Continuation methods for dissipative partial differential equations. Theory.

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Overview

- Equilibria and periodic orbits of PDEs
- Newton-Krylov continuation methods
- Inexact Newton methods
- Iterative linear solvers and GMRES
- Stability
- An example

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 regims 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.

Continuation of zeros of a nonlinear system of equations

Consider a system of nonlinear equations depending on a parameter p

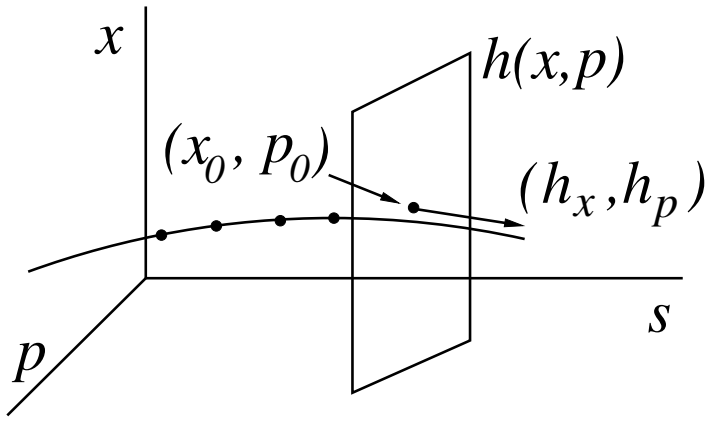
$$H(x,p)=0, \quad (x,p)\in\mathcal{U}\subset\mathbb{R}^m\times\mathbb{R}$$

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

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 $\delta p = \delta D$,

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

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* $x^* \subset \mathbb{R}^n$. *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* $x^* \subset \mathbb{R}^n$. *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 neiborhood 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*

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

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 algebra.

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

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

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:

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

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 $V_k = [v_1, \ldots, v_k]$. Then if $x = x_0 + V_k y \in x_0 + \mathcal{K}_k$ with $y \in \mathbb{R}^k$ and

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

The orthonormal basis is found by means of the Arnoldi factorization.

1. Start: Choose as initial unitary vector $v_1 = r_0/\|r_0\|$, and set $\beta = \|r_0\|$.
2. Set the $(k+1) \times k$ matrix $\tilde{H}_k = \{h_{i,j}\}$ to zero.
3. Iterate: for $j = 1, 2, \ldots, k$ do
   (a) compute Av_j
   (b) $h_{i,j} = \langle Av_j, v_i \rangle$, $i = 1, 2, \ldots, j$
   (c) $w_j = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$ (Gram-Schmidt orthogonalization)
   (d) $h_{j+1,j} = \|w_j\|$, if $h_{j+1,j} = 0$ stop
   (e) $v_{j+1} = w_j/\|w_j\|$

If $V_k = [v_1, \ldots, v_k]$ 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 $\tilde{H}_k$ is the $(k+1) \times k$ matrix whose nonzero entries are the $h_{i,j}$ then

$$AV_k = V_{k+1} \tilde{H}_k \quad \text{or} \quad AV_k = V_{k+1} H_k + w_k e_k^\top$$

  where $w_k = h_{k+1} v_{k+1}$, and H_k is $\tilde{H}_k$ without the last row.

Now

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

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

The complete restarted version of the algorithm GMRES(m) is then

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) Set the $(k + 1) \times k$ matrix $\tilde{H}_k = \{h_{i,j}\}$ to zero.
   (c) Iterate: for $j = 1, 2, \ldots, k$ do
   (d) compute Av_j
   (e) $h_{i,j} = \langle Av_j, v_i \rangle$, $i = 1, 2, \ldots, j$,
   (f) $w_j = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$, (Gram-Schmidt orthogonalization)
   (g) $h_{j+1,j} = \|w_j\|$, if $h_{j+1,j} = 0$ stop
   (h) $v_{j+1} = w_j/\|w_j\|$
   (i) find y_k the minimizer of $\|\beta e_1 - \tilde{H}_k y\|_2$
   (j) set $\rho = \|\beta e_1 - \tilde{H}_k y_k\|_2$
4. if $\rho < \varepsilon$ then set $x_k = x_0 + V_k y_k$ as approximate solution and exit
5. if $l > l_{max}$ (to many iterations without convergence) exit
6. if $k = m$ set $x_0 = x_k$, $r_0 = b - Ax_0$ 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 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,

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

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

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

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

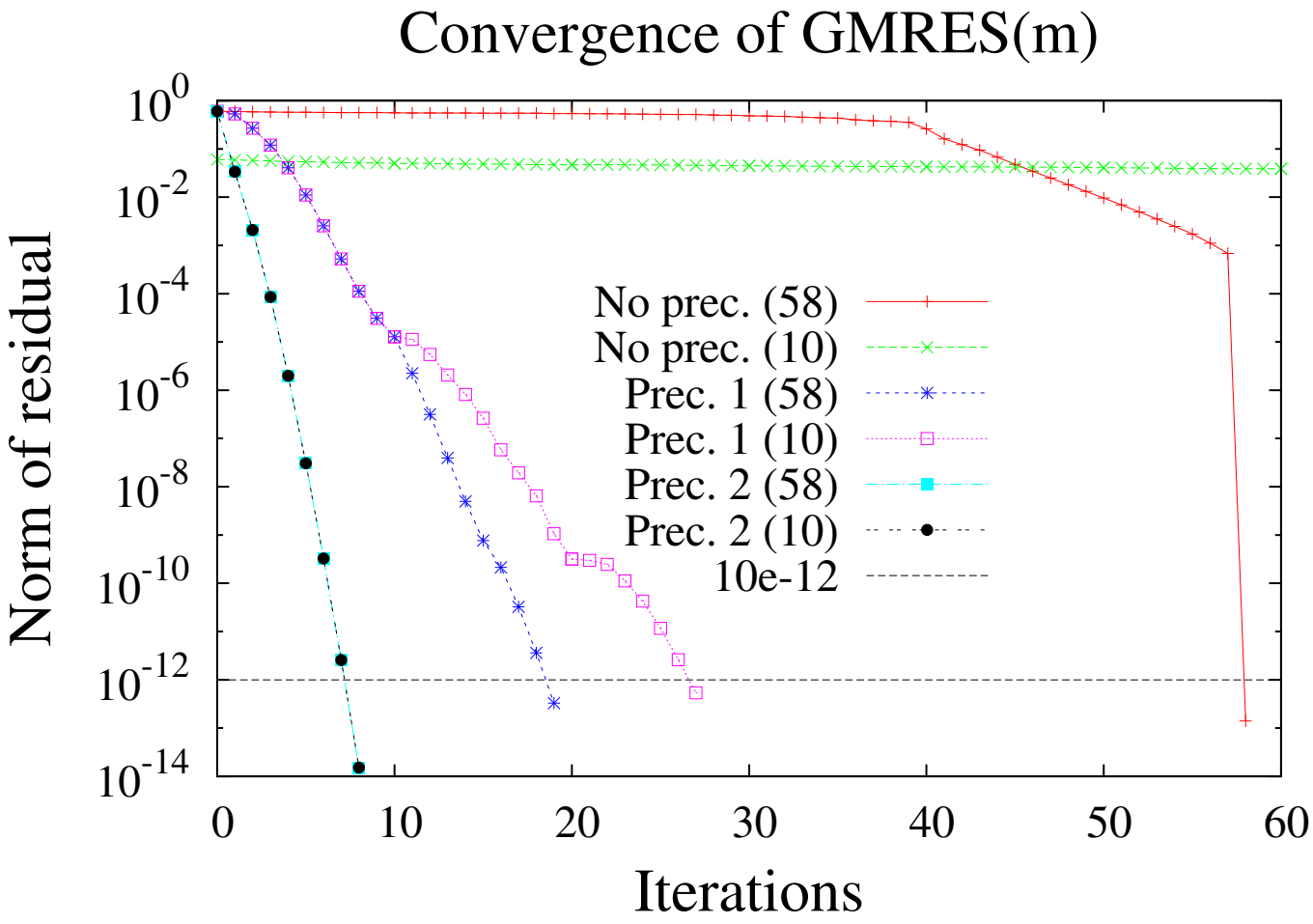
Two possible preconditioners are

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

and

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

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 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.

Eigenvalue problems

Two main methods ar available to obtain the leading (largest magnitude) eigenvalues of a $n \times n$ large-scale $(n \gg 1)$ matrix A.

Subspace iteration (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. For I=1,. . . , k do
   (a) Compute $Z_m = AV_m$
   (b) Orthonormalize Z_m by computing $Z_m = Q_m R_m$, and set $V_m = Q_m$
3. Form $B_m = V_m^T A V_m$ and compute the eigenpairs (λ_i, z_i), $i = 1, \cdots, m$ of B_m by the QR method (LAPACK).
4. Test for convergence of eigenvalues and/or eigenvectors
5. 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. If not go to 2.

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 k is large enough, then 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 $\varepsilon_{i,k} = 0$.

Eigenvalue problems

Arnoldi's method (implemented, for instance, in ARPACK).

1. Start: Choose an initial unitary vector v_1.
2. Iterate: Until convergence do:
   (a) Compute the Arnoldi factorization $AV_m = V_m H_m + w_m e_m^T$ 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 $H_m = V_m^T A V_m$ 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 $A - \xi I$.

The Arnoldi factorization

1. Start: Choose an initial unitary vector v_1.
2. Iterate: for $j = 1, 2, \ldots, m$ compute
   (a) $h_{i,j} = \langle Av_j, v_i \rangle$, $i = 1, 2, \ldots, j$,
   (b) $w_j = Av_j - \sum_{i=1}^{j} h_{i,j} v_i$, (Gram-Schmidt orthogonalization)
   (c) $h_{j+1,j} = \|w_j\|$, if $h_{j+1,j} = 0$ stop
   (d) $v_{j+1} = w_j / h_{j+1,j}$

If $V_m = [v_1, \ldots, v_m]$ then

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

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

Proposition. *Let $y_{i,m}$ be an eigenvector of H_m associated with the eigenvalue $\lambda_{i,m}$, and $u_{i,m} = V_m y_{i,m}$ the Ritz approximate eigenvector of A. Then,*

$$(A - \lambda_{i,m} I) u_{i,m} = h_{m+1,m} e_m^T y_{i,m} v_{m+1}$$

and, therefore

$$\|(A - \lambda_{i,m} I) u_{i,m}\|_2 = h_{m+1,m} |e_m^T y_{i,m}|.$$

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 $\sigma = \rho + i\theta$,

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

- 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 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

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

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

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

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

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,

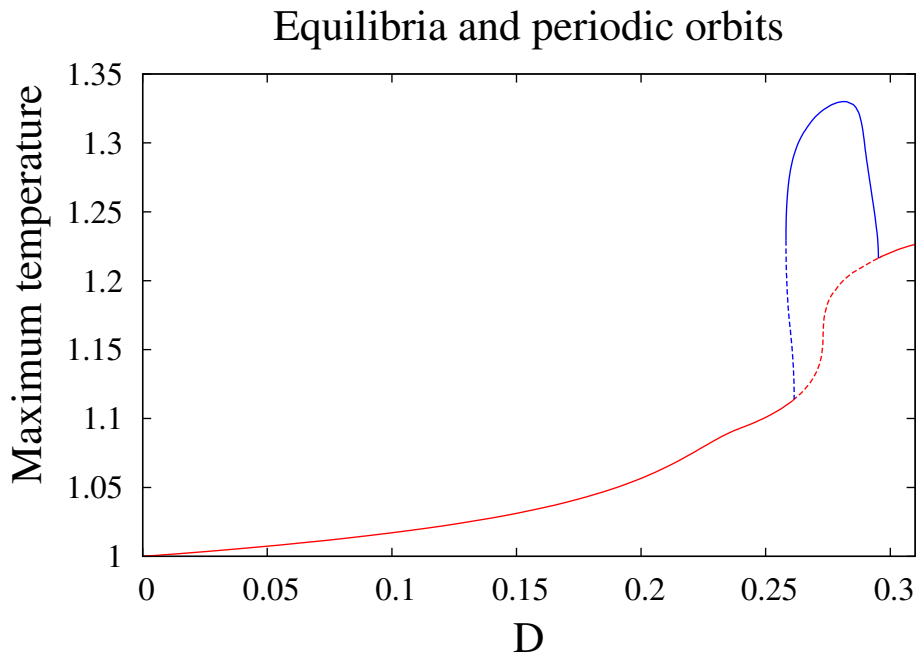
$$\begin{aligned} \dot{y} &= f(y,p) \\ \dot{y}_1 &= D_y f(y,p)y_1 + D_p f(x,p)\delta p \end{aligned} \qquad \text{with initial conditions} \qquad \begin{aligned} y(0) &= x \\ y_1(0) &= \delta x. \end{aligned}$$

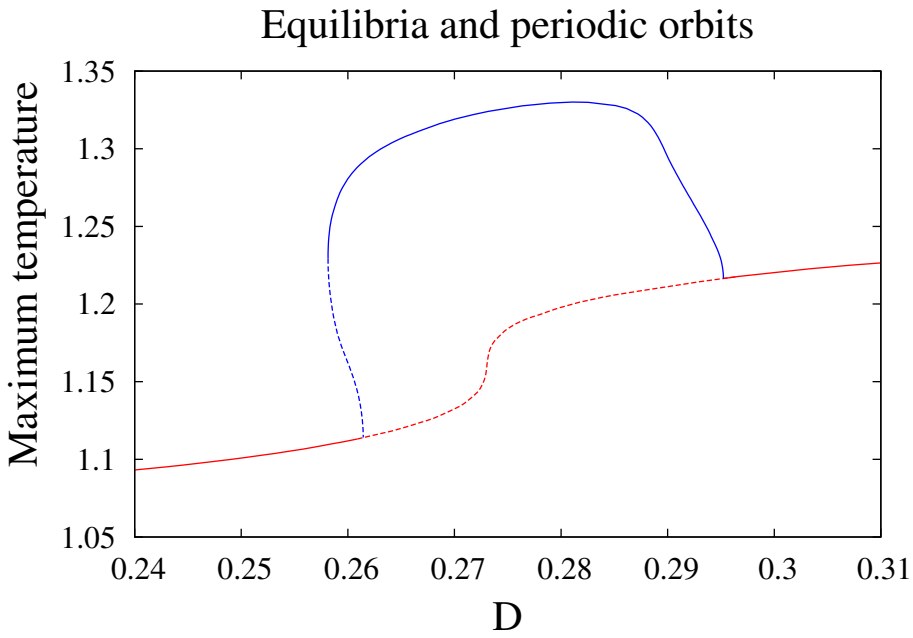
Finally

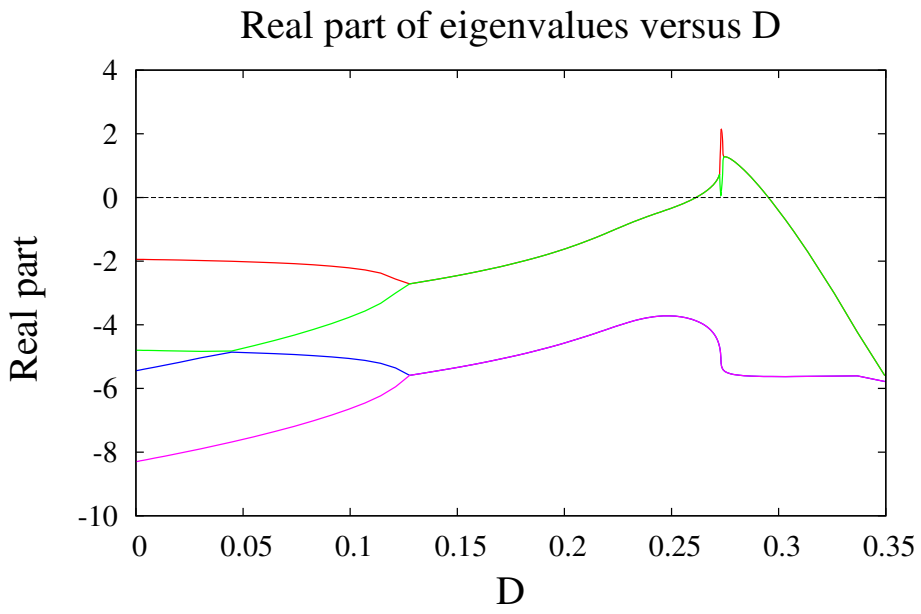
$$D_x\varphi(T,x,p)\delta x + D_p\varphi(T,x,p)\delta p = y_1(T).$$

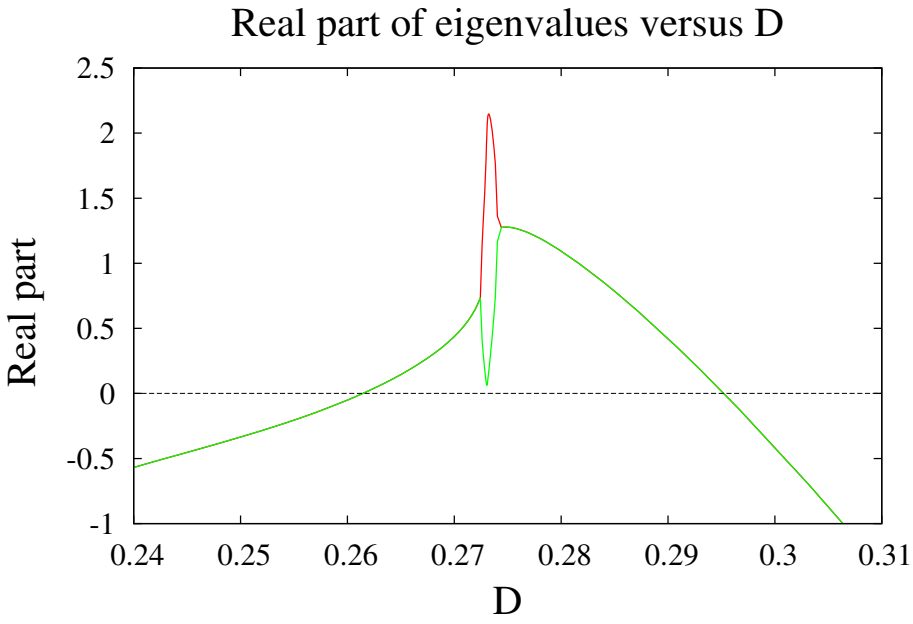
Results for the HP problem

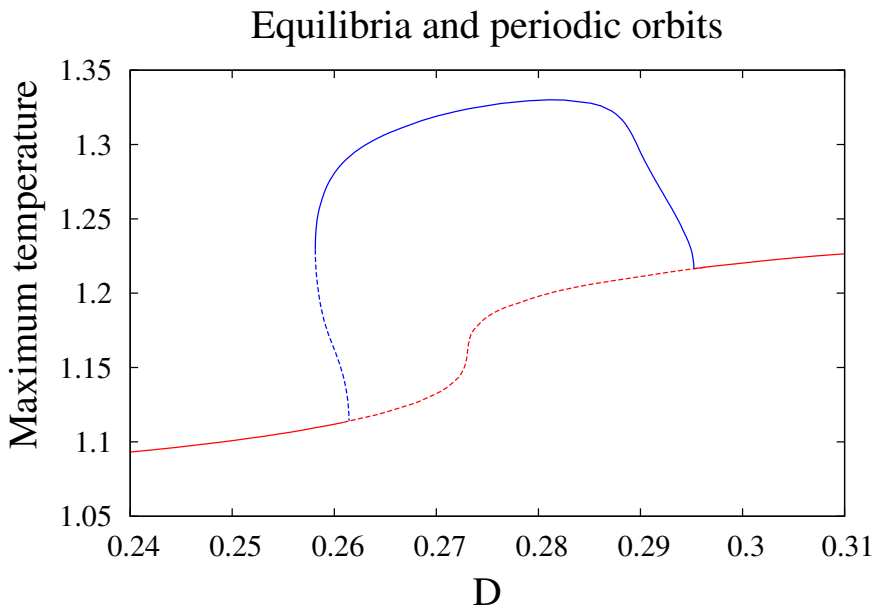
In this example $Pe_m = Pe_h = 5$, $B = 0.5$, $\gamma = 25$, $\beta = 3.50$, and $\theta_r = 1$.










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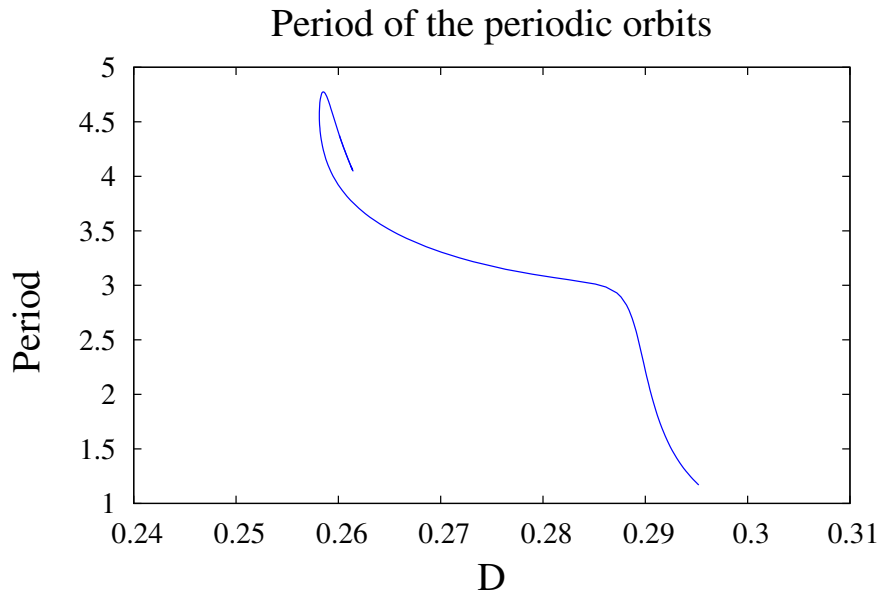
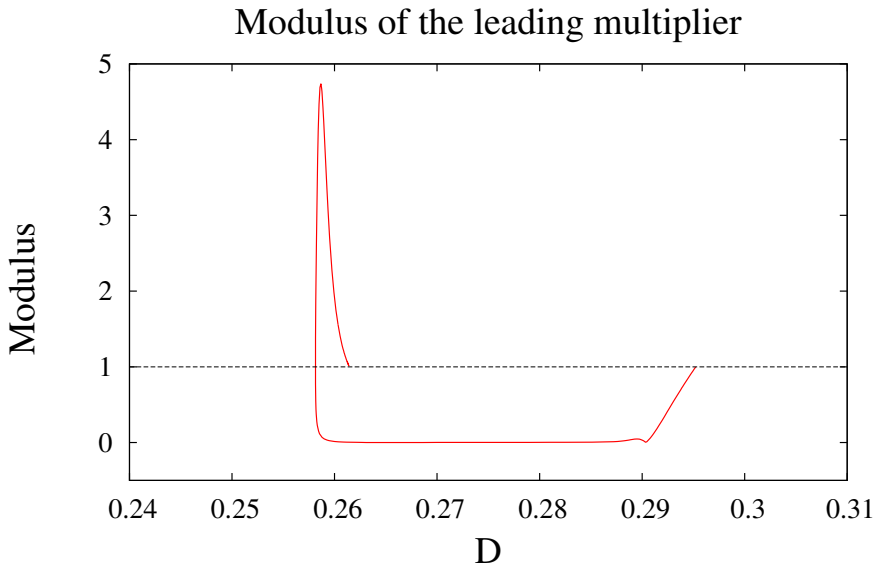
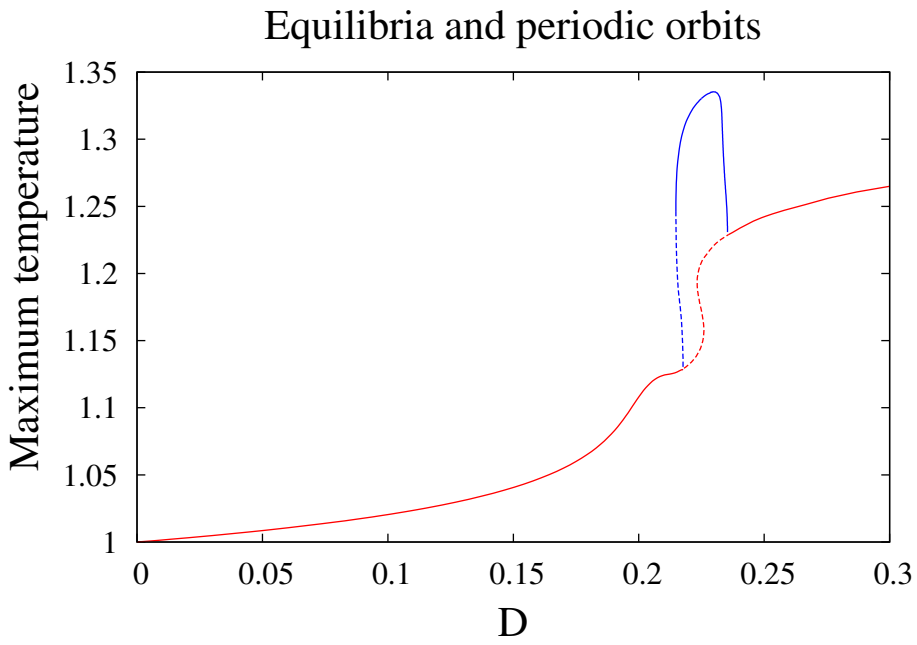
1.3
1.25
1.2
1.15
1.1
1.05
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
D

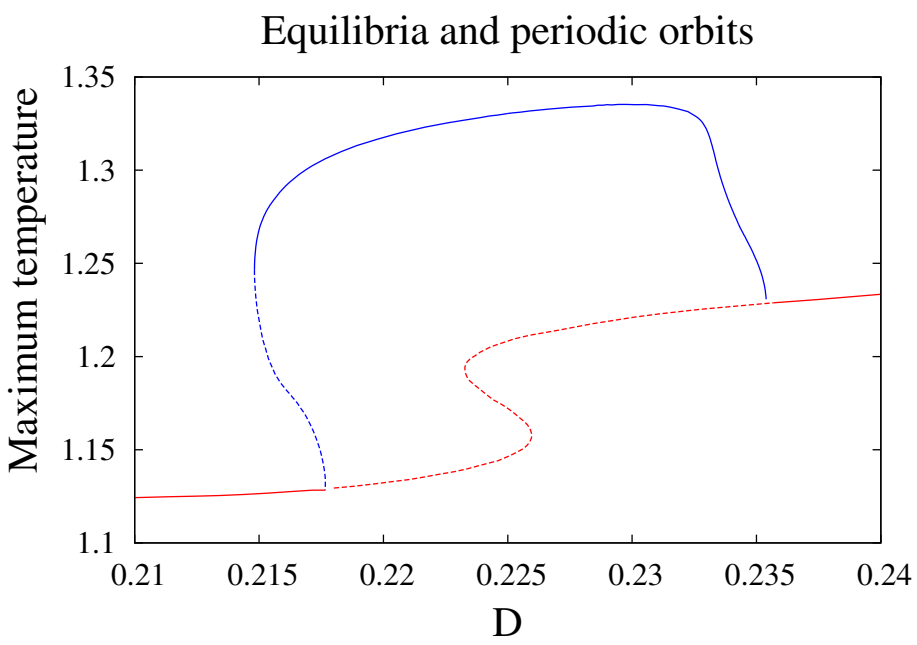

Period of the periodic orbits
Period
5
4.5
4
3.5
3
2.5
2
1.5
1
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
D

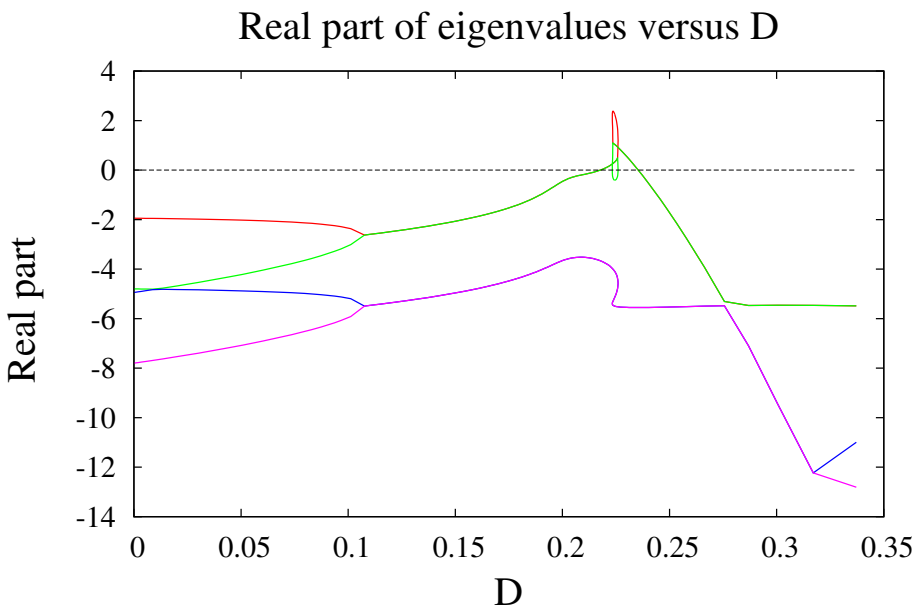

Modulus of the leading multiplier
Modulus
5
4
3
2
1
0
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
D

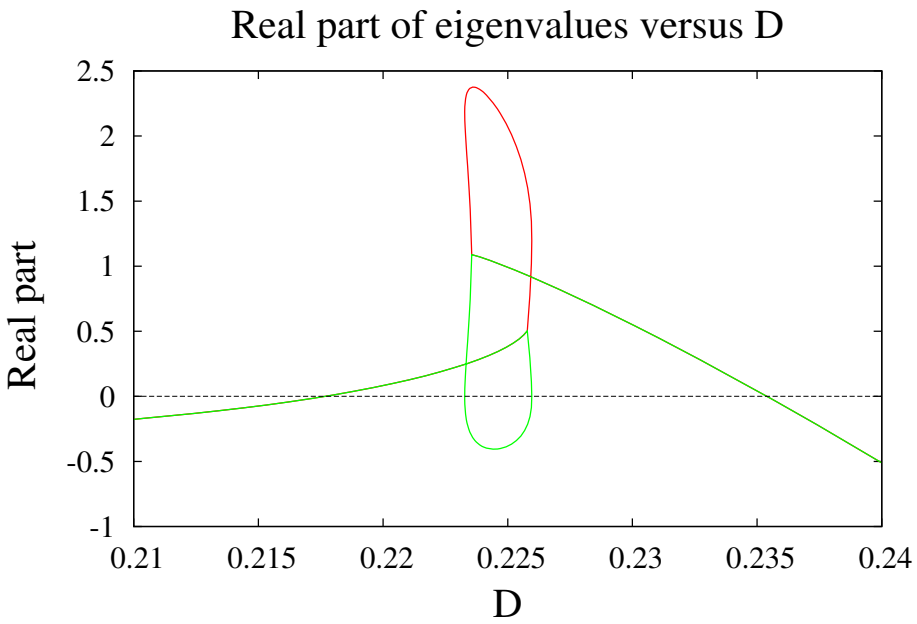
Results for the HP problem

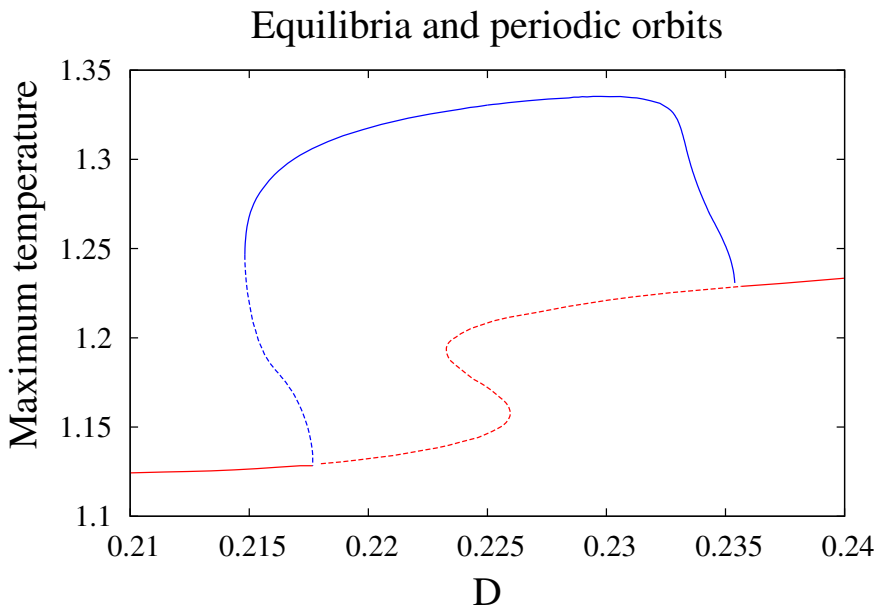
In this example $Pe_m = Pe_h = 5$, $B = 0.5$, $\gamma = 25$, $\beta = 3.00$, and $\theta_r = 1$.

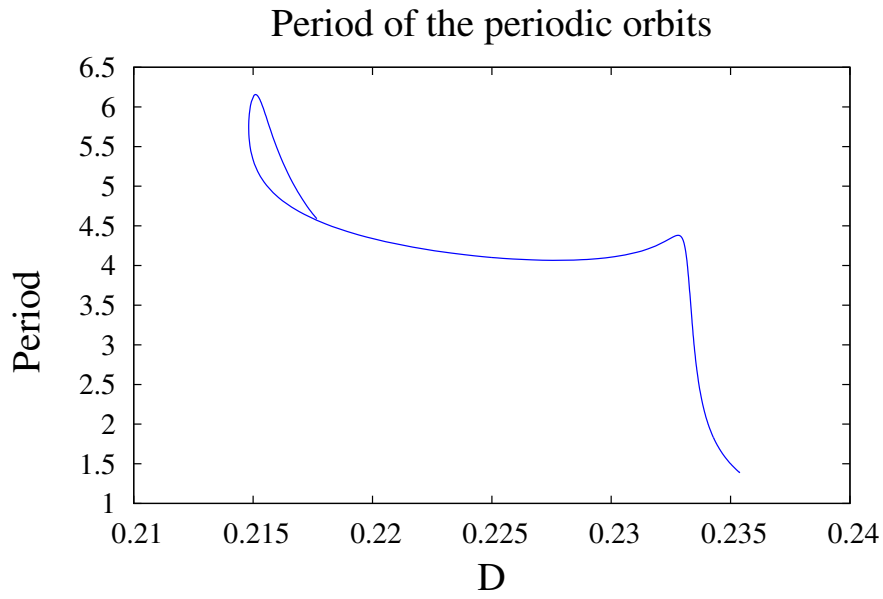


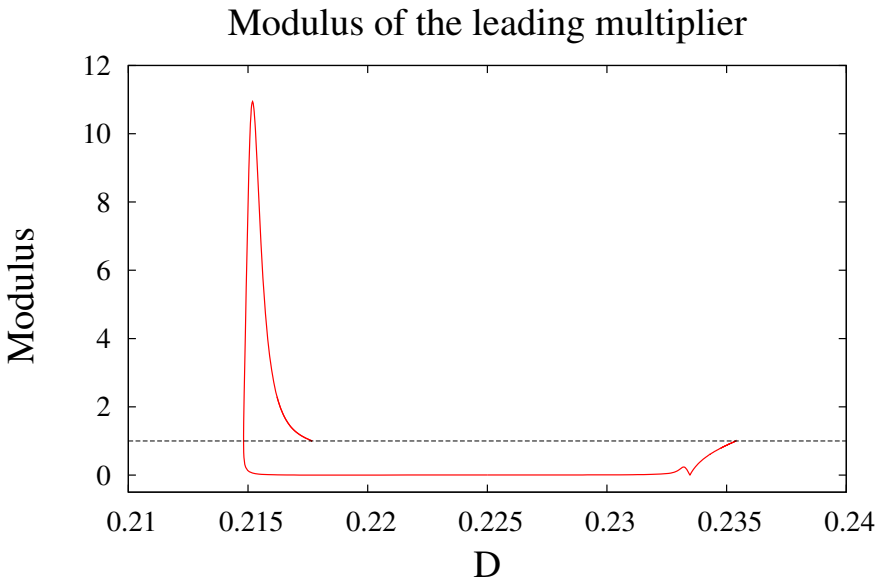







Equilibria and periodic orbits
Maximum temperature
1.35
1.3
1.25
1.2
1.15
1.1
0.21
0.215
0.22
0.225
0.23
0.235
0.24
D


Period of the periodic orbits
Period
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
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

Other objects which have been computed by Newton-Krylov methods

- Periodic orbits by multiple shooting.
- Two-dimensional invariant tori.
- Curves of codimension-one bifurcations of equilibria and periodic orbits.

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