A Framework for the Numerical Computation and a Posteriori Verification of Invariant Objects of Evolution Equations

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Abstract

We develop a theoretical framework for computer-assisted proofs of the existence of invariant objects in semilinear PDEs. The invariant objects considered in this paper are equilibrium points, traveling waves, periodic orbits and invariant manifolds attached to fixed points or periodic orbits. The core of the study is writing down the invariance condition as a zero of an operator. These operators are in general not continuous, so one needs to smooth them by means of preconditioners before classical fixed point theorems can be applied. We develop in detail all the aspects of how to work with these objects: how to precondition the equations, how to work with the nonlinear terms, which function spaces can be useful, and how to work with them in a computationally rigorous way. In two companion papers, we present two different implementations of the tools developed in this paper to study periodic orbits.

Keywords

Evolution equation · Periodic Orbits · Contraction mapping
Invariant Manifolds · Rigorous Computations · Interval Analysis

Mathematics Subject Classification (2010)

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1 Introduction

This paper establishes the theoretical background for the computation and rigorous verification of different types of invariant solutions for evolution PDEs. It is accompanied by two papers [26, 45] providing independent implementations for periodic orbits for the Kuramoto-Sivashinsky PDE. The choices of spaces, algorithms and implementations are different. Moreover, paper [45] shows how to perform continuation with respect to parameters while paper [26] establishes lower bounds of analyticity of solutions.

The goal of this paper is to present an approach to the existence of invariant objects in evolution partial differential equations which can be used to obtain computer-assisted proofs validating numerical computations. In this paper we only present some unified strategy that works in several problems. Of course, in concrete problems one needs to present many more details, but we hope that the unified remarks can be used as a systematic guide to understand seemingly disparate papers.

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We consider fixed points, periodic traveling waves, periodic solutions and invariant manifolds attached to them. Eventually, the study of invariant manifolds could lead to the study of homoclinic or heteroclinic connections.

The general philosophy is that we formulate the existence of these invariant objects as the existence of solutions of a functional equation. These functional equations are shown to have solutions by applying a constructive version of a fixed point theorem (e.g. contraction mapping in this paper). The main ingredients of the theorem is the existence of an approximate fixed point, as well as some non-degeneracy conditions. One of the byproducts of the application of such results is local uniqueness.

The approximate solutions can be the product of a numerical computation. It is then important that one can verify the conditions of the theorem with a finite computation with finite precision. If these computations are carried out on an actual computer, we can validate the computation and obtain a *computer-assisted proof.*

From the point of view of computer-assisted proofs, it is important that the conditions of the theorem can be verified by a finite computation. This entails, in particular, reducing the problem to a finite dimensional problem and devising theoretically explicit estimates for the truncation errors. These studies of the truncation depend very much on the structure of the operators and the spaces on which we consider them acting. Hence, we present only some cases.

Similar strategies have been already applied in different contexts. Constructive fixed point theorems were used in the study of Renormalization Group operators [16, 24], and in finite dimensional invariant manifolds in [52, 66, 72].

In this paper we show how to give constructive proofs (computer-assisted) of existence of some special orbits (fixed points, traveling waves, periodic orbits and some stable/unstable manifolds) of parabolic equations of the form

$$\partial_t u = Lu + N(u), \tag{1}$$

where L is an elliptic operator and N is a semilinear operator (of lower order than L). Without loss of generality (using translations in u and redefining L), we assume $N(0) = 0$, $DN(0) = 0$. We make it precise later on in what sense DN should be understood. In the theoretical development, the unknown u could take values in $\mathbb{R}^n$, even if the main examples here are with $n = 1$.

This evolution equation is supplemented with boundary conditions. We impose boundary conditions by considering equation (1) as defined in an appropriate Banach space of functions satisfying the boundary conditions. Indeed the choice of spaces is very important (see Section 4). Sometimes, we require the existence of a scalar product defined in the space. From the more theoretical point of view, the spaces encode not only the boundary conditions but also the regularity properties of the solutions obtained. To perform the analysis, we require that the norm of the spaces is such that one can study comfortably the operators that appear in the problem (differential operators, their inverses, etc) and that they are Banach algebras under multiplication. To be able to do efficient numerical analysis, we also require that the norms of vectors and of linear operators can be computed accurately and efficiently, and that truncations are easy to estimate. Some choices of spaces that satisfy these theoretical and practical requirements are discussed in Section 4. At some point, we find it useful to use the *two spaces approach* of [33].

A concrete example of equation (1) that is worth keeping in mind and which is used in the concrete numerical implementations, see [26, 45], is the Kuramoto-Sivashinsky equation [15, 40, 43, 62],

$$\partial_t u = \alpha \partial_x^2 u + \partial_x^4 u + u \partial_x u, \tag{2}$$

which we supplement with periodic boundary conditions in x (possibly also with the requirement that the solution is odd in x). The real number α is a parameter of the problem. In the literature, one can find different forms of the equation which are equivalent to this one by changing the units of space, time and u.

Note that the evolution equation (1) is infinite dimensional and that both L and N are unbounded (in the case of (2), $L(u) = (\alpha \partial_x^4 + \partial_x^2)u$ and $N(u) = u\partial_x u$). Hence, one cannot directly apply the methods of ordinary differential equations, and even existence of a semi-flow requires methods appropriate for PDEs [33, 59–61].

However, it is worth remarking that, since we are only aiming at obtaining some particular solutions, we do not need that the evolution is defined nor well-posed. Indeed, methods similar to the ones in this paper have been applied to obtain existence of some specific solutions in some ill-posed equations such as the Boussinesq equation and the Boussinesq system [6, 12, 23, 27] (numerical computations for some of these problems is work in progress). Similar ideas work for delay differential equations, neutral delay equations (with advanced and retarded delays) and for fractional evolution PDEs. The study of some specific solutions such as traveling waves, even in ill-posed equations, has been common-place for a while.

It is important to mention that the methods considered here are not the only possibilities. Indeed, periodic orbits of equation (2) have been considered in [41, 42] and methods for computer-assisted proofs based on topological methods appeared in [18, 19, 71] and other functional methods based on propagating and finding fixed points for the time T map appeared in [3]. Each method has its own set of practical difficulties, e.g. propagation methods have difficulties with stiffness, Fourier discretizations have difficulties when the solutions develop shocks. All methods share the *curse of dimensionality*. Hence, it is important that our methods use only functions of the same number of variables than the objects they aim to compute.

Let us conclude by mentioning a short list of problems of invariant objects in PDEs that are not treated in this paper but we believe could be interesting to attack. These objects consist of quasi-periodic tori, normally hyperbolic invariant manifolds, connecting orbits, inertial manifolds and invariant foliations.

The rest of the paper is organized as follows. In Section 2, we present general fixed point theorems for functional equations. In Section 3, we reduce the existence of the dynamical objects to a functional equation and show how to manipulate them in such a way that they are reduced to a constructive fixed point theorem. In Section 4, we introduce some basis, spaces and norms which are useful to perform the analysis. In Section 5, we present some guidelines for the implementation of the computer-assisted verification of the invariant objects following the framework presented in this paper.

2 Fixed point theorems for functional equations

In this section we present general fixed point theorems for functional equations. These theorems are useful for the implementation of numerical schemes and rigorous computer-assisted proofs of the invariance equations for the different invariant objects treated in this paper.

Fixed point theorems are classical in the literature. In this section we present them tailored for the equations we want to work with. Also, in this section, we present some other tools that we need while working with the invariance equations. Sometimes, these equations are underdetermined, so we impose extra conditions to have local uniqueness of solutions. Also, while imposing conditions for the attached invariant manifolds, eigenvalue problems arise, which we transform into a fixed point equation.

2.1 Lipschitz theorems with preconditioning

Here we describe some rather general manipulations that are frequently used in the constructive study of nonlinear equations. We begin by describing the manipulations formally and postpone the discussions about ranges, domains and boundedness of the operators for later.

We start with an equation

$$F(u) = 0. \tag{3}$$

Given any injective operator M equation (3) is equivalent to

$$T(u) = u + MF(u) = u. \tag{4}$$

Remark 2.1. Notice that we only need that M, often called the *preconditioner*, is injective and not boundedly invertible.

It is important to note that the above manipulations could make sense even when F and M are unbounded. The only thing that we need is that MF is a well defined C^2 operator.

A case that we consider is $F(u) = Lu + N(u)$, where both L and N are differential operators, hence unbounded. More precisely, L is an invertible elliptic linear operator and N is another (nonlinear) differential operator. If the order of L is higher than that of N (the semilinear case), the operator $L^{-1}N$ is bounded (indeed compact). The choice of M is rather flexible and there are many choices. In this case $M = L^{-1}$ is suitable, but sometimes more convenient approximations are considered.

The next two theorems provide sufficient conditions to prove that an operator is a contraction, and therefore that it has a unique fixed point. Also, this theorem provides estimates of the size of the correction term δu.

Theorem 2.2. *Consider the operator F in equation (3) defined in $\overline{B_\rho(\bar{u})} = \{u : \|u - \bar{u}\| \le \rho\}$, with $\rho > 0$. Denote $N_{\bar{u}}$ the nonlinear part of the operator F at the point $\bar{u}$, that is*

$$N_{\bar{u}}(z) = F(\bar{u} + z) - F(\bar{u}) - DF(\bar{u})z.$$

Let B be a linear operator such that $BDF(\bar{u})$, BF and $BN_{\bar{u}}$ are continuous operators. If, for some $b, K > 0$ we have:

(a) $\|I - BDF(\bar{u})\| = \alpha < 1$;

(b) $\|B\,(F(\bar{u}) + N_{\bar{u}}(z))\,\| \le b$ *whenever* $\|z\| \le \rho$;

(c) $Lip_{\|z\|\le\rho} BN_{\bar{u}}(z) < K$;

(d) $\frac{b}{1-\alpha} < \rho$;

(e) $\frac{K}{1-\alpha} < 1$.

then there exists δu such that $\bar{u} + \delta u$ is in $\overline{B_\rho(\bar{u})}$ and is a unique solution of equation (4), with $\|\delta u\| \le \frac{\|BF(\bar{u})\|}{1-\alpha-K}$.

The proof is based on a standard application of the Banach fixed point theorem. We include it for the sake of completeness.

Proof. We should check that the map

$$u \to \bar{u} - (BDF(\bar{u}))^{-1}B(F(\bar{u}) + N_{\bar{u}}(u - \bar{u})) \tag{5}$$

applies the ball $\overline{B_\rho(\bar{u})}$ to itself and is contracting. A fixed point of this map is equivalent to a solution of the equation

$$F(u + \bar{u}) = 0.$$

Condition (a) implies that the linear operator $BDF(\bar{u})$ is invertible, and the norm of its inverse is bounded above by $\frac{1}{1-\alpha}$. Condition (d) implies that the map maps $\overline{B_\rho(\bar{u})}$ to itself, and condition (e) that it is a contraction with Lipschitz constant $\frac{K}{1-\alpha}$.

Finally, the Banach fixed point theorem assures that there is a unique solution $u_* = \bar{u} + \delta u$ in $\overline{B_\rho(\bar{u})}$. The last assertion follows from the fact that if we iterate the contracting map (5) starting from the point $u_0 = \bar{u}$, then

$$\|\delta u\| = \|u_0 - u_*\| \le \frac{1}{1 - \frac{K}{1-\alpha}}\|u_0 - u_1\| = \frac{1}{1 - \frac{K}{1-\alpha}}\|(BDF(\bar{u}))^{-1}BF(\bar{u})\| \le \frac{1}{1-\alpha-K}\|BF(\bar{u})\|.$$

$\square$

2.1.1 The radii polynomial approach

It may appear at first that Theorem 2.2 is not suitable for numerical computations because is it not readily clear how to find ρ. However there are explicit choices for the constants in the theorem. One example of how to choose the constants is provided by the classical Newton-Kantorovich Theorem. Another example, that is a refinement of the latter, is the *radii polynomial* approach [21, 29, 30].

Theorem 2.3. *Let T in (4) be C^1, let $\rho > 0$ and $\overline{B_\rho(\bar{u})} = \{u : \|u - \bar{u}\| \leq \rho\}$. Consider bounds ε and $\kappa = \kappa(\rho)$ satisfying*

$$\|T(\bar{u}) - \bar{u}\| \leq \varepsilon \tag{6}$$

$$\sup_{w \in \overline{B_\rho(\bar{u})}} \|DT(w)\| \leq \kappa(\rho). \tag{7}$$

If

$$\varepsilon + \rho\kappa(\rho) < \rho \tag{8}$$

then $T : \overline{B_\rho(\bar{u})} \to \overline{B_\rho(\bar{u})}$ is a contraction with constant $\kappa(\rho) < 1$. Moreover, the linear operator M is injective and therefore $F = 0$ has a unique solution in $\overline{B_\rho(\bar{u})}$.

Proof. By (7), $\|DT(\bar{u})\| = \|Id - MDF(\bar{u})\| \leq \kappa(\rho) < 1$. Using Neumann series, we conclude that M is injective. Hence, fixed points of T are in a one-to-one correspondence with the zeros of F. Given any $x \neq y \in B_{\bar{u}}(\rho)$, there exists $z = tx + (1-t)y \in B_{\bar{u}}(\rho)$ with $t \in [0, 1]$ such that

$$\|T(x) - T(y)\| = \|DT(z)(x - y)\| \leq \|DT(z)\|\|x - y\| < \kappa(\rho)\|x - y\|.$$

That shows that T is a contraction. It remains to prove that T maps $\overline{B_\rho(\bar{u})}$ into itself given $x \in \overline{B_\rho(\bar{u})}$.

$$\|T(x) - \bar{u}\| \leq \|T(x) - T(\bar{u})\| + \|T(\bar{u}) - \bar{u}\| \leq \kappa(\rho)\|x - \bar{u}\| + \varepsilon \leq \varepsilon + \rho\kappa(\rho) < \rho,$$

follows by (8). The contraction mapping theorem yields a unique fixed point u_* of T in $\overline{B_\rho(\bar{u})}$ and therefore a unique solution of $F = 0$ in $\overline{B_\rho(\bar{u})}$. □

Once the bounds (6) and (7) are computed, the main hypothesis of Theorem 2.3 is to verify the existence of a radius $\rho > 0$ such that inequality (8) is satisfied. We may use the notion of radii polynomials to find such $\rho > 0$. The philosophy of the radii polynomial approach is to leave the radius ρ of the closed ball $\overline{B_\rho(\bar{u})}$ variable in case that the nonlinearities of T are polynomials.

We can derive analytic estimates (using the fact that the function space is a Banach algebra) and use interval arithmetic computations to obtain a polynomial bound for the right hand side of (7) of the form $\kappa(\rho) = \kappa_1 + \kappa_2\rho + \kappa_3\rho^2 + \cdots + \kappa_N\rho^{N-1}$, where the coefficients κ_i ($i = 1, \ldots, N$) are nonnegative and typically N is the degree of the polynomial nonlinearity in the problem under investigation. The term κ_1 should be small, thanks to the fact that T is a Newton-like operator at $\bar{u}$ and the term ε should be small if $\bar{u}$ is a good enough numerical approximation. Then, we can define the *radii polynomial* by

$$p(\rho) = \sum_{j=2}^{N} \kappa_j\rho^j + (\kappa_1 - 1)\rho + \varepsilon. \tag{9}$$

Let

$$\mathcal{I} = \{\rho > 0 \ : \ p(\rho) < 0\}.$$

If the hypothesis (8) of Theorem 2.3 holds, then $\mathcal{I} \neq \emptyset$. This implies that $\kappa_1 - 1 < 0$, as otherwise we would not be able to find $\rho > 0$ such that $p(\rho) < 0$. By Descartes' rule of signs, the radii polynomial (9) has exactly two positive real zeros that we denote by $\rho_- < \rho_+$. This implies that $\mathcal{I}$ is an open interval.

Heuristically, since we aim at finding small radii, that is $0 < \rho \ll 1$, then for ρ small $p(\rho) \approx \kappa_2\rho^2 + (\kappa_1 - 1)\rho + \varepsilon$. If $(\kappa_1 - 1)^2 - 4\varepsilon\kappa_2 > 0$, then there should exist an open interval $\mathcal{I} = (\rho_-, \rho_+)$ such that for every $\rho \in \mathcal{I}$, $p(\rho) < 0$. This approach yields a *continuum* of balls of the form $\overline{B_\rho(\bar{u})}$ (with $\rho \in \mathcal{I}$)

that contain a unique solution of $F = 0$. The existence of the interval $\mathcal{I}$ yields information that may be useful. For instance, if we are interested in localizing the solutions in the smallest possible ball, then the set $\overline{B_{\rho_-}(\bar{u})}$ provides that information. On the other hand, we may sometimes be interested in getting a large isolating ball containing the unique solution. In this case, this information would be given by the set $\overline{B_{\rho_+}(\bar{u})}$. Finally, another information that may be useful is that the set $\overline{B_{\rho_+}(\bar{u})} \setminus \overline{B_{\rho_-}(\bar{u})}$ does not contain any solution of $F = 0$. This provides a set of non existence of solutions of $F = 0$.

2.2 Extra equations

Across the paper we encounter several times functional equations that are underdetermined. They have many solutions which are nevertheless physically equivalent (e.g. when looking for a parameterization of a periodic orbit, we have the choice of any point on the orbit to correspond to $t = 0$ in the parameterization). So, extra normalizing conditions are needed to obtain a unique solution. There are several alternatives that can be chosen. Some of them are:

- *Fixed point in phase space*: This extra condition arises when we force the solution u to lie on a codimension 1 subspace. In the evolution language, this is equivalent to fixing a Poincaré section. This condition is stated in algebraic terms as

$$\langle u, v\rangle = 0 \tag{10}$$

  for some v. Note that we require the scalar product $\langle \cdot, \cdot \rangle$ to be a differentiable operator in the Banach space we are considering. For example, the L^2 scalar product satisfies this property in the space of differentiable functions. See Section 4 for a detailed treatment of this fact.

- *Fixed phase*: This extra condition impose that the correction $u - \bar{u}$ is perpendicular to the initial guess $\bar{u}$. This is done by imposing that

$$\langle u - \bar{u}, \bar{u}\rangle = 0. \tag{11}$$

  This condition is useful when we want to eliminate a translation.

2.3 A general eigenvalue-eigenvector equation

During the exposition we encounter several times eigenvalue-eigenvectors equations of the form

$$Lv + Av = \lambda v, \tag{12}$$

where L and A are linear operators such that $L^{-1}A$ is a bounded operator. This equation is underdetermined, but after imposing an extra scalar equation (for example $\langle v, v\rangle = 1$), it can be transformed into a fixed point equation for the unknowns (λ, v). In more concrete terms, after adding this last condition we obtain that the pair (λ, v) satisfies the system of equations

$$F(\lambda, v) = \begin{pmatrix} Lv + Av - \lambda v \\ \langle v, v\rangle - 1 \end{pmatrix} = 0. \tag{13}$$

In all problems in this paper, the linear operator L is easily invertible, and satisfies that both L^{-1} and $L^{-1}A$ are continuous operators. Following the formulation as in Subsection 2.1, we multiply equation (13) by the operator

$$M = \begin{pmatrix} L^{-1} & 0 \\ 0 & 1 \end{pmatrix}.$$

Remark 2.4. Notice that the nonlinear (in fact quadratic) part of the last system is easily treatable.

Remark 2.5. In the literature the extra condition in terms of norms is classic, see for instance [37]. Other choices are also possible. For example, in [13] the authors use the condition of fixing the value of one of the coefficients. Again, we need that the extra constraint is differentiable in the Banach space considered. We also need that the condition given by the extra equation leads to a good preconditioning with (hopefully) not too large norm.

3 Invariance equations and formulation as a fixed point

In this section we reduce the existence of the dynamical objects to functional equations and show how to manipulate them in such a way that they are reduced to a constructive fixed point problem. The manipulations are largely formal (we ignore issues such as the domain of unbounded operators and assume invertibility when needed, etc). These are addressed when we specify the spaces.

Unstable manifolds attached to invariant objects, due to the dissipative character of the evolution equation (1), are finite dimensional. In this paper we present only the case of one-dimensional attached manifolds. To see how to deal with higher dimensional ones the reader should consult [10].

Along all the presentation of all the problems, we follow the notation in Subsection 2.1, we specify the operator F and the linear preconditioner M. If necessary, we discuss the nonlinear term $N_{\bar{u}}$.

3.1 Equilibrium points

In this section, we show how to use our framework to compute equilibrium points of an evolution equation. The example to keep in mind is that of a parabolic PDE. In this case, the equilibrium point is the solution of an elliptic PDE. There is an extensive literature on the a posteriori verification of solutions of elliptic PDE, notably for finite element discretizations (see e.g. [8, 53, 56, 58] and the references therein). The presentation in this section is more geared towards spectral discretizations, which is also used for the other objects we discuss later, and to obtain computer-assisted proofs in very smooth norms.

A function u is an equilibrium (time independent solution) of (1) if

$$F(u) = Lu + N(u) = 0. \tag{14}$$

In our applications, L is an elliptic operator, N is a nonlinear differential operator of smaller order than L, and $L^{-1}N$ is a compact operator when considered acting on appropriate spaces. Hence, the operator M considered in Subsection 2.1 is $-L^{-1}$. A discussion of suitable spaces appears in Section 4. If the operator is compact then finite dimensional approximations have a good chance of working.

In some cases, the operator L is not invertible but $L + \lambda I$ is (this happens for instance for elliptic operators and for most $\lambda \in \mathbb{C}$). Moreover, adding the parameter λ may be numerically advantageous even if L is invertible since the operator $MF + I$ may be more numerically stable, with $M = (L + \lambda I)^{-1}$. Indeed, $(L + \lambda I)^{-1}$ may be easier to reliably compute than L^{-1}.

In practical applications, further preconditioning by finite dimensional matrices may be advantageous. Specially when the operator $L^{-1}N$ is compact.

3.2 Traveling waves

Traveling waves are solutions of (1) of the form $u(x, t) = \phi(x - ct)$ (x can be n dimensional but the displacement c is one dimensional). Hence, to find a traveling wave (using that the operators L and N are time independent) we obtain an operator equation for c and ϕ of the form

$$c\phi' + L\phi + N(\phi) = 0. \tag{15}$$

This equation is underdetermined, since leaving c unmodified and shifting ϕ along x also gives a solution of (15). So we add the extra scalar condition $\langle \phi, \phi \rangle = 1$ to obtain the system of equations

$$F(\phi, c) = \begin{pmatrix} c\phi' + L\phi + N(\phi) \\ \langle \phi, \phi \rangle - 1 \end{pmatrix} = 0.$$

For this equation we obtain that the preconditioner is

$$M = \begin{pmatrix} (L + c\partial_x)^{-1} & 0 \\ 0 & 1 \end{pmatrix}.$$

Remark 3.1. In order to obtain a complete formulation, one should specify the space of functions to which the function ϕ belongs.

In practice, this method works only for periodic traveling waves. Clearly, Dirichlet boundary conditions or odd periodic conditions do not allow non-trivial traveling waves.

The problem of traveling waves on the whole line with conditions at infinity are not considered here. The study of these [63] is mathematically very challenging since the spectral properties of the linearization are difficult (e.g. one has continuous spectrum). Moreover, this study could be conducted as homoclinic orbits [52, 66].

Remark 3.2. When the space variable x is one-dimensional, the study of existence of traveling waves reduces to the study of periodic solutions of the one parameter family of differential equations

$$c\phi' + L\phi + N(\phi) = 0,$$

and hence ODE techniques can be applied.

3.3 Periodic orbits

Periodic orbits are solutions of equation (1) of the form $u(x,t) = u(x, t+T)$, with $T > 0$. The period T is also an unknown of the problem. To write down the functional equation (u, T) satisfy, we parametrize them by $v(x,\theta) = u(x, \frac{\theta}{a})$, obtaining

$$a\partial_\theta v = Lv + N(v), \tag{16}$$

where $0 \leq \theta \leq 2\pi$ and $v(x, \theta + 2\pi) = v(x, \theta)$.

Notice that the frequency a is now another unknown of the problem equivalent to T. Hence, we proceed again as in the traveling wave case and add an extra scalar equation. The most suitable one is fixing the phase of the parameterization.

More concretely, given an approximate solution $(\bar{a}, \bar{v})$ of equation (16), we look for a correction (α, w) satisfying the system of equations

$$F(\alpha, w) = \begin{pmatrix} (\bar{a}+\alpha)\partial_\theta(\bar{v}+w) - L(\bar{v}+w) - N(\bar{v}+w) \\ \langle \partial_\theta \bar{v}, w\rangle \end{pmatrix} = 0. \tag{17}$$

A good preconditioner for equation (17) is

$$M = \begin{pmatrix} (\bar{a}\partial_\theta - L)^{-1} & 0 \\ 0 & 1 \end{pmatrix}.$$

3.4 One dimensional manifolds attached to fixed points

Given a fixed point u_0 that satisfies equation (14), we are seeking a function $U(s,x)$ that satisfies

$$\lambda s \partial_s U(s,x) = LU(s,x) + N(U(s,x)), \tag{18}$$

where L and N are differential operators in x.

It is clear that if we find a solution that satisfies (18), then

$$u(t,x) = U(e^{\lambda t}, x) \tag{19}$$

satisfies the evolution equation (1).

We can think geometrically of U as providing a parameterization of a one dimensional manifold invariant under the semiflow. For each value of s, $U(s,\cdot)$ is a point in a function space. Hence, as s traces an interval, we obtain a line segment in the function space. The dynamics of the evolution equation (1) moves along the curve with exponential dynamics.

At first (18) may looks similar to equation (14) for functions of two variables. We can indeed write it as

$$\tilde{L}U + N(U) = 0$$

where $\tilde{L} = -\lambda s\partial_s + L$. Nevertheless, there are two important differences:

- We emphasize that in (18), the unknowns are both the (real) number λ and the function of two variables U.
- We also note that the equation (18) does not admit a unique solution. If (λ, U) is a solution of (18), and σ is any number, then (λ, U_σ), with $U_\sigma(s, x) = U(s\sigma, x)$, is also a solution of (18).

Despite the above important differences, we are able to reduce the problem to a fixed point problem, but we need some extra steps. Our first goal is to use the techniques already developed in Sections 2.3 and 3.1 to obtain approximate solutions of (18). In particular, we have to find λ. Then, we show how to start a fixed point algorithm based on these approximate solutions. See the following subsections for a discussion of the method.

More detailed and more general results along these lines appear in [9, 10, 22]. In particular, there are results for manifolds of dimension higher than one.

3.4.1 Approximate solutions of the parameterization equation up to first order

Proceeding heuristically for the moment, we seek U as a power series in s with coefficients which are functions of x

$$U(s, x) = \sum_{n\geq 0} u_n(x) s^n.$$

We also assume that the operator N is differentiable. Of course, all this needs to be verified later with the appropriate definitions of Banach spaces, but in this section, we just describe the numerical algorithm.

In a first step, we obtain that u_0 should satisfy the equilibrium equation (14) discussed in Section 3.1. In the second step, we obtain that the coefficient u_1 and λ satisfy

$$\lambda u_1 = L u_1 + DN(u_0) u_1. \tag{20}$$

Equation (20) is precisely an eigenvalue equation of the type discussed in Section 2.2. Picking an eigenvalue determines uniquely the manifold to be computed. While (20) determines λ uniquely, u_1 is only determined up to a multiple.

As it turns out, this choice of the multiple of the eigenvector corresponds to the non-uniqueness pointed out in Section 2.2. Once we fix the length of the eigenvector, the (local) uniqueness is settled. This can be used as a normalization to obtain uniqueness.

3.4.2 Approximate solutions of the parameterization equation to order higher than one

If we continue solving equation (18) to orders (in s) higher than one, we see that equating the coefficients of s^n on both sides of (18) we obtain

$$n\lambda u_n = (L + DN(u_0)) u_n + R_n(u_0, u_1, \dots, u_{n-1}), \tag{21}$$

where R_n is an expression (polynomial in $u_1, \dots, u_{n-1}$) which can be readily computed substituting the expansion already computed in the Taylor expansion of N. See [32] for a detailed exposition on the numerical aspects.

If

$$n\lambda \notin \mathrm{Spec}(L + DN(u_0)), \tag{22}$$

one can find u_n and proceed. On the other hand, if (22) fails and $n\lambda \in \mathrm{Spec}(L + DN(u_0))$, it is not hard to construct examples of non-linearities N for which the invariance equation (18) has no solution.

For the Kuramoto-Sivashinsky equation (2), the spectrum of $L + DN(u_0)$ accumulates to $-\infty$, hence a negative λ is rather problematic. On the other hand, positive λ are tractable because the spectrum of $L + DN(u_0)$ only contains a finite number of positive eigenvalues. In particular, the most unstable eigenvalue automatically satisfies the non-resonance condition (22).

3.4.3 Preconditioning the fixed point equation

Given the periodic orbit u_0 and the eigenpair (λ, u_1), we can write the functional equation (3) for the high order $s^2 g(x,s) = U(x,s) - u_0(x) - u_1(x)s$ as

$$F(g) = \lambda s \partial_s(u_0 + u_1 s + g s^2) - L(u_0 + u_1 s + g s^2) - N(u_0 + u_1 s + g s^2) = 0.$$

Then, we apply the existence theorems of Section 2 with the approximation of g computed using the method of Section 3.4.2 and with preconditioner

$$M = (\lambda s \partial_s - L)^{-1}.$$

Remark 3.3. As stated in Section 3.4.2, the existence of the parameterization of the invariant manifold depends on the absence of resonances in (22). This absence is equivalent to finding the operator B required in Theorem 2.2. In general, the proof of absence of resonances is a delicate question, since we should prove that $n\lambda$ does not accumulate in the spectrum. There are however easier cases, for instance in the case of the fast (strong) unstable manifold.

3.5 One dimensional invariant manifolds attached to periodic orbits

Similar to the case of invariant manifolds attached to fixed points, manifolds attached to periodic orbits are parameterized by $U(x,\theta,s) = u_0(x,\theta) + \sum_{n\geq 1} u_n(x,\theta)s^n$, where $u_0(x,\theta)$ is the parameterization of the periodic orbit, hence satisfying equation (16). The functional equation for $U(x,\theta,s)$ is

$$a\partial_\theta U(x,\theta,s) + \lambda s \partial_s U(x,\theta,s) = LU(x,\theta,s) + N(U(x,\theta,s)). \tag{23}$$

As in Section 3.4, the eigenpair (λ, u_1) satisfies a linear equation,

$$a\partial_\theta u_1 + \lambda u_1 = L u_1 + DN(u_0)u_1,$$

and it is solved as explained in Section 2.3.

Then, once the eigenpair (λ, u_1) is determined, the term $g(x,\theta,s) = \sum_{n\geq 2} u_n(x,\theta)s^{n-2}$ satisfies the functional equation

$$F(g) = a\partial_\theta(u_0 + u_1 s + g s^2) + \lambda s \partial_s(u_0 + u_1 s + g s^2) - L(u_0 + u_1 s + g s^2) - N(u_0 + u_1 s + g s^2) = 0.$$

This equation is then preconditioned by multiplying it by the linear operator

$$M = (a\partial_\theta + \lambda s \partial_s - L)^{-1}.$$

Again, we refer to [9, 10, 22] for results on higher dimensions in this case.

4 Functional analysis considerations

In this section we present some spaces which are useful to perform the analysis. The choice of spaces is dictated by the need to have effective estimates for the operators we are considering. We want to make explicit the considerations that lead to the choices and provide several elementary lemmas. There are other choices which are also possible which may be preferable if the considerations change. We also present some of these possible choices and, indeed present some of the shortcomings of the different choices.

In the exposition we consider the simplest case of functions of one variable. The case of functions of several variables can be reduced to this one by expanding the functions in Fourier (or Taylor) series with respect one of the variables and considering the coefficients of this expansion as functions of the other variables. This process is recursive and very easy to implement in computer languages which support overloading.

4.1 Choice of basis

We consider expansions in Fourier (or Taylor) series of eigenfunctions $\phi_n(x)$ of L. In practice Fourier series of functions satisfy the boundary and symmetry conditions. For our purposes these are useful when dealing with differential operators. Indeed, since the constant coefficients differential operators are diagonal it is easy to estimate truncations.

Recent years have witnessed several successful attempts in combining Fourier series with computer-assisted estimates to prove existence of solutions of finite and infinite dimensional dynamical systems. Rigorous results about periodic solutions of ODEs, delay equations and PDEs [3,4,35,44,71,73], dynamics of infinite dimensional maps [19,20], equilibria of PDEs [2,28–30,34,39] and global dynamics of parabolic PDEs [18,48] have been obtained using Fourier series. By now there are many efficient implemented algorithms handling Fourier series. In fact, there is specialized hardware (GPU) carrying out operations with Fourier coefficients. The main (well known) shortcoming of Fourier series is that they are not adaptive and that they are computationally hard if one is dealing with phenomena that present singularities or high oscillations in small regions of the phase space.

There is an extensive literature on the a posteriori verification of solutions of elliptic PDE, notably for finite element discretizations [1, 8, 11, 25, 38, 53, 55, 56, 58, 67]. Among them, methods involving rigorous enclosure of eigenvalues of nonlinear operators are used in [8,58] to prove existence of solutions of second-order elliptic boundary value problems. In [53, 54], a technique combining the Schauder fixed point theorem and a priori error estimates for finite element approximations in Sobolev spaces is applied to prove the existence of solutions of elliptic problems.

Splines interpolations have also led to rigorous existence results for PDEs [31], boundary value problems [69], connecting orbits [46, 46, 66] and localized solutions of reaction-diffusion PDEs [65].

There are, several works on theoretical estimates [14] or on numerical work with wavelets [68] but we are not aware of rigorous computer-assisted estimates.

Interpolation with Chebyshev polynomials has received a great deal of attention [57] and there are computer-assisted estimates [17, 47, 64]. Note that Chebyshev polynomials are closely related to Fourier series.

Taylor methods have led to rigorous integrators of flows of ODEs [5, 36, 49, 70] and rigorous enclosure of invariant manifolds [50–52] leading to effective computation of connecting orbits.

4.2 Choices of norms

We consider spaces of functions (indexed by the parameter μ)

$$u(x) = \sum a_n \phi_n(x)$$

with

$$\|u\|_\mu = \sum |a_n| W_n^\mu$$

for conveniently chosen weights W_n^μ. We say that this space is a *w*eigthed ℓ^1 norm.

There are several reasons to take weighted ℓ^1 spaces rather than other spaces such as weighted ℓ^2, which have interesting properties such as being a Hilbert space or other ℓ^p spaces, which have nice properties such as being reflexive Banach spaces.

- The norms can be evaluated more reliably in finite precision computation and in interval arithmetic than those involving higher powers.

  The main reason is that the round off is much more dramatic when we are adding modes of different sizes. Since the squares of numbers have a bigger spread of sizes than the numbers themselves, adding numbers is less affected by rounding than adding their squares.

- Sensitivity to round off is not the only numerical criterion. Note that while the ℓ^∞ norm is insensitive to the roundoff, it is insensitive to many changes in the function.

- It is easy to compute numerically the norm of an operator.

  As we see in (24), the norm of a matrix of size N can be estimated rigorously in N^2 operations. (The estimates are accurate up to round off).

- The space ℓ^1 is not reflexive, but at least its dual ℓ^∞ is explicit and rather manageable.

Some weights that we consider are of the form

$$W_n^{\mu_1,\mu_2} = (1+|n|)^{\mu_1} e^{\mu_2|n|}$$

for $\mu_1, \mu_2 \geq 0$. Note that the case $\mu_2 > 0$ automatically ensures analyticity of the solutions, while the case $\mu_1 > d$ ensures that the functions are C^d.

With these norms, operator norms are easy to compute. Given an operator T with coefficients $T_{n,m}$ associated to the base $\{\phi_n\}$, its norm is

$$\|T\|_{\mu\to\mu'} = \sup_m \frac{\sum_n |T_{n,m}| W_n^\mu}{W_m^{\mu'}}. \tag{24}$$

When the target space coincides with the definition space, we denote $\|T\|_{\mu\to\mu}$ by $\|T\|_\mu$.

Sometimes there is the need to compute the norm of the composition of two operators, let us say A and B, such that A is a compact operator and B is unbounded, but with AB bounded. Suppose that the norm of both operators can be computed but the norm of their composition cannot. Then, it is useful to use *the two spaces approach* appearing in [33]. This consists on bounding the norm $\|AB\|_\mu$ by the product of the norms $\|A\|_{\mu'\to\mu}$ and $\|B\|_{\mu\to\mu'}$.

Another space that we consider for the solutions

$$u(x) = \sum a_n \phi_n(x)$$

is ℓ^∞ with a weighted norm. More precisely, given a sequence $a = \{a_n\}_n$ and a decay rate $s > 1$, we define the norm

$$\|a\|_s = \sup_n \{|a_n| \omega_n^s\},$$

where the weight ω_n^s is defined by $\omega_{n_i}^{q_i}$, with

$$\omega_n^s = \begin{cases} 1, & \text{if } n = 0 \\ |n|^s, & \text{if } n \neq 0. \end{cases}$$

Using this norm we define the Banach space

$$X = \{a : \|a\|_s < \infty\},$$

of algebraically decaying sequences with decay rate s. The Banach space $(X, \|\cdot\|_s)$ with $s > 1$ is an algebra under discrete convolution, but it is not directly a Banach algebra. However, it is possible to use analytic estimates to obtain $C = C(s)$ such that $\|a * b\|_s \leq C(s)\|a\|_s\|b\|_s$ [7, 30]. With the new norm $\|\cdot\|_X = C(s)\|\cdot\|_s$, $(X, \|\cdot\|_X)$ is a Banach algebra under discrete convolutions.

5 Implementation of the verification method

In this section we present the general ideas for the implementation of the computer-assisted verification of the invariant objects, that is, how to solve in practice problem (3). Usually the need for proving the existence of an invariant object comes from the fact that there is evidence of its existence. This evidence could come from different sources. For example, some non-rigorous numerical computations, or heuristic perturbative arguments. Thus, we have an approximation of the object of interest and we want to give a rigorous proof of its existence. The main steps for the proof of the existence of these objects are the following:

- Compute a good approximation $\bar{u}$ of the invariant object, that is, an approximate solution of (3). The proof to be produced assures the existence of a nearby invariant object, with explicit estimates in terms of norms of how close it is to the approximation $\bar{u}$.

- Construct the preconditioned equation (4). The preconditioner M is problem dependent, so we should detect the operator L that must be preconditioned (M will be its inverse). As stated in all the cases, the inverse of this operator is easily stated, since it is expected that it has the form of $P(D_1, \cdots, D_n)$, where P is a polynomial with constant coefficients and D_i are differential operators of the form ∂_x, ∂_θ, and so on.

- Once the preconditioned equation (4) is constructed, we apply one of the fixed points Theorems 2.2 or 2.3. Choosing which one must be used is more a matter of taste. Both are equivalent and provide similar qualitative information about the fixed point.

- Finally, for the application of the fixed point theorem one must evaluate the quantities required in the theorems. These quantities are bounds on the error of the approximation $F(\bar{u})$, on the derivative of T and on the Lipschitz constant of the derivative of T around the approximation. The evaluation of these three quantities are problem dependent, and must be treated in a case by case basis.

In general, one must split the problem into two subproblems, a finite dimensional one and an infinite dimensional one. This splitting is done in accordance to how the functional equation deals with the finite dimensional part and the infinite dimensional part. The finite dimensional part is handled with the aid of a computer, while the infinite dimensional part must be dealt with by hand. Although a priori this may sound very challenging, this is actually a treatable problem. The action of the contraction operator on the modes of the infinite dimensional part can be managed since, hopefully, the linearization of the operator is compact. The choice of truncations seems to be different depending on the problem.

6 Concluding remarks

In this paper we present rather general methods for the computation and rigorous verification of several invariant objects arising in the study of PDEs. We specify the functional equations that these invariant objects must satisfy, and describe how them can be rigorously computed. All these functional equations have the property that the linearization around their zeros have a spectral gap around zero. This allows us to set up a contraction mapping problem that leads to the rigorous verification of the computed objects.

In two companion papers we present two different implementations of the method presented in this paper to rigorously verify the existence of time periodic orbits for the Kuramoto-Sivashinsky equation (2).

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