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SMOOTH SCHUR FACTORIZATIONS IN THE CONTINUATION OF SEPARATRICES

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ABSTRACT. Numerical computation of separatrices as general connecting orbits in dynamical systems is performed, and their continuation as problem parameters vary is approached via a direct application of smooth block Schur factorizations of Jacobians and monodromy matrix functions. Several numerical examples are presented to illustrate the effectiveness of the algorithms used.

1. INTRODUCTION

The importance of constant matrix factorizations cannot be overstressed. They are very useful not only within matrix computations and linear algebra contexts, but they have also found several applications in areas beyond mathematics. The factorization of more general matrices depending on some parameters is by no means less important. In particular, it has been proved to be essential for the computation and continuation of special solutions in dynamical systems, among other applications. We mention the work by Dieci and Eirola [1] as a main source of such factorizations, where a thorough study of several orthogonal decompositions of matrix functions is made, including Schur, QR and SVD, and potential applications are pointed out such as orthonormalization for boundary value problems, computation of Lyapunov exponents, solution of Riccati equations and continuation of connecting orbits. Based on [1], an algorithm for the continuation of invariant subspaces is developed in [2], by applying smooth block Schur factorizations.

In [3], a sound theoretical study is presented, establishing connecting orbits in dynamical systems as solutions of well-posed problems. As a direct application of the work in [2], and using the theory developed in [3], a general algorithm for the computation and continuation of connecting orbits between hyperbolic equilibria and periodic orbits in dynamical systems is constructed in [4], and a truncation error analysis is provided. Following the work in [4], several types of traveling waves (pulses, traveling fronts, etc) solutions to partial differential equations are computed in [5] within the framework of parametrized ordinary differential equations, after appropriate changes of coordinates, and several applications are considered.

Although numerical computation and continuation can readily be performed for point-to-point connections (e.g. [6]), the general numerical computation of homoclinic and heteroclinic connections between periodic orbits is relatively new. The implementation of the algorithms proposed in [4], which deal with connections between equilibria and connecting orbits, have been improved here (see details below), allowing continuation for larger variations of the parameters, and are used in this work to perform such computations. In addition, some

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connections will be monitored through continuation as parameters vary, providing us with a tool for the detection of qualitative behavior changes of some periodic orbits, as illustrated in the numerical examples.

The computation of general connecting orbits establishes the existence of separatrices in the phase portrait of the dynamical system, providing a better understanding of the global behavior of solutions. In addition, the information provided by the computed periodic orbits and the continuation of both solutions through smooth block Schur matrix factorizations are essential for the qualitative description of solutions of parametrized dynamical systems.

2. Smooth block Schur factorizations

Matrix factorizations play a central role in matrix computations and linear algebra in general, and orthogonal matrices are the ideal matrices to be used in numerical computations due to its stability properties, which oversimplifying means errors are not magnified. We are interested in block Schur (orthogonal) factorizations of real matrices that depend on a real parameter; that is, given a smooth matrix function \( A : \mathbb{R} \to \mathbb{R}^{m \times m} \), we want to find smooth matrix functions \( Q(\lambda) \) and \( R(\lambda) \) such that \( A(\lambda) = Q(\lambda)R(\lambda)Q^T(\lambda) \), with \( Q \) orthogonal and \( R \) block upper triangular.

These factorizations become an essential tool when solving the boundary value problems that define connecting orbits. This is so, because the imposed projection boundary conditions will require us to find a set of vectors that span the center-stable or center-unstable vector subspaces of the Jacobian at an equilibrium point, or that of the monodromy matrix associated with a periodic orbit. Once the Jacobian and/or monodromy matrices are computed, we find not just a spanning set of vectors of those subspaces, but one with orthonormal vectors. These orthonormal sets of vectors (the columns of the matrix function \( Q \) above, with \( A \) playing the role of the Jacobian or the monodromy matrix) are found precisely with block Schur factorizations of the Jacobian and/or the monodromy matrices.

The precise statement about smooth block Schur factorizations and the proofs (for general complex matrix functions) can be found in [1]. We remark that two conditions are required for such a factorization to exist: there has to exist an initial factorization of the required form, and the eigenvalues of the matrix \( A \) have to be split in two disjoint sets for all values around the initial parameter. This is in fact not much to require from a matrix function that arises from a hyperbolic equilibrium point or a hyperbolic periodic orbit.

**Theorem 2.1.** ([1]) Let \( A \in C^k(\mathbb{R}, \mathbb{R}^{m \times m}) \). Assume that for some initial \( \lambda = \lambda_0 \) there exists an orthogonal matrix \( Q_0 \) such that \( Q_0^T A(\lambda_0) Q_0 = \begin{pmatrix} R_{11}(\lambda_0) & R_{12}(\lambda_0) \\ 0 & R_{22}(\lambda_0) \end{pmatrix} \). Assume also that \( A(\lambda) \) has two disjoint sets \( \sigma_1(\lambda), \sigma_2(\lambda) \) of eigenvalues for all \( \lambda \) around \( \lambda_0 \). Then, \( A(\lambda) \) has a \( C^k \)-block Schur factorization, for all \( \lambda \) around \( \lambda_0 \), with the blocks corresponding to those two groups of eigenvalues, i.e. there is an orthogonal \( Q(\lambda) \in C^k(\mathbb{R}, \mathbb{R}^{m \times m}) \) such that

\[
Q(\lambda)^T A(\lambda) Q(\lambda) = \begin{pmatrix} R_{11}(\lambda) & R_{12}(\lambda) \\ 0 & R_{22}(\lambda) \end{pmatrix}
\]

with \( Q(\lambda_0) = Q_0 \), and \( \text{eig}(R_{11}(\lambda)) = \sigma_1(\lambda), \text{eig}(R_{22}(\lambda)) = \sigma_2(\lambda) \).
Remark 2.2. The Schur factorization above can in fact be implemented as an ordered factorization, in the sense that it can be performed in such a way that the block \( R_{11}(\lambda) \) contains the eigenvalues we are interested in.

The main ingredient in the proof of Theorem 2.1 is to associate the factorization with the solution of the following system of differential algebraic equations (DAEs)

\[
\begin{align*}
\dot{R} &= Q^T \dot{A}Q + RH - HR \\
\dot{Q} &= QH \\
R_{21} &= 0, \quad H^T = -H
\end{align*}
\]

(2.2)

where \( H = Q^T \dot{Q} \). By eliminating the algebraic part, this DAEs are then reduced to a standard system of differential equations. It can be proved that \( H = \begin{pmatrix} 0 & H_{12} \\ -H_{12}^T & 0 \end{pmatrix} \), and that \( H_{12} \) is solution of the Sylvester equation

\[
R_{22}H_{12}^T - H_{12}^T R_{11} = (Q^T \dot{A}Q)_{21}.
\]

Thus, the existence of the Schur factors of \( A(\lambda) \) is guaranteed as smooth solutions of (2.2).

Remark 2.3. In general, a block Schur factorization is preferred over a simple Schur factorization due to the fact that numerical difficulties can be expected when two or more eigenvalues become close.

2.1. CIS Algorithm. Recall that we are interested in computing a set of vectors that span the center-stable or center-unstable subspaces of an equilibrium point or a periodic orbit. Through the factorization given in (2.1), we can locate the desired eigenvalues in \( R_{11}(\lambda) \), then block the matrix \( Q(\lambda) = [Q_1(\lambda) \ Q_2(\lambda)] \), and from \( AQ = QR \) we realize that the columns of \( Q_1(\lambda) \) span the desired subspace.

An algorithm for computing such Schur factors was proposed in [2], which takes into account their existence as smooth solutions of (2.2). It is a predictor-corrector type algorithm, and it is called Continuation of Invariant Subspaces (CIS) algorithm. We refer the reader to [2] for full details; here we just briefly mention the main ideas.

We need to compute a smooth and orthogonal \( Q(\lambda) = [Q_1(\lambda) \ Q_2(\lambda)] \in \mathbb{R}^{m \times m} \), with \( Q_1(\lambda) \in \mathbb{R}^{m \times n} \), \( Q_2(\lambda) \in \mathbb{R}^{m \times (m-n)} \) so that \( Q_1(\lambda) \) spans the invariant subspace associated with the eigenvalues of \( R_{11}(\lambda) \) in (2.1). Consider the initial factorization as in Theorem 2.1. The idea is to perform iterative orthogonal corrections of the form

\[
Q(\lambda) = Q(0) U(\lambda), \quad \text{with} \quad U(0) = I,
\]

and \( U \) given by

\[
U(s) = \left[ \begin{pmatrix} I \\ Y \end{pmatrix} (I + YY^T)^{-1/2} \begin{pmatrix} -Y^T \\ I \end{pmatrix} (I + YY^T)^{-1/2} \right],
\]

where \( Y \) is minimum norm solution of the Riccati equation

\[
\dot{R}_{22}Y - Y \dot{R}_{11} = -E_{21} + Y \dot{R}_{12} Y
\]

(which is solved by Newton's method). The terms \( \dot{R}_{ij} \) and \( E_{21} \) are obtained from

\[
Q(0)^T A(s) Q(0) = \begin{bmatrix} \dot{R}_{11} & \dot{R}_{12} \\ E_{21} & \dot{R}_{22} \end{bmatrix}.
\]
This CIS algorithm will be used when setting up the boundary conditions in the system of differential equations to be solved. We will need to compute certain matrices denoted by $L_{-c}(\lambda)$ and $L_{+c}(\lambda)$ (which span the center-stable and center-unstable subspaces of the invariant sets). These matrices will be obtained through this algorithm implemented as a "black box" subroutine within the main program. Suitable matrices $Q(\lambda)$ which span a subspace related to the spectrum of $R_{11}(\lambda)$ will give us the corresponding matrices $L_{-}(\lambda)$, and smoothness with respect to the parameter $\lambda$ will be guaranteed. Some more details are given in the section on numerical examples.

**Remark 2.4.** A number of modifications within the subroutine CIS have been made to the original codes in [4] including: larger number of arguments, Newton refinement in the computation of $(I + Y^T Y)^{-1/2}$, and a new subroutine to solve the Sylvester equations.

3. Connecting Orbits and Projection Boundary Conditions

Let us consider dynamical systems of the form

\[
\dot{x} = f(x, \lambda), \quad x(t) \in \mathbb{R}^m, \quad \lambda \in \mathbb{R}^p,
\]

where $f : \mathbb{R}^m \times \mathbb{R}^p \rightarrow \mathbb{R}^m$ is assumed to be sufficiently smooth, and $\lambda$ is a vector of parameters. We are interested mainly in the cases of point-to-periodic and periodic-to-periodic connections. Then, let $M_{-}(\lambda)$ be either a hyperbolic\(^1\) equilibrium $y_{-}(\lambda)$ of (3.1), or a hyperbolic\(^2\) periodic orbit $\gamma_{-}(\lambda)$ of (3.1), and let $M_{+}(\lambda)$ be a hyperbolic periodic orbit $\gamma_{+}(\lambda)$ of (3.1). We will use the notation $y_{+}(t, \lambda)$ to denote the periodic solution corresponding to $\gamma_{+}(\lambda)$, and similarly $y_{-}(t, \lambda)$ will be the periodic solution relative to $\gamma_{-}(\lambda)$, if $M_{-}(\lambda) = \gamma_{-}(\lambda)$. A solution $x(t, \lambda), t \in \mathbb{R}$ of (3.1) is called a connecting orbit from $M_{-}(\lambda)$ to $M_{+}(\lambda)$ if

\[
\text{dist} (x(t, \lambda), M_{\pm}(\lambda)) \rightarrow 0 \quad \text{as} \quad t \rightarrow \pm \infty.
\]

Since we consider autonomous systems, a connecting orbit is not unique: if $x(t, \lambda)$ is a solution, so is $x(t + c, \lambda)$ for any $c$. To fix the solution, we will impose a so called phase condition

\[
\psi(x, y_{-}, y_{+}, \lambda) = 0.
\]

The topic of connecting orbits as solutions of dynamical systems has several important applications. To mention a few: semiconductors [7], celestial mechanics [8], biology and chemistry [5], etc. The theoretical foundations for the computation of connecting orbits are established in [3] and a numerical example is presented. The work in [2] provides an algorithm for smooth continuation of solutions. Based on these two works, a general numerical algorithm for computation and continuation of point-to-periodic and periodic-to-periodic connections is given in [4].

The main idea in computing connecting orbits is to truncate the real line to a finite, but sufficiently large, interval $[T_{-}, T_{+}]$, $T_{-} < 0 < T_{+}$, and impose boundary conditions at $T_{\pm}$. An appropriate choice for these boundary conditions can be obtained by using the fact that the connecting orbit leaves $M_{-}(\lambda)$ along its unstable manifold and enters $M_{+}(\lambda)$ along its stable manifold. These manifolds are tangent to the unstable subspace $E^{u}_{-}(\lambda)$ of $M_{-}(\lambda)$ and to the stable subspace $E^{s}_{+}(\lambda)$ of $M_{+}(\lambda)$, respectively.

\(^1\)No eigenvalue of $f_{x}(y_{-}(\lambda))$ is on the imaginary axis

\(^2\)Only one Floquet multiplier is on the unit circle
For each \( \lambda \), the numbers \( m^u_-, m^c_- \), and \( m^c_+ \), will denote the dimensions of the unstable, center, and stable manifolds respectively of \( M_-(\lambda) \), and analogously we will write \( m^u_+, m^c_+ \), and \( m^c_- \) respectively to \( M_+(\lambda) \). Here, \( m^c_\pm \) are the dimensions of \( M_\pm(\lambda) \). For an equilibrium point we have \( m^c_\pm = 0 \) and for a (hyperbolic) periodic orbit, we have \( m^c_\pm = 1 \).

Following [4], we will impose projection boundary conditions and will compute the connecting orbits by considering the following boundary value problem

\[
\begin{align*}
\dot{x} &= f(x, \lambda), \quad T_- \leq t \leq T_+ \\
L_-(\lambda)(x(T_-) - y_-(s(T_-))) &= 0, \quad L_+(\lambda)(x(T_+) - y_+(s(T_+))) = 0, \\
\psi(x, y_-, y_+, \lambda) &= 0,
\end{align*}
\]

where \( L_- : \mathbb{R}^p \to \mathbb{R}^{m^c_- + m^c_-} \) and \( L_+ : \mathbb{R}^p \to \mathbb{R}^{m^c_+ + 1} \) are smooth functions of \( \lambda \) (these are the matrix functions that result from Schur factorization of Jacobians or monodromy matrices) and span the center-stable subspace \( E^c_- (\lambda) \) of \( \gamma_- (\lambda) \), and the center-unstable subspace \( E^c_+ (\lambda) \) of \( \gamma_+(\lambda) \). Also, in (3.3), \( \psi \) corresponds to the truncated version of the phase condition.

We let \( W^c_- (\lambda) \), respectively \( W^c_+ (\lambda) \), be the center-unstable manifold of \( M_- (\lambda) \), respectively the center-stable manifold of \( M_+ (\lambda) \). The manifold \( W^c_- \) has dimension \( m^c_- + m^u_- + p \) and \( W^c_+ \) has dimension \( 1 + m^u_+ + p \). Suppose that there is a connecting orbit \( \gamma \), connecting \( M_- \) and \( M_+ \), then, we must have \( \gamma \subset W^c_- \cap W^c_+ \). The connecting orbit \( \gamma \) is isolated if for the tangent spaces at \( z(t) \) we have

\[
T_{z(t)} W^c_- \cap T_{z(t)} W^c_+ = T_{z(t)} \gamma = \text{span } \{ \dot{z}(t) \}, \quad \forall \ t \in \mathbb{R},
\]

and is persistent if the intersection is \textit{transversal}, i.e.

\[
T_{z(t)} W^c_- + T_{z(t)} W^c_+ = \mathbb{R}^{m^u_- + p}, \quad \forall \ t \in \mathbb{R},
\]

where \( z = (x, \lambda) \). The main result in [3] states that the connecting orbit problem

\[
\begin{align*}
\dot{x} &= f(x, \lambda), \quad -\infty < t < \infty, \\
\lim_{t \to -\infty} \text{dist}(x(t, \lambda), M_-(\lambda)) &= 0, \quad \lim_{t \to +\infty} \text{dist}(x(t, \lambda), M_+(\lambda)) = 0, \\
\psi(x, y_-, y_+, \lambda) &= 0,
\end{align*}
\]

where the phase condition satisfies a nondegeneracy requirement \(^3\), is well posed if and only if the manifolds \( W^c_- \) and \( W^c_+ \) intersect transversally in the sense of (3.4)-(3.5).

### 3.1. Truncation to a finite interval.

Summarizing the results in [4], we establish the solvability of (3.3) and the exponentially decaying errors resulting from applying the projection boundary conditions. We use the spaces

\[
W := C^1(J, \mathbb{R}^m) \times \mathbb{R}^p, \quad Z := C(J, \mathbb{R}^m) \times \mathbb{R}^{m^c_- + m^c_+} \times \mathbb{R}^{m^c_- + 1}.
\]

For \( \alpha, \beta > 0 \), their norms are defined as

\[
\| (x, \lambda) \|_W = \sup_{t \in J_-} \| x(t) \| e^{\alpha t} + \sup_{t \in J_+} \| x(t) \| e^{-\beta t} + \| \lambda \|,
\]

where

\[
\psi(x, y_-, y_+; \lambda) = 0, \quad \frac{\partial \psi}{\partial x} (\dot{x}_- + \frac{\partial \psi}{\partial y_-} (\dot{y}_- + \frac{\partial \psi}{\partial y_+} \dot{y}_+ \neq 0
\]

\[\[\]\]

\[\[\]\]
\[ \left\| (y, r_-) \right\|_{Z_1} = \sup_{t \in J_-} \left\| y(t) \right\| e^{\epsilon t} + \left\| r_- \right\|, \quad \text{and} \]
\[ \left\| (y, r_+) \right\|_{Z_2} = \sup_{t \in J_+} \left\| y(t) \right\| e^{-\beta t} + \left\| r_+ \right\|, \quad \| \cdot \| = \| \cdot \|_{\infty}, \]
and \( J_- = [T_-, 0] \) and \( J_+ = [0, T_+] \). With these norms, \( W \) and \( Z \) become Banach spaces. Anticipating the asymptotic convergence of \( x(t) \) to \( y(t) \) with rate \( \epsilon > 0 \) we impose the condition that for some constant \( C \), \( \| x(t) - y_{\pm}(t) \| \leq Ce^{-\epsilon |t|} \), as \( t \to \pm \infty \).

**Theorem 3.1.** Let (3.4), (3.5) hold, and let \((\hat{x}, \hat{\lambda})\) be an orbit connecting either a hyperbolic equilibrium point \( y_-(\hat{\lambda}) \) or a hyperbolic periodic orbit \( \gamma_-(\hat{\lambda}) \), to a hyperbolic periodic orbit \( \gamma_+(\hat{\lambda}) \). Consider (3.3) and assume that \( f \in C^2(\mathbb{R}^{m+P}, \mathbb{R}^{m}) \), and that \( L_{\pm} \) are \( C^1 \) (in \( \lambda \)).

Then, there exists \( \delta > 0 \) sufficiently small and \( C > 0 \), such that for sufficiently large \( J = [T_-, T_+] \), the boundary-value problem (3.3) has a unique solution \((x_J, \lambda_J)\) in \( \mathcal{K}_{\delta} = \{(x, \lambda) : \| (x, \lambda) - (\hat{x}, \hat{\lambda}) \|_{W} \leq \delta \} \). Moreover, the following estimate holds
\[ \| (x_J, \lambda_J) - (\hat{x}, \hat{\lambda}) \|_{W} \leq C e^{-2 \min(\mu_-|T_-, \mu_+T_+)} \]
where \( 0 < \mu_- < \text{Re} \mu \), for all unstable eigenvalues \( \mu \) of the Jacobian \( f_x(y_-(\hat{\lambda})) \) (if \( M_-(\hat{\lambda}) = y_-(\hat{\lambda}) \)), or all unstable Floquet exponents of the monodromy matrix relative to \( \gamma_-(\hat{\lambda}) \) (if \( M_-(\hat{\lambda}) = \gamma_-(\hat{\lambda}) \)). Also, \( 0 < \mu_+ < -\text{Re} \mu \), for all stable Floquet exponents \( \mu \) associated to the periodic orbit \( \gamma_+(\hat{\lambda}) \).

### 3.2. Main algorithm.
We consider only the point-to-periodic connection; the modifications for the point-to-point and periodic-to-periodic cases should be obvious. One of the main ideas in the algorithm is to split the problem in two parts, the first one to compute the connecting orbit, and the second, as a subroutine of the first, to compute the periodic orbits and the associated monodromy matrices. After rescaling to the interval \([0, 1]\), this can be expressed as
\[ \begin{cases} 
\dot{x} = (T_+ - T_-)f(x, \lambda), & 0 \leq t \leq 1, \\
L_-(\lambda)(x(0, \lambda) - y_-(\lambda)) = 0, \\
L_+(\lambda)(x(1, \lambda) - y_+(0, \lambda)) = 0, 
\end{cases} \]
and
\[ \begin{cases} 
f(y_+(\hat{\lambda})) = 0, \\
\dot{y}_+ = \tau_+ f(y_+, \hat{\lambda}), & 0 \leq t \leq 1, \\
y_+(0) = y_+(1), \\
\sigma(y_+, \hat{\lambda}) = 0, 
\end{cases} \]
where \( \sigma = 0 \) is a phase condition for the periodic orbit, serving the role of \( \psi = 0 \) in (3.3), and where \( L_-(\lambda) \in \mathbb{R}^{m_L,m_L} \), \( L_+(\lambda) \in \mathbb{R}^{m_L+1,m_L} \). Also, observe that the value of the parameter \( \hat{\lambda} \) is fixed within the subroutine that computes the periodic orbit.

We define \( L_- \) and \( L_+ \) in such a way that they depend smoothly on \( \lambda \), not only because of the theoretical restriction imposed by Theorem 3.1, but also because it is crucial for the success of the numerical methods. Typically (3.3) is solved by a discretization method for boundary value problems, say collocation, coupled with Newton's method. Failure to have
smooth functions $L_{\pm}$ will mean trouble with convergence of the Newton iteration. This is where the smooth block Schur factorization plays a key role. For the continuation of solutions, we will make use of the smooth continuation of invariant subspaces (CIS) algorithm in [2].

If $A(\lambda)$ is the Jacobian or the monodromy matrix that is being factored in the form (2.1), then we block $Q$ according to the dimensions of $R$:

$$Q(\lambda) = [Q_1(\lambda) \quad Q_2(\lambda)], \quad R(\lambda) = \begin{bmatrix} R_{11}(\lambda) & R_{12}(\lambda) \\ 0 & R_{22}(\lambda) \end{bmatrix},$$

where $R_{11}(\lambda)$ contains the eigenvalues of interest (say, the eigenvalues with negative real part, for a stable subspace of an equilibrium point). In this setting, the columns of $Q_1(\lambda)$ span the desired subspace (say, the stable subspace), i.e. we take $L(\lambda) = Q_1(\lambda)$. See Section 2 and [4] for more details on this approach.

In this work, a collocation code is used for solving (3.10), and multiple shooting is used for solving (3.11), which is called as a subroutine of the code for (3.10) when imposing the boundary conditions. Some Lapack (http://www.netlib.org/lapack) routines have been used.

4. Numerical Examples

In this section we illustrate the key role that smooth block Schur factorization plays in the computation and continuation of special solutions of dynamical systems of the form (3.3) through selected examples. The special solutions we are interested in are heteroclinic connections between an equilibrium point and a periodic orbit and those between two periodic orbits. Once such connections are computed, we perform continuation as problem parameters vary by using block Schur factorization of the matrices $L_{-}(\lambda)$ and $L_{+}(\lambda)$ in (3.10), via the continuation of invariant subspaces (CIS) algorithm. The algorithms used allow for a monitoring of the eigenvalues of the Jacobian and monodromy matrices, which in turn help explain the stability properties of such invariant sets. For example, by monitoring the eigenvalues we can observe whether a periodic orbit may gain or lose stability or hyperbolicity.

Remark 4.1. As a consequence of the modifications made to the codes in [4], a clearly better performance of the algorithms is observed. Besides the modifications made to the subroutines within CIS and other modifications to several other subroutines, we have also allowed the size of the integration interval $T = T_+ - T_- \in (3.10)$ to vary with continuation, and we have used second order approximations to derivatives. This gives a better accuracy of the solutions.

4.1. Lorenz equations. For continuation of separatrices as point-to-periodic heteroclinic connections we consider the well-known Lorenz equations. This is a system that has been extensively studied because of the wide range of solution behaviors it shows, including chaotic solutions as well as homoclinic and heteroclinic orbits. In particular, this system was studied in [4], where a bifurcation analysis was followed by the computation of a heteroclinic connection from an equilibrium point to a periodic orbit. The system is

$$\begin{align*}
\dot{x}_1 &= \sigma (x_2 - x_1) \\
\dot{x}_2 &= \lambda x_1 - x_2 - x_1 x_3 \\
\dot{x}_3 &= x_1 x_2 - b x_3,
\end{align*}$$

(4.1)
where we take \( \sigma = 10, \beta = \frac{8}{3} \) and treat \( \lambda \) as a free parameter. For these values, a bifurcation analysis shows that at \( \lambda = 1.0 \) there is a pitchfork bifurcation from the trivial equilibrium and a Hopf bifurcation point at \( \lambda = 24.7368 \) along both pitchfork branches. From each of these Hopf points, one can continue in \( \lambda \) a branch of hyperbolic periodic orbits.

There exists a connection from the origin to a periodic orbit as the result of the transversal intersection of the one-dimensional unstable manifold of the origin with the two-dimensional center-stable manifold of the periodic orbit for \( \lambda = 24.0579003223 \). The computed periodic orbit has period \( \tau = 0.6771717981 \) and Floquet multipliers \( \mu_1 = 1, \mu_2 = 1.0293329333, \mu_3 = 0.0000929367 \). Continuation was also performed in [4] to obtain a branch of point-to-periodic connections as the parameter \( b \) varies. There, it was possible to extend the continuation up to \( b = 5.2366666666 \) and \( \lambda = 41.4875170876 \), almost doubling the original value of \( \lambda \).

**Remark 4.2.** However, with the codes in [4] it was not possible to perform continuation beyond these values.

The modifications and improvements to the implementation of the original algorithms in [4] now allow to perform continuation for much larger values of \( \lambda \) and \( b \), which clearly shows the robustness of the algorithms. The geometrical shapes of the connections and periodic orbits in the phase portrait change dramatically in scale as the parameters increase, and due to this difference in scale, it is not possible anymore to see the initial connecting orbit (the one computed for the smallest parameter value) together with the final one in one single picture. The initial one (and even the final one in [4]) would be as tiny as a single point next to the final connecting orbit computed here. This time we have reached the values \( b = 13.4416464434 \) and \( \lambda = 4829.6606254594 \).

In Figures 1 through 4 we show branches of heteroclinic connecting orbits obtained by smooth continuation. Observe that the connecting orbits with smallest magnitude in Figures 2 through 4 correspond to the connecting orbits with the largest magnitude in the corresponding previous figure. One should compare the solutions obtained here with the ones in [4]. We also show in Table 1 the evolution of the period and the Floquet multipliers of the orbits as the parameter varies. Observe that the hyperbolicity of the periodic orbits is preserved.

For completeness, we show the Jacobian matrix \( J \) at the origin \((0,0,0)\) and its block Schur factorization involved in the computation of the connecting orbit for \( \lambda = 2.7566666666 \). See (2.1).

\[
Q^T J Q = Q^T \begin{bmatrix}
-10 & 10 & 0 \\
\lambda & -1 & 0 \\
0 & 0 & -\frac{8}{3}
\end{bmatrix} Q = \begin{bmatrix}
-12.41495963 & 0.00000000 & -7.24333333 \\
0.00000000 & -2.66666666 & 0.00000000 \\
0.00000000 & 0.00000000 & 1.41495963
\end{bmatrix},
\]

where

\[
Q = [Q_1 \quad Q_2] = \begin{bmatrix}
-0.97205634 & 0.00000000 & 0.23474768 \\
0.23474768 & 0.00000000 & 0.97205634 \\
0.00000000 & 1.00000000 & 0.00000000
\end{bmatrix}.
\]

Then, the matrix \( L(\lambda) := Q_1 \) spans the stable subspace of the equilibrium point \((0,0,0)\) at \( \lambda = 2.7566666666 \).
4.2. Coupled Oscillators. We consider the system

\[
\begin{align*}
\dot{x}_1 &= x_1 + \beta y_1 - x_1(x_1^2 + y_1^2) + \lambda (x_2 - x_1 + y_2 - y_1) \\
\dot{y}_1 &= -\beta x_1 + y_1 - y_1(x_1^2 + y_1^2) + \lambda (x_2 - x_1 + y_2 - y_1) \\
\dot{x}_2 &= x_2 + \beta y_2 - x_2(x_2^2 + y_2^2) + \lambda (x_1 - x_2 + y_1 - y_2) \\
\dot{y}_2 &= -\beta x_2 + y_2 - y_2(x_2^2 + y_2^2) + \lambda (x_1 - x_2 + y_1 - y_2).
\end{align*}
\]

The system (4.2) can be simplified by introducing the linear subspaces

\[
\Gamma = \{(x_1, y_1, x_2, y_2) \in \mathbb{R}^4 : x_1 = x_2, \; y_1 = y_2\}, \quad \text{and}
\]

\[
\Pi = \{(x_1, y_1, x_2, y_2) \in \mathbb{R}^4 : x_1 = -x_2, \; y_1 = -y_2\}.
\]

Then, we introduce coordinates relative to $\Gamma$ and $\Pi$ by defining
In these coordinates, the governing equations become

\[
\begin{align*}
\dot{u}_1 &= u_1 + \beta v_1 - u_1^3 - 3u_1u_2^2 - u_1(v_1^2 + v_2^2) - 2v_1v_2u_2 \\
\dot{v}_1 &= -\beta u_1 + v_1 - v_1^3 - 3v_1v_2^2 - v_1(u_1^2 + u_2^2) - 2u_1u_2v_2 \\
\dot{u}_2 &= (1 - 2\lambda)u_2 + (\beta - 2\lambda)v_2 - u_2^3 - 3u_2u_1^2 - u_2(v_1^2 + v_2^2) - 2v_1v_2u_1 \\
\dot{v}_2 &= -(\beta + 2\lambda)u_2 + (1 - 2\lambda)v_2 - v_2^3 - 3v_2v_1^2 - v_2(u_1^2 + u_2^2) - 2u_1u_2v_1
\end{align*}
\]
Observe that on $\Gamma$ we have $u_2 = v_2 = 0$, while on $\Pi$ we have $u_1 = v_1 = 0$, so that the flow restricted to these manifolds reduces to the governing equations for the uncoupled oscillators. For small $\lambda$, two persistent periodic orbits can be explicitly given as (see [9])

$$
\omega_\pi(t) = (0, 0, \rho(t) \cos \theta(t), \rho(t) \sin \theta(t)), \quad \omega_0(t) = (\cos \beta t, -\sin \beta t, 0, 0),
$$

where

$$
\dot{\rho} = (1 - 2\lambda - 2\lambda \sin 2\theta)\rho - \rho^3 \quad \text{and} \quad \dot{\theta} = -\beta - 2\lambda \cos 2\theta.
$$

Observe that $\omega_\pi$ lies in $\Pi$, whereas $\omega_0$ lies in $\Gamma$. Here we compute and then perform smooth continuation of a connecting orbit from $\omega_\pi$ to $\omega_0$. In Figures 6 through 9 we show 3-dimensional views of the connecting orbit, where we have actually plotted $(u_1, v_1, \sqrt{u_2^2 + v_2^2})$ and $(u_2, v_2, \sqrt{u_1^2 + v_1^2})$ respectively.

<table>
<thead>
<tr>
<th>$b$</th>
<th>$\lambda$</th>
<th>Period</th>
<th>Floquet multipliers</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.7566666666</td>
<td>24.4872943345</td>
<td>0.6633333236</td>
<td>0.0001055321</td>
</tr>
<tr>
<td>5.2766666666</td>
<td>41.9064116742</td>
<td>0.4301691358</td>
<td>0.0003875710</td>
</tr>
<tr>
<td>8.9766662563</td>
<td>151.9179506324</td>
<td>0.2206728489</td>
<td>0.0081105622</td>
</tr>
<tr>
<td>11.9766664585</td>
<td>861.7281515695</td>
<td>0.1304312721</td>
<td>1.5012230948</td>
</tr>
<tr>
<td>13.441644434</td>
<td>4829.660625494</td>
<td>0.100748120</td>
<td>9.5770852838</td>
</tr>
</tbody>
</table>

Table 1. Periods and multipliers for (4.1)
In Table 2 we show the evolution of the multipliers of the periodic orbit $\omega_\pi$ as $\lambda$ varies. Observe especially how the unstable multiplier grows fast, and how this is reflected in the shape of the connecting orbit leaving $\omega_\pi$ in Figures 6 through 11.

**Remark 4.3.** The codes in [4] have been also tested in this problem, and it was not possible to do continuation beyond $\lambda = 0.19$.

4.3. Michelson equations. Here we consider the Kuramoto-Sivashinsky PDE

\[ u_t + u_{xxx} + u_{xx} + uu_x = 0, \]
which is used to describe spatio-temporal evolution of a flame front. We start by performing a change of variables in the form \( u(x,t) = v(x) - s^2t \), \( y = v' \) from which we obtain \( y'' + y' + \frac{1}{2} y^2 - s^2 = 0 \), which in turn can be written as
\[
\begin{align*}
\dot{u}_1 &= u_2 \\
\dot{u}_2 &= u_3 \\
\dot{u}_3 &= s^2 - \frac{1}{2} u_1^2 - u_2.
\end{align*}
\]  
(4.7)

This set of ODEs is known as Michelson’s system. The existence of several periodic solutions as well as heteroclinic connections between equilibria and periodic orbits for these equations has been proved in [10], and a heteroclinic orbit connecting two periodic orbits \((P_1 \text{ and } P_2 \text{ in Figure 12})\) has been numerically computed in [5] for \( s = 1 \), with periods \( \tau_1 = 9.29958014 \)
and $\tau_2 = 6.64993366$ respectively. Starting with this periodic-to-periodic connection, here we perform continuation of solutions as $s$ increases, to obtain a branch of heteroclinic connections. Observe the interesting fact that as $s$ increases, the periodic orbits $P_1$ and $P_2$ as well as their periods approach each other to the point that geometrically the periodic orbits look as lying on top of each other. See Figures 13 through 15. However, their monodromy matrices have different eigenvalues (Floquet multipliers). See Table 3.
<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>Period</th>
<th>Floquet multipliers, $\omega_\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>12.26300000</td>
<td>0.3909E-08  0.3009E-08  10.39383656</td>
</tr>
<tr>
<td>0.14</td>
<td>13.27268967</td>
<td>0.2687E-06  0.5006E-08  31.49315169</td>
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<tr>
<td>0.19</td>
<td>15.80206826</td>
<td>0.2649E-05  0.3092E-08  191.78655953</td>
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<tr>
<td>0.24</td>
<td>23.39980488</td>
<td>0.4448E-04  0.3050E-10  3457.95142789</td>
</tr>
</tbody>
</table>

Table 2. Period and multipliers of $\omega_\pi$ for (4.5)

**Figure 12.** Periodic orbits of (4.7) for $s = 1$.

It is equally important to observe the evolution of both, the stable and the unstable Floquet multipliers of the periodic orbit $P_1$. At $s = 1$, they are $\mu_1 = -0.0315000$ and $\mu_2 = -31.65554783$, and as $s$ increases, $\mu_1$ approaches $-1.0$ from the right, and $\mu_2$ approaches $-1.0$ from the left, and hyperbolicity is lost at approximately $s = 1.26599$. For $s = 1.2660$ the multipliers of $P_2$ are complex and are located at on unit circle (the multipliers of $P_1$ remain real). Thus, as the parameter $s$ approaches $s = 1.26599$, the monodromy matrix corresponding to $P_2$ has no longer a single eigenvalue of magnitude 1, and hyperbolicity is lost.

**Remark 4.4.** The ability to track eigenvalues with continuation and detect qualitative changes in the solution is a very important feature in this numerical method.
\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig13.png}
\caption{Periodic-to-periodic connections of (4.7)}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig14.png}
\caption{Periodic-to-periodic connections of (4.7).}
\end{figure}

5. Conclusions

In this work we have applied smooth block Schur factorizations of matrix functions to the numerical computation of separatrices in dynamical systems, as heteroclinic orbits connecting equilibria and periodic orbits. The implementation of the numerical algorithms in [4] have been modified increasing reliability and allowing better performance in continuation;
in particular, we have been able to perform continuation on the Lorenz system for significantly large values of the parameter. The continuation of invariant subspaces algorithm has been used to implement the Schur factorizations. Monitoring eigenvalues of Jacobians and monodromy matrices through smooth continuation was used to detect qualitative behavior changes in the solutions been computed, such as the loss of hyperbolicity. Generalizations and adaptations of these methods and algorithms to e.g. nonhyperbolic connections, delay differential equations, $n$-body problems and general infinite dimensional systems are very interesting directions for future research, with several potential applications.
REFERENCES


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