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Computer Assisted Proof of Transverse Saddle-to-Saddle Connecting Orbits for First Order Vector Fields

Jean-Philippe Lessard · Jason D. Mireles James · Christian Reinhardt

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Abstract In this paper we introduce a computational method for proving the existence of generic saddle-to-saddle connections between equilibria of first order vector fields. The first step consists of rigorously computing high order parametrizations of the local stable and unstable manifolds. If the local manifolds intersect, the Newton–Kantorovich theorem is applied to validate the existence of a so-called short connecting orbit. If the local manifolds do not intersect, a boundary value problem with boundary values in the local manifolds is rigorously solved by a contraction mapping argument on a ball centered at the numerical solution, yielding the existence of a so-called long connecting orbit. In both cases our argument yields transversality of the corresponding intersection of the manifolds. The method is applied to the Lorenz equations, where a study of a pitchfork bifurcation with saddle-to-saddle stability is done and where several proofs of existence of short and long connections are obtained.

Keywords Computer assisted proof · Invariant manifolds · Parameterization method · Connecting orbits · Contraction mapping · Transversality

1 Introduction

Equilibria of vector fields and connecting orbits between them are among the fundamental objects of study in the qualitative theory of dynamical systems. On the one hand these

J.-P. Lessard
Département de Mathématiques et de Statistique, Université Laval, 1045 avenue de la Médecine, Québec, QC G1V0A6, Canada
e-mail: jean-philippe.lessard@mat.ulaval.ca

J. D. Mireles James
Department of Mathematics, Rutgers University, 110 Frelinghuysen Rd, Piscataway, NJ 08854, USA
e-mail: jmireles@math.rutgers.edu

C. Reinhardt (✉)
Technische Universität München, Boltzmannstr. 3, 85747 Garching, Germany
e-mail: reinhard@ma.tum.de

objects provide a basic heuristic skeleton of the global dynamics for a particular system. On the other hand the equilibria and connecting orbits comprise the building blocks of more powerful qualitative tools such as Morse's Theory for the homology of manifolds and dynamical forcing theorems such as Smale's Tangle theorem [37], and the Shilnikov theorem on heteroclinic tangencies [30]. Since it is usually impossible to find closed form expressions for connecting orbits, it is natural to use the computer in order to construct finite numerical approximations. Once this is done, it is equally natural to ask if the computer can be used in order to pass from good numerical approximations to abstract existence results and rigorous error bounds.

In the present work we develop a computer aided method for proving the existence of generic saddle-to-saddle connections for nonlinear differential equations. The method is constructive, so that in addition to obtaining abstract existence results we also obtain precise information about the location and transversality of the connecting orbit. In order to formalize the discussion let $g\colon \mathbb{R}^n \to \mathbb{R}^n$ be a vector field and $p_1, p_2 \in \mathbb{R}^n$ be equilibria of the differential equation $\frac{du}{dt} = g(u)$. We make the following assumptions.

A1: The vector field g is real analytic in some neighborhoods of p_1 and p_2.

A2: The equilibria p_1 and p_2 are *generic connectable saddles*, that is we assume that $Dg(p_1)$ and $Dg(p_2)$ are diagonalizable, that $Dg(p_1)$ has $n_u \leq n$ eigenvalues with positive real part, that $Dg(p_2)$ has $n_s \leq n$ eigenvalues with negative real parts, and that the non-degeneracy condition $n_s + n_u = n + 1$ is satisfied (the reason for this, quite standard non-degeneracy assumption, will become clear as we proceed). Let $\lambda_1^u, \ldots, \lambda_{n_u}^u$ and $\lambda_1^s, \ldots, \lambda_{n_s}^s$ denote the unstable and stable eigenvalues of $Dg(p_1)$ and $Dg(p_2)$ respectively. Similarly let $\xi_1^u, \ldots, \xi_{n_u}^u$ and $\xi_1^s, \ldots, \xi_{n_s}^s$ denote a fixed choice of associated eigenvectors. Let Λ_u and Λ_s be the $n_u \times n_u$ and $n_s \times n_s$ diagonal matrices with the unstable and stable eigenvalues on the diagonal respectively, and $A_u = [\xi_1^u | \ldots | \xi_{n_u}^n]$ and $A_s = [\xi_1^s | \ldots | \xi_{n_s}^s]$ denote the matrices whose columns are the above mentioned eigenvectors.

A3: There are real analytic chart maps for the local unstable (resp. stable) manifold at p_1 (resp. at p_2) denoted by $W^u_{\text{loc}}(p_1)$ (resp. by $W^s_{\text{loc}}(p_2)$). More precisely, we assume that there are neighborhoods of the origin $V_{\nu_u} \subset \mathbb{R}^{n_u}$, $V_{\nu_s} \subset \mathbb{R}^{n_s}$ and analytic injections $P\colon V_{\nu_u} \to \mathbb{R}^n$ and $Q\colon V_{\nu_s} \to \mathbb{R}^n$ so that

$$P(0) = p_1, \qquad Q(0) = p_2,$$
$$DP(0) = A_u, \qquad DQ(0) = A_s,$$

and

$$P\left[V_{\nu_u}\right] = W^u_{\text{loc}}(p_1) \qquad Q\left[V_{\nu_s}\right] = W^s_{\text{loc}}(p_2).$$

Moreover we assume that these chart maps conjugate the dynamics on the local unstable and stable manifolds to the dynamics in the parameter space given by the linear vector fields Λ_u and Λ_s respectively. Explicitly this means that if $\Phi\colon \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is the flow generated by g then we assume that

$$\Phi\left(P(\theta), t\right) = P\left(e^{\Lambda_u t}\theta\right) \qquad \text{for all} \quad \theta \in V_{\nu_u} \quad \text{and} \quad t \leq 0, \tag{1.1}$$

and that

$$\Phi\left(Q(\phi), t\right) = Q\left(e^{\Lambda_s t}\phi\right) \qquad \text{for all} \quad \phi \in V_{\nu_s} \quad \text{and} \quad t \geq 0. \tag{1.2}$$

Remark 1 Assumption **A3** appears as a strong assumption, but is in fact met for generic sets of eigenvalues. P and Q are discussed in greater detail as we proceed.

Remark 2 Strictly speaking assumption **A3** is stated correctly only for real eigenvalues and has to be modified slightly when there are complex conjugate pairs. This can be done in a quite standard way and, as will be seen in the applications, the presence of complex eigenvalues presents no obstruction to our methods. The complex case does however introduce notational complications and for the sake of simplicity in the introduction we take **A3** as written and treat the technicalities only as they arise.

Assume that assumptions **A1–A3** are satisfied. A heteroclinic connection $u(t)$ from p_1 to p_2 is a solution of the differential equation $\frac{du}{dt} = g(u)$ satisfying

$$\lim_{t \to -\infty} u(t) = p_1 \qquad \text{and} \qquad \lim_{t \to \infty} u(t) = p_2.$$

Since p_1 and p_2 are hyperbolic saddle points we refer to this as a saddle-to-saddle connection. Denoting by $W^u(p_1)$ the n_u-dimensional unstable manifold of p_1 and $W^s(p_2)$ the n_s-dimensional stable manifold of p_2, we note that

$$u(t) \in W^u(p_1) \cap W^s(p_2) \qquad \text{for all } t \in \mathbb{R},$$

by definition. Then finding heteroclinic orbits is equivalent to finding intersections of the stable and unstable manifolds. With this in mind we consider separately the two cases which can occur.

Suppose first that the local unstable and local stable manifolds parameterized by P and Q intersect in phase space, that is assume that

$$\text{image}[P] \cap \text{image}[Q] \neq \emptyset.$$

Taking a point $q \in \text{image}[P] \cap \text{image}[Q]$, we have that the orbit of q is a heteroclinic orbit from p_1 to p_2. In this case we say that there is a *short-connection* from p_1 to p_2 in order to emphasize that the heteroclinic orbit is determined by the local data. Note that the connection is *short* only with respect to the local manifolds, that is with respect to a fixed choice of parameterizations P and Q, but we consider these to be fixed throughout.

We now define $F_{\text{short}} \colon V_{\nu_u} \times V_{\nu_s} \to \mathbb{R}^n$ by

$$F_{\text{short}}(\theta, \phi) = P(\theta) - Q(\phi) \tag{1.3}$$

and observe that if (θ_0, ϕ_0) satisfies $F_{\text{short}}(\theta_0, \phi_0) = 0$, then the orbit of

$$q_0 \overset{\text{def}}{=} P(\theta_0) = Q(\phi_0)$$

is a heteroclinic orbit from p_1 to p_2. We refer to the map in (1.3) as the *short-connection operator* and to the problem of finding zeros of (1.3) as *the short-connection problem.*

The second case is when the intersection of the local unstable manifold $W^u_{\text{loc}}(p_1)$ and the local stable manifold $W^s_{\text{loc}}(p_2)$ parameterized respectively by P and Q is empty. In this case we seek an orbit segment whose initial condition lies in $W^u_{\text{loc}}(p_1)$, and which terminates after some finite time $L > 0$ in $W^s_{\text{loc}}(p_2)$. These conditions are summarized explicitly by the boundary value problem

$$\begin{cases} \dfrac{d}{dt} u(t) = g(u(t)), \ t \in [0, L] \\ u(0) \in W^u_{\text{loc}}(p_1), \ u(L) \in W^s_{\text{loc}}(p_2). \end{cases}$$

We note that this is essentially the classical method of projected boundary conditions of [4,14,17]. We say that any such $u([0, L])$ is a *long-connection* from p_1 to p_2, in order to emphasize that we must now solve a boundary value problem for an orbit which begins and ends on the local manifolds.

Let $X = \mathbb{R}^n \times C([0, 1], \mathbb{R}^n)$, where $C([0, 1], \mathbb{R}^n)$ is the space of continuous function from $[0, 1]$ to $\mathbb{R}^n$. Using again the chart maps P and Q and rewriting the differential equation in integrated form with time rescaled by L leads to the operator $F_{\text{long}} : V_{\nu_u} \times V_{\nu_s} \times C([0, 1], \mathbb{R}^n) \to X$ defined by

$$F_{\text{long}}(\theta, \phi, u)(t) = \begin{pmatrix} Q(\phi) - \left(P(\theta) + L \int_0^1 g[u(\tau)]\, d\tau \right) \\ P(\theta) + L \int_0^t g[u(\tau)] d\tau - u(t) \end{pmatrix}. \tag{1.4}$$

If (θ_0, ϕ_0, u_0) satifies $F_{\text{long}}(\theta_0, \phi_0, u_0) = 0$ then u_0 is a heteroclinic connection from p_1 to p_2. The map (1.4) is called the *long-connection operator* and the problem of finding zeros of (1.4) is called the *long-connection problem*. A fundamental question follows.

Question 1 *Suppose we are given a "good enough" approximate zero of either operator* (1.3) *or* (1.4)*. Can we conclude the existence of a true solution? If yes, then how far from the approximate solution is the true solution? Is the resulting intersection transverse?*

To this end we introduce other assumptions. For the short-connection problem, suppose

A4s: that we are given $(\hat{\theta}, \hat{\phi}) \in V_{\nu_u} \times V_{\nu_s}$ so that $F_{\text{short}}(\hat{\theta}, \hat{\phi}) \approx 0$,
A5s: that g is real analytic in some neighborhood of image$[P] \cup$ image$[Q]$,

and for the long-connection problem, suppose

A4ℓ: that we are given $(\hat{\theta}, \hat{\phi}) \in V_{\nu_u} \times V_{\nu_s}$ and $\hat{u} \in C([0, 1], \mathbb{R}^n)$ so that $F_{\text{long}}(\hat{\theta}, \hat{\phi}, \hat{u}) \approx 0$,
A5ℓ: that g is real analytic in some neighborhood of image$[P] \cup$ image$[Q] \cup \hat{u}([0, 1])$.

Assumptions **A5** (s and ℓ) are redundant when g is real analytic on all of $\mathbb{R}^n$ (for example polynomial). The remainder of the present work is devoted to crafting a-posteriori techniques for the short and long-connection problems. The a-posteriori techniques allow us to address Question 1 under the assumptions **A1–A5**. Several remarks are in order.

Remark 1 (a) The definitions of F_{short} and F_{long} require knowing explicitly the chart maps P and Q. For this we follow the previous work of authors one and two with van den Berg and Mischaikow in [3,26] and exploit the so-called parameterization method for invariant manifolds [5–7]. This method facilitates the computation of polynomial approximations of the chart maps to any desired finite order and provides rigorous error bounds on the truncation errors. Moreover using the parameterization method we are able to exploit analytic properties of the chart maps in order to bound derivatives of the truncation errors as well. These polynomial approximations and their error bounds play a critical role in the a-posteriori analysis of the connecting orbit operators developed in the sequel.

(b) F_{short} is a finite dimensional map and, with the aid of the estimates mentioned in (a), we prove the existence of solutions using a boilerplate Newton–Kantorovich argument in finite dimension. On the other hand since F_{long} is an infinite dimensional operator, we must consider a finite dimensional projection. In this case the a-posteriori analysis is more delicate and it is advantageous to develop a contraction mapping argument which heavily exploits the particular form of the operator as well as the givens of the problem. We use the method of radii polynomials (e.g. see [13]) in order to obtain a sheaf of existence proofs, giving not only lower bounds on the approximation errors (distance from the approximation to the true solution) but also isolation bounds for the solution, that is lower and upper bounds on the size of the balls about $\hat{x}$ in function space where the solution is unique.

(c) A useful feature of our method is that transversality of the intersection of the stable and unstable manifolds comes *for free* from the existence proof of the connections. This is because for both short and long-connection problems we formulate our existence results in terms of showing that a given Newton-like operator is a contraction. (For the short connection problem this formulation is buried in the proof of the Newton–Kantorovich theorem). When we verify the hypotheses of the contraction mapping theorem, we have to show that a certain non-degeneracy condition is strictly less than one. In both the finite and infinite dimensional cases this will automatically yield that the differential of the Newton-like operator is boundedly invertible at the true solution. Since we will show that the bounded invertibility of the differential of the operator implies the transversality of the orbit itself, the transversality comes for free once the existence proof is completed. Compare this to topological methods of rigorous proof of connecting orbits (such as [2,8,25,41,44]) where the existence of an orbit is first treated by an index argument while the transversality is treated separately by either a cone-condition argument or another index argument in the tangent bundle.

(d) The advantage of using high-order approximations of the stable/unstable manifolds is that it allows us to solve the short/long connection operators in regions of phase space which are far from the equilibria. We can often arrange that the distance between the equilibrium and the boundary of the local manifold given by the image of the parameterization polynomial is one or more, with error bounds which are two or three hundred multiples of double precision machine epsilon. Compare this to the approximation by eigenspaces, where this same distance would have to be about 10^{-7} in phase space in order to obtain approximation errors of this magnitude.
Using the parameterization method we do not spend floating point operations integrating the orbit near the equilibria, where the dynamics are both slow and well understood. When we solve the boundary value problem for the connecting orbit we contend only with the global dynamics. Compare this to related methods such as [10,11,22,33,38] where both the global and local dynamics are studied simultaneously using a single operator equation. Note also that if we formulate our short and long connecting operators using the linear approximation of the invariant manifolds by their eigenspaces (with rigorous error bounds), then our method also reduces to a single operator equation both for the local and global dynamics.
The high order approximation of the invariant manifolds is like a *pre-conditioning* of the connecting operator which stabilizes the numerics by shortening the integration time along the approximate orbit, reducing so-called *wrapping effects* (or eliminating them entirely in the case of the short connections). This remark is worth stressing because we must not forget that while our final goal is to obtain abstract existence results, our methods are a-posteriori hence only work as well as the underlying non-rigorous numerics. Any pre-conditioning which improves the numerics allows us to push the rigorous component of the work further.

(e) While the boundary value problem for the connection is solved far from from the equilibria, our method also provides accurate information about the asymptotics of the connecting orbit. This is seen by considering the conjugacy conditions given by (1.1) and (1.2). Suppose for example that (θ_0, ϕ_0) is a solution of the short-connection problem $F_{\text{short}} = 0$. A finite orbit segment in parameter space is obtained by choosing any $T > 0$, and computing the parameter space segments

$$\gamma_u = e^{\Lambda_u[-T,0]}\theta_0 \subset V_{\nu_u} \text{ and } \gamma_s = e^{\Lambda_s[0,T]}\phi_0 \subset V_{\nu_s}.$$

For long enough T these orbits come as close as we like to the origins in their respective parameter spaces. By lifting the parameter arcs into phase space we obtain the orbit segment $u[-T,T] = P(\gamma_u) \cup Q(\gamma_s)$, which again begins and ends as close as we like to the equilibria. While the dynamics in parameter space are linear and hence easy to compute, the real advantage of using this conjugacy is that the dynamics in parameter space are either purely stable (in case of Λ_s) or purely unstable (in case of Λ_u). The hyperbolicity of the fixed points has in a sense been factored out of the problem, in the sense that the numerical errors which accumulate in parameter space never push $u[-T,T]$ away from the fixed points p_1 and p_2. Contrast this to the situation where we simply integrate the initial condition $P(\theta_0) = Q(\phi_0)$ in phase space. Since p_1 and p_2 are saddles the errors introduced by the numerical integration eventually drive the numerical orbit away from the neighborhood of the equilibria. Similar comments hold for long connections.

(f) Notice that the operators defined in (1.3) and in (1.4) are underdetermined. For example F_{short} maps a subset of $\mathbb{R}^{n_s+n_u} = \mathbb{R}^{n+1}$ into $\mathbb{R}^n$. This can be understood geometrically by realizing that any time shift of a finite heteroclinic orbit segment is again a heteroclinic orbit segment. The usual remedy to this situation is to introduce a *phase condition* which reduces the number of unknowns by one. In fact the set up of the operator equations using chart maps facilitates a natural choice of phase conditions in either the parameter space V_{ν_u} or V_{ν_s} (the situation is similar for the long-connection operator). This technical matter is postponed for the sake of the clarity of the present introduction, but is treated in detail below.

In practice locating the approximate heteroclinic connections even numerically can be one of the most difficult part of our method. Indeed locating connecting orbits numerically remains an active area of research (e.g. see [15,16,21,23] and the references therein). One situation where we may find saddle-to-saddle connections with little difficulty is just after a pitchfork bifurcation. If the bifurcation results in equilibria with saddle type stability, then the desired saddle-to-saddle heteroclinic connections are likely. In this setting a natural strategy is to look for short-connections just after the bifurcation has occurred (when the fixed points are still close to each other) and to follow the intersection of the local manifolds using parameter continuation. During this continuation scheme, the fixed points may move far enough apart so that the local manifolds no longer intersect, at which point the switch to the long-connection approach is appropriate.

This is the strategy we utilize in Sect. 7 of the present work. In fact it is interest in pitchfork bifurcations which motivates the entire short-connection/long-connection distinction. Therefore we note that while we do not peruse rigorous parameter continuation in the present work, the bifurcation setting both minimizes the difficulty of the non-rigorous numerical portion of the problem while also illustrating the utility of our approach in a context which is often of interest in applications. That being said, we stress again that this bifurcation setting is a convenience; our method depends only on having a "good enough" numerical approximation in hand (where much of the technicalities to follow arise in making precise the meaning of the term "good enough").

In order to illustrate the applicability of our method we consider the Lorenz equations

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} \sigma(y-x) \\ x(\rho - z) - y \\ xy - \beta z \end{pmatrix}, \tag{1.5}$$

which has an equilibrium solution $p_0 = (0, 0, 0)^T$, as well as a pair of real distinct equilibria $p_\pm = \left(\pm\sqrt{\beta(\rho-1)}, \pm\sqrt{\beta(\rho-1)}, \rho-1\right)$ when $\rho > 1$. We prove the following theorem.

Theorem 1 *Let $\sigma = -2.2$, $\beta = 8/3$, $U_1 = \{\rho_i = 1.33 + 0.01(i-1) : 1 \le i \le 187\}$ and $U_2 = \{\rho_i = 3.2 + 0.01(i-1) : 1 \le i \le 101\}$. For each $\rho \in U_1 \cup U_2$, the system (1.5) has a transverse, heteroclinic, saddle-to-saddle connection beginning at p_+ and terminating at p_0. By symmetry, there is also connection from p_- to p_0 for each $\rho \in U_1 \cup U_2$.*

The result is discussed more thoroughly in Sects. 7.1 and 7.2. However we note for the expert that the unorthodox choice of $\sigma < 0$ is so that the pitchfork bifurcation, which occurs a $\rho = 1$, results in the desired saddle-to-saddle stability. With the classical choice of $\sigma > 0$ the $\rho > 1$ bifurcation results in saddle-sink type stability, which is considerably easier to treat than the saddle-to-saddle connections treated here. (Saddle-sink connections simply require following the unstable manifold of the saddle into a trapping region of the sink. This situation, while very important, is somewhat less delicate as the stable manifold of the sink is a full neighborhood of the equilibria).

Before proceeding, a few remarks about the literature are in order. As already indicated above, substantial effort over the last quarter of a century has gone into the development of numerical methods for studying connecting orbits on the computer. The literature is vast, however the interested reader might consult [4,14,17] and the references therein. In more recent years a number of researchers have examined the problem of validating the results of classical numerical computations of connecting orbits. Therefore we stress that this work is by no means the first to develop a method for computer assisted proof of the existence of connecting orbits for differential equations. Since a thorough survey of the relevant literature would fall far outside the scope of the present work, we present only a brief sketch. It is our hope that by consulting the works cited here the interested reader might gain a clearer picture of the entire field.

The first computer assisted proof of the existence for connecting orbits that we know of is the work of [29]. Here a method for verifying the transverse intersection of stable and unstable manifolds of hyperbolic fixed points is implemented for a two dimensional discrete time dynamical system. Since then many powerful and general techniques have emerged for rigorous computer assisted study of connecting orbits. For example [10,11,22,33,38] develop methods for validating the existence of connecting orbits of both continuous and discrete time dynamical systems by solving boundary value problems on non-compact intervals (the real line or the integers depending on wether the system is continuous or discrete). These methods exploit shadowing results based on the theory of exponential dichotomies to analyze the behavior of the orbits as time goes to plus or minus infinity (that is to control the connecting orbit in the neighborhood of an equilibria).

Rigorous methods for studying invariant manifolds and connecting orbits between them based on smooth topological arguments in phase space (i.e. finite dimensional Brouwer degree theory and cone conditions) are developed in [18,19,44]. These methods are implemented as efficient numerical algorithms for validating connecting dynamics and chaotic motions (e.g. see [39–42]). Though we know of no examples of these methods being used to compute saddle-to-saddle connections between equilibria of differential equations without symmetry, it is clear that they could be so modified.

Other topological methods for proving existence of connecting orbits are based on Conley index theory, that is they are based on algebraic rather than differential topology. For a theoretical discussion of the Conley index in the context of differential equations see [9]. The so-called connection matrix of Conley theory can be used to prove existence of connecting orbits (e.g. see [25]). Some applications of Conley theoretic methods for studying connecting orbits with numerical implementations are found in [2,12,27].

Finally we mention the works of [3,28,31,43] as these are most closely related to the present work. These works treat rigorous numerics for solutions of boundary value problems using a-posteriori functional analytic arguments applied to some Newton-like operators. Specifically we remark that our work has much in common with the computer assisted proof of the existence of a homoclinic tangency in a one parameter family of planar vector fields that is implemented in [31] (note that this is a degenerate/non-transverse orbit and one must solve also for the parameter). Even closer to the present work is [3] where one finds a computer assisted proof scheme of the existence of symmetric homoclinic orbits in second order systems of ordinary differential equations (this method also incorporates the parameterization method in order to control the projected boundary conditions in a systematic way, but the intersections are not transverse, and the second order equations are more regular than the equations studied in the present work). The scheme of [3] is implemented in order to prove the existence of symmetric homoclinic connections at 30 distinct parameter values in the four dimensional Gray–Scott system.

The paper is organized as follows. In Sect. 2 we discuss the notation and background material used throughout the paper. In particular in Sect. 2.3 we review the parameterization method for invariant manifolds with an emphasis on rigorous numerics, and in Sect. 2.4 we recall some elementary results from the theory of differential equations. In Sect. 3 we develop two complementary validation methods, one based on the Newton–Kantorovich Theorem and the other based on the method of radii polynomials for infinite dimensional problems. In Sect. 4 we apply the Newton–Kantorovich Theorem to formulate an a-posteriori validation result for the short-connection problem. We go on to apply the method of radii polynomials to validate solutions to the long-connection problem in Sect. 5.

In Sect. 6 we demonstrate how the methods of proof in Sects. 4 and 5 in particular imply the transverse intersection of the stable and unstable manifolds. In Sect. 7 we discuss numerical examples and prove Theorem 1. The proofs at the parameter values $\rho \in U_1$ are done using the short-connection method in Sect. 7.1. The proofs at the remaining parameter values $\rho \in U_2$ are done using long-connections in Sect. 7.2. Finally some technical estimates and formulas used in the numerical implementation of the method are discussed in the appendices.

2 Background

This section serves as a review of the background material necessary for the rest of the paper. After introducing the spaces we work on in Sect. 2.1, we summarize some analytic results used in the a-posteriori analysis in Sect. 2.2. One main ingredient for this analysis is the parametrization method for invariant manifolds [5–7] which we treat in Sect. 2.3. We finish this preparatory section by recalling some basic facts from the theory of ordinary differential equations.

2.1 Spaces and Norms

We endow the spaces $\mathbb{R}$ and $\mathbb{C}$ with the usual real and complex absolute values and write $|x|$ for $x \in \mathbb{R}$ and $|z| = |x + iy| = \sqrt{x^2 + y^2}$ for $z \in \mathbb{C}$. If $x \in \mathbb{R}^2$ we have the Euclidean norm $\|x\|_2 = \sqrt{x_1^2 + x_2^2}$. For the finite dimensional vector spaces $\mathbb{C}^n$ and $\mathbb{R}^n$ we use several different norms depending on the situation.

- For $z \in \mathbb{C}^n$ we use the supremum norm

$$\|z\|_\infty = \max_{i=1,\ldots,n} |z_i|.$$

  Since this choice is used consistently we are safe with the abbreviation $\|z\|_\infty = |z|$ when it is clear from context that $z \in \mathbb{C}^n$.
- When $x \in \mathbb{R}^n$ is a point in the phase space of a real vector field we also use the supremum norm

$$\|x\|_\infty = \max_{i=1,\ldots,n} |x_i|.$$

  When it is clear from context that $x \in \mathbb{R}^n$ is a phase space variable we sometimes write $\|x\|_\infty = |x|$.
- When we formulate connecting orbit operators for real dynamical systems we deal with parameterizations having domain $\mathbb{R}^k$ and range $\mathbb{R}^n$ with $k \leq n$. Suppose $l, m \in \mathbb{N}$ with $l + 2m = k$. Then for $x \in \mathbb{R}^k$ we define the (l, m)-*cylindrical norm* on $\mathbb{R}^k$ to be

$$|x|_{(l,m)} = \max_{1\leq i\leq l} \max_{1\leq j\leq m} \left(|x_i|, \|(x_{l+2j-1}, x_{l+2j})\|_2\right).$$

We prefer to use the supremum norms when possible as they are easy to evaluate on the computer, introduce no extra rounding errors, and often minimizes the complexity of hand derived estimates. However for reasons which will be made clear in Sect. 2.3 the cylindrical norm is sometimes natural. For $\nu > 0$ the norms above induce the following neighborhoods.

- The *Euclidean* ν*-disk* centered at $x_0 \in \mathbb{R}^2$ is defined to be

$$D_\nu(x_0) = \left\{x \in \mathbb{R}^2 : \|x - x_0\|_2 < \nu\right\}.$$

- The *complex* ν*-polydisc* centered at $z_0 \in \mathbb{C}^m$ is defined to be

$$\mathbb{B}_\nu(z_0) = \left\{z \in \mathbb{C}^n : \|z - z_0\|_\infty < \nu\right\}.$$

- The *real* ν*-polydisk* (n-or cube) centered at $x_0 \in \mathbb{R}^n$ is defined to be

$$B_\nu(x_0) = \left\{x \in \mathbb{R}^n : \|x - x_0\|_\infty < \nu\right\}.$$

- For $l, m \in \mathbb{N}$ with $l + 2m = k$ the *real* ν*-polycylinder* centered at $x_0 \in \mathbb{R}^k$ is defined to be

$$V_\nu(x_0) = \left\{x \in \mathbb{R}^k : |x - x_0|_{(l,m)} < \nu\right\}.$$

We choose the name polycylinder as when $x_0 \in \mathbb{R}^3$ and $l = m = 1$, the set $V_\nu(x_0)$ is the usual cylinder centered at x_0. For sake of simplicity of the presentation, we introduce the notation $\mathbb{B}_\nu$ to denote $\mathbb{B}_\nu(0)$, the notation B_ν to denote $B_\nu(0)$, and the notation V_ν to denote $V_\nu(0)$. Note that

$$V_\nu = [-\nu, \nu]^l \times D_\nu^m,$$

which if $m = 0$ is a product of k intervals and if $l = 0$ is a product of $m/2$ Euclidian disks.

In preparation for the error analysis of the parametrization computation we topologize the space of analytic functions $f : \mathbb{B}_\nu \subset \mathbb{C}^m \to \mathbb{C}^n$ with the norm

$$\|f\|_\nu = \sup_{z\in\mathbb{B}_\nu} \|f(z)\|_\infty.$$

In addition, considering a power series expansion of f on $\mathbb{B}_\nu$ given by

$$f(z) = \sum_{|k|=0}^{\infty} b_k z^k, \quad (b_k \in \mathbb{C}^n),$$

where $k = (k_1, \ldots, k_m)$ is a multi-index, $|k| = \sum_{i=1}^m k_i$ and $z^k = \prod_{i=1}^m z_i^{k_i}$, define the norm

$$\|f\|_{\Sigma,\nu} = \sum_{|k|\geq 0}^{\infty} \|b_k\|_\infty \nu^{|k|}.$$

Note that $\|.\|_{\Sigma,\nu}$ is efficiently computable if f is a polynomial and that $\|f\|_\nu \leq \|f\|_{\Sigma,\nu}$. These facts will be exploited in our computations. In the a-posteriori analysis for the short and long-connections we will also have to control derivatives of the parametrizations. Therefore for matrix valued analytic functions $A : \mathbb{B}_\nu \subset \mathbb{C}^m \to \mathbb{C}^{n,n}$ we set

$$\|A\|_{M,\nu} = \sup_{z\in\mathbb{B}_\nu} \sup_{\|w\|_\infty=1} \|A(z)w\|_\infty.$$

The long-connection operator F_{long} given by (1.4) will be defined on the Banach space $X = \mathbb{R}^n \times C([0, 1], \mathbb{R}^n)$ which we endow with the norm

$$\|(\vartheta, u)\| = \max\left\{\|\vartheta\|_\infty, \|u\|_{C^0}\right\}$$

where $\vartheta \in \mathbb{R}^n$, $u = ([u]_1, [u]_2, \ldots, [u]_n)^T \in C([0, 1], \mathbb{R}^n)$ and $\|u\|_{C^0} = \max_{l=1,\ldots,n} \max_{t\in[0,1]} |[u]_l(t)|$.

2.2 Analytic Preliminaries

The following result, whose proof can be found in [26], allows estimating the derivatives of an analytic function of several complex variables given a bound on the supremum of the function itself, but on strictly smaller domain disks. The size of the bounds depends on how much domain we are *willing to give up*.

Lemma 1 (Cauchy Bounds) *Suppose that* $f : \mathbb{B}_\nu \subset \mathbb{C}^m \to \mathbb{C}^n$ *is bounded and analytic. Then for any* $0 < \sigma \leq 1$ *we have that*

$$\|\partial_i f\|_{\nu e^{-\sigma}} \leq \frac{2\pi}{\nu\sigma}\|f\|_\nu \quad \textit{so that} \quad \|Df\|_{M,\nu e^{-\sigma}} \leq \frac{2\pi m}{\nu\sigma}\|f\|_\nu,$$

as well as

$$\|\partial_i\partial_j f\|_{\nu e^{-\sigma}} \leq \frac{4\pi^2}{\nu^2\sigma^2}\|f\|_\nu \quad \textit{so that} \quad \left\|D^2 f\right\|_{\nu e^{-\sigma}} \leq \frac{4\pi^2 m^2}{\nu^2\sigma^2}\|f\|_\nu.$$

2.3 Parameterization of Invariant Manifolds

The present discussion is aimed at addressing the claims of **A3** in Sect. 1. To this end we review the necessary elements of the parameterization method for stable and unstable manifolds of hyperbolic equilibria of vector fields. We also discuss in detail how we obtain a real manifold when there are complex conjugate eigenvalues. For the full development in all generality see [5–7].

Recall that the general goal is to develop a rigorous computational method for the existence of a connecting orbit from p_1 to p_2. We restrict our attention to the computation of the stable manifold of p_2. The unstable manifold of p_1 can be obtained by time reversal. For ease of notation we will write $p = p_2$ and omit the script s (denoting the stable manifold) where no confusion results. Let $\lambda_1, \ldots, \lambda_{n_s}$ be as in assumption **A1** in Sect. 1. Without loss of generality there are l real eigenvalues $\lambda_1, \ldots, \lambda_l$ and m pairs of complex conjugate eigenvalues $\lambda_i, \bar{\lambda}_i$ for $i = 1, \ldots, m$. Note that $n_s = l + 2m$. We are looking for the parametrization $Q : V_\nu \subset \mathbb{R}^{n_s} \to \mathbb{R}^n$ having

$$Q[V_\nu] = W^s_{\text{loc}}(p).$$

The choice of the polycylinder V_ν as the domain will become clear momentarily.

For technical reasons it is preferable to work with holomorphic functions, so we begin by considering consider a complex valued extension

$$f : \mathbb{B}_\nu \subset \mathbb{C}^{n_s} \to \mathbb{C}^n$$

having that

$$f(0) = p, \quad Df(0) = \mathcal{A}, \tag{2.1}$$

where $\mathcal{A}$ is the matrix whose columns $\zeta_1, \ldots, \zeta_{n_s}$ are the possibly complex eigenvectors corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_{n_s}$. As in [3,5–7] we require that

$$g(f(z)) = Df(z)\Lambda z, \quad \text{for all} z \in \mathbb{B}_\nu, \tag{2.2}$$

where we recall that g is the vector field and $\Lambda \in \mathbb{C}^{n_s, n_s}$ is the diagonal matrix with the eigenvalues on the diagonal. Since g is real analytic we extend g to accept complex input in the usual way: namely by simply replacing the real variables in the power series expansion of g with complex variables. Equation (2.2) is referred to as the *invariance equation* for the chart map f. The parameterization method is built on the observation that if f is a solution of Eq. 2.2 satisfying the constraints of Eq. (2.1), then f is a chart map for the stable manifold. This is checked by differentiating (1.2) with respect to time and taking the limit as $t \to 0$ (with f replacing Q of course).

Once we have the parameterization $f : \mathbb{B}_\nu \to \mathbb{C}^n$ of the complex stable manifold we define the map Q in a real domain $V_\nu \subset \mathbb{R}^{n_s}$ by making the complex conjugate change of variables

$$\begin{aligned} Q(\phi_1, \ldots, \phi_l, \phi_{l+1}, \phi_{l+2}, \ldots, \phi_{l+2m-1}, \phi_{l+2m}) = f(\phi_1, \ldots, \phi_l, \phi_{l+1} \\ + i\phi_{l+2}, \phi_{l+1} - i\phi_{l+2}, \ldots, \phi_{l+2m-1} + i\phi_{l+2m}, \phi_{l+2m-1} - i\phi_{l+2m}). \end{aligned} \tag{2.3}$$

(So if $m = 0$ then Q is just the restriction of f to the real line and there is no complication). This change of variables makes it clear that the polydisk topology on $\mathbb{C}^{n_s}$ induces the polycylinder topology in $\mathbb{R}^{n_s}$, and is the reason that $V_\nu \subset \mathbb{R}^{n_s}$ is the natural domain of Q. It is also clear that the image of Q is a subset of the complex stable manifold of g. We will see in a moment why Q is real valued, and hence why the image of Q is the real local stable manifold as required by condition **A3** of the introduction.

Note that (2.2) is a system of first order partial differential equations with analytic data and first order constraints. The general formal approach is to consider the expansion

$$f(z) = \sum_{|k|=0}^{\infty} b_k z^k, \tag{2.4}$$

where $b_k \in \mathbb{C}^n$, $k = (k_1, \ldots, k_{n_s}) \in \mathbb{N}^{n_s}$ is a multi-index, z^k is given by $\Pi_{i=1}^{n_s} z_i^{k_i}$ and $|k| = \sum_{j=1}^{n_s} k_j$. The first order constraints give that

$$b_0 = p \qquad \text{and} \qquad b_{(0,\ldots,1,\ldots,0)} = \zeta_i,$$

where the 1 in $(0, \ldots, 1, \ldots, 0)$ is in the i-th position. The remaining coefficients are worked out by plugging the unknown power series (2.4) into the invariance Eq. (2.2), matching like powers and isolating the highest order terms in order to obtain recurrence relations for the k-th coefficient. It can be shown that this formal computation results in the linear system of equations

$$\left[Dg(p) - (k_1\lambda_1 + \ldots + k_{n_s}\lambda_{n_s})I\right] b_k = s_k, \tag{2.5}$$

which is known as the *homological equation* for the parameterization coefficients. Here s_k is a function of only multi-indices $\bar{k}$ with $|\bar{k}| < |k|$. The specific form of s_k is determined by the nonlinearity of g. In Appendix 1 we provide explicit formulas for the case where g is the Lorenz vector field.

Suppose that $m > 0$ and $1 \leq j \leq m$. Consider a multi-index

$$\alpha = (\alpha_1, \ldots, \alpha_{l+2j-1}, \alpha_{l+2j}, \ldots, \alpha_{l+2m}),$$

and define

$$\text{conj}_j(\alpha) = (\alpha_1, \ldots, \alpha_{l+2j}, \alpha_{l+2j-1}, \ldots, \alpha_{l+2m}).$$

Now one can check that, due to the symmetry properties of the homological Eq. (2.5), the power series coefficients of f satisfy

$$b_{\text{conj}_j(\alpha)} = \overline{b_\alpha},$$

where the bar denotes complex conjugate. In other words for every complex coefficient which appears in the power series expansion of f, its complex conjugate appears as well. Then evaluating f on complex conjugate variables results in a real value and the image of Q is real.

Let f_M be the M-th order polynomial approximation of f obtained by solving the homological equations (2.5) up to order M and let Q_M be the M-th order polynomial defined by the same complex conjugate change of variables as in Eq. (2.3). We now want to ascertain the quality of the approximation. The philosophy of a-posteriori analysis is the following: given the approximate parametrization Q_M, prove that there is an exact parametrization Q nearby. More precisely we will try to find a parameter disk $V_\nu \subset \mathbb{R}^{n_s}$ and a $\delta > 0$ such that

$$\|Q(\phi) - Q_M(\phi)\|_\infty < \delta, \quad \text{for all} \quad \phi \in V_\nu.$$

Theorem 4.2 in [3] provides numerically verifiable sufficient conditions under which this is possible. In the following we describe the necessary ingredients. Given an approximate solution $f_M : \mathbb{B}_\nu \subset \mathbb{C}^{n_s} \to \mathbb{C}^n$ to (2.2) fulfilling the constraints (2.1) with

$$f_M(z) = \sum_{|k|=0}^{M} b_k z^k, \tag{2.6}$$

we derive error bounds which by construction carry over to the real valued restriction given by (2.3). We define the following validation values.

Definition 1 *(Validation Values)* The collection of positive constants $\nu, \epsilon_{tol}, C_1, C_2, \rho', \rho$ and μ are called validation values if they possess the following properties.

1. $\|g \circ f_M - Df_M \Lambda\|_{\Sigma,\nu} < \epsilon_{tol}$.
2. $\|f_M\|_\nu \leq \rho' < \rho$.
3. $\|Dg(f_M)\|_{M,\nu} \leq C_1$.

4. $\max_{|\alpha|=2} \max_{1\leq j\leq n} \sup_{|z-p_0|\leq\rho} |\partial^\alpha g_j(p_0+z)| \leq C_2$.
5. $\max_{1\leq i\leq n_s} Re(\lambda_i) < -\mu$.

It is important that all these values can be computed rigorously using interval arithmetic. The following theorem is the basis of the a-posteriori analysis. We use as shorthand notation

$$N_g = \max_{j=1,\ldots,n} \#\{(k,l)|1 \leq k,l \leq n \quad \text{such that} \quad \partial^k\partial^l g_j \not\equiv 0\},$$

and suppose we are given constants such that

$$M_1 \geq N_g,$$
$$M_2 \geq \frac{n(n+2)^{n+2}}{(n+1)^{n+1}}.$$

Theorem 2 [Theorem 4.2 in [3]] *Suppose that for an approximation f_M in the sense of (2.6) we are given validation values as in Definition (1). Assume that M and δ fulfill*

$$(M+1)\mu - C_1 > 0,$$
$$\delta > \frac{2\epsilon_{tol}}{(M+1)\mu - C_1},$$
$$\delta < \min\left\{\frac{(M+1)\mu - C_1}{C_2 M_1 M_2}, \frac{\rho-\rho'}{n+2}\right\}.$$

Then there exists a unique solution $f : \mathbb{B}_\nu \to \mathbb{C}^n$ to (2.2) fulfilling the initial value constraints (2.1) such that

$$\|f - f_M\|_\nu \leq \delta. \tag{2.7}$$

Furthermore the series coefficients for $|k| > M$ satisfy the growth bounds $\|a_k\|_\infty \leq \frac{\delta}{\nu^{|k|}}$.

In particular it follows from (2.7) that

$$\|Q(\phi) - Q_M(\phi)\|_\infty < \delta, \quad \text{for all} \quad \phi \in V_\nu,$$

as we wished.

We remark that the proof actually shows that the truncation error $H(z) = f(z) - f_M(z)$ is itself an analytic function on $\mathbb{B}_\nu$ with $\|e\|_\nu \leq \delta$. In particular we know that $h(\phi) = Q(\phi) - Q_M(\phi)$ is a real analytic function with

$$\|h(\phi)\|_\infty \leq \delta, \quad \text{for all } \phi \in V_\nu.$$

Furthermore we can use classical estimates of complex analysis in order to obtain bounds on the derivatives of the truncation error on smaller disks. This observation is useful when formulating a-posteriori validation theorems for connecting orbits. When some of the eigenvalues occur in complex conjugate pairs we require the following adaption of the Cauchy bounds.

Remark 1 (Bounds on Derivatives When There Are Complex Conjugate Eigenvalue Pairs) Recall that in the case of complex conjugate pairs of eigenvalues $\lambda_{j+1} = \overline{\lambda}_j$ of $Dg(p)$, the parameterization of the real stable manifold is given by the complex conjugate change of variable in Eq. (2.3). If we think of this change of variable as a composition of functions then it is clear that in order to obtain bounds on derivatives of the real parameterization we must employ the chain rule.

In particular suppose for a component function $H\colon \mathbb{B}_\nu \subset \mathbb{C}^2 \to \mathbb{C}$, that $H(z, \bar{z}) \subset \mathbb{R}$ for each $z \in B_\nu$, and that $\|H\|_\nu \le \delta$. Let $h\colon V_\nu \subset \mathbb{R}^2 \to \mathbb{R}$ be defined by $h(\phi_1, \phi_2) = H(\phi_1 + i\phi_2, \phi_1 - i\phi_2)$. For $j = 1, 2$ we have

$$\frac{\partial}{\partial \phi_j} h(\phi_1, \phi_2) = -i^{j+1}\left(\frac{\partial}{\partial z} H(z, \bar{z}) + (-1)^{j+1}\frac{\partial}{\partial \bar{z}} H(z, \bar{z})\right). \tag{2.8}$$

Then for any $0 < \sigma \le 1$, applying Lemma 1 gives the bound

$$\left\|\frac{\partial}{\partial \phi_j} h\right\|_{\nu e^{-\sigma}} \le 2\left\|\partial_j H\right\|_{\nu e^{-\sigma}} \le \frac{4\pi}{\nu\sigma}\delta. \tag{2.9}$$

Taking another derivative requires applying the chain rule to both terms in Eq. (2.8), leading to four terms which must be bound, so that

$$\left\|\frac{\partial^2}{\partial \phi_j \partial \phi_k} h\right\|_{\nu e^{-\sigma}} \le \frac{16\pi^2}{\nu^2\sigma^2}\delta, \qquad \text{for} \qquad j, k = 1, 2. \tag{2.10}$$

Finally suppose that $f = f_M + H$ is the complex parameterization of a n_s dimensional real stable manifold given by Theorem 2. Suppose that there are l real distinct stable eigenvalues and m pairs of complex conjugate stable eigenvalues. Suppose that we have the bound $\|H\|_\nu \le \delta$ from Theorem 2. Then the parameterization of the real stable manifold is given by $Q = Q_M + h$ where Q_M and h are defined through the complex conjugate variables given in Eq. (2.3). Counting complex conjugate pairs of variables and applying the componentwise estimates given by Eqs. (2.9) and (2.10) gives by definition of $\|.\|_\nu$

$$\|DQ\|_{\nu e^{-\sigma}} \le \|DQ_M\|_\nu + \frac{(2l + 4m)\pi}{\nu\sigma}\delta, \tag{2.11}$$

and

$$\left\|D^2 Q\right\|_{\nu e^{-\sigma}} \le \|DQ_M\|_\nu + \frac{(2l + 4m)^2\pi}{\nu^2\sigma^2}\delta, \tag{2.12}$$

for any loss of domain parameter $0 < \sigma \le 1$. We note that for the applications to the two dimensional stable and unstable manifolds associated with a single complex conjugate pair of eigenvalues in the Lorenz equations considered in the present work we have that $l = 0$ and $m = 1$.

2.4 Flows and Vector Fields

In this section, we recall some elementary results from the theory of differential equations. Consider an analytic vector field $g\colon \mathbb{R}^n \to \mathbb{R}^n$ and $\Phi : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ the flow associated to the differential equation $\frac{du}{dt} = g(u)$. Given $\hat{z} \in \mathbb{R}^n$, let $\text{orbit}(\hat{z}) \overset{\text{def}}{=} \{\Phi(\hat{z}, t) \mid t \in \mathbb{R}\}$. The following result is classical.

Lemma 2 *Consider $\hat{z} \in \mathbb{R}^n$ and suppose that the set orbit$(\hat{z})$ is bounded in $\mathbb{R}^n$. Then the orbit of $\hat{z}$ defined by $\Phi(\hat{z}, t)$ is analytic at each $t \in \mathbb{R}$. Moreover, the flow operator $\Phi(\hat{z}, t)$ is a diffeomorphism for each $t \in \mathbb{R}$.*

Proof The proof that $\Phi(\hat{z}, t)$ is analytic at each $t \in \mathbb{R}$ is omitted. We show only that $\Phi(\hat{z}, t)$ is a diffeomorphism for each $t \in \mathbb{R}$. First notice that the differential

$$M(\hat{z}, t) \overset{\text{def}}{=} D\Phi(\hat{z}, t) \tag{2.13}$$

is solution of the variational equation

$$\frac{d}{dt}M(\hat{z},t) = Dg[\Phi(\hat{z},t)]M(\hat{z},t), \qquad M(\hat{z},0) = I.$$

But $Dg[\Phi(\hat{z},t)]$ is a matrix of functions which are analytic for all $t \in \mathbb{R}$. So this is just another analytic vector field. Then the solution $M(\hat{z},t)$ exists and is analytic. This means that the flow is differentiable at all points along orbit$(\hat{z})$. Note that we have

$$\Phi(\hat{z},t) = \hat{z} + \int_0^t g[\Phi(\hat{z},\tau)]\,d\tau,$$

and

$$M(\hat{z},t) = I + \int_0^t Dg[\Phi(\hat{z},\tau)]M(\hat{z},\tau)d\tau.$$

The flow has the semi-group property and for each $t \in \mathbb{R}$ we have the inverse

$$\Phi^{-1}(\hat{z},t) = \Phi(\hat{z},-t).$$

Let us now show that $[M(\hat{z},t)]^{-1}$ exists for all t. First, $\Phi^{-1}(\hat{z},t)$ exists for all time as it is just orbit$(\hat{z})$ with time reversed. Then $D[\Phi^{-1}(\hat{z},t)]$ exists for all $t \in \mathbb{R}$ by the same argument that was used to show that $M(\hat{z},t) = D\Phi(\hat{z},t)$ exists. Also, the implicit function theorem gives the invertibility of M. In fact we have that

$$\Phi^{-1}(\hat{z},t) = \hat{z} - \int_0^t g[\Phi(\hat{z},-\tau)]d\tau,$$

and

$$D\Phi^{-1}(\hat{z},t) = I - \int_0^t Dg[\Phi(\hat{z},-\tau)]M^{-1}(\hat{z},t)\,d\tau.$$

This can be used to give an explicit formula for $[D\Phi(\hat{z},t)]^{-1} = [M(\hat{z},t)]^{-1}$. That shows that the flow operator $\Phi(\hat{z},t)$ is a diffeomorphism for each $t \in \mathbb{R}$. □

Now let $p_1, p_2 \in \mathbb{R}^n$. Then the stable (unstable) manifold theorem gives that $W^u(p_1)$ and $W^s(p_2)$ are immersed real analytic n_u and n_s dimensional manifolds respectively.

Lemma 3 *Suppose that $W^u(p_1) \cap W^s(p_2)$ is transverse at $\hat{z} \in \mathbb{R}^n$. Then the intersection is transverse and nonempty at $\Phi(\hat{z},t)$ for each $t \in \mathbb{R}$.*

Proof If $\hat{z}$ is on both manifolds then orbit$(\hat{z})$ is a heteroclinic connection from p_1 to p_2. As such it is contained in some compact set D. Then the flow Φ is a diffeomorphism along the orbit of $\hat{z}$ by Lemma (2). Since the intersection is transverse at $\hat{z}$ the tangent spaces $T_{\hat{z}}W^u(p_1)$ and $T_{\hat{z}}W^s(p_2)$ span $\mathbb{R}^n$ at $\hat{z}$. Let A be a matrix whose columns span $T_{\hat{z}}W^u(p_1)$ and B be a matrix whose columns span $T_{\hat{z}}W^s(p_2)$ (that is we pick bases for the tangent spaces at $\hat{z}$). Then if $C = [A|B]$ is the matrix obtained by concatenating the columns of A and B, we have that the columns of C span $\mathbb{R}^n$ by transversality.

Recalling (2.13), one has that the invariance of $W^u(p_1)$ and $W^s(p_2)$ gives that $M(\hat{z},t)A$ and $M(\hat{z},t)B$ transport the basis at $\hat{z}$ to $T_{\Phi(\hat{z},t)}W^u(p_1)$ and $T_{\Phi(\hat{z},t)}W^s(p_2)$ respectively for any $t \in \mathbb{R}$. Since Φ is a diffeomorphism along orbit$(\hat{z})$ it follows that the matrix $[M(\hat{z},t)A|M(\hat{z},t)B]$ spans $\mathbb{R}^n$. But then $W^u(p_1) \cap W^s(p_2)$ is transverse at $\Phi(\hat{z},t)$ (precisely because the tangent spaces span $\mathbb{R}^n$ there). Since t was arbitrary we have the transversality of any finite orbit segment. □

3 Validation of Solutions to Operator Equations

In Sect. 1 we showed that finding connecting orbits between equilibria $p_{1,2}$ is equivalent to finding zeros of the operators F_{short} defined in (1.3) for short, respectively F_{long} defined in (1.4) for long connections. Our goal in this section is to describe general validation methods for solutions to operator equations of the form

$$F(x) = 0, \qquad x \in X, \tag{3.1}$$

where X is a possibly infinite dimensional Banach space and F is a Fréchet differentiable mapping. We start with the classical Newton–Kantorovich Theorem that we will apply in order to validate solutions to the finite dimensional Eq. (1.3). While being valid in infinite dimensional settings like in Eq. (1.4), its numerical application bears some hurdles that we circumvent by using the method of radii polynomials described in the sequel. In both cases we obtain results that guarantee that the derivative $DF(\hat{x})$ at a solution $\hat{x}$ of (3.1) is invertible, hence yielding transversality of the orbits (see Sect. 6).

3.1 Newton–Kantorovich Theorem

The Newton–Kantorovich Theorem is a classical result in nonlinear analysis giving information about the convergence behavior of the Newton iteration. Stated in the following way we can use it to validate solutions to (3.1) in the sense that we find a ball around an approximate solution x_* in which we can guarantee a unique genuine solution $\hat{x}$ to exist.

Theorem 3 (Newton–Kantorovich Theorem) *Let $(X, \|\cdot\|_X)$ be a Banach space and $F : X \to X$ be a Fréchet differentiable mapping. Consider $x_* \in X$, $r > 0$ and $B_r(x_*) \subset X$ the closed ball of radius r centered at x_*. Let $B(X)$ be the space of bounded linear operators on X with the operator norm $\|\cdot\|_{B(X)}$. Assume that*

(i) $DF(x_*)$ has a bounded inverse, and
(ii) $\|DF(x) - DF(y)\|_{B(X)} \leq \kappa \|x - y\|_X$ for all $x, y \in B_r(x_*)$,

for $\kappa \geq 0$. If

(I)

$$\epsilon_{NK} \geq \left\| DF(x_*)^{-1} F(x_*) \right\|_X,$$

(II)

$$\epsilon_{NK} \leq \frac{r}{2},$$

and

(III)

$$4\epsilon_{NK}\, \kappa \left\| DF(x_*)^{-1} \right\|_{B(X)} \leq 1,$$

then there is a unique $\hat{x} \in B_r(x_*)$ so that $F(\hat{x}) = 0$.

A proof of Newton–Kantorovich Theorem can be found in [32]. In order to use Theorem 3 to validate a numerical approximation to a solution of (3.1) defined on a finite dimensional space X we take the following steps:

1. Check if $\|DF^{-1}(x_*)\|_{B(X,Y)}$ is bounded.
2. Compute ϵ_{NK} such that

$$\left\|DF(x_*)^{-1}F(x_*)\right\|_X \leq \epsilon_{NK} \tag{3.2}$$

3. Set $r = 2\epsilon_{NK}$.
4. Compute κ for this r.
5. Check if

$$4\epsilon_{NK}\kappa \left\|DF^{-1}(x_*)\right\|_{B(X)} \leq 1. \tag{3.3}$$

By using interval arithmetic we can check the strict inequality in (3.3). The benefit is that we can exploit the following lemma to ascertain invertibility of $DF(\hat{x})$.

Corollary 1 (Bounded Invertibility of the Inverse) *Let x_*, ϵ_{NK}, κ, $\|DF(x_*)^{-1}\|_{B(X)}$, r, and $\hat{x}$ be as Theorem 3. In addition suppose that $r \leq 4\epsilon_{NK}$ and that the strict inequality*

$$4\epsilon_{NK}\kappa \left\|DF(\hat{x})^{-1}\right\|_{B(X)} < 1,$$

is satisfied. Let M be any constant with $4\epsilon_{NK}\kappa\|DF(x_*)^{-1}\|_{B(X)} \leq M < 1$. Then $DF(\hat{x})$ is invertible and

$$\|DF(\hat{x})^{-1}\|_{B(X)} \leq \frac{\|DF(x_*)^{-1}\|_{B(X)}}{1-M}.$$

Proof Apply a Neumann Series argument to the expression

$$DF(\hat{x}) = DF(x_*)\left[I - DF(x_*)^{-1}\left(DF(x_*) - DF(\hat{x})\right)\right]. \qquad \square$$

Note that since $r = 2\epsilon_{NK}$ step 3 above we always have $r \leq 4\epsilon_{NK}$ as needed for the Lemma. Then if in step 5 we actually have strict inequality the invertibility follows directly from the Lemma. (We note that it is unlikely bordering on impossible that exact equality will occur in this step using interval arithmetic).

The point distinguishing the finite from the infinite dimensional setting is that in the finite dimensional case we can estimate ϵ_{NK} and κ directly by evaluating F and DF using interval arithmetic. When working on infinite dimensional spaces the additional error produced by discretizing X has to be taken into account. Hence, it is more difficult to get estimates for ϵ_{NK} and κ, as we can neither evaluate the operator F nor its derivative DF numerically. One strategy to cope with this problem raised by infinite dimensionality is to use the method of radii polynomials that we shall describe in the next section.

3.2 Method of Radii Polynomials

The notion of the radii polynomials provides an efficient means of determining a domain on which the contraction mapping theorem is applicable in order to validate a numerical solution to an equation of the form (3.1). These polynomials were originally developed to compute rigorously equilibria of partial differential equations in [13]. In particular this method is suitable for establishing the existence of a unique solution to Eq. (3.1) on an *infinite dimensional* Banach space X, providing additionally rigorous error bounds on the approximate solution. The fundamental strategy consists in considering a splitting

$$X = X_k \oplus X_\infty,$$

into a k-dimensional rounding space $X_k \cong \mathbb{R}^k$ with corresponding norm $\|\cdot\|_{X_k}$ and an infinite dimensional error space X_∞ with norm $\|\cdot\|_{X_\infty}$ induced by $\|\cdot\|$. Note that $\left(X_k, \|\cdot\|_{X_k}\right)$ and $\left(X_\infty, \|\cdot\|_{X_\infty}\right)$ are assumed to be Banach spaces and denote by 0_k the zero in X_k and 0_∞ the zero in X_∞. Let $\Pi_k : X \to X_k$ and $\Pi_\infty : X \to X_\infty$ be the generically induced projections. For $x \in X$ we write $x = (x_k, x_\infty)$, with $x_k \stackrel{\text{def}}{=} \Pi_k x$ and $x_\infty \stackrel{\text{def}}{=} \Pi_\infty x$. Furthermore we have the splitting of the operator

$$F = F_k \oplus F_\infty \stackrel{\text{def}}{=} \Pi_k F \oplus \Pi_\infty F. \tag{3.4}$$

To find a solution of (3.1), we compute a finite dimensional approximate solution $x_* \in X$ such that $F_k(x_*) \approx 0$, and show that within a certain set $B_{x_*}(r)$ there is a unique solution to $F = 0$. More precisely the set is given by $B_{x_*}(r) = x_* + B(r, \omega)$, where

$$B(r, \omega) \stackrel{\text{def}}{=} \{x \in X : \|x_k\|_{X_k} \leq r \quad \text{and} \|x_\infty\|_{X_\infty} \leq \omega r\}, \tag{3.5}$$

with a fixed parameter ω that can be used to control the infinite dimensional error. Note that the dependence of the set $B_{x_*}(r)$ on the variable radius r is a-priori unknown, and that the idea of the method of radii polynomials is to solve for a suitable r_* such that a corresponding fixed point operator T is a contraction on $B_{x_*}(r)$. Using the contraction mapping theorem this leads to the existence of a unique solution of (3.1) in $B_{x_*}(r)$.

Before turning to the explicit definition of the fixed point operator T we elaborate more about the numerical setup. Consider an isomorphism $i : \mathbb{R}^k \to X_k$ and define $F^k = i^{-1} \circ F_k \circ \tau$, where the embedding $\tau : \mathbb{R}^k \to X_k \oplus \{0_\infty\}$ is defined by $x \mapsto (i(x), 0_\infty)$. For sake of simplicity we identify X_k and $\mathbb{R}^k$, as well as $x_k \in X_k$ and $i^{-1}(x_k) \in \mathbb{R}^k$. In particular we write $x = (x_k, x_\infty) = ([x_k]_1 \ldots, [x_k]_k, x_\infty)$. Note that $F^k : \mathbb{R}^k \to \mathbb{R}^k$ and we can use standard numerical techniques (e.g. Newton's method, continuation techniques) in order to compute an approximate solution x_k^* of

$$F^k(x_k) = 0. \tag{3.6}$$

From the above construction, one has that $x_* = \tau(x_k^*)$ is an approximate solution of (3.6). In order to define T, assume first that the following assumptions (**RP**) are fulfilled.

- **RP1.** We have computed an approximate solution $x_* = (x_k^*, 0_\infty)$ for (3.6), that is there exists a *small* $\epsilon > 0$ such that $\|F^k(x_k^*)\|_{X_k} \leq \epsilon$.
- **RP2.** We have computed the Fréchet derivative $A_k = DF^k(x_k^*)$.
- **RP3.** We have computed an approximate inverse $A_k^\dagger$ for A_k.
- **RP4.** $A_k^\dagger$ is injective.

Then define the fixed point operator $T : X \to X$ to be

$$T(x) = (x_k - A_k^\dagger F_k(x)) \oplus (F_\infty(x) + x_\infty). \tag{3.7}$$

Lemma 4 *Let $x \in X$. Then $F(x) = 0$ if and only if $T(x) = x$.*

Proof Assume $F(x) = 0$. By (3.4), one has that $F_k(x) = 0_k$ and $F_\infty(x) = 0_\infty$. Therefore $T(x) = x_k \oplus x_\infty = x$. On the other hand if $T(x) = x$ it follows that $A_k^\dagger F_k(x) = 0_k$ and by injectivity of $A_k^\dagger$ this amounts to $F_k(x) = 0_k$. Furthermore we have $F_\infty(x) = 0_\infty$ and by (3.4) it follows that $F(x) = 0 \in X$. □

We are now in the position to explain what we mean by finding a suitable radius r_* and how it is determined. Since we aim at applying the contraction mapping theorem to $B_{x_*}(r)$, we have to show that $T(B_{x_*}(r)) \subset B_{x_*}(r)$ and that T is a contraction on $B_{x_*}(r)$. In order to do so, we consider the residual function

$$y \stackrel{\text{def}}{=} T(x_*) - x_* = -A_k^\dagger F_k(x_*) \oplus F_\infty(x_*). \tag{3.8}$$

First let us assume that we are given positive constants $Y_1, \dots, Y_k$ and Y_∞ such that

$$|\,[\Pi_k y]_l\,| \le Y_l, \quad \text{for all} \quad l = 1, \dots, k \tag{3.9}$$

and

$$\|\Pi_\infty y\|_{X_\infty} \le Y_\infty. \tag{3.10}$$

To show that T is a contraction, we introduce, for $x_1, x_2 \in B(r, \omega)$, the quantity

$$z(x_1, x_2) \stackrel{\text{def}}{=} DT(x_* + x_1)x_2. \tag{3.11}$$

Realize that $z(x_1, x_2)$ is linear in x_2. Assume further that we are given polynomials bounds $Z_1(r), \dots, Z_k(r)$ and $Z_\infty(r)$ satisfying

$$\sup_{x_1, x_2 \in B(r,\omega)} |[\Pi_k(z(x_1, x_2))]_l| \le Z_l(r), \quad \text{for all} \quad l = 1, \dots, k, \tag{3.12}$$

and

$$\sup_{x_1, x_2 \in B(r,\omega)} \|\Pi_\infty(z(x_1, x_2))\|_{X_\infty} \le Z_\infty(r). \tag{3.13}$$

Using the above ingredients we define the radii polynomials.

Definition 2 Assume we are given bounds as in (3.9) and (3.10) and polynomial bounds as in (3.12) and (3.13). Then define for $l = 1, \dots, k$ the finite radii polynomials

$$p_l(r) = Y_l + Z_l(r) - r$$

and, given a number $\omega > 0$, define the tail radii polynomial

$$p_\infty(r) = Y_\infty + Z_\infty(r) - \omega r.$$

Let us now state the main result, whose proof can be found in [3].

Theorem 4 [Theorem 2.6 in [3]] *If there exists an $r_* > 0$ such that $p_l(r_*) < 0$ for all $l = 1, \dots, k$ and $p_\infty(r_*) < 0$ then T is a contraction on $B_{x_*}(r_*)$ and hence there exists a unique zero $\hat{x}$ of (3.1) in $B_{x_*}(r_*)$.*

Remark 3 The bounds $Y_1, \dots, Y_k$ and $Z_1(r), \dots, Z_k(r)$ defined in (3.9) and (3.12) are the direct analogues of ϵ_{NK} and κ that are also found numerically. The additional bounds Y_∞ and $Z_\infty(r)$ are introduced in order to control the truncation error introduced by discretization.

Just as in the Newton–Kantorovich context we have the following lemma that assures invertibility of the derivative $DF(\hat{x})$ at a zero of (3.1) found by using the method of radii polynomials.

Corollary 2 *Assume that the hypotheses of Theorem 4 are satisfied and consider $\hat{x}$ the unique fixed point of T within $B_{x_*}(r) = x_* + B(r, \omega)$. Then the linear operator $DF(\hat{x}) : X \to X$ is invertible.*

Proof Recalling (5.2) and (5.3), we define a norm on X as follows. Given $x \in X$, consider the weighed norm on X by

$$\|x\|_X = \max\left\{\|\Pi_k x\|_{X_k}\ ,\ \frac{1}{\omega}\|\Pi_\infty x\|_{X_\infty}\right\}. \tag{3.14}$$

Recalling (3.5), the closed unit ball in X with respect to norm (3.14) is $B(1,\omega)$. Then, letting x_* be the center of the ball $B_{x_*}(r)$, there exists $x_1 \in B(r,\omega)$ such that $\hat{x} = x_* + x_1$. Recalling (3.12) and (3.13) and from the fact that each radii polynomial $p_l(r) < 0$, we then get that

$$\begin{aligned}\|DT(\hat{x})\|_X &= \sup_{x\in B(1,\omega)} \|DT(\hat{x})x\|_X = \frac{1}{r}\sup_{x\in B(1,\omega)} \|DT(x_*+x_1)xr\|_X \\ &= \frac{1}{r}\sup_{x\in B(1,\omega)}\left\{\max\left\{\|\Pi_k DT(x_*+x_1)xr\|_{X_k}\ ,\ \frac{1}{\omega}\|\Pi_\infty DT(x_*+x_1)wr\|_{X_\infty}\right\}\right\} \\ &\le \max\left\{\frac{Z_0}{r},\frac{Z_1}{r},\frac{Z_2}{r},\ldots,\frac{Z_{n(m+2)}}{r},\frac{Z_\infty}{r}\right\} \\ &< 1.\end{aligned}$$

Using Neumann series, we get that the operator $I - DT(\hat{x}) : X \to X$ is invertible. Since

$$T(x) = (\Pi_k - A_k^\dagger \Pi_k F)(x) + \Pi_\infty(F(x)+(x)) = x - A_k^\dagger \Pi_k F(x) + \Pi_\infty F(x),$$

then

$$I - DT(\hat{x}) = -A_k^\dagger \Pi_k DF(\hat{x}) + \Pi_\infty DF(\hat{x}).$$

Suppose that there exists $y \in X$ such that $DF(\hat{x})y = 0$. Then $\Pi_k DF(\hat{x})y = 0$ ($\overset{A_k^\dagger \text{ invertible}}{\Longleftrightarrow}$ $-A_k^\dagger \Pi_k DF(\hat{x})y = 0$) and $\Pi_\infty DF(\hat{x})y = 0$. Hence

$$[I - DT(\hat{x})]y = -A_k^\dagger \Pi_k DF(\hat{x})y + \Pi_\infty DF(\hat{x})y = 0$$

which implies that $y = 0$ by invertibility of $I - DT(\hat{x})$. That implies that $DF(\hat{x})$ is injective. We want to show that $DF(\tilde{x})$ is surjective. Consider $w \in X$ (we want to construct $y \in X$ such that $w = DF(\hat{x})y$). Let $w_k \overset{\text{def}}{=} \Pi_k w$ and $w_\infty \overset{\text{def}}{=} \Pi_\infty w$. Define $z_k = -A_k^\dagger w_k$, $z_\infty = w_\infty$ and $z = z_k + z_\infty \in X$. We know by surjectivity of $I - DT(\hat{x})$ that there exists $y \in X$ such that

$$z = [I - DT(\hat{x})]y = -A_k^\dagger \Pi_k DF(\hat{x})y + \Pi_\infty DF(\hat{x})y.$$

Hence, $z_k = \Pi_k z = -A_k^\dagger \Pi_k DF(\hat{x})y$ and $z_\infty = \Pi_\infty z = \Pi_\infty DF(\hat{x})y$. The invertibility of $A_k^\dagger$ (see **RP4** above) implies that $w_k = -(A_k^\dagger)^{-1} z_k = \Pi_k DF(\hat{x})y$. We can therefore conclude that $w = w_k + w_\infty = \Pi_k DF(\hat{x})y + \Pi_\infty DF(\hat{x})y = DF(\hat{x})y$. ◻

4 Rigorous Numerics for Short Connections

We now turn the five step method for checking the hypotheses of the Newton–Kantorovich Theorem discussed in Sect. 3.1 into a validation method for the short-connection problem. In order to achieve this we need to introduce a phase condition that we describe in the next section. Using Cauchy bounds, we formulate an a-posteriori validation theorem for the short-connection problem.

Throughout this section we assume that assumptions **A1–A3** and **A4**s–**A5**s of Sect. (1) are satisfied. To ease notation we let $F = F_{\text{short}}$.

4.1 Phase Condition

In order to interpret the heteroclinic connection from p_1 to p_2 as an *isolated* zero of an operator we need to introduce a phase condition for F. The reason for this is that from **A2**, we know that F maps a subset of $\mathbb{R}^{n+1}$ into $\mathbb{R}^n$, that is $F\colon V_{\nu_u} \times V_{\nu_s} \subset \mathbb{R}^{n_u+n_s} = \mathbb{R}^{n+1} \to \mathbb{R}^n$. Hence, we cannot expect $DF(\theta, \phi)$ to be invertible or in other words there are no isolated zeros of F as currently defined. To remedy the situation we exploit the chart map formulation or the short-connection operator which allows us to impose a generic phase condition in parameter space.

Let $\Theta_\nu\colon B_1 \subset \mathbb{R}^{n_u-1} \to \text{int}\left(V_{\nu_u}\right) \subset \mathbb{R}^{n_u}$ be an immersion of the $(n_u - 1)$-sphere of radius ν, where we recall that B_1 is the unit euclidean ball of radius 1. Moreover we require that image(Θ_ν) is transverse to the linear vector field Λ_u in unstable parameter space. This transversality condition insures that for any $\alpha \in B_1$ the columns of $D\Theta_\nu(\alpha)$ and the single vector $\Lambda_u\Theta_\nu(\alpha)$ are a linearly independent set of vectors which span $\mathbb{R}^{n_u}$. Then the columns of $DP[\Theta_\nu(\alpha)]\Theta_\nu(\alpha)$ and the vector $DP[\Theta_\nu(\alpha)]\Lambda_u\Theta_\nu(\alpha)$ span $T_{P[\Theta_\nu(\alpha)]}W^u(p_1)$. Note that since the dynamics on the manifold are conjugate to the linear dynamics in parameter space we know that $DP[\Theta_\nu(\alpha)]\Lambda_u\Theta_\nu(\alpha)$ is the tangent vector to the orbit through $P[\Theta_\nu(\alpha)]$. Then the columns of $DP[\Theta_\nu(\alpha)]D\Theta_\nu(\alpha)$ span the subspace of $T_{P[\Theta_\nu(\alpha)]}W^u(p_1)$ perpendicular to the orbit.

We thus redefine F by $F\colon B_1 \times V_{\nu_s} \subset \mathbb{R}^{n_u-1} \times \mathbb{R}^{n_s} = \mathbb{R}^n \to \mathbb{R}^n$ given by

$$F(\alpha, \phi) = P[\Theta_\nu(\alpha)] - Q(\phi). \tag{4.1}$$

with the effect that F maps $\mathbb{R}^n$ into itself and the Newton–Kantorovich technique is applicable.

Remark 4 In practice we can take Θ_ν to be a parameterization of the $(n_u - 1)$-dimensional sphere with radius ν small enough so that the sphere is contained in V_{ν_u}.

4.2 Validation

Let F be the modified short-connection operator defined by (4.1). We combine the notation of assumptions **A1–A3** and **A4**s–**A5**s of Sect. 1 with the results of Sect. 2.3 and see that in practice the parameterizations $P\colon V_{\nu_u} \subset \mathbb{R}^{n_u} \to \mathbb{R}^n$ and $Q\colon V_{\nu_s} \subset \mathbb{R}^{n_s} \to \mathbb{R}^n$ have the form

$$P(\theta) = P_N(\theta) + h_u(\theta), \qquad Q(\phi) = Q_M(\phi) + h_s(\phi),$$

where P_N and Q_M are known N-th and M-th order polynomials respectively, and h_u, h_s are analytic functions on $V_{\nu_u} \subset \mathbb{R}^{n_u}$ and $V_{\nu_s} \subset \mathbb{R}^{n_s}$ respectively. We suppose that there are l_s, l_u real distinct stable and unstable eigenvalues, and m_s, m_u pair of complex conjugate pair of stable and unstable eigenvalues associated with p_1 and p_2.

Moreover we have known constants $\delta_u, \delta_s > 0$ so that

$$\sup_{\theta \in V_{\nu_u}} |h_u(\theta)| \leq \delta_u \qquad \text{and} \qquad \sup_{\phi \in V_{\nu_s}} |h_s(\phi)| \leq \delta_s.$$

We expand (4.1) as

$$\begin{aligned} F(\alpha,\phi) &= P[\Theta_\nu(\alpha)] - Q(\phi) \\ &= P_N[\Theta_\nu(\alpha)] + h_u[\Theta_\nu(\alpha)] - Q_M(\phi) - h_s(\phi) \\ &= P_N[\Theta_\nu(\alpha)] - Q_M(\phi) + (h_u[\Theta_\nu(\alpha)] - h_s(\phi)) \\ &=: F_{(M,N)}(\alpha,\phi) + H(\alpha,\phi), \end{aligned} \tag{4.2}$$

and note that

$$\begin{aligned} DF(\alpha,\phi) &= DF_{(M,N)}(\alpha,\phi) + DH(\alpha,\phi) \\ &= [DP_N(\Theta_\nu(\alpha))D\Theta_\nu(\alpha)| - DQ_M(\phi)] \\ &\quad + [Dh_u(\Theta_\nu(\alpha))D\Theta_\nu(\alpha)| - Dh_s(\phi)], \end{aligned} \tag{4.3}$$

so that

$$\begin{aligned} D^2F[\alpha,\phi](u,v) &= D^2F[\alpha,\phi]((u_1,u_2),(v_1,v_2)) \\ &= D^2P_N[\Theta_\nu(\alpha)](D\Theta_\nu(\alpha)u_1, D\Theta_\nu(\alpha)v_1) + DP_N(\Theta_\nu(\alpha))D^2\Theta_\nu(\alpha)(u_1,v_1) \quad (4.4) \\ &\quad + D^2h_u[\Theta_\nu(\alpha)](D\Theta_\nu(\alpha)u_1, D\Theta_\nu(\alpha)v_1) + Dh_u(\Theta_\nu(\alpha))D^2\Theta_\nu(\alpha)(u_1,v_1) \\ &\quad + D^2Q_M(\phi)(u_2,v_2) + D^2h_s(\phi)(u_2,v_2). \end{aligned}$$

We interpret assumption **A4**s as having an approximate zero of $F_{(M,N)}$. Our strategy is to treat this as an approximate zero of the full operator F and then apply Theorem 3 a-posteriori. In order to formalize this notion we make the following definition.

Definition 3 (Short-connections validation values) We call $\alpha_* \in B_1 \subset \mathbb{R}^{n_u-1}$, $\phi_* \in B_{\nu_s} \subset \mathbb{R}^{n_s}$ and the positive constants $\epsilon, \sigma_u, \sigma_s, C_1, C_2, \tilde{C}_1, \tilde{C}_2, \tilde{C}_3, \tilde{C}_4, \hat{C}_1, \hat{C}_2, M$, and r *validation values for the short-connection problem* if

(i)

$$|\Theta_\nu(\alpha_*)|_{l_u,m_u} < \nu_u \quad \text{and} \quad |\phi_*|_{l_s,m_s} < \nu_s,$$

(ii)

$$\sigma_u \le -\ln\left(\frac{|\Theta_\nu(\alpha_*)|_{l_u,m_u}}{\nu_u}\right) \quad \text{and} \quad \sigma_s \le -\ln\left(\frac{|\phi_*|_{l_s,m_s}}{\nu_s}\right),$$

(iii)

$$\left|F_{(M,N)}(\alpha_*,\phi_*)\right| \le \epsilon,$$

(iv)

$$\left\|[DF_{(M,N)}(\alpha_*,\phi_*)]^{-1}\right\|_M \le C_1,$$

(v)

$$\|D\Theta_\nu(\alpha_*)\|_M \le C_2,$$

(vi)

$$\pi C_1\left(\frac{(2l_u+4m_u)C_2}{\nu_u\sigma_u}\delta_u + \frac{2l_s+4m_s}{\nu_s\sigma_s}\delta_s\right) \le M,$$

(vii)

$$\frac{2C_1}{1-M}(\epsilon + \delta_u + \delta_s) \le r,$$

(viii)

$$\sup_{|\alpha-\alpha_*|<r} \|DP_N(\Theta_\nu(\alpha))\|_M \le \tilde{C}_1, \qquad \sup_{|\alpha-\alpha_*|<r} \left\|D^2 P_N(\Theta_\nu(\alpha))\right\|_M \le \tilde{C}_2,$$

$$\sup_{|\alpha-\alpha_*|<r} \|D\Theta_\nu(\alpha)\|_M \le \tilde{C}_3, \qquad \sup_{|\alpha-\alpha_*|<r} \left\|D^2 \Theta_\nu(\alpha)\right\|_M \le \tilde{C}_4,$$

(ix)

$$\sup_{|\phi-\phi_*|<r} \|DQ_M(\phi)\|_M \le \hat{C}_1, \qquad \sup_{|\phi-\phi_*|<r} \left\|D^2 Q_M(\phi)\right\|_M \le \hat{C}_2.$$

Theorem 5 (A-posteriori existence of a short-connection) *Suppose that α_*, ϕ_*, ϵ, σ_u, σ_s, C_1, C_2, $\tilde{C}_1$, $\tilde{C}_2$, $\tilde{C}_3$, $\tilde{C}_4$, $\hat{C}_1$, $\hat{C}_2$, M, and r are validation values for the short-connection problem in the sense of Definition 3. Suppose that $M < 1$ and that*

(h1)

$$0 < \hat{\sigma}_u \le -\ln\left(\frac{|\Theta[B_r(\alpha_*)]|_{l_u,m_u}}{\nu_u}\right),$$

(h2)

$$0 < \hat{\sigma}_s \le -\ln\left(\frac{|B_r(\phi_*)|_{l_s,m_s}}{\nu_s}\right),$$

(h3) we define

$$\varepsilon_{NK} = \frac{r}{2},$$

(h4) we define

$$\delta_\kappa = \frac{\pi^2(2l_u+4m_u)^2}{\nu_u^2\hat{\sigma}_u^2}\delta_u\tilde{C}_3^2 + \frac{\pi(2l_u+4m_u)}{\nu_u\hat{\sigma}_u}\delta_u\tilde{C}_4 + \frac{\pi^2(2l_s+4m_s)^2}{\nu_s^2\hat{\sigma}_s^2}\delta_s,$$

(h5) and we define

$$\kappa = \tilde{C}_2\tilde{C}_3^2 + \tilde{C}_1\tilde{C}_4 + \hat{C}_2 + \delta_\kappa.$$

If

$$\frac{4\varepsilon_{NK}\kappa C_1}{1-M} \le 1, \tag{4.5}$$

then there exist a unique $(\hat{\alpha}, \hat{\phi}) \in B_r(\alpha_*) \times B_r(\phi_*)$ so that $F(\hat{\alpha}, \hat{\phi}) = 0$, with $F = F_{\text{short}}$ given by (4.1).

It follows from the discussion of the previous sections that $\hat{x} \stackrel{\text{def}}{=} Q(\hat{\phi}_*)$ is a point in the intersection $W^u_{\text{loc}}(p_1) \cap W^s_{\text{loc}}(p_2)$. Then there is a unique heteroclinic orbit from p_1 to p_2 passing through $Q[B_r(\phi_*)] \cap P[\Theta_\nu(B_r(\alpha_*))] \subset \mathbb{R}^n$. We have the error bound

$$|(\alpha_*, \phi_*) - (\hat{\alpha}, \hat{\phi})| < r,$$

in parameter space. Moreover, defining $x_* = Q(\phi_*)$*, and*

$$\hat{r} = \min\left(diam(Q[B_r(\phi_*)]), diam(P[\Theta_\nu(B_r(\alpha_*))])\right)$$

we obtain a phase space bound of the form

$$|x_* - \hat{x}| \le \hat{r}.$$

Proof First we note that by condition (iii) of Definition 3 we have

$$\begin{aligned} \|F(\alpha_*, \phi_*)\| &\le \|F_{(M,N)}(\alpha_*, \phi_*)\| + \|H(\alpha_*, \phi_*)\| \\ &\le \epsilon + \delta_u + \delta_s. \end{aligned} \tag{4.6}$$

Using the Cauchy Bounds on the first derivatives we see that

$$\begin{aligned} &\|DF_{(M,N)}(\alpha_*, \phi_*)^{-1} DH(\alpha_*, \phi_*)\| \\ &\le C_1 \left(\|Dh_u(\Theta_\nu(\alpha_*)) D\Theta_\nu(\alpha_*)\| + \|Dh_s(\phi_*)\|\right) \\ &= C_1 \left(\|Dh_u\|_{e^{-\sigma_u}\nu_u} \|D\Theta_\nu(\alpha_*)\| + \|Dh_s\|_{e^{-\sigma_s}\nu_s}\right) \\ &\le C_1 \left(\frac{(2l_u + 4m_u)\pi}{\nu_u \sigma_u} \delta_u \|D\Theta_\nu(\alpha_*)\| + \frac{(2l_s + 4m_s)\pi}{\nu_s \sigma_s} \delta_s\right) \\ &\le M, \end{aligned} \tag{4.7}$$

where we have used conditions (i), (ii), (iv), (v), and (vi) of Definition 3. Combining this with (4.3), the hypothesis that $M < 1$, and the Neumann Series we obtain the bound

$$\begin{aligned} \left\|[DF(\alpha_*, \theta_*)]^{-1}\right\| &= \left\|\left[DF_{(M,N)}(\alpha_*, \phi_*) + DH(\alpha_*, \phi_*)\right]^{-1}\right\| \\ &= \left\|\left[I + DF_{(M,N)}(\alpha_*, \phi_*)^{-1} DH(\alpha_*, \phi_*)\right]^{-1} DF_{(M,N)}(\alpha_*, \phi_*)^{-1}\right\| \\ &\le \frac{1}{1-M} \left\|DF_{(M,N)}(\alpha_*, \phi_*)^{-1}\right\|, \end{aligned} \tag{4.8}$$

which also shows that $DF(\alpha_*, \phi_*)$ is invertible, so that condition (i) of Theorem 3 is satisfied. Now we are able to estimate

$$\left\|DF(\alpha_*, \phi_*)^{-1} F(\alpha_*, \phi_*)\right\| \le \frac{C_1}{1-M}(\epsilon + \delta_u + \delta_s)$$

using (4.6) and (4.8). Then by *(h3)* of Theorem 5 and condition (vii) of Definition 3 we have that

$$\left\|DF(\alpha_*, \phi_*)^{-1} F(\alpha_*, \phi_*)\right\| \le \varepsilon_{NK}$$

and $\varepsilon_{NK} \le r/2$ so that conditions *(I)* and *(II)* of Theorem 3 are satisfied.

Now we note that if $w, v \in B_r(\alpha_*) \times B_r(\phi_*)$ then

$$\|DF(w) - DF(v)\| \le \left\|D^2 F\right\|_{B_r(\alpha_*) \times B_r(\phi_*)} \|w - v\|$$

by the mean value theorem. Standard estimates applied to (4.4) give

$$\left\|D^2 F\right\|_{B_r(\alpha_*) \times B_r(\phi_*)} \le \kappa,$$

by definition of κ in *(h5)* (here we take into account the definition of δ_κ in *(h4)*, the Cauchy Bounds on the second derivatives of h_u and h_s on the disks $B_{e^{-\sigma_{u,s}}\nu_{u,s}} \subset B_{\nu_{u,s}}$, as well as the conditions (xiii) and (ix) in Definition 3). Then condition (ii) of Theorem 3 is satisfied. The hypothesis given by (4.5) insures that the final necessary condition *(III)* of Theorem 3 is satisfied, which completes the proof. □

5 Rigorous Numerics for Long Connections

Our next goal is to apply the method of radii polynomials to the long-connection problem defined on the infinite dimensional space $\mathbb{R}^{n+1} \times C([0,1],\mathbb{R}^n)$. In analogy to the short-connection problem we first need to impose a phase condition that we shortly describe in the next section. Then we go on to construct the necessary estimates in order to apply Theorem 4 for the validation of long connections. Throughout this section let the assumptions **A1–A3** and **A4ℓ–A5ℓ** of Sect. 1 be satisfied and set $F = F_{\text{long}}$.

5.1 Phase Condition

The considerations of Sect. 4.1 apply here as well and we are led to redefine the nonlinear operator given in (1.4) to $F\colon B_1 \times V_{\nu_u} \times C([0,1],\mathbb{R}^n) \to X$ with

$$F(\alpha,\phi,u)(t) = \begin{pmatrix} Q(\phi) - \left(P(\Theta_\nu(\alpha)) + L\int_0^1 g[u(\tau)]\,d\tau \right) \\ P(\Theta_\nu(\alpha)) - L\int_0^t g[u(\tau)]\,d\tau - u(t) \end{pmatrix}. \tag{5.1}$$

Since $\mathbb{R}^n \cong B_1 \times V_{\nu_u}$, we can think of F as an operator from X to itself, and we are in the setting where the contraction mapping theorem may be applied.

5.2 Validation

Recalling the definition of F given in (5.1), we introduce in this section, the ingredients to solve the problem $F(x) = 0$, where $x = (\alpha,\phi,u) \in X = \mathbb{R}^n \times C([0,1],\mathbb{R}^n)$.

In order to rigorously validate the existence of the long connecting orbit we apply the concept of radii polynomials, as introduced in Sect. (3.2).

Construction of the splitting $X = X_k \oplus X_\infty$:

In order to obtain the splitting $X = X_k \oplus X_\infty$ we have to discretize $C([0,1],\mathbb{R}^n)$. To do this we use linear splines for every component function. More concretely define the mesh $\Delta : 0 = t_0 < t_1 < \ldots < t_m = 1$, denote $\mathcal{S}_h$ the space of linear splines subordinate to the grid Δ and consider the linear spline projection $\Pi_h : C([0,1],\mathbb{R}) \to \mathcal{S}_h \cong \mathbb{R}^{m+1}$ consisting of computing the linear interpolation of u with respect to the mesh Δ. For $u \in C([0,1],\mathbb{R}^n)$ define $u_h = (\Pi_h)^n u = (\Pi_h u_1,\ldots,\Pi_h u_n) \in (\mathcal{S}_h)^n \cong \mathbb{R}^{n(m+1)}$. Define $X_k = \mathbb{R}^n \times (\mathcal{S}_h)^n$ and the finite dimensional projection $\Pi_k : X \to X_k : (\alpha,\phi,u) \mapsto (\alpha,\phi,(\Pi_h)^n u)$. By using the complementary projection $I - \Pi_h$ we get that $X_\infty = 0 \times (I-\Pi_h)^n C([0,1],\mathbb{R}^n)$, where $(I-\Pi_h)^n u = ((I-\Pi_h)u_1,\ldots,(I-\Pi_h)u_n)$. The associated projection $\Pi_\infty : X \to X_\infty$ is given by $(\alpha,\phi,u) \mapsto (0,(I-\Pi_h)^n u)$. Hence, we obtain that

$$F_k(x) = \begin{pmatrix} Q(\phi) - \left(P(\Theta_\nu(\alpha)) + L\int_0^1 g[u(\tau)]\,d\tau \right) \\ (\Pi_h)^n \left(P(\Theta_\nu(\alpha)) + L\int_0^t g[u(\tau)]d\tau - u(t) \right) \end{pmatrix}$$

and

$$F_\infty(x) = \begin{pmatrix} 0 \\ (I-\Pi_h)^n \left(P(\Theta_\nu(\alpha)) + L\int_0^t g[u(\tau)]d\tau - u(t) \right) \end{pmatrix}.$$

Assuming now that we are given approximate parametrizations

$$P_N(\theta) = \sum_{k=0}^{N} a_k^u \theta^k \quad \text{and} \quad Q_M(\phi) = \sum_{k=0}^{M} a_k^s \phi^k,$$

we define the operator $F^{k,N,M} : B_1 \times V_{\nu_u} \times \mathbb{R}^{n(m+1)} \to \mathbb{R}^n \times \mathbb{R}^{n(m+1)}$ by

$$F^{k,N,M}(\alpha, \phi, u_h) = \begin{pmatrix} Q_M(\phi) - \left(P_N(\Theta_\nu(\alpha)) + L \int_0^1 g(u_h(\tau))d\tau \right) \\ f^{k,N}(\alpha, u_h) - u_h \end{pmatrix},$$

where $f^{k,N} = (f_1^{k,N}, \ldots, f_n^{k,N})$ and $f_i^{k,N}(\alpha, u_h)$ is given component-wise by

$$\left[f_i^{k,N}(\alpha, u_h) \right]_j = [P_N(\Theta_\nu(\alpha))]_i + L \int_0^{t_j} g_i(u_h(\tau))d\tau.$$

Note that the finite dimensional operator $F^{k,N,M}$ can be rigorously evaluated using interval arithmetic and that the operator F^k differs from $F^{k,N,M}$ by the exact parametrizations. Let us now define the norms

$$\|\Pi_k(\alpha, \phi, u)\|_{X_k} = \max\{\|\alpha\|_\infty, \|\phi\|_\infty, \|\Pi_h u_1\|_\infty, \ldots, \|\Pi_h u_n\|_\infty\} \tag{5.2}$$

and

$$\|\Pi_\infty(\alpha, \phi, u)\|_{X_\infty} = \max_{l=1,\ldots,n} \sup_{t\in[0,1]} |(I - \Pi_h)[u]_l(t)|, \tag{5.3}$$

which qualify the pairs $(X_k, \|.\|_{X_k})$ and $(X_\infty, \|.\|_{X_\infty})$ as Banach spaces.

Construction of the bounds $Y_1, \ldots, Y_k, Y_\infty$ *and* $Z_1(r), \ldots, Z_k(r), Z_\infty(r)$:

We wish to construct the bounds $Y_1, \ldots, Y_k$ and Y_∞ as specified in (3.9) and (3.10) as well as $Z_1, \ldots, Z_k(r)$ and $Z_\infty(r)$ given by (3.12) and (3.13). Assume that the four assumptions (**RP**) of Sect. 3.2 are satisfied, in particular we assume an approximate solution $(\alpha_*, \phi_*, u_h^*)$ such that $\|F^k(\alpha_*, \phi_*, u_h^*)\|_{X_k} \le \epsilon$, for a given *small* $\epsilon > 0$. Furthermore let $\delta_s, \delta_u \ge 0$ and validation neighborhoods V_{ν_s}, V_{ν_u} such that

$$\|Q(\phi) - Q_M(\phi)\|_\infty < \delta_s, \quad \text{for all } \phi \in V_{\nu_s},$$
$$\|P(\theta) - P_N(\theta)\|_\infty < \delta_u, \quad \text{for all } \theta \in V_{\nu_u}.$$

Let $\delta = \max\{\delta_u, \delta_s\}$. It is important to test that $\Theta_\nu(B_1) \subset V_{\nu_u}$ in order to guarantee the validity of the above estimate after imposing the phase condition, as introduced in Sect. 5.1. If this is not the case, then we can reduce the radius ν of the sphere $\Theta_\nu(B_1)$ and start over. Let us compute the bounds $Y_1, \ldots, Y_k$. We use the splitting

$$\begin{aligned} F^k(\alpha, \phi, u_h) &= F^{k,N,M}(\alpha, \phi, u_h) + \begin{pmatrix} (Q(\phi) - Q_M(\phi)) + (P_N(\Theta_\nu(\alpha)) - P(\Theta_\nu(\alpha))) \\ [P_N(\Theta_\nu(\alpha)) - P(\Theta_\nu(\alpha))]_1 \, \mathbf{1}_{m+1} \\ \vdots \\ [P_N(\Theta_\nu(\alpha)) - P(\Theta_\nu(\alpha))]_n \, \mathbf{1}_{m+1} \end{pmatrix} \\ &= F^{k,N,M}(\alpha, \phi, u_h) + E(\alpha, \phi), \end{aligned}$$

where $E(\alpha, \phi) := F^k(\alpha, \phi, u_h) - F^{k,N,M}(\alpha, \phi, u_h)$ is independent of u_h and where $\mathbf{1}_{m+1} \in \mathbb{R}^{m+1}$ is a vector with components all equal to 1. Choose $Y_1, \ldots, Y_k$ such that

$$Y_1 \geq \left| \left[A_k^\dagger F^k(x_*) \right]_1 \right| + 2 \left\| A_k^\dagger \right\|_\infty \delta \text{ and } Y_j \geq \left| \left[A_k^\dagger F^k(x_*) \right]_j \right| + \left\| A_k^\dagger \right\|_\infty \delta, \tag{5.4}$$

for $j = 2, \ldots, k$. All quantities involved in (5.4) can be evaluated rigorously using interval arithmetic. Let us now turn to Y_∞.

Lemma 5 *Let $x_* = (\alpha_*, \phi_*, u_h^*)$. If we define*

$$Y_\infty \geq \max_{l=1,\ldots,n} \max_{i=1,\ldots,m} \frac{(t_i - t_{i-1})^2}{8} \sup_{t \in [t_{i-1}, t_i]} \left| \frac{d^2}{dt^2} L \int_0^t g(u_h^*(\tau)) d\tau \right|$$

then, recalling (3.8), one has that

$$\|\Pi_\infty y\|_{X_\infty} = \|F_\infty(x_*)\|_{X_\infty} \leq Y_\infty.$$

Proof One has that

$$\begin{aligned} \|F_\infty(x_*)\|_{X_\infty} &= \left\| (I - \Pi_h)^n (P(\Theta_\nu(\alpha_*)) + L \int_0^t g(u_h^*(\tau)) d\tau - u_h^*) \right\|_{C^0} \\ &= \left\| (I - \Pi_h)^n L \int_0^t g(u_h^*(\tau)) d\tau \right\|_{C_0}. \end{aligned}$$

We now apply Theorem 2.6 form [36] to obtain

$$\|F_\infty(x_*)\|_{X_\infty} \leq \max_{l=1,\ldots,n} \max_{i=1,\ldots,m} \frac{(t_i - t_{i-1})^2}{8} \sup_{t \in [t_{i-1}, t_i]} |\frac{d^2}{dt^2} L \int_0^t g(u_h^*(\tau)) d\tau|$$

The results follows immediately. □

We remark that the quantities involved in the Lemma 5 can be computed rigorously using interval arithmetic. We now compute the polynomial bounds $Z_1(r), \ldots, Z_k(r)$ and $Z_\infty(r)$. Recalling (3.11), $z(x_1, x_2) = DT(x_* + x_1)x_2$, where T is defined in (3.7) and $x_1, x_2 \in B(r, \omega)$. In particular we can write $x_{1,2} = r\tilde{x}_{1,2}$ where $\tilde{x}_{1,2} = (\tilde{\alpha}_{1,2}, \tilde{\phi}_{1,2}, \tilde{u}_{1,2}) \in B(1, \omega)$. Let us start with $Z_1(r), \ldots, Z_k(r)$. Realize that we have

$$\begin{aligned} \Pi_k z(x_1, x_2) &= \left(I - A_k^\dagger DF_k(x_* + x_1) \right) x_2 \\ &= \left(I - A_k^\dagger DF_k(x_*) \right) x_2 + \left(A_k^\dagger DF_k(x_*) - A_k^\dagger DF_k(x_* + x_1) \right) x_2. \end{aligned} \tag{5.5}$$

If one defines

$$\eta(s) = F_k(x_* + r\tilde{x}_1 + s\tilde{x}_2) - F_k(x_* + s\tilde{x}_2),$$

then (5.5) can be rewritten as

$$\Pi_k z(x_1, x_2) = \left(I - A_k^\dagger DF(x_*) \right) r\tilde{x}_2 - A_k^\dagger \eta'(0) r.$$

Hence we have to estimate $\left[\eta'(0)\right]_l$ for $l = 1, \ldots, k$. We begin with $l = 1, \ldots, n$. First,

$$\begin{aligned}\{[\eta(s)]_l\}_{l=1,\ldots,n} =& -(P_N(\Theta_\nu(\alpha_* + r\tilde{\alpha}_1 + s\tilde{\alpha}_2)) - P_N(\Theta_\nu(\alpha_* + s\tilde{\alpha}_2)))\\ &+ Q_M(\phi_* + r\tilde{\phi}_1 + s\tilde{\phi}_2) - Q_M(\phi_* + s\tilde{\phi}_2)\\ &- \left(L\int_0^1 \left[g(u_h^*(\tau) + r\tilde{u}_1(\tau) + s\tilde{u}_2(\tau)) - g(u_h^*(\tau) + s\Pi_h\tilde{u}_2(\tau))\right]d\tau\right)\\ &+ \left(E(\alpha_* + r\tilde{\alpha}_1 + s\tilde{\alpha}_2, \phi_* + r\tilde{\phi}_1 + s\tilde{\phi}_2) - E(\alpha_* + s\tilde{\alpha}_2, \phi_* + s\tilde{\phi}_2)\right)\\ =:& -\beta_1(s) + \beta_2(s) - \beta_3(s) + \beta_4(s).\end{aligned}$$

Let us consider the $\beta_i(s) \in \mathbb{R}^n$ $(i = 1, 2, 3, 4)$ separately. Denote by $e_l \in \mathbb{R}^n$ the l-th canonical basis vector. We start with $\beta_1'(0)$:

$$\begin{aligned}\beta_1'(0) &= \frac{d}{ds}\left[\sum_{|k|=0}^{N} a_k^u(\Theta_\nu(\alpha_* + r\tilde{\alpha}_1 + s\tilde{\alpha}_2)^k - \Theta_\nu(\alpha_* + s\tilde{\alpha}_2)^k)\right]\Big|_{s=0}\\ &= \sum_{|k|=1}^{N} a_k^u\left(\sum_{\substack{l=1\\k_l>0}}^{n_u} k_l\Theta_\nu(\alpha_* + r\tilde{\alpha}_1)^{k-e_l}(D\Theta_\nu(\alpha_* + r\tilde{\alpha}_1)\tilde{\alpha}_2)^{e_l} - k_l\Theta_\nu(\alpha_*)^{k-e_l}(D\Theta_\nu(\alpha_*)\tilde{\alpha}_2)^{e_l}\right).\end{aligned}$$

Now we use the intermediate value theorem component-wise to rewrite the difference in the inner sum

$$\begin{aligned}&\beta_1'(0)\\ &= \sum_{|k|=1}^{N} a_k^u\sum_{\substack{l=1\\k_l>0}}^{n_u} k_l\left(\sum_{\substack{n=1\\k_l>\delta_{l,n}}}^{n_u}(k_n - \delta_{l,n})\Theta_\nu(\sigma^{l,u})^{k-e_l-e_n}(D\Theta_\nu(\sigma^{l,u})\tilde{\alpha}_2)^{e_n}(D\Theta_\nu(\sigma^{l,u})\tilde{\alpha}_2)^{e_l}\right)r\\ &\quad + \sum_{|k|=1}^{n_s} a_k^u\left(\sum_{\substack{l=1\\k_l>0}}^{n_u} k_l\Theta_\nu(\sigma^{l,u})^{k_l-e_l}(D^2\Theta_\nu(\sigma^{l,u})\tilde{\alpha}_1\tilde{\alpha}_2)^{e_l}\right)r, \qquad (5.6)\end{aligned}$$

where $\delta_{l,n}$ is the Kronecker's delta, $\sigma^{l,u} = \alpha_* + \xi_l^u r \in \mathbb{R}^{n_u-1}$, with $\xi_l^u \in (0, 1)$ for $l = 1, \ldots, n_u$. Let us fix an a priori bound r_*^u such that for all $r \le r_*^u$ one has that $\Theta_\nu(\sigma^{1,u}), \ldots, \Theta_\nu(\sigma^{n_u,u}) \in V_{\nu_u}$, and such that

$$\left[\sigma^{l,u}\right]_j \in \left([\alpha_*]_j - r_*^u, [\alpha_*]_j + r_*^u\right),$$

for $j = 1, \ldots, n_u - 1$ and for $l = 1, \ldots, n_u$. Thus we can estimate $\beta_1'(0)$ as

$$\|\beta_1'(0)\|_\infty \le \|\Sigma_1\|_\infty + \|\Sigma_2\|_\infty,$$

with

$$\Sigma_1 = \sum_{|k|=1}^{N} a_k^u \sum_{\substack{l=1 \\ k_l>0}}^{n_u} k_l \left(\sum_{\substack{n=1 \\ k_l>\delta_{l,n}}}^{n_u} (k_n - \delta_{l,n}) \Theta_\nu(\sigma^{l,u})^{k-e_l-e_n} (D\Theta_\nu(\sigma^{l,u})\tilde{\alpha}_2)^{e_n} (D\Theta_\nu(\sigma^{l,u})\tilde{\alpha}_2)^{e_l} \right),$$

$$\Sigma_2 = \sum_{|k|=1}^{n_u} a_k^u \left(\sum_{\substack{l=1 \\ k_l>0}}^{n_u} k_l \Theta_\nu(\sigma^{l,u})^{k_l-e_l} (D^2\Theta_\nu(\sigma^{l,u})\tilde{\alpha}_1\tilde{\alpha}_2)^{e_l} \right).$$

Using interval arithmetic and the fact that $\|\tilde{\alpha}_i\|_\infty \leq 1$ $(i = 1, 2)$ one can derive rigorous bounds $\Lambda^u_{\Sigma,1}, \Lambda^u_{\Sigma,2} \in \mathbb{R}^n$ such that with $\Lambda^u_\Sigma = \Lambda^u_{\Sigma,1} + \Lambda^u_{\Sigma,2}$

$$|[\beta_1'(0)]_l| \leq [\Lambda^u_\Sigma]_l r, \quad \text{for} \quad l = 1, \ldots, n.$$

By a similar argument based on the intermediate value theorem we obtain

$$\beta_2'(0) = \sum_{|k|=1}^{M} a_k^s \sum_{\substack{l=1 \\ k_l>0}}^{n_s} k_l \tilde{\phi}_2^{e_l} \left(\sum_{\substack{n=1 \\ k_n>\delta_{l,n}}}^{n_s} (k_n - \delta_{l,n}) \tilde{\phi}_1^{e_n} (\sigma^{l,s})^{k-e_l-e_n} \right) r, \tag{5.7}$$

where $\sigma^{l,s} = \phi_* + \xi_l^s r \in \mathbb{R}^{n_s}$ with $\xi_l^s \in (0, 1)$ for $l = 1, \ldots, n_s$. Fixing an a priori bound r_*^s such that for all $r \leq r_*^s$, one has that $\sigma^{1,s}, \ldots, \sigma^{n_s,s} \in V_{\nu_s}$. Again using the fact that

$$[\sigma^{l,s}]_j \in ([\phi_*]_j - r_*^s, [\phi_*]_j + r_*^s), \quad \text{for} \quad j, l = 1, \ldots, n_s,$$

together with $\|\tilde{\phi}_i\|_\infty \leq 1$ $(i = 1, 2)$ one can derive via interval arithmetic rigorous bounds $\Lambda^s_\Sigma \in \mathbb{R}^n$ such that for $l = 1, \ldots, n$

$$|[\beta_2'(0)]_l| \leq [\Lambda^s_\Sigma]_l r.$$

Also, we have that

$$\beta_3'(0) = \frac{d}{ds} \left[L \int_0^1 \left[g(u_h^*(\tau) + r\tilde{u}_1(\tau) + s\tilde{u}_2(\tau)) - g(u_h^*(\tau) + s(\Pi_h)^n \tilde{u}_2(\tau)) \right] d\tau \right] \Bigg|_{s=0}$$
$$= L \int_0^1 \left[Dg(u_h^*(\tau) + r\tilde{u}_1(\tau))\tilde{u}_2(\tau) - Dg(u_h^*(\tau))(\Pi_h)^n \tilde{u}_2(\tau) \right] d\tau.$$

We assume for the moment that we can write

$$Dg(u_h^* + r\tilde{u}_1)\tilde{u}_2 - Dg(u_h^*)(\Pi_h)^n \tilde{u}_2 = \sum_{d=1}^{D} v_d r^{d-1} \tag{5.8}$$

for vector functions $v_d = v_d(u_h^*, \tilde{u}_1, \tilde{u}_2) \in \mathbb{R}^n$ and a suitable $D \in \mathbb{N}$. In general, in case the analytic vector field g is polynomial, D will be the degree of polynomial. We will elaborate on how to compute the expansion (5.8) for the Lorenz equations in Appendix 2. Under this assumption we obtain bounds $\Gamma_d \in \mathbb{R}^n$ such that component-wise

$$\int_0^1 |[v_d]_l(\tau)| d\tau \leq [\Gamma_d]_l, \quad \text{for} \quad l = 1, \ldots, n.$$

The bounds Γ_d depend on the form of the vector field. We refer to Appendix 2 for a specific derivation in the case of the Lorenz equations. Hence, we obtain that

$$|[\beta_3'(0)]_l| \leq L \sum_{d=1}^{D} [\Gamma_d]_l r^{d-1}, \quad \text{for } l = 1, \ldots, n.$$

Finally let us consider $\beta_4'(0)$. Using Cauchy bounds discussed in Lemma 1 we can derive bounds Λ_C^u, Λ_C^s such that for $l = 1, \ldots, n$

$$|[\beta_4'(0)]_l| \leq [\Lambda_C^u + \Lambda_C^s]_l r.$$

Defining $\Lambda^u = \Lambda_\Sigma^u + \Lambda_C^u$ and $\Lambda^s = \Lambda_\Sigma^s + \Lambda_C^s$ we obtain in total:

$$|[\eta'(0)]_l| \leq \left[(\Lambda^s + \Lambda^u) r + L \sum_{d=1}^{D} \Gamma_d r^{d-1} \right]_l, \quad \text{for } l = 1, \ldots, n.$$

Note that we have bounds on the first n components. Let us do the same for the remaining $n(m+1)$ components. Fix an index $i \in \{1, \ldots, n\}$. Then we obtain

$$\begin{aligned}
&\{[\eta(s)]_l\}_{l=n+(i-1)(m+1)+1,\ldots,n+i(m+1)} \\
&= \left[P_N(\Theta_\nu(\alpha_* + r\tilde{\alpha}_1 + s\tilde{\alpha}_2)) - P_N(\Theta_\nu(\alpha_* + s\tilde{\alpha}_2)) \right]_i \mathbf{1}_{m+1} \\
&\quad + L \int_0^{t_{\iota(l)}} [g_l(u_h^*(\tau) + r\tilde{u}_1(\tau) + \tilde{u}_2(\tau)) - g_l(u_h^*(\tau) + s\tilde{u}_2(\tau))] d\tau \\
&\quad - \left[(\Pi_h)^n (u_h^* + r\tilde{u}_1 + s\tilde{u}_2) - (\Pi_h)^n (u_h^* + s\tilde{u}_2) \right]_i \\
&= \left[P_N(\Theta_\nu(\alpha_* + r\tilde{\alpha}_1 + s\tilde{\alpha}_2)) - P_N(\Theta_\nu(\alpha_* + s\tilde{\alpha}_2)) \right]_i \mathbf{1}_{m+1} \\
&\quad + L \int_0^{t_{\iota(l)}} [g_l(u_h^*(\tau) + r\tilde{u}_1(\tau) + \tilde{u}_2(\tau)) - g_l(u_h^*(\tau) + s\tilde{u}_2(\tau))] d\tau - (\Pi_h)^n r\tilde{u}_1 \\
&=: \gamma_1(s) + \gamma_2(s) - \gamma_3,
\end{aligned}$$

where we define $\iota(l) = (l - (n+1)) mod (i-1) \in \{0, \ldots, m\}$. Consider $\gamma_1(s)$. Using the above calculations and assuming that $r \leq r_*^u$ we obtain uniformly in l

$$|[\gamma_1'(0)]_l| \leq [\Lambda^u]_i r$$

For $\beta_2(s)$ we obtain for $l = n + (i-1)(m+1) + 1, \ldots, n + i(m+1)$ in the same way as above

$$|[\beta_2'(0)]_l| \leq L \sum_{d=1}^{D} [\Gamma_d^i]_{\iota(l)} r^{n-1},$$

where for $i = 1, \ldots, n$, the bound $\Gamma_d^i \in \mathbb{R}^{m+1}$ is defined so that

$$\int_0^{t_j} |[v_d]_i(s)| ds \leq [\Gamma_d^i]_j$$

for the v_d ($d = 1, \ldots, D$) specified in (5.8). In summary this leads to

$$|[\eta'(0)]_l| \leq [\Lambda^u]_l r + L \sum_{d=1}^{D} [\Gamma_d^i]_{\iota(l)} r^{d-1}$$

for $l = n + (i-1)(m+1) + 1, \dots, n + i(m+1)$. If we define $\tilde{V}_d \in \mathbb{R}^{n(m+2)}$ for $d \neq 2$ as

$$\tilde{V}_d = (\Gamma_d, \Gamma_d^1, \dots, \Gamma_d^n)$$

and for $d = 2$ and $i = 1, \dots, n$

$$\{[\tilde{V}_2]_l\}_{l=1,\dots,n} = \Lambda^u + \Lambda^s + L\Gamma_2,$$
$$\{[\tilde{V}_2]_l\}_{l=n+(i-1)(m+1)+1,\dots,n+i(m+1)} = [\Lambda^u]_i + [\Lambda^s]_i + L[\Gamma_2^i]_{\iota(l)},$$

we arrive at

$$|[\eta'(0)r]_l| \leq \sum_{d=1}^{D} [\tilde{V}_d]_l r^d$$

for $l = 1, \dots, d(m+2)$. Now using that $\|\tilde{x}_2\|_\infty \leq 1$,

$$\begin{aligned} |[\Pi_k z(x_1, x_2)]_l| &\leq \left| \left[[(I - A_k^\dagger DF^k(x_*))\Pi_k \tilde{x}_2] r - A_k^\dagger \eta'(0) r \right]_l \right| \\ &\leq \|I - A_k^\dagger DF^k\|_\infty r + \|A_k^\dagger\|_\infty \sum_{d=1}^{D} [\tilde{V}_d]_l r^d \end{aligned}$$

for $l = 1, \dots, d(m+2)$. Set

$$\begin{aligned} V_1 &= \|I - A_k^\dagger DF^k\|_\infty \mathbf{1}_n + \|A_k^\dagger\|_\infty \tilde{V}_1, \\ V_d &= \|A_k^\dagger\|_\infty \tilde{V}_d, \quad \text{for} \quad d \neq 1, \end{aligned}$$

where $\mathbf{1}_n = (1, \dots, 1) \in \mathbb{R}^n$. By assumption **RP4.** we can assume that there is a small ϵ_I such that

$$\|I - A_k^\dagger DF^k\|_\infty \leq \epsilon_I.$$

Then with

$$Z_l(r) = \sum_{n=1}^{D} [V_n]_l r^n$$

and $r \leq r_* = \max\{r_*^s, r_*^u\}$, the inequality

$$\sup_{x_1, x_2 \in B(r,\omega)} |[\Pi_k z(x_1, x_2)]_l| \leq Z_l(r)$$

is fulfilled. Concerning the bound $Z_\infty(r)$ we have to compute the following:

$$\begin{aligned} &\|\Pi_\infty z(x_1, x_2)\|_{X_\infty} \\ &\quad = \|(I - \Pi_h)^n (D[P(\Theta(\alpha_* + r\tilde{\alpha}_1)) + L \int_0^t g(u_h^*(\tau) + r\tilde{u}_1(\tau)) d\tau] r\tilde{u}_2)\|_{C^0}. \end{aligned}$$

In order to estimate this we use the next result.

Lemma 6 *Let x_1, x_2 be specified as above. If we define*

$$Z_\infty(r) \geq \left[\max_{l=1,\dots,d} \max_{i=1,\dots,m} \frac{t_i - t_{i-1}}{2} \sup_{t \in [t_{i-1}, t_i]} |LDg_l(u_h^*(t) + r\tilde{u}_1(t))\tilde{u}_2(t)| \right] r$$

then $\|\Pi_\infty z(x_1, x_2)\|_{X_\infty} \leq Z_\infty(r)$.

Proof By definition we obtain

$$\begin{aligned}
&\|\Pi_\infty z(x_1,x_2)\|_{X_\infty} \\
&= \|(I-\Pi_h)^n (L\int_0^t Dg(u_h^*(s)+r\tilde{u}_1(s))r\tilde{u}_2(s)ds)\|_{C^0} \\
&\le \left[\max_{l=1,\dots,n}\max_{i=1,\dots,m}\frac{t_i-t_{i-1}}{2}\sup_{t\in[t_{i-1},t_i]}|LDg_l(u_h^*(t)+r\tilde{u}_1(t))\tilde{u}_2(t)|\right] r
\end{aligned}$$

where we used a result from [36] for the inequality. The assertion now follows. □

This completes the construction of the bounds and puts us in the position to apply the method to a concrete problem which will be done in Sect. 7.2. In Appendix 2 we complement the discussion by giving concrete formulas concerning the Lorenz equations.

6 Transversality

As shown in Sect. 3 the rigorous numerical methods of Sects. 4 and 5 by construction not only assure the existence of a unique genuine zero $\hat{x}$ of the respective operator F but, under suitable mild assumptions, also the invertibility of $DF(\hat{x})$. In this section we show that invertibility of $DF(\hat{x})$ in both cases implies the transversality of the intersection of $W^u(p_1)$ and $W^s(p_2)$. We start with the case of short connections in Sect. 6.1 and treat long connections in Sect. 6.2.

6.1 Short Connections

Suppose that $(\hat{\alpha},\hat{\phi}) \in B_r(\alpha_*)\times B_r(\phi_*) \subset B_1\times V_{\nu_s} \subset \mathbb{R}^{n_u-1}\times\mathbb{R}^{n_s} = \mathbb{R}^n$ satisfies $F(\hat{\alpha},\hat{\phi}) = 0$ where F is given by (4.1). Define $D_r = B_r(\alpha_*)\times B_r(\phi_*)$. If we set $\hat{x} = Q(\hat{\phi}) \in \mathbb{R}^n$, then orbit$(\hat{x})$ is heteroclinic from p_1 to p_2.

Theorem 6 *Suppose that the hypotheses of Theorem 5 are satisfied. If in addition the inequality given by* (4.5) *is strict, i.e. if*

$$\frac{4\epsilon_{NK}\kappa C_1}{1-M} < 1,$$

then the connecting orbit from p_1 to p_2 through $\hat{x}\in\mathbb{R}^n$ is transverse.

Proof Note that by the definition of ϵ_{NK} in Theorem 5 we have that $r = 2\epsilon_{NK} < 4\epsilon_{NK}$. Since the inequality in (4.5) is strict we see that the hypotheses of Corollary 1 are satisfied, and it follows that $DF(\hat{\alpha},\hat{\phi})$ is invertible. We now show that the invertibility of $DF(\hat{\alpha},\hat{\phi})$ implies that the stable and unstable manifolds intersect transversally.

Recall that $F(\alpha,\phi) = P[\Theta_\nu(\alpha)] - Q(\phi)$. Combining this with the preceding paragraph we have that,

$$DF(\hat{\alpha},\hat{\phi}) = \left[DP\left(\Theta_\nu(\hat{\alpha})\right)D\Theta_\nu(\hat{\alpha}) \,|\, -DQ(\hat{\phi})\right]$$

is invertible. Note that $P[\Theta_\nu(\hat{\alpha})] = Q(\hat{\phi})$ and denote $\hat{x}(t)$ the orbit through $\hat{x}$. Then

$$\hat{x}'(0) = g[\hat{x}] = g[P(\Theta_\nu(\hat{\alpha}))] = DP(\Theta_\nu(\hat{\alpha}))\Lambda_u\Theta_\nu(\hat{\alpha}),$$

(the last equality is the invariance equation for the parameterization) and also

$$\hat{x}'(0) = g[\hat{x}] = g[Q(\hat{\phi})] = DQ(\hat{\phi})\Lambda_s\hat{\phi}.$$

Then the vector

$$DQ(\hat{\phi})\Lambda_s\hat{\phi} = DP(\Theta_\nu(\hat{\alpha}))\Lambda_u\Theta_\nu(\hat{\alpha}) \tag{6.1}$$

lies in both $T_{\hat{x}}W^u(p_1)$ and $T_{\hat{x}}W^s(p_2)$ (as this vector is tangent to the heteroclinic orbit itself, which is in the intersection of the manifolds). Also, since image(Θ) is transverse to the linear vector field Λ_u, we have that $DP[\Theta_\nu(\hat{\alpha})]D\Theta_\nu(\hat{\alpha})$ spans the linear subspace of $T_{\hat{x}}W^u(p_1)$ perpendicular to $DP(\Theta_\nu(\hat{\alpha}))\Lambda_u\Theta_\nu(\hat{\alpha})$. In other words, the columns of the matrix $[DP(\Theta_\nu(\hat{\alpha}))D\Theta_\nu(\hat{\alpha}) \mid DP(\Theta_\nu(\hat{\alpha}))\Lambda_u\Theta_\nu(\hat{\alpha})]$ are linearly independent and span $T_{\hat{x}}W^u(p_1)$. Similarly, the columns of the matrix $-DQ(\hat{\phi})$ spans $T_{\hat{x}}W^s(p_2)$. Since the vector $DQ(\hat{\phi})\Lambda_s\hat{\phi} \in T_{\hat{x}}W^s(p_2)$ it is in the span of the columns of the matrix $-DQ(\hat{\phi})$. Then $DQ(\hat{\phi})\Lambda_s\hat{\phi} = DP(\Theta_\nu(\hat{\alpha}))\Lambda_u\Theta_\nu(\hat{\alpha})$ lies in the span of the columns of the matrix $-DQ(\hat{\phi})$. Then the vector defined by (6.1) is redundant and the remaining columns of the matrix $DF(\hat{\alpha},\hat{\phi}) = [DP(\Theta_\nu(\hat{\alpha}))D\Theta_\nu(\hat{\alpha})| - DQ(\hat{\phi})]$ are linearly independent and span both $T_{\hat{x}}W^u(p_1)$ and $T_{\hat{x}}W^s(p_2)$. Since $DF(\hat{\alpha},\hat{\phi})$ is invertible, its columns span $\mathbb{R}^n$. Hence $T_{\hat{x}}W^u(p_1)$ and $T_{\hat{x}}W^s(p_2)$ span $\mathbb{R}^n$, which shows that $\hat{x}$ is a point of transverse intersection of the manifolds. By Lemma 3 orbit($\hat{x}$) is a transverse heteroclinic orbit. □

6.2 Long Connections

Suppose that $(\hat{\alpha},\hat{\phi},\hat{u}) \in X$ is a zero of the operator F given by (5.1). We require the Fréchet derivative of the operator $F\colon X \to X$. Consider $(\alpha_1,\phi_1,u_1) \in X$. Computing the difference

$$F(\hat{\alpha}+\alpha_1,\hat{\phi}+\phi_1,\hat{u}+u_1) - F(\hat{\alpha},\hat{\phi},\hat{u}),$$

and neglecting the terms which are quadratic in (α_1,ϕ_1,u_1) leads to

$$DF[\hat{\alpha},\hat{\phi},\hat{u}](\alpha_1,\phi_1,u_1) = \begin{pmatrix} DQ(\hat{\phi})\phi_1 - DP(\Theta_\nu(\hat{\alpha}))D\Theta_\nu(\hat{\alpha})\alpha_1 - L\int_0^1 Dg[\hat{u}(\tau)]u_1(\tau)\,d\tau \\ u_1(t) - DP(\Theta_\nu(\hat{\alpha})D\Theta_\nu(\hat{\alpha})\alpha_1 - L\int_0^t Dg[\hat{u}(\tau)]u_1(\tau)\,d\tau \end{pmatrix}. \tag{6.2}$$

As in the case of transversality of short-connections, we formulate the long-connection transversality condition without stating any additional assumptions. As a preparation we formulate the following result characterizing the kernel of DF.

Lemma 7 *One has that $(\alpha_1,\phi_1,u_1) \in ker(DF(\alpha,\phi,u))$ if and only if*

$$u_1'(t) = LDg[u(t)]u_1(t), \tag{6.3}$$

$$u_1(0) = DP(\Theta_\nu(\alpha)D\Theta_\nu\alpha)\alpha_1 \quad \text{and} \quad u_1(1) = DQ(\phi)\phi_1. \tag{6.4}$$

Proof The proof follows by rewriting (6.3) in integral form and taking the boundary conditions (6.4) at $t = 0$ and at $t = 1$ into account. □

Theorem 7 *Suppose that $(\hat{\alpha},\hat{\phi},\hat{u}) \in X$ is a zero of F, and that $DF(\hat{\alpha},\hat{\phi},\hat{u})$ is invertible. Then the intersection of $W^u(p_1)$ and $W^s(p_2)$ is non-empty and transverse on orbit$(Q[\hat{\phi}])$.*

Proof Let $\hat{z} = P(\Theta_\nu(\hat{\alpha})) \in W^u(p_1)$ and define $\hat{y} = \Phi(\hat{z},1) = \hat{u}(1)$. Then by the fact $F(\alpha_*,\hat{\theta},\hat{u}) = 0$ it follows $\hat{y} = Q(\hat{\phi}) \in W^s(p_2)$. Furthermore it follows from the flow invariance of $W^u(p_1)$ and $W^s(p_2)$ that orbit$(\hat{z})$ = orbit$(\hat{y}) \subset W^u(p_1) \cap W^s(p_2)$, so that the intersection is non-empty.

$\Phi(\hat{z}, t) \in W^u(p_1)$ for any $t \in \mathbb{R}$, and by the chain rule

$$D_\alpha \Phi(P(\Theta_\nu(\hat{\alpha})), t) = D\Phi(\hat{z}, t) DP(\Theta_\nu(\hat{\alpha})) D\Theta_\nu(\hat{\alpha}).$$

Then the columns of this matrix span the linear subspace of $T_{\Phi(\hat{z},t)} W^u(p_1)$ perpendicular to the orbit of $\hat{z}$ for any $t \in [0, 1]$. Since the columns of $-DQ(\hat{\phi})$ span $T_{\hat{y}} W^s(p_2)$ (and since the orbit passes through $\hat{y}$) we have that the columns of the matrix

$$[D\Phi(\hat{z}, 1) DP(\Theta_\nu(\hat{\alpha})) D\Theta_\nu(\alpha) \mid -DQ(\hat{\phi})]$$

span $T_{\hat{y}} W^u(p_1)$ and $T_{\hat{y}} W^s(p_2)$.

Assume for the sake of contradiction that the intersection $W^u(p_1) \cap W^s(p_2)$ is not transverse at $\hat{y}$. Then $T_{\hat{y}} W^u(p_1)$ and $T_{\hat{y}} W^s(p_2)$ do not span $\mathbb{R}^n$ and there is a non-zero vector $\xi = (\xi_1, \xi_2) \in \mathbb{R}^{n_u - 1} \times \mathbb{R}^{n_s} = \mathbb{R}^n$ so that

$$[D\Phi(\hat{z}, 1) DP(\Theta_\nu(\hat{\alpha})) D\Theta_\nu(\hat{\alpha}) \mid -DQ(\hat{\phi})]\xi = 0.$$

or

$$M(\hat{z}, 1) DP(\Theta_\nu(\hat{\alpha})) D\Theta_\nu(\hat{\alpha})\xi_1 = DQ(\hat{\phi})\xi_2,$$

where $M(\hat{z}, t)$ is the solution of the variational equation

$$\frac{d}{dt} M(\hat{z}, t) = L\, Dg[\hat{u}(t)] M(\hat{z}, t) \qquad M(\hat{z}, 0) = I.$$

If we define $\alpha_1 = \xi_1$, $\phi_1 = \xi_2$, and take $u_1 \colon [0, 1] \to \mathbb{R}^n$ to be

$$u_1(t) = M(\hat{z}, t) DP(\Theta_\nu(\hat{\alpha})) D\Theta_\nu(\hat{\alpha})\alpha_1 \qquad \text{for all} \qquad t \in [0, 1],$$

then (α_1, ϕ_1, u_1) solves the boundary value problem (6.3). Thus $0 \neq (\alpha_1, \phi_1, u_1) \in ker(DF(\hat{\alpha}, \hat{\phi}, \hat{u}))$ which is a contradiction as we assumed $DF(\hat{\alpha}, \hat{\phi}, \hat{u})$ to be invertible. □

7 Numerical Examples of Computer Assisted Proofs

In this section we discuss some explicit example computations including the proof of Theorem 1. The MATLAB/INTLAB codes for our implementation of these computations and proofs can be downloaded from [24].

7.1 Proof of the Existence of Transverse Heteroclinic Connections in the Lorenz Equations Using Short Connections

We begin by discussing a computer assisted proof of the existence of "short" saddle-to-saddle connections in some detail. The numerical implementation of this example can be found in the MATLAB program `paperCodeEx1.m` at [24]. Consider then the Lorenz equations with parameters $\sigma = -2.2$, $\beta = 8/3$, and $\rho = 1.33$. The choice of $\sigma < 0$ is in order to obtain saddle-to-saddle stability as discussed in Sect. 1 (beyond this the choice of -2.2 is arbitrary). The choice of β is *classical*, while the choice of ρ is determined by the fact that we need $\rho > 1$ in order that there are three distinct fixed points, and we choose $\rho - 1$ small so that we are close to the pitchfork bifurcation at 0, which happens at $\phi = 1$. Hence, $\rho = 1.33$

is a reasonable starting point. For these parameter values we focus on the two equilibria given by

$$p_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

and

$$p_1 = \begin{pmatrix} \sqrt{\beta(\rho-1)} \\ \sqrt{\beta(\rho-1)} \\ \rho - 1 \end{pmatrix} \in B\left[\begin{pmatrix} 0.938083151964686 \\ 0.938083151964686 \\ 0.330 \end{pmatrix}, 1.2 \times 10^{-16}\right].$$

The Jacobian at the origin has eigenvalues

$$\begin{aligned} \lambda_1^{p_0} &\in B(-2.666666666666667, 1.2 \times 10^{-16}) \\ \lambda_2^{p_0} &\in B(0.6 - i0.604979338490167, 1.163 \times 10^{-15}) \\ \lambda_3^{p_0} &\in B(0.6 + i0.604979338490167, 1.163 \times 10^{-15}), \end{aligned}$$

while the Jacobian at the secondary equilibria p_1 has eigenvalues

$$\begin{aligned} \lambda_1^{p_1} &\in B(1.573023115184390, 6.662 \times 10^{-16}) \\ \lambda_2^{p_1} &\in B(-1.519844890925528 - 0.389324796755971i, 1.966 \times 10^{-15}) \\ \lambda_3^{p_1} &\in B(-1.519844890925528 + 0.389324796755971i, 1.966 \times 10^{-15}). \end{aligned}$$

We see that, as claimed above, it is reasonable to look for a saddle-to-saddle connection from p_0 (the origin) to p_1. Again we defer to the notation established in Sect. 1 and let $\lambda_1^u = \lambda_2^{p_0}$, $\lambda_2^u = \lambda_3^{p_0}$, $\lambda_1^s = \lambda_2^{p_1}$, and $\lambda_2^s = \lambda_3^{p_1}$ and stress that the unstable and stable eigenvalues are now associated with different fixed points. We also choose associated eigenvectors (the reader interested in the values of the eigenvector can consult the MATLAB program).

Now we compute polynomial approximations of the two dimensional invariant manifolds to order $N = 45$ at p_0 and $M = 35$ at p_1. We call the resulting approximations $P_N(\phi)$ and $Q_M(\theta)$. Note that we compute the unstable manifold to higher order as the unstable eigenvalues are close to degenerate, that is the real parts are closer to zero. Note that since $l_s = l_u = 0$ the norm in parameter space is just the Euclidean norm. We choose $\nu_u = 0.725$ and $\nu_s = 0.575$ and check (using the notation of Definition 1) that the *a-posteriori* errors have

$$\|f \circ Q_M - DQ_M \Lambda_s\|_{\Sigma,\nu_s} \le 6.29 \times 10^{-14}$$

and

$$\|f \circ P_N - DP_N \Lambda_u\|_{\Sigma,\nu_u} \le 1.09 \times 10^{-13}.$$

From Theorem 2 there are analytic M and N-tails $h_s \colon V_{\nu_s} \to \mathbb{R}^n$ and $h_u \colon V_{\nu_u} \to \mathbb{R}^n$ such that

$$\|h_s\|_{\nu_s} \le \delta_s < 3.5 \times 10^{-14} \qquad \text{and} \qquad \|h_u\|_{\nu_u} \le \delta_u < 3.3 \times 10^{-14},$$

and such that

$$P(\theta) = P_N(\theta) + h_u(\theta) \qquad \text{and} \qquad Q(\phi) = Q_M(\phi) + h_s(\phi).$$

We remark that the rigorous bound on h_u is actually better than the bound on the a-posteriori error. This is because we have taken N large enough so that the denominator of the estimate

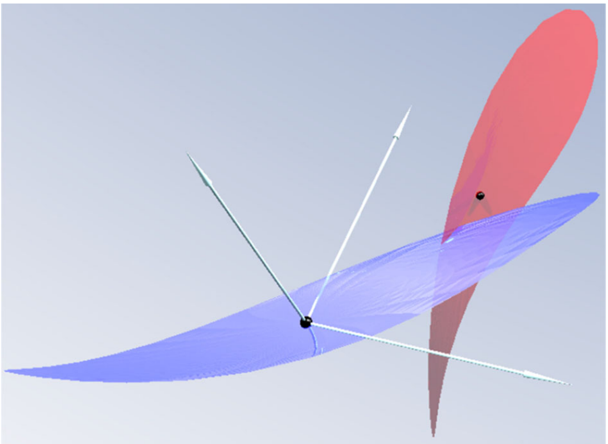

Fig. 1 Local stable (*blue*) and local unstable (*red*) manifolds for Lorenz when $\sigma = -2.2$, $\beta = 8/3$ and $\rho = 1.33$. *Black spheres* denote the location of the fixed points. Note that even though these are polynomial images of circles the local manifolds are stretched and bent substantially. This suggests that there are *fast* and *slow* direction due to the full nonlinearities of the flow rather than just the linearization at the equilibria and highlights the utility of the parameterization method for capturing the effects of the nonlinearities on the local manifolds (Color figure online)

given by the second inequality in Theorem 2 is greater than two. A plot of the resulting local stable and unstable manifolds is shown in Fig. 1, and the figure suggests that the local manifolds do in fact intersect transversally in phase space.

Since the two dimensional manifolds are associated with complex conjugate eigenvalues the dynamics in parameter space are conjugated by the dynamics generated by these complex numbers. In other words the dynamics are linear rotation and contraction in the stable parameter space, and linear rotation and expansion in the unstable parameter space. Because of the expansion/contraction the linear vector field is never tangent to a circle about the origin in parameter space. Then we choose the phase function $\Theta_\nu : \mathbb{S}^1 \to V_{\nu_u}$ given by

$$\Theta_\nu(\alpha) = \nu \begin{pmatrix} \cos(\alpha) \\ \sin(\alpha) \end{pmatrix}$$

with $\nu = 0.70796507495989$. This mysterious value of ν, as well as the values of ν_s and ν_u come from a non-rigorous approximate solution obtained by a classical Newton scheme.

We now have enough information to define the short-connection operator of (4.1). We obtain, via the non-rigorous Newton iteration alluded to above, that

$$\alpha_* = -1.08544433208255 \quad \text{(radians)}$$

and

$$\phi_* = (-0.018554373780656, 0.548268655433034)$$

give an approximate zero of (4.1) with

$$|F_{\text{short}}(\alpha_*, \phi_*)| < 2.25 \times 10^{-14}.$$

We verified that $|\Theta_\nu(\alpha_*)|_2 < \nu_u = 0.725$, and $|\phi_*|_2 < \nu_s = 0.575$ using interval arithmetic. This shows our solution parameters are interior to the domains of definition of P and Q, so that σ_u, σ_s from Definition 3 are well defined. In other words there is a small amount of

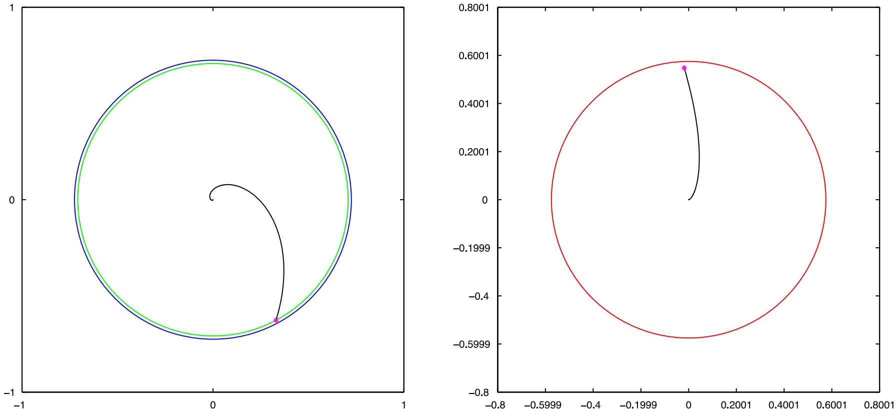

Fig. 2 The solution of the short-connection problem in stable and unstable parameter spaces when $\sigma = -2.2$, $\beta = 8/3$ and $\rho = 1.33$. The *blue circle* (*left*) and *red circle* (*right*) represent the boundaries of the unstable and stable parameter spaces respectively. The *green circle* in the stable parameter space represents the phase circle. The *pink star* on the left represents the validated solution parameters $(\bar{\phi}_1, \bar{\phi}_2)$ of the short-connection problem in stable parameter space while the *pink star* on the right represents the validated solution parameters $(\bar{\theta}_1, \bar{\theta}_2)$ in unstable parameter space. The *black lines* show the linear flow of the validated solution parameters in parameter space. The flow of the parameters is computed using the exponential matrix (Color figure online)

domain in each parameter space that we can give up in order to estimate derivatives of the truncation errors h_u and h_s.

We now validate the approximate solution of the short-connection operator using Theorem 5, and obtain that there exists at true solution in $(\hat{\alpha}, \hat{\phi})$ with

$$(\hat{\alpha}, \hat{\phi}) \in B\left[(\alpha_*, \phi_*), 2.72 \times 10^{-12}\right],$$

and also that the resulting intersection is transverse.

We can integrate the approximate solution in parameter space in order to obtain a representation of the entire saddle-to-saddle connecting orbit on parameter space. This integration is especially easy because the dynamics in phase space are generated by the eigenvalues, hence this ‘integration’ is just complex multiplication, that is the flow is explicitly known, and can be easily evaluated using interval arithmetic. The resulting orbits in parameter space are shown in Fig. 2, along with the validated parameters θ_*, ϕ_* and the phase circle in unstable parameter space. If we now lift, via the unstable and stable parameterizations, the validated solution along with the integrated parameter orbits into phase space we obtain a representation of the connecting orbit. The result is shown in Fig. 3 along with the phase condition projected onto the local manifold.

An interesting way to benchmark the result is to ask the following question: If we approximate the local stable and unstable manifolds using only the linear approximation given by the eigenspaces (i.e if we use the classical method of projected boundary conditions of [4,14,17]), then how ‘long’ would the resulting orbit be? More precisely: for how many time units would we have to integrate the orbit in order to make the flight from the unstable eigenspace to the stable eigenspace? A reasonable answer is provided by a simple back of the envelope calculation.

We have approximated the manifolds to high order and obtained errors on the order of 10^{-14}. In order to obtain the same accuracy with only the linear approximation we should restrict to a neighborhood on the order to 10^{-7} of the origin in the stable and unstable

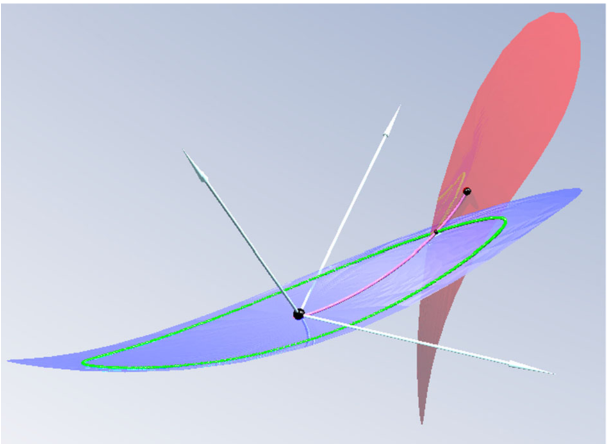

Fig. 3 Validated *short connecting orbits* for Lorenz when $\sigma = -2.2$, $\beta = 8/3$ and $\rho = 1.33$. The image of the phase condition Φ is shown as a *green circular arc* on the local stable manifold. The solution of the short-connection operator is shown as a *black dot* on the intersection of the manifolds and the *green phase arc*. The *pink arc* is the image under the parameterizations of the flow in parameter space (Color figure online)

parameter space. The magnitude of the approximate solution parameters $\Theta_\nu(\alpha_*)$ and ϕ_* are roughly 0.72 and 0.54 in unstable and stable parameter space respectively. The linear flow expands/contracts the parameters at a rate given by

$$\|e^{\Lambda_u t}\theta\| = e^{0.6t}\|\theta\|, \qquad \text{and} \qquad \|e^{\Lambda_s t}\phi\| \approx e^{-1.52t}\|\phi\|,$$

respectively. The unstable and stable parameters can be flown into a 10^{-7} neighborhood of their respective origins in parameter space in

$$-26.3 \approx \frac{1}{0.6}\ln\left(\frac{10^{-7}}{0.72}\right) \qquad \text{and} \qquad 10.19 \approx \frac{-1}{1.52}\ln\left(\frac{10^{-7}}{0.54}\right),$$

time units respectively, so that the “time of flight” of the connecting orbit (with respect to the eigenspace approximation of the local stable and unstable manifolds) would be approximately 36 units of time. Using the *rk45* integrator in MatLab, suppose we now integrate the initial condition

$$q = P\left[e^{-\Lambda_u 26.3}\theta_*\right],$$

for 36 time units. We denote the numerical flow by $\Phi_{\text{numerical}}$. The initial distance between the origin and q is $\|q\| \leq 1.45 \times 10^{-7}$ as desired. The numerical orbit of q does in fact begin to converge to the equilibria p_1, and we find that $\|p_1 - \Phi_{\text{numerical}}(q, 31.5)\| \approx 3.5 \times 10^{-4}$ minimizes the distance between the numerical orbit and p_1. However for times greater than $t = 32$ the numerical orbit begins to diverge along the unstable manifold of p_1 and we see that the terminal point on the numerical orbit has $\|p_1 - \Phi_{\text{numerical}}(q, 36)\| \approx 0.59$. In other words 36 is a sufficient number of time units to allow numerical errors to *kick* the integrated orbit off of the actual connecting orbit. On the other hand Fig. 3 shows the results of the same integration carried out in parameter space and then lifted into phase space, and here the orbit remains always on the manifolds. This illustrates a numerical advantage of working with the high order manifolds: namely that the parameterizations capture the asymptotics of the orbits in a natural and accurate way, which is also immune to the any unstable dynamics near the equilibria.

Table 1 Data for the proofs of the *short connections* for Lorenz with $\sigma = -2.2$, $\beta = 8/3$ and $\rho = 1.33$

M	N	δ_u	δ_s	R	Proof time
10	13	4.2×10^{-5}	2.88×10^{-7}	Failed	NA
10	15	4.2×10^{-6}	2.9×10^{-7}	1.4×10^{-4}	17 (s)
15	20	1.9×10^{-8}	2.1×10^{-11}	5.5×10^{-7}	31 (s)
20	25	8.9×10^{-11}	6.3×10^{-14}	2.6×10^{-9}	48.4 (s)
20	35	4.2×10^{-14}	6.3×10^{-14}	3.6×10^{-12}	1.3 (min)
35	45	3.3×10^{-14}	3.5×10^{-14}	2.55×10^{-12}	2.6 (min)

The first line of the table shows the results of a failed proof. Increasing the order of approximation of the unstable manifold by one results in a successful proof. Line two shows the results of the simplest possible proof for these parameters. Note that we only obtain the location of the intersection to within three decimal places. The last line of the table is recalls the performance data for the proof discussed in detail above. In the last two lines of the table note that the increased parameterization order doubles the computation time but results in roughly twice the accuracy of the previous computation, while the previous increases in order lead to improvements of several orders of magnitude. This suggests that the last two proofs are close to optimal, for double precision computations

We record that in this example the computation of the coefficients of P_N and Q_M using rigorous interval arithmetic take roughly 13.2 and 8.2 seconds respectively. Validating the manifolds takes 25.95 and 14.2 seconds. The proof of the existence of the connecting orbit takes another 91 seconds. The entire computer assisted proof takes roughly 2.55 minutes. However we remark that this proof has been optimized for accuracy rather than runtime. Table 1 shows the results of the same computer assisted proof for several different choices of parameterization order. We see that if we are willing to sacrifice accuracy, that is if we care more about abstract existence results than about localizing the orbit, then the proof can succeed in much less time. We also remark that the high order approximation aids us because we are near the bifurcation at $\rho = 1$, hence the problem is shomewhat degenerate (note that the eigenvalues are all close to the imaginary axis).

The technique described above can be used to prove the existence of short-connections for many nearby parameter values. Fixing σ and β and increasing ρ moves the fixed points farther from one another. In the program `paperCode_shortCont.m` [24] we implement a simple continuation scheme which finds and validates 187 short-connections for $1.33 \leq \rho \leq 3.2$. This results in the proof of the connecting orbits associated with the parameter set U_1 reported in Theorem 1.

The continuation begins with $\rho = 1.33$, $\nu_u = 0.725$, $\nu_s = 0.575$, and a phase circle fixed at $r = 0.70796507495989$. Each step of the continuation increases the previous value of ρ by 0.01, the previous value of ν_u by 0.0079, the previous value of ν_s by 0.0108, and the previous value of r by 0.0079. In each computation the value of N and M are held at 30. For each value of the parameters the origin p_0 has two dimensional unstable manifold and the secondary equilibria p_1 has two dimensional stable manifold, both with complex conjugate eigenvalues. Some of the the results are sumarized in Table 2, and seven of the resulting orbits are illustrated in Fig. 4. It takes about three and a half hours for all 187 proofs to complete. (The proofs reported in Table 2 can be produced by running the program `paperCode_shortContinuationII.m` [24] without computing all 187 parameter values. This program runs in a much shorter time).

We remark that the computations only illustrate the use of our scheme and should not be seen as a definitive test of limits of the method. No attempt is made to optimize the proofs in the individual continuation steps, nor to push the continuation as far as possible. For example

Table 2 Proof of short-connections for sixteen different values of ρ

ρ	δ_u	δ_s	R	Proof time (s)
1.35	2.26×10^{-13}	2.78×10^{-14}	1.36×10^{-11}	86.5
1.45	3.03×10^{-13}	4.00×10^{-14}	2.86×10^{-12}	87.1
1.55	4.83×10^{-13}	3.70×10^{-14}	3.00×10^{-12}	87.2
1.65	8.49×10^{-13}	3.89×10^{-14}	4.87×10^{-12}	87.0
1.75	1.54×10^{-12}	5.55×10^{-14}	8.65×10^{-12}	87.1
1.85	2.88×10^{-12}	6.33×10^{-14}	1.60×10^{-11}	87.0
1.95	5.47×10^{-12}	7.70×10^{-14}	3.05×10^{-11}	87.0
2.05	1.05×10^{-11}	8.53×10^{-14}	5.84×10^{-11}	87.1
2.15	2.03×10^{-11}	1.13×10^{-13}	1.15×10^{-10}	87.3
2.25	3.98×10^{-11}	1.23×10^{-13}	2.28×10^{-10}	89.5
2.35	7.95×10^{-11}	1.54×10^{-13}	4.62×10^{-10}	95.5
2.45	1.59×10^{-10}	1.72×10^{-13}	9.39×10^{-10}	102.6
2.55	3.16×10^{-10}	2.15×10^{-13}	1.91×10^{-9}	104.5
2.65	6.20×10^{-10}	2.37×10^{-13}	3.84×10^{-9}	96.8
2.75	1.20×10^{-9}	2.78×10^{-13}	7.58×10^{-9}	91.1
2.85	2.27×10^{-9}	3.34×10^{-13}	1.50×10^{-8}	91.2

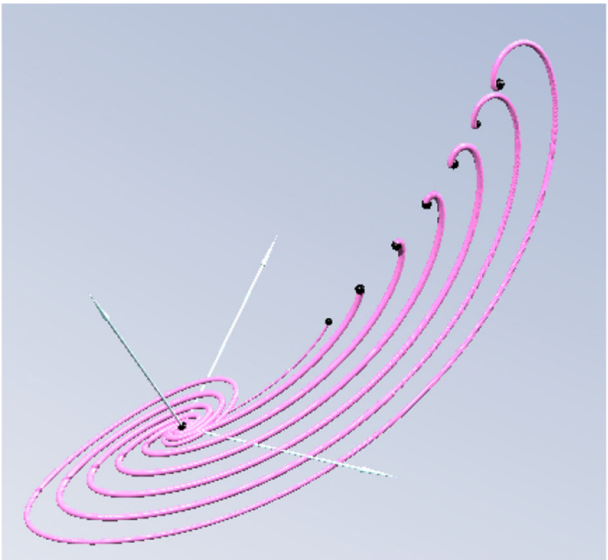

Fig. 4 Seven validated *short connecting orbits* for Lorenz with $\sigma = -2.2$, $\beta = 8/3$ and ρ taking the values 1.35, 1.55, 1.75, 2.05, 2.25, 2.55, and 2.75

the loss of accuracy seen in column 4 of Table 2 as a function of ρ is due to the fact that set up of the proof was optimized by hand at the first step of the continuation, and that the choices made at the first step become less and less optimal as ρ is adjusted. It is possible to optimize each of the proofs 'by hand' and obtain much better results. In fact by carefully choosing the proof parameters we have been able to validate short connecting orbits for parameters as high as $\rho = 4$. However the design of a self-optimizing continuation scheme is outside the scope of the present work. Here our aim is to provide only a satisfactory 'proof of concept'.

7.2 Proof of the Existence of Transverse Heteroclinic Connections in the Lorenz Equations Using Long Connections

Consider again the Lorenz equations, this time with $N = 35$, $M = 30$, $\nu_s = 1.75$, $\nu_u = 1.5$, $\beta = 8/3$, $\sigma = -2.2$, and $\rho = 3.2$. For these parameters we again have two dimensional saddles at the equilibria with complex conjugate eigenvalues. We note that the manifold validation in the long connection case proceeds exactly as in the short connection case. We computed validated bounds for the local unstable and stable manifolds of $\delta_u = 1.48 \times 10^{-13}$ and $\delta_s = 2.75 \times 10^{-14}$ and find (by graphical inspection) that the local stable and unstable manifolds do not intersect in phase space. We then define the long-connection operator with $L = 0.5$ and discretize $C^0\left([0, 1], \mathbb{R}^3\right)$ using piecewise linear splines with 500 uniformly spaced grid points. We run a classical Newton iteration scheme and obtain an approximate orbit with non-rigorous defect of 9×10^{-16}.

This approximate orbit is validated using the program `performance_rho3p2.m`. We obtain the existence of a unique solution of the long-connection operator about the approximate numerical solution in a 5.11×10^{-5} neighborhood of the approximation. Using the radii polynomial method we also obtain isolation in a neighborhood whose radius is not more than 0.041. Transversality follows as discussed in Sect. 6.2. The proof takes 44 seconds. The results are illustrated in Fig. 5. (Note we have fixed phase condition in the stable rather than the unstable parameter space but this makes no difference to the argument). The figure

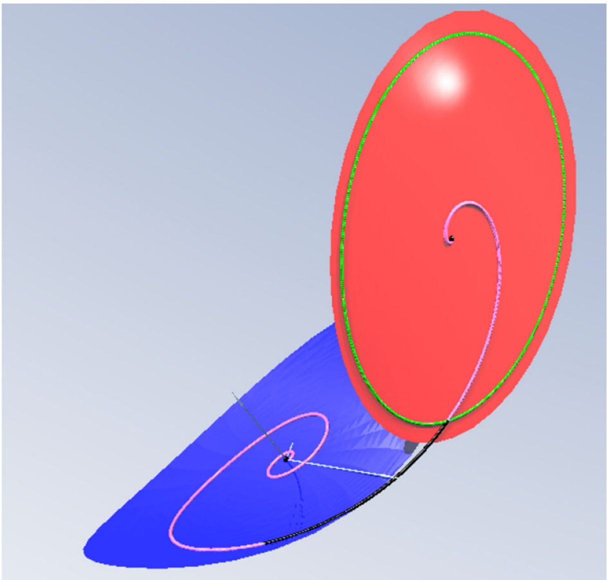

Fig. 5 Validated *long connecting orbit* for Lorenz when $\sigma = -2.2$, $\beta = 8/3$ and $\rho = 3.2$. The image of the phase condition Φ is shown as a *green circular arc* on the local stable manifold. The solution of the long-connection operator is shown as a *black arc*. The *pink arcs* are the image under the parameterizations of the boundary points in parameter space. The manifolds intersect transversally along the *black arc* (Color figure online)

Table 3 Performance data for seven proofs of long-connections for Lorenz with $\beta = 8/3$, $\sigma = -2.2$ and $\rho = 3.2$

M	N	Grid	δ_u	δ_s	R	Proof time
20	25	125	3.09×10^{-11}	4.34×10^{-14}	[0.00127, 0.04144]	14 (s)
20	25	250	3.09×10^{-11}	4.34×10^{-14}	[0.00023, 0.04145]	20 (s)
20	25	500	3.09×10^{-11}	4.34×10^{-14}	[0.00005, 0.04145]	36 (s)
20	25	1000	3.09×10^{-11}	4.34×10^{-14}	[0.00001, 0.04146]	1.4 (min)
20	25	2000	3.09×10^{-11}	4.34×10^{-14}	$[2.93 \times 10^{-6}, 0.04146]$	15 (min)

Table 4 Proof of long-connections for eight different values of ρ

ρ	δ_u	δ_s	R	Proof time (s)
3.2	1.48×10^{-13}	2.75×10^{-14}	[0.00005, 0.04145]	44
3.3	1.88×10^{-13}	3.33×10^{-14}	[0.00006, 0.04298]	45
3.4	3.33×10^{-13}	4.20×10^{-14}	[0.00006, 0.04101]	44
3.5	4.81×10^{-13}	5.40×10^{-14}	[0.00007, 0.03992]	44
3.6	1.27×10^{-12}	6.52×10^{-14}	[0.00007, 0.03843]	44
3.7	5.81×10^{-13}	7.20×10^{-14}	[0.00007, 0.03286]	44
3.8	3.73×10^{-11}	1.01×10^{-13}	[0.00007, 0.02995]	44
3.9	3.21×10^{-10}	1.21×10^{-13}	[0.00008, 0.02703]	44
4.0	3.31×10^{-9}	1.39×10^{-13}	[0.00008, 0.02395]	44
4.1	3.86×10^{-8}	2.05×10^{-13}	[0.00009, 0.02056]	44
4.2	5.14×10^{-6}	2.52×10^{-13}	[0.0001, 0.01509]	44

All manifolds computed to order $N = 25$ and $M = 20$ and spline discretization of 600 grid points

clearly illustrates that the local stable and unstable manifolds do not intersect in phase space, and shows both the spline approximation of the long-connection and the asymptotic orbit segments obtained by applying the linear flow to the boundary points in parameter space. Table 3 tabulates performance results for the same proof at $\rho = 3.2$ for several different parameterization orders and grid discretizations.

To prove Theorem 1 for $\rho \in U_2$ we implemented a simple continuation scheme for the long-connection operator. This implementation can be found in the program `continuation_rho3p2.m`. The results are reported in Table 4. Again, all of these parameter values result in manifolds with complex conjugate pair of eigenvalues. We reiterate that better results can be obtained by finely tuning each computation by hand, and that one can push the value of ρ substantially further. Nevertheless we hope that the results presented here illustrate the utility of the method.

Appendices

Appendix 1: Parameterization Method for Lorenz

Consider $\dot{u} = g(u)$ given by the Lorenz equations (1.5). Let p denote one of the fixed points, λ_1 and λ_2 denote two eigenvalues of $Dg(p)$ with similar stability (either both stable or both unstable), and a_1, a_2 be two associated eigenvectors. In the above considered setting

$\lambda_1 = \bar{\lambda}_2$ and $a_{1,2}$ are complex eigenvectors. Let P denote the parameterization of the invariant manifold (whether stable or unstable) and $\Lambda \in \mathbb{C}^{2,2}$ denote the matrix with λ_1 and λ_2 as diagonal entries. Then in this case the power series is

$$P(\theta) = f(\theta_1 + i\theta_2, \theta_1 - i\theta_2) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} p_{(n_1,n_2)} (\theta_1 + i\theta_2)^{n_1} (\theta_1 - i\theta_2)^{n_2},$$

with $p_{(n_1,n_2)} \in \mathbb{C}^3$ for each $n_1, n_2 \geq 0$ and $f(z) = f(z_1, z_2) : \mathbb{C}^2 \to \mathbb{C}^3$. The linear constraints give that $p_{(0,0)} = p$, $p_{(0,1)} = a_1$, and $p_{(1,0)} = a_2$. The coefficients for $n_1+n_2 \geq 2$ are worked out by considering the functional equation

$$\begin{bmatrix} \sigma(f_2(z) - f_1(z)) \\ \rho f_1(z) - f_1(z) f_3(z) - f_2(z) \\ f_1(z) f_2(z) - \beta f_3(z) \end{bmatrix} = \begin{bmatrix} z_1\lambda_1\partial_{z_1} f_1(z) + z_2\lambda_2\partial_{z_2} f_1(z) \\ z_1\lambda_1\partial_{z_1} f_2(z) + z_2\lambda_2\partial_{z_2} f_2(z) \\ z_1\lambda_1\partial_{z_1} f_3(z) + z_2\lambda_2\partial_{z_2} f_3(z) \end{bmatrix}.$$

The right hand side expands as

$$\begin{bmatrix} z_1\lambda_1\partial_{z_1} f_1(z) + z_2\lambda_2\partial_{z_2} f_1(z) \\ z_1\lambda_1\partial_{z_1} f_2(z) + z_2\lambda_2\partial_{z_2} f_2(z) \\ z_1\lambda_1\partial_{z_1} f_3(z) + z_2\lambda_2\partial_{z_2} f_3(z) \end{bmatrix} = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} (n_1\lambda_1 + n_2\lambda_2) \begin{bmatrix} p^1_{(n_1,n_2)} \\ p^2_{(n_1,n_2)} \\ p^3_{(n_1,n_2)} \end{bmatrix} z_1^{n_1} z_2^{n_2},$$

while the left hand side is

$$\begin{bmatrix} \sigma(f_2(z) - f_1(z)) \\ \rho f_1(z) - f_1(z) f_3(z) - f_2(z) \\ f_1(z) f_2(z) - \beta f_3(z) \end{bmatrix}$$
$$= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \begin{bmatrix} \sigma\left(p^2_{(n_1,n_2)} - p^1_{(n_1,n_2)}\right) \\ \rho\, p^1_{(n_1,n_2)} - p^2_{(n_1,n_2)} - \sum_{k=0}^{n_2} \sum_{j=0}^{n_1} p^1_{(n_1-j,n_2-k)} p^3_{(j,k)} \\ -\beta\, p^3_{(n_1,n_2)} + \sum_{k=0}^{n_2} \sum_{j=0}^{n_1} p^1_{(n_1-j,n_2-k)} p^2_{(j,k)} \end{bmatrix} z_1^{n_1} z_2^{n_2}.$$

Matching like powers of z and solving for the higher order terms in terms of the lower order terms gives the homological equation

$$\begin{pmatrix} \sigma - (n_1\lambda_1 + n_2\lambda_2) & \sigma & 0 \\ \rho - p^3_{(0,0)} & -1 - (n_1\lambda_1 + n_2\lambda_2) & -p^1_{(0,0)} \\ p^2_{(0,0)} & p^1_{(0,0)} & -\beta - (n_1\lambda_1 + n_2\lambda_2) \end{pmatrix} \begin{bmatrix} p^1_{(n_1,n_2)} \\ p^2_{(n_1,n_2)} \\ p^3_{(n_1,n_2)} \end{bmatrix}$$
$$= \sum_{k=0}^{n_2} \sum_{j=0}^{n_1} \begin{bmatrix} 0 \\ \bar{p}^1_{(n_1-j,n_2-k)} \bar{p}^3_{(j,k)} \\ -\bar{p}^1_{(n_1-j,n_2-k)} \bar{p}^2_{(j,k)} \end{bmatrix},$$

where

$$\bar{p}_{(j,k)} = \begin{cases} 0 & \text{if either} \quad i = j = 0 \quad \text{or} \quad i = n_1, j = n_2 \\ p_{(i,j)} & \text{otherwise.} \end{cases}$$

The homological equation has the form

$$[\, Dg(p) - (n_1\lambda_1 + n_2\lambda_2) I \,]\, p_{(n_1,n_2)} = s_{(n_1,n_2)},$$

with s depending only on lower order terms. Moreover the matrix is a characteristic matrix for $Dg(p)$ and is invertible as long as $n_2\lambda_1 + n_2\lambda_2 \neq \lambda_\ell$ for any $n_1 + n_2 \geq 2$ and either of $\ell = 1, 2$. When $\lambda_{1,2}$ are a complex conjugate pair this non-resonance condition holds for all $n_1 + n_2 \geq 2$. If $\lambda_{1,2}$ were real distinct and $\lambda_1 < \lambda_2$ then if $n_2\lambda_2 < \lambda_1$, it follows that $n_1\lambda_1 + n_2\lambda_2 < \lambda_\ell$, $\ell = 1, 2$. So there are no resonances for any multi-index (n_1, n_2) with $n_1 + n_2 \geq \lambda_1/\lambda_2$. Once we check that there are no resonances for multi-indices smaller than this then we rule out resonances to all orders.

Appendix 2: Radii Polynomial Estimates and Formulas for Lorenz

First notice that

$$Dg(x, y, z) = \begin{pmatrix} -\sigma & \sigma & 0 \\ \rho - z & -1 & -x \\ y & x & -\beta \end{pmatrix}. \tag{7.1}$$

Let us start with the computation of the vector functions $v_d(u_h^*, \tilde{u}_1, \tilde{u}_2)$ $(d = 1, \ldots, D)$ defined in (5.8). Recall that we seek an expression of the form

$$Dg(u_h^*(s) + r\tilde{u}_1(s))\tilde{u}_2(s) - Dg(u_h^*(s))(\Pi_h)^n\tilde{u}_2(s) = \sum_{d=1}^{D} v_d r^{d-1}.$$

Let $x_i = (\theta_i, \alpha_i, u_i) = r\tilde{x}_i$,$\tilde{x}_i \in B(1, \omega)$, $i = 1, 2$ as defined in (3.5). This in particular implies that

$$\begin{aligned} \|\tilde{u}_i\|_{C_0} &\leq 1 + \omega \\ \|\tilde{u}_i - (\Pi_h)^3\tilde{u}_i\|_{C_0} &\leq \omega \end{aligned} \tag{7.2}$$

Denoting $u_h^* = ([u_h^*]_1, [u_h^*]_2, [u_h^*]_3)$, $\tilde{u}_i = ([\tilde{u}_i]_1, [\tilde{u}_i]_2, [\tilde{u}_i]_3)$ $(i = 1, 2)$ and applying (7.1) we can write (5.8) as follows.

$$\begin{aligned} &Dg(u_h^*(s) + r\tilde{u}_1(s))\tilde{u}_2(s) - Dg(u_h^*(s))(\Pi_h)^3\tilde{u}_2(s) \\ &= \begin{pmatrix} -\sigma([\tilde{u}_2]_1 - \Pi_h[\tilde{u}_2]_1) + \sigma([\tilde{u}_2]_2 - \Pi_h[\tilde{u}_2]_2) \\ \rho([\tilde{u}_2]_1 - \Pi_h[\tilde{u}_2]_1) - [u_h^*]_3([\tilde{u}_2]_1 - \Pi_h[\tilde{u}_2]_1) - ([\tilde{u}_2]_2 \\ -\Pi_h[\tilde{u}_2]_2) - [u_h^*]_1([\tilde{u}_2]_3 - \Pi_h[\tilde{x}_2]_3) \\ [u_h^*]_2([\tilde{u}_2]_1 - \Pi_h[\tilde{u}_2]_1) + [u_h^*]_1([\tilde{u}_2]_2 - \Pi_h[\tilde{u}_2]_2) - \beta([\tilde{u}_2]_3 - \Pi_h[\tilde{u}_2]_3) \end{pmatrix} \\ &\quad + r\begin{pmatrix} 0 \\ [\tilde{u}_1]_3[\tilde{u}_2]_1 - [\tilde{u}_1]_1[\tilde{u}_2]_3 \\ 2[\tilde{u}_1]_2[\tilde{u}_2]_1 \end{pmatrix} \\ &:= v_1(u_h^*, \tilde{u}_1, \tilde{u}_2) + rv_2(u_h^*, \tilde{u}_1, \tilde{u}_2). \end{aligned}$$

In particular $D = 2$ in this case. Now using (7.2) we can compute $\Gamma_{1,2} \in \mathbb{R}^3$ by applying the following estimates on the subintervals. For $i = 1, \ldots, m$

$$\begin{aligned} &\int_{t_{i-1}}^{t_i} |v_1(u_h^*(s), \tilde{u}_1(s), \tilde{u}_2(s))| ds \\ &\quad \leq \begin{pmatrix} 2|\sigma| \\ \max_{t\in[t_{i-1},t_i]}\{|\rho - [u_h^*]_3(t)| + 1 + |[u_h^*]_1(t)|\} \\ \max_{t\in[t_{i-1},t_i]}\{|[u_h^*]_2(t)| + |[\hat{x}_h]_1(t)| + |\beta|\} \end{pmatrix} \omega(t_i - t_{i-1}) \end{aligned} \tag{7.3}$$

where the absolute value is to be understood component-wise. Similarly

$$\int_{t_{i-1}}^{t_i} |v_2(u_h^*(s), \tilde{u}_1(s), \tilde{u}_2(s))| ds \leq \begin{pmatrix} 0 \\ 2 \\ 2 \end{pmatrix} (t_i - t_{i-1})(1+\omega)^2. \tag{7.4}$$

Splitting the integral from 0 to 1 into the sum of the integrals over the subintervals $[t_{i-1}, t_i]$ $(i = 1, \ldots, m)$ we can use (7.3) and (7.4) to compute $\Gamma_{1,2}$. More explicitely

$$\Gamma_1 = \omega \sum_{i=1}^{m} \begin{pmatrix} 2|\sigma| \\ \max_{t\in[t_{i-1},t_i]}\{|\rho - [u_h^*]_3(t)| + 1 + |[u_h^*]_1(t)|\} \\ \max_{t\in[t_{i-1},t_i]}\{|[u_h^*]_2(t)| + |[u_h^*]_1(t)| + |\beta|\} \end{pmatrix}$$

and

$$\Gamma_2 = (1+\omega)^2 \begin{pmatrix} 0 \\ 2 \\ 2 \end{pmatrix}.$$

By a similar reasoning we can compute $\Gamma_{1,2}^i \in \mathbb{R}^{m+1}$ for $i = 1, 2, 3$. The bounds $\Lambda_{s,u}$ were derived in general in (5.6) and (5.7). Therefore we have all the ingredients to compute the bounds $Z_l(r)$ $(l = 1, \ldots, 3(m+2))$.

We continue to derive explicit expressions for Y_∞ and $Z_\infty(r)$. Recall that

$$(u_h^*)'(t)|_{(t_{i-1},t_i)} = \frac{1}{t_i - t_{i-1}} \Delta u_i^*,$$

where $u_i^* = u_h^*(t_i)$ for $i = 0, \ldots, m$ and $\Delta u_i^* = u_i^* - u_{i-1}^*$.
$\underline{Y_\infty}$: Let $i = 1, \ldots, m$:

$$Dg(u_h^*)(u_h^*)'|_{(t_{i-1},t_i)} = \frac{1}{t_i - t_{i-1}} \begin{pmatrix} -\sigma & \sigma & 0 \\ \rho - [u_h^*]_3|_{(t_{i-1},t_i)} & -1 & -[u_h^*]_1|_{(t_{i-1},t_i)} \\ [u_h^*]_2|_{(t_{i-1},t_i)} & [u_h^*]_1|_{(t_{i-1},t_i)} & -\beta \end{pmatrix} \Delta u_i^*.$$

Hence we obtain:

$$\left|\frac{d^2}{dt^2} h^1(t)|_{(t_{i-1},t_i)}\right| \leq \frac{L}{t_i - t_{i-1}} \sigma \left|\Delta[u_i^*]_2 - \Delta[u_i^*]_1\right|$$

$$\left|\frac{d^2}{dt^2} h^2(t)|_{(t_{i-1},t_i)}\right| \leq \frac{L}{t_i - t_{i-1}} \left|(\rho - [u_h^*]_3\big|_{(t_{i-1},t_i)})\Delta[u_i^*]_1 - \Delta[u_i^*]_2 - [u_h^*]_1\big|_{(t_{i-1},t_i)} \Delta[u_i^*]_3\right|$$

$$\left|\frac{d^2}{dt^2} h^3(t)|_{(t_{i-1},t_i)}\right| \leq \frac{L}{t_i - t_{i-1}} \left|[u_h^*]_2|_{(t_{i-1},t_i)} \Delta[u_i^*]_1 + [u_h^*]_1\big|_{(t_{i-1},t_i)} \Delta[u_i^*]_2 - \beta\Delta[u_i^*]_3\right|.$$

Using interval arithmetic we are able to evaluate $[u_h^*]_i|_{(t_{i-1},t_i)}$ for $i = 1, 2, 3$ and finalize the computations for Y_∞ using Lemma 5.
$\underline{Z_\infty}$: Using (7.1) one obtains after computing

$$Dg(u_h^* + r\tilde{u}_1)\tilde{u}_2 = \begin{pmatrix} -\sigma[\tilde{u}_2]_1 + \sigma[\tilde{u}_2]_1 \\ \rho[\tilde{u}_2]_2 - [u_h^*]_3[\tilde{u}_2]_1 - r[\tilde{u}_1]_3[\tilde{u}_2]_1 - [\tilde{x}_2]_2 - [u_h^*]_1[\tilde{u}_2]_|3 - r[\tilde{x}_1]_1[\tilde{u}_2]_3 \\ [u_h^*]_2[\tilde{x}_2]_1 + r[\tilde{x}_1]_2[\tilde{u}_2]_1 + [u_h^*]_1[\tilde{u}_2]_2 + r[\tilde{x}_1]_2[\tilde{u}_2]_2 - \beta[\tilde{u}_2]_3 \end{pmatrix}$$

that

$$|Dg^1(u_h^* + r\tilde{u}_1)\tilde{u}_2| \leq 2\sigma(1+\omega)$$
$$|Dg^2(u_h^* + r\tilde{u}_1)\tilde{u}_2| \leq (\rho + 1 + |[u_h^*]_3| + |[u_h^*]_1| + 2r)(1+\omega)^2$$
$$|Dg^3(u_h^* + r\tilde{u}_1)\tilde{u}_2| \leq (\beta + |[u_h^*]_2| + |[\hat{x}_h]_1| + 2r)(1+\omega)^2.$$

Using Lemma 6 by evaluating the above bounds with interval arithmetic on the subintervals (t_{i-1}, t_i) $(i = 1, \ldots, m)$ we can use this finalize the computation of $Z_\infty(r)$.

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