Numerical methods for large-scale dissipative dynamical systems.

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Equilibria and periodic orbits of PDEs

Equilibria and periodic orbits of ODEs

Suppose

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

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

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

x being a point of the periodic orbit selected by the phase condition $g(x, p) = 0$ 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.

Newton-Krylov continuation methods

Continuation of zeros of a nonlinear system of equations

Consider a system of nonlinear equations depending on a parameter p

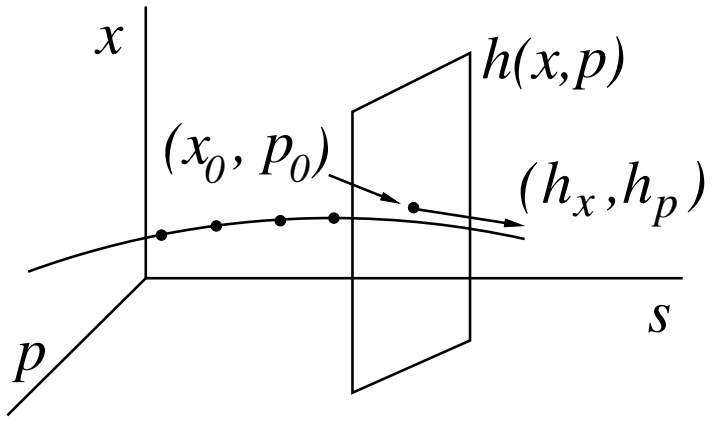
$$H(x,p)=0, \quad (x,p)\in\mathcal{U}\subset\mathbb{R}^m\times\mathbb{R}$$

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 solutions. 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 $h(x,p)=h_x^\top(x-x_0)+h_p(p-p_0)$, 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 points.



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, FOM, TFQMR, 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
FOM	=	Full Orthogonalization Method
TFQMR	=	Transpose-Free Quasi-Minimal Residual

An example of a matrix-free product

Consider the system of PDEs

$$\partial_\tau c = (1/Pe_m)\partial^2_{ss} c - \partial_s c - Dc\exp(\gamma(1-1/\theta))$$
$$\partial_\tau \theta = (1/Pe_h)\partial^2_{ss}\theta - \partial_s\theta - \beta(\theta-\theta_r) + BDc\exp(\gamma(1-1/\theta)),$$

modelling a tubular exotermic chemical reactor (Heinemann and Poore 1981), with $s \in [0,1]$, and where c, θ and τ are the non-dimensional concentration of a reactant, temperature and time, respectivelly. Pe_m, Pe_h, D, β, B, θ_r and γ are non-dimensional parameters of the problem.

Suppose that all of them are fixed except D that will be our control parameter (p in the previous slides), and that our state variable is $x = (c, \theta)$.

Let

$$H(x,p) = \begin{pmatrix} (1/Pe_m)\partial^2_{ss} c - \partial_s c - Dc\exp(\gamma(1-1/\theta)) \\ (1/Pe_h)\partial^2_{ss}\theta - \partial_s\theta - \beta(\theta-\theta_r) + BDc\exp(\gamma(1-1/\theta)) \end{pmatrix}.$$

Then, if $\delta x = (\delta c, \delta\theta)$ and $\delta p = \delta D$,

$$D_x H(x,p)\delta x + D_p H(x,p)\delta p =$$
$$\begin{pmatrix} (1/Pe_m)\partial^2_{ss}\delta c - \partial_s\delta c - \exp(\gamma(1-1/\theta))(D\delta c + Dc(\gamma/\theta^2)\delta\theta + \delta Dc) \\ (1/Pe_h)\partial^2_{ss}\delta\theta - \partial_s\delta\theta - \beta\delta\theta + B\exp(\gamma(1-1/\theta))(D\delta c + Dc(\gamma/\theta^2)\delta\theta + \delta Dc) \end{pmatrix}.$$

Inexact Newton's methods

Types of convergence

Iterative methods can be classified by their rate of convergence.

Definition. *Let $\{x_k\} \subset \mathbb{R}^n$ and $x^* \in \mathbb{R}^n$. Then*

- *$x_k \to x^*$ q-quadratically if $x_k \to x^*$ and there is $K > 0$ such that*

$$\|x_{k+1} - x^*\| \leq K\|x_k - x^*\|^2.$$

- *$x_k \to x^*$ q-superlinearly with q-order $\alpha > 1$ if $x_k \to x^*$ and there is $K > 0$ such that*

$$\|x_{k+1} - x^*\| \leq K\|x_k - x^*\|^\alpha.$$

- *$x_k \to x^*$ q-superlinearly if*

$$\lim_{n\to\infty} \|x_{k+1} - x^*\|/\|x_k - x^*\| = 0.$$

- *$x_k \to x^*$ q-linearly with q-factor $\sigma \in (0, 1)$ if*

$$\|x_{k+1} - x^*\| \leq \sigma\|x_k - x^*\|.$$

Definition. *Let $\{x_k\} \subset \mathbb{R}^n$ and $x^* \in \mathbb{R}^n$. Then $x_k \to x^*$ r-(quadratically, superlinearly, linearly) if there is a sequence $\{\xi_k\} \subset \mathbb{R}$ converging q-(quadratically, superlinearly, linearly) to zero such that*

$$\|x_k - x^*\| \leq \xi_k,$$

and $x_k \to x^*$ r-superlinearly with r-order $\alpha > 1$ if the sequence $\xi_k \to 0$ q-superlinearly with q-order α.

Newton's method

Suppose we seek to solve the system

$$F(x) = 0$$

with $x, F(x) \in \mathbb{R}^n$, and assume the following *standard* conditions hold

- $F(x) = 0$ has a solution x^*,
- There is a neighborhood of x^*, $\Omega \subset \mathbb{R}^N$, such that $DF : \Omega \to \mathbb{R}^{N \times N}$ is Lipschitz continuous with Lipschitz constant $\gamma > 0$, i.e.,

  $$\|DF(x) - DF(y)\| \leq \gamma \|x - y\|$$

  for all $x, y \in \Omega$,
- $DF(x^*)$ is nonsingular.

Theorem. *Under the above assumptions there is a $\delta > 0$ such that if $\|x_0 - x^*\| < \delta$ the Newton iteration*

$$x_{k+1} = x_k + s_k, \quad \textit{with} \quad DF(x_k)s_k = -F(x_k)$$

converges q-quadratically to x^*, i.e., there is a $K > 0$ such that

$$\|x_{k+1} - x^*\| \leq K \|x_k - x^*\|^2.$$

Inexact Newton methods

Suppose now that instead of solving

$$DF(x_k)s_k = -F(x_k)$$

exactly, the linear system is solved by an iterative method with stopping criteria

$$\|DF(x_k)s_k + F(x_k)\| \leq \eta_k \|F(x_k)\|.$$

Theorem. *Let the standard conditions hold. Then there exists $\delta > 0$ such that if $\|x_0 - x^*\| < \delta$, and $\{\eta_k\} \subset [0, \eta]$ with $\eta < \bar{\eta} < 1$, then the inexact Newton iteration*

$$x_{k+1} = x_k + s_k, \quad \text{with} \quad \|DF(x_k)s_k + F(x_k)\| \leq \eta_k \|F(x_k)\|,$$

converges q-linearly to x^* with respect to the norm $\|\cdot\|_* = \|DF(x^*)\cdot\|$. Moreover

- *if $\eta_k \to 0$ the convergence is q-superlinear, and*
- *if $\eta_k \leq K_\eta \|F(x_k)\|^p$ for some $K_\eta > 0$ the convergence is q-superlinear with q-order 1+p.*

Proposition. *Under the standard conditions, and if $x_k \to x^*$, $\|x_k - x^*\|_* \to 0$ q-linearly if and only if $\|F(x_k)\|$ does.*

Iterative linear solvers and GMRES

Krylov methods for linear systems

Large-scale non-symmetric 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 satisfies

$$||b - Ax_k||_2 = \inf_{x \in x_0 + \mathcal{K}_k} \|b - Ax\|_2.$$

It minimizes the norm $||b - Ax||_2$ 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

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

It follows that

$$\begin{aligned} r_k =& b - Ax_k = b - A(x_0 + z_k) = r_0 - Az_k = \\ &= Ir_0 - A(\alpha_1 r_0 + \alpha_2 Ar_0 + \cdots + \alpha_k A^{k-1} r_0) \\ &= (I - \alpha_1 A - \alpha_2 A^2 - \cdots - \alpha_k A^k) r_0 = p_k(A) r_0 \end{aligned}$$

p_k being a polynomial of degree k, with $p_k(0) = 1$.

Now, by using that

- If $A = V\Lambda V^{-1}$ then $A^l = V\Lambda^l V^{-1}$ and $p(A) = Vp(\Lambda)V^{-1}$
- If $\Lambda = diag(\lambda_1, \ldots, \lambda_n)$ then $p(\Lambda) = diag(p(\lambda_1), \ldots, p(\lambda_n))$
- $\|p(A)\|_2 \leq \|p(\Lambda)\|_2 \|V\|_2 \|V^{-1}\|_2 = \kappa_2(V)\|p(\Lambda)\|_2$, with $\kappa_2(V) = \|V\|_2\|V^{-1}\|_2$ the norm-2 condition number of V.
- If $\Lambda = diag(\lambda_1, \ldots, \lambda_n)$ then $\|p(\Lambda)\|_2 = \max_{i=1,\ldots,n} |p(\lambda_i)|$

the following result is obtained.

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*

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

Proof:

$$\|b - Ax_k\|_2 = \inf_{\substack{p \in P_k \\ p(0)=1}} \|p(A)r_0\| \leq \kappa_2(V) \inf_{\substack{p \in P_k \\ p(0)=1}} \max_{i=1,\ldots,n} |p(\lambda_i)| \|b - Ax_0\|_2.$$

The Arnoldi's factorization

It is used in the solution of linear systems, eigenvalue problems (Arnoldi's method), and to find reduced order models by the dynamic mode decomposition (DMD).

Let $\langle ., . \rangle$ be the euclidean dot product. Given a matrix A and an initial unitary vector v_1

Iterate: for $j = 1, 2, \ldots, k$ compute

1. $h_{i,j} = \langle Av_j, v_i \rangle$, for $i = 1, 2, \ldots, j$
2. $w_j = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$ (this is classical Gram-Schmidt orthogonalization)
3. $h_{j+1,j} = \|w_j\|_2$, if $h_{j+1,j} = 0$ stop
4. $v_{j+1} = w_j / h_{j+1,j}$

If $V_k = [v_1, \ldots, v_k]$ is the matrix with columns $v_1, \ldots, v_k$ then

- The columns of V_k form an orthonormal basis of $\mathcal{K}_k = \{v_1, Av_1, A^2 v_1, \ldots, A^{k-1} v_1\}$.
- If H_k is the $k \times k$ upper Hessenberg matrix whose nonzero entries are the $h_{i,j}$ then

$$AV_k = V_k H_k + w_k e_k^\top, \quad \text{and} \quad V_k^\top A V_k = H_k,$$

  with $w_k = h_{k+1,k} v_{k+1}$, and $e_k^\top = (0, \ldots, 0, 1) \in \mathbb{R}^k$.

- If $\tilde{H}_k$ is the $(k+1) \times k$ matrix whose nonzero entries are the $h_{i,j}$ then

$$AV_k = V_{k+1} \tilde{H}_k.$$

The matrix H_k is $\tilde{H}_k$ without its last row.

$AV_k = V_k H_k + h_{k+1,k} v_{k+1} e_k^\top$:

$$A[v_1, \ldots, v_k] = [v_1, \ldots, v_k] \begin{bmatrix} h_{1,1} & h_{1,2} & h_{1,3} & \cdots & h_{1,k} \\ h_{2,1} & h_{2,2} & h_{2,3} & \cdots & h_{2,k} \\ 0 & h_{3,2} & h_{3,3} & \cdots & h_{3,k} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & h_{k,k-1} & h_{k,k} \end{bmatrix} + h_{k+1,k}[0, \ldots, 0, v_{k+1}]$$

$AV_k = V_{k+1} \tilde{H}_k$:

$$A[v_1, \ldots, v_k] = [v_1, \ldots, v_k, v_{k+1}] \begin{bmatrix} h_{1,1} & h_{1,2} & h_{1,3} & \cdots & h_{1,k} \\ h_{2,1} & h_{2,2} & h_{2,3} & \cdots & h_{2,k} \\ 0 & h_{3,2} & h_{3,3} & \cdots & h_{3,k} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & h_{k,k-1} & h_{k,k} \\ 0 & \cdots & \cdots & 0 & h_{k+1,k} \end{bmatrix}$$

Practical implementation of the Arnoldi's factorization

Given a matrix A and an initial unitary vector v_1 Iterate: for $j = 1, 2, \ldots, k$ compute

1. $w = Av_j$
2. for $i = 1, 2, \ldots, j$ do (this is modified Gram-Schmidt orthogonalization)
   (a) $h_{i,j} = \langle w, v_i \rangle$
   (b) $w \leftarrow w - h_{i,j} v_i$
3. $h_{j+1,j} = \|w\|_2$, if $h_{j+1,j} = 0$ stop
4. $v_{j+1} = w/h_{j+1,j}$

To complete GMRES, it remains to solve the minimizing problem

$$\inf_{x \in x_0 + \mathcal{K}_k} \|b - Ax\|_2.$$

Suppose that $v_1, \ldots, v_k$ form an orthonormal basis of $\mathcal{K}_k$ and let $V_k = [v_1, \ldots, v_k]$. It is found by means of the Arnoldi factorization with $v_1 = r_0/\|r_0\|$. Then

$$x \in x_0 + \mathcal{K}_k \implies x = x_0 + V_k y \quad \text{with} \quad y \in \mathbb{R}^k,$$

and

$$\inf_{x \in x_0 + \mathcal{K}_k} \|b - Ax\|_2 = \inf_{y \in \mathbb{R}^k} \|b - A(x_0 + V_k y)\| = \inf_{y \in \mathbb{R}^k} \|r_0 - AV_k y\|.$$

Now, since $AV_k = V_{k+1}\tilde{H}_k$,

$$\|r_0 - AV_k y\|_2 = \|r_0 - V_{k+1}\tilde{H}_k y\|_2 = \|V_{k+1}^\top(\beta v_1 - V_{k+1}\tilde{H}_k y)\|_2 = \|\beta e_1 - \tilde{H}_k y\|_2$$

with $\beta = \|r_0\|$, $e_1 = (1, 0, \ldots, 0)^\top \in \mathbb{R}^{k+1}$ and $y \in \mathbb{R}^k$.

Therefore

$$\inf_{x \in x_0 + \mathcal{K}_k} \|b - Ax\|_2 = \inf_{y \in \mathbb{R}^k} \|\beta e_1 - \tilde{H}_k y\|_2.$$

The latter is a least-squares problem without restrictions in $\mathbb{R}^k$.

One wants to solve the system in a small number of iterations to avoid the matrix V_k to grow too much and then in practice $k \ll n$.

The restarted GMRES(m) algorithm

The complete restarted version of the algorithm GMRES(m) is , given x_0, and $r_0 = b - Ax_0$,

1. Set $l = 0$.
2. Start: Choose as initial unitary vector $v_1 = r_0/\|r_0\|$, set $\rho = \beta = \|r_0\|$, $k = 0$.
3. do while $\rho > \varepsilon$, $k < m$, and $l < l_{max}$:
   (a) set $k = k + 1$ and $l = l + 1$
   (b) compute the Arnoldi's factorization $AV_k = V_{k+1}\tilde{H}_k$
   (c) find y_k the minimizer of $\|\beta e_1 - \tilde{H}_k y\|_2$
   (d) set $\rho = \|\beta e_1 - \tilde{H}_k y_k\|_2$ (remember that $\inf_{x \in x_0 + \mathcal{K}_k} \|b - Ax\|_2 = \inf_{y \in \mathbb{R}^k} \|\beta e_1 - \tilde{H}_k y\|_2$)
4. if $\rho < \varepsilon$ then set $x_k = x_0 + V_k y_k$ as approximate solution and exit
5. if $l > l_{max}$ (too many iterations without convergence) exit
6. if $k = m$ set $x_0 \leftarrow x_0 + V_k y_k$ and restart the algorithm (go to 2).

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 the 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.

Spatial discretization of the HP problem

Consider the system of PDEs

$$\partial_\tau c = (1/Pe_m)\partial^2_{ss} c - \partial_s c - Dc\exp(\gamma(1-1/\theta))$$
$$\partial_\tau \theta = (1/Pe_h)\partial^2_{ss} \theta - \partial_s \theta - \beta(\theta-\theta_r) + BDc\exp(\gamma(1-1/\theta)),$$

in the interval $s \in [0,1]$, with boundary conditions

$$\partial_s c = Pe_m(c-1) \quad \text{at} \quad s=0, \qquad \partial_s c = 0 \quad \text{at} \quad s=1,$$
$$\partial_s \theta = Pe_h(\theta-1) \quad \text{at} \quad s=0, \qquad \partial_s \theta = 0 \quad \text{at} \quad s=1.$$

To implement the boundary conditions easily we substitute $c = \bar{c}+1$, $\theta = \bar{\theta}+1$ in the equations and boundary conditions to obtain, after removing the overbars the equations

$$\partial_\tau c = (1/Pe_m)\partial^2_{ss} c - \partial_s c - D(c+1)\exp(\gamma\theta/(\theta+1)))$$
$$\partial_\tau \theta = (1/Pe_h)\partial^2_{ss} \theta - \partial_s \theta - \beta(\theta-\theta_r+1) + BD(c+1)\exp(\gamma\theta/(\theta+1))),$$

with boundary conditions

$$\partial_s c = Pe_m c \quad \text{at} \quad s=0, \qquad \partial_s c = 0 \quad \text{at} \quad s=1,$$
$$\partial_s \theta = Pe_h \theta \quad \text{at} \quad s=0, \qquad \partial_s \theta = 0 \quad \text{at} \quad s=1.$$

If $D=0$ and $\theta_r = 1$ then $c=0$ and $\theta = 0$ is a solution of the problem.

We use collocation methods in a Gauss-Lobatto mesh. Let $s_i = 0.5(1 - \cos(\pi i/n_d))$, $i = 0, \ldots, n_d$ and $D^{(l)} = \{d^{(l)}_{i,j}\}$ the $(n_d + 1) \times (n_d + 1)$ matrices which approximate the derivatives on the mesh, i.e,

$$f^{(l)}(s_i) \approx \sum_{j=0}^{n_d} d^{(l)}_{i,j} f(s_j), \quad i = 0, \ldots, n_d.$$

Let $c_i = c(s_i)$, $\theta_i = \theta(s_i)$ and approximate the boundary conditions (of c, for instance) by

$$\sum_{j=0}^{n_d} d^{(1)}_{0,j} c_j = Pe_m c_0, \qquad \sum_{j=0}^{n_d} d^{(1)}_{n_d,j} c_j = 0.$$

From these two equations the values at the end points can be obtained as a linear combination of the values at the inner points,

$$c_0 = \sum_{j=1}^{n_d-1} \alpha_{0,j} c_j, \quad c_{n_d} = \sum_{j=1}^{n_d-1} \alpha_{n_d,j} c_j.$$

And then, for instance,

$$\partial^2_{ss} c(s_i) \approx \sum_{j=1}^{n_d-1} (d^{(2)}_{i,j} + d^{(2)}_{i,0}\alpha_{0,j} + d^{(2)}_{i,n_d}\alpha_{n_d,j}) c_j = \sum_{j=1}^{n_d-1} \tilde{d}^{(2)}_{i,j} c_j, \quad i = 1 \ldots, n_d - 1$$

and $\tilde{D}^{(2)} = \{\tilde{d}^{(2)}_{i,j}\}$ is the $(n_d - 1) \times (n_d - 1)$ matrix which approximates ∂^2_{ss} incorporating the boundary conditions and acting only on the values at the inner points.

After the spatial discretization of

$$\partial_\tau c = (1/Pe_m)\partial^2_{ss} c - \partial_s c - D(c+1)\exp(\gamma\theta/(\theta+1)))$$
$$\partial_\tau \theta = (1/Pe_h)\partial^2_{ss}\theta - \partial_s \theta - \beta(\theta - \theta_r + 1) + BD(c+1)\exp(\gamma\theta/(\theta+1))),$$

the following *stiff* system of ODEs of dimension $2(n_d - 1)$ is obtained

$$\dot{c}_i = \sum_{j=1}^{n_d-1} \left((1/Pe_m)\tilde{d}^{(2)}_{i,j} - \tilde{d}^{(1)}_{i,j}\right) c_j - D(c_i+1)\exp(\gamma\theta_i/(\theta_i+1)))$$
$$\dot{\theta}_i = \sum_{j=1}^{n_d-1} \left((1/Pe_h)\tilde{d}^{(2)}_{i,j} - \tilde{d}^{(1)}_{i,j} - \beta\delta_{i,j}\right) \theta_j - \beta(1-\theta_r) + BD(c_i+1)\exp(\gamma\theta_i/(\theta_i+1))),$$
$$i = 1, \ldots, n_d - 1$$

which is integrated with the subroutine DLSODPK from the ODEPACK library.

Effect of the preconditioner in the HP problem

In all the following examples we have taken $n_d = 30$ and therefore the dimension of the dynamical system is $n = 2(n_d - 1) = 58$.

For the next examples $Pe_m = Pe_h = 5$, $B = 0.5$, $\gamma = 25$, $\beta = 3.5$, $\theta_r = 1$, and D will be the free parameter.

If $\delta x = (\delta c, \delta\theta)$ then,

$$D_x H(x,p)\delta x = \begin{pmatrix} (1/Pe_m)\partial^2_{ss}\delta c - \partial_s \delta c - N \\ (1/Pe_h)\partial^2_{ss}\delta\theta - \partial_s\delta\theta - \beta\delta\theta + BN \end{pmatrix},$$

with $N = \exp(\gamma\theta/(\theta+1))D(\delta y + (y+1)(\gamma/(\theta+1)^2)\delta\theta)$

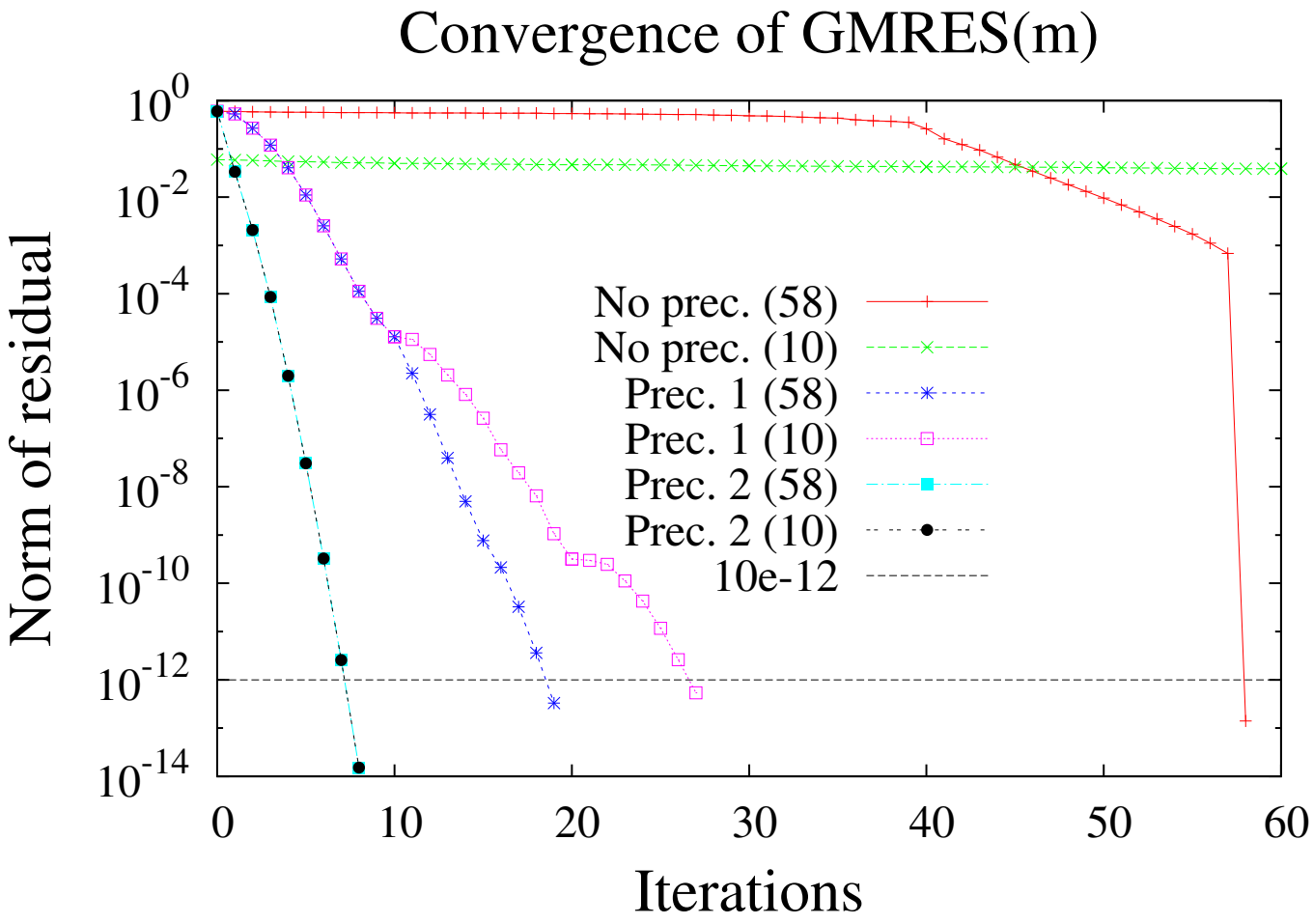
Two possible preconditioners are

$$M_1 = \begin{pmatrix} (1/Pe_m)\partial^2_{ss} & 0 \\ 0 & (1/Pe_h)\partial^2_{ss} \end{pmatrix},$$

and

$$M_2 = \begin{pmatrix} (1/Pe_m)\partial^2_{ss} - \partial_s & 0 \\ 0 & (1/Pe_h)\partial^2_{ss} - \partial_s - \beta I \end{pmatrix}.$$

The following figure shows the convergence of GMRES at the first Newton iteration for $D = 0.1$ starting with $c = 0$ and $\theta = 0$. The size of the linear system is $n = 58$, and the dimension of the Krylov subspace was $m = 10$ or $m = 58$. Norm of the residual $= \|b - Ax_k\|_2$.



Stability

Stability of fixed points (equilibria)

Given an autonomous system of ODE $\dot{x} = f(x)$, with $f : \mathcal{U} \subset \mathbb{R}^n \to \mathbb{R}^n$ (which we will assume to be at least C^1), let $\varphi(t, x)$ its solution with initial condition x.

Let x_* be a fixed point (or equilibrium) of the system of EDOs, i.e., $f(x_*) = 0$.

Definition. *The fixed point is said to be Lyapunov stable if for every neighborhood N of x_* there is a neighborhood $M \subset N$ of x_* such that if $x \in M$, then $\varphi(t, x) \in N$ for all $t \geq 0$.*

An equilibrium that is not stable is called unstable.

Definition. *The fixed point is said to be asymptotically stable if it is Lyapunov stable and there is a neighborhood N of x_* such if $x \in N$ then $\lim_{t\to\infty} \|\varphi(t, x) - x_*\| = 0$.*

Definition. *The fixed point said to be exponentially stable if it is asymptotically stable and there exist $\alpha > 0$, and $\beta > 0$, and a neighborhood N of x_* such that if $x \in N$, then $\|\varphi(t, x) - x_*\| \leq \alpha\|x - x_*\|e^{-\beta t}$, for $t \geq 0$.*

Theorem. *If f is of class C^1 and x_* is a fixed point such that all the eigenvalues of $Df(x_*)$ have strictly negative real parts, then x_* is exponentially stable (and hence asymptotically stable). If at least one eigenvalue has strictly positive real part, then x_* is unstable.*

The eigenvalues of $Df(x_*)$ close the imaginary axis have to be computed to detect bifurcations of fixed points.

Stability of periodic orbits

Definition. *A set Λ is said to be invariant under the flow $\varphi(t,x)$ if $\varphi(t,\Lambda)=\Lambda$ for all t; that is, for each $x\in\Lambda$, $\varphi(t,x)\in\Lambda$ for any t.*

Definition. *The invariant set is said to be stable if for every neighborhood N of Λ there is a subset $M\subset N$ of Λ such that if $x\in M$, then $\varphi(t,x)\in N$ for all $t\geq 0$.*

An set that is not stable is called unstable.

Definition. *The invariant set is said to be asymptotically stable if it is stable and there is a neighborhood N of Λ such if $x\in N$ then, then $\lim_{t\to\infty}\rho(\varphi(t,x),\Lambda)=0$, with $\rho(x,\Lambda)=\inf_{y\in\Lambda}(\|x-y\|)$.*

A trajectory $x(t)=\varphi(t,x)$ is a periodic orbit if there is a minimal $T>0$ such that $\varphi(T,x)=x$.

Consider the first variational equation $\dot{M}=Df(x(t))M$ about the periodic orbit $x(t)$, with initial condition $M(0)=I$. The solution at time T is called the monodromy matrix $M(T)$. Its eigenvalues are called the Floquet multipliers of the periodic orbit.

Theorem. *The monodromy matrix $M(T)$ always has a unit eigenvalue with eigenvector $\dot{x}(0)=\dot{x}(T)=f(x(0))$.*

This unit eigenvalue is named the trivial eigenvalue of the periodic orbit.

Theorem. *If $x(t)$ is a periodic orbit of a C^2 flow $\varphi(t,x)$ that is linearly asymptotically stable (its monodromy matrix has all the eigenvalue inside the unit circle except the trivial one), then it is asymptotically stable.*

The eigenvalues of $M(T)$ of largest magnitude have to be computed to detect bifurcations of the periodic orbits.

Subspace iteration and Arnoldi methods

Eigenvalue problems

Rayleigh-Ritz method.
Assume A is a real matrix of dimension $n \times n$ $(n \gg 1)$, and that V_m is of dimension $n \times m$ $(m \ll n)$ such that $V_m^\top V_m = I_m$ (I_m identity of dimension m) and

$$AV_m = V_m B_m$$

with B_m of dimension $m \times m$. This expressions says that the columns of V_m span an invariant subspace of A of dimension m. Moreover,

$$\text{if} \quad (\lambda, u) \quad \text{eigenpair of} \quad B_m \quad (B_m u = \lambda u) \implies (\lambda, V_m u) \quad \text{eigenpair of} \quad A:$$

$$AV_m u = V_m B_m u = \lambda V_m u.$$

If the identity $AV_m = V_m B_m$ is not exact, the pairs $(\lambda, V_m u)$ are called Ritz values and vectors of A, respectively.

It is clear that since $V_m^\top V_m = I_m$ then $B_m = V_m^\top A V_m$.

There are two main methods to obtain approximate bases, V_m, of the subspace corresponding to the leading (largest magnitude) eigenvalues of a large-scale matrix A, **subspace iteration** and **Arnoldi's method**.

Subspace iteration

Subspace iteration is implemented, for instance, in LOPSI and SRRIT.

1. Start: Choose an initial system of orthonormal vectors $V_m = [v_1, \ldots, v_m]$, $(m \ll n)$
2. Iterate: Until convergence do:
   (a) For l=1,. . . , k do
      i. Compute $Z_m = AV_m$
      ii. Orthonormalize Z_m by computing $Z_m = Q_m R_m$, with $Q_m^\top Q_m = I$ and R_m upper-triangular, and set $V_m = Q_m$
   (b) Form $B_m = V_m^\top A V_m$ and compute the eigenpairs (λ_i, z_i), $i = 1, \cdots, m$ of B_m by the QR method (LAPACK)
   (c) Test for convergence of eigenvalues and/or eigenvectors
3. Stop: When satisfied, compute the approximate eigenvectors of A as $x_i = V_m z_i$, $i = 1, \cdots, m$. The λ_i, $i = 1, \cdots, m$ are the approximate eigenvalues.

Theorem. *Suppose that the n eigenvalues of A are ordered by decreasing modulus as follows: $|\lambda_1| \geq |\lambda_2| \geq \cdots |\lambda_m| > |\lambda_{m+1}| \geq \cdots \geq |\lambda_n|$. If the initial set of vectors V_m is not deficient in the eigenvectors corresponding to $\lambda_1, \cdots, \lambda_m$, and if the total number of iterations taken, k, is large enough, then the previous algorithm computes approximations $\hat{\lambda}_{i,k}$ to λ_i $(i = 1, \ldots, m)$ with*

$$|\hat{\lambda}_{i,k} - \lambda_i| = O\left(\left|\frac{\lambda_{m+1}}{\lambda_i}\right| + \varepsilon_{i,k}\right)^k, \qquad \lim_{k\to\infty} \varepsilon_{i,k} = 0.$$

Moreover, if λ_i is simple, then $\varepsilon_{i,k} = 0$.

Arnoldi's method

Arnoldi's method is implemented, for instance, in ARPACK.

1. Start: Choose an initial unitary vector v_1.
2. Iterate: Until convergence do:
   (a) Compute the Arnoldi factorization $AV_m = V_m H_m + w_m e_m^\top$ of length m. The columns of V_m form an orthonormal basis of $\mathcal{K}_m = \{v_1, Av_1, A^2v_1, \ldots, A^{m-1}v_1\}$.
   (b) Compute the eigenpairs (λ_i, z_i), $i = 1, \cdots, m$ of $H_m = V_m^\top AV_m$ by the QR method (LAPACK).
   (c) Test for convergence of eigenvalues and/or eigenvectors. If not converged select a new initial vector v_1 from the Arnoldi factorization.
3. Stop: When satisfied, compute approximate eigenvectors of A as $x_i = V_m z_i$, $i = 1, \cdots, m$. The λ_i, $i = 1, \cdots, m$ are the approximate eigenvalues.

Theorem. *Suppose that the n eigenvalues of A are simple and that $\lambda_2, \ldots, \lambda_n$ are enclosed by a circle centered at ξ and passing through λ_2, and that $\hat{\lambda}_1$ is the approximation to λ_1 obtained by Arnoldi's method, then*

$$|\hat{\lambda}_1 - \lambda_1| \leq c \left| \frac{\lambda_2 - \xi}{\lambda_1 - \xi} \right|^{m-1},$$

with c a constant. This gives the same error bound as $m-1$ steps of the power method applied to $A - \xi I$.

From the Arnoldi's decomposition

$$AV_m = V_m H_m + w_m e_m^\top, \quad \text{with} \quad w_m = h_{m+1,m} v_{m+1},$$

it is easy to find the residual $\|(A - \lambda_i I)x_i\|_2$.

Proposition. *Let z_i be an eigenvector of H_m associated with the eigenvalue λ_i, and $x_i = V_m z_i$ the Ritz approximate eigenvector of A. Then,*

$$(A - \lambda_i I)x_i = h_{m+1,m}(e_m^\top z_i)v_{m+1}$$

and, therefore

$$\|(A - \lambda_i I)x_i\|_2 = h_{m+1,m}|e_m^\top z_i|.$$

Proof:

$$AV_m z_i = V_m H_m z_i + h_{m+1,m} v_{m+1} e_m^\top z_i$$

$$Ax_i - \lambda_i x_i = h_{m+1,m}(e_m^\top z_i)v_{m+1}$$

and v_{m+1} is unitary.

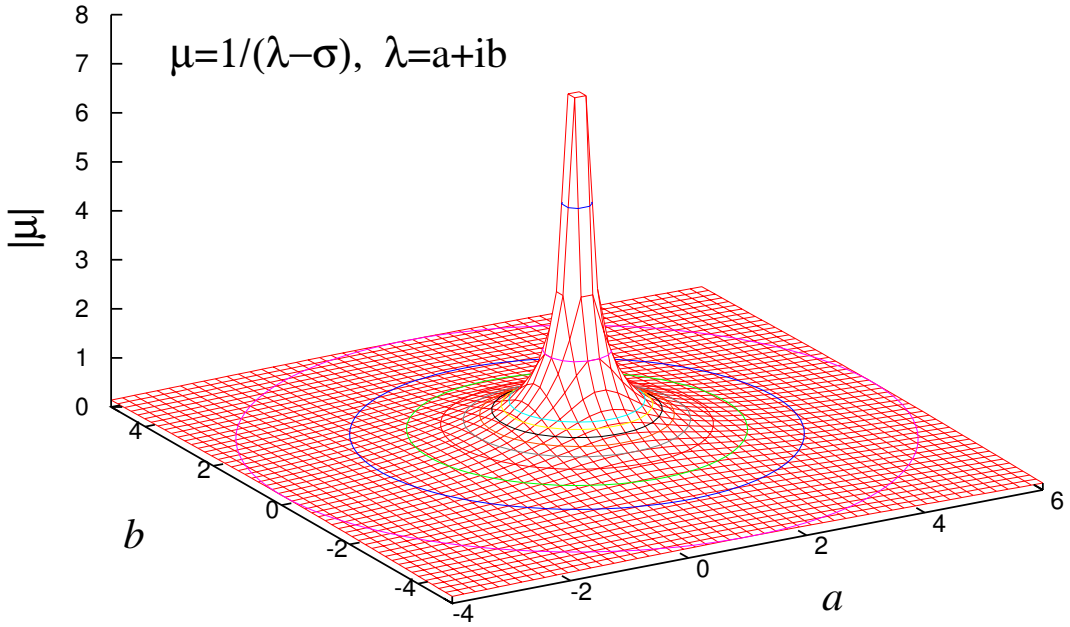
Eigenvalue Transformations

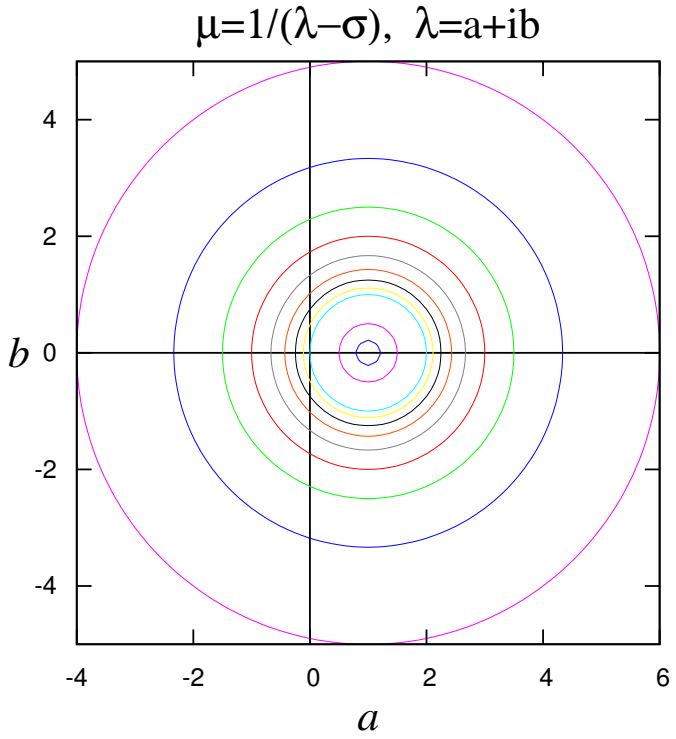
To find the leading (maximal real part) eigenvalues of $Av = \lambda v$ the following transformations can be used:

Shift-invert with real or complex shift:

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

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

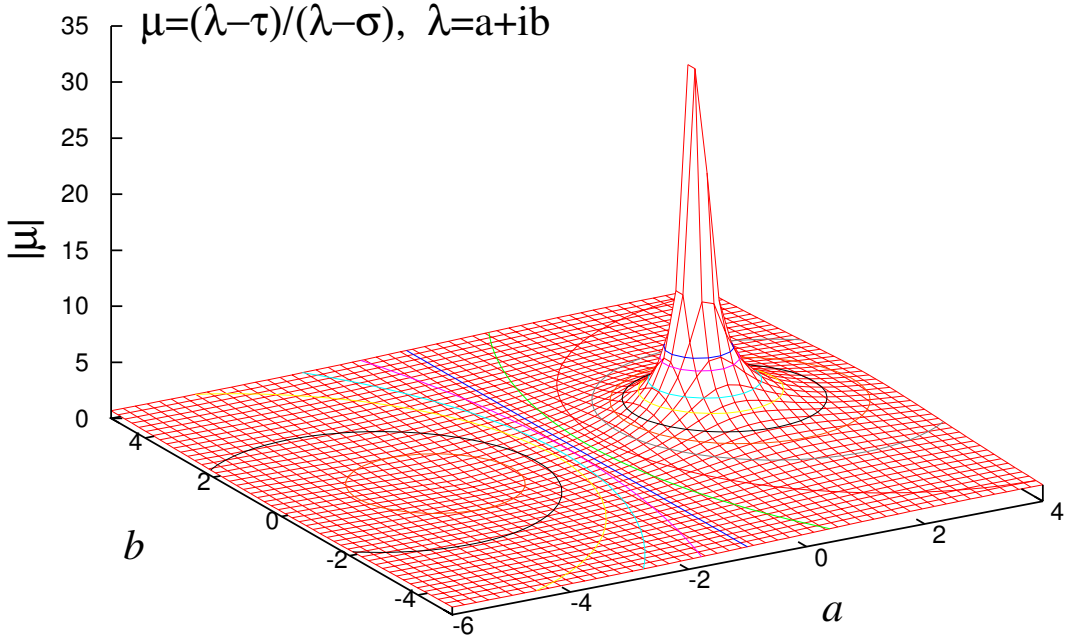


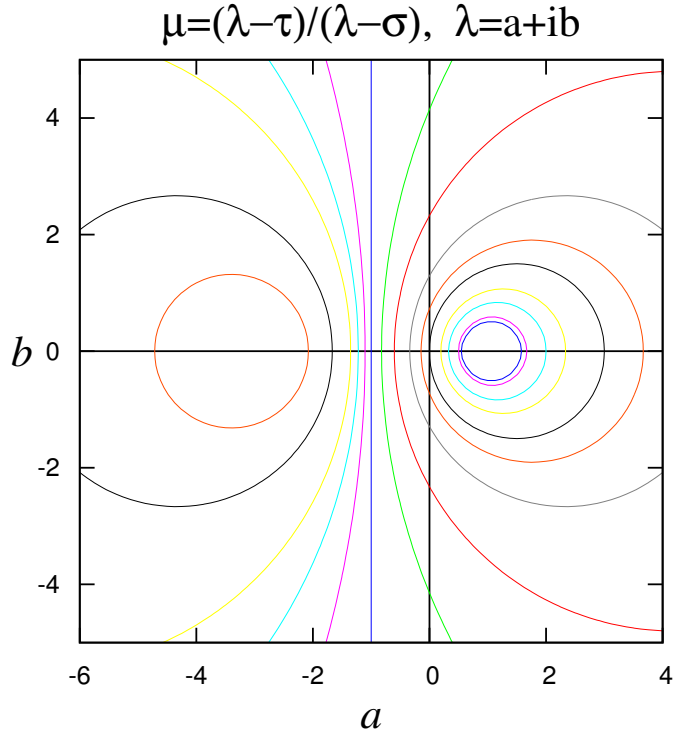


Generalized Cayley transformation:

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

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.

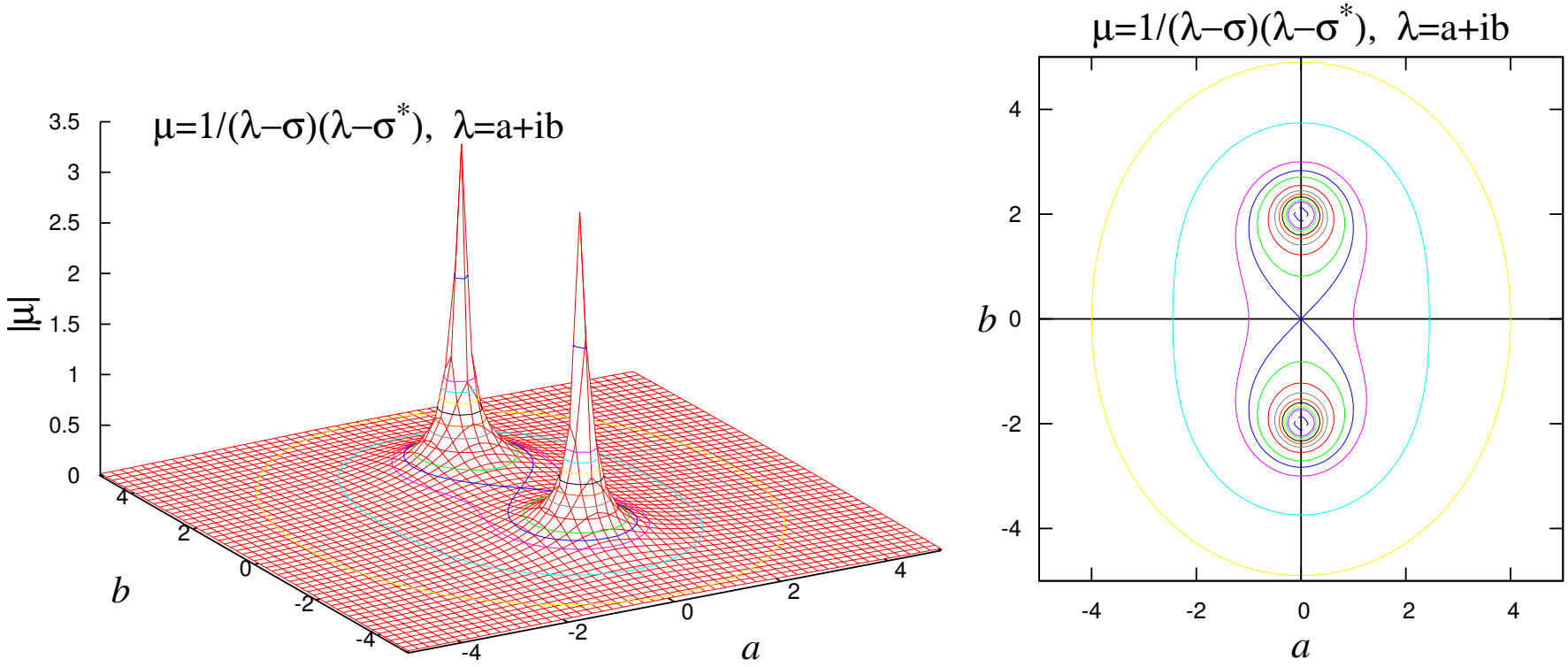




Double complex shift: If $\sigma = \rho + i\theta$,

$$Av = \lambda v \implies (A - \sigma I)^{-1}(A - \bar{\sigma} I)^{-1} v = \mu v \quad \text{with} \quad \mu = 1/((\lambda - \rho)^2 + \theta^2).$$

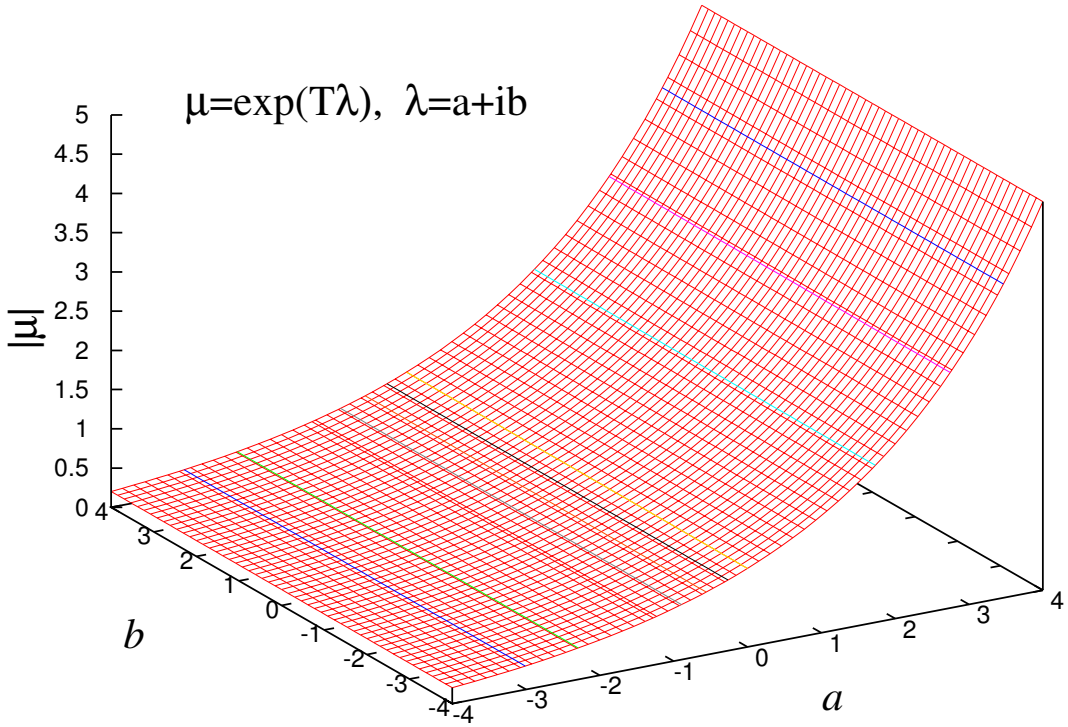
Systems with matrix $(A - \sigma I)(A - \bar{\sigma} I) = (A - \rho I)^2 + \theta^2 I$ have to be solved.

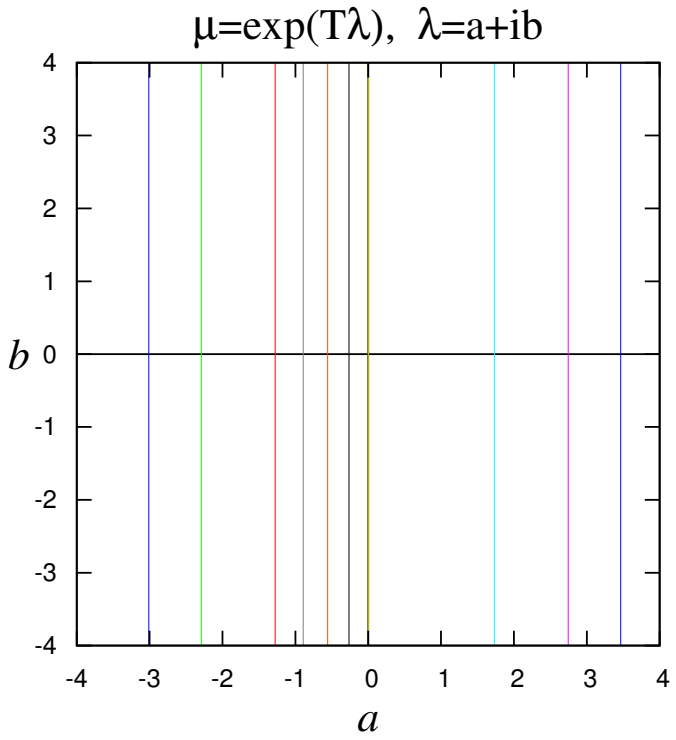


Exponential:

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

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.





By taking logarithms, and using that $\lambda = \langle v, Av\rangle / \langle v, v\rangle$ to recover the undetermined imaginary part, λ can be obtained from μ.

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

Continuation of fixed points of ODEs

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

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

  In the previous example (HP problem) we used an approximation of the form

$$\mathcal{M} = \begin{pmatrix} M & 0 \\ 0 & 1 \end{pmatrix}.$$

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

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

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

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

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

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

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

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

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

Continuation of fixed points of ODEs by time evolution

The equilibria of the system of ODEs

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

can also be obtained as fixed points of the map

$$x \to \varphi(T, x, p)$$

$\varphi(t, x, p)$ being the solution of the ODEs with initial condition x, because

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

The arbitrary time T must be large enough to have most of the spectrum of $D_x\varphi(T, x, p)$ 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

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

Then

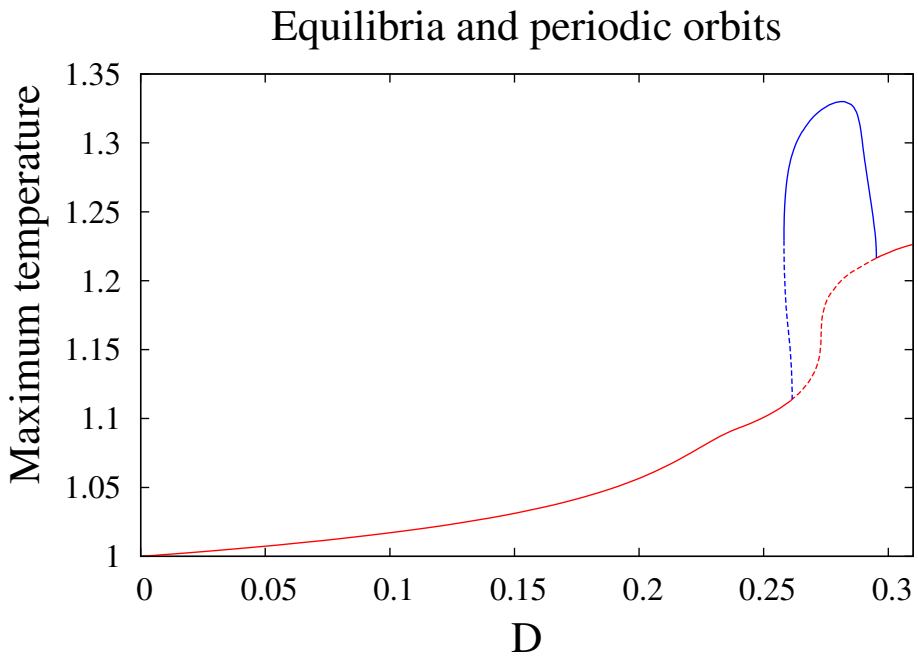
$$D_x\varphi(T, x, p)\delta x + D_p\varphi(T, x, p)\delta p = y(T).$$

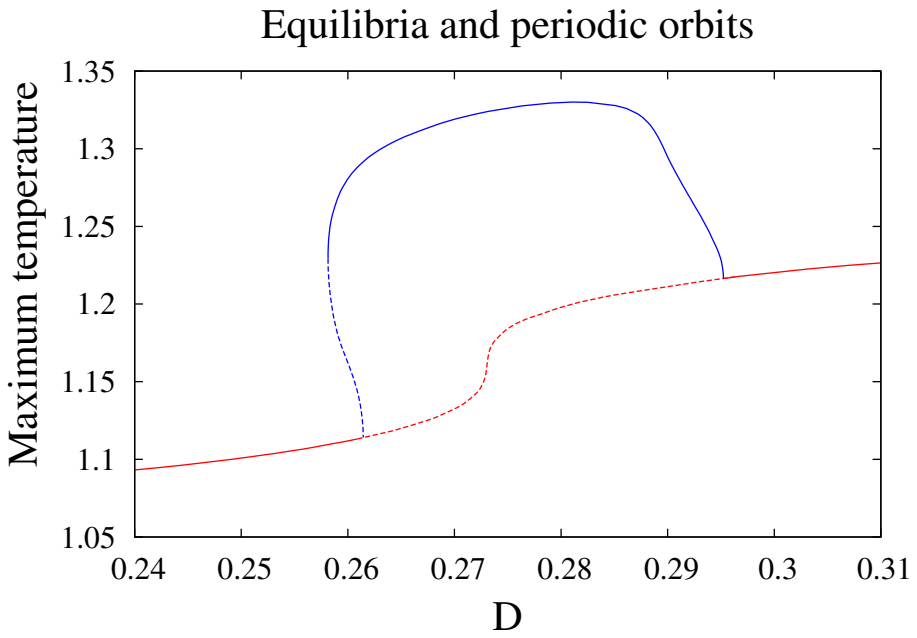
This method can be used as a second option, for instance, when the continuation method applied to $f(x, p)$ fails due to the lack a good preconditioner for the linear systems or the eigenvalue problems.

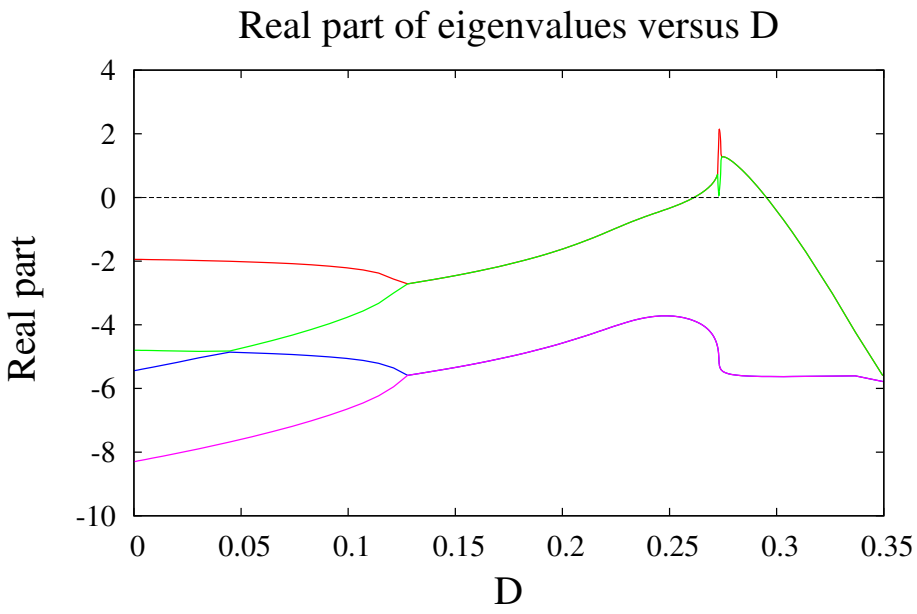
Examples and exercises

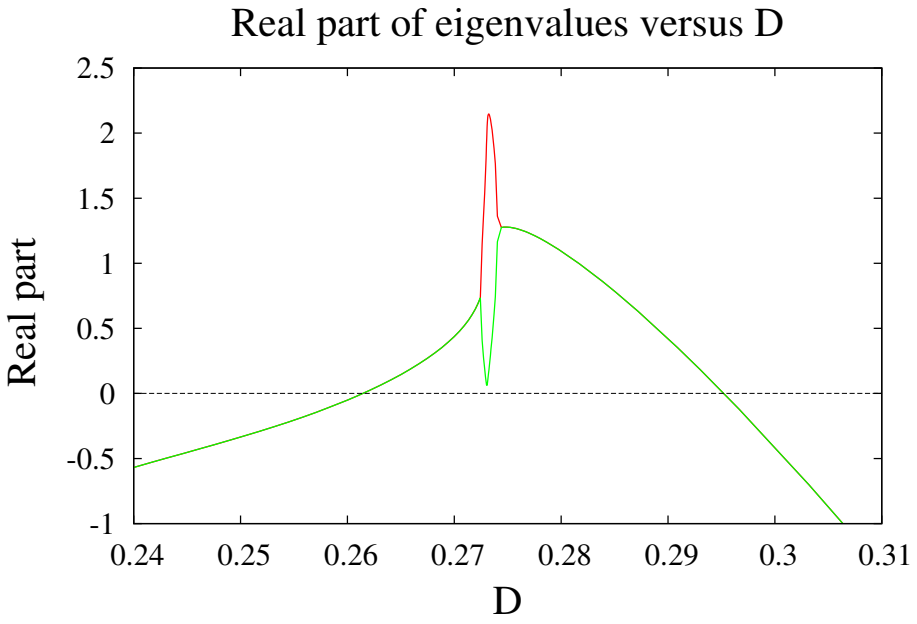
Results for the HP problem

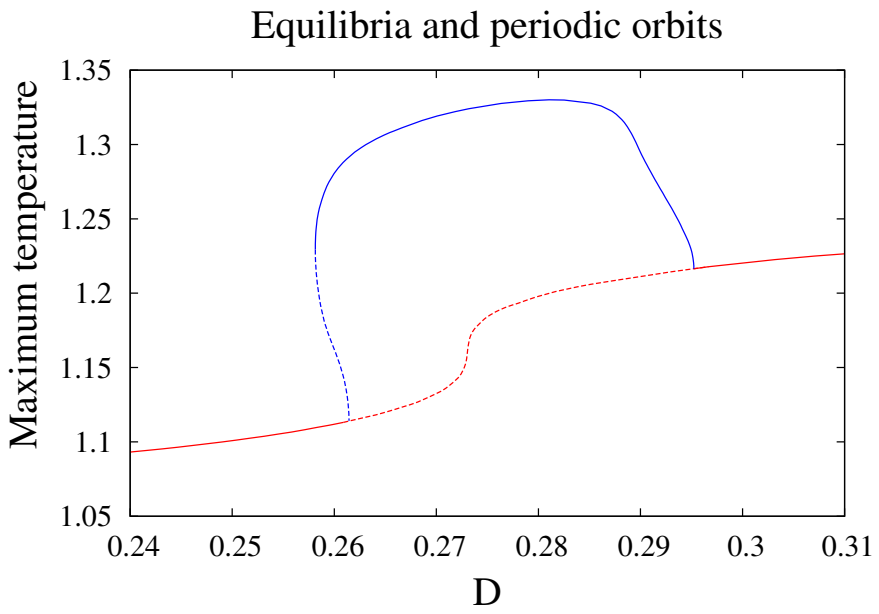
In this example $Pe_m = Pe_h = 5$, $B = 0.5$, $\gamma = 25$, $\beta = 3.50$, and $\theta_r = 1$.

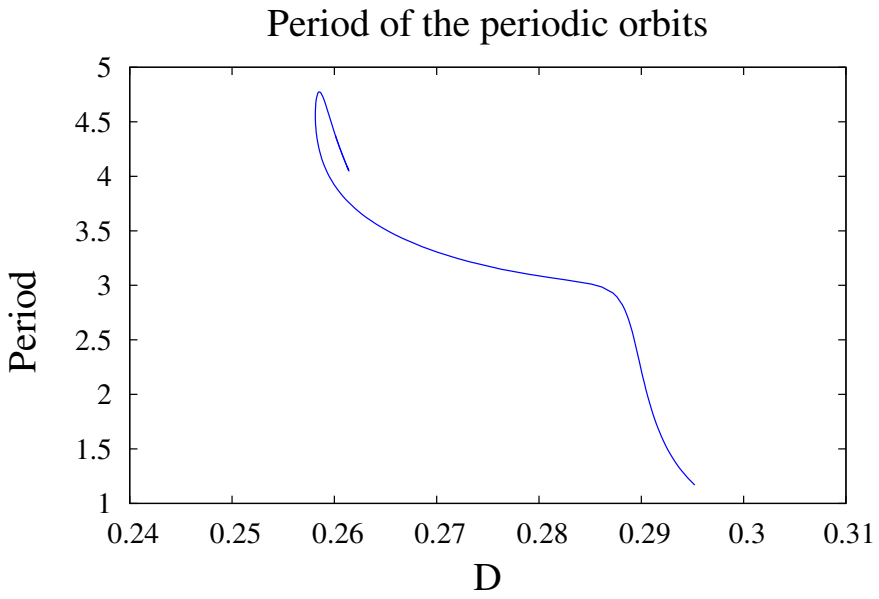


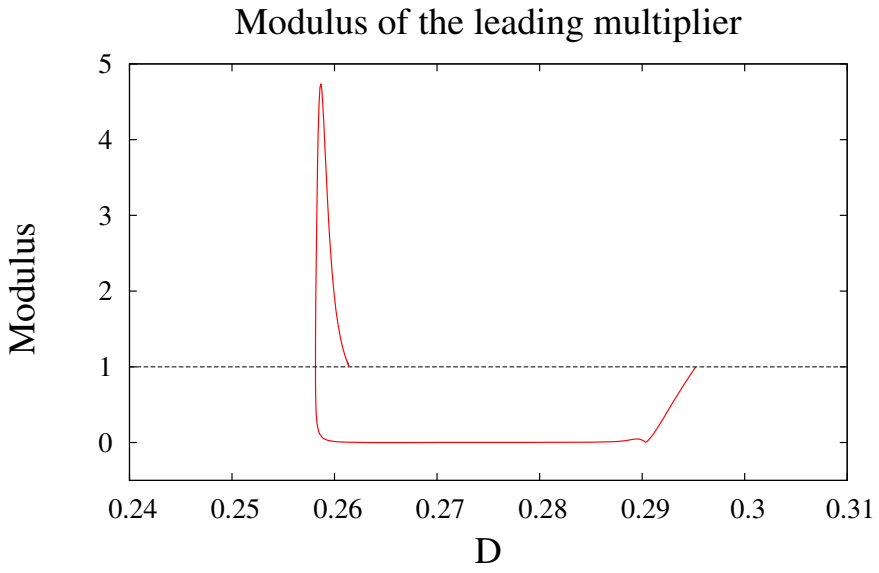




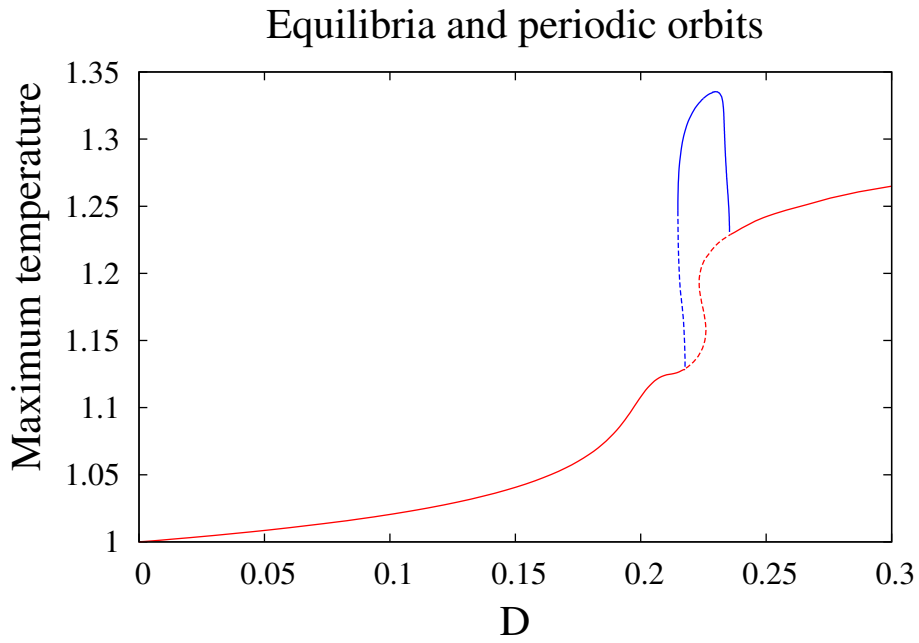


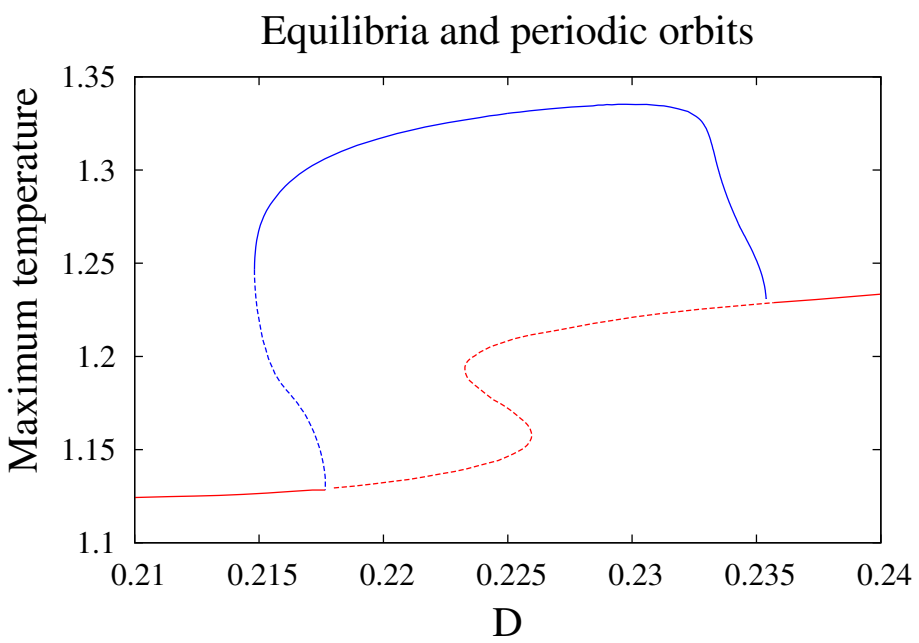

Equilibria and periodic orbits
Maximum temperature
1.35
1.3
1.25
1.2
1.15
1.1
1.05
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
D

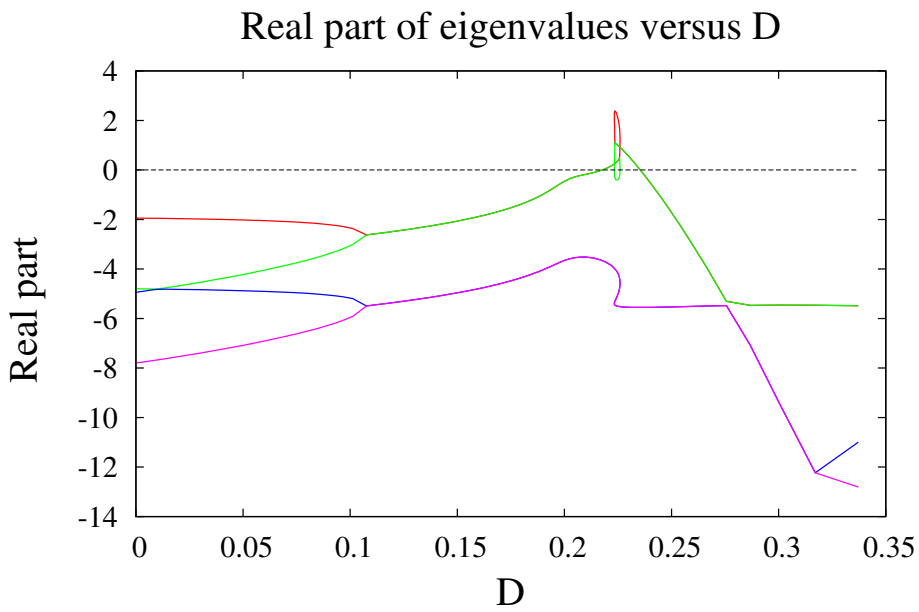

Period of the periodic orbits
Period
5
4.5
4
3.5
3
2.5
2
1.5
1
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
D

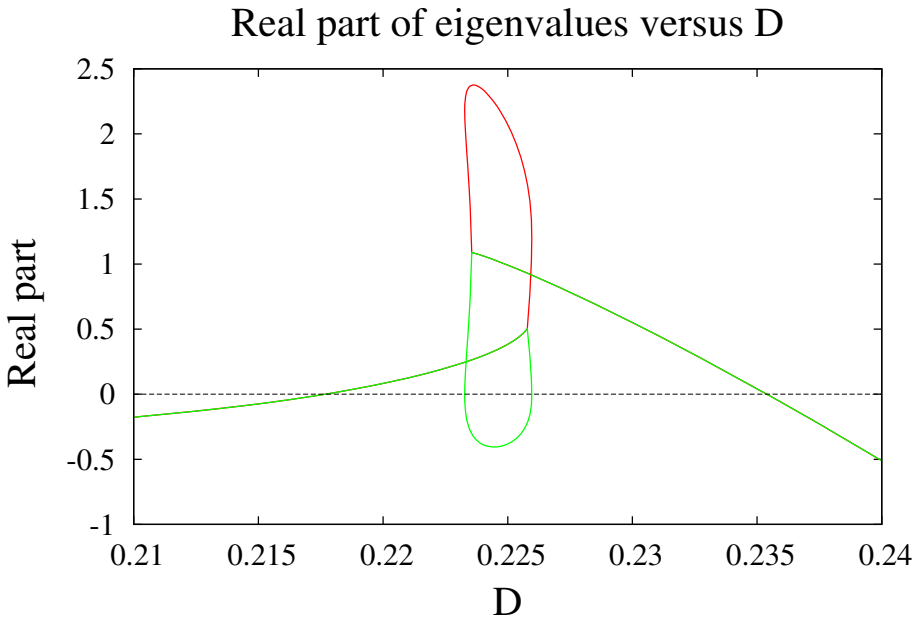

Modulus of the leading multiplier
Modulus
5
4
3
2
1
0
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
D

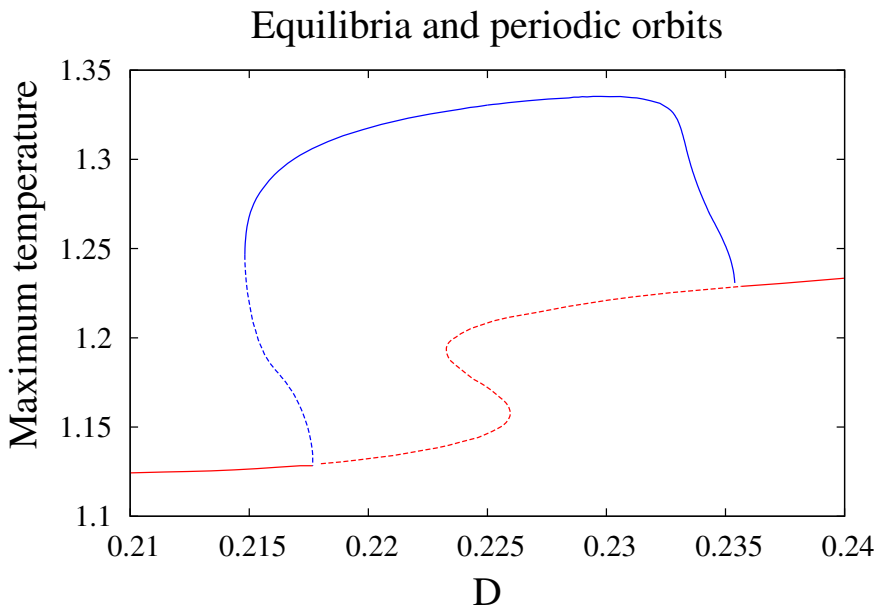
In this example $Pe_m = Pe_h = 5$, $B = 0.5$, $\gamma = 25$, $\beta = 3.00$, and $\theta_r = 1$.

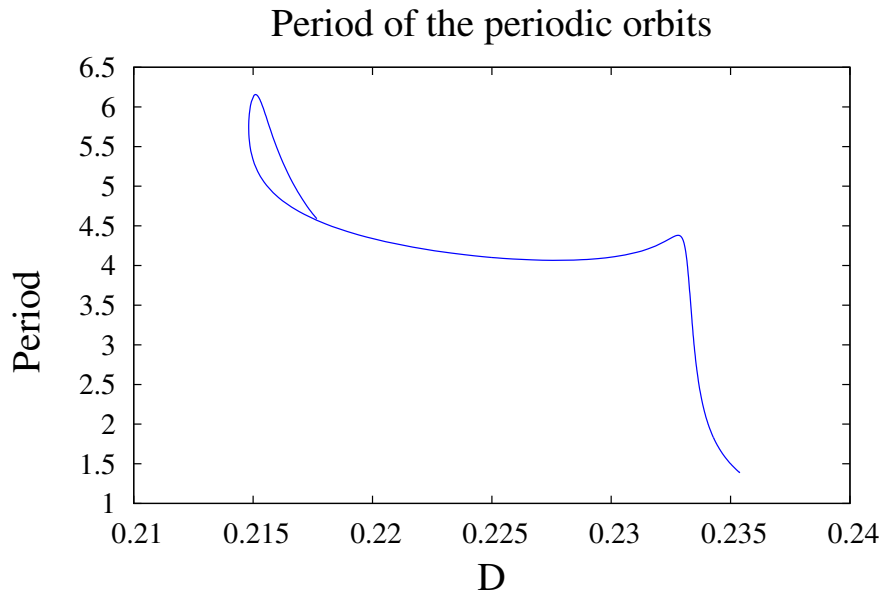









Equilibria and periodic orbits
Maximum temperature
1.35
1.3
1.25
1.2
1.15
1.1
0.21
0.215
0.22
0.225
0.23
0.235
0.24
D


Period of the periodic orbits
Period
6.5
6
5.5
5
4.5
4
3.5
3
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2
1.5
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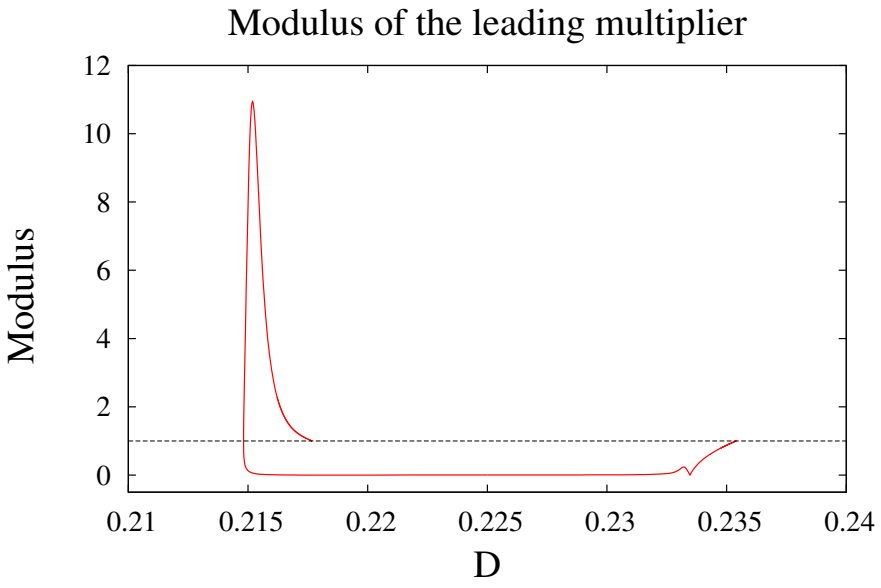
0.21
0.215
0.22
0.225
0.23
0.235
0.24
D


Modulus of the leading multiplier
Modulus
12
10
8
6
4
2
0
0.21
0.215
0.22
0.225
0.23
0.235
0.24
D

The one-dimensional Brusselator

Consider the system of PDEs

$$\partial_t X = (D_X/L^2)\partial^2_{zz} X + X^2 Y - (B+1)X + A$$
$$\partial_t Y = (D_Y/L^2)\partial^2_{zz} Y - X^2 Y + BX,$$

in the interval $z \in [0,1]$, with boundary conditions

$$X(0) = X(1) = A$$
$$Y(0) = Y(1) = B/A.$$

For any value of the parameters the problem has the trivial constant solution $X = A$ and $Y = B/A$. It undergoes Hopf bifurcations for

$$L_k = k\pi\sqrt{\frac{D_X + D_Y}{B - A^2 - 1}}, \quad k = 1, 2 \ldots.$$

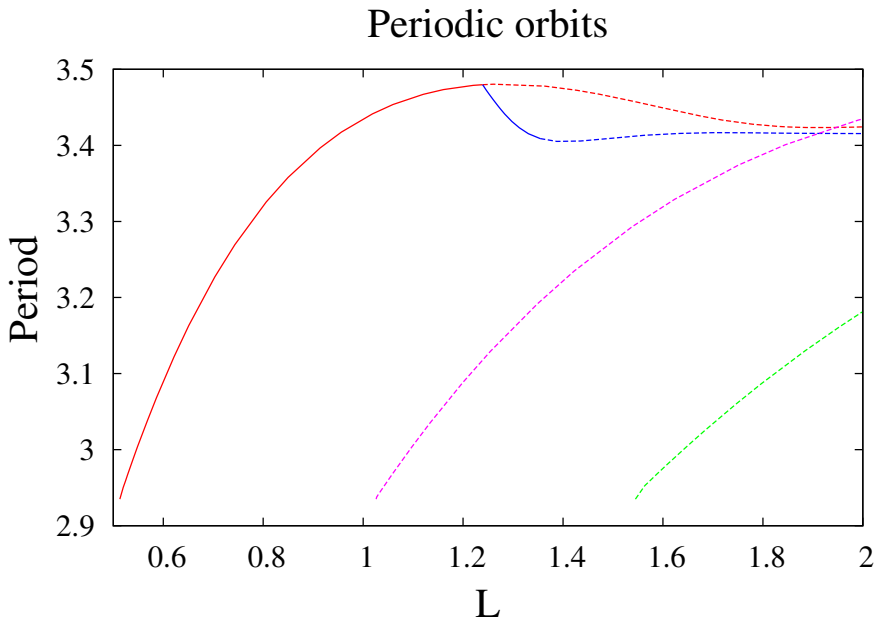
If $D_X = 0.008$, $D_Y = 0.004$, $A = 2$, $B = 5.45$ then $L_k \approx 0.5130k$.

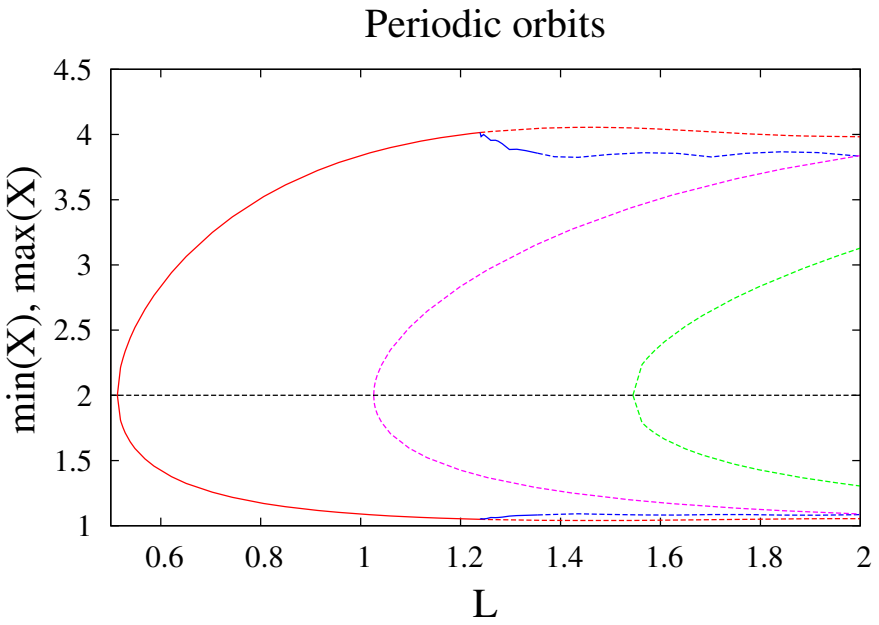
To implement the boundary conditions we substitute $X = \bar{X} + A$, $Y = \bar{Y} + B/A$ in the equations and boundary conditions to obtain, after removing the overbars the equations

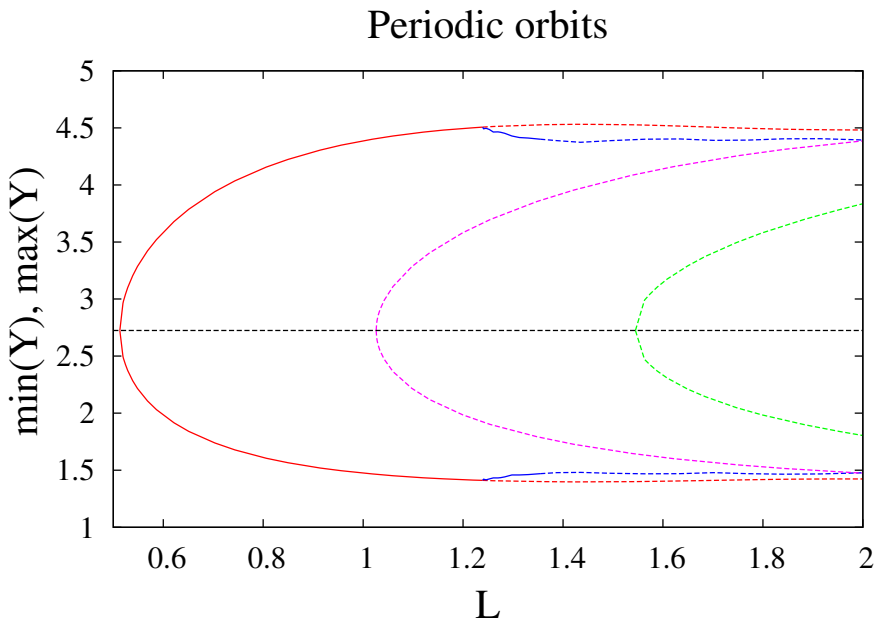
$$\partial_t X = (D_X/L^2)\partial^2_{zz} X + X^2 Y + (B/A)X^2 + 2AXY + A^2 Y + (B-1)X, \quad X(0) = X(1) = 0,$$
$$\partial_t Y = (D_Y/L^2)\partial^2_{zz} Y - X^2 Y - (B/A)X^2 - 2AXY - A^2 Y - BX, \quad Y(0) = Y(1) = 0.$$

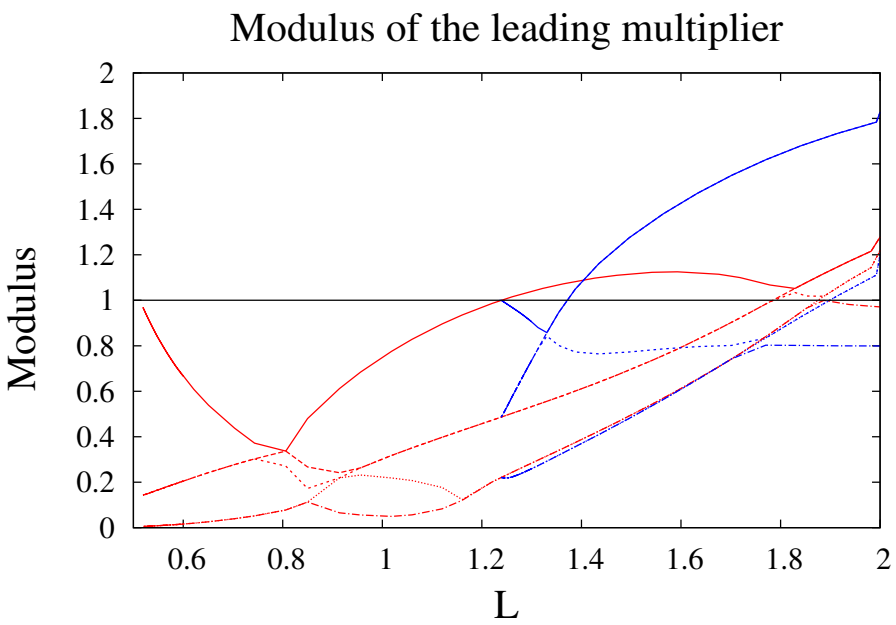
Results for the Brusselator problem

In this example $D_X = 0.008$, $D_Y = 0.004$, $A = 2$, $B = 5.45$ and L is the continuation parameter.

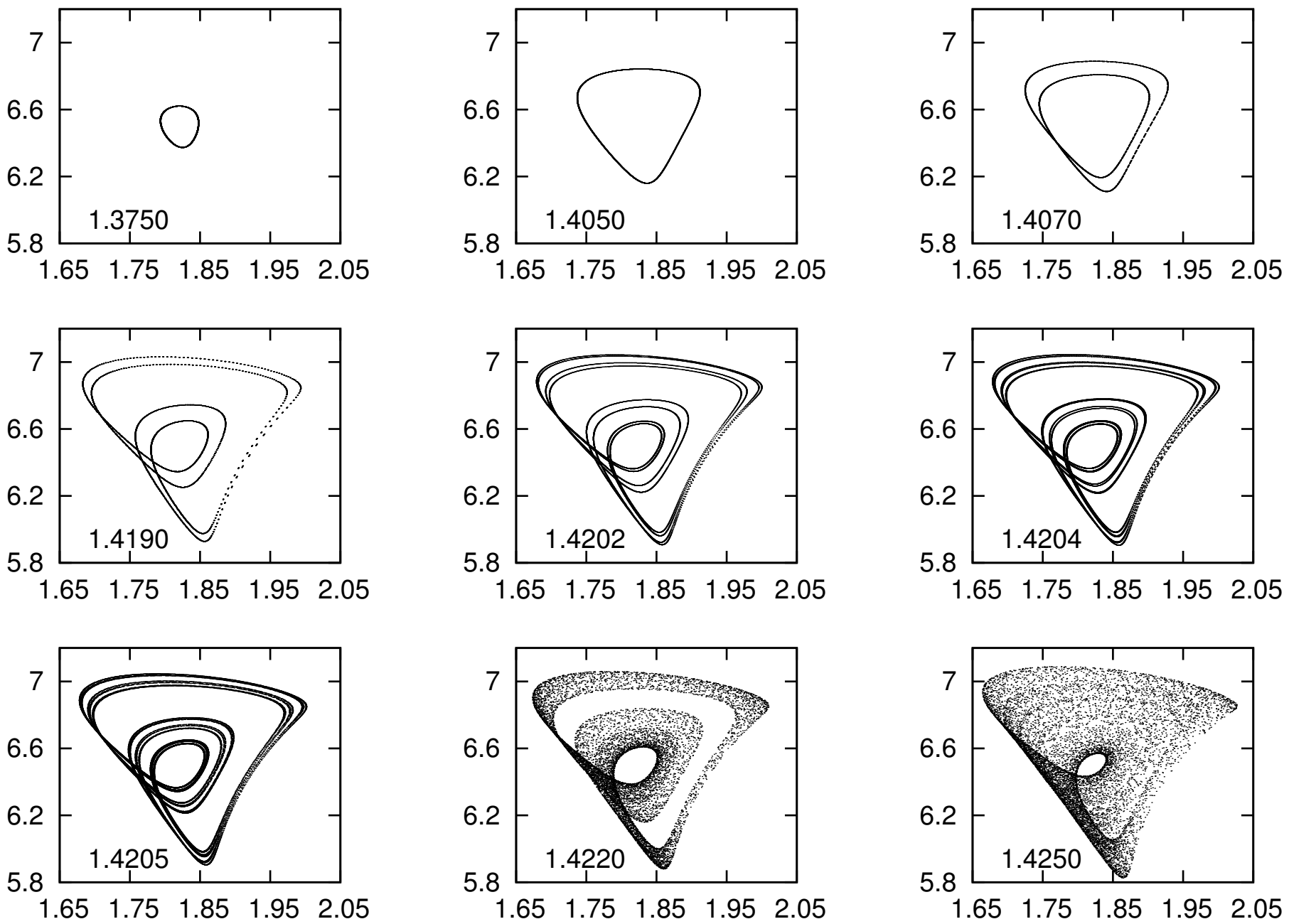








A period doubling cascade or tori in the Brusselator problem



Continuation of codimension-one bifurcation points of equilibria and periodic orbits

Continuation of bifurcation curves

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:

- `fun(X,h)` which computes $h = H(X)$ from X, and
- `dfun(X,`δ`X,`δ`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

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

- $g(x) = 0$ is a phase condition to select a single point on the periodic orbit. We use $g(x) = \langle v_\pi, x - x^{(\pi)} \rangle = 0$.
- $f = f(x, p)$ 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

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

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

$$
\begin{aligned}
\dot{y} &= f(y,p), & y(0) &= x\\
\dot{y}_1 &= D_y f(y,p)y_1, & y_1(0) &= u\\
\dot{y}_2 &= D_y f(y,p)y_2 + D_p f(y,p)\delta p, & y_2(0) &= \delta x\\
\dot{y}_3 &= D_y f(y,p)y_3 + D^2_{yy} f(y,p)(y_1,y_2) + D^2_{yp} f(y,p)(y_1,\delta p), & y_3(0) &= 0\\
\dot{y}_4 &= D_y f(y,p)y_4, & y_4(0) &= \delta u.
\end{aligned}
$$

Neimark-Sacker bifurcations

The Hopf bifurcations of periodic orbits with multiplier $e^{i\theta}$ and eigenvector $u+iv$ are solutions of the system $H(x,u,v,T,\theta,p)=0$ given by

$$\begin{aligned} x-\varphi(T,x,p) &= 0,\\ g(x) &= 0,\\ u\cos\theta - v\sin\theta - D_x\varphi(T,x,p)u &= 0,\\ u\sin\theta + v\cos\theta - D_x\varphi(T,x,p)v &= 0,\\ \langle u,u\rangle + \langle v,v\rangle &= 1,\\ \langle u,v\rangle &= 0. \end{aligned}$$

- $g(x)=0$ is the phase condition $g(x)=\langle v_\pi, x-x^{(\pi)}\rangle = 0$.
- The third and fourth equations are the real and imaginary parts of

$$e^{i\theta}(u+iv) - D_x\varphi(T,x,p)(u+iv) = 0.$$

- The two last equations uniquely determine the eigenvector $u+iv$.

Now $X=(x,u,v,T,\theta,p)$ has dimension $3n+4$, and the $3n+3$ equations define the curve of solutions.

Pitchfork bifurcations

If the initial system is $\mathcal{T}$-invariant, $f(\mathcal{T}x, p) = \mathcal{T}f(x, p)$ with $\mathcal{T}^2 = I$, and $\mathcal{T}x = x$, the pitchfork bifurcation points of periodic orbits are solutions of the system $H(x, u, T, \xi, p) = 0$ are given by

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

- The slack variable ξ and the third equation are introduced to make the system regular. Moreover $\xi = 0$ at the solution.
- $g(x) = 0$ is the phase condition $g(x) = \langle v_\pi, x - x^{(\pi)}\rangle = 0$.
- ϕ is a given antisymmetric vector, $\mathcal{T}\phi = -\phi$.
- The last equation uniquely determines the eigenvector u.

Now $X = (x, u, T, \xi, p)$ has dimension $2n + 4$, and the $2n + 3$ equations define the curve of solutions.

Thermal convection in binary fluid mixtures

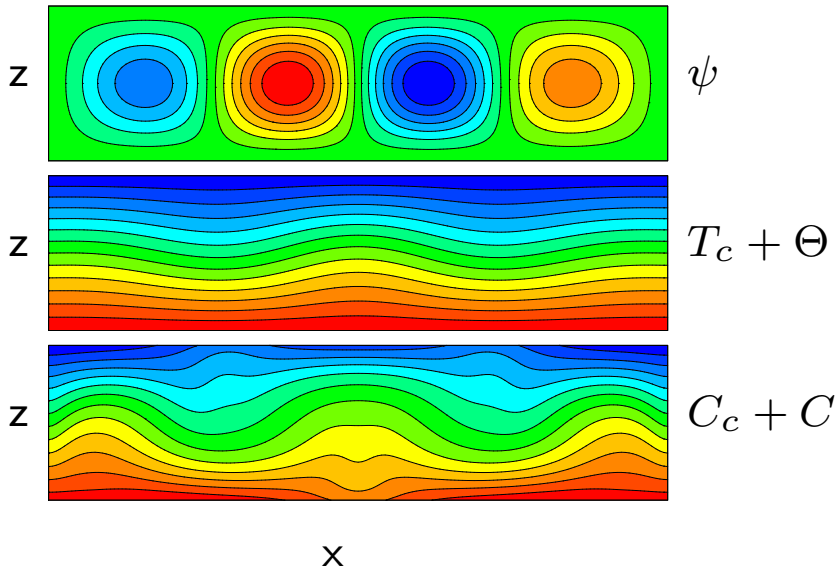
The equations in $\Omega = [0, \Gamma] \times [0, 1]$ for the perturbation of the basic state ($\mathbf{v}_c = 0$, $T_c = T_c(0) - z$, and $C_c = C_c(0) - z$) in non-dimensional form are

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

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

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

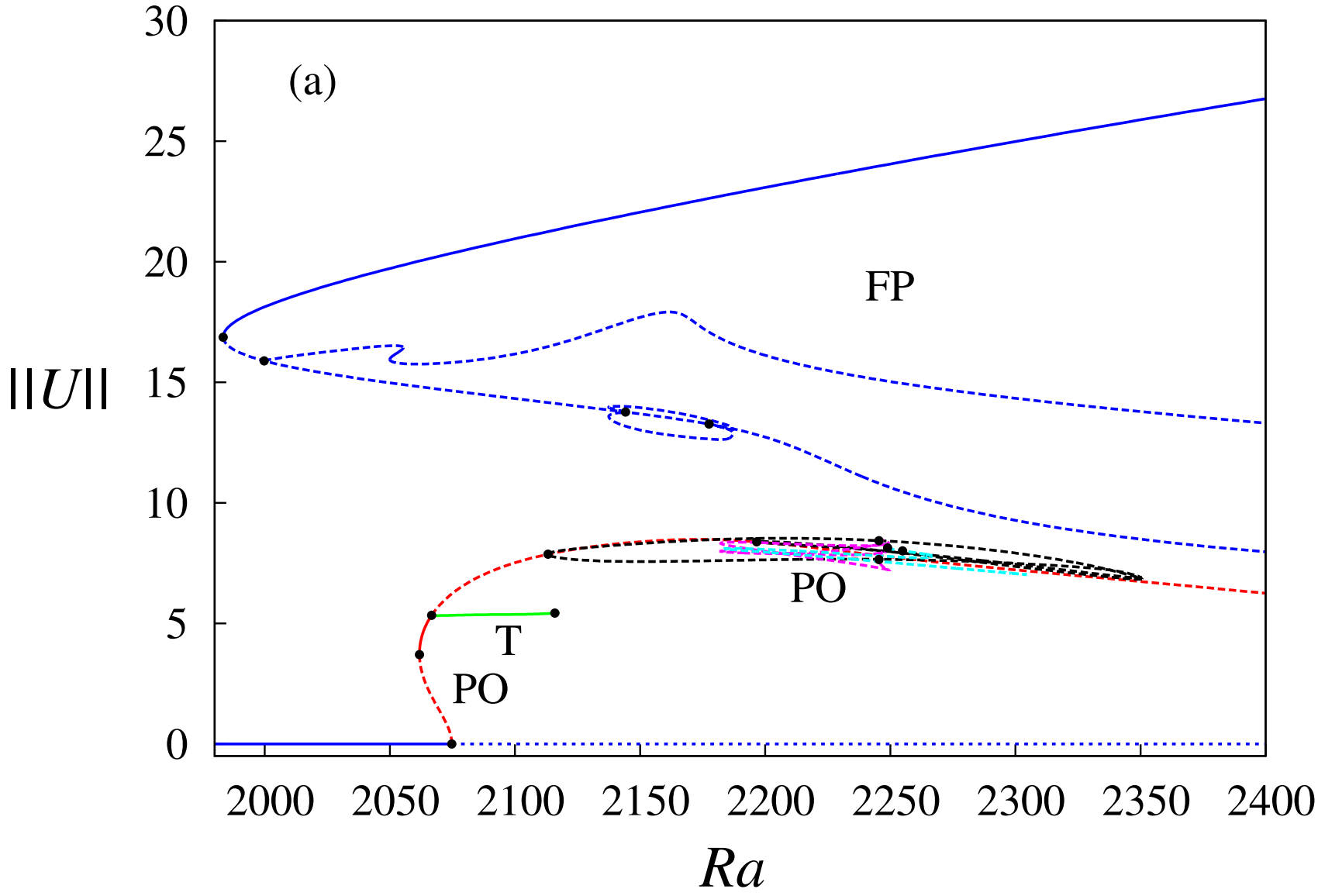
with $u = (\psi_{ij}, \Theta_{ij}, \eta_{ij})$.

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

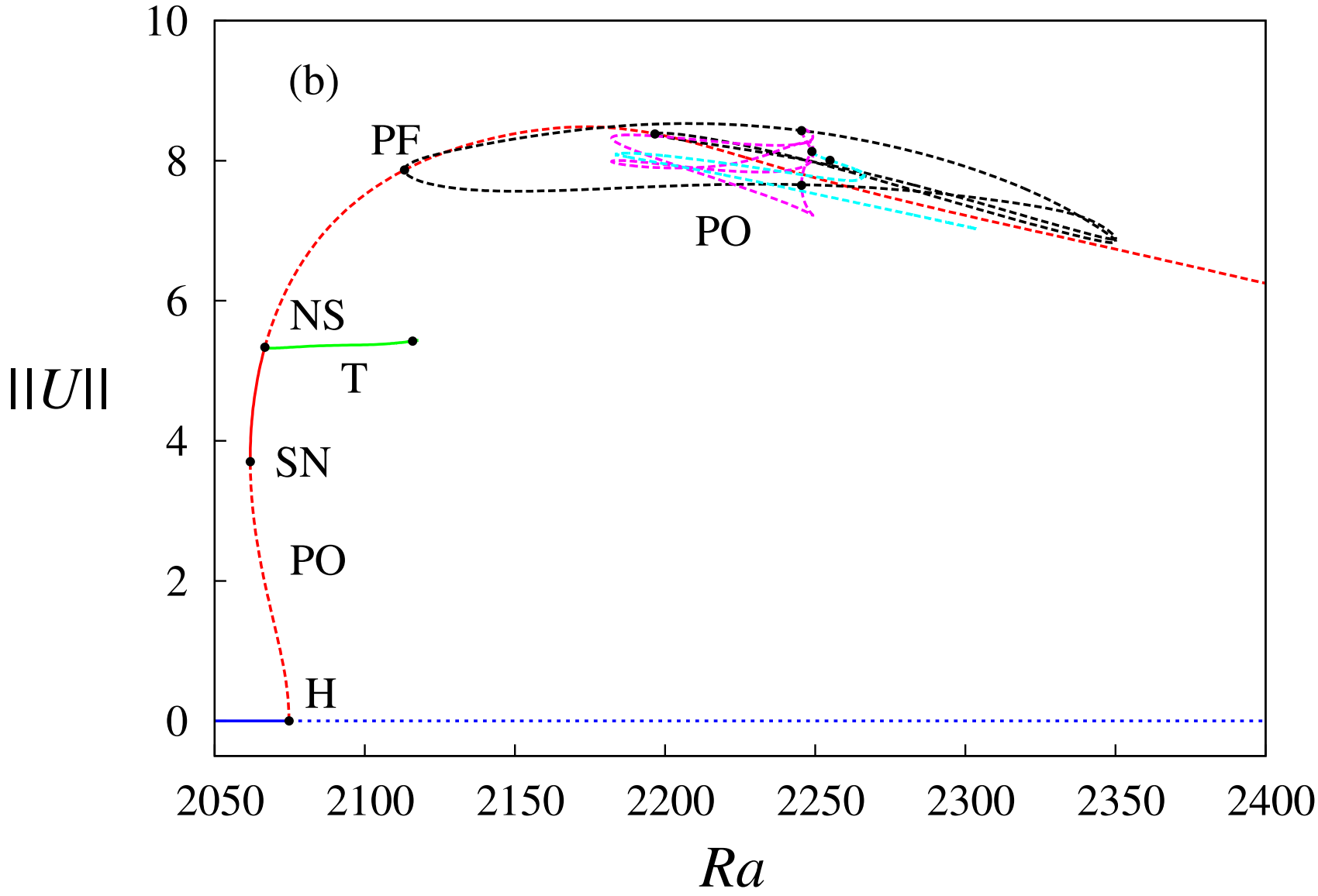
$$\frac{1}{\Delta t} B \left(\gamma_0 u^{n+1} - \sum_{i=0}^{k-1} \alpha_i u^{n-i} \right) = \sum_{i=0}^{k-1} \beta_i N(u^{n-i}) + L u^{n+1}.$$

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

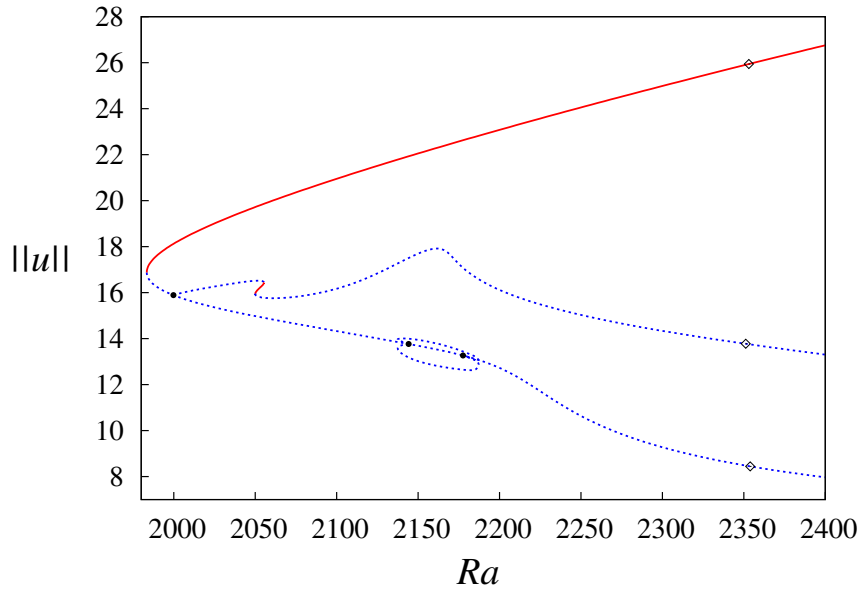
Some results for $\sigma = 0.6$

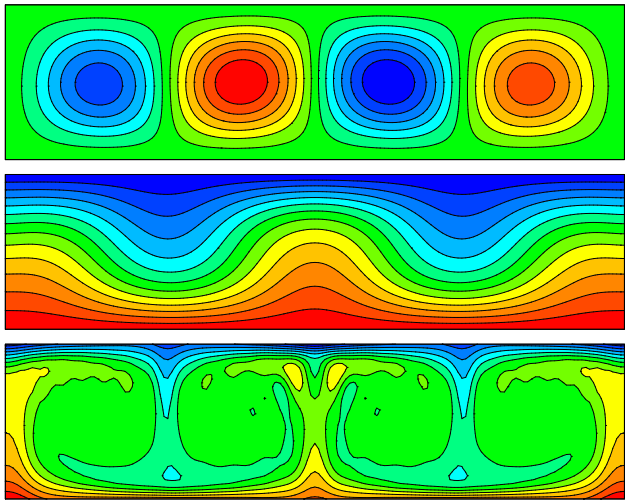


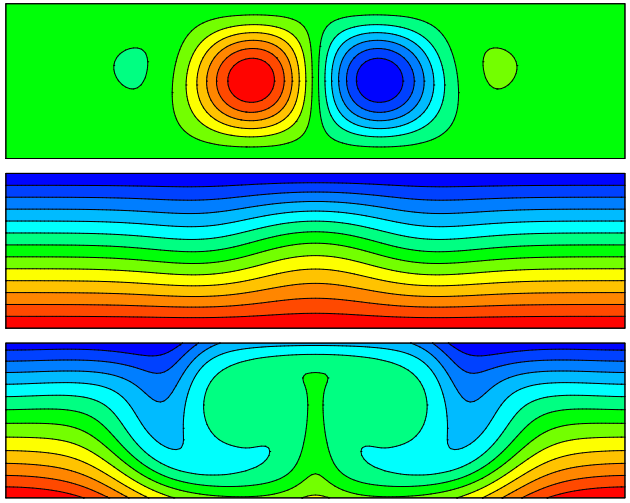
Some results for $\sigma = 0.6$

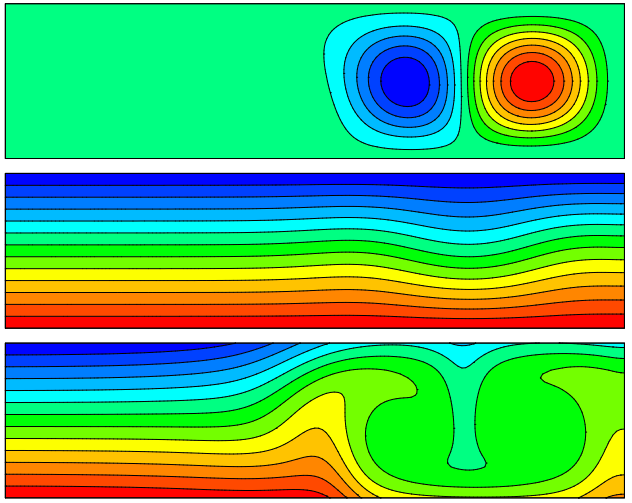


Fixed points

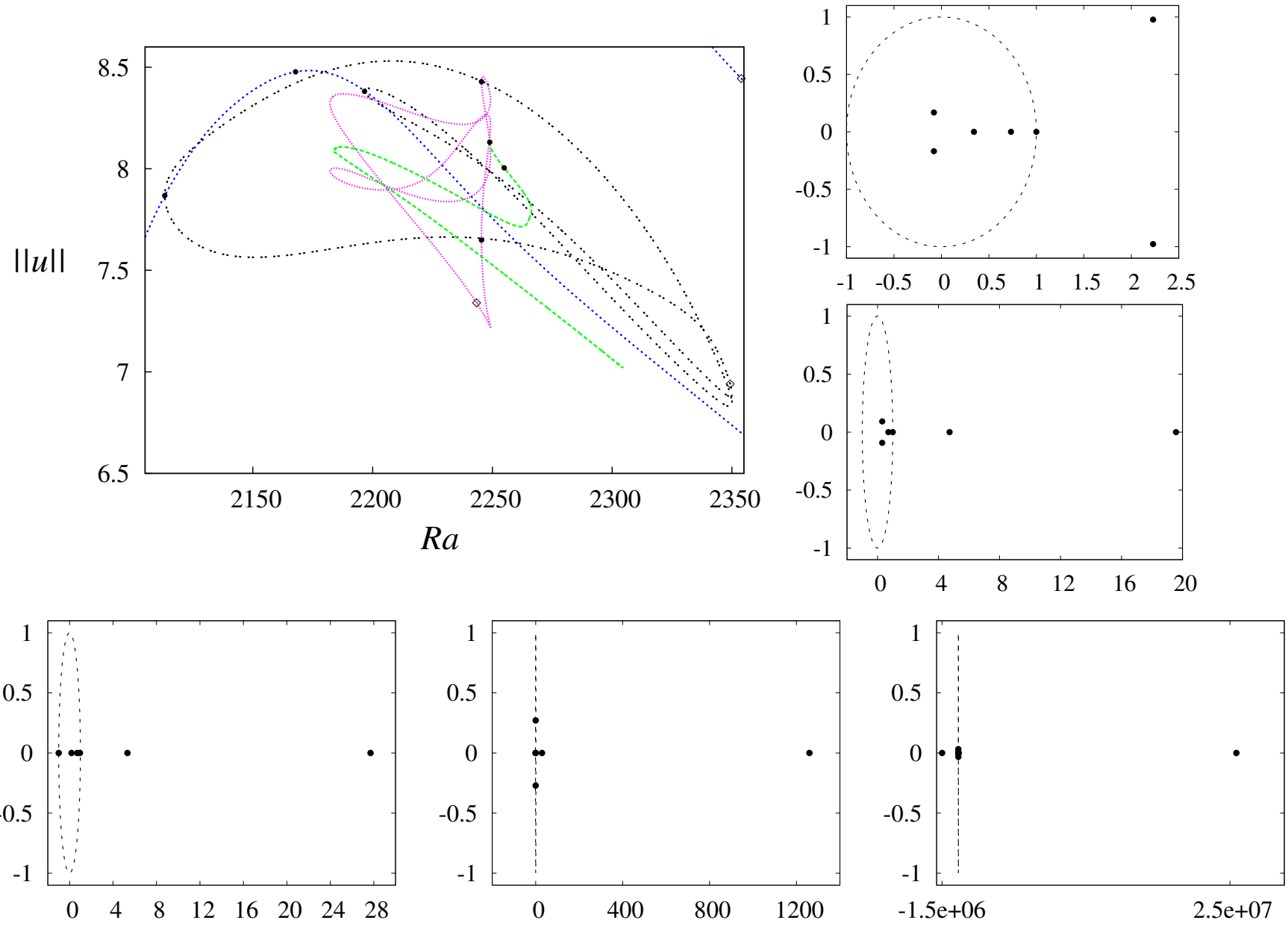




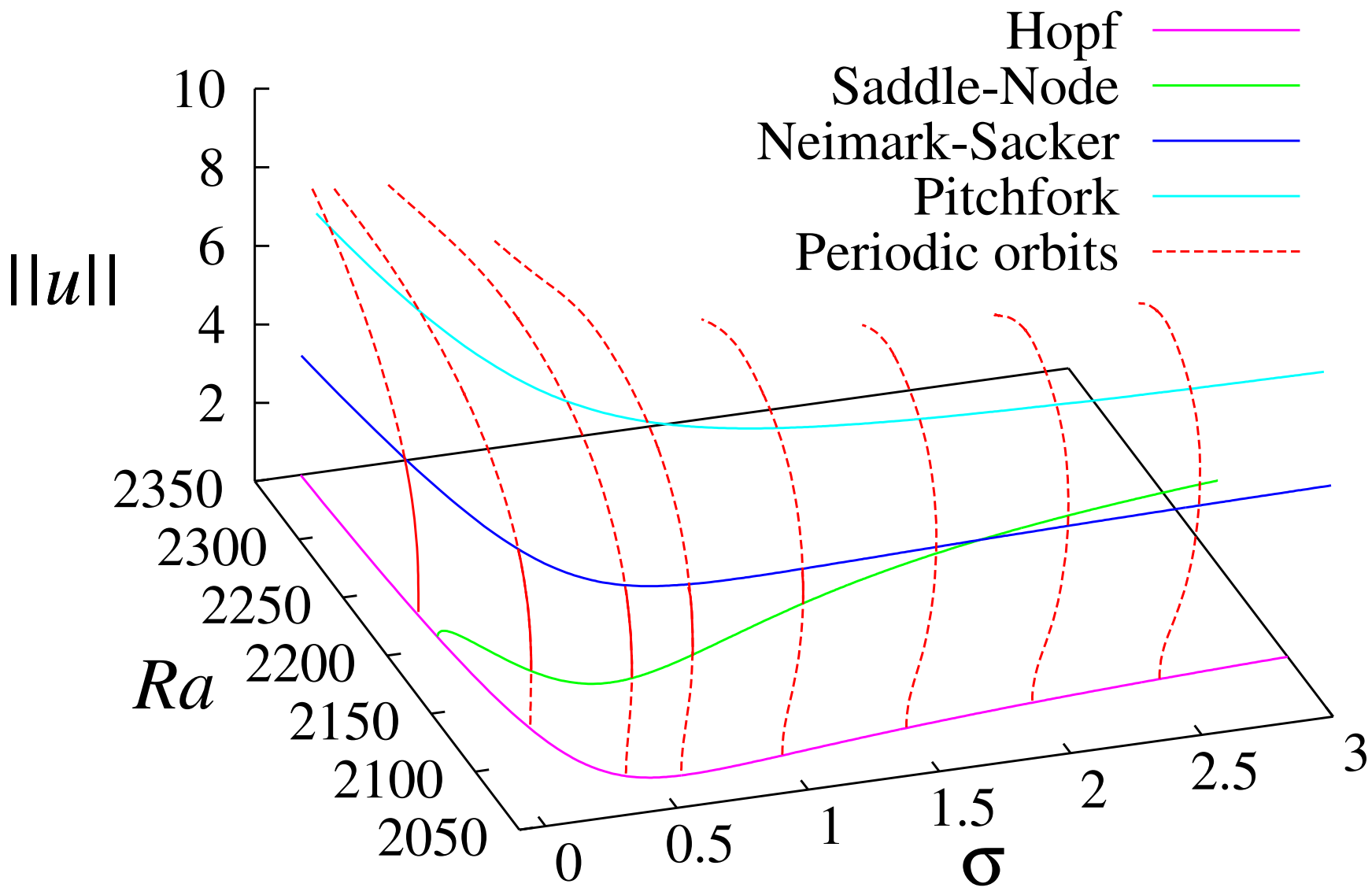




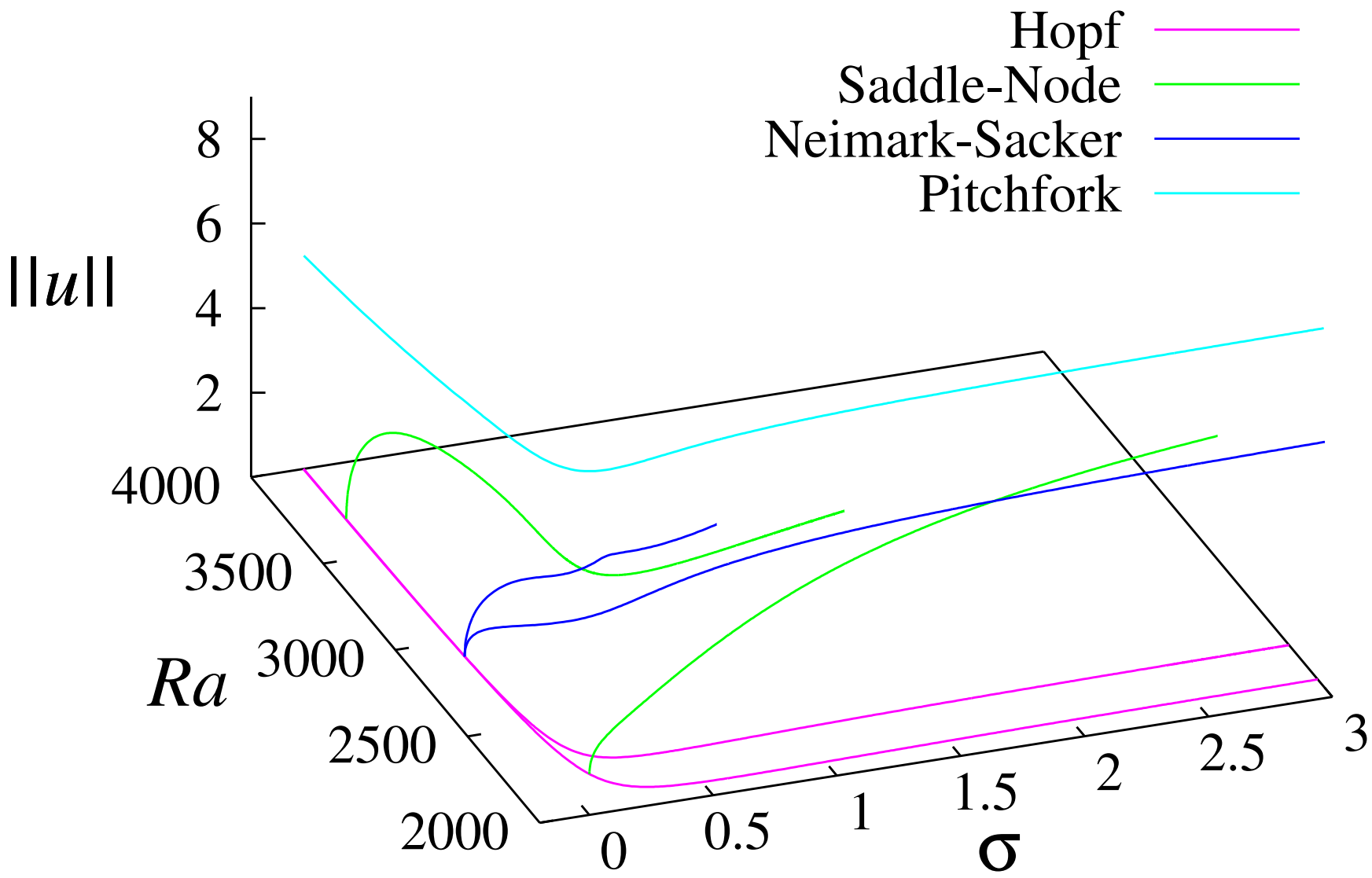
Periodic orbits



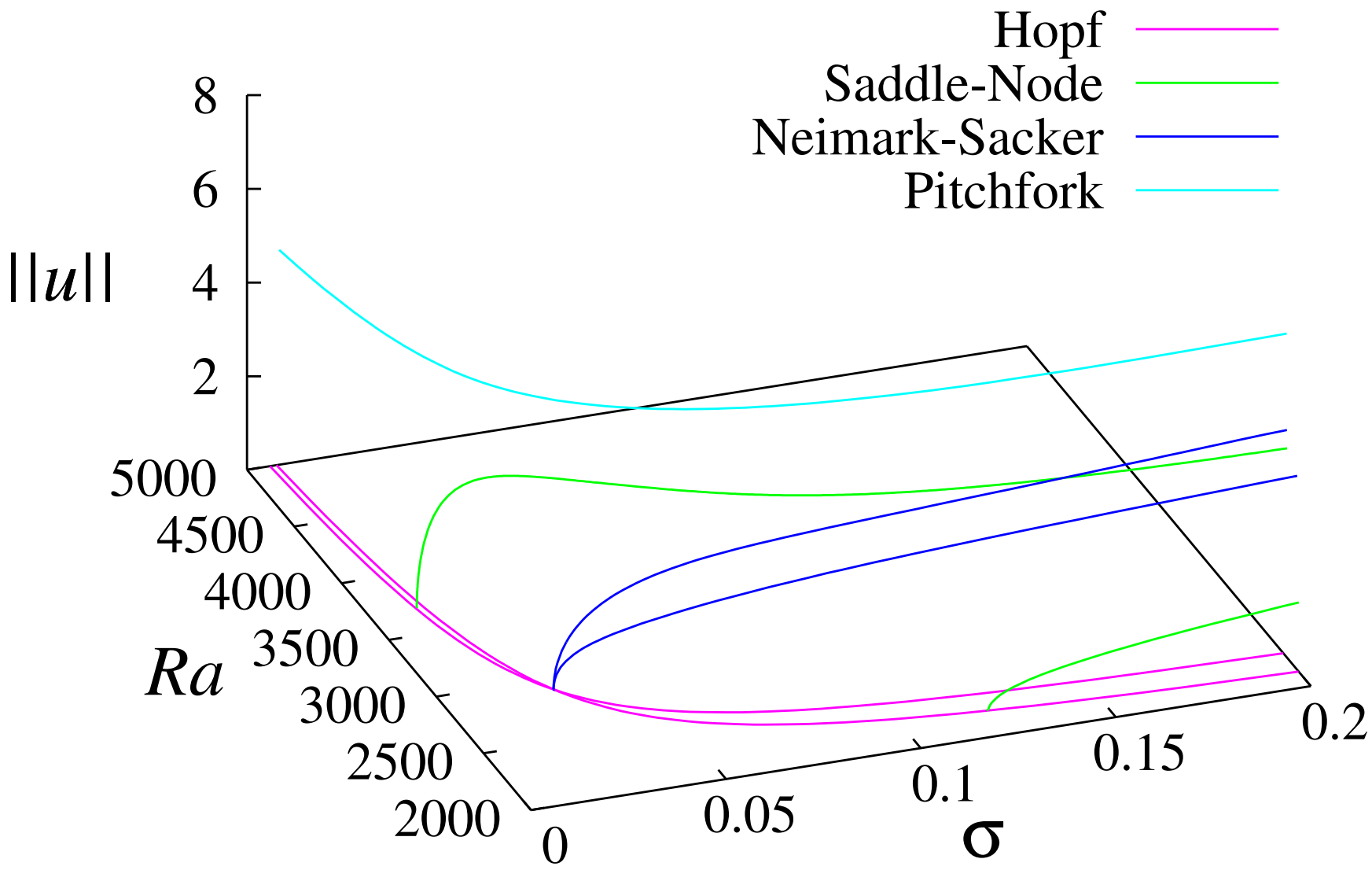
Curves of bifurcations



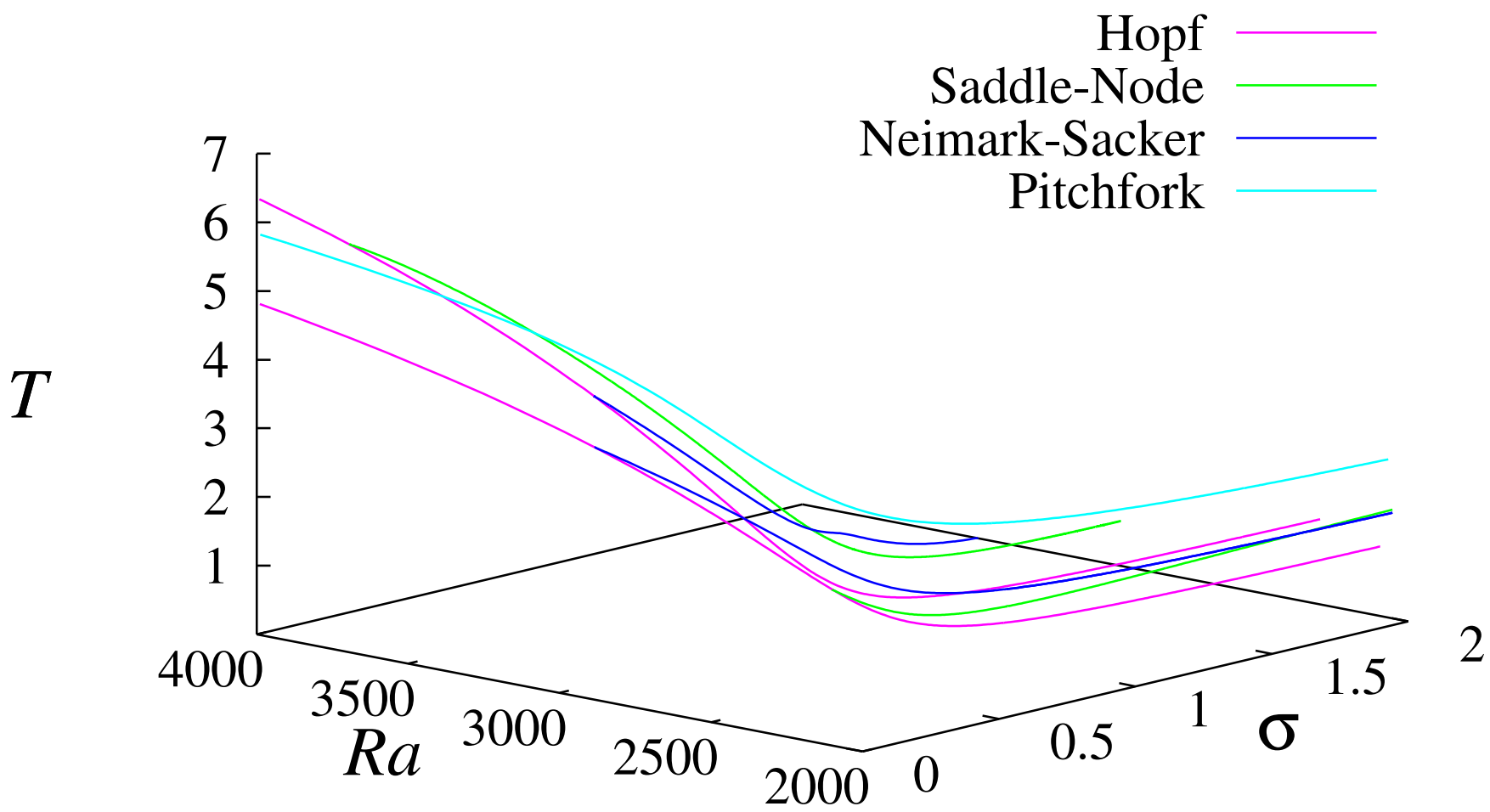
Curves of bifurcations



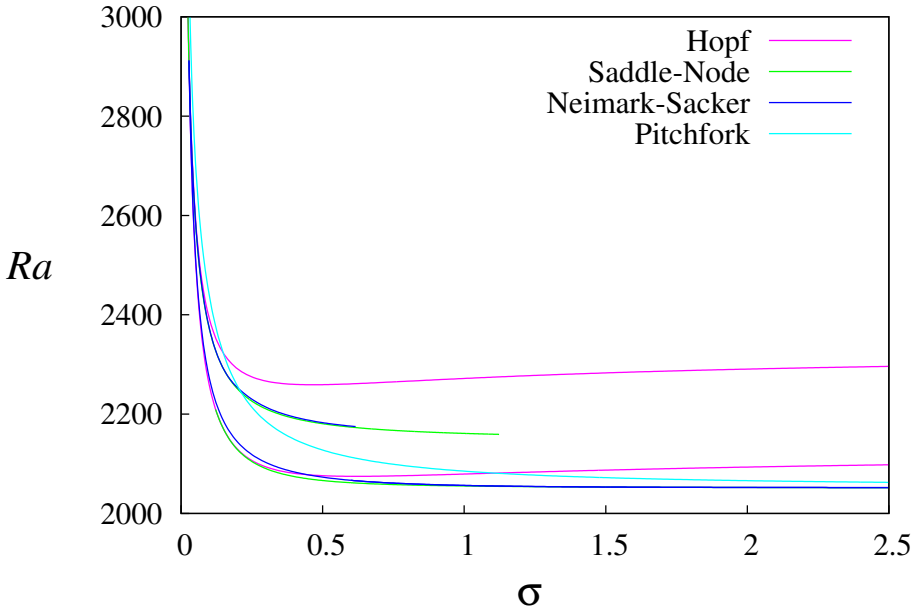
Curves of bifurcations

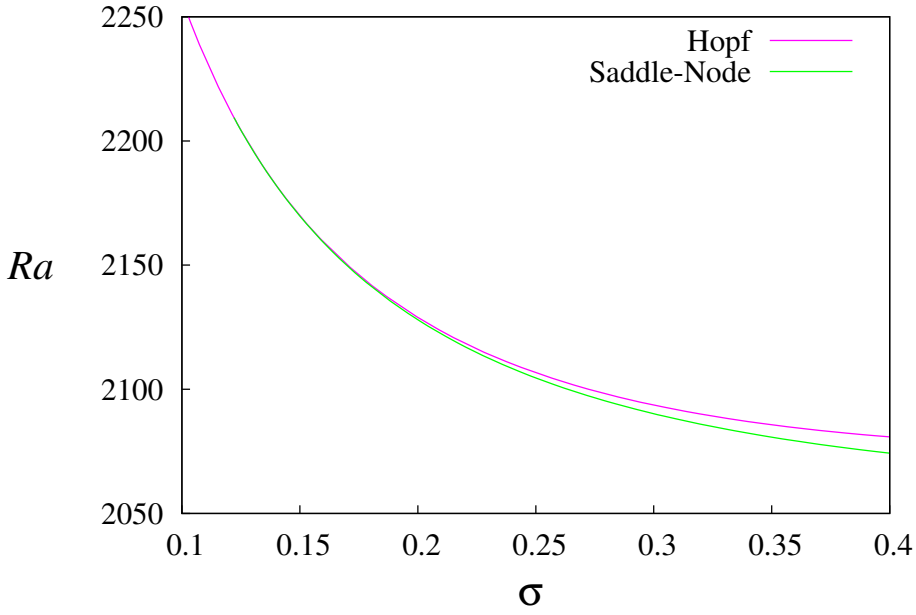


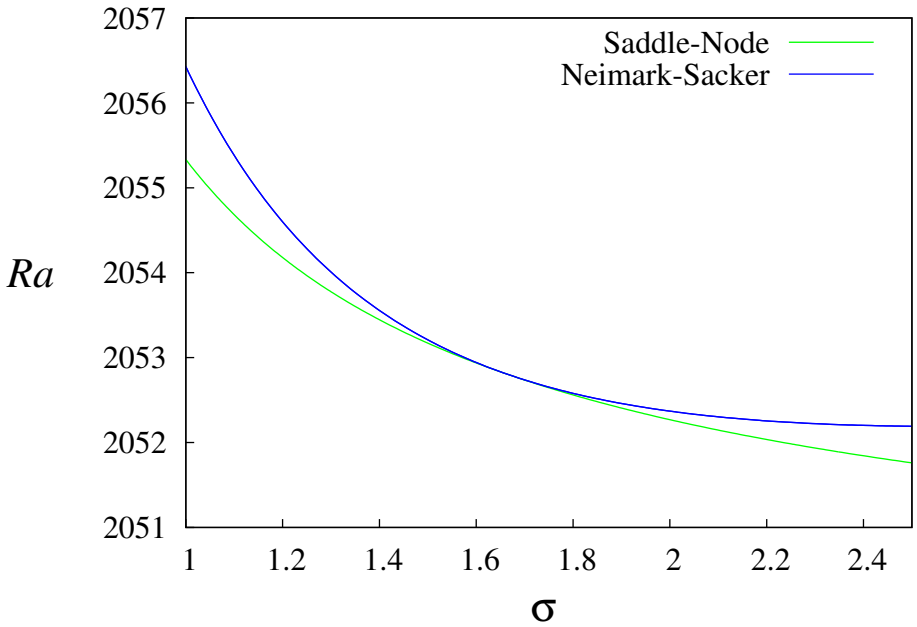
Period

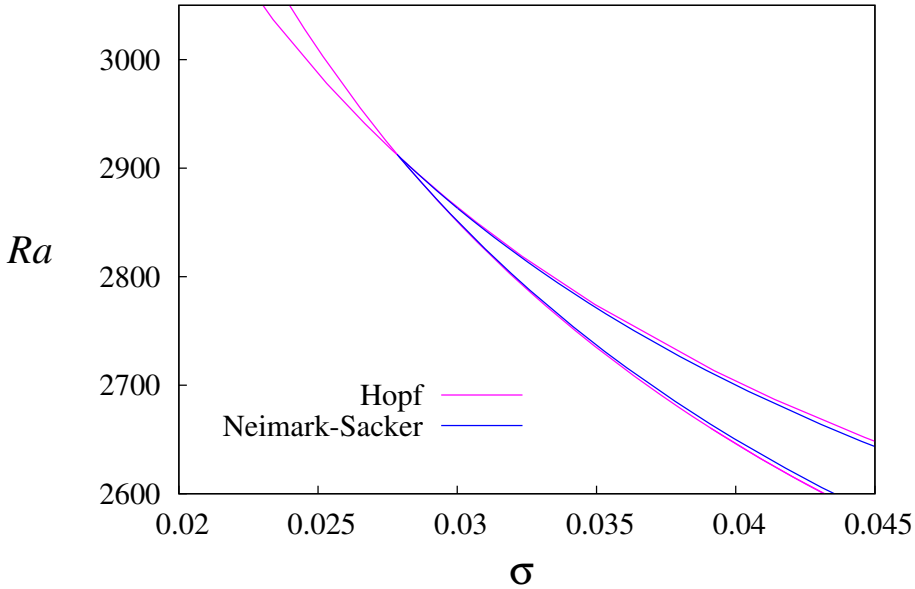

Hopf
Saddle-Node
Neimark-Sacker
Pitchfork
T
7
6
5
4
3
2
1
4000
3500
3000
2500
2000
Ra
0
0.5
1
1.5
2
σ

Codimension-two points

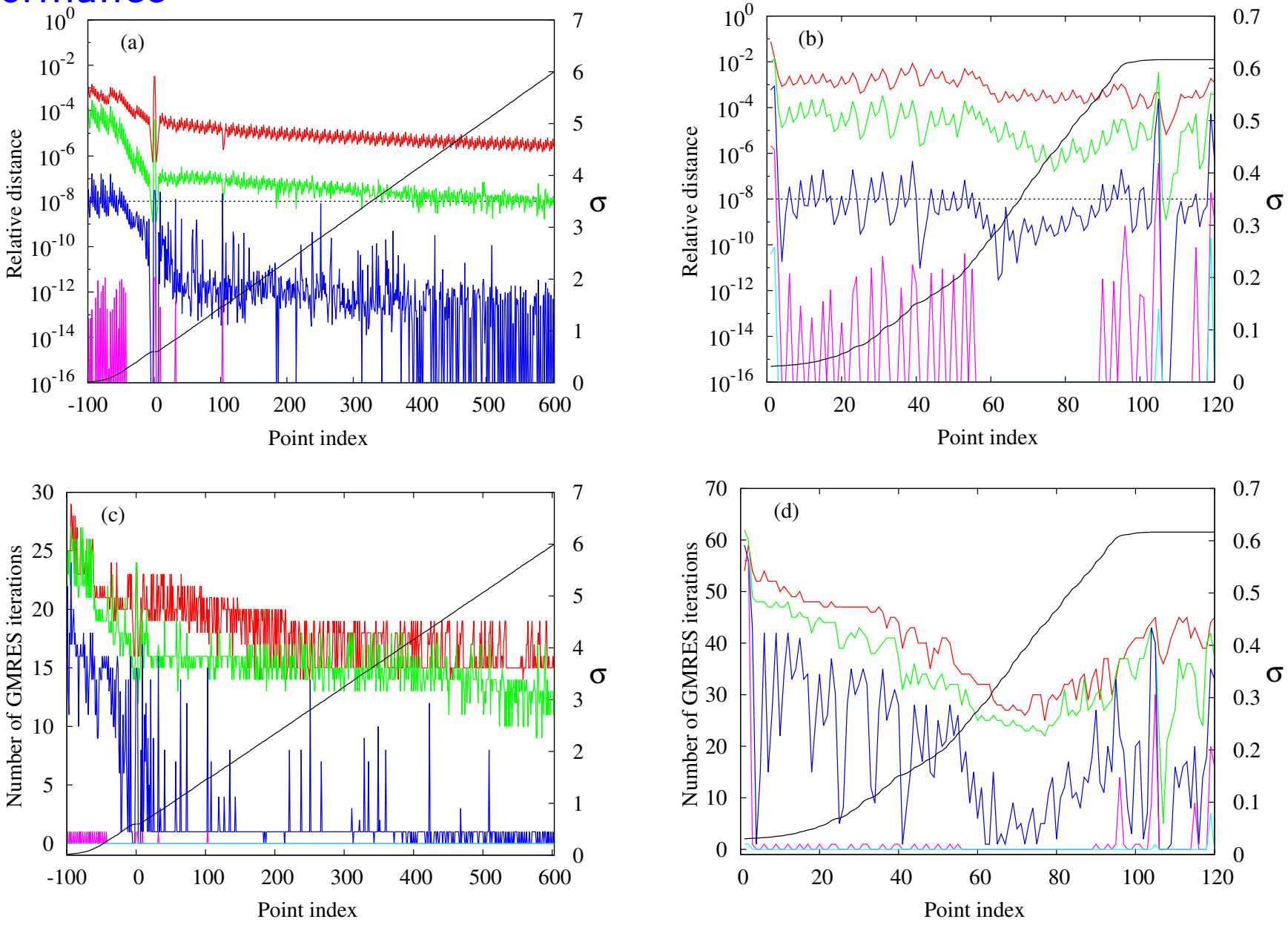








Performance



Relative distance between Newton iterates and number of GMRES iterations for the pitchfork and one of the Neimark-Sacker curves.

Continuation of invariant tori

Poincaré maps and its derivatives

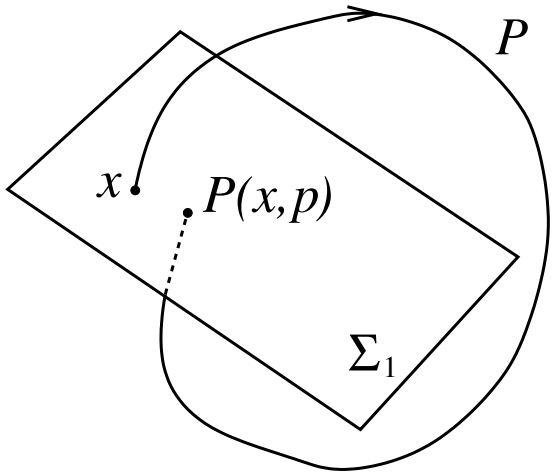
Given the system of ODEs

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

let $\varphi(t,x,p)$ is its solution with initial condition x at $t=0$ for a fixed value of p ($\varphi(0,x,p)=x$), and suppose there is a periodic orbit which cuts transversely a hyperplane Σ_1 given by

$$\Sigma_1 = \left\{ y \in \mathbb{R}^n \,/\, \langle v_1, y - x_1^{\Sigma} \rangle = 0 \right\}.$$

Let $\mathcal{V} \subset \Sigma_1$ be a neighborhood of the intersection. The Poincaré map $P : \mathcal{V} \subset \Sigma_1 \to \Sigma_1$ is defined as



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

$t(x,p)$ being the first positive time for which

$$\varphi(t(x,p),x,p) \in \Sigma_1$$

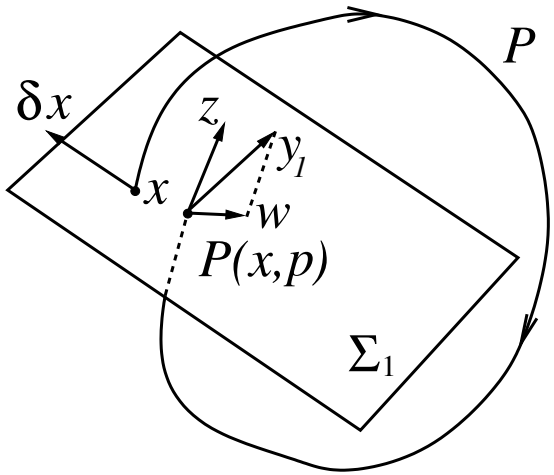
with

$$\operatorname{sign}\langle v_1, f(x,p)\rangle = \operatorname{sign}\langle v_1, f(P(x,p),p)\rangle.$$

The action of the Jacobian of $P(x,p) = \varphi(t(x,p),x,p)$ on $(\delta x, \delta p)$ with $\langle v_1, \delta x\rangle = 0$ is

$$w = D_x P(x,p)\delta x + D_p P(x,p)\delta p = y_1 - \frac{\langle v_1, y_1\rangle}{\langle v_1, z\rangle} z,$$

where $z = f(P(x,p),p)$, y_1 is the solution, at the arrival time, $t(x,p)$, of the first variational equation



$$\dot{y} = f(y,p)$$
$$\dot{y_1} = D_y f(y,p) y_1 + D_p f(y,p)\delta p$$

with initial conditions

$$y(0) = x$$
$$y_1(0) = \delta x.$$

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

To see that

$$D_x P(x,p)\delta x + D_p P(x,p)\delta p = y_1 - \frac{\langle v_1, y_1\rangle}{\langle v_1, z\rangle} z,$$

first differentiate $P(x,p) = \varphi(t(x,p),x,p)$ to obtain

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

if

$$\begin{aligned} y_1(t) =& D_x\varphi(t,x,p)\delta x + D_p\varphi(t,x,p)\delta p, \\ c =& D_x t(x,p)\delta x + D_p t(x,p)\delta p \in \mathbb{R}, \\ z =& f(\varphi(t(x,p),x,p),p) \end{aligned}$$

Then

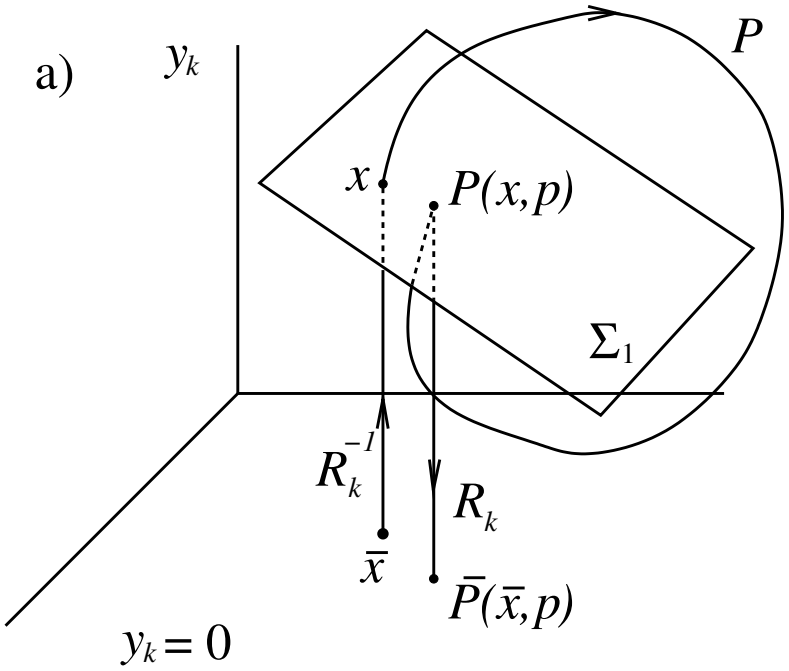
- y_1 satisfies $\dot{y}_1 = D_y f(y,p)y + D_p f(y,p)\delta p$ and $y_1(0) = \delta x$ (because $\varphi(0,x,p) = x$), $y(t) = \varphi(t,x,p)$ being the solution of $\dot{y} = f(y,p)$ with $y(0) = x$.
- Since $h_1(x,p) \equiv \langle v_1, P(x,p) - x_1^\Sigma\rangle = 0\ \forall x \in \mathcal{V}$ and p, and then

$$D_x h_1(x,p)\delta x + D_p h_1(x,p)\delta p = \langle v_1, y_1\rangle + c\langle v_1, z\rangle = 0$$

Continuation of periodic orbits of ODEs

The periodic orbits $\dot{y} = f(y, p)$ can be computed as fixed points of a parameterized version of the Poincaré map.

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



The parameterized map

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

and its fixed points verifying

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

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

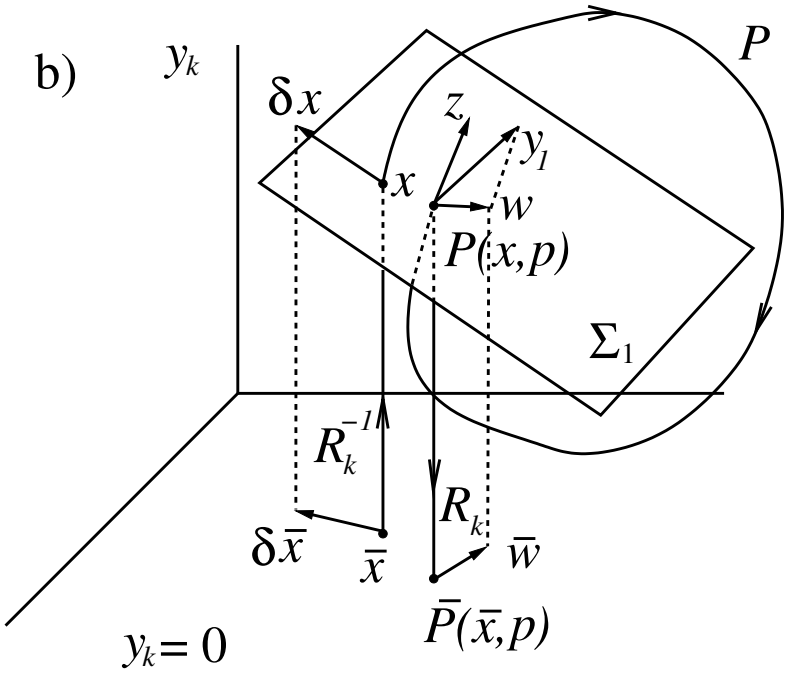
By applying the chain rule to $\bar{P}(\bar{x},p) = R_k(P(R_k^{-1}(\bar{x}),p))$

$$D_{\bar{x}}\bar{P}(\bar{x},p)\delta\bar{x} + D_p\bar{P}(\bar{x},p)\delta p = R_k\left(D_xP(x,p)DR_k^{-1}(\bar{x})\delta\bar{x} + D_pP(x,p)\delta p\right) = R_k w$$

whith

$$w = D_xP(x,p)\delta x + D_pP(x,p)\delta p = y - \frac{< v_1, y >}{< v_1, z >} z,$$

where $\delta x = DR_k^{-1}(\bar{x})\delta\bar{x}$, $z = f(P(x,p),p)$, and y_1 is the solution, at the arrival time, $t(x,p)$, of the first variational equation



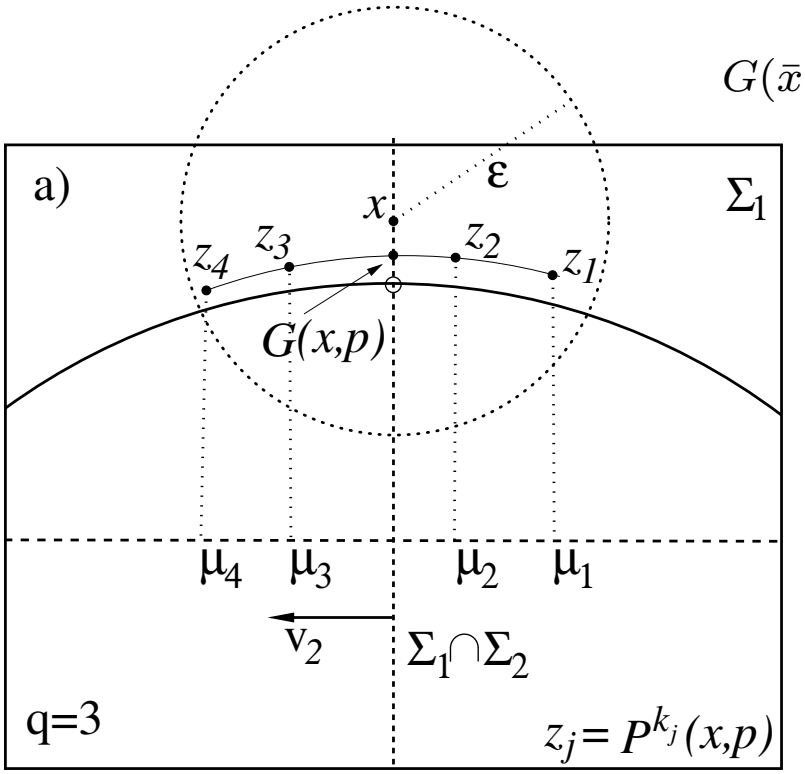
$$\dot{x} = f(x,p)$$
$$\dot{y}_1 = D_xf(x,p)y_1 + D_pf(x,p)\delta p$$

with initial conditions

$$x(0) = x = R_k^{-1}(\bar{x})$$
$$y_1(0) = \delta x = DR_k^{-1}(\bar{x})\delta\bar{x}.$$

'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 $\langle v_2, x - x_2^{\Sigma} \rangle = 0$, transversal to both Σ_1 and the invariant 2-tori. Fix ε, and define the map $G(\bar{x}, p) : \mathcal{U} \subset \mathbb{R}^{n-2} \times \mathbb{R} \to \mathbb{R}^{n-2}$ as follows. If $R : \Sigma_1 \cap \Sigma_2 \to \mathbb{R}^{n-2}$ is a parameterization of $\Sigma_1 \cap \Sigma_2$ and $\bar{x} \in \mathcal{U}$ let $x = R^{-1}(\bar{x})$ and $z_j = P^{k_j}(x, p)$, $j = 1, \ldots, q+1$ be the first $q+1$ powers of P on x such that $\|P^{k_j}(x, p) - x\| < \varepsilon$. Then



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

where the l_j are the Lagrange interpolation polynomials of degree q associated to the mesh of points

$$\mu_j = \langle v_2, P^{k_j}(x, p) - x_2^{\Sigma} \rangle, \quad j = 1, \cdots, q+1$$

$$l_j(\mu) = \prod_{\substack{i=1 \\ i \neq j}}^{q+1} \frac{\mu - \mu_i}{\mu_j - \mu_i},$$

evaluated at $\mu = 0$.

Then $\bar{x} - G(\bar{x}, p) = 0$ is solved.

The fixed points of the map $G(\bar{x}, p)$ 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 radius ε defining G must be varied adaptively during the 'continuation' process.

The action of the Jacobian of $G(\bar{x},p) = R(\sum_{j=1}^{q+1} l_j(0) P^{k_j}(R^{-1}(\bar{x}),p))$, on a $(\delta\bar{x},\delta p)$ reduces to the case of the differential of the Poincaré map

$$D_{\bar{x}}G(\bar{x},p)\delta\bar{x} + D_pG(\bar{x},p)\delta p = R\sum_{j=1}^{q+1}\Big[\, l_j(0)\big(D_xP^{k_j}(x,p)\delta x + D_pP^{k_j}(x,p)\delta p\big) + P^{k_j}(x,p)\sum_{i=1}^{q+1}\partial_{\mu_i} l_j(0)\langle v_2, D_xP^{k_i}(x,p)\delta x + D_pP^{k_i}(x,p)\delta p\rangle\Big],$$

with $x = R^{-1}(\bar{x})$ and $\delta x = D_{\bar{x}}R^{-1}(\bar{x})\delta\bar{x}$, and where

$$\langle v_2, D_xP^{k_i}(x,p)\delta x + D_pP^{k_i}(x,p)\delta p\rangle = D_x\mu_i\delta x + D_p\mu_i\delta p.$$

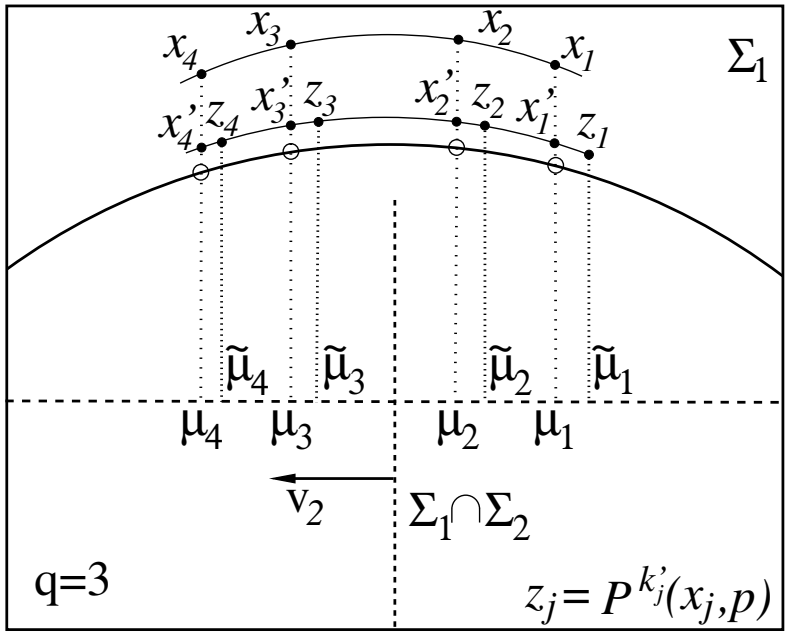
The derivatives $\partial_{\mu_i} l_j(0)$ of

$$l_j(0) = \prod_{\substack{i=1\\ i\neq j}}^{q+1}\frac{\mu_i}{\mu_i - \mu_j}$$

are trivial.

'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 $\langle v_2, x - x_2^{\Sigma} \rangle = 0$, 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 $x = x_2^{\Sigma} + \mu v_2$. Fix ε, and define the map $G(X,p) : \mathcal{U} \subset \mathbb{R}^{(n-1)(q+1)} \times \mathbb{R} \to \mathbb{R}^{(n-1)(q+1)}$ as follows. If $X = (x_1, \cdots, x_{q+1}) \in \mathcal{U}$ let $z_j = P^{k'_j}(x_j, p)$ be the first power of P on x_j such that $\|P^{k'_j}(x_j,p) - x_j\| < \varepsilon$ for $j = 1, \ldots, q+1$. Then



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

$X' = (x'_1, \cdots, x'_{q+1})$, $Z(X,p) = (z_1, \cdots, z_{q+1})$,

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 $\tilde{\mu}_j = \langle v_2, P^{k'_j}(x_j,p) - x_2^{\Sigma} \rangle, \quad j = 1, \cdots, q+1$ respectively.

The fixed points of the map $G(X,p)$ approximate an arc 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

$$DG(X,p)(\delta X, \delta p) = \left[DZ(X,p)(\delta X, \delta p) - Z(X,p)\tilde{V}(X,p)^{-1} D\tilde{V}(X,p)(\delta X, \delta p)\right] \tilde{V}(X,p)^{-1} V$$

where

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

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

and $\eta_j = \langle v_2, DP^{k'_j}(x_j,p)(\delta x_j, \delta p)\rangle$. 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.

Comparison of the two methods to compute invariant tori

Assuming the same degree q of interpolation is used to approximate the invariant curve:

- The first method requires computing increasing powers $k_1 < k_2 < \cdots < k_{q+1}$ of the Poincaré map of a single initial condition x. This is a sequential process.
- The second requires the first returning powers k'_j for a collection of initial conditions x_j. They can be computed in parallel. If the x_j are close enough all the k'_j will be the same.
- If the two methods are applied to the same problem with the same ε, and close initial conditions, one can expect $k'_1 = \cdots = k'_{q+1} = k_1$. Therefore if parallelism is used in the second method the wall-clock time to compute the map or the action by the Jacobian is reduced by a factor k_{q+1}/k_1.
- If the number of iterations of Newton's method and the linear solver are the same for both methods, the time (wall-clock) to do the continuation will be reduced essentially by a factor k_{q+1}/k_1.
- If $k_2 \approx 2k_1, \cdots, k_{q+1} \approx (q+1)k_1$ then $k_{q+1}/k_1 \approx q+1$.
- If $k'_1 = \cdots = k'_{q+1}$ the speed-up of the second method (time sequential/time parallel) is essentially $q+1$.
- Since the second method requires, in principle, lower powers of the Poincaré map, it should be best suited for the computation of weakly unstable invariant tori.

Thermal convection in binary fluid mixtures

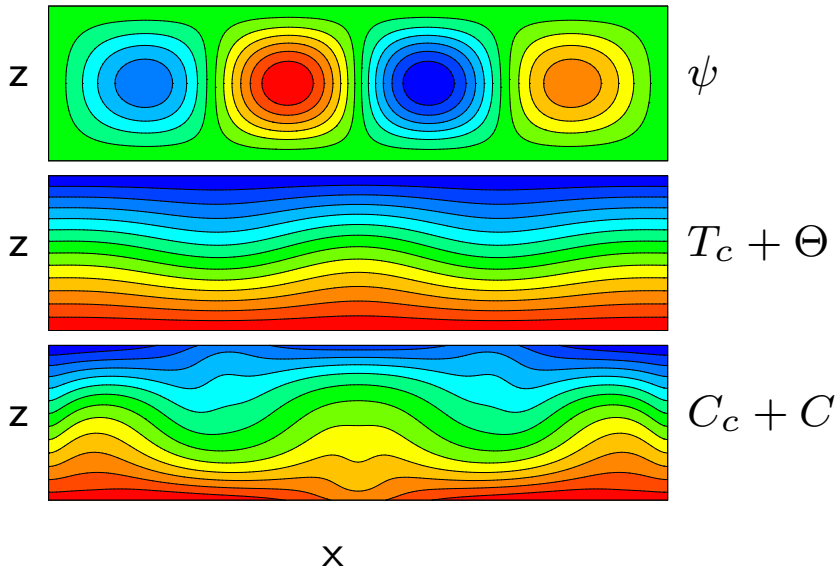
The equations in $\Omega = [0, \Gamma] \times [0, 1]$ for the perturbation of the basic state ($\mathbf{v}_c = 0$, $T_c = T_c(0) - z$, and $C_c = C_c(0) - z$) in non-dimensional form are

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

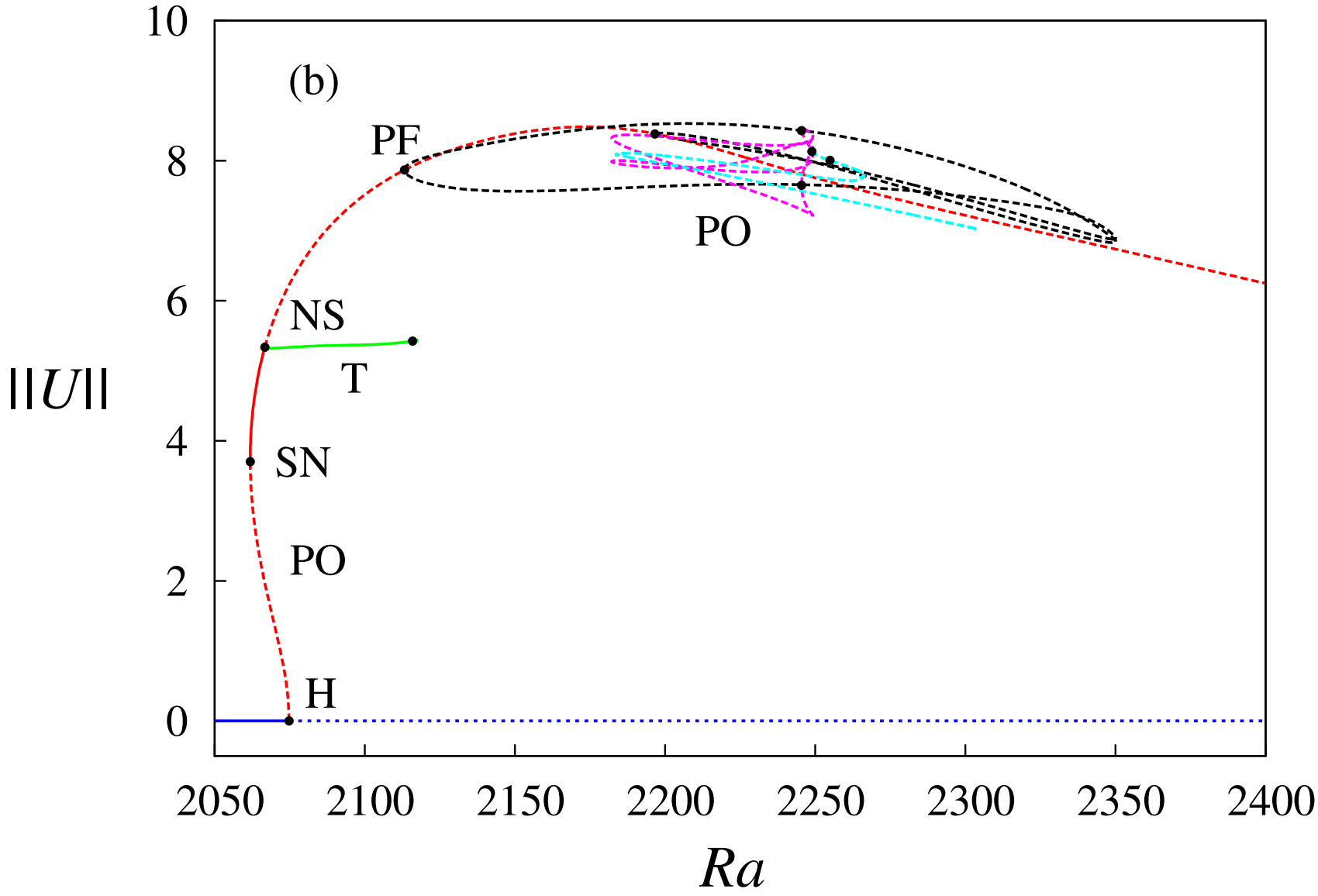
The boundary conditions are non-slip for $\mathbf{v}$, constant temperatures at top and bottom and insulating lateral walls for $\Theta = T - T_c$, and impermeable boundaries for C.

The parameters are

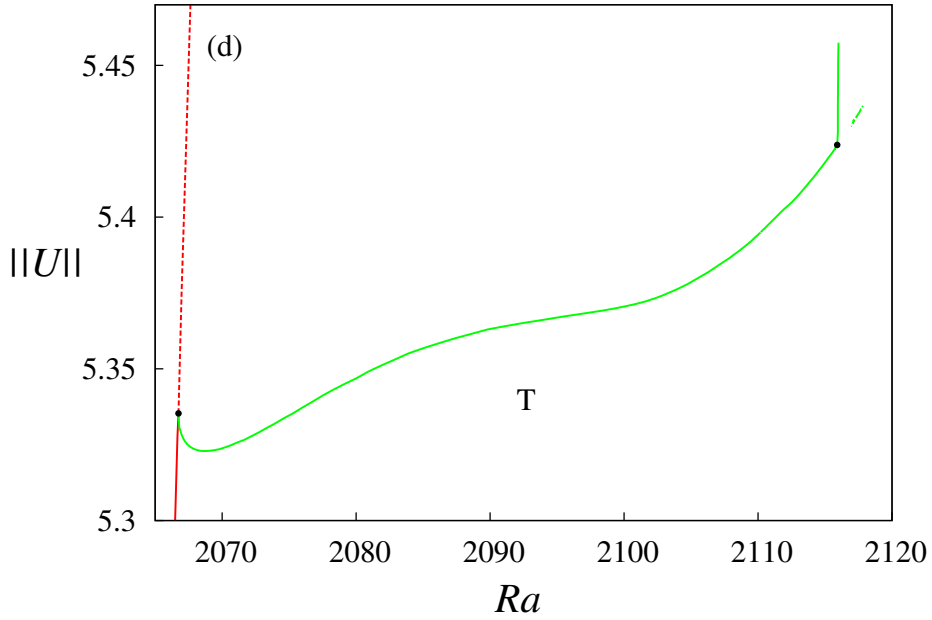
Γ	Aspect ratio (4)
S	Separation ratio (-0.1)
L	Lewis number (0.03)
σ	Prandtl number (control)
Ra	Rayleigh number (control)

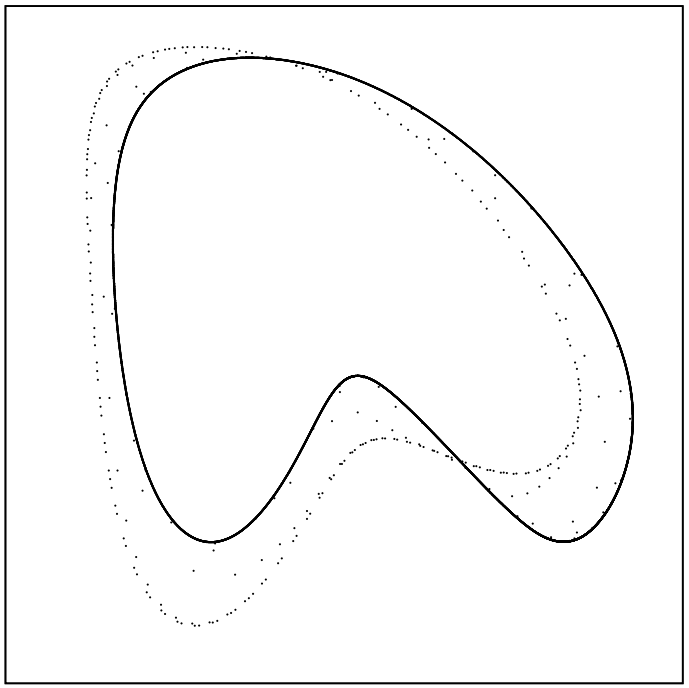


Some results for $\sigma = 0.6$



Invariant tori for $\sigma = 0.6$





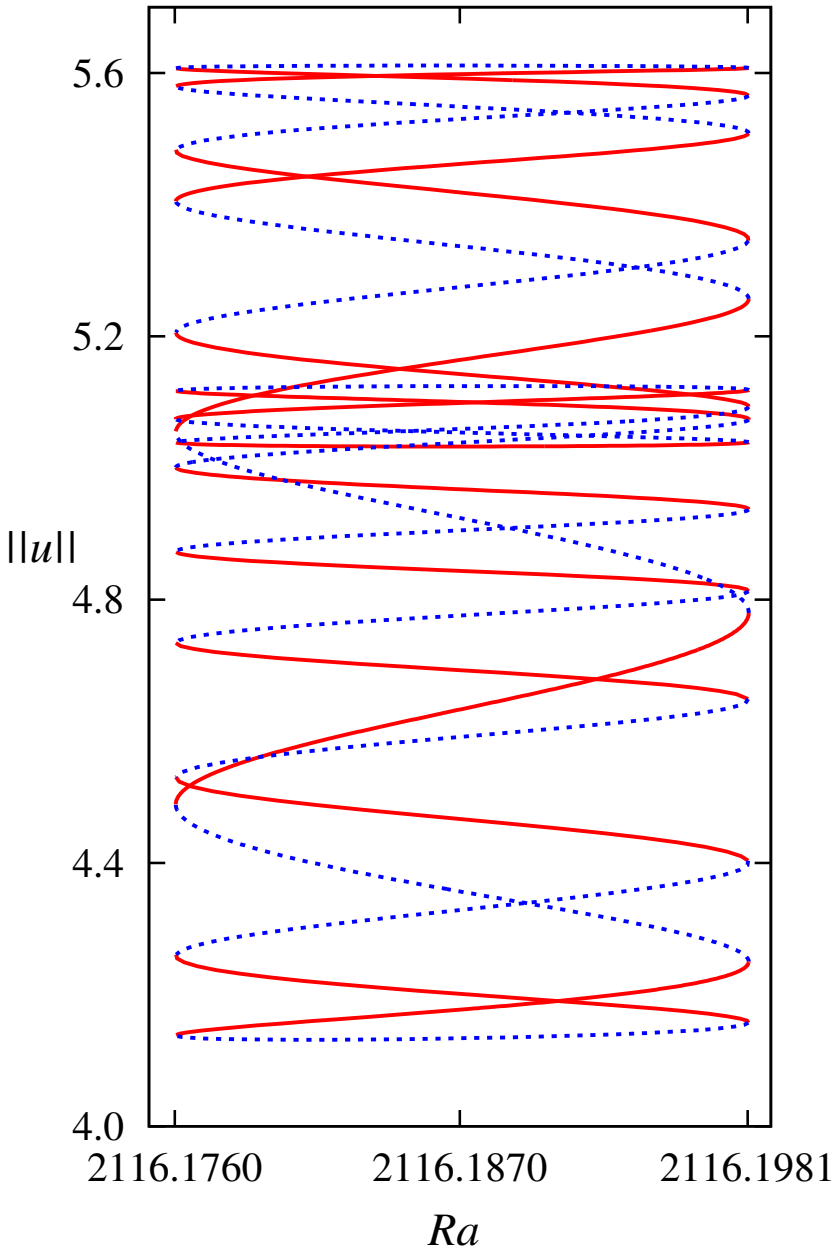
- Beginning of the branch: $Ra = 2066.74$
- $1/7$–resonance interval $2102.79 < Ra < 2102.80$
- Pitchfork bifurcation $Ra \approx 2115.92$
- $1/8$–resonance interval $2116.18 \leq Ra \leq 2116.20.$
- First period doubling $Ra \approx 2118.40$
- Second period doubling $Ra \approx 2118.55$
- Breakdown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

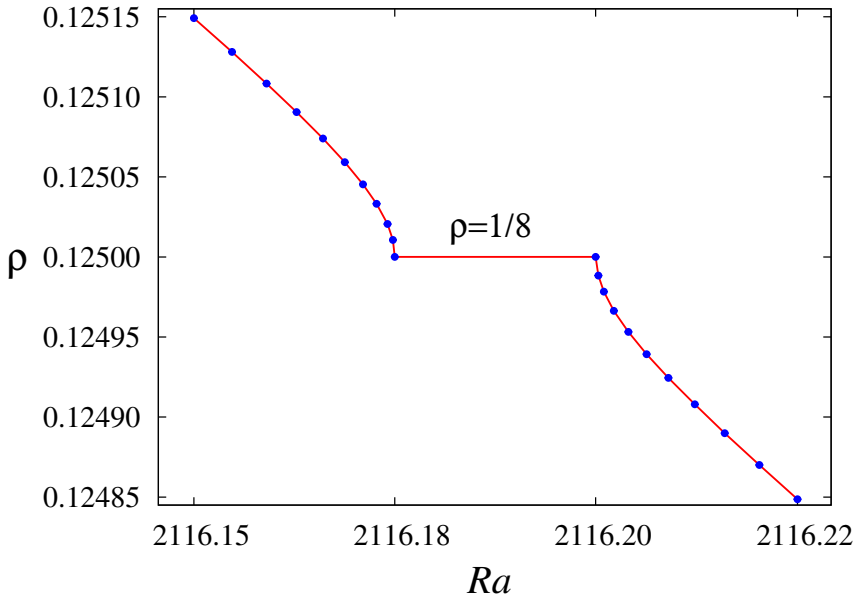
Comparison of the two methods to compute invariant tori

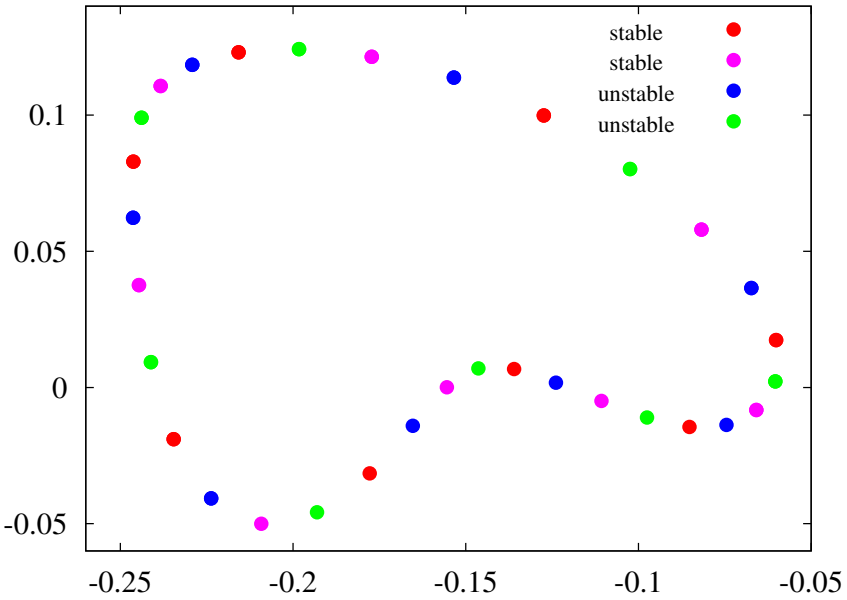
Meth.	Version	q	Time	N. sol.	Time/N. sol.	Ratio_1	Ratio_2
1	serial	2	3725	19	196	4.97	4.71
1	serial	3	3960	19	208	5.27	4.99
1	serial	4	5019	19	264	7.34	7.34
1	serial	5	5664	19	298	7.97	7.97
2	serial	2	2255	18	125	3.01	3.01
2	serial	3	2830	18	157	3.76	3.76
2	serial	4	3563	19	188	5.21	5.21
2	serial	5	4333	19	228	6.09	6.09
2	parallel	2	749	18	42	1.00	1.00
2	parallel	3	752	18	42	1.00	1.00
2	parallel	4	684	19	36	0.91	0.87
2	parallel	5	711	19	37	0.95	0.90

Comparison of the wall-clock times for the different algorithms, implementations, and interpolation degrees. The continuation corresponds to the interval $Ra \in [210, 2115]$.

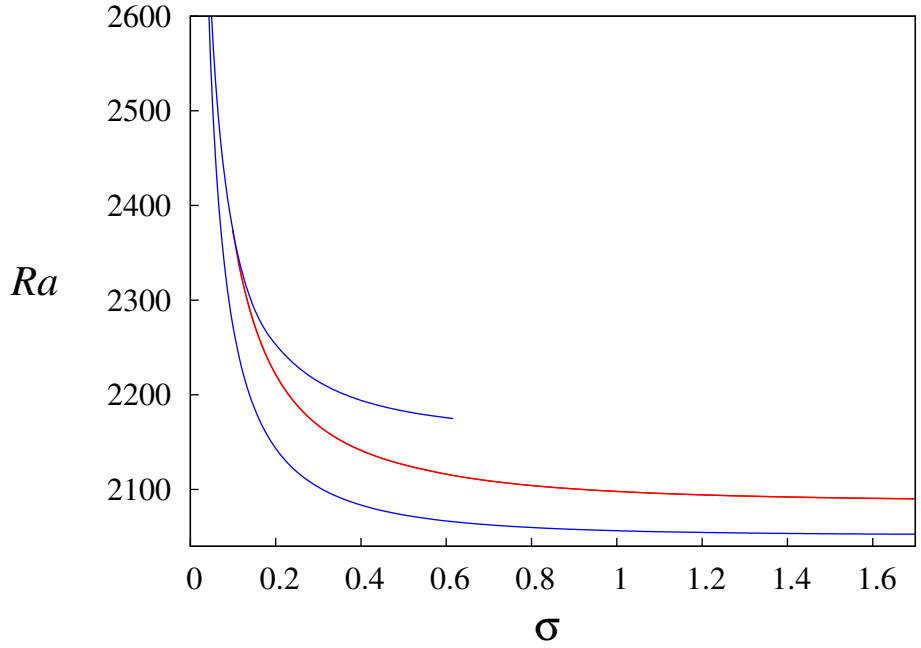
The Arnold's tongue of $\rho = 1/8$ ($\sigma = 0.6$)

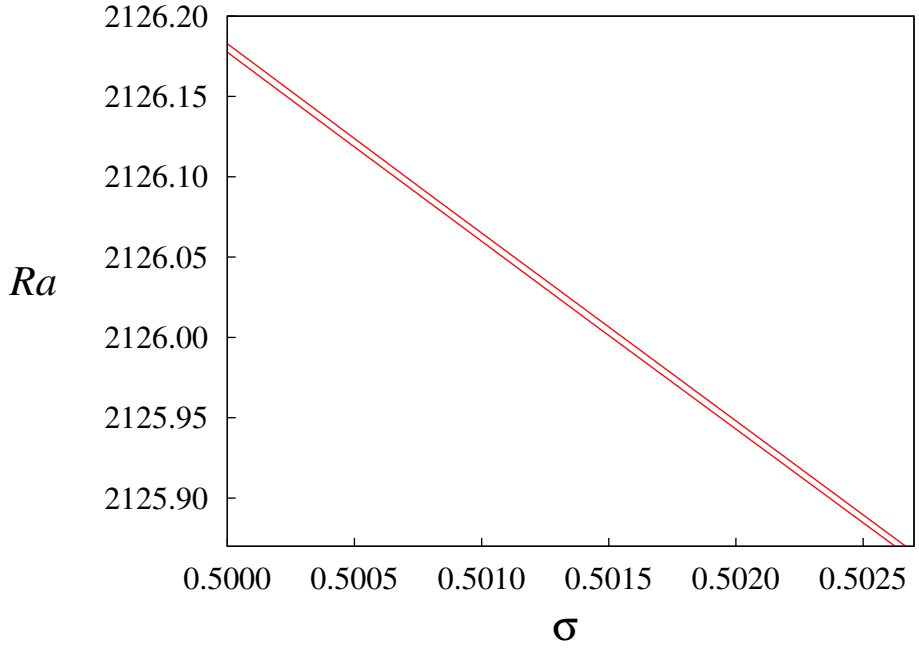


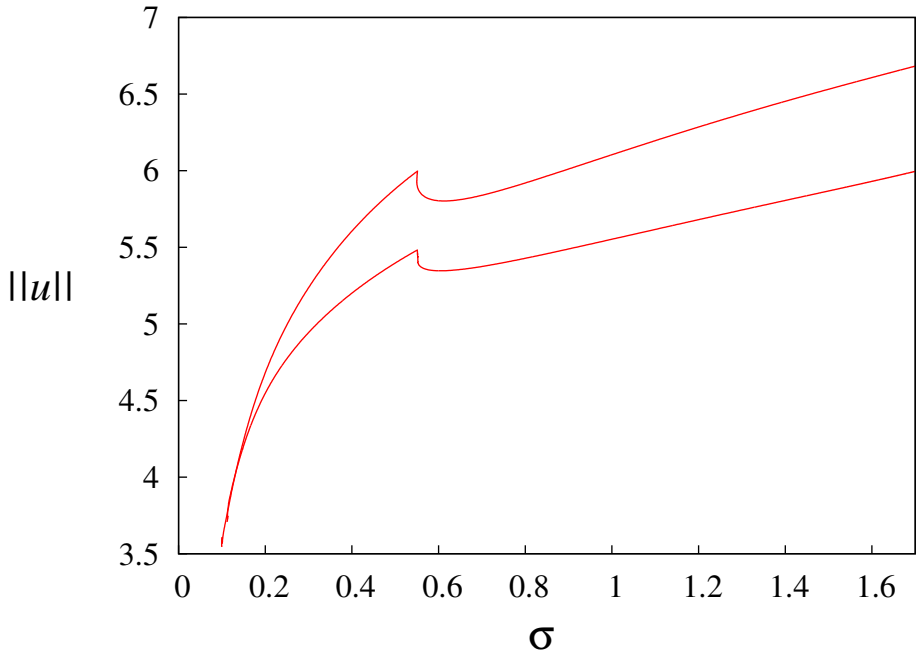


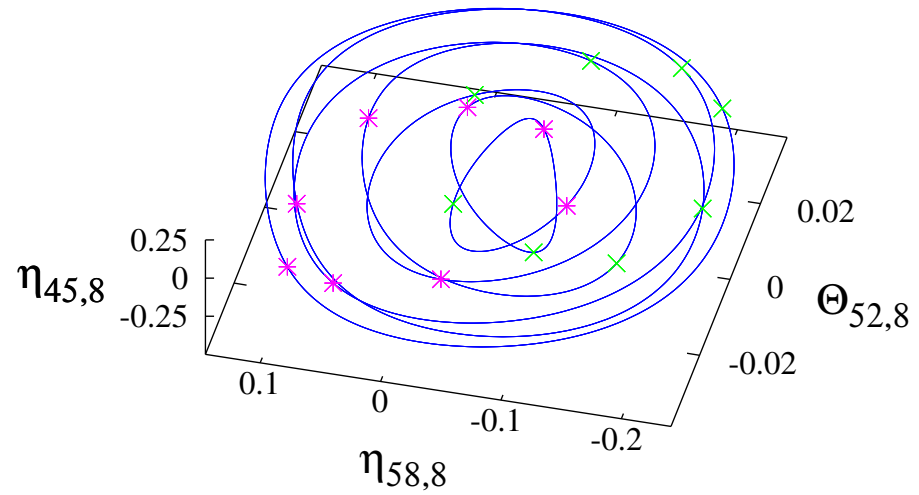


Computation of the limits of the $1/8$ tongue









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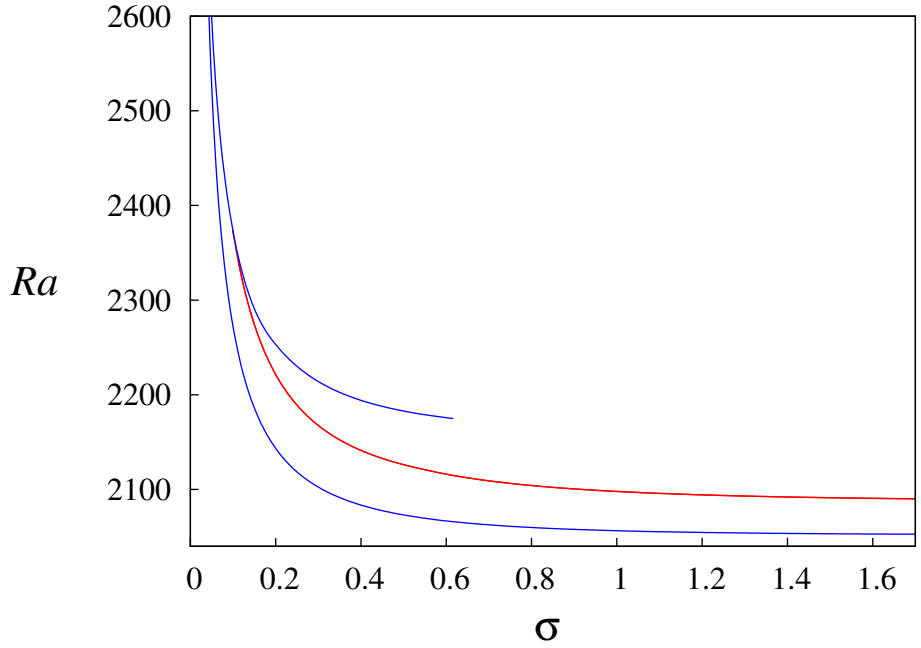
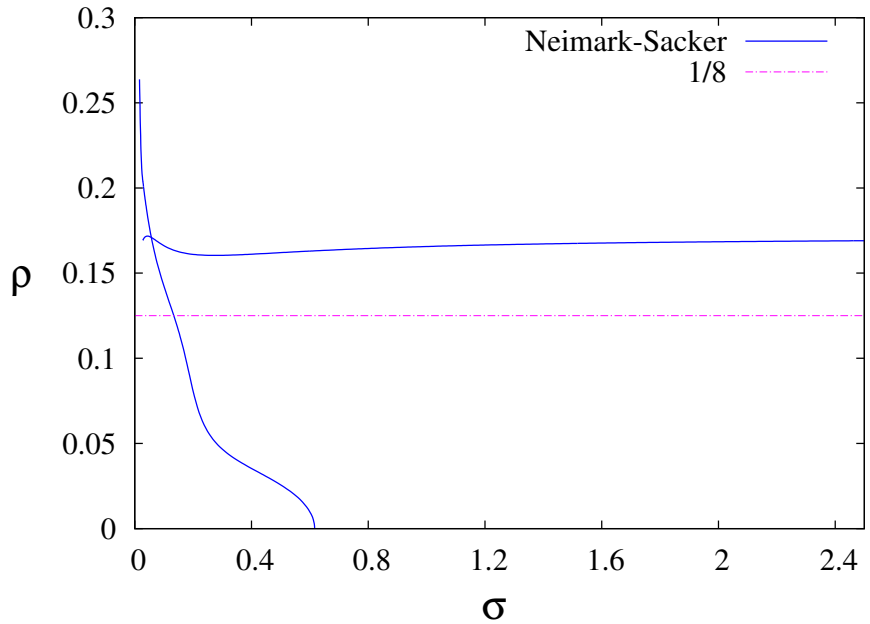
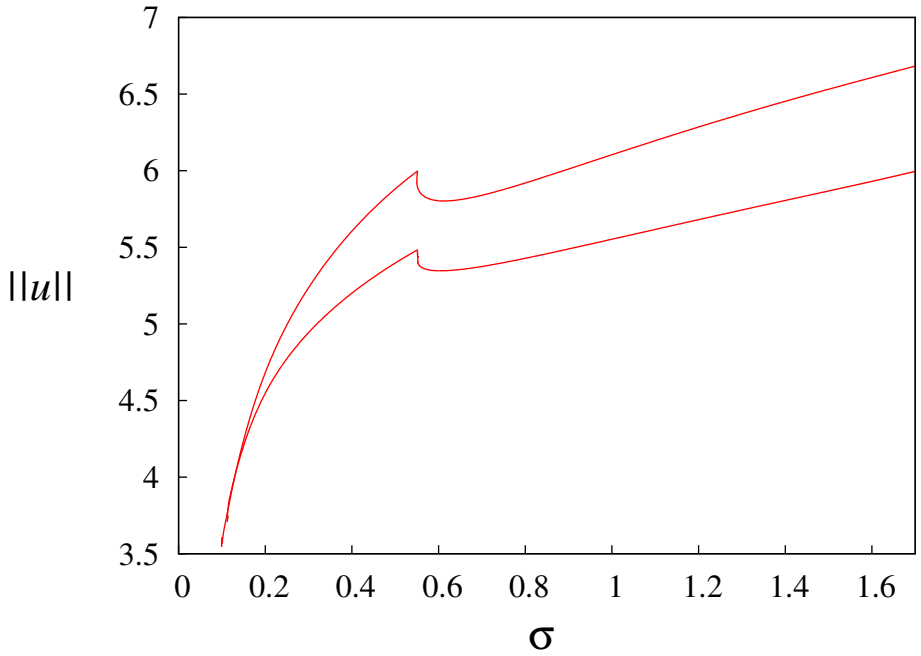
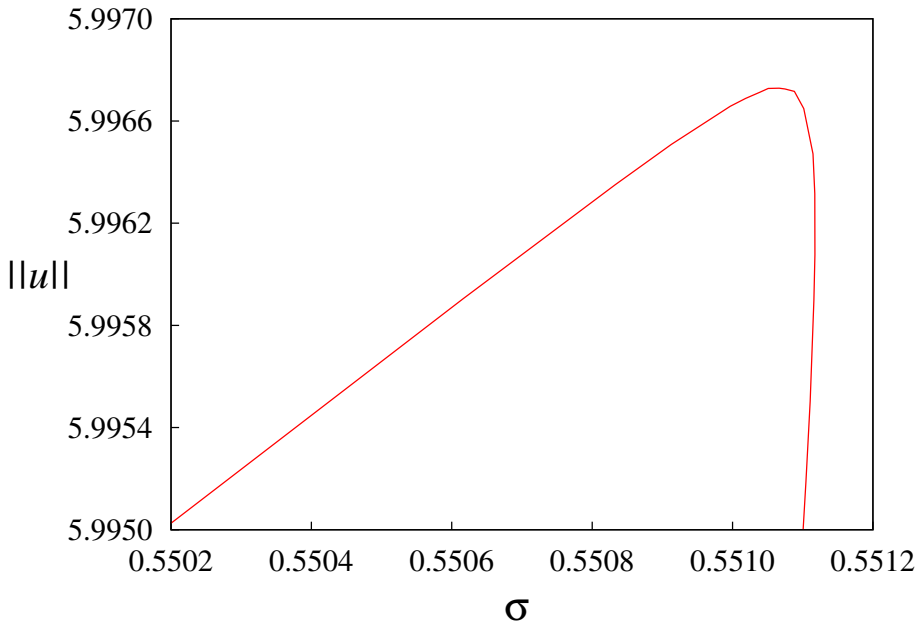








Continuation of periodic orbits by multiple shooting

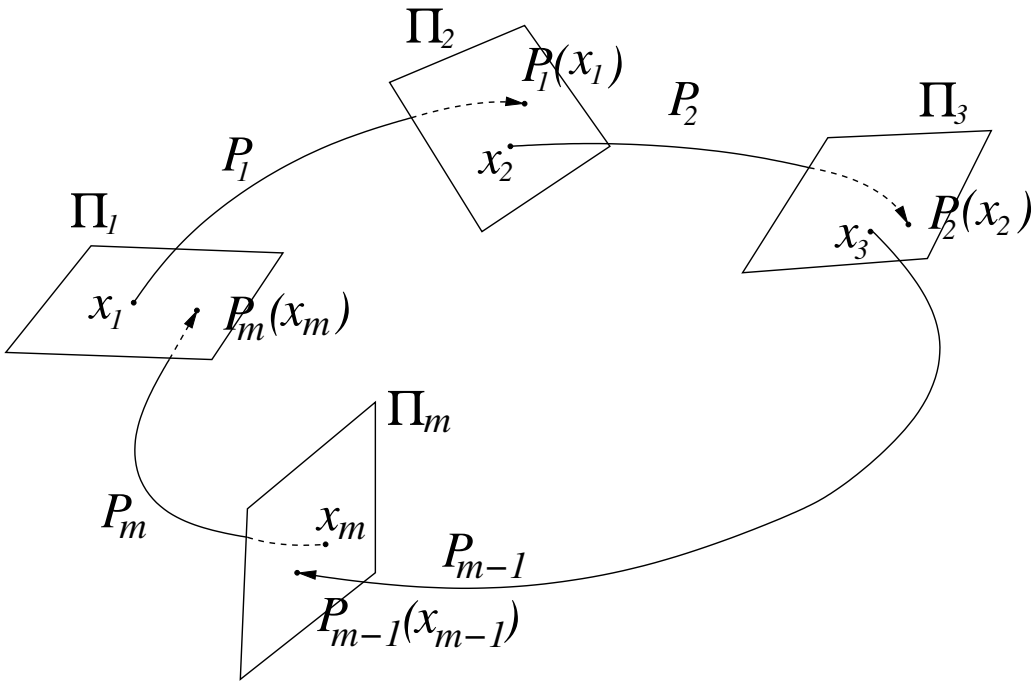
Computation of periodic orbits by parallel multiple shooting

Consider a system of autonomous differential equations

$$\dot{x} = f(x,p), \quad (x,p) \in \mathcal{U} \times I \subset \mathbb{R}^{n+1},$$

m hyperplanes Π_i intersecting transversally an initial periodic orbit, the partial Poincaré maps P_i $(i = 1 \cdots, m)$, and the Poincaré map on Π_1, P. They satisfy

$$P(x_1,p) = (P_m \circ P_{m-1} \circ \cdots \circ P_1)(x_1,p),$$



if $x_{i+1} = P_i(x_i,p)$, $i = 1, \cdots, m-1$,

$$D_x P(x_1,p) = D_x P_m(x_m,p) D_x P_{m-1}(x_{m-1},p) \cdots D_x P_1(x_1,p).$$

We also define $X = (x_1, \cdots, x_m) \in \mathbb{R}^{mn}$, and the map $\mathcal{G}$ as

$$\mathcal{G}(X,p) = (x_1 - P_m(x_m,p), x_2 - P_1(x_1,p), \cdots, x_m - P_{m-1}(x_{m-1},p)).$$

The points $x_1, \cdots, x_m$ are on a periodic orbit if $\mathcal{G}(X,p) = 0$.

Continuation and the Newton-Krylov method

The equation $\mathcal{G}(X,p)=0$ is completed with

$$U^\top (X-X_0)+u_p(p-p_0)=0,$$

(X_0,p_0) being the prediction of a new point on the curve of solutions, and (U,u_p) an approximation of the tangent with $U=(u_1,\cdots,u_m)$. Setting $U=0$ and $u_p=1$ leads to parameter continuation.

The system is solved by Newton's method and the linear systems by Krylov matrix-free methods (GMRES in our case), which only require computing the action by the Jacobian of the system

$$\begin{pmatrix} D_X\mathcal{G} & D_p\mathcal{G} \\ U^\top & u_p \end{pmatrix} = \begin{pmatrix} I & \dots & \dots & 0 & -A_m & -b_m \\ -A_1 & I & & \vdots & 0 & -b_1 \\ 0 & \ddots & \ddots & & \vdots & \vdots \\ & & & & & \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & -A_{m-1} & I & -b_{m-1} \\ u_1^\top & \dots & u_{m-2}^\top & u_{m-1}^\top & u_m^\top & u_p \end{pmatrix},$$

with $A_i = D_x P_i(x_i,p)$, and $b_i = D_p P_i(x_i,p)$.

The computation of

$$\mathcal{G}(X,p) = (x_1 - P_m(x_m,p), x_2 - P_1(x_1,p), \cdots, x_m - P_{m-1}(x_{m-1},p)).$$

involves the time integration of $\dot{x} = f(x,p)$ with m initial conditions $x(0) = x_i$.

The computation of the action of $D\mathcal{G}(X,p)$ on $(V,\mu) = (v_1, \cdots, v_m, \mu)$,

$$D\mathcal{G}(X,p)(V,\mu) =$$
$$(v_1 - DP_m(x_m,p)(v_m,\mu), v_2 - DP_1(x_1,p)(v_1,\mu), \cdots, v_m - DP_{m-1}(x_{m-1},p)(v_{m-1},\mu))$$

is also trivially parallelizable, and involves the time integration of the system of first variational equations (for a vector)

$$\dot{v} = D_x f(x,p)v + D_p f(x,p)\mu,$$

with initial conditions $v(0) = v_i$, together with the original system $\dot{x} = f(x,p)$, with initial conditions $x(0) = x_i$.

Only systems of at most $2n$ equations must be integrated.

Speedup and efficiency

Let $T(m,k)$ be the wall-clock time required to do a continuation with m sections, with each partial shoot computed on a different processor, and using a preconditioner (to be defined later) based on an invariant subspace of dimension mk ($k=0$ means no preconditioning).

The (absolute) speedup is defined as

$$S(m,k) = T_{ref}/T(m,k), \quad \text{(the goal is} \quad S(m,k) = m)$$

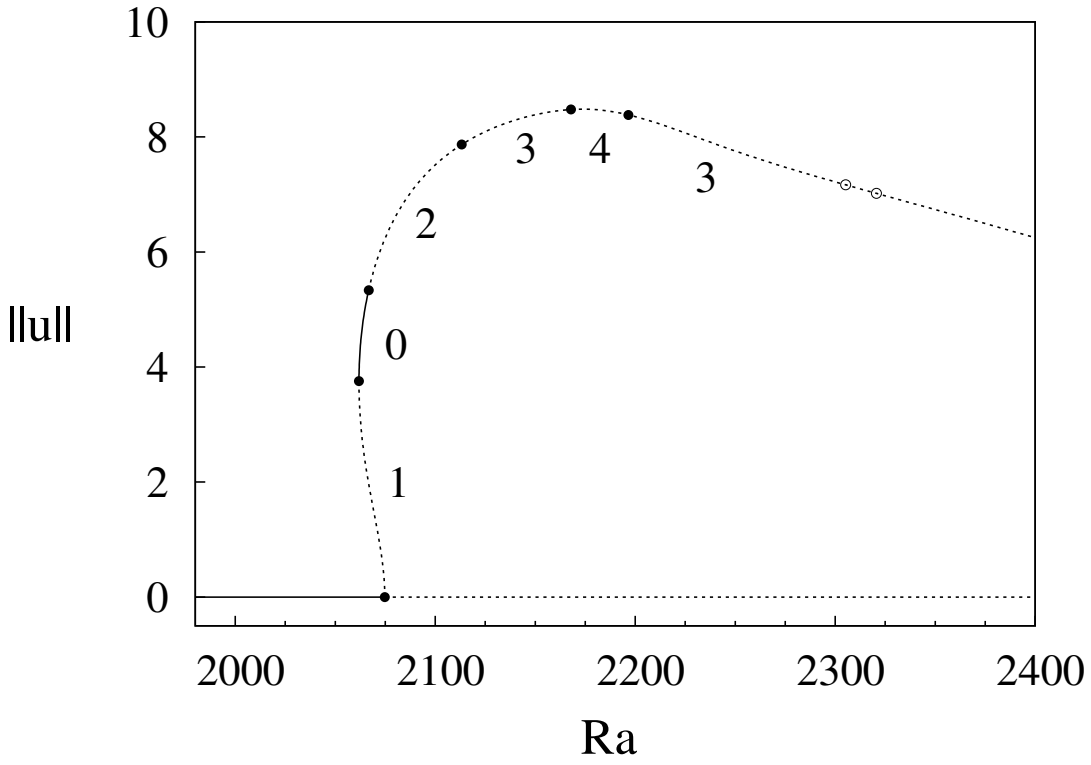
T_{ref} being the wall-clock time of the best algorithm without using parallelism. We have taken $T_{ref} = T(1,0)$.

The efficiency is

$$E(m,k) = S(m,k)/m \quad \text{(the goal is} \quad E(m,k) = 1).$$

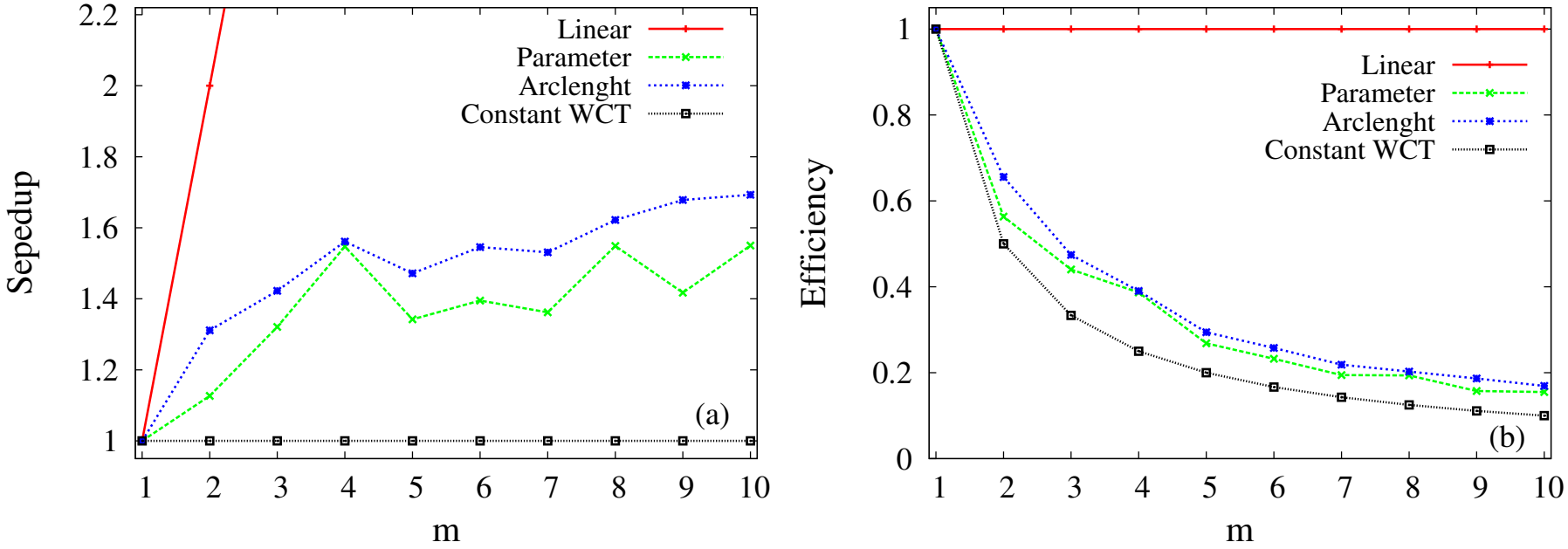
Bifurcation diagram (main branch of periodic orbits)

The full circles indicate bifurcation points, and the empty circles the point at which the continuation is started in the numerical experiments ($Ra = 2320$), and that at which the preconditioner has been computed ($Ra = 2305$).



Solid and dashed lines mean stable and unstable branches, respectively. The labels beside the branch of periodic orbits indicate the number of multipliers outside the unit circle.

Results for the unpreconditioned computations



(a) Speedup, and (b) efficiency versus the number of sections m corresponding to the computation of five points without preconditioning, and starting at $Ra = 2320$.

Block cyclic matrices I

Consider the matrices

$$\mathcal{A} = \begin{pmatrix} 0 & \dots & \dots & 0 & A_m \\ A_1 & \ddots & & & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & A_{m-1} & 0 \end{pmatrix},$$

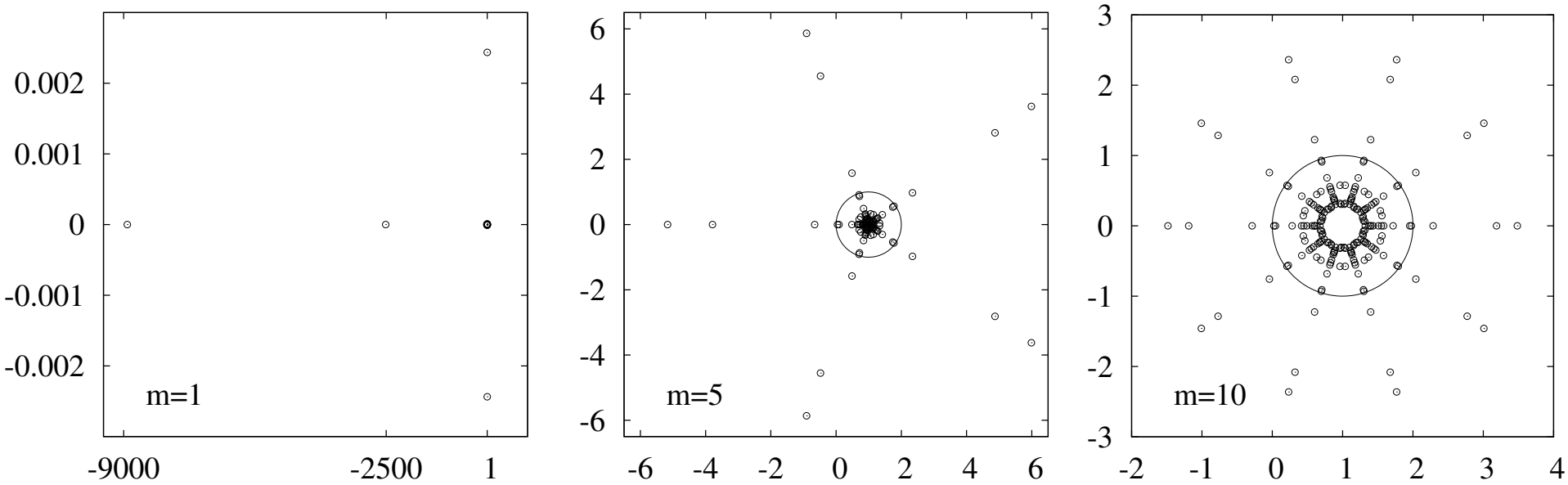
$A = A_m A_{m-1} \cdots A_1$, with $\mathcal{A} \in \mathbb{R}^{mn \times mn}$, and $A_i \in \mathbb{R}^{n \times n}$.

Proposition. *If A and $\mathcal{A}$ are defined as above then*

a) if (μ, V) is an eigenpair of $\mathcal{A}$, with $\mu \in \mathbb{C}$, and $V = (v_1, \cdots, v_m)^\top$ with $v_i \in \mathbb{C}^n$ $(i = 1, \cdots, m)$, then (μ^m, v_1) is an eigenpair of A.

b) if (λ, u_1) is an eigenpair of A, with $\lambda \in \mathbb{C}$ and $u_1 \in \mathbb{C}^n$, and if $\mu^m = \lambda$, then (μ, V), with $V = (\mu^{m-1}u_1, \mu^{m-2}u_2, \cdots, \mu u_{m-1}, u_m)^\top$, and $u_{i+1} = A_i u_i$ $(i = 1, \cdots, m-1)$, is an eigenpair of $\mathcal{A}$.

This result states that the eigenvalues of $\mathcal{A}$ are placed on circles centered at the origin, and then, those of $\mathcal{I} - \mathcal{A}$ on circles centered at $+1$.



Leading eigenvalues of $\mathcal{I} - \mathcal{A}$ for $m = 1$, $m = 5$, and $m = 10$ at $Ra = 2305$. The closed curve is the unit circle centered at $+1$.

Preconditioners based on leading invariant subspaces (deflation)

Let $Cx = b$ be a linear system with non-singular matrix $C \in \mathbb{R}^{n\times n}$. We look for a right preconditioner, M such that the convergence of the iterative methods applied to

$$CM^{-1}y = b, \quad x = M^{-1}y,$$

be faster. We assume that most of the spectrum of C is clustered around $+1$.

Let the columns of $Q = [q_1, \cdots, q_k] \in \mathbb{R}^{n\times k}$ form an orthonormal basis of an invariant subspace of C corresponding to the first k leading (maximal distance to $+1$) eigenvalues of C, with $Q^\top Q = I_k$, and $k \ll n$. The matrix Q verifies

$$CQ = QR, \quad \text{and} \quad C^{-1}Q = QR^{-1},$$

with R an invertible $k \times k$ matrix. Then, we define $M = QRQ^\top + (I - QQ^\top)$.

- $M^{-1} = QR^{-1}Q^\top + (I - QQ^\top)$
- $M^\top = QR^\top Q^\top + (I - QQ^\top)$, and $(M^\top)^{-1} = Q(R^\top)^{-1}Q^\top + (I - QQ^\top)$
- $CM^{-1} = QQ^\top + C(I - QQ^\top)$
- If $z = z_1 + z_2$ with $z_1 \in Span\{q_1, \cdots, q_k\}$, and $z_2 \in Span\{q_1, \cdots, q_k\}^\perp$,

$$CM^{-1}z = z_1 + Cz_2.$$

In the case of multiple shooting we need a preconditioner for $(\mathcal{I} - \mathcal{A})X = B$.

Block cyclic matrices II

Proposition. *Let the matrix $Q_1 \in \mathbb{R}^{n\times k}$, with $Q_1^\top Q_1 = I_k$, be such that $AQ_1 = Q_1 R$ is a partial real Schur decomposition of $A = A_m A_{m-1}\cdots A_1$. Let $Q_{i+1} \in \mathbb{R}^{n\times k}$, and $R_i \in \mathbb{R}^{k\times k}$, $i = 1, \cdots, m-1$, form a partial periodic real Schur decomposition of A, defined by*

$$A_i Q_i = Q_{i+1} R_i, \quad \text{and}$$

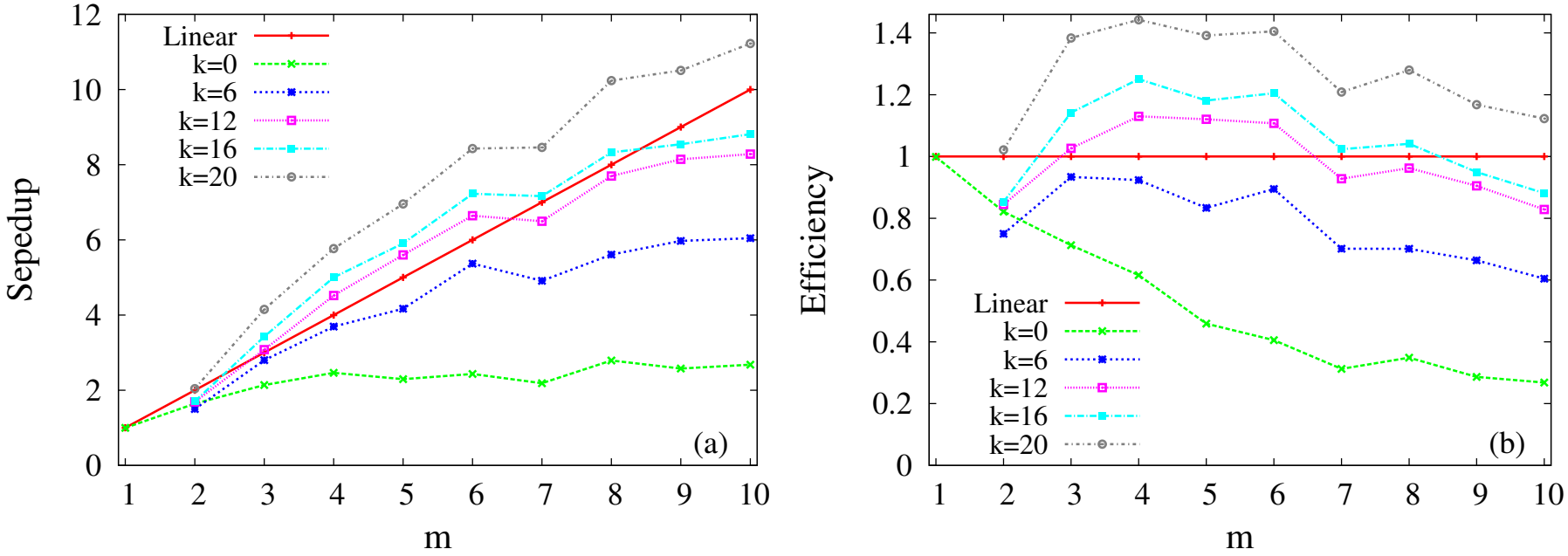
$$R_m = Q_1^\top A_m Q_m.$$

Then it follows that $R = R_m R_{m-1}\cdots R_2 R_1$, and if

$$\mathcal{Q} = \begin{pmatrix} Q_1 & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & Q_m \end{pmatrix}, \quad \text{and} \quad \mathcal{R} = \begin{pmatrix} 0 & \cdots & \cdots & 0 & R_m \\ R_1 & \ddots & & & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & R_{m-1} & 0 \end{pmatrix},$$

with $\mathcal{Q} \in \mathbb{R}^{mn\times mk}$ and $\mathcal{R} \in \mathbb{R}^{mk\times mk}$, then $\mathcal{A}\mathcal{Q} = \mathcal{Q}\mathcal{R}$ and $(\mathcal{I} - \mathcal{A})\mathcal{Q} = \mathcal{Q}(\mathcal{I} - \mathcal{R})$, i.e., the columns of $\mathcal{Q}$ form an orthonormal basis of an invariant subspace, of dimension mk, of $\mathcal{A}$ and of $\mathcal{I} - \mathcal{A}$.

Results for the preconditioned computations



Parameter continuation of an interval of 15 units in Ra without limitation of the step size. (a) Speedup, and (b) efficiency.

Preconditioners for the multiple shooting

The matrices of the linear systems corresponding to pseudo-arclength and parameter continuation are

$$\begin{pmatrix} D_X\mathcal{G} & D_p\mathcal{G} \\ U^\top & u_p \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} D_X\mathcal{G} & 0 \\ 0 & 1 \end{pmatrix},$$

with $D_X\mathcal{G} = \mathcal{I} - \mathcal{A}$. If M is a preconditioner for $D_X\mathcal{G}$ the systems can be preconditioned with

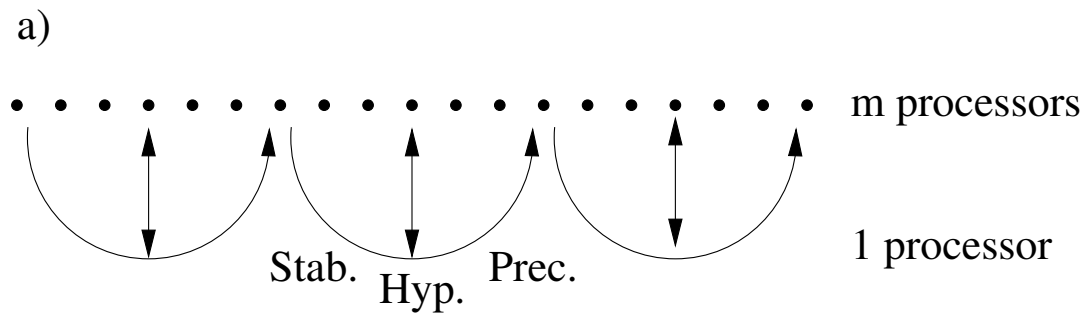
$$\begin{pmatrix} M & D_p\mathcal{G} \\ U^\top & u_p \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} M & 0 \\ 0 & 1 \end{pmatrix}.$$

The former is a bordered system, which can be solved in a stable way by the BEM algorithm. It requires solving systems with M and $M^\top$, and to know explicitly the column $D_p\mathcal{G} = -D_p\mathcal{P}$. It can be obtained by integrating the first variational equations with initial conditions $v(0) = 0$, and $\mu(0) = 1$.

The continuation and preconditioning process

There are two possible straightforward ways of linking the continuation and the updating of the preconditioner processes.

a) m processors are used to compute the periodic orbits and another one is updating the preconditioner.



b) The m processors are used to do both tasks.