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Finite element approximation of invariant manifolds by the parameterization method

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Abstract A new method for approximating unstable manifolds for parabolic PDEs is introduced, which combines the parameterization method for invariant manifolds with finite element analysis and formal Taylor series expansions, and is applicable to problems posed on irregular spatial domains. The parameterization method centers on an infinitesimal invariance equation for the unstable manifold, which we solve via a power series anzats. A power matching argument leads to linear elliptic PDEs – the so called homological equations – describing the jets of the manifold. These homological equations are solved recursively to any desired order using finite element approximation. The end result is a polynomial expansion of the manifold whose coefficients lie in an appropriate finite element space. We implement the method for a variety of example problems having both polynomial and non-polynomial nonlinearities posed on non-convex two dimensional polygonal domains. The parameterization method admits a natural notion of a-posteriori error and we provide numerical evidence in support of the claim that the manifolds are computed accurately.

1 Introduction

For a parabolic partial differential equation (PDE) generating a compact semi-flow on a function space an important problem is to understand any compact flow invariant sets. This problem is especially challenging in the presence of strong nonlinearities. One good computational strategy is to numerically integrate a sufficiently large ensemble of initial conditions for sufficiently long that the structure of the global attractor is illuminated. Yet, as is well known, numerical simulation is not effective at locating invariant objects

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with saddle type stability. Moreover simulations provide only limited information about the connections between invariant objects.

Another technique for studying parabolic PDEs is to project onto a countable basis of eigenfunctions. This has the effect of reducing the problem to a countable system of coupled ordinary differential equations (ODEs) and makes available entire cannon of computational methods for ODEs. The difficulty with this approach is that it works best when the eigenvalues and eigenfunctions are explicitly known, and this usually happens only for particularly simple spatial domains. For example problems posed on one dimensional/cubical/toroidal domains with Dirichlet /Neuman/Robin/periodic boundary conditions are amenable to Fourier series methods. In the present work we are interested in problems formulated on more general irregular spatial domains where the eigenfunctions are not explicitly known. We are also interested in invariant structures with some unstable directions.

The parameterization method for invariant manifolds, introduced in a series of three papers by Cabré, Fontich, and de la Llave [8, 9, 10], provides a general functional analytic framework for studying invariant manifolds. The main idea is to study an invariance equation conjugating the desired manifold to simpler polynomial (or even linear) dynamics. The references [8, 9, 10] prove that, under mild non-resonance assumptions, there exist solutions to the invariance equation. Moreover the solution is unique up to the choice of the scalings of eigenvectors, and the parameterization is as regular as the mapping. The method is constructive and leads to efficient computational schemes.

Another feature of the parameterization method is that, since it studies a conjugacy equation, it recovers the dynamics on the manifold in addition to the embedding. Moreover the parameterization is not required to be the graph of a function and hence can follow folds in the embedding. Since the desired parameterization is required to solve a functional equation, the method lends itself to a-posteriori analysis of errors and even to computer assisted proofs of existence.

Following its introduction in the works just mentioned, the parameterization method has been expanded and applied to a wide variety of problems such as invariant manifolds attached to parabolic fixed points [2], invariant manifolds for periodic orbits of ODEs [33, 15, 45, 32] computation of invariant tori and their whiskers [27, 26, 28], computation of invariant manifolds for difference equations [41], KAM theory without action angle variables for maps, flows, and PDEs, for non-autonomous systems, and for dissipative perturbations of symplectic maps [40, 22, 42, 11, 32], and computer assisted proof for KAM [19], to study normally hyperbolic invariant tori and their breakdown [14, 12, 13], to study quasi-periodic solutions of state dependent delay differential equations [30, 29]. Work closely related to the present study includes recent applications to the dynamics of infinite dimensional systems like computation of unstable manifolds attached to fixed points of compact infinite dimensional maps [24], and also unstable manifolds of equilibrium solutions of delay differential equations and one dimensional PDEs [24, 44], as well as the studies of periodic solutions of parabolic PDEs in [18, 23, 20]. Much more complete introduction and thorough discussion of the literature is found in the recent book of [25] on the topic.

In the present work we adapt the parameterization method to the study of unstable manifolds attached to equilibrium solutions of parabolic partial differential equations. In contrast to the earlier work of [44], our approach works for problems formulated on spatial domains of more than one dimension where a countable basis of eigenfunctions is not available. Instead we project the function space onto a suitable basis of finite elements. We illustrate the use of the method for equations with both polynomial and non-polynomial nonlinearities, and apply it to problems formulated on non-convex spatial domains. Though the method in this paper applies to problems on any number of spatial dimensions, the present work focuses on planar polygonal domains.

The approach exploits formal series expansions which require some preliminary pen and paper calculations to set up. The formal calculations lead to a system of recursive linear elliptic PDEs describing the jets of the local unstable manifold parameterization. Solving these equations is a standard problem in numerical analysis, well suited for finite element methods (FEM).

Before concluding this informal introduction, a few words on the technical assumptions of the paper are in order. We focus on parabolic partial differential equations since, as is well known, they generate compact semi-flows under sectorial assumptions on the associated elliptic operator. In particular, the usual situation is that the spectrum of the linearized equation at an equilibrium solution has at most finitely many unstable eigenvalues of finite multiplicity. It follows that the attached unstable manifold is finite dimensional, hence well suited to numerical approximation. We refer to [58,31,1,59] for more complete discussion of the dynamics of parabolic PDEs.

If in addition the linearized equation at the equilibrium solution generates an analytic semi-group then the local unstable manifold is itself analytic. In this case we are justified in looking for an analytic local parameterization. This observation informs the use of power series methods throughout the present work. It must be stressed that the present work does not here treat convergence of the formal series. Rather, our exposition is example driven with each problem chosen to highlight a particular facet of the procedure. We consider the following models.

- **Fisher Equation:** scalar reaction/diffusion equation with logistic nonlinearity. This pedagogical example illustrates the main steps of our procedure in the easiest possible setting.
- **Ricker Equation:** a modification of the Fisher equation with a more realistic exponential nonlinearity. We use ideas from automatic differentiation for formal power as an example of how to treat non-polynomial problems.
- **Kurramoto-Shivisinsky Equation:** a scalar parabolic PDEs with the bi-harmonic Laplacian as the leading term and lower order derivatives in the nonlinearities. The system is a toy model of fluid dynamics. This example requires the use of higher order elements and we utilize the Argyris element.

The remainder of the paper is organized as follows. In Section 2 we review some basic notions from the theory of finite elements. In Section 3 we describe the parameterization method. Section 4 contains the main calculations of the paper, where we derive the homological equations for each of the chosen example problems. . Some conclusions and reflections are found in Section 6.

2 Finite element method

The FEM is numerical framework for accurate and efficient approximation of solutions of PDEs. The method employs piecewise polynomial approximation of functions on an appropriate triangulation of the domain. It has many advantages over the finite difference method, especially when solutions are of (a-priori) low regularity. The method mainly consists of three steps:

1. Discretizing the domain Ω by an admissible triangulation.
2. Constructing basis elements for the solution space and projecting the infinite dimensional problem onto a finite dimensional vector space. The basis functions should be supported on a small number of triangles so that their matrix representations are sparse.
3. Solving the sparse linear system for the weak formulation of the PDE projected onto the finite dimensional space.

Throughout the present work for the sake of simplicity we consider $\Omega \subset \mathbb{R}^2$, where Ω need not to be convex or even simply connected. We will however assume that Ω is a polygonal domain. The various domains Ω used in this paper are illustrated in Fig. 1.

For a detailed mathematical analysis of FEM we refer the reader to any of the well written books on the subject, for example [16,6,4]. Here, in order that the present work be more self contained, we present a brief overview of the FEM for elliptic PDEs. Consider a uniformly elliptic linear PDE of the form

$$\mathscr{L}u = f \text{ in } \Omega,$$

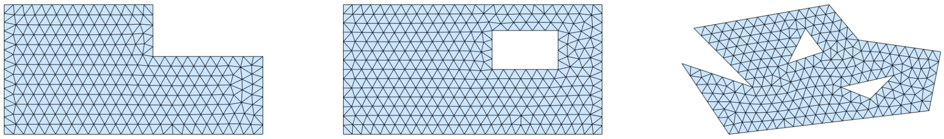

Fig. 1 Some non-convex, non-simply connected domains considered in the examples in Section 4.

with boundary conditions $\{B_i(u)|_{\partial\Omega} = g_i\}$ where the B_i's are the boundary operators. Multiplying the differential equation by test functions and then integrating over the domain Ω we obtain a weak formulation. The weak formulation is interpreted as a variational problem as follows:

$$\text{Find} \quad u \in V \quad \text{such that} \quad a(u,v) = f(v) \quad \forall v \in V. \tag{1}$$

The *Lax-Milgram Lemma* guarantees that the variational problem has a unique solution u over a Hilbert space V whenever a is a continuous V-elliptic bilinear form and $f \in V^*$ [16,6].

To approximate the solution of the variational problem, we first discretize the domain Ω as

$$\Omega = \bigcup_{i=1}^{ne} T_i,$$

where T_i is the i^{th} triangle, and ne is the number of triangular elements. We say that the triangulation $\{T_i\}_{i=1}^{ne}$ forms an admissible partition of the domain Ω provided that the intersection $T_i \bigcap T_j$ occurs only at a common vertex or an edge. Next, we construct finite dimensional subspace $V_h \subset V$ as the span of component-wise bounded basis with "small" compact support. These basis functions are typically chosen to be piecewise polynomials. We use linear basis functions when approximating the solutions of the second order Fisher and Ricker equations, and use the Argyris basis functions to solve the fourth order Kurramoto-Shivisinsky equation. The Argyris elements, which uses the degree 5 polynomials for the finite elements are discussed in detail in section 4.6.

For each triangle T, denote the finite elements by $E = [z_1, \cdots, z_{nn}] \subset T$ where the z_i are control points and the $S_i := \{L_{ij} : 1 \leq j \leq s_i\}$ corresponding sets of control operators evaluated at z_i. Here nn stands for "number of nodes". We write $lnb := \sum_{k=1}^{nn} s_i$ to denote the total number of operators associated with the element E. These letters appropriately stand for "local number of basis" since these operators are used to determine the basis elements associated with T_i. This means that once a basis space $\mathbb{B} \subset V$ is chosen, letting $S = \bigcup_{i=1}^{nn} S_i = \{L_i : 1 \leq i \leq lnb\}$ for each k, the system $L(\phi) := (L_1(\phi), \cdots, L_{lnb}(\phi)) = e_k$ has a unique solution in $\mathbb{B}$. Here e_k is the k^{th} elementary basis vector in $\mathbb{R}^{lnb}$. Usually $\mathbb{B}$ is chosen to be $\mathbb{P}_k := \{\phi : \phi \ \text{ is a polynomial of degree } \ k\}$.

For instance, choosing $\mathbb{P}_1$ leads to elements of the form $E = [n_1, n_2, n_3]$, where the n_i's are the vertices of the triangle T, and $S_i = \{Id\}$ for all T's. Similarly choosing $\mathbb{P}_5$ leads to elements of the form $E = [z_1, z_2, z_3, z_{12}, z_{23}, z_{13}]$, where the z_i's are the vertices of the triangle T and $z_{ij} = (z_i + z_j)/2$ are the midpoints of the sides. Then 5^{th} degree polynomial can be uniquely determined by

$$S_i = \{\phi(z_j), \partial_x\phi(z_j), \partial_y\phi(z_j), \partial_{xx}\phi(z_j), \partial_{xy}\phi(z_j), \partial_{yy}\phi(z_j) \text{ for } j = 1,2,3 \text{ and } \partial_n\phi(z_{12}), \partial_n\phi(z_{23}), \partial_n\phi(z_{13})\},$$

for all T's.

This is a Lagrange interpolation of the function f over the finite element E with control set $\{S_i\}$, and can be expressed as

$$\Pi_E(f) = \sum_{i=1}^{lnb} L_i(f)(z_{n(i)})\frac{det(A_i)}{det(A)},$$

where $L_i \in S = \bigcup_{i=1}^{nn} S_i$, and the index $n(i) = k$ is such that $s_0 + \cdots s_{k-1} + 1 \leq i \leq s_0 + \cdots s_k$. Moreover $A_{ij} = \Big(L_i(x^m y^n)(z_{n(i)})\Big)$, and $(A_k)_{ij} = (1-\delta_{ki})A_{ij} + \delta_{ki}L_i(x^m y^n)$, where $j = \frac{(m+n)(m+n+1)}{2} + (n+1)$. We let $S_0 := \emptyset$ for convenience in writing the expressions for $n(i)$. Notice that the $\phi_i = \frac{det(A_i)}{det(A)}$ are precisely the desired basis functions. For each i, the basis in $\Phi_i := \{\phi_{ij} : 1 \leq j \leq s_i\}$ will have support equal to $\mathscr{N}(z_i) := \{\bigcup T_k : z_i \in T_k\}$.

Finally we define the interpolation space $V_h := \mathrm{span}\{\phi_i\}_{i=1}^{nb} \subset V$, where nb is the total number of basis elements. Notice that while working in $\mathbb{P}_k$ we must have $lnb = \frac{(k+1)(k+2)}{2}$. Regularity conditions imposed on the solution u will carry further restrictions on the elements.

Let h denotes the discretization parameter, that is the mesh (triangulation) size. The smaller the h, the larger the dimension of the finite dimensional vector space V_h. After constructing the basis functions, we approximate the solution $u \in V$ of Equation (1) in the subspace V_h by solving the projected, or discrete weak formulation of the problem given by

$$\text{Find } \; u_h \in V_h \; \text{ such that } \; a(u_h, v_h) = f(v_h) \;\; \forall v_h \in V_h. \tag{2}$$

It is a standard result that the approximate solution $u_h \in V_h$ converges to the unique solution $u \in V$ as $h \to 0$. See for example [4,6,16].

Now let $V = H^{k+1}(\Omega)$ and $V_h \subset \mathbb{P}_k$ for some $k \geq 1$. It is a consequence of the *Bramble-Hilbert Lemma*, as in [16,6,4], that the convergence rate is

$$\|u - u_h\|_{H^1(\Omega)} = O(h^k).$$

Since $u_h = \sum_{i=1}^{nb} c_i\phi_i$, the discrete weak formulation (2) is equivalent to the linear system of equations

$$\sum_{j=1}^{nb} c_j a(\phi_j, \phi_i) = f(\phi_i),$$

which we abreviate as $Ax = b$. Here the matrix $A_{ij} = a(\phi_j, \phi_i)$ is the so called stiffness matrix and is invertible for all V_h-elliptic bilinear forms a. The vector $b_i = f(\phi_i) = \int_\Omega f\phi_i$ is the so called load vector.

For low order polynomial basis it is feasible to evaluate the necessary integrals exactly. For high order basis on the other hand it is more practical to use quadrature rules of sufficiently high degree to approximate the integrals. We write

$$\int_\Omega f = \sum_{i=1}^{ne}\int_{T_i} f \approx \sum_{i=1}^{ne}\sum_{j=i}^{nq} w_j^{T_i} f(q_j^{T_i}),$$

where nq is the degree of the quadrature rule, $q_j^{T_i}$ are the quadratures points and $w_j^{T_i}$ are the corresponding weights. These approximations lead to

$$\Big(a_q(\phi_j, \phi_i)\Big)c_q = \Big(f_q(\phi_i)\Big),$$

where a_q is a the quadrature approximated bilinear form. Note that if a is V-elliptic then it is necessarily V_h-elliptic which in turn implies that $\left(a(\phi_j,\phi_i)\right)$ is invertible. The V-elliptic property of a is studied via the Sobolev embedding theorems. For polynomial basis we certainly have $a_q(\phi_j,\phi_i) = a(\phi_j,\phi_i)$ for nq large enough. Notice that in this case $\|c_q - c\| \leq \|f_q - f\| \|a_q^{-1}\|$. For $f(\phi) = \int_\Omega g\phi$ approximating $g = p + \varepsilon$ with a polynomial p provides the rough estimate $\|f_q - f\| \leq 2\sup(\varepsilon)\|\mathbb{1}\|$ where $\mathbb{1}(\phi) = \int_\Omega \phi$ whenever nq is sufficiently large.

3 The parameterization method for unstable manifolds of equilibria

Let $\mathscr{H}$ be a Hilbert (or Banach) space and $F\colon \mathscr{H} \to \mathscr{H}$ be a smooth map, which need be only densely defined. Consider the initial value problem

$$\frac{\partial}{\partial t} u(t) = F(u(t)), \qquad \text{with } u(0) = \bar{u} \in \mathscr{H} \text{ given.}$$

Suppose that $u_0 \in \mathscr{H}$ is an equilibrium solution, so that

$$F(u_0) = 0,$$

and assume that $A = DF(u_0)$ generates a compact semi-group e^{At} so that the Morse index of A is finite – that is: we have that there are at most finitely many unstable eigenvalues of A, each with only finite multiplicity.

Let $\lambda_1, \ldots, \lambda_M$ denote the unstable eigenvalues ordered so that

$$0 < \mathrm{real}(\lambda_1) \leq \ldots \leq \mathrm{real}(\lambda_M).$$

Suppose for the sake of simplicity that each unstable eigenvalue has multiplicity one (though this assumption can be removed – see [8,3]), and let $\xi_1, \ldots, \xi_M \in \mathscr{H}$ be an associated choice of eigenvectors, so that

$$DF(u_0)\xi_j = \lambda_j \xi_j, \qquad 1 \leq j \leq M.$$

An orbit or *solution curve* for F is a smooth curve $\gamma\colon (a,b) \to \mathscr{H}$ having that

$$\frac{d}{dt}\gamma(t_0) = F(\gamma(t_0)),$$

for each $t_0 \in (a,b)$. Suppose that u_0 is an equilibrium solution and that $\gamma\colon (-\infty, 0]$ is a solution curve. Given $u \in \mathscr{H}$ we say that γ is an infinite pre-history for u, accumulating at u_0 if

$$\gamma(0) = u, \qquad \text{and} \qquad \lim_{t \to -\infty} \gamma(t) = u_0.$$

The unstable manifold attached to u_0, denoted $W^u(u_0)$, is the set of all $u \in \mathscr{H}$ which have an infinite backwards time orbit accumulating at u_0. The intersection of $W^u(u_0)$ with a small neighborhood of u_0 is a local unstable manifold for u_0, and is the set of all points near u_0 which have well-defined backwards history remaining in a neighborhood of u_0 for all time $t \leq 0$.

Let $\mathbb{B} = [-1,1]^M$ denote the M-dimensional unit hypercube. We seek a parameterization $P\colon \mathbb{B} \to \mathscr{H}$ having that

$$P(0) = u_0, \tag{3}$$

$$\partial_j P(0) = \xi_j, \qquad 1 \leq j \leq M, \tag{4}$$

and that

$$P\left([-1,1]^M\right) \subset W^u(u_0).$$

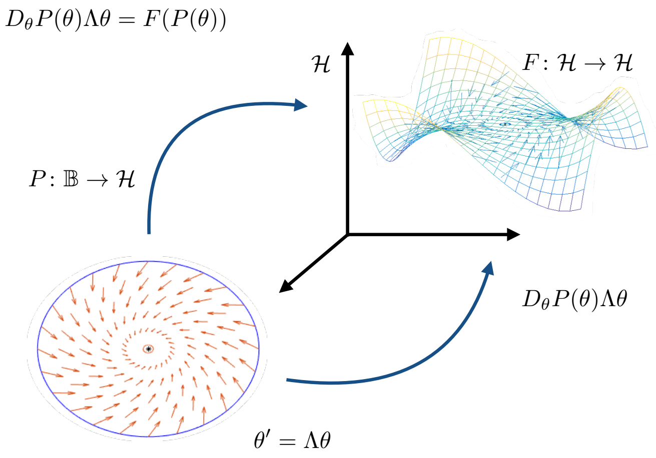

Fig. 2 Schematic representation of the invariance equation.

Any such P parameterizes a local unstable manifold at u_0. Since any reparameterization of P is again a parameterization of an unstable manifold, the problem has infinitely many freedoms and we need to impose an additional (infinite dimensional) constraint to isolate a single parameterization.

Write

$$\Lambda = \begin{pmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_M \end{pmatrix}.$$

In the context of the present work, the parameterization method seeks a P which, in addition to satisfying the constraint Equations (3) and (4), is also a solution of the *invariance equation*

$$F(P(\theta)) = DP(\theta)\Lambda\theta, \qquad \text{for all } \theta \in \mathbb{B} = [-1,1]^M. \tag{5}$$

Figure 2 illustrates the geometry behind Equation (5), which says that the push forward of the linear vector field Λ by DP matches the vector field F restricted to the image of P. Loosely speaking, since the two vector fields match on the image of P they must generate the same dynamics – with the dynamics generated by Λ well understood. It is natural to expect that P maps orbits of Λ in $\mathbb{B}$ to orbits of F on the image of P. Since P maps orbits to orbits, Equation (5) is also called an infinitesimal conjugacy equation. The orbit correspondence is illustrated in Figure 3, and the observations of the preceding paragraph are made precise in the following lemma.

Lemma 1 (Orbit correspondence) *Assume that the unstable eigenvalues $\lambda_1,\dots,\lambda_M$ are real and distinct. Suppose that $P\colon [-1,1]^M \to \mathscr{H}$ satisfies the first order constraints of Equations* (3) *and* (4)*, and that P is a smooth solution of Equation* (5) *on $\mathbb{B} = (-1,1)^M$. Then P parameterizes a local unstable manifold for u_0.*

Proof First observe that the image of P is a smooth disk, as its domain $\mathbb{B}$ is a topological disk and P is smooth. Also observe that the constraint given in Equation (4) implies that P is tangent to the unstable eigenspace of $DF(u_0)$ at u_0.

Now fix a $\theta \in (-1,1)^M$ and define the curve $\gamma_\theta\colon (-\infty,0] \to \mathscr{H}$ by

$$\gamma_\theta(t) = P\left(e^{\Lambda t}\theta\right).$$

Our first claim is that γ_θ is a solution curve for F. To see this first observe that for all $t \in (-\infty, 0]$ we have that

$$\hat{\theta} := e^{\Lambda t}\theta \in \mathbb{B},$$

as the entries of Λ are unstable, real, and distinct. Then consider

$$\begin{aligned}
\frac{d}{dt}\gamma_\theta(t) &= \frac{d}{dt}P\left(e^{\Lambda t}\theta\right) \\
&= DP\left(e^{\Lambda t}\theta\right)\Lambda e^{\Lambda t}\theta \\
&= DP\left(e^{\Lambda t}\theta\right)\Lambda e^{\Lambda t}\theta \\
&= DP(\hat{\theta})\Lambda\hat{\theta} \\
&= F(P(\hat{\theta})) \\
&= F(P(e^{\Lambda t}\theta)) \\
&= F(\gamma_\theta(t)),
\end{aligned}$$

as desired.

In addition to being a solution curve, we have also that γ_θ accumulates at u_0 in backward time. Indeed

$$\begin{aligned}
\lim_{t\to-\infty}\gamma_\theta(t) &= \lim_{t\to-\infty} P\left(e^{\Lambda t}\theta\right) \\
&= P\left(\lim_{t\to-\infty} e^{\Lambda t}\theta\right) \\
&= P(0) \\
&= u_0,
\end{aligned}$$

where we have used the assumption that P is smooth and hence continuous on $(-1,1)^M$. Since θ was arbitrary, we see that every point $P(\theta)$ on the image of P has a backward orbit which accumulates at u_0. That is

$$\text{image}(P) \subset W^u(u_0).$$

Since image(P) is an M-dimensional disk containing u_0 and contained in the unstable manifold we have that image(P) is a local unstable manifold as desired.

We remark that if F generates a flow Φ near u_0, then Lemma 1 says that P satisfies the flow conjugacy

$$P(e^{\Lambda t}\theta) = \Phi(P(\theta), t),$$

for all t such that $e^{\Lambda t}\theta \in (-1,1)^M$. That is, P conjugates the flow generated by Λ to the flow generated by F.

Remark 1 (Complex conjugate unstable eigenvalues) When there are complex conjugate eigenvalues one proceeds just as in the finite dimensional case, as discussed at length in [39]. The main idea is to find associated complex conjugate eigenfunctions in the complexified Hilbert space and looks for a parameterization $P(z_1, \ldots, z_M)$ with complex variables $z_1, \ldots, z_M$.

Suppose for example that the only pair complex conjugate eigenvalues are $\lambda_1, \lambda_2 \in \mathbb{C}$. That is, assume that $\lambda_2 = \overline{\lambda_1}$. Then we take complex conjugate variables $z_1 = \theta_1 + i\theta_2$ and $z_2 = \theta_1 - i\theta_2$ and arrange, just as in [39], that $P(\theta_1 + i\theta_2, \theta_1 - i\theta_2, \theta_3, \ldots, \theta_M)$ is real for all $\theta \in [-1,1]^M$. This is because the Taylor coefficients of P inherit the same complex conjugate symmetry imposed on the eigenfuncitons. Of course if there are additional complex conjugate pairs of eigenvalues we treat them in exactly the same way. Since complex conjugate eigenvalues do not appear in the examples treated in the present work we only refer the interested reader to the reference already cited for more complete discussion.

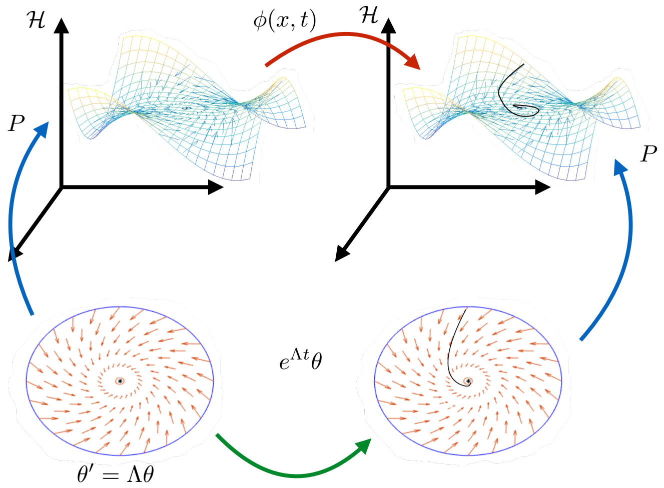

Fig. 3 The orbit correspondence induced by the invariance Equation. The orbits generated by the vector field Λ accumulate in backwards time to the origin in $\mathbb{B}$. Then P lifts these orbits to orbits in $\mathscr{H}$ which accumulate at the equilibrium u_0. From this it follows that image of P is a local unstable manifold. (5)

3.1 Formal power series and the homological equations for parabolic PDEs

In this section we narrow the discussion to focus a specific class of example problems. The discussion in this section generalizes to parabolic equations involving more general elliptic operators, higher dimensional domains, more general boundary conditions, and even to systems of PDEs. Our goal is not to describe the most general possible setting but rather to illustrate the application parameterization method, and especially the solution of Equation (5), for an interesting class of PDEs. To this end let $\Omega \subset \mathbb{R}^2$ a bounded, planar, polygonal domain and $f\colon \mathbb{R} \times \Omega \to \mathbb{R}$ be a smooth function. We consider the class of scalar parabolic PDEs given by

$$\frac{\partial}{\partial t} u(t,x,y) = \Delta u(t,x,y) + f(u(t,x,y),x,y), \tag{6}$$

with the Neumann boundary conditions

$$\frac{\partial}{\partial \mathbf{n}} u(t,x,y) = 0 \quad \text{for } (x,y) \in \partial\Omega.$$

Let $\mathscr{H} = H^1(\Omega)$ and suppose that $u_0\colon \Omega \to \mathbb{R}$ is in $\mathscr{H}$ ands is a weak solution of the elliptic nonlinear boundary value problem

$$\Delta u_0(x,y) + f(u_0(x,y),x,y) = 0,$$

subject to the Neumann boundary conditions. Moreover, suppose that $\lambda_1, \ldots, \lambda_M \in (0,\infty)$ and $\xi_1, \ldots, \xi_M\colon \Omega \to \mathbb{R}$ are weak solutions in $\mathscr{H}$ of the eigenvalue problems

$$\Delta \xi_j + \partial_1 f(u_0)\xi_j = \lambda_j \xi_j,$$

again subject to the boundary conditions.

We look for $P\colon [-1,1]^M \to \mathscr{H}$ given by a formal power series

$$P(\theta_1, \ldots, \theta_M, x, y) = \sum_{n_1=0}^{\infty} \cdots \sum_{n_M=0}^{\infty} p_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1} \ldots \theta_M^{n_M},$$

and solving the invariance equation (5). Here each $p_{n_1,\ldots,n_M}(x,y) \in \mathscr{H}$ is required to satisfy the boundary conditions. Moreover, imposing the constraints of Equations (3) and (4) gives that the first order coefficients of P will have

$$p_{0,\ldots,0}(x,y) = u_0(x,y),$$

and

$$p_{1,\ldots,0}(x,y) = \xi_1(x,y), \qquad \ldots \qquad p_{0,\ldots,1}(x,y) = \xi_M(x,y).$$

To work out the remainder of the coefficients we proceed as follows. We calculate the push forward of Λ by DP on the level of power series and find that

$$DP(\theta,x,y)\Lambda\theta = \sum_{n_1=0}^{\infty}\ldots\sum_{n_M=0}^{\infty}(n_1\lambda_1^{n_1}+\ldots+n_M\lambda_M^{n_M})p_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M}.$$

Observe that the value of this series at $\theta = 0$ is zero.

Now define the vector field $F\colon \mathscr{H} \to \mathscr{H}$ by

$$F(u) = \Delta u + f(u,x,y),$$

and consider

$$F(P(\theta,x,y)) = \Delta P(\theta,x,y) + f(P(\theta,x,y),x,y)$$

Formally we have that

$$\Delta P(\theta,x,y) = \sum_{n_1=0}^{\infty}\ldots\sum_{n_M=0}^{\infty}\Delta p_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M}.$$

If f is analytic then it admits a power series representation. If f is of only C^k regularity then it has a Taylor series expansion to order k and the argument below is modified accordingly. Focusing on the analytic case we suppose that

$$f(P(\theta,x,y),x,y) = \sum_{n_1=0}^{\infty}\ldots\sum_{n_M=0}^{\infty}q_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M},$$

where the $q_{n_1,\ldots,n_M}$ are the formal Taylor coefficients of the composition depending on the coefficients of P. Efficient computation of the $q_{n_1,\ldots,n_M}$ is a calculation best illustrated through examples. For the moment we only remark that for any given multi-index $(n_1,\ldots,n_M) \in \mathbb{N}^M$ the dependence of $q_{n_1,\ldots,n_M}$ on $p_{n_1,\ldots,n_M}$ has

$$q_{n_1,\ldots,n_M} = D_1 f(u_0(x,y),x,y)p_{n_1,\ldots,n_M} + S_{n_1,\ldots,n_M}.$$

where $S_{n_1,\ldots,n_M}$ depends only on coefficients of P of lower order.

Matching like powers in Equation (5) leads to

$$\begin{aligned}(n_1\lambda_1^{n_1}+\ldots+n_M\lambda_M^{n_M})p_{n_1,\ldots,n_M}(x,y) &= \Delta p_{n_1,\ldots,n_M}(x,y) + q_{n_1,\ldots,n_M} \\ &= \Delta p_{n_1,\ldots,n_M}(x,y) + D_1 f(u_0(x,y),x,y)p_{n_1,\ldots,n_M} + S_{n_1,\ldots,n_M},\end{aligned}$$

so that

$$\Delta p_{n_1,\ldots,n_M}(x,y) + D_1 f(u_0(x,y),x,y)p_{n_1,\ldots,n_M} - (n_1\lambda_1^{n_1}+\ldots+n_M\lambda_M^{n_M})p_{n_1,\ldots,n_M}(x,y) = -S_{n_1,\ldots,n_M},$$

or more succulently

$$\left(DF(u_0) - (n_1\lambda_1^{n_1}+\ldots+n_M\lambda_M^{n_M})\mathrm{Id}_{\mathscr{H}}\right)p_{n_1,\ldots,n_M}(x,y) = -S_{n_1,\ldots,n_M}. \qquad (7)$$

Equation (7) is referred to as *the homological equation* for the unstable manifold for F at u_0. Observe that Equation (7) is a linear elliptic PDE with the same boundary conditions as the original reaction/diffusion equation (6). The moral of the story is that each Taylor coefficient of P is the solution of a linear problem no more complicated than the linearized equation at u_0, and these equations are amiable to finite element analysis under mild assumptions on the domain Ω.

Remark 2 (Non-resonance conditions and existence of a formal solution) Observe that Equation (7) has a unique solution if and only if the *non-resonance condition*

$$n_1\lambda_1^{n_1} + \ldots + n_M\lambda_M^{n_M} \notin \mathrm{spec}(DF(u_0)), \tag{8}$$

is satisfied. Since $\lambda_1, \ldots, \lambda_M$ are the only unstable eigenvalues of $DF(u_0)$, and since $DF(u_0)$ generates a compact semi-group, we have that the countably many remaining eigenvalues are stable. Since the $n_1, \ldots, n_M$ are all positive, there are only finitely many opportunities for $n_1\lambda_1^{n_1} + \ldots + n_M\lambda_M^{n_M}$ to be an eigenvalue. If Equation (8) is satisfied for all multi-indices $(n_1, \ldots, n_M) \in \mathbb{N}^M$ with $n_1 + \ldots + n_M \geq 2$ then we say that the unstable eigenvalues are *non-resonant*, and in this case we have that the parameterization P is formally well defined to all orders. That is, Equation (5) has a well defined formal series solution satisfying the first order constraints of Equations (3) and (4).

Remark 3 (Uniqueness up to rescaling of the first order data) The unique solvability of the homological equations, assuming non-resonance of the unstable eigenvalues, gives that the solution P at u_0 is unique up to the choice of the scalings of the eigenvectors. The choice of the scaling of the eigenvector directly effects the decay of the coefficients $p_{n_1,\ldots,n_M}$ as discussed in [5,44]. For this reason we always fix the domain of the parameterization to be $\mathbb{B} = [-1,1]^M$, and choose the scaling of the eigenvectors so that we have small errors on this domain. Of course while choosing smaller scalings for the eigenvectors provides faster coefficient decay, it also means that the image of $\mathbb{B}$ is smaller in $\mathscr{H}$. That is, smaller scalings stabilize the numerics but reveal a smaller portion of the local unstable manifold. In practice we must strike a balance between the polynomial order of the calculation (at what order do we truncate the formal series?) the scaling of the eigenvectors and the size of the local unstable manifold we compute.

3.2 Automatic differentiation of power series

The most challenging step in the formal calculations of the previous section is to work out the power series coefficients $q_{n_1,\ldots,n_M}$ of $f(P(\theta,x,y),x,y)$ in terms of the coefficients $p_{n_1,\ldots,n_M}$ of P. This challenge reduces to repeated application of the Cauchy product formula of $f(\cdot,x,y)$ has polynomial nonlinearity.

For example consider the case where f is a quadratic function of the form

$$f(u,x,y) = a(x,y)u^2.$$

Then

$$\begin{aligned}
f(P(\theta,x,y),x,y) &= a(x,y)\left(\sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty} p_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M}\right)\left(\sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty} p_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M}\right) \\
&= a(x,y)\sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty}\left(\sum_{k_1=0}^{n_1}\cdots\sum_{k_M=0}^{n_M} p_{n_1-k_1,\ldots,n_M-k_M}(x,u)p_{k_1,\ldots,k_M}(x,y)\right)\theta_1^{n_1}\ldots\theta_M^{n_M} \\
&= \sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty}\left(\sum_{k_1=0}^{n_1}\cdots\sum_{k_M=0}^{n_M} a(x,y)p_{n_1-k_1,\ldots,n_M-k_M}(x,y)p_{k_1,\ldots,k_M}(x,y)\right)\theta_1^{n_1}\ldots\theta_M^{n_M} \\
&= \sum_{k_1=0}^{n_1}\cdots\sum_{k_M=0}^{n_M} q_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M},
\end{aligned}$$

and we see that

$$\begin{aligned} q_{n_1,\dots,n_M}(x,y) &= \sum_{k_1=0}^{n_1}\dots\sum_{k_M=0}^{n_M} a(x,y)p_{n_1-k_1,\dots,n_M-k_M}(x,y)p_{k_1,\dots,k_M}(x,y) \\ &= 2a(x,y)p_{0,\dots,0}(x,y)p_{n_1,\dots,n_M}(x,y) + \text{“lower order terms”} \\ &= 2\frac{\partial}{\partial u}f(u_0,x,y)p_{n_1,\dots,n_M}(x,y) + \text{“lower order terms”}, \end{aligned}$$

as promised above. Indeed the “lower order terms” have the explicit form

$$S_{n_1,\dots,n_M} = \sum_{k_1=0}^{n_1}\dots\sum_{k_M=0}^{n_M} \hat{\delta}_{n_1,\dots,n_M}^{k_1,\dots,k_M} a(x,y)p_{n_1-k_1,\dots,n_M-k_M}(x,y)p_{k_1,\dots,k_M}(x,y)$$

where the coefficient

$$\hat{\delta}_{n_1,\dots,n_M}^{k_1,\dots,k_M} = \begin{cases} 0 & \text{if } k_1 = \dots = k_M = 0 \\ 0 & \text{if } k_1 = n_1, \dots, k_M = n_M \\ 1 & \text{otherwise} \end{cases},$$

appears in the sum to indicate that both of the $p_{n_1,\dots,n_M}(x,y)$ have been removed.

When f contains non-polynomial terms the calculation of the $q_{n_1,\dots,n_M}$ are more delicate. We employ a semi-numerical technique based on the idea that many typical nonlinearities appearing in applications are themselves solutions of polynomial differential equations. This fact can be exploited to develop fast recursion schemes.

Consider for example the case of

$$f(u,x,y) = a(x,y)e^{-u}.$$

Let

$$P(\theta,x,y) = \sum_{n_1=0}^{\infty}\dots\sum_{n_M=0}^{\infty} p_{n_1,\dots,n_M}(x,y)\theta_1^{n_1}\dots\theta_M^{n_M},$$

and write

$$f(P(\theta,x,y),x,y) = Q(\theta,x,y) = \sum_{n_1=0}^{\infty}\dots\sum_{n_M=0}^{\infty} q_{n_1,\dots,n_M}(x,y)\theta_1^{n_1}\dots\theta_M^{n_M}. \tag{9}$$

Following the procedure discussed in Chapter 2 of [25] we define the *radial gradient* to be the first order partial differential operator given by

$$\nabla_\theta = \theta_1\frac{\partial}{\partial\theta_1} + \dots + \theta_M\frac{\partial}{\partial\theta_M}.$$

Applying the radial gradient to both sides of Equation (9) leads to

$$\nabla_\theta f(P(\theta,x,y),x,y) = \nabla_\theta Q(\theta,x,y).$$

That is

$$\begin{aligned} &\nabla_\theta f(P(\theta,x,y),x,y) \\ &= \theta_1\frac{\partial}{\partial u}f(u,x,y)\big|_{u=P(\theta,x,y)}\frac{\partial}{\partial\theta_1}P(\theta,x,y) + \dots + \theta_M\frac{\partial}{\partial u}f(u,x,y)\big|_{u=P(\theta,x,y)}\frac{\partial}{\partial\theta_M}P(\theta,x,y) \\ &= -a(x,y)e^{-P(\theta,x,y)}\left(\theta_1\frac{\partial}{\partial\theta_1}P(\theta,x,y) + \dots + \theta_M\frac{\partial}{\partial\theta_M}P(\theta,x,y)\right) \\ &= -Q(\theta,x,y)\nabla_\theta P(\theta,x,y) \end{aligned}$$

$$= -\left(\sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty} q_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M}\right)\left(\sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty}(n_1+\ldots+n_M)p_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M}\right)$$

$$= -\sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty}\left(\sum_{k_1=0}^{n_1}\cdots\sum_{k_M=0}^{n_M}(k_1+\ldots+k_M)q_{n_1-k_1,\ldots,n_M-k_M}p_{k_1,\ldots,k_M}\right)\theta_1^{n_1}\ldots\theta_M^{n_M},$$

on the left, and

$$\nabla_\theta Q(\theta,x,y) = \sum_{n_1=0}^{\infty}\cdots\sum_{n_M=0}^{\infty}(n_1+\ldots+n_M)q_{n_1,\ldots,n_M}(x,y)\theta_1^{n_1}\ldots\theta_M^{n_M},$$

on the right. Matching like powers and isolating $q_{n_1,\ldots,n_M}$ leads to

$$q_{n_1,\ldots,n_M} = \frac{-1}{n_1+\ldots+n_M}\sum_{k_1=0}^{n_1}\cdots\sum_{k_M=0}^{n_M}(k_1+\ldots+k_M)q_{n_1-k_1,\ldots,n_M-k_M}p_{k_1,\ldots,k_M}.$$

The implication is that the complexity of computing the power series coefficients of $a(x,y)e^{-P(\theta,x,y)}$ is the same as the complexity of a single Cauchy product. The additional cost is that the coefficients of Q have to be stored. In the applications considered in the present work the additional use of memory resources is never prohibitive.

Such methods for formal series manipulations are referred to by many authors as *automatic differentiation for power series*, and they facilitate rapid computation of the formal series coefficients of compositions with all the elementary functions. A classic reference which includes an in depth historical discussion is found in Chapter 4, Section 6 of [36]. See also the discussion of software implementations found in [35].

4 Applications

4.1 A first worked example: Fisher's Equation

As a first example consider the parabolic PDE

$$\frac{\partial}{\partial t}u = \Delta u + \alpha u(1-u),$$

with Neumann boundary conditions on the L-shaped domain Ω (leftmost domain in Fig. 1). This reaction-diffusion equation was introduced by Ronald Fisher in the context of population dynamics as a toy model for the propagation of advantageous genes [21]. To find an equilibrium solution we set the left hand side to zero and solve the equation

$$\Delta u + \alpha u(1-u) = 0.$$

The weak formulation follows by multiplying the steady state equation with a test function $\phi \in H^1(\Omega)$ and then integrating over Ω. Using Green's identity we get,

$$-\int_\Omega \nabla u\cdot\nabla\phi + \int_\Omega \alpha u(1-u)\phi = 0.$$

We now triangulate Ω and solve for the projection $u_h = \sum_{j=1}^{nb} c_j\phi_j$ of u to a finite dimensional vector space with linear basis functions ϕ_j defined as:

$$\phi_j(n_i) = \begin{cases} 1 & j = i \\ 0 & j \neq i \end{cases}.$$

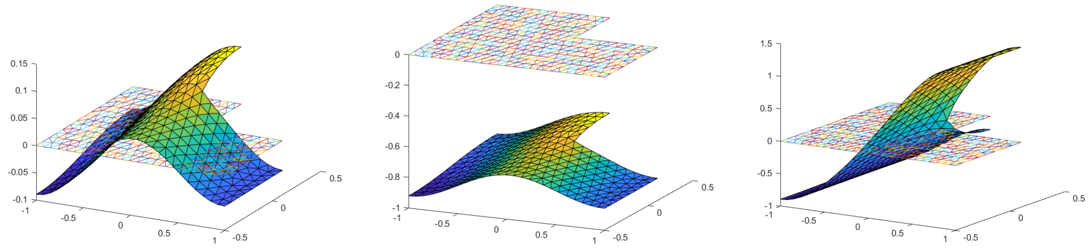

Fig. 4 Left: Equilibrium solution u_0, ne=515. Center: Eigenfunction for $\lambda_1 = 9.04$. Right: Eigenfunction for $\lambda_2 = 7.16$.

Here n_i is the i^{th} vertex , and the number of basis nb is the number of nodes in the triangulation.

Letting $\phi = \phi_i$ for $1 \le i \le nb$ leads to the nb by nb system

$$F_i(c) = -\int_\Omega \left(\sum_{j=1}^{nb} c_j \nabla \phi_j \right) \cdot \nabla \phi_i + \int_\Omega \alpha \left(\sum_{j=1}^{nb} c_j \phi_j \right) \left(1 - \sum_{j=1}^{nb} c_j \phi_j \right) \phi_i = 0,$$

which we solve using the Newton's Method where $F = (F_1, ..., F_{nn})$ and

$$c^{(k)} - c^{(k-1)} = -DF\left(c^{(k-1)}\right)^{-1} F\left(c^{(k-1)}\right).$$

Here

$$DF(c) = -\left(\int_\Omega \nabla \phi_j \cdot \nabla \phi_i \right) + \alpha \left(\int_\Omega \frac{\partial \left(\sum_{j=1}^{nb} c_j \phi_j \right) \left(1 - \sum_{j=1}^{nb} c_j \phi_j \right)}{\partial c_j} \phi_i \right).$$

Solving $F(c) = 0$ by Newton's Method with $ne = 515$ linear finite elements, we obtain the equilibrium solution $u_0 = \sum_{j=1}^{nb} c_j \phi_j$ illustrated in the left frame of Fig 4.

Next, we proceed to solve the linearized eigenvalue problem at the equilibrium u_0,

$$\Delta \xi + \alpha(1 - 2u_0)\xi - \lambda \xi = 0,$$

and again solve for the projection $\xi = \sum_{j=1}^{nb} c_j \phi_j$ in the weak formulation leading to

$$-\int_\Omega \left(\sum_{j=1}^{nb} c_j \nabla \phi_j \right) \cdot \nabla \phi_i + \int_\Omega \alpha(1 - 2u_0) \left(\sum_{j=1}^{nb} c_j \phi_j \right) \phi_i = \int_\Omega \lambda \left(\sum_{j=1}^{nb} c_j \phi_j \right) \phi_i \quad i = 1, \ldots, nb$$

$$\left(-\int_\Omega \nabla \phi_j \cdot \nabla \phi_i + \alpha(1 - 2u_0)\phi_j \phi_i \right) c = \lambda \left(\int_\Omega \phi_j \phi_i \right) c \quad i = 1, \ldots, nb.$$

We obtain two positive eigenvalues, and the corresponding eigenfunctions illustrated in the middle and right frames of Fig 4.

Having found the equilibrium solution $u_0(x,y)$ as well as the the unstable eigenvalues λ_1 and λ_2 and corresponding eigenfunctions $\xi_1(x,y)$ and $\xi_2(x,y)$, we now solve the invariance equation (5) specialized to the present situation. That is, we consider

$$F(P(\theta)) = \lambda_1 \theta_1 \frac{\partial}{\partial \theta_1} P(\theta) + \lambda_2 \theta_2 \frac{\partial}{\partial \theta_2} P(\theta),$$

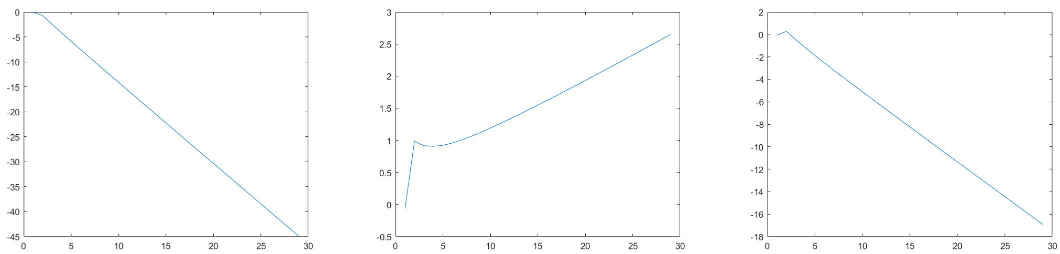

Fig. 5 Left: The scaling of the eigenvector is too small and only a few coefficients contribute to the computation. Center: The chosen eigenvector scaling is now too large and the $p_{m,n}$'s do not decay. Right: The scaling is chosen so that the last coefficient in P is of machine precision order.

where

$$P(\theta) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} p_{m,n}(x,y)\theta_1^m \theta_2^n,$$

with $p_{0,0} = u_0$, $p_{1,0} = \xi_1$ and $p_{0,1} = \xi_2$. Comparing powers in the weak formulation, and taking the projection $p_{m,n} = \sum_{i=1}^{nb} c_i^{(m,n)} \phi_i$ we obtain

$$\Big(-\int_\Omega \nabla\phi_j \cdot \nabla\phi_i + \alpha(1 - 2u_0 - m\lambda_1 - n\lambda_2)\phi_j\phi_i \Big)\Big(c_i^{(m,n)}\Big) = \Big(\int_\Omega s_{(m,n)}\phi_i\Big)$$

$$\Big(DF(u_0) - (\lambda_1 m + \lambda_2 n)\int_\Omega \phi_j\phi_i\Big)c^{(m,n)} = \Big(\int_\Omega s_{(m,n)}\phi_i\Big),$$

for $m+n \geq 2$ with

$$s_{(m,n)} = \alpha \sum_{i=0}^{m}\sum_{j=0}^{n} \delta(i,j) p_{i,j} p_{m-i,n-j}.$$

Here

$$\delta(i,j) = \begin{cases} 0 & (i,j) = (0,0) \text{ or } (i,j) = (m,n) \\ 1 & otherwise \end{cases},$$

is a coefficient which expresses the fact that the terms of order (m,n) have been removed from the sum. As expected, the homological equations are elliptic PDE which we solve recursively to any desired order using the Finite Element Method. A numerical representation of the fast and slow unstable manifolds obtained by evaluating the sub-parameterizations $P(\theta_1, 0)$ and $P(0, \theta_2)$ are illustrated in Figure 6.

The effect of the non-uniqueness of the solution P on the decay of the coefficients is shown in Figure 5. Recall that the non-uniqueness is due only to the freedom of the choice in scalings for the eigenvectors. The important observation is that a poor choice of scaling leads to either too rapid growth or too rapid decay of the power series coefficients. When computing P to a desired polynomial order N we always choose the scaling so that the N-th coefficients are below some prescribed tolerance. A good rule of thumb is that the magnitude of the truncation error – measured on the domain $[-1,1]^M$ – has the same order as the magnitude of the N-the coefficients. Even better heuristics are obtained by looking at the exponential best fit applied to all the coefficients. Algorithms for choosing the best scalings in an automatic way are treated in [5].

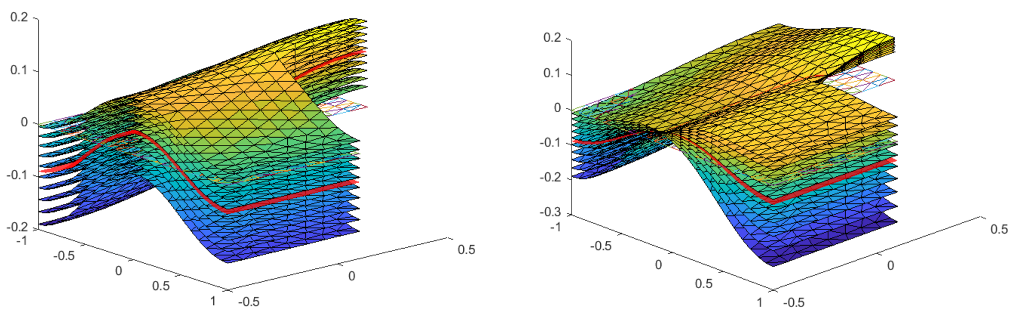

Fig. 6 Left: 10 pts on the fast manifold, $N = 30$, L^2 error on the invariance equation 1.09e-08 Right: 10 pts on the slow manifold, $N = 30$, L^2 error on the invariance equation 2.99e-07

4.2 A reaction diffusion equation with non-polynomial nonlinearity: one unstable eigenvalues

In this section we derive the homological equations for a non-polynomial problem. We consider the following reaction diffusion equation with exponential nonlinearity, sometimes referred to as a Ricker nonlinearity

$$u_t = \Delta u + \alpha u \left(0.5 - e^{-u}\right).$$

The equilibrium solutions solve

$$F_i(c) = -\int_\Omega \left(\sum_{j=1}^{nb} c_j \nabla\phi_j\right) \cdot \nabla\phi_i + \int_\Omega \alpha \left(\sum_{j=1}^{nb} \phi_j\right) \left(0.5 - \exp\{\sum_{j=1}^{nb} c_j\phi_j\}\right) \phi_i = 0,$$

and the corresponding eigenvalue-eigenfunction problem is

$$DF(u_0)c = \lambda \left(\int_\Omega \phi_j\phi_i\right) c.$$

Assume that an unstable eigenvalue λ and corresponding eigenfunction ξ are known and write $P(\theta) = \sum_{n=0}^{\infty} p_n\theta^n$. The Invariance Equation (5) is

$$\sum_{n=0}^{\infty} \Delta p_n\theta^n + \alpha \left(\sum_{n=0}^{\infty} p_n\theta^n\right) \left(0.5 - \exp\{-\sum_{n=0}^{\infty} p_n\theta^n\}\right) = \lambda \sum_{n=0}^{\infty} np_n\theta^n.$$

To obtain an equivalent polynomial problem we use automatic differentiation as discussed in Section 3.2.

That is we define $Q(\theta) := e^{-P(\theta)} = \sum_{n=0}^{\infty} q_n\theta^n$, and observe that $Q' = -QP'$. Comparing like powers leads to

$$(n+1)q_{n+1} = -\sum_{j=0}^{n} (j+1)p_{j+1}q_{n-j},$$

and isolating the n-th term gives that

$$q_n = -p_n q_0 - \frac{1}{n}\sum_{j=0}^{n-2} (j+1)p_{j+1}q_{n-1-j},$$

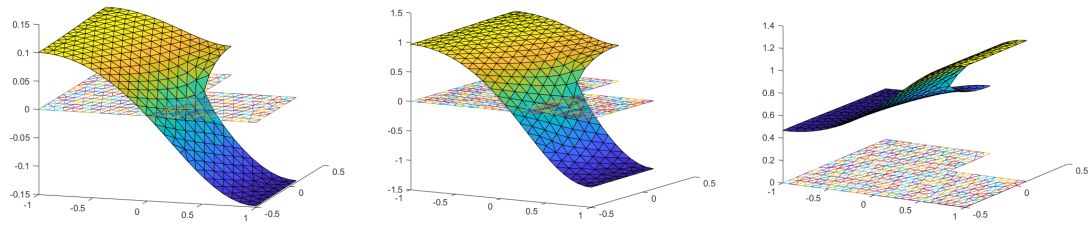

Fig. 7 Left: Equilibrium solution, ne=515. Center: Eigenfunction ξ_1 with $\lambda_1 = 2.34$. Right: Eigenfunction ξ_2 with $\lambda_2 = 0.07$.

a relation allowing us to compute q_n to any desired order.

Returning to the Invariance Equation we now exploit th formula for q_n just derived, so that

$$\Delta p_n + \alpha(0.5 - q_0 - \lambda n)p_n - \alpha p_0 q_n = \alpha \sum_{j=1}^{n-1} p_j q_{n-j},$$

$$\Delta p_n + \alpha(0.5 - q_0 + p_0 q_0 - \lambda n)p_n = s_n,$$

with

$$s_n = \alpha \sum_{j=1}^{n-1} p_j q_{n-j} - \frac{\alpha p_0}{n} \sum_{j=0}^{n-2} (j+1) p_{j+1} q_{n-1-j},$$

or

$$\left(DF(u_0) - \lambda n \int_\Omega \phi_j \phi_i \right) c^{(n)} = \left(\int_\Omega s_n \phi_i \right).$$

Notice that s_n only depends on p_k's and q_k's with $k < n$, and with p_0, q_0 and p_1 computed a-priori. Then p_n is computed to any desired order using this recursion.

4.3 A reaction diffusion equation with non-polynomial nonlinearity: two unstable eigenvalues

A simple modification of the method just discussed is used in the case of higher dimensional manifolds for problems with non-polynomial nonlinearities. Consider again

$$\frac{\partial}{\partial t} u = \Delta u + \alpha u(0.5 - e^{-u}),$$

and assume the Equilibrium, λ_1 and λ_2 are computed along with the corresponding ξ_1 and ξ_2.

The Invariance Equation (5) is

$$F(P(\theta)) = \lambda_1 \theta_1 \frac{\partial}{\partial \theta_1} P(\theta) + \lambda_2 \theta_2 \frac{\partial}{\partial \theta_2} P(\theta),$$

with

$$P(\theta) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} p_{m,n}(x,y) \theta_1^m \theta_2^n,$$

and where $p_{m,n}$ are to be determined. As per the discussion of the radial gradient in Section 3.2 we define

$$Q := \exp\{-P(\theta)\} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{m,n}(x,y) \theta_1^m \theta_2^n,$$

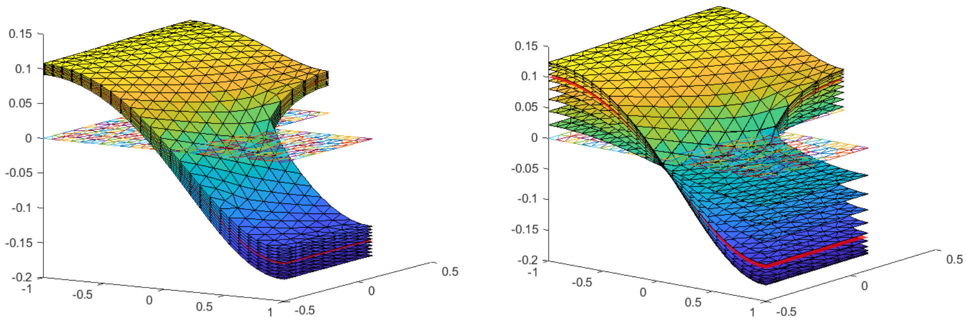

Fig. 8 Left: Fast manifold with $N = 30$. L^2 error on the invariance equation 4.08e-08. Right: Slow manifold with $N = 30$. L^2 error on the invariance equation 1.68e-06

and consider

$$\nabla_\theta Q(\theta) = \nabla_\theta \exp(P(\theta)),$$

so that

$$\theta_1 \frac{\partial}{\partial \theta_1} Q + \theta_2 \frac{\partial}{\partial \theta_2} Q = -Q(\theta_1 \frac{\partial}{\partial \theta_1} P + \theta_2 \frac{\partial}{\partial \theta_2} P).$$

Comparing like powers leads to

$$\sum_{m,n \geq 1} (m+n) q_{m,n} \theta_1^m \theta_2^n = -\Big(\sum_{m,n \geq 1} (m+n) p_{m,n} \theta_1^m \theta_2^n \Big) \Big(\sum_{m,n \geq 0} q_{m,n} \theta_1^m \theta_2^n \Big),$$

$$q_{m,n} = -\frac{1}{(m+n)} \sum_{i=1}^{m} \sum_{j=1}^{n} (i+j) p_{i,j} q_{m-i,n-j},$$

a recursive expression for the q_{mn}.

Returning to the Invariance Equation and using the recursive formula for $q_{m,n}$ we obtain

$$\Delta p_{m,n} + \alpha(0.5 - q_{0,0} - \lambda_1 m - \lambda_2 n) p_{m,n} - \alpha p_{0,0} q_{m,n} = \alpha \sum_{i=0}^{m} \sum_{j=0}^{n} q_{i,j} p_{m-i,n-j} \delta(i,j)$$

$$\Delta p_{m,n} + \alpha(0.5 - q_{0,0} + p_{0,0} q_{0,0} - \lambda_1 m - \lambda_2 n) p_{m,n} = s_{m,n}$$

with

$$s_{m,n} = \alpha \sum_{i=0}^{m} \sum_{j=0}^{n} q_{i,j} p_{m-i,n-j} \delta(i,j) - \frac{\alpha p_{0,0}}{(m+n)} \sum_{i=1}^{m-1} \sum_{j=1}^{n-1} (i+j) p_{i,j} q_{m-i,n-j},$$

or

$$\Big(DF(u_0) - (\lambda_1 m + \lambda_2 n) \int_\Omega \phi_j \phi_i \Big) c^{(m,n)} = \Big(\int_\Omega s_n \phi_i \Big)$$

and solve to any desired order. Numerical results are illustrated in Figure 8.

4.4 Higher order PDEs: Kuramoto-Sivashinsky type equation

In this section we demonstrate the use of our methods for a higher order PDE, and consider a problem whose diffusion operator is bi-harmonic Laplacian rather than the Laplacian. The Kuramoto-Sivashinsky equation is such an equation, and models the propagation of a flame front. It is known to exhibit complicated dynamics like periodic oscillations, heteroclinic/homoclinic connecting orbits and spatiotemporal chaos. We refer to [38,34,63,54,37] for more complete discussion of the equation and its dynamical properties.

Define

$$F(u) = -\Delta^2 u - \Delta u - 0.5|\nabla u|^2.$$

The difference between this example and the previous ones is that higher order Finite Elements are now required. To simplify the location of equilibrium solutions, we modify the KS equation and view it as a perturbation of the Fisher's equation with natural boundary conditions. This facilitates computation of the equilibrium solutions by continuation from the Fisher problems already considered. We stress that this is a computational convenience rather than a fundamental limitation of the method.

So, let

$$F(u) = \alpha\Delta^2 u + \beta\Delta u + \gamma|\nabla u|^2 + \varepsilon u(1-u), \tag{10}$$

or

$$F(u) = \alpha\Delta^2 u + \beta\Delta u + N(u),$$

with $N(u) = \gamma|\nabla u| + \varepsilon u(1-u)$. We will refer to the corresponding 4th order equation as Kuramoto-Sivashinsky-Fisher (KSF). We use the Argyris elements which guarantee C^1 solutions and offer high convergence rate. We refer to [16] for the mathematical theory of the Argyris elements and to [17] for a useful discussion of the numerical implementation.

The Argyris basis are first order polynomials in two space variable constructed as follows: Define the operators $L_1 = Id, L_2 = \partial_{10}, L_3 = \partial_{01}, L_4 = \partial_{20}, L_5 = \partial_{11}$ and $L_6 = \partial_{02}$. For an element $[n_1, n_2, n_3, m_1, m_2, m_3]$ with nodes n_1, n_2 and n_3 and midpoints m_1, m_2 and m_3, the nodal basis $\phi_k^{n_i}$ are defined by

$$L_\ell(\phi_k^{n_i}(n_j)) = \delta_{ij}\delta_{\ell k}.$$

$$\frac{\partial}{\partial n}\phi_k^{n_i}(m_j) = 0,$$

and the basis associated to the midpoints by

$$\frac{\partial}{\partial n}\phi^{m_i}(m_j) = \delta_{ij},$$

$$L_\ell\phi^{m_i}(n_j) = 0,$$

where $1 \le i, j \le 3$ and $1 \le k, \ell \le 6$.

These are 21 constraints for each ϕ which uniquely defines a fifth order polynomials in x, y that is

$$\phi(x,y) = \sum_{0 \le i+j \le 5} c_{ij} x^i y^j.$$

We solve a 21×21 linear system $Ac = b$ for the coefficients c_{ij} for each of the 21 basis associated with an element. In practice, we only do this for a reference triangle and transfer these basis to an arbitrary element using the method of Dominguez and Sayas [17]. Indeed, our implementation is very similar to that described in the reference just cited.

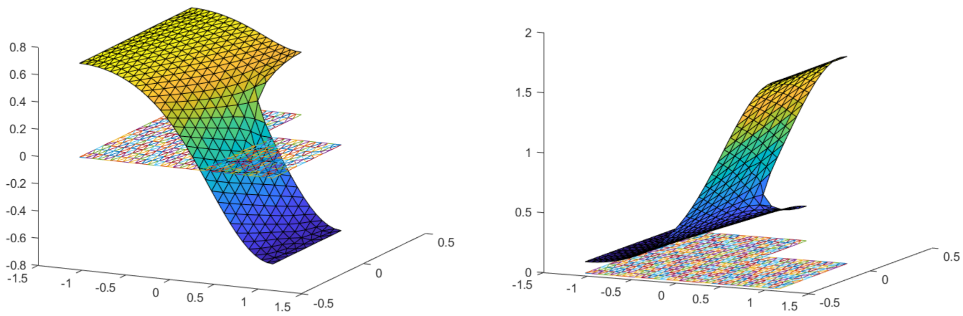

Fig. 9 Left: Equilibrium solution, ne=705. Right: Eigenfunction ξ with $\lambda = 3.57$.

In the notation presented earlier, $S_i = \{L_k : 1 \leq k \leq 6\}$ for $i = 1,2,3$ and $S_i = \{\frac{\partial}{\partial n}\}$ for $i = 4,5,6$ and after indexing $\bigcup_i S_i = \{L_k\}$

$$\phi_i = \frac{det(A_i)}{det(A)},$$

for $1 \leq i \leq 21$. The global representation of u becomes:

$$u = \sum_{k=1}^{6} \sum_{\text{all } n_i} c_k^{n_i} \phi_k^{n_i} + \sum_{\text{all } m_i} c^{m_i} \phi^{m_i}.$$

Going back to the KSF equation, we derive the weak formulation. Starting with

$$\int_\Omega \alpha \left(\Delta^2 u\right) \phi + \int_\Omega \beta(\Delta u)\phi + \int_\Omega N(u)\phi = 0,$$

apply Green's formula to obtain

$$\int_\Omega -\alpha \nabla(\Delta u) \cdot \nabla \phi + \oint_{\partial\Omega} \alpha(\nabla(\Delta u) \cdot n)\phi - \int_\Omega \beta \nabla u \cdot \nabla \phi + \oint_{\partial\Omega} \beta(\nabla u \cdot n)\phi + \int_\Omega N(u)\phi = 0.$$

Assume the boundary integrals vanish and apply Green's formula again so that

$$\int_\Omega \alpha \Delta u \Delta \phi - \oint_{\partial\Omega} \alpha(\nabla\phi \cdot n)\Delta u - \int_\Omega \beta \nabla u \cdot \nabla \phi + \int_\Omega N(u)\phi = 0.$$

Again imposing the the boundary conditions leads to

$$\int_\Omega \alpha \Delta u \Delta \phi - \int_\Omega \beta \nabla u \cdot \nabla \phi + \int_\Omega N(u)\phi = 0.$$

From this expression we solve for the projection

$$u = \sum_{j=1}^{nb} c_j \phi_j,$$

with $nb = 6nv + ned$, where nv is the number of vertices and ned is the number of edges in the triangulation.

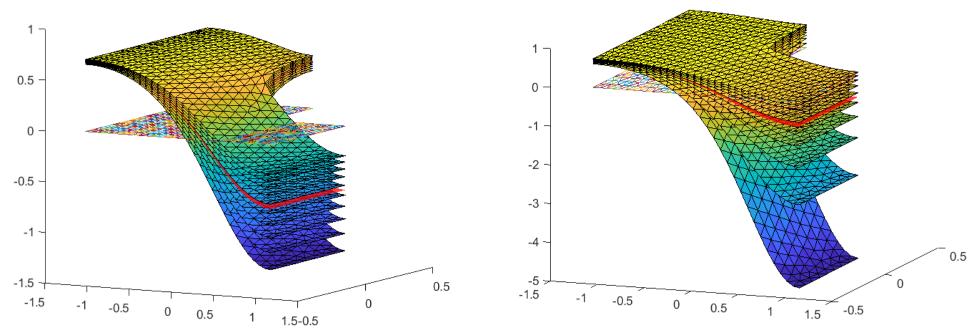

Fig. 10 Unstable manifolds for the KSF equation. Left: 10 points on the 1d manifold, $N = 30$. L^2 error on the invariance equation 1.06e-07. Right: 10 points on the 1d manifold, $N = 120$. L^2 error on the invariance equation 2.14e-07

After computing an equilibrium solution and eigendata λ and ξ we proceed to solve Equation (5) in the case of Morse index one so that

$$F(P(\theta)) = \lambda\theta\frac{\partial P}{\partial\theta},$$

where

$$P(\theta) = \sum_{n=0}^{\infty} p_n\theta^n.$$

Comparing powers and solving for

$$p_n = \sum_{j=1}^{nb} c_j^{(n)}\phi_j,$$

leads to

$$\alpha\Delta^2 p_n + \beta\Delta p_n + 2\gamma\left(\frac{\partial p_0}{\partial x}\frac{\partial p_n}{\partial x} + \frac{\partial p_0}{\partial y}\frac{\partial p_0}{\partial y}\right) + \varepsilon(1-2p_0)p_n - \lambda p_n = s_n,$$

where

$$s_n = -\gamma\left(\sum_{k=1}^{n-1}\frac{\partial p_k}{\partial x}\frac{\partial p_{n-k}}{\partial x} + \frac{\partial p_k}{\partial y}\frac{\partial p_{n-k}}{\partial y}\right) + \varepsilon\sum_{k=1}^{n-1} p_k p_{n-k},$$

and the weak formulation of the homological equation is

$$\left(DF(u_0) - \lambda n\int_\Omega \phi_j\phi_i\right)c^{(n)} = \left(\int_\Omega s_n\phi_i\right).$$

Figure 10 illustrates the resulting numerical approximation of the unstable manifold when $\alpha =$?, ... It is interesting to note that the equilibrium solution the Fisher equation persist for a relatively large range of ε.

5 Some additional examples and performance results

Figure 11 illustrates two additional unstable manifold calculations for an equilibrium solution of the KSF equation posed on other domains. The results show that the method works in principle on non-convex, not simply connected domains.

The tables below show the effect of decreasing the mesh size of the triangulation on the conjugacy equation error.

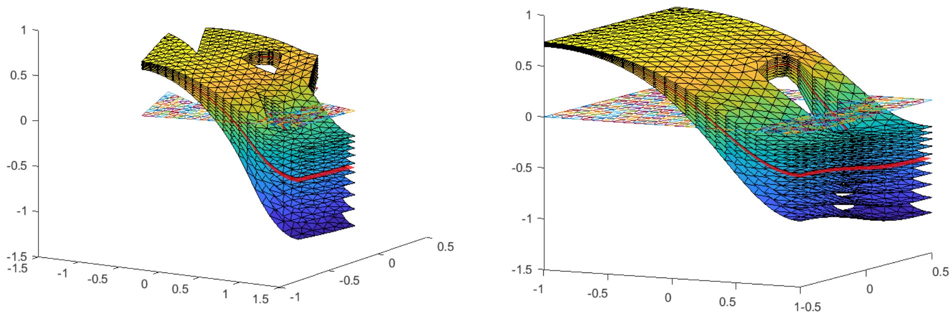

Fig. 11 Unstable manifolds for the Kuramoto-Fisher type equation posed on non-convex domains with holes (middle and right domains illustrated in Figure 1). Left: 10 points on the 1d manifold, $N = 30$. L^2 error on the invariance equation 1.40e-06. Right: 10 points on the 1d manifold, $N = 30$. L^2 error on the invariance equation 1.45e-07

ne	Fisher 1d manifolds	Fisher 2d manifolds
515	2.65e-08	5.20e-08
984	1.44e-08	2.41e-08
1963	6.53e-09	1.32e-08

Table 1 L^2 norms of the error in the conjugacy equation for 1d and 2d manifolds in the Fisher equation.

ne	Fisher-Ricker 1d manifolds	Fisher-Ricker 2d manifolds
515	1.53e-07	1.03e-06
984	2.39e-08	5.88e-07
1963	1.01e-08	2.38e-07

Table: L^2 norms of the error in the conjugacy equation for 1d and 2d manifolds in the Fisher equation with exponential nonlinearity.

ne	KSF on L domain	ne	KSK on domain 3	ne	KSF on domain 2
100	6.62e-07	122	5.57e-07	123	8.23e-07
200	3.46e-07	214	3.43e-07	260	3.21e-07
423	1.74e-07	443	2.44e-07	522	1.71e-07

Table: L^2 norms of the error in the conjugacy equation for 1d manifolds in the Kuramoto-Sivashinsky-Fisher equation over several irregular domains.

We also compared the L_2 errors in the conjugacy equation of the second order Fisher equation using linear and Argyris basis. Using linear basis we obtained an error of 2.65e-08, while using Argyris basis we approached machine precision errors.

6 Conclusions

We have combined the parameterization method with finite element analysis to obtain a new approximation method for unstable manifolds of equilibrium solutions for parabolic PDEs. The method works for PDEs defined on planar polygonal domains and is implemented for number of example problems with both polynomial and non-polynomial nonlinearities, for unstable manifolds of dimension one and two, for a number of non-convex and non-simply connected domains, and for problems involving both Laplacian and bi-harmonic Laplacian diffusion operators. The method is easy to implement for computing the approximation to arbitrary order: the same code that computes the second order approximation will compute the approximation to order 50 – this is just a matter of changing a loop variable. The method is amenable to a-posteriori analysis of errors and we employ these indicators to show that our calculations are accurate far from the equilibrium solution.

Interesting future projects would be to apply the method to problems with other boundary conditions such as Dirichlet or Robin, to apply it to problems formulated on spatial domains of dimension 3 or more, to extend the method for the computation of unstable manifolds attached to periodic solutions of parabolic PDEs, or to extend the method to study invariant manifolds attached to equilibrium or periodic solutions of systems of parabolic PDEs.

Finally we mention that there is a thriving literature on mathematically rigorous computer assisted proof for elliptic PDEs based on finite element analysis. See for example the works of [46,52,48,47,49, 51,62,50,53,7,57,56,43,61,60,55] for validated numerical methods for solving nonlinear elliptic PDE (equilibrium solutions of parabolic PDEs) and their associated eigenvalue/eigenfunction problems. We refer also the references just cited for more complete review of this literature. From the point of view of the present discussion the important point is this: that the present work reduces the problem of computing jets of unstable manifolds to the problem of solving elliptic boundary value problems – and moreover that a number of authors have developed powerful methods of computer assisted proof for solving such problems. A very interesting line of future research would be to combine the results of the present work validated numerical methods for elliptic BVPs.

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