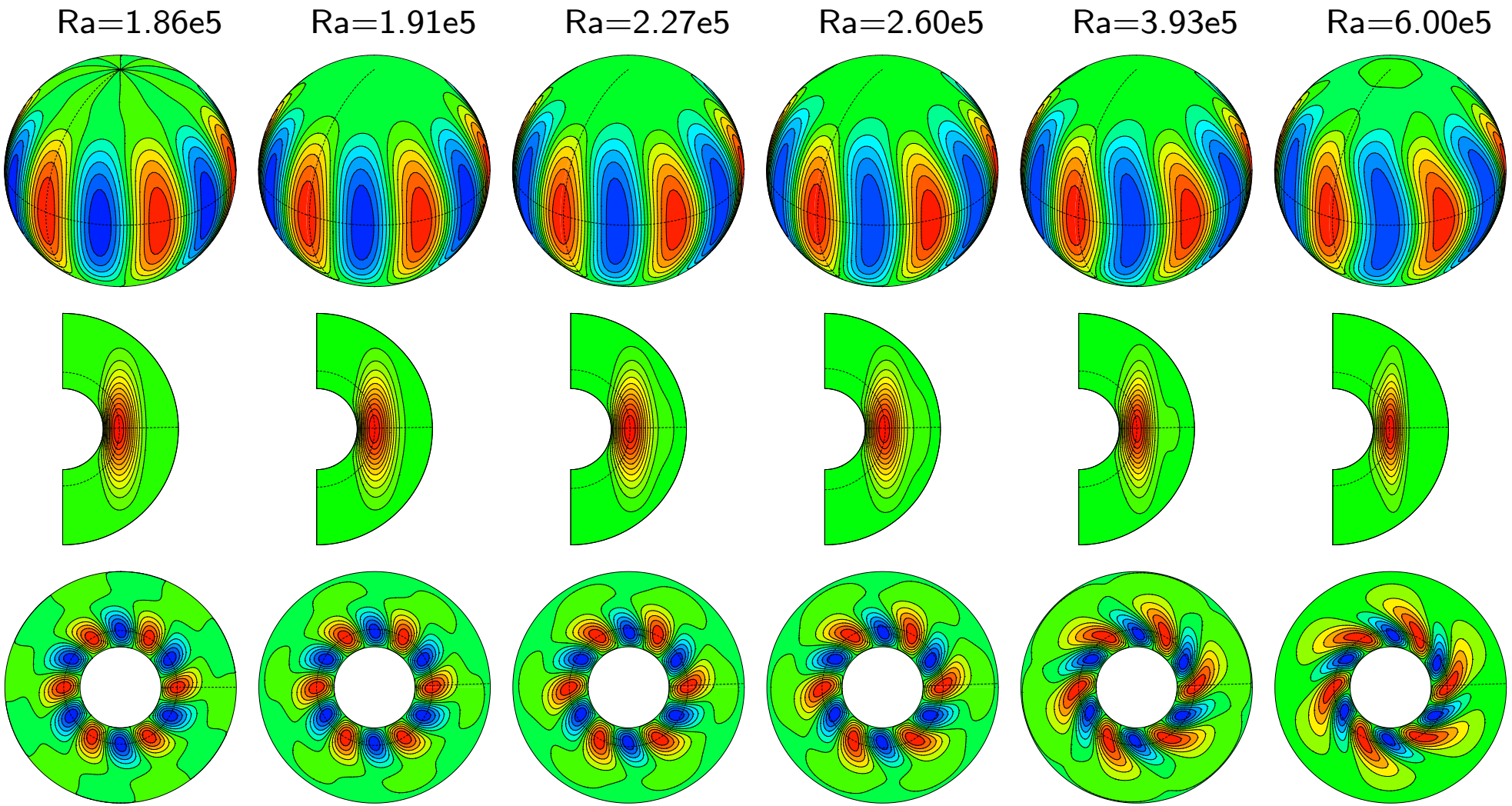
To apply the inverse matrix on a vector is equivalent to solving with $(L_0^{-1}D_uF(u)-\beta I)$, but the convergence is very slow. So we precondition with the tridiagonal part of the matrix minus βI, $L_0^{-1}(L+\omega L_0\partial_{\tilde{\varphi}}-\beta I)$.

Bifurcation diagram for $\eta = 0.35$

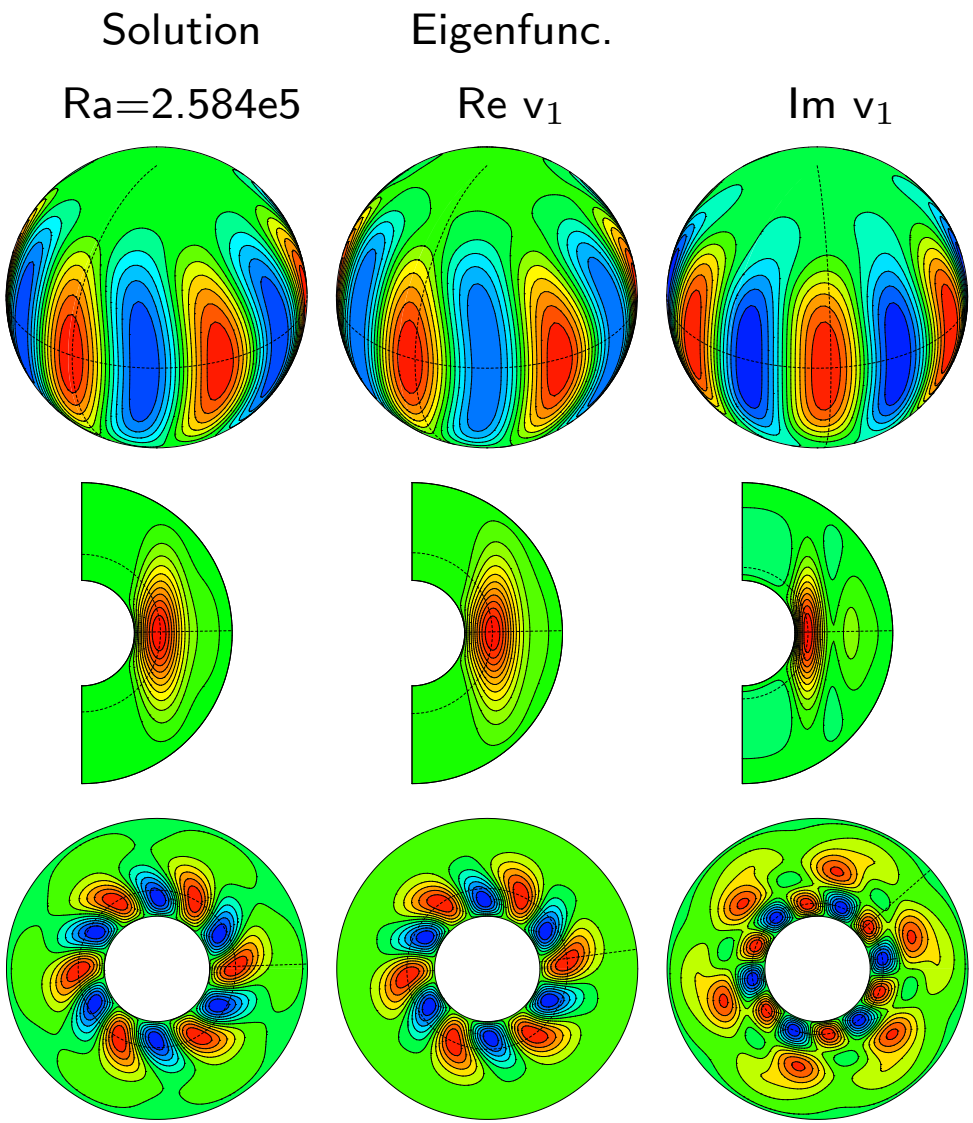


Norm and frequency versus Ra for $\eta = 0.35$, $\sigma = 0.1$, and $E = 10^{-4}$.

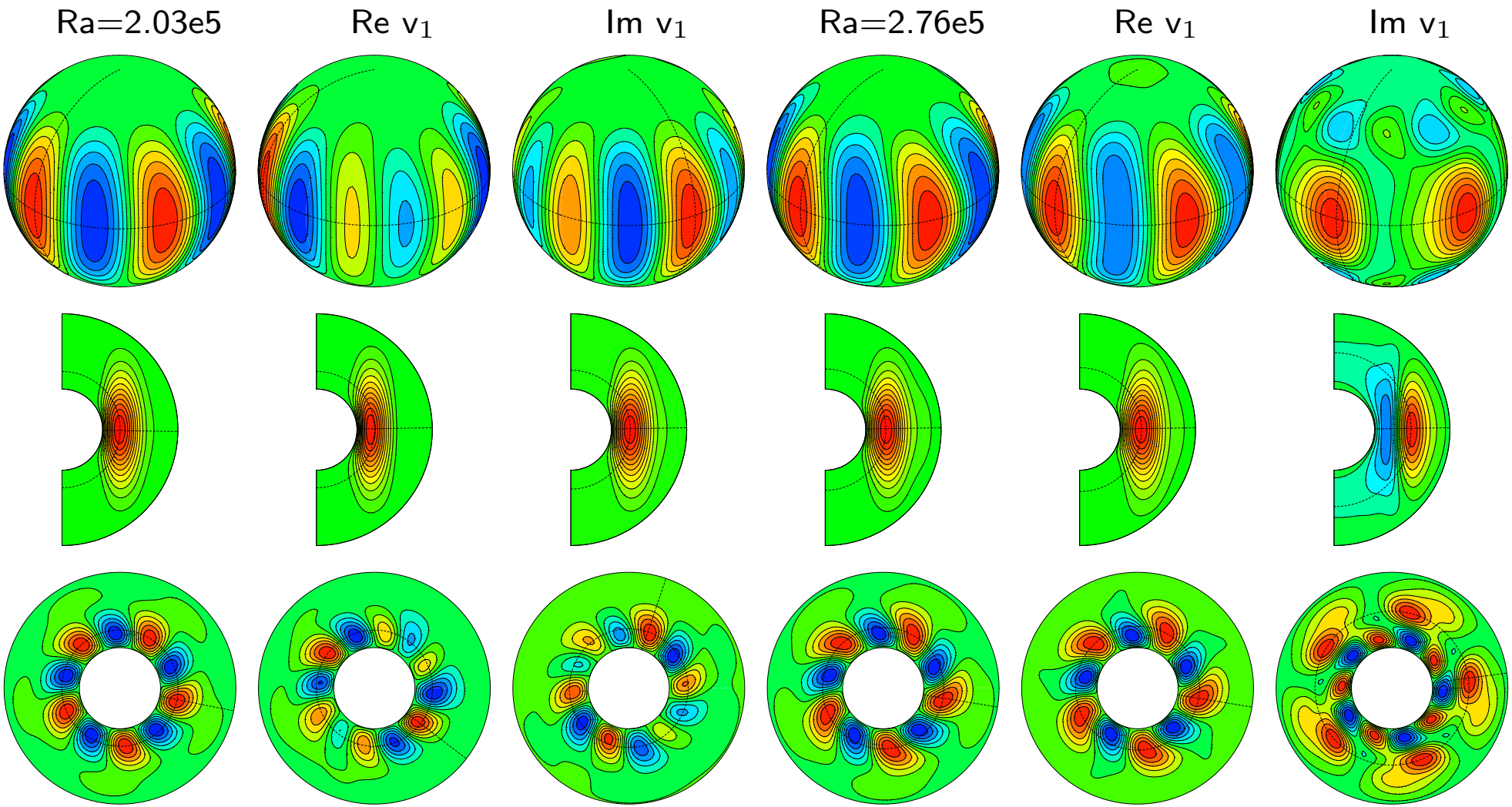
Solutions along the m=6 branch



Eigenfunctions at the bifurcation from the m=6 wave



Eigenfunctions at the bifurcation from the m=5 wave



Modulated rotating waves

The instability of the rotating waves gives rise to modulated rotating waves of the system

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

These modulated waves are solutions for which there exist a minimal time $\tau > 0$ and a precession velocity ω such that

$$u(t + \tau, r, \theta, \varphi) = u(t, r, \theta, \varphi - \omega\tau) \quad \forall t.$$

The time τ is the period of the modulation in the frame of reference at which only the oscillations due to the modulation are observed, and ω is the angular velocity of this frame of reference (relative to the spheres).

In this case, taking into account that the modulated rotating waves can be written as $u(t, r, \theta, \varphi) = \tilde{u}(t, r, \theta, \varphi - \omega t)$ and that again we call $\tilde{\varphi} = \varphi - \omega t$, by deriving, it results that $\partial_t u = \partial_t \tilde{u} - \omega \partial_{\tilde{\varphi}} \tilde{u}$. So, they can be computed as periodic orbits of the system

$$L_0 \partial_t u = \omega L_0 \partial_{\tilde{\varphi}} u + L(p)u + B(u, u).$$

Now, the unknows are $X = (u, \tau, \omega, p)$, so two additional phase conditions $g_1(u) = 0$, $g_2(u) = 0$ are needed to define a curve of solutions. As before, we suppose the pseudo-arclength condition included in the continuation code.

The conditions $g_1(u) = 0$ and $g_2(u) = 0$ are selected to fix the two undetermined phases of the modulated wave. We use the conditions $g_1(u) =< u, \partial_\varphi u_c >= 0$ and $g_2(u) =< u, \partial^3_\varphi u_c >= 0$, where u_c is a reference solution (the eigenvector, $u_c = v_c$, at $p = p_c$, a previously computed solution, or the extrapolated value of u at the first iteration). The former determines the azimuthal phase and the second the phase of the modulation.

So, we look for solutions of the system

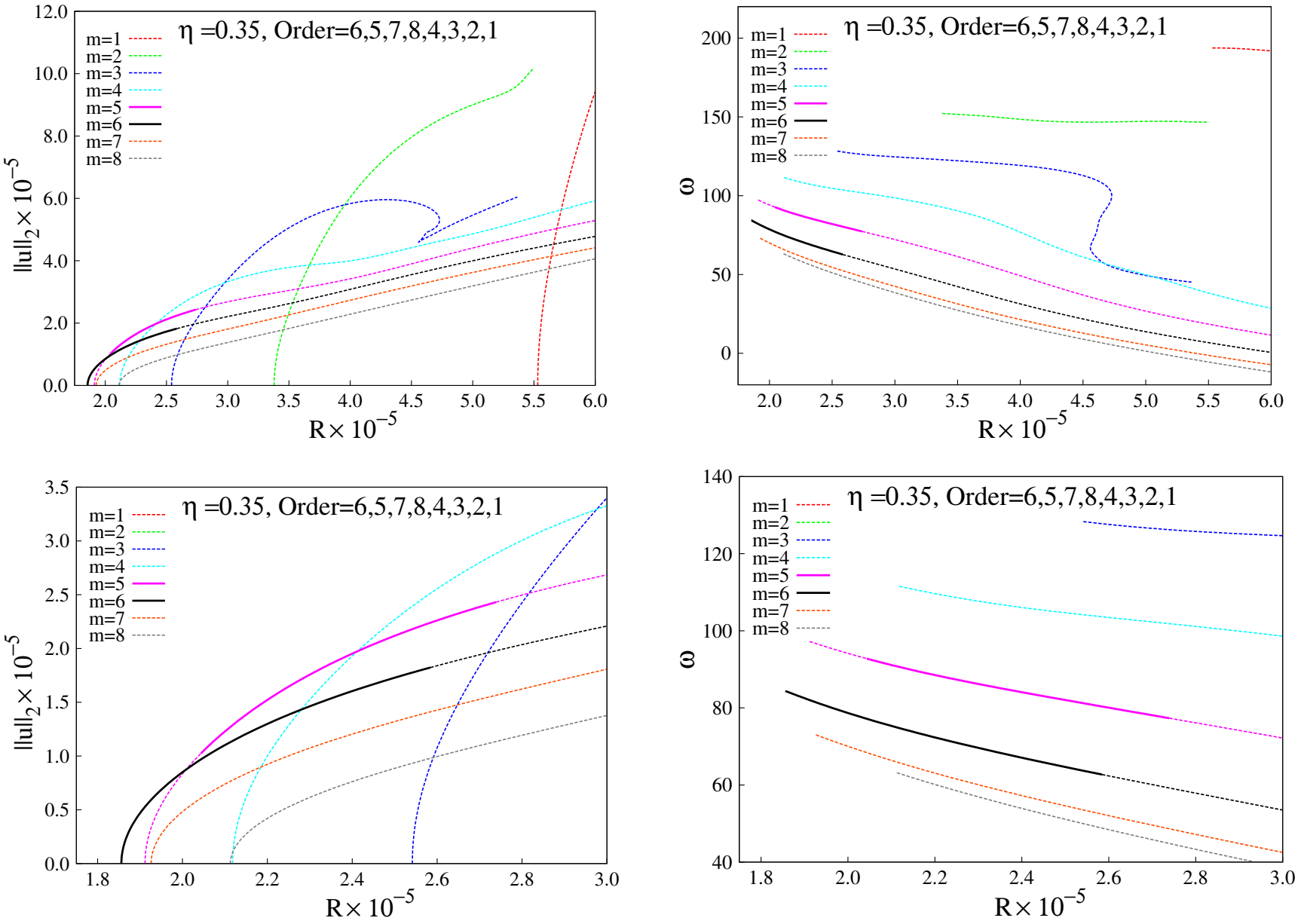
$$H(u, \omega, \tau, p) = \begin{pmatrix} u - \phi(\tau, u, \omega, p) \\ < u, \partial_\varphi u_c > \\ < u, \partial^3_\varphi u_c > \end{pmatrix} = 0,$$

$\phi(\tau, u, \omega, p)$ being the solution of

$$L_0 \partial_t u = \omega L_0 \partial_{\tilde{\varphi}} u + L(p)u + B(u, u)$$

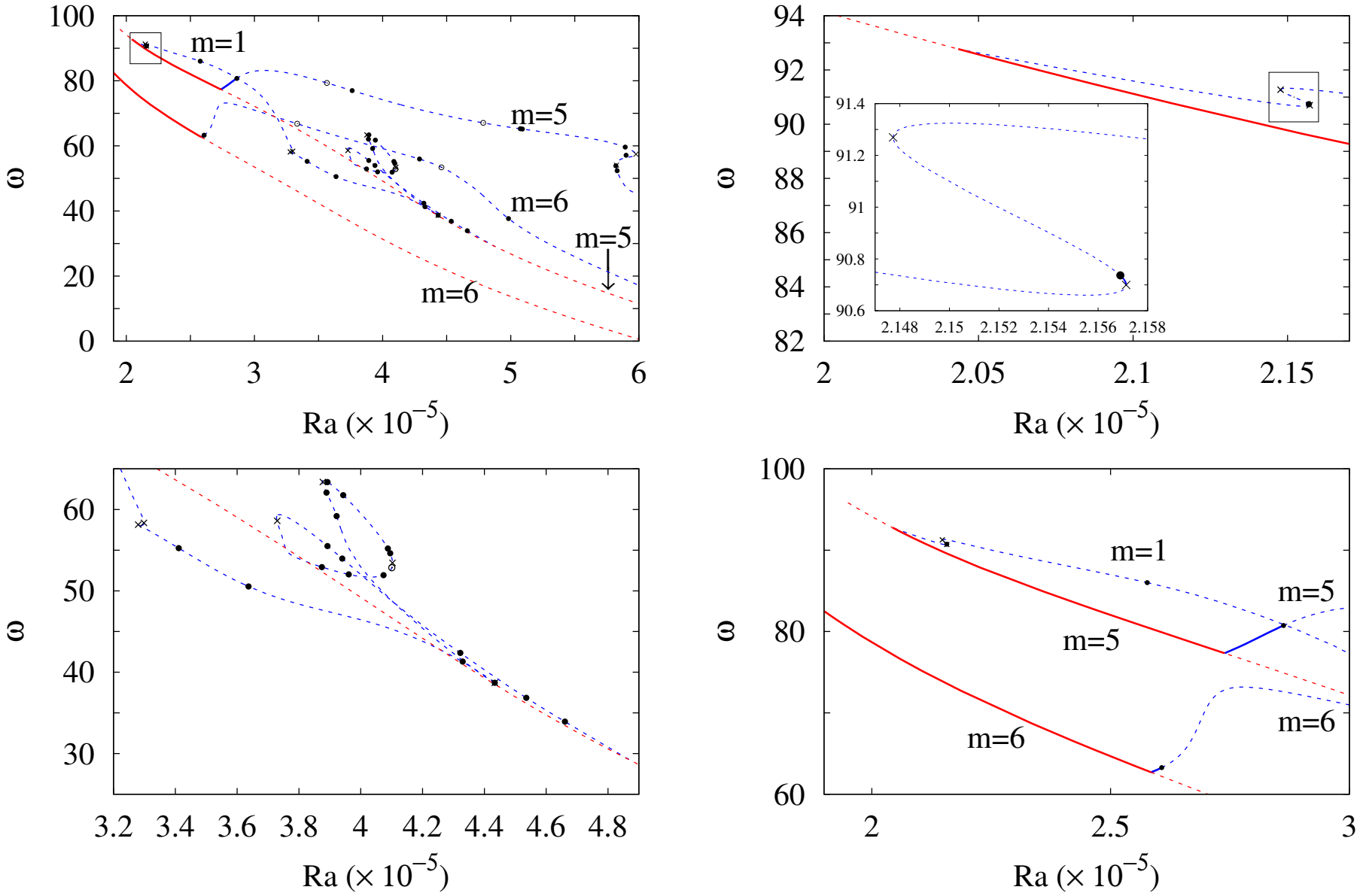
at time τ with initial condition u at $t = 0$, and for fixed ω and p (the continuation parameter).

Bifurcation diagram for $\eta = 0.35$



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

Bifurcation diagram of ω versus Ra



Travelling waves (red), modulated waves (blue). Stable (solid line), unstable (dashed-line). The parameters are $\sigma = 0.1$, and $E = 10^{-4}$.

Some conclusions for this problem

- With continuation techniques we have been able to find branches of travelling as well as modulated waves which are impossible to detect with just time integrations. Regions of multistability of two and three different waves have been identified.
- We have obtained branches of stable modulated waves in a small Rayleigh number range, one of them, without any azimuthal symmetry at $Ra/Ra_c = 1.16$, i.e, very close to the onset of convection.
- The $m = 1, 5, 6$ modulated waves give rise to three-frequency stable solutions via tertiary Hopf bifurcations. The symmetry of the latter is seen from the eigenfunctions of the stability problem.
- To find a single modulated wave with relative tolerances of 10^{-8} the Newton-Krylov method typically converges in roughly 4 Newton iterations. Each of them requires a function evaluation, i.e, one time integration of an ODE system of dimension $n = 0(10^5 - 10^6)$ plus an average of 15 GMRES iterations, i.e, 15 additional time integrations of an ODE system of dimension $2n$ are needed. Close to bifurcation points the convergence slows down. Efficient and accurate (high-order) time integration is essential.

Other kind of computations

Already studied:

- Computation of periodic orbits by multiple shooting in parallel with each shoot on a different processor and preconditioned to obtain a linear speed-up.
- Invariant 2-tori, computing a single point on the invariant curve on a Poincaré section.
- Invariant 2-tori, computing a collection of points approximating a segment of the invariant curve on a Poincaré section.
- Computation of boundaries of Arnold's tongues.
- Computation of the coefficients of a normal form close to a multicritical periodic orbit only known numerically.

To do:

- Continuation of some codimension-two bifurcations. Some require the vanishing of a normal form coefficient. Are there alternative formulations without the need of adjoint problems?
- Delay ODEs or PDEs.
- Software. Write a driver for the most common computations (equilibria, periodic orbits and branching at codimension-one bifurcations), letting to the user the spatial discretization and time integration.
- etc.

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