# Rigorous numerics for nonlinear differential equations using Chebyshev series

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**Abstract**

A computational method based on Chebyshev series to rigorously compute solutions of initial and boundary value problems of analytic nonlinear vector fields is proposed. The idea is to recast solutions as fixed points of an operator defined on a Banach space of rapidly decaying Chebyshev coefficients and to use the so-called radii polynomials to show the existence of a unique fixed point nearby an approximate solution. As applications, solutions of initial value problems in the Lorenz equations and symmetric connecting orbits in the Gray-Scott equation are rigorously computed. The symmetric connecting orbits are obtained by solving a boundary value problem with one of the boundary values in the stable manifold.

## 1 Introduction

In this paper, we propose a rigorous numerical method based on the Chebyshev polynomials to compute solutions of nonlinear differential equations. More explicitly, the field of rigorous numerics develops algorithms that provide approximate solutions to a problem together with precise bounds within which exact solutions are guaranteed to exist in the mathematically rigorous sense. In this context, the main idea of our proposed approach is to expand the solution of a given differential equation using its Chebyshev series, plug the expansion in the equation, obtain an equivalent infinite dimensional problem of the form $f(x) = 0$ to solve in a Banach space of rapidly decaying Chebyshev coefficients and to get the existence, via a fixed point argument, of a genuine solution of $f(x) = 0$ nearby a numerical approximation of a finite dimensional projection of $f$. The fixed point argument is solved by using the radii polynomials (e.g. see [1]), which provide an efficient way of constructing a set on which the contraction mapping theorem is applicable.

Before proceeding further, it is worth mentioning that a similar approach based on Fourier series is widely used in the field of rigorous numerics to compute solutions of differential equations with periodic profiles. For instance, time periodic solutions of ODEs [2, 3], stationary solutions of PDEs with periodic or Neumann boundary conditions [4, 5, 6, 7], time periodic solutions of delay differential equations [8, 9] and invariant sets of infinite dimensional maps [10] have been successfully computed using Fourier series and rigorous numerics. However, to the best of our knowledge, this is the first time that a method based on Chebyshev series is presented to rigorously compute solutions of nonlinear differential equations. Since a large class of solutions of differential equations

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are non periodic (e.g. solutions of initial value problems (IVPs) and boundary value problems (BVPs) with non periodic boundary values), we believe that our proposed approach is a valuable contribution to the field of rigorous numerics. Also, since Chebyshev series are Fourier series *in disguise* [11], the mathematical machinery developed in the last ten years to prove existence of solutions with periodic profiles can directly be transferred to prove existence of non periodic solutions. To give a few examples, the analytic estimates introduced in [4, 6, 10, 12] and the Banach space of rapidly decaying coefficients used in [3, 4] can be used here. Finally, let us mention the work [13] where the authors develop Chebyshev interpolation polynomial-based tools for rigorous computing. However, it seems that they have not yet applied their methods to rigorously solve nonlinear differential equations.

In the present work, we focus our attention to analytic vector fields of the form

$$\frac{du}{dt} = \Psi(u), \quad \Psi : \mathbb{R}^n \to \mathbb{R}^n, \tag{1}$$

where we aim at computing rigorously solutions of IVPs and BVPs associated to (1). Even if we present the method in this context, we strongly believe that a similar approach could be adapted to directly prove existence of solutions of higher order differential equations.

The Chebyshev polynomials are defined by $T_0(t) = 1$, $T_1(t) = t$ and $T_{k+1}(t) = 2tT_k(t) - T_{k-1}(t)$ for $k \geq 1$. They lead to an analogue of the Fourier expansion for non periodic functions on an interval and, as mentioned earlier, they are Fourier series *in disguise*, as $T_k(\cos\theta) = \cos(k\theta)$. The following standard result can be found in [14].

**Theorem 1.1.** *Every Lipschitz continuous function $v : [-1, 1] \to \mathbb{R}$ has a unique representation as an absolutely and uniformly convergent series $v(t) = \sum_{k=0}^{\infty} a_k T_k(t)$.*

The following result, which can also be found in [14], shows that the coefficients $a_k$ of the Chebyshev series of an analytic function $v$ decay exponentially fast to zero.

**Theorem 1.2.** *Let a function $v$ analytic in $[-1, 1]$ be analytically continuable to the open $\rho$-ellipse $E_\rho$ for some $\rho > 1$ where it satisfies $|v(z)| \leq M$ for all $z \in E_\rho$ for some $M$. Then its Chebyshev coefficients satisfy $|a_k| \leq 2M\rho^{-k}$, with $|a_0| \leq M$ in the case $k = 0$.*

$E_\rho$ (with foci at $\pm 1$) is defined by fixing $\rho > 1$ and considering the image of the circle with radius $\rho$ in the complex plane $\mathbb{C}$ under the map $w = \frac{1}{2}(z + z^{-1})$. This consequence of Theorem 1.1 and Theorem 1.2 plays a fundamental role in the design of our approach.

**Corollary 1.1.** *Assume that $\Psi : \mathbb{R}^n \to \mathbb{R}^n$ is real analytic and let $u : [-1, 1] \to \mathbb{R}^n$ be a solution of (1). Then each component $u_j$ of $u$ is real analytic and has a unique representation as an absolutely and uniformly convergent series of the form $u_j(t) = \sum_{k=0}^{\infty} (a_j)_k T_k(t)$. Also, for each $j \in \{1, \ldots, n\}$, the sequence of Chebyshev coefficients $\{(a_j)_k\}_{k\geq 0}$ of $u_j$ decreases to zero faster than any algebraic decay, that is, for any decay rate $s > 1$, there exists a constant $C_j = C_j(s) < \infty$ such that $|(a_j)_k| \leq \frac{C_j}{k^s}$, for $k \geq 1$.*

Consider a Chebyshev expansion of a solution $u$ of the analytic vector field (1)

$$u(t) = a_0 + 2\sum_{k\geq 1} a_k T_k(t), \tag{2}$$

where $a_k = \big((a_1)_k, (a_2)_k, \cdots, (a_n)_k\big)^T \in \mathbb{R}^n$. Letting $\|a_k\|_\infty = \max_{j=1,\ldots,n}\{|(a_j)_k|\}$ and defining the weights

$$\omega_k^s \stackrel{\text{def}}{=} \begin{cases} 1, & \text{if } k = 0 \\ |k|^s, & \text{if } k \neq 0, \end{cases} \tag{3}$$

one has by Corollary 1.1 that for any given $s > 1$

$$\|a\|_s \stackrel{\text{def}}{=} \sup_{k\geq 0}\{\|a_k\|_\infty \omega_k^s\} < \infty. \tag{4}$$

The philosophy of our method is therefore to rigorously compute solutions $u$ of an IVP or a BVP associated to (1) first by recasting them as solutions of an operator equation

$$F(u) = 0, \tag{5}$$

and then to use Chebyshev series to transform (5) into an equivalent problem of the form

$$f(x) = 0, \tag{6}$$

to solve in a Banach space $X^s$ of algebraically decaying Chebyshev coefficients. We now introduce the operators (5) and (6), first for IVPs and then for BVPs.

**Initial value problems.** The first class of problems we address in the present work are initial value problems associated to the vector field (1). Integrating (1) from $-1$ to $t$, one has that finding a solution $u$ with initial condition $u(-1) = p_0 \in \mathbb{R}^n$ is equivalent to finding a solution $u$ of $F(u) = 0$, where the nonlinear operator $F$ is given by

$$F(u)(t) \stackrel{\text{def}}{=} p_0 + \int_{-1}^{t} \Psi(u(s))ds - u(t), \quad t \in [-1, 1]. \tag{7}$$

The fact that $t \in [-1, 1]$ is not a restriction since in the autonomous vector field (1), a re-scaling of time could be considered. The goal is to develop a rigorous computational method based on Chebyshev series to compute solutions of (7). Given the Chebyshev expansion (2) of $u$ with $a = (a_k)_{k\geq 0}$ the infinite vector of Chebyshev coefficients, consider the Chebyshev expansion of $\Psi(u)$ given by

$$\Psi(u(t)) = c_0 + 2\sum_{k\geq 1} c_k T_k(t), \tag{8}$$

where $c_k = c_k(a) = \big((c_1)_k, (c_2)_k, \cdots, (c_n)_k\big)^T \in \mathbb{R}^n$. In particular, if $\Psi(u)$ is a polynomial vector field, then since Chebyshev polynomials satisfy $T_k(\cos\theta) = \cos(k\theta)$, $c_k$ is given by discrete convolutions involving the coefficients of $a$. Plugging (2) and (8) in (7), and using the properties $T_k(-1) = (-1)^k$ and $T_k(1) = 1$ for all $k$, $\int T_0(s)ds = T_1(s)$, $\int T_1(s)ds = (T_2(s) + T_0(s))/4$ and $\int T_k(s)ds = \frac{1}{2}\left(\frac{T_{k+1}(s)}{k+1} - \frac{T_{k-1}(s)}{k-1}\right)$ for $k \geq 2$, one gets that

$$F(u)(t) = \tilde{f}_0 + 2\sum_{k\geq 1} \tilde{f}_k T_k(t),$$

where $\tilde{f}_0 \stackrel{\text{def}}{=} p_0 - a_0 + c_0 - \frac{c_1}{2} - 2\sum_{j\geq 2} \frac{(-1)^j}{j^2-1} c_j$ and $\tilde{f}_k \stackrel{\text{def}}{=} \frac{c_{k-1} - c_{k+1}}{2k} - a_k$, for $k \geq 1$. Denote $x = a$ and define $f(x) = (f_k(x))_{k\geq 0}$ component-wise by

$$f_k(x) \stackrel{\text{def}}{=} \begin{cases} p_0 - a_0 + c_0 - \dfrac{c_1}{2} - 2\displaystyle\sum_{j\geq 2} \frac{(-1)^j}{j^2-1} c_j, & k = 0, \\ 2ka_k + c_{k+1} - c_{k-1}, & k \geq 1. \end{cases} \tag{9}$$

Note that $f_k = -2k\tilde{f}_k$ for $k \geq 1$. $f$ given by (9) is called the *IVP-operator* and finding a solution $u$ of the initial value problem (7) is equivalent to finding a zero of the IVP-operator.

**Boundary value problems.** A second class of problems that we address in the present work are boundary value problems associated to the vector field (1), that is solutions $u$ satisfying the differential equations (1) in $[-1,1]$ while satisfying the boundary condition

$$\mathcal{G}(u(-1),u(1))=0, \tag{10}$$

where $\mathcal{G}:\mathbb{R}^{2n}\to\mathbb{R}^p$ is an affine map, with $p$ the *number* of boundary conditions. Letting $p_1=u(1)$, integrating the vector field (1) from $t$ to 1 and appending the boundary condition (10) results in the integral operator defined by

$$F(\theta,u)(t)\overset{\text{def}}{=}\begin{pmatrix}\mathcal{G}(u(-1),u(1))\\ u(t)+\displaystyle\int_t^1\Psi(u(s))ds-p_1\end{pmatrix}, \tag{11}$$

where $\mathcal{G}(u(-1),u(1))$ and/or $p_1$ depend on a parameter $\theta\in\mathbb{R}^p$ which ensures that the operator (11) is not overdetermined. Denote by $x=(\theta,a)$ the infinite dimensional vector of unknowns. Following the same approach as the one used to derive the IVP-operator, we plug (2) and (8) in (11), use standard properties of the Chebyshev polynomials and then we define the operator $f(x)=(f_k(x))_{k\geq -1}$ given component-wise by

$$f_k(x)=\begin{cases}\eta(\theta,a), & k=-1,\\ a_0+c_0+\dfrac{c_1}{2}-2\displaystyle\sum_{j\geq 2}\frac{1}{j^2-1}c_j-p_1, & k=0,\\ 2ka_k+c_{k+1}-c_{k-1}, & k\geq 1,\end{cases} \tag{12}$$

where $\eta\in\mathbb{R}^p$ is a function of $a=(a_k)_{k\geq 0}$ and possibly of $\theta$ that represents the boundary condition (10) expressed using the Chebyshev expansion of $u$. We call the operator $f(x)=(f_k(x))_{k\geq -1}$ given by (12) the *BVP-operator*. Hence, finding a solution $u$ of the boundary value problem (11) is equivalent to finding a zero of the BVP-operator.

Let us introduce the notation $x=(x_k)_{k\geq k_0}$ and $f=(f_k)_{k\geq k_0}$, with $k_0\in\{-1,0\}$. If $x$ is the vector of unknown of the IVP-operator (9), then $k_0=0$ and $x=(x_k)_{k\geq k_0}$, with $x_k=a_k\in\mathbb{R}^n$ for $k\geq 0$. If $x$ is the vector of unknown of the BVP-operator (12), then $k_0=-1$ and $x=(x_k)_{k\geq k_0}$, with $x_{-1}=\theta\in\mathbb{R}^p$ and $x_k=a_k\in\mathbb{R}^n$ for $k\geq 0$. Similarly, if $f$ is the IVP-operator (9), then $k_0=0$ and if $f$ is the BVP-operator (12), then $k_0=-1$ and $f=(f_k)_{k\geq k_0}$, with $f_{-1}=\eta\in\mathbb{R}^p$.

Given $\theta\in\mathbb{R}^p$, let $\|\theta\|_\infty=\max\{|\theta_1|,|\theta_2|,\ldots,|\theta_p|\}$. Recall the weights (3). As a consequence of Corollary 1.1, we define the IVP-operator and the BVP-operator on the Banach space of decaying Chebyshev coefficients given by

$$X^s=\{x=(x_k)_{k\geq k_0}:\|x\|_s\overset{\text{def}}{=}\sup_{k\geq k_0}\{\|x_k\|_\infty\omega_k^s\}<\infty\}, \tag{13}$$

with $k_0=0$ in case of the IVP-operator and with $k_0=-1$ in case of the BVP-operator. The rest of the paper aims at introducing the rigorous method to prove existence of solutions of $f(x)=0$ within $X^s$ using the notion of the radii polynomials.

The paper is organized as follows. In Section 2, we introduce the rigorous computational method to prove existence of solutions of $f(x)=0$ within $X^s$, where $f$ is either the IVP-operator (9) or the BVP-operator (12). In Section 3, we present some applications. In Section 3.1, rigorous computations of IVPs in the Lorenz equations are introduced while in Section 3.2, we compute symmetric connecting orbits for the Gray-Scott equation. Note that the symmetric connecting orbits are obtained by computing solutions of a BVP with one of the boundary values in the stable manifold. We conclude the paper in Section 4 by presenting some possible extensions and improvements.

## 2 Rigorous computations

In this section, we introduce the rigorous computational method to compute $x \in X^s$ that are solutions of $f(x) = 0$, where the operator $f$ is either the IVP-operator (9) or the BVP-operator (12). Let us formalize the definition of the operator $f$ on $X^s$.

**Lemma 2.1.** *Consider the Banach space $X^s$ with $s > 1$, the vector field (1), let $x = (x_k)_{k\geq k_0} \in X^s$ and define $u(t) = a_0 + 2\sum_{k\geq 1} a_k T_k(t)$, where $a_k = x_k$ for $k \geq 0$. Assume that the coefficients $(c_k)_{k\geq 0}$ of the Chebyshev series of $\Psi(u)$ given by (8) satisfy*

$$\|c\|_s = \sup_{k\geq 0}\{\|c_k\|_\infty \omega_k^s\} < \infty. \tag{14}$$

*Consider $f$ either the IVP-operator (9) or the BVP-operator (12). Then, $f : X^s \to X^{s-1}$. Also, if $x \in X^s$ is a solution of $f(x) = 0$, then $x \in X^{s_0}$ for any $s_0 > 1$. Finally, $u(t) = a_0 + 2\sum_{k\geq 1} a_k T_k(t)$ is a solution of $F = 0$ where $F$ is the integral operator (7) (respectively (11)) if and only if $x = (x_k)_{k\geq k_0} \in X^s$ solves $f(x) = 0$ where $f$ is the IVP-operator (9) (respectively the BVP-operator (12)).*

Before presenting the proof of Lemma 2.1, it is important to remark that the hypothesis (14) is met for all polynomial vector fields, since for any $s > 1$, $\Omega^s \stackrel{\text{def}}{=} \{a = (a_k)_{k\in\mathbb{N}} : a_k \in \mathbb{R},\ \|a\|_s < \infty\}$ is an algebra under the discrete convolution. More precisely for any $a, b \in \Omega^s$, there exists a constant $\alpha = \alpha(a, b) < \infty$ such that $|(a * b)_k| = |\sum_{\substack{k_1+k_2=k \\ k_i\in\mathbb{Z}}} a_{|k_1|} b_{|k_2|}| \leq \frac{\alpha}{\omega_k^s}$ (e.g. see [4] for the case $s \geq 2$ and see [15] for the case $s \in (1, 2)$). This implies that $a * b \in \Omega^s$, and hence that $(\Omega^s, *)$ is an algebra. For ease of notation we will henceforth omit the $*$.

*Proof.* (of Lemma 2.1) Consider $x = (x_k)_{k\geq k_0} \in X^s$ and define $u(t) = a_0 + 2\sum_{k\geq 1} a_k T_k(t)$, with $a_k = x_k$ for $k \geq 0$. In case $k_0 = -1$, one clearly has that $\|f_{k_0}(x)\|_\infty = \|\eta(x)\|_\infty < \infty$. Consider the Chebyshev coefficients $(c_k)_{k\geq 0}$ of $\Psi(u)$ that satisfy $\|c\|_s < \infty$. Hence, $\|c_k\|_\infty \leq \frac{\|c\|_s}{\omega_k^s}$ and therefore $\|\sum_{j\geq 2} \frac{c_j}{j^2-1}\|_\infty \leq \|c\|_s \sum_{j\geq 2} \frac{1}{j^s(j^2-1)} < \infty$. That implies that $\|f_0(x)\|_\infty < \infty$. Now, there exists a constant $\alpha_1 < \infty$ such that $\|f_k(x)\|_\infty = \|2ka_k + c_{k+1} - c_{k-1}\|_\infty \leq \frac{2\|a\|_s}{\omega_k^{s-1}} + \frac{\|c\|_s}{\omega_{k+1}^s} + \frac{\|c\|_s}{\omega_{k-1}^s} \leq \frac{\alpha_1}{\omega_k^{s-1}}$ for all $k \geq 1$. It follows that $\|f(x)\|_{s-1} < \infty$ and therefore that $f(x) \in X^{s-1}$.

Assume now that $x \in X^s$ is a solution of $f(x) = 0$. Hence, for any $k \geq 1$, $f_k(x) = 2ka_k + c_{k+1} - c_{k-1} = 0$ which implies that $a_k = -\frac{1}{2k}(c_{k+1} - c_{k-1})$. Since $c = (c_k)_{k\geq 0}$ satisfies (14), there exists a constant $\alpha_2 < \infty$ such that

$$\sup_{k\geq 1}\{\|a_k\|_\infty \omega_k^{s+1}\} \leq \sup_{k\geq 1}\{\frac{1}{2k}(\|c_{k+1}\|_\infty + \|c_{k-1}\|_\infty)\omega_k^{s+1}\} \leq \alpha_2.$$

That shows that $x = (x_k)_{k\geq k_0} \in X^{s+1}$. Repeating the same argument inductively and using the fact that $X^{s_1} \subset X^{s_2}$ for any $s_1 \geq s_2$, one gets that $x \in X^{s_0}$ for all $s_0 > 1$. Finally, the fact that $u(t) = a_0 + 2\sum_{k\geq 1} a_k T_k(t)$ is a solution of $F = 0$ where $F$ is the integral operator (7) (resp. (11)) if and only if $x = (x_k)_{k\geq k_0} \in X^s$ solves $f(x) = 0$ where $f$ is the IVP-operator (9) (resp. the BVP-operator (12)) is trivial by construction. □

A consequence of Lemma 2.1 is that if one shows the existence of $x \in X^s$ such that $f(x) = 0$ (for some $s > 1$) where $f$ is the IVP-operator (9) (resp. the BVP-operator (12)), then the coefficients $(a_k)_k$ decay faster than any algebraic decay and $u(t)$ given by (2) is a solution of the initial value problem (7) (resp. the boundary value problem (11)).

The strategy to find solutions of (6) is to consider an equivalent fixed point operator $T : X^s \to X^s$ whose fixed point are in one-to-one correspondence with the zeros of $f$. More precisely, the operator $T$ is a Newton-like operator about an approximate solution $\bar{x}$ of $f$. In order to compute this numerical approximation we introduce a Galerkin projection. Let $m > 1$ and define the finite dimensional projection $\Pi_m : X^s \to X^s_m$ by $\Pi_m x = (x_k)_{k=k_0}^{m-1}$. The Galerkin projection of $f$ is defined by

$$f^{(m)} : X^s_m \to X^s_m : x_F \mapsto \Pi_m f(x_F, 0_\infty), \tag{15}$$

where $0_\infty = (I - \Pi_m)0$. Identifying $(x_F, 0_\infty)$ with $x_F \in X^s_m \cong \mathbb{R}^{p+nm}$ we think of $f^{(m)} : \mathbb{R}^{p+nm} \to \mathbb{R}^{p+nm}$. Now assume that we have computed $\bar{x}_F \in \mathbb{R}^{p+nm}$ such that $f^{(m)}(\bar{x}_F) \approx 0$ and let $\bar{x} = (\bar{x}_F, 0_\infty) \in X^s$. Let $B_{\bar{x}}(r) = \bar{x} + B(r)$, the closed ball in $X^s$ of radius $r$ centered at $\bar{x}$, where

$$B(r) = \left\{ x \in X^s : \ \|x\|_s = \sup_{k \geq k_0} \{\|x_k\|_\infty \omega_k^s\} \leq r \right\} = \prod_{k \geq k_0} \left[ -\frac{r}{\omega_k^s}, \frac{r}{\omega_k^s} \right]^{d(k_0)}, \tag{16}$$

where $d(-1) = p$ and $d(k) = n$ for $k \geq 0$. In order to define the fixed point operator $T$, we introduce $A_m \approx \left(Df^{(m)}(\bar{x}_F)\right)^{-1}$ a numerical inverse of $Df^{(m)}(\bar{x}_F)$. Assume that the finite dimensional matrix $A_m$ is invertible (this hypothesis can be rigorously verified with interval arithmetic). Define the linear invertible operator $A : X^s \to X^{s+1}$ by

$$(Ax)_k = \begin{cases} (A_m(\Pi_m x))_k, & k = k_0, \ldots, m-1 \\ \left(\frac{1}{2k}\right) x_k, & k \geq m. \end{cases} \tag{17}$$

Finally define the Newton-like operator $T : X^s \to X^s$ about the numerical solution $\bar{x}$ by

$$T(x) = x - Af(x). \tag{18}$$

The goal is to determine (if possible) a positive radius $r$ of the ball $B_{\bar{x}}(r)$ so that $T : B_{\bar{x}}(r) \to B_{\bar{x}}(r)$ is a contraction. Assuming that such $r > 0$ exists, an application of the contraction mapping theorem yields the existence of a unique fixed point $\tilde{x}$ of $T$ within the closed ball $B_{\bar{x}}(r)$. By invertibility of the linear operator $A$, one can conclude that $\tilde{x}$ is the unique solution of $f(x) = 0$ in the ball $B_{\bar{x}}(r)$. By construction, this unique solution represents a solution $u(t)$ of the IVP-operator (7) or the boundary value problem (11), depending on the situation. Hence, all we need to do is to find $r > 0$ such that $T : B_{\bar{x}}(r) \to B_{\bar{x}}(r)$ is a contraction. This task is achieved with the notion of the radii polynomials (originally introduced in [1] to compute equilibria of PDEs), which provide an efficient way of constructing a set on which the contraction mapping theorem is applicable. Their construction depends on some bounds that we introduce shortly. Before that, we introduce the notation $\preceq$ to denote component-wise inequality, that is given two vectors $u, v$, $u \preceq v$ if and only if $u_k \leq v_k$ for all $k$. The same notation holds for $\prec$. Consider now the bound $Y = (Y_k)_{k \geq k_0}$ satisfying

$$\left| \left[ T(\bar{x}) - \bar{x} \right]_k \right| \preceq Y_k, \quad k \geq k_0, \tag{19}$$

where $Y_k \in \mathbb{R}^n_+$ for $k \geq 0$. If $k_0 = -1$, then $Y_{k_0} \in \mathbb{R}^p_+$. Consider the bound $Z(r) = (Z_k(r))_{k \geq k_0}$ satisfying

$$\sup_{\xi_1, \xi_2 \in B(r)} \left| \left[ DT(\bar{x} + \xi_1)\xi_2 \right]_k \right| \preceq Z_k(r), \quad k \geq k_0, \tag{20}$$

where $Z_k(r) \in \mathbb{R}^n_+$ for $k \geq 0$. If $k_0 = -1$, then $Z_{k_0}(r) \in \mathbb{R}^p_+$. If the vector field (1) is polynomial, then it is possible to obtain a polynomial expansion in $r$ for $Z_k(r)$. As a matter of fact, in this case, the degree of the polynomial $Z_k(r)$ is the same than the degree of the polynomial vector field $\Psi(u)$. Otherwise, that is if the analytic vector field $\Psi(u)$ is not polynomial, a Taylor expansion can be considered in order to obtain a polynomial expression in $r$ for $Z_k(r)$. We make now the following important assumption. Assume that there exists a number $M \geq m$ where $m$ is the *dimension* of the Galerkin projection (15) such that the bounds $Y$ and $Z$ satisfying (19) and (20) are such that

**A1.** $Y_k = 0 \in \mathbb{R}^n$ for all $k \geq M$.

**A2.** There exists a *uniform* polynomial bound $\bar{Z}_M(r) \in \mathbb{R}^n_+$ such that for all $k \geq M$,

$$Z_k(r) \preceq \frac{\bar{Z}_M(r)}{\omega_k^s}. \tag{21}$$

Before introducing the radii polynomials, let us briefly talk about the two above assumptions. If the vector field $\Psi(u)$ is polynomial, then the nonlinear terms $c_k(\bar{a})$ are convolutions terms of the form $(\bar{a}_{(j_1)}\bar{a}_{(j_2)}\cdots\bar{a}_{(j_\ell)})_k$ which are eventually equal to zero for large enough $k$ since $\bar{a}_k = 0$ for $k \geq m$. Hence, by construction of $A$ defined in (17) and of the bound $Y$ as in (19), there exists $M$ such that $Y_k$ can be defined to be $0 \in \mathbb{R}^n$ for $k \geq M$. Again in case the vector field $\Psi(u)$ is polynomial, there are some analytic convolution estimates (e.g. the ones developed in [4]) that allow computing $\bar{Z}_M(r)$ satisfying (21). The computation of the uniform polynomial bound $\bar{Z}_M(r)$ is presented explicitly in the examples of Section 3.

**Defintion 2.1.** *Denote by* $\mathbf{1_n} \in \mathbb{R}^n$ *the vector whose components are all* 1. *We define the finite radii polynomials* $(p_k(r))_{k\geq k_0}^{M-1}$ *by*

$$p_k(r) = Y_k + Z_k(r) - \frac{r}{\omega_k^s}\mathbf{1_n}, \quad k = k_0, \ldots, M-1, \tag{22}$$

*and the tail radii polynomial by*

$$p_M(r) = \bar{Z}_M(r) - r\mathbf{1_n}. \tag{23}$$

The following result justifies the construction of the radii polynomials of Definition 2.1.

**Theorem 2.1.** *If there exists* $r > 0$ *such that* $p_k(r) \prec 0$ *for all* $k = k_0, \ldots, M$, *then* $T : B_{\bar{x}}(r) \to B_{\bar{x}}(r)$ *is a contraction and therefore there exists a unique* $\tilde{x} \in B_{\bar{x}}(r)$ *such that* $T(\tilde{x}) = \tilde{x}$. *Hence, there exists a unique* $\tilde{x} \in B_{\bar{x}}(r)$ *such that* $f(\tilde{x}) = 0$.

*Proof.* See Corollary 3.6 in [4]. □

The strategy to rigorously compute solutions of the IVP-operator $f$ given in (7) and the BVP-operator $f$ given in (11) is therefore to construct the radii polynomials of Definition 2.1, to verify (if possible) the hypothesis of Theorem 2.1, and to use the result of Lemma 2.1 to conclude that $u(t) = a_0 + 2\sum_{k\geq 1} a_k T_k(t)$ is a solution of $F = 0$ where $F$ is either the integral operator given by (7) or the operator given by (11)

While the computation of the bound $Y$ satisfying (19) is rather straightforward, the computation of the polynomial bound $Z(r)$ satisfying (20) is more involved. In order to simplify its computation, we introduce the linear invertible operator $A^\dagger : X^s \to X^{s-1}$ by

$$(A^\dagger x)_k = \begin{cases} (Df^{(m)}(\bar{x}_F)(\Pi_m x))_k, & k = k_0, \ldots, m-1 \\ (2k)\, x_k, & k \geq m. \end{cases} \tag{24}$$

and we use the factorization $T(x) = x - Af(x) = (I - AA^\dagger)x - A(f(x) - A^\dagger x)$. Letting $\xi_1 = wr$, $\xi_2 = vr$ with $w, v \in B(1)$, one has that

$$\begin{aligned} DT(\bar{x} + \xi_1)\xi_2 &= (I - AA^\dagger)\xi_2 - A\left(Df(\bar{x} + \xi_1)\xi_2 - A^\dagger\xi_2\right) \\ &= \left[(I - AA^\dagger)v\right] r - A\left(Df(\bar{x} + wr)vr - A^\dagger vr\right), \end{aligned} \tag{25}$$

where the first term is of the form $\epsilon r$, for $\epsilon = (I - AA^\dagger)v \in X^s$ very small, and where the coefficient of $r$ in $[Df(\bar{x}+wr)vr - A^\dagger vr]_k$ should be small as the dimension of the Galerkin projection $m$ is large. Hence, for $m$ large enough, the coefficient in $r$ of $Z_k(r)$ should be small. That should increase the chances of the coefficient of $r$ in the radii polynomials defined in Definition 2.1 to be negative, and therefore increase the chances of verifying the hypothesis of Theorem 2.1. We are now ready to present some applications.

# 3 Applications

In this section, we present two applications. The first application, presented in Section 3.1, concerns initial value problems in the Lorenz equations. More precisely, we use the notion of radii polynomials to compute rigorously solutions of the IVP-operator $f$ given by (9). This yields rigorous enclosures of solutions of the integral operator (7), where $\Psi(u)$ is the vector field arising in the Lorenz equations. The second application, presented in Section 3.2, concerns projected boundary value problems in the Gray-Scott equation. More precisely, we use the notion of radii polynomials to compute rigorously solutions of the BVP-operator $f$ given by (12) where one of the boundary value is in the stable manifold of a steady state. This yields rigorous enclosures of several symmetric connecting orbits for the Gray-Scott equation.

## 3.1 Initial value problem in the Lorenz equations

Consider the Lorenz equations re-scaled by a time factor $L$ given by

$$\frac{du}{dt} = \Psi(u) = L \begin{pmatrix} \sigma(u_2 - u_1) \\ \rho u_1 - u_2 - u_1 u_3 \\ u_1 u_2 - \beta u_3 \end{pmatrix} \tag{26}$$

at the classical parameter values $\sigma = 10$, $\rho = 28$ and $\beta = 8/3$.

The Chebyshev coefficients (8) of (26) are given explicitly by

$$c_k = L \begin{pmatrix} \sigma((a_2)_k - (a_1)_k) \\ \rho(a_1)_k - (a_2)_k - (a_1 a_3)_k \\ (a_1 a_2)_k - \beta(a_3)_k \end{pmatrix} \tag{27}$$

with

$$(a_n a_m)_k = \sum_{\substack{k_1 + k_2 = k \\ k_i \in \mathbb{Z}}} (a_n)_{|k_1|}(a_m)_{|k_2|}$$

for $n = 1$, $m = 1, 2$ and $k \geq 0$. Given an initial condition $p_0$, this results in an explicit expression $f(x)$ for the IVP-operator (9). We now present rigorous numerical results illustrating the performance of our method.

**Theorem 3.1.** *Consider*

$$p_0^1 = (8.102574164767477, 9.551574461919124, 24.429705657930224)$$
$$p_0^2 = (-0.3074083926082352, 0.3943349846945122, 0)$$
$$p_0^3 = (4.102702069909453, 8.936495309135337, 0.5789130478426856).$$

*Let $s = 2$. For $p_0 \in \{p_0^1, p_0^2, p_0^3\}$ consider the IVP-operator $f$ given by (9) with $c_k$ as in (27). For each $L$ in Table 1 or Table 2 corresponds a unique solution $\tilde{x} \in X^s$ of $f(x) = 0$ in a ball $B_{\bar{x}}(r_{p_0^{1,2,3}}) \subset X^s$ of radius $r_{p_0^{1,2,3}}$ centered at an approximate solution $\bar{x}$.*

| $L$ | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.54 |
|---|---|---|---|---|---|---|
| $m_{p_0^2}$ | 300 | 300 | 300 | 300 | 300 | 300 |
| $r_{p_0^2}$ | $2.01 \times 10^{-12}$ | $3.21 \times 10^{-12}$ | $5.80 \times 10^{-11}$ | $1.95 \times 10^{-10}$ | $5.12 \times 10^{-9}$ | $4.52 \times 10^{-8}$ |

Table 1: Given $p_0^2$ and for a fix $L$, these are corresponding values of the Galerkin projection dimension $m_{p_0^2}$ and the radius $r_{p_0^2}$ around the approximate solution $\bar{x}$ in $X^s$ for which the radii polynomials approach was successful.

| $L$ | 0.5 | 1 | 1.5 | 2 | 2.5 | 3 |
|---|---|---|---|---|---|---|
| $m_{p_0^1}$ | 50 | 100 | 200 | 250 | 300 | 500 |
| $m_{p_0^3}$ | 150 | 200 | 300 | 400 | 500 | 600 |
| $r_{p_0^1}$ | $2.61 \times 10^{-9}$ | $1.27 \times 10^{-8}$ | $2.85 \times 10^{-8}$ | $8.77 \times 10^{-8}$ | $4.53 \times 10^{-7}$ | $1.03 \times 10^{-6}$ |
| $r_{p_0^3}$ | $1.07 \times 10^{-7}$ | $1.31 \times 10^{-7}$ | $6.29 \times 10^{-7}$ | $1.09 \times 10^{-6}$ | $1.40 \times 10^{-6}$ | $5.17 \times 10^{-6}$ |

Table 2: Given $p_0^{1,3}$ and for a fix $L$, these are corresponding values of the Galerkin projection dimension $m_{p_0^{1,3}}$ and the radius $r_{p_0^{1,3}}$ around the approximate solution $\bar{x}$ in $X^s$ for which the radii polynomials approach was successful.

Before we discuss the proof via an application of Theorem 2.1 we comment on the choice of the initial conditions. $p_0^1$ is chosen to lie approximately on the unstable manifold of the *positive eye* equilibrium $(\sqrt{\beta(\rho-1)}, \sqrt{\beta(\rho-1)}, \rho-1)$, $p_0^2$ lies approximately on the unstable manifold of the origin whereas $p_0^3$ is taken randomly. As one can see in Tables 1 and 2, the data of the verification method depends strongly on the choice of the initial condition. We assume that this stems from the presence of poles of the complex extension of the solutions $u : [-1, 1] \to \mathbb{R}^3$ of (26) whose position in the complex plane changes depending on the initial condition and the scaling factor $L$. By Theorem 1.2 this influences the decay rate of the Chebychev coeffcients. This is illustrated in Figure 1. We refer to Figure 2 for a representation in phase space of two solutions of Theorem 3.1.

The proof of Theorem 3.1 can be found in the MATLAB programs *proofLorenz1.m*, *proofLorenz2.m* and *proofLorenz3.m* at [16]. It relies on Theorem 2.1 and uses the package Intlab [17] for the interval computations and the package Chebfun [18]. In order to apply Theorem 2.1 the construction of the radii polynomials as defined in (22) and (23) is crucial. After the following remark we aim to give some details about the derivation of the bounds defined in (19), (20) and (21) involved in the construction of the polynomials.

**Remark 3.1.** *Consider an approximate solution $\bar{x}$ and a corresponding unique genuine solution $\tilde{x} \in B_{\bar{x}}(r) \subset X^s$ of $f(x) = 0$ for a decay rate $s > 1$ and a radius $r > 0$. Via the expansion (2) the sequences of Chebyshev coefficients $\bar{x}$ and $\tilde{x}$ correspond to*

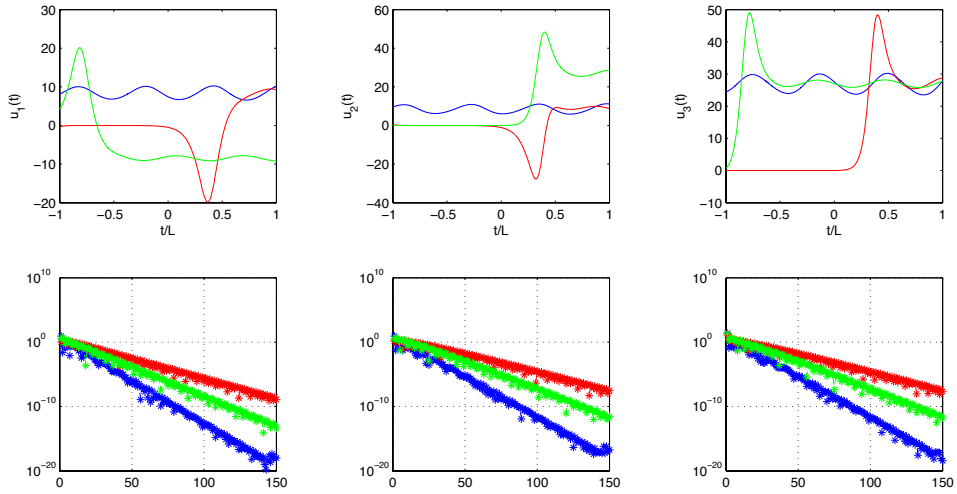
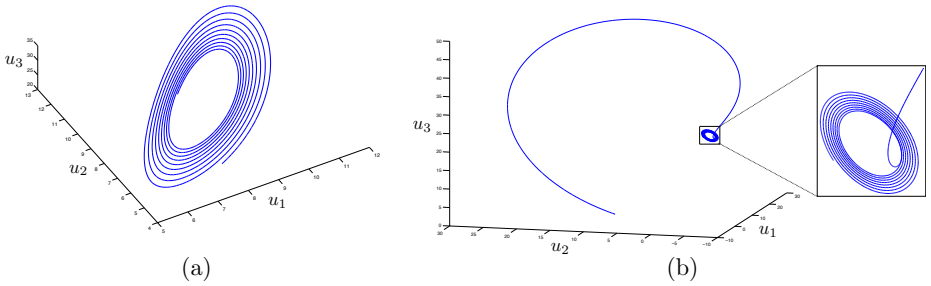



Figure 1: Comparison of the componentwise solution profiles of a solution $u : [-1, 1] \to \mathbb{R}^3$ of the Lorenz equations for the initial condition $p_0^1$ (blue), $p_0^2$ (red) and $p_0^3$ (green) for $L = 1$ and of the decay rates of their Chebyshev coefficient sequences.




(a) (b)

Figure 2: Profile in phase space of the solution $(u_1, u_2, u_3)$ of the Lorenz equations starting at (a) the initial condition $p_0^1$; (b) the initial condition $p_0^3$.

*functions* $\bar{u}$ *and* $\tilde{u}$ *respectively, where* $\tilde{u}$ *solves* (26) *with respective initial condition* $p_0$. *The following reasoning translates the inequality* $\|\bar{x} - \tilde{x}\|_s \leq r$ *into an upper bound for* $\|\bar{u} - \tilde{u}\|_{C^0} \stackrel{\text{def}}{=} \sup_{t\in[-1,1]} \|\bar{u}(t) - \tilde{u}(t)\|_\infty$. *For every* $t \in [-1, 1]$ *and every* $s > 1$ *we have*

$$\|\bar{u}(t) - \tilde{u}(t)\|_\infty \leq \|\bar{a}_0 - \tilde{a}_0\|_\infty + 2\sum_{k=1}^{\infty} \|\bar{a}_k - \tilde{a}_k\|_\infty \underbrace{|T_k(t)|}_{\leq 1} \leq \left(1 + 2\sum_{k=1}^{\infty} \frac{1}{\omega_k^s}\right) r$$

$$\leq \left(3 + \frac{2}{s-1}\right) r.$$

*Hence by taking the supremum over all* $t \in [-1, 1]$ *we obtain* $\|\bar{u} - \tilde{u}\|_{C^0} \leq \left(3 + \frac{2}{s-1}\right) r$.

We now turn to the computations of the bounds involved in the construction of the radii polynomials.

### 3.1.1 Derivation of the bounds required to construct the radii polynomials

Note here that $k_0 = 0$, $p = 0$ and $n = 3$. Choose a time scaling factor $L$. Consider $f$ the IVP-operator (9) with $c_k$ given in (27). Recalling (15), consider a Galerkin projection dimension $m$ and an approximate solution $\bar{x} = \bar{a} = (\bar{a}_F, 0_\infty)$, that is $f^{(m)}(\bar{a}_F) \approx 0$. Set the computational parameter $M$ arising in hypotheses **A1** and **A2** to $M = 2m - 1$. With this choice, **A1** is fulfilled and we can directly compute $Y_0, \dots, Y_{M-1}$ from (19) using interval arithmetic. Concerning the computation of $Z_1(r), \dots, Z_{M-1}(r)$ satisfying (20) and $\bar{Z}_M(r)$ satisfying (21), the first step is to use (25) and to compute polynomials $z_k(r) = z_1^k r + z_2^k r^2$ for $k \geq 0$ with $z_l^k \in \mathbb{R}^3$, such that $\left[Df(\bar{x} + rw)rv - A^\dagger rv\right]_k = z_k(r)$, where $w, v \in B(1)$. Note that $B(1)$ is given by (16) with $r = 1$. The derivation of an upper bound for $|z_k(r)|$ is a major step to obtain $Z_k(r)$ and is postponed to a separate consideration. We remark that we have to distinguish the cases $k = 0$, $1 \leq k \leq m-1$ and $m \leq k$. A straightforward calculation leads to the expressions summarized in Table 3. Note that $v_i^I$ is defined for $i = 1, 2, 3$ by

$$(v_i^I)_k = \begin{cases} 0, & k = 0, \dots, m-1 \\ (v_i)_k, & k \geq m. \end{cases}$$

| | |
|---|---|
| | $k = 0$ |
| $z_1^0$ | $L \left[ \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1^I)_0 - (\bar{a}_1 v_3^I)_0 \\ (\bar{a}_1 v_2^I)_0 + (\bar{a}_2 v_2^I)_0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1^I)_1 - (\bar{a}_1 v_3^I)_1 \\ (\bar{a}_1 v_2^I)_1 + (\bar{a}_2 v_2^I)_1 \end{pmatrix} - 2 \sum_{j=2}^{m-1} \frac{1}{j^2 - 1} \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1^I)_j - (\bar{a}_1 v_3^I)_j \\ (\bar{a}_1 v_2^I)_j + (\bar{a}_2 v_2^I)_j \end{pmatrix} - 2 \sum_{j=m}^{M-1} \frac{1}{j^2 - 1} \left[ \begin{pmatrix} \sigma((v_2)_j - (v_1)_j) \\ \rho(v_1)_j - (v_2)_j \\ -\beta(v_3)_j \end{pmatrix} + \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1)_j - (\bar{a}_1 v_3)_j \\ (\bar{a}_1 v_2)_j + (\bar{a}_2 v_2)_j \end{pmatrix} \right] - 2 \sum_{j=M}^{\infty} \frac{1}{j^2 - 1} \left[ \begin{pmatrix} \sigma((v_2)_j - (v_1)_j) \\ \rho(v_1)_j - (v_2)_j \\ -\beta(v_3)_j \end{pmatrix} + \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1)_j - (\bar{a}_1 v_3)_j \\ (\bar{a}_1 v_2)_j + (\bar{a}_2 v_2)_j \end{pmatrix} \right] \right]$ |
| $z_2^0$ | $L \left[ \begin{pmatrix} 0 \\ -(w_3 v_1)_0 - (w_1 v_3)_0 \\ (w_1 v_2)_0 + (w_2 v_1)_0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 \\ -(w_3 v_1)_0 - (w_1 v_3)_0 \\ (w_1 v_2)_0 + (w_2 v_1)_0 \end{pmatrix} - 2 \sum_{j=2}^{\infty} \frac{1}{j^2 - 1} \begin{pmatrix} 0 \\ -(w_3 v_1)_j - (w_1 v_3)_j \\ (w_1 v_2)_j + (w_2 v_1)_j \end{pmatrix} \right]$ |
| | $k = 1, \dots, m-1$ |
| $z_1^k$ | $L \left[ \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1^I)_{k+1} - (\bar{a}_1 v_3^I)_{k+1} \\ (\bar{a}_1 v_2^I)_{k+1} + (\bar{a}_2 v_2^I)_{k+1} \end{pmatrix} - \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1^I)_{k-1} - (\bar{a}_1 v_3^I)_{k-1} \\ (\bar{a}_1 v_2^I)_{k-1} + (\bar{a}_2 v_2^I)_{k-1} \end{pmatrix} \right]$ |
| $z_2^k$ | $L \left[ \begin{pmatrix} 0 \\ -(w_3 v_1)_{k+1} - (w_1 v_3)_{k+1} \\ (w_1 v_2)_{k+1} + (w_2 v_1)_{k+1} \end{pmatrix} - \begin{pmatrix} 0 \\ -(w_3 v_1)_{k-1} - (w_1 v_3)_{k-1} \\ (w_1 v_2)_{k-1} + (w_2 v_1)_{k-1} \end{pmatrix} \right]$ |
| | $k \geq m$ |
| $z_1^k$ | $L \left[ \left[ \begin{pmatrix} \sigma((v_2)_{k+1} - (v_1)_{k+1}) \\ \rho(v_1)_{k+1} - (v_2)_{k+1} \\ -\beta(v_3)_{k+1} \end{pmatrix} + \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1)_{k+1} - (\bar{a}_1 v_3)_{k+1} \\ (\bar{a}_1 v_2)_{k+1} + (\bar{a}_2 v_2)_{k+1} \end{pmatrix} \right] - \left[ \begin{pmatrix} \sigma((v_2)_{k-1} - (v_1)_{k-1}) \\ \rho(v_1)_{k-1} - (v_2)_{k-1} \\ -\beta(v_3)_{k-1} \end{pmatrix} + \begin{pmatrix} 0 \\ -(\bar{a}_3 v_1)_{k-1} - (\bar{a}_1 v_3)_{k-1} \\ (\bar{a}_1 v_2)_{k-1} + (\bar{a}_2 v_2)_{k-1} \end{pmatrix} \right] \right]$ |
| $z_2^k$ | $L \left[ \begin{pmatrix} 0 \\ -(w_3 v_1)_{k+1} - (w_1 v_3)_{k+1} \\ (w_1 v_2)_{k+1} + (w_2 v_1)_{k+1} \end{pmatrix} - \begin{pmatrix} 0 \\ -(w_3 v_1)_{k-1} - (w_1 v_3)_{k-1} \\ (w_1 v_2)_{k-1} + (w_2 v_1)_{k-1} \end{pmatrix} \right]$ |

Table 3: Formulas for $z_k^l$

Our next goal is to compute polynomials $\tilde{Z}_k(r) = \tilde{Z}_1^k r + \tilde{Z}_2^k r^2 \in \mathbb{R}^3$ such that

$$\left| z_l^k \right| \preceq \tilde{Z}_l^k, \quad \text{for } \; l = 1, 2 \; \text{ and } \; k = 0, \dots, M-1 \tag{28}$$

and $\tilde{Z}_M(r) = \tilde{Z}_1^M r + \tilde{Z}_2^M r^2 \in \mathbb{R}^3$ such that

$$|z_l^k| \preceq \frac{\tilde{Z}_l^M}{\omega_k^s}, \quad \text{for } \; l = 1, 2 \; \text{ and } \; k \geq M. \tag{29}$$

To obtain the bounds $\tilde{Z}_1^k$ for $k = 0, \dots, M-1$ define the finite sums

$$\Sigma_i^{k,I} \stackrel{\text{def}}{=} \sum_{k_1=-m+1}^{m-1} (|\bar{a}_i|)_{|k_1|} \frac{1}{\omega_{k-k_1}^{s,I}}, \quad \text{for} \quad k=0,\dots,M-1,$$
$$\Sigma_i^{k} \stackrel{\text{def}}{=} \sum_{k_1=-m+1}^{m-1} (|\bar{a}_i|)_{|k_1|} \frac{1}{\omega_{k-k_1}^{s}}, \quad \text{for} \quad k=0,\dots,M,$$

where

$$\omega_k^{s,I} \stackrel{\text{def}}{=} \begin{cases} 0, & 0 \le k \le m-1 \\ \omega_k^s, & k \ge m. \end{cases}$$

To define the uniform bound $\tilde{Z}_1^M$ for $k \ge M$ we set for $i=1,2,3$

$$\Sigma_i^{M-1} = (|\bar{a}_i|)_0 + \sum_{k_1=1}^{m-1} (|\bar{a}_i|)_{k_1} \left(1 + \frac{1}{(1-\frac{k_1}{M-1})^s}\right).$$

In order to compute $\tilde{Z}_2^k$ for $k=0,\dots,M$ and $\tilde{Z}_2^M$ we employ estimates whose detailed explanation can be found in [4]. For $M \ge 6$ and $s \ge 2$, define the constant

$$\gamma_M = 2\left(\frac{M}{M-1}\right)^s + \left(\frac{4\ln(M-2)}{M} + \frac{\pi^2-6}{3}\right)\left(\frac{1}{M}+\frac{1}{2}\right)^{s-2},$$

and in addition define

$$\alpha_k^{2,M} = \begin{cases} 1 + 2\sum_{k_1=1}^{M} \frac{1}{\omega_{k_1}^{2s}} + \frac{2}{M^{2s-1}(2s-1)}, & k=0 \\ \sum_{k_1=1}^{M} \frac{2k^s}{\omega_{k_1}^s \omega_{k+k_1}^s} + \frac{2k^s}{(k+M+1)^s(M-1)^s(s-1)} + 2 + \sum_{k_1=1}^{M} \frac{2k^s}{\omega_{k_1}^s \omega_{k-k_1}^s}, & 1 \le k \le M-1 \\ 2 + 2\sum_{k_1=1}^{M} \frac{1}{\omega_{k_1}^s} + \frac{2}{M^{s-1}(s-1)} + \gamma_M, & k \ge M. \end{cases}$$

This yields that

$$\left| \sum_{k_1+k_2=k} \frac{1}{\omega_{k_1}\omega_{k_2}} \right| \le \frac{\alpha_k^{2,M}}{\omega_k^s}, \quad \text{for} \quad k \ge 0.$$

Combining these definitions a direct reasoning leads to the bounds of Table 4.

We are now in position to take the last step in defining $Z_k(r) = Z_1^k r + Z_2^k r^2$ for $k=0,\dots,M-1$ specified in (20) and $\bar{Z}_M(r) = \bar{Z}_1^M r + \bar{Z}_2^M r^2$ given by (21). As previously mentioned, by definition of $A$ and $A^\dagger$, there is a small $\epsilon$ such that for all $k \ge 0$,

$$\left|\left[(I - AA^\dagger)rv\right]_k\right| \preceq r\epsilon \mathbf{1_3}.$$

In particular for $k \ge m$ we have $\epsilon = 0$ by definition of $A$ and $A^\dagger$ given respectively by (17) and (24). We let $V_l = (\tilde{Z}_l^0, \dots, \tilde{Z}_l^{m-1}) \in \mathbb{R}^{3m}$ for $l=1,2$ to obtain for $k=0,\dots,m-1$

$$\begin{aligned} Z_1^k &= [|A_m|V_1]_k + \epsilon \mathbf{1_3} \\ Z_2^k &= [|A_m|V_2]_k, \end{aligned} \tag{30}$$

| | |
|---|---|
| | $k=0$ |
| $\tilde{Z}_1^0$ | $L\left[\begin{pmatrix}\Sigma_3^{0,I}+\Sigma_1^{0,I}\\ \Sigma_1^{0,I}+\Sigma_2^{0,I}\end{pmatrix}+\frac{1}{2}\begin{pmatrix}\Sigma_3^{1,I}+\Sigma_1^{1,I}\\ \Sigma_1^{1,I}+\Sigma_2^{1,I}\end{pmatrix}+2\sum_{j=2}^{m-1}\frac{1}{j^2-1}\begin{pmatrix}\Sigma_3^{j,I}+\Sigma_1^{j,I}\\ \Sigma_3^{j,I}+\Sigma_1^{j,I}\end{pmatrix}\right.$ $\left.+2\sum_{j=m}^{M-2}\frac{1}{j^2-1}\left[\frac{1}{\omega_j^s}\begin{pmatrix}2\lvert\sigma\rvert\\ \lvert\rho\rvert+1\\ \lvert\beta\rvert\end{pmatrix}+\begin{pmatrix}\Sigma_3^{j}+\Sigma_1^{j}\\ \Sigma_2^{j}+\Sigma_2^{j}\end{pmatrix}\right]+\frac{2}{((M-1)^2-1)(s-1)(M-2)^{s-1}}\left[\begin{pmatrix}2\lvert\sigma\rvert\\ \lvert\rho\rvert+1\\ \lvert\beta\rvert\end{pmatrix}+\begin{pmatrix}\Sigma_3^{M-1}+\Sigma_1^{M-1}\\ \Sigma_1^{M-1}+\Sigma_2^{M-1}\end{pmatrix}\right]\right]$ |
| $\tilde{Z}_2^0$ | $L\left[\frac{2\alpha_0^{2,M}}{\omega_0^s}+\frac{\alpha_1^{2,M-1}}{\omega_1^s}+2\sum_{j=2}^{M-1}\frac{2\alpha_j^{2,M-1}}{(j^2-1)\omega_j^s}+\frac{4\alpha_{M-1}^{2,M-1}}{((M-1)^2-1)(s-1)(M-2)^{s-1}}\right]\begin{pmatrix}0\\1\\1\end{pmatrix}$ |
| | $k=1,\dots,m-1$ |
| $\tilde{Z}_1^k$ | $L\left[\begin{pmatrix}\Sigma_3^{k+1,I}+\Sigma_1^{k+1,I}\\ \Sigma_1^{k+1,I}+\Sigma_2^{k+1,I}\end{pmatrix}+\begin{pmatrix}\Sigma_3^{k-1,I}+\Sigma_1^{k-1,I}\\ \Sigma_1^{k-1,I}+\Sigma_2^{k-1,I}\end{pmatrix}\right]$ |
| $\tilde{Z}_2^k$ | $L\left[\frac{\alpha_{k+1}^{2,M-1}}{\omega_{k+1}^s}+\frac{\alpha_{k-1}^{2,M-1}}{\omega_{k-1}^s}\right]\begin{pmatrix}0\\2\\2\end{pmatrix}$ |
| | $k=m,\dots,M-1$ |
| $\tilde{Z}_1^k$ | $L\left[\frac{1}{\omega_{k+1}^s}\begin{pmatrix}2\lvert\sigma\rvert\\ \lvert\rho\rvert+1\\ \lvert\beta\rvert\end{pmatrix}+\begin{pmatrix}\Sigma_3^{k+1}+\Sigma_1^{k+1}\\ \Sigma_1^{k+1}+\Sigma_2^{k+1}\end{pmatrix}\right]+L\left[\frac{1}{\omega_{k-1}^s}\begin{pmatrix}2\lvert\sigma\rvert\\ \lvert\rho\rvert+1\\ \lvert\beta\rvert\end{pmatrix}+\begin{pmatrix}\Sigma_3^{k-1}+\Sigma_1^{k-1}\\ \Sigma_1^{k-1}+\Sigma_2^{k-1}\end{pmatrix}\right]$ |
| $\tilde{Z}_2^k$ | $L\left[\frac{\alpha_{k+1}^{2,M-1}}{\omega_{k+1}^s}+\frac{\alpha_{k-1}^{2,M-1}}{\omega_{k-1}^s}\right]\begin{pmatrix}0\\2\\2\end{pmatrix}$ |
| | $k\geq M$ |
| $\tilde{Z}_1^M$ | $L\left[(1+(\frac{M}{M-1})^s)\begin{pmatrix}2\lvert\sigma\rvert\\ \lvert\rho\rvert+1\\ \lvert\beta\rvert\end{pmatrix}+(1+(\frac{M}{M-1})^s)\begin{pmatrix}\Sigma_3^{M-1}+\Sigma_1^{M-1}\\ \Sigma_1^{M-1}+\Sigma_2^{M-1}\end{pmatrix}\right]$ |
| $\tilde{Z}_2^M$ | $L\left[(1+(\frac{M}{M-1})^s)\alpha_{M-1}^{2,M-1}\right]\begin{pmatrix}0\\2\\2\end{pmatrix}$ |

Table 4: Formulas for $\tilde{Z}_k^l$

where the absolute value is taken component-wise and for $k=m,\dots,M-1$

$$Z_l^k=\frac{1}{2k}\tilde{Z}_l^k,\quad \text{for } \ l=1,2. \tag{31}$$

Finally we set

$$\bar{Z}_l^M=\frac{1}{2M}\tilde{Z}_l^M,\quad \text{for } \ l=1,2. \tag{32}$$

Combining the bounds $Y_0,\dots Y_{M-1}$ and the bounds (30), (31) and (32) completes the construction of the radii polynomials defined in (22) and (23).

## 3.2 The Gray-Scott equation

Consider the Gray-Scott equation re-scaled by a time factor $L$ given by

$$\begin{cases} v_1''=L^2\left(v_1v_2^2-\lambda(1-v_1)\right)\\ v_2''=L^2\left(\frac{1}{\gamma}(v_2-v_1v_2^2)\right),\end{cases} \tag{33}$$

where $\gamma$ and $\lambda$ are real parameters. The Gray-Scott model serves as a model for a continuously fed unstirred autocatalytic reaction. The homoclinic solutions we seek represent non-trivial stationary spatial patterns in the form of pulses. See [19] and the references therein for more details on the significance of the equation. Letting $u_1=v_1$, $u_2=v_1'$, $u_3=v_2$, $u_4=v_2'$ and $u=(u_1,u_2,u_3,u_4)^T$, we re-write (33) as the vector field

$$\frac{du}{dt}=\Psi(u)=\begin{pmatrix}u_2\\ L^2\left(\lambda u_1+u_1u_3^2-\lambda\right)\\ u_4\\ L^2\left(\frac{1}{\gamma}u_3-\frac{1}{\gamma}u_1u_3^2\right)\end{pmatrix}. \tag{34}$$

Hence, the Chebyshev coefficients (8) of (34) are given explicitly by

$$c_k = \begin{pmatrix} (a_2)_k \\ L^2\left(\lambda(a_1)_k + (a_1 a_3^2)_k - \lambda\delta_{k,0}\right) \\ (a_4)_k \\ L^2\left(\frac{1}{\gamma}(a_3)_k - \frac{1}{\gamma}(a_1 a_3^2)_k\right) \end{pmatrix}, \tag{35}$$

where $\delta_{k,0}$ is the Kronecker delta function and where

$$(a_1 a_3^2)_k = \sum_{\substack{k_1+k_2+k_3=k \\ k_i\in\mathbb{Z}}} (a_1)_{|k_1|}(a_3)_{|k_2|}(a_3)_{|k_3|}.$$

We are interested in computing symmetric homoclinic orbits at $p = (1,0,0,0)^T$. Consider $P(\theta)$ to be a parameterization of the local stable manifold $W^s_{\text{loc}}(p)$ at the steady state $p$. In order to compute $P$ we employ the parametrization method developed in [20], [21] and [22]. The philosophy is to use a power series expansion to solve an invariance equation for $P$ and thereby compute a multivariate polynomial approximation $P_N$ to $P$. In addition the a-posteriori verification enables to find a domain $V$ and a bound $\delta$ such that $\|P(\theta) - P_N(\theta)\|_\infty < \delta$ for all $\theta \in V$. For details on the implementation and the a-posterori verification we refer the reader to [23].

We interpret symmetric homoclinic orbits as solutions of a BVP with the boundary value $u(1) = P(\theta)$, that is $u(1) \in W^s_{\text{loc}}(p)$. We impose the even symmetry condition of the orbit $(v_1, v_2)$ with $v_1'(-1) = u_2(-1) = 0$ and $v_2'(-1) = u_4(-1) = 0$. Hence, the boundary condition (10) reads as $\mathcal{G}(u(-1), u(1)) = (u_2(-1), u_4(-1))^T \in \mathbb{R}^2$, $p_1 = P(\theta)$ and then the operator (11) is given by

$$F(\theta, u)(t) = \begin{pmatrix} u_2(-1) \\ u_4(-1) \\ u(t) + \displaystyle\int_t^1 \Psi(u(s))ds - P(\theta) \end{pmatrix}. \tag{36}$$

To obtain the first component $\eta$ of (12), we use that $T_k(-1) = (-1)^k$ for all $k \geq 0$ to get

$$\eta(\theta, a) = \left((a_2)_0 + 2\sum_{k=1}^{\infty}(-1)^k(a_2)_k, (a_4)_0 + 2\sum_{k=1}^{\infty}(-1)^k(a_4)_k\right)^T. \tag{37}$$

Together with (35) we obtain an explicit expression $f(x) = f_{\gamma,\lambda}(x)$ for the BVP-operator (12) tailored to the problem of finding even homoclinics in the Gray-Scott system (34).

It is shown in [19] that for parameter values $\gamma\lambda = 1$ and $\lambda > 4$ there exists a family of even symmetric homoclinics. More precisely for all $(\lambda, \gamma)$ in the parameter set

$$\mathcal{C}_0 = \left\{(\gamma, \frac{1}{\gamma}) : \ 0 < \gamma < \frac{2}{9}\right\},$$

the functions given by

$$v_1(t) = 1 - \frac{3\gamma}{1 + Q\cosh(\frac{t}{\sqrt{\gamma}})} \quad \text{and} \quad v_2(t) = \frac{3}{1 + Q\cosh(\frac{t}{\sqrt{\gamma}})}, \tag{38}$$

with $Q(\gamma) = \sqrt{1 - \frac{9\gamma}{2}}$, are even symmetric homoclinic orbits of (34). Furthermore in Theorem C of [19] it is ensured that the homoclinics persist if $\lambda\gamma = 1 + \epsilon$ for some

small $\epsilon$ and in [23] to a certain extent the magnitude of $\epsilon$ for $\gamma = 0.15$ is investigated. More concretely the authors of [23] show in Theorem 1.1 the existence of 30 homoclinic orbits on the line $\gamma = 0.15$ in parameter space. We take a similar approach but extend the considered region in parameter space. Before presenting the result, note that there is a theoretical constraint in using the parameterization method to compute $W^s_{\text{loc}}(p)$ in parameter space. This constraint comes from the presence of resonances between the eigenvalues $\pm\frac{L}{\sqrt{\gamma}}$ and $\pm\sqrt{\lambda}L$ of $D\Psi(p)$. A resonance occurs when $\lambda\gamma = n^2$ or $\lambda\gamma = (1/n)^2$ for some $n \in \mathbb{N}$. Denote $\mathcal{C}_n \stackrel{\text{def}}{=} \{(\lambda,\gamma) : \lambda\gamma = (n+1)^2\}$ for $n \geq 0$ and $\mathcal{C}_{1/n} \stackrel{\text{def}}{=} \{(\lambda,\gamma) : \lambda\gamma = (1/n)^2\}$ for $n \geq 2$. The parameterization method uses a power series representation of $W^s_{\text{loc}}(p)$ and will fail to converge at resonances. As a matter of fact our rigorous numerical method combining Chebyshev series and the parameterization method will necessarily fail at those parameter values located on $\mathcal{C}_n$ $(n \geq 1)$ and $\mathcal{C}_{1/n}$ $(n \geq 2)$.

Let us now formulate a result guaranteeing the existence of 297 homoclinics at the parameter values $\gamma = 0.14$, $\gamma = 0.15$ and $\gamma = 0.16$, and for several different values of $\lambda$.

**Theorem 3.2.** *Define*

$$\Lambda^{\pm}_{\mathcal{I},\Delta_\lambda}(\gamma) = \left\{(\gamma,\lambda) : \lambda = \frac{1 \pm k\Delta_\lambda}{\gamma},\ \ k \in \mathcal{I}\right\},$$

*over an index set $\mathcal{I}$. Let $\Delta_\lambda = 0.03$ and $\gamma_i = 0.14 + (i-1)0.01$ for $i = 1,2,3$. Set $\mathcal{I}^+(\gamma_i) = \{1,\dots,90\}$ for $i = 1,2,3$ and $\mathcal{I}^-(\gamma_i) = \{1,\dots,K^-(\gamma_i)\}$ where $K^-(\gamma_i)$ is specified in Table 5 for $i = 1,2,3$. If*

$$(\lambda,\gamma) \in \bigcup_{i=1}^{3} \Lambda^{+}_{\mathcal{I}^+(\gamma_i),\Delta_\lambda}(\gamma_i) \cup \Lambda^{-}_{\mathcal{I}^-(\gamma_i),\Delta_\lambda}(\gamma_i),$$

*there exists a ball $B_{\bar{x}}(r_{\gamma,\lambda}) \subset X^s$ (with $f_{\gamma,\lambda}(\bar{x}) \approx 0$) containing a unique solution $\tilde{x} = (\tilde{\theta},\tilde{a})$ of $f_{\gamma,\lambda}(x) = 0$ corresponding to an even homoclinic solution of (33).*

For a geometric representation of the result of Theorem 3.2, we refer to Figure 3 and Figure 4.

Beside these rigorously verified homoclinic solutions we investigated a bigger region in parameter space by constructing the radii polynomials $p_1(r),\dots,p_M(r)$ without interval arithmetic and finding an $r > 0$ such that $p_i(r) \prec 0$ for all $i = 1,\dots M$. The results are marked in black in Figure 5. More precisely set $\Delta_\lambda = 0.03$ and $\gamma_i = 0.10 + (i-1)0.1$ for $i = 1,\dots,11$ and let $K^{\pm}(\gamma_i)$ be specified by Table 5. Define $\mathcal{I}^+_{\text{nr}}(\gamma_i) = \{1,\dots,90\} \cup \{110,\dots,K^+(\gamma_i)\}$ for $i \in \{1,2,3,4,5,8,9,10,11\}$, $\mathcal{I}^+_{\text{nr}}(\gamma_i) = \{110,\dots,K^+(\gamma_i)\}$ for $i = 6,7,8$ and $\mathcal{I}^-_{\text{nr}}(\gamma_i) = \{1,\dots,K^-(\gamma_i)\}$. Note that "nr" stands for non rigorous. We found symmetric homoclinic solutions for

$$(\gamma,\lambda) \in \bigcup_{i=1}^{11} \left(\Lambda^{+}_{\mathcal{I}^+_{\text{nr}}(\gamma_i),\Delta_\lambda}(\gamma_i) \cup \Lambda^{-}_{\mathcal{I}^-_{\text{nr}}(\gamma_i),\Delta_\lambda}(\gamma_i)\right).$$

These computations are carried out by the MATLAB program *nonrigoroushomoclinics.m*. The rigorous verification of Theorem 3.2 can be found in the MATLAB programs *proofLambdaplus$\gamma$.m* and *proofLambdaminus$\gamma$.m* with $\gamma = 014, 015, 016$, and relies on Theorem 2.1. All codes can be downloaded from [16]. The programs make use of the package Intlab [17] for the interval computations and of the package Chebfun [18]. Chebfun is used to compute the Chebyshev coefficients of the exact solutions (38) from which a continuation is performed. The main prerequisite for applying Theorem 2.1 is the construction of the radii polynomials (22) and (23). We now give some details on their derivation.

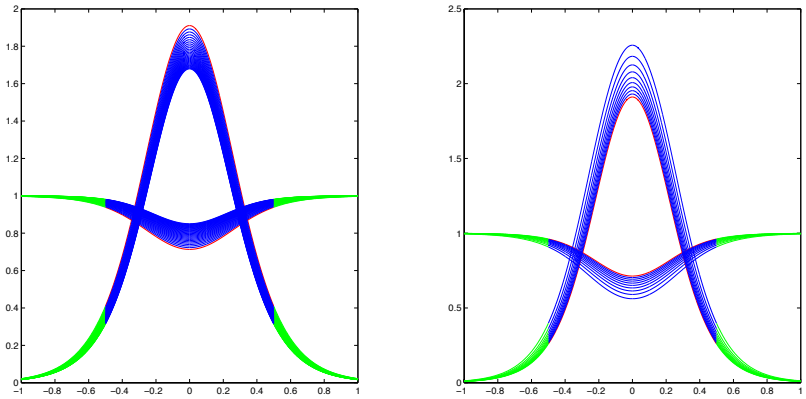


Figure 3: Thirty-nine homoclinics from Theorem 3.2, where $(\lambda,\gamma) \in \Lambda^{+}_{\{1,\dots,30\},0.03}(0.15)$ on the left and $(\lambda,\gamma) \in \Lambda^{-}_{\{1,\dots,9\},0.03}(0.15)$ on the right. The red solution corresponds to the exact homoclinic given by (38). Each couple $(v_1, v_2)$ is the center of a ball in function space in which an exact solution is guaranteed to exist. The blue part over $[0, \frac{1}{2}]$ corresponds to the interval $[-1, 1]$ for the operator (36), which in turn corresponds to the rescaling of $[0, L^{\pm}(0.15)]$. The green part is added by using the conjugacy relation (see equation (57) in [23]) fulfilled by the parametrization $P$ of $W^s_{\mathrm{loc}}(p)$, where we integrate for 2 time units on the time scale of (36) and then rescale $[-1, 3]$ to the interval [0,1]. The part over $[-1, 0]$ is obtained using the symmetry.

| $\gamma$ | 0.10 | 0.11 | 0.12 | 0.13 | 0.14 | 0.15 | 0.16 | 0.17 | 0.18 | 0.19 | 0.20 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $L^+(\gamma)$ | 0.45 | 0.50 | 0.55 | 0.60 | 0.60 | 0.60 | 0.65 | 0.70 | 0.75 | 0.75 | 0.75 |
| $L^-(\gamma)$ | 0.50 | 0.55 | 0.55 | 0.55 | 0.60 | 0.70 | 0.65 | 0.65 | 0.70 | 0.70 | 0.7 |
| $K^+(\gamma)$ | 114 | 128 | 143 | 158 | 172 | 187 | 202 | 217 | 231 | 246 | 261 |
| $K^-(\gamma)$ | 18 | 16 | 15 | 12 | 11 | 9 | 7 | 6 | 3 | 2 | 1 |

Table 5: Values of the rescaling factor $L$ and the number of steps $K^{\pm}$ we take in the $\lambda$ direction in dependence of the different values of $\gamma$.

### 3.2.1 Derivation of the bounds required to construct the radii polynomials

We are in the case $k_0 = -1$, $p = 2$ and $n = 4$. Consider a dimension $m$ for the Galerkin projection (15) and an approximation $\bar{x} = (\bar{\theta}, \bar{a}) = (\bar{\theta}, \bar{a}_F, 0_\infty)$ such that $f^{(m)}(\bar{\theta}, \bar{a}_F) \approx 0$, where $f$ is the BVP-operator (12), $c_k$ is given in (35) and the boundary conditions $\eta : X^s \to \mathbb{R}^p$ is given by (37). For instance if $(\gamma,\lambda) \in \Lambda^{+}_{\mathcal{I}^+(0.15),\Delta_\lambda}$ we choose $m = 37$ and set $L = 0.6$. For $(\gamma,\lambda) \in \Lambda^{-}_{\mathcal{I}^-(0.15),\Delta_\lambda}$ we choose $m = 47$ and let $L = 0.7$. Note that if we set $M = 3m - 2$ assumption **A1** is satisfied and $Y_1, \dots, Y_M$ can be computed by (19). The strategy to construct the bounds $Z_1(r), \dots, Z_{M-1}(r)$ and $\bar{Z}_M(r)$ defined in (20) and (21) is analogue to the Lorenz example. Note that $\xi_1, \xi_2$ in (25) are now given by $\xi_1 = r(\theta, w)$ and $\xi_2 = r(\phi, v)$ with $(\theta, w), (\phi, v) \in B(1) \subset X^s$. In addition we assume that we have a bound $\Lambda \in \mathbb{R}^4_+$ such that for every $\theta, \phi$ corresponding to $\xi_{1,2}$

$$|DP(\bar{\theta} + r\theta)\phi| \preceq \Lambda$$

for all $r$ with $0 < r < r_*$, where $r_*$ is an apriori bound on $r$ that we set to $r_* = 0.004$. The explicit construction of $\Lambda$ in the context of the Gray-Scott equations is presented in Section 5 in [23]. In particular, at $(\gamma,\lambda) \in \Lambda^{+}_{\mathcal{I}^+(0.15),\Delta_\lambda}$ we choose $N = 13$ as the order of the polynomial approximation $P_N$ and at $(\gamma,\lambda) \in \Lambda^{-}_{\mathcal{I}^-(0.15),\Delta_\lambda}$, we choose $N = 15$.

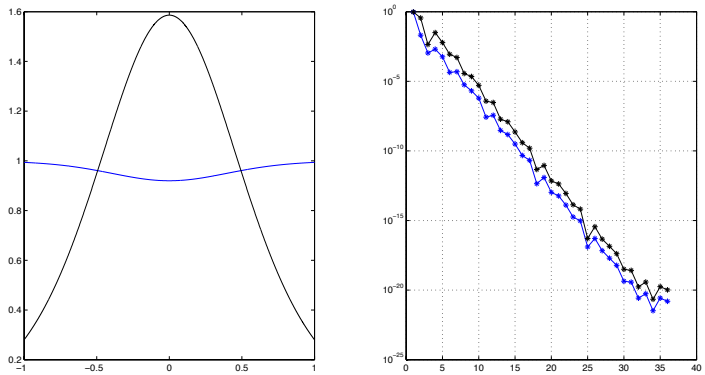


Figure 4: **(Left)** Components $v_1$ (black) and $v_2$ (blue) of the homoclinic solution of Theorem 3.2 corresponding to the parameter value $(\gamma, \lambda) = (0.15, \frac{1+89(0.03)}{0.15}) \in \Lambda^+_{\mathcal{I}^+(0.15),0.03}(0.15)$. The interval $[0,1]$ corresponds to the rescaled interval $[-1,1]$ of (36), corresponding itself in turn to a rescaling of $[0, 0.6]$. The interval $[-1,0]$ is added by symmetry. **(Right)** The Chebyshev coefficients of $v_1$ (black) and $v_2$ (blue). Notice the fast decay of the coefficients to zero.

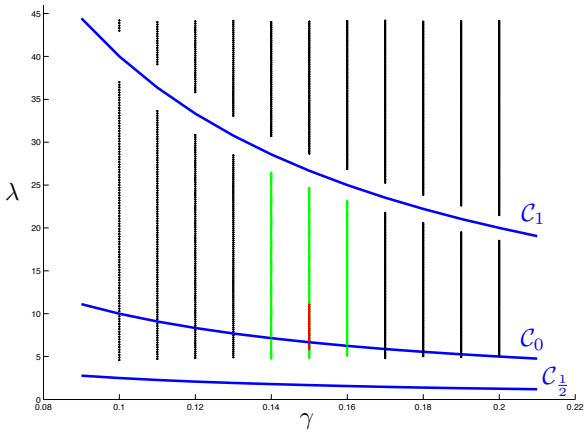



Figure 5: The green points indicate the region in parameter space at which the rigorous proof of existence of symmetric homoclinics was obtained by computing the radii polynomials with interval arithmetic. The red points indicate the region investigated in [23]. The black points are investigated using the radii polynomials computed without the use of interval arithmetic. Based on the discussion about resonances, we portrait the curve $\mathcal{C}_1$ and $C_{\frac{1}{2}}$ at which our rigorous method will necessarily fail. Note that $\mathcal{C}_0$ is the curve on which the exact homoclinics (38) exist.

For more details on the choice of $m$ and $N$ at $\gamma = 0.14, 0.16$ we refer to the code at [16]. A central step is to compute the polynomials $\tilde{Z}_k(r) = \sum_{l=1}^3 \tilde{Z}_l^k r^l \in \mathbb{R}^4$ and $\tilde{Z}_M(r) = \sum_{l=1}^3 \tilde{Z}_l^M r^l \in \mathbb{R}^4$ fulfilling the analogue of (28) and (29). We only present $\tilde{Z}_l^k$ and $\tilde{Z}_l^M$ for $k = 0, \ldots, M-1$ and $l = 1, 2, 3$ in Tables 6 and 7 in the Appendix.

Our main technical tool to compute these bounds is given by the following Lemma which is a simplified combination of Lemmas A.3 and A.4 in [4]. In order to explain its usefulness in our context, we recall that given three sequences $a, b, c \in \Omega^s$, the cubic

convolution sums $(abc)_k$ can be split as

$$(abc)_k = (abc)_k^M + \sum_{\substack{k_1+k_2+k_3=k \\ \max\{|k_1|,|k_2|,|k_3|\}\geq M \\ k_i\in\mathbb{Z}}} a_{|k_1|}b_{|k_2|}c_{|k_3|},$$

where

$$(abc)_k^M \stackrel{\text{def}}{=} \sum_{\substack{k_1+k_2+k_3=k \\ |k_i|\leq M, i=1,2,3 \\ k_i\in\mathbb{Z}}} a_{|k_1|}b_{|k_2|}c_{|k_3|}.$$

One of the aims of the following result is to bound the infinite tail sum.

**Lemma 3.1.** *Let $a, b, c \in \Omega^s$ and $M \geq 6$. Set $A = \|a\|_s$, $B = \|b\|_s$ and $C = \|c\|_s$. Then there exist computable numbers $\varepsilon_k^{(3)} = \varepsilon_k^{(3)}(M)$ for $k = 0, \ldots, M$ such that*

$$\sum_{\substack{k_1+k_2+k_3=k \\ \max\{|k_1|,|k_2|,|k_3|\}|\geq M+1 \\ k_i\in\mathbb{Z}}} |a|_{|k_1|}|b|_{|k_2|}|c|_{|k_3|} \leq 3(ABC)\varepsilon_k^{(3)}.$$

*In addition there is a computable number $\alpha_{M-1}^{(3)}$ such that for $k \geq M-1$*

$$\sum_{\substack{k_1+k_2+k_3=k \\ k_i\in\mathbb{Z}}} |a|_{|k_1|}|b|_{|k_2|}|c|_{|k_3|} \leq (ABC)\frac{\alpha_{M-1}^{(3)}}{\omega_k^s}.$$

For a proof and for details on the computation see [4] as well as the code at [16]. Defining $A_{1,3} = \|\bar{a}_{1,3}\|_s$ and for $i = 1, 3$ and $j = 3$

$$\Sigma_{ij}^{M-1} = \sum_{k_1=-m+1}^{m-1}\sum_{k_2=-m+1}^{m-1} (|\bar{a}_i|)_{|k_1|}(|\bar{a}_j|)_{|k_2|} \max\left\{\frac{M^s}{(M-1-k_1-k_2)^s}, 1\right\}$$

completes the ingredients for Tables 6 and 7.

# 4 Conclusion

Let us conclude this paper by presenting some potential extensions and improvements of our proposed rigorous computational method to solve IVPs and BVPs of ODEs.

First, our method could probably be generalized to compute rigorously solutions of higher-order differential equations without re-writing them as first order vector fields. For example, we believe that computing solutions of BVPs associated to the Gray-Scott equations (33) could be obtained by integrating twice each equation which could then be solved rigorously by moving to the space of Chebyshev coefficients. The improvement would be twofold. First, the linear part of the equations would grow as $O(k^2)$ (as opposed to $O(k)$ in the BVP-operator (12)), hence facilitating the use of a contraction mapping argument based on a Newton-like operator. Second, the size of the finite dimensional projection would be twice smaller. A downside is that we would obtain more complicated formulas of the Chebyshev expansions of the equations resulting from the double integration.

A second extension of the method would be to use a multiple shooting approach to solve the integral operators over long periods of time. Indeed, the theory of the Chebyshev series presented in Section 1 suggests that integrating over long periods of time (e.g. compute solutions with large scaling factor $L$) has the disadvantage of bringing the (potentially existing) poles closer to the $\rho$-ellipse mentioned in Theorem 1.2. This implies that the Chebyshev coefficients of the solutions decay to zero at a slow rate. Therefore, an advantage of a multiple shooting approach based on integrating over many short intervals (with corresponding short scaling factor $L$) would push away the poles, hence bringing a faster decay rate to the Chebyshev coefficients of the solutions. We could then potentially take smaller Galerkin projection dimensions to perform our rigorous computations, thanks to the fast decay rates of the solutions on each sub-intervals. The downside would again be a more complicated formulation of the operators which would need to take care of solving simultaneously many parallel problems.

A third extension of the method would be to combine the rigorous pseudo arc length continuation method of [15, 24] to compute global smooth branches of solutions of BVPs.

A fourth and slightly more challenging improvement consists of modifying the proposed approach to vector fields with nonlinearities that are non polynomial. That would require extending the already existing convolution estimates to the non polynomial case.

A final and most ambitious extension would be to attempt to rigorously compute solutions of spatially periodic PDEs combining a Chebyshev series expansion in time and a Fourier series expansion in space.

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# A Formulas for $\tilde{Z}_k$ for $k = -1, \ldots, M$ in the Gray-Scott equations

We give an overview of the bounds $\tilde{Z}_k$ for $k = -1, \ldots, M$ involved in the construction of the radii polynomials for the proof of Theorem 3.2.

| | $k = -1$ |
|---|---|
| $\tilde{Z}_1^{-1}$ | $(s-1)\begin{pmatrix} \frac{1}{(m-1)^{s-1}} \\ \frac{1}{(m-1)^{s-1}} \end{pmatrix}$ |
| | $k = 0$ |
| $\tilde{Z}_1^0$ | $\left[\begin{pmatrix} L^2((\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_0^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_0^M) \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_0^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_0^M\right] \end{pmatrix} + \varepsilon_0^{(3)}\begin{pmatrix} L^2(A_3 + 2A_1A_3) \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix} + \frac{1}{2}\begin{pmatrix} L^2((\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_1^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_1^M) \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_1^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_1^M\right] \end{pmatrix} + \frac{\varepsilon_1^{(3)}}{2}\begin{pmatrix} L^2(A_3 + 2A_1A_3) \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix} + 2\sum_{j=2}^{m-1}\frac{1}{j^2-1}\left(\begin{pmatrix} L^2(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_j^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_j^M \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_j^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_j^M\right] \end{pmatrix} + \varepsilon_j^{(3)}\begin{pmatrix} L^2(A_3 + 2A_1A_3) \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix}\right) + \sum_{j=m}^{M-2}\frac{1}{j^2-1}\left(\begin{pmatrix} \frac{1}{\omega_j^s}\begin{pmatrix} L^2\lambda \\ 1 \\ \frac{L^2}{\gamma} \end{pmatrix} \end{pmatrix} + \begin{pmatrix} L^2((\lvert\bar{a}_3\rvert^2\lvert v_1\rvert)_j^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3\rvert)_j^M) \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert)_j^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3\rvert)_j^M\right] \end{pmatrix} + \varepsilon_j^{(3)}\begin{pmatrix} L^2(A_3 + 2A_1A_3) \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix}\right) + \frac{2}{((M-1)^2-1)(s-1)(M-2)^{s-1}}\left(\begin{pmatrix} L^2\lambda \\ 1 \\ \frac{L^2}{\gamma} \end{pmatrix} + \begin{pmatrix} L^2(\Sigma_{33}^{M-1} + 2\Sigma_{13}^{M-1}) \\ \frac{L^2}{\gamma}(\Sigma_{33}^{M-1} + 2\Sigma_{13}^{M-1}) \end{pmatrix}\right)\right] + \Lambda$ |
| $\tilde{Z}_2^0$ | $\left[\begin{pmatrix} L^2(2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_0^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_0^{M-1} + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_0^M) \\ \frac{L^2}{\gamma}\left[2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_0^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_0^{M-1} + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_0^M\right] \end{pmatrix} + 2\varepsilon_0^{(3)}\begin{pmatrix} L^2(4A_3 + 2A_1) \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix} + \frac{1}{2}\begin{pmatrix} L^2(2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_1^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_1^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_1^M) \\ \frac{L^2}{\gamma}\left[2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_1^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_1^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_1^M\right] \end{pmatrix} + \varepsilon_1^{(3)}\begin{pmatrix} L^2(4A_3 + 2A_1) \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix} + 2\sum_{j=2}^{M-2}\frac{1}{j^2-1}\left(\begin{pmatrix} L^2(2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_j^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_j^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_j^M) \\ \frac{L^2}{\gamma}\left[2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_j^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_j^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_j^M\right] \end{pmatrix} + 2\varepsilon_j^{(3)}\begin{pmatrix} L^2(4A_3 + 2A_1) \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix}\right) + \frac{2\alpha_{M-1}^{(3)}}{((M-1)^2-1)(s-1)(M-2)^{s-1}}\begin{pmatrix} L^2(4A_3 + 2A_1) \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix}\right]$ |
| $\tilde{Z}_3^0$ | $\left[\begin{pmatrix} L^2((\lvert w_3\rvert^2\lvert v_3\rvert)_0^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_0^M) \\ \frac{L^2}{\gamma}\left[(\lvert w_3\rvert^2\lvert v_3\rvert)_0^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_0^M\right] \end{pmatrix} + 9\varepsilon_0^{(3)}\begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{1}{\gamma} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} L^2((\lvert w_3\rvert^2\lvert v_3\rvert)_1^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_1^M) \\ \frac{L^2}{\gamma}\left[(\lvert w_3\rvert^2\lvert v_3\rvert)_1^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_1^M\right] \end{pmatrix} + \frac{9}{2}\varepsilon_1^{(3)}\begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix} + 2\sum_{j=2}^{M-2}\frac{1}{j^2-1}\left(\begin{pmatrix} L^2((\lvert w_3\rvert^2\lvert v_3\rvert)_j^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_j^M) \\ \frac{L^2}{\gamma}\left[(\lvert w_3\rvert^2\lvert v_3\rvert)_j^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_j^M\right] \end{pmatrix} + 9\varepsilon_j^{(3)}\begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix}\right) + \frac{6\alpha_{M-1}^{(3)}}{((M-1)^2-1)(s-1)(M-2)^{s-1}}\begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix}\right]$ |

Table 6: Formulas for $\tilde{Z}_l^k$, $k = -1, 0$

| | |
|---|---|
| | $k = 1, \dots, m-1$ |
| $\tilde{Z}_1^k$ | $\left[\begin{pmatrix} 0 \\ L^2((\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_{k+1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_{k+1}^M\right] \end{pmatrix} + \varepsilon_{k+1}^{(3)} \begin{pmatrix} 0 \\ L^2(A_3 + 2A_1A_3) \\ 0 \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix} + \begin{pmatrix} 0 \\ L^2((\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_{k-1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert^I)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3^I\rvert)_{k-1}^M\right] \end{pmatrix} + \varepsilon_{k-1}^{(3)} \begin{pmatrix} 0 \\ L^2(A_3 + 2A_1A_3) \\ 0 \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix}\right]$ |
| $\tilde{Z}_2^k$ | $\left[\begin{pmatrix} 0 \\ L^2(2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M + 2(\lvert\bar{a}_3\rvert w_1\rvert\lvert v_3\rvert)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M\right] \end{pmatrix} + 2\varepsilon_{k+1}^{(3)} \begin{pmatrix} 0 \\ L^2(4A_3 + 2A_1) \\ 0 \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix} + \begin{pmatrix} 0 \\ L^2(2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M + 2(\lvert\bar{a}_3\rvert w_1\rvert\lvert v_3\rvert)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M + 2(\lvert\bar{a}_3\rvert w_1\rvert\lvert v_3\rvert)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M\right] \end{pmatrix} + 2\varepsilon_{k-1}^{(3)} \begin{pmatrix} 0 \\ L^2(4A_3 + 2A_1) \\ 0 \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix}\right]$ |
| $\tilde{Z}_3^k$ | $\left[\begin{pmatrix} 0 \\ L^2((\lvert w_3\rvert^2\lvert v_3\rvert)_{k+1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_{k+1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert w_3\rvert^2\lvert v_3\rvert)_{k+1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_{k+1}^M\right] \end{pmatrix} + 9\varepsilon_{k+1}^{(3)} \begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix} + \begin{pmatrix} 0 \\ L^2((\lvert w_3\rvert^2\lvert v_3\rvert)_{k-1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_{k-1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert w_3\rvert^2\lvert v_3\rvert)_{k-1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_{k-1}^M\right] \end{pmatrix} + 9\varepsilon_{k-1}^{(3)} \begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix}\right]$ |
| | $m \le k \le M-1$ |
| $\tilde{Z}_1^k$ | $\left[\frac{1}{\omega_{k+1}^s} \begin{pmatrix} 1 \\ L^2\lambda \\ 1 \\ \frac{L^2}{\gamma} \end{pmatrix} + \begin{pmatrix} 0 \\ L^2((\lvert\bar{a}_3\rvert^2\lvert v_1\rvert)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3\rvert)_{k+1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3\rvert)_{k+1}^M\right] \end{pmatrix} + \varepsilon_{k+1}^{(3)} \begin{pmatrix} 0 \\ L^2(A_3 + 2A_1A_3) \\ 0 \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix} + \frac{1}{\omega_{k-1}^s} \begin{pmatrix} 1 \\ L^2\lambda \\ 1 \\ \frac{L^2}{\gamma} \end{pmatrix} + \begin{pmatrix} 0 \\ L^2((\lvert\bar{a}_3\rvert^2\lvert v_1\rvert)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3\rvert)_{k-1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert\bar{a}_3\rvert^2\lvert v_1\rvert)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert\bar{a}_3\rvert\lvert v_3\rvert)_{k-1}^M\right] \end{pmatrix} + \varepsilon_{k-1}^{(3)} \begin{pmatrix} 0 \\ L^2(A_3 + 2A_1A_3) \\ 0 \\ \frac{L^2}{\gamma}(A_3 + 2A_1A_3) \end{pmatrix}\right]$ |
| $\tilde{Z}_2^k$ | $\left[\begin{pmatrix} 0 \\ L^2(2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M + 2(\lvert\bar{a}_3\rvert w_1\rvert\lvert v_3\rvert)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_{k+1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k+1}^M\right] \end{pmatrix} + 2\varepsilon_{k+1}^{(3)} \begin{pmatrix} 0 \\ L^2(4A_3 + 2A_1) \\ 0 \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix} + \begin{pmatrix} 0 \\ L^2(2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M + 2(\lvert\bar{a}_3\rvert w_1\rvert\lvert v_3\rvert)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[2(\lvert\bar{a}_3\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M + 2(\lvert\bar{a}_3\rvert\lvert w_1\rvert\lvert v_3\rvert)_{k-1}^M + 2(\lvert\bar{a}_1\rvert\lvert w_3\rvert\lvert v_1\rvert)_{k-1}^M\right] \end{pmatrix} + 2\varepsilon_{k-1}^{(3)} \begin{pmatrix} 0 \\ L^2(4A_3 + 2A_1) \\ 0 \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix}\right]$ |
| $\tilde{Z}_3^k$ | $\left[\begin{pmatrix} 0 \\ L^2((\lvert w_3\rvert^2\lvert v_3\rvert)_{k+1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_{k+1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert w_3\rvert^2\lvert v_3\rvert)_{k+1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_{k+1}^M\right] \end{pmatrix} + 9\varepsilon_{k+1}^{(3)} \begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix} + \begin{pmatrix} 0 \\ L^2((\lvert w_3\rvert^2\lvert v_3\rvert)_{k-1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_{k-1}^M) \\ 0 \\ \frac{L^2}{\gamma}\left[(\lvert w_3\rvert^2\lvert v_3\rvert)_{k-1}^M + 2(\lvert w_1\rvert\lvert w_3\rvert\lvert v_3\rvert)_k^M\right] \end{pmatrix} + 9\varepsilon_{k-1}^{(3)} \begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix}\right]$ |
| | $k = M$ |
| $\tilde{Z}_1^M$ | $(1 + (\frac{M}{M-1})^s) \left[\begin{pmatrix} 1 \\ L^2\lambda \\ 1 \\ \frac{L^2}{\gamma} \end{pmatrix} + \begin{pmatrix} 0 \\ L^2(\Sigma_{33}^{M-1} + 2\Sigma_{13}^{M-1}) \\ 0 \\ \frac{L^2}{\gamma}(\Sigma_{33}^{M-1} + 2\Sigma_{13}^{M-1}) \end{pmatrix}\right]$ |
| $\tilde{Z}_2^M$ | $(1 + (\frac{M}{M-1})^s)\alpha_{M-1}^{(3)} \begin{pmatrix} 0 \\ L^2(4A_3 + 2A_1) \\ 0 \\ \frac{L^2}{\gamma}(4A_3 + 2A_1) \end{pmatrix}$ |
| $\tilde{Z}_3^M$ | $(1 + (\frac{M}{M-1})^s)3\alpha_{M-1}^{(3)} \begin{pmatrix} 0 \\ L^2 \\ 0 \\ \frac{L^2}{\gamma} \end{pmatrix}$ |

Table 7: Formulas for $\tilde{Z}_l^k$, $k = 1, \dots, M$