CONNECTING ORBITS IN NONLINEAR SYSTEMS

VICI grant proposal

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1 REGISTRATION FORM (BASIC DETAILS)

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1B Title of Research Proposal

Connecting Orbits in Nonlinear Systems

1C Summary of Research Proposal

Patterns are all around us: our fingerprints, the red spots typical for measles, the stripes on zebras, and the convection rolls in the atmosphere and oceans which shape our climate. It is a formidable challenge to understand and predict the large contrasts featured in these patterns. Much is known about how such patterns start to develop from a homogeneous state, but we are still unable to predict or analyze the features of fully developed patterns. These fascinating nonlinear problems require the integration of computations with topology.

Numerical simulation produces clear pictures of the dynamics, but the information it provides is local and non-rigorous, since in scientific computing one selects an approximate version of the problem, and computes on this prototype. The fundamental novelty of the proposed research lies in developing topological tools that unequivocally link the outcome of such calculations with the true problem. My goal is to create topologically validated computational machinery for finding the pivotal objects of interest in large amplitude pattern formation: the paths along which dynamical systems change from one state into another.

These connections play an organizing role. First, connecting orbits describe localized patterns such as pulses and boundary layers. Second, they act as building blocks from which more complicated, sometimes chaotic, patterns can be constructed. Third, the transitions between different patterns, and their emergence from a homogeneous background, are connections between structured and trivial equilibrium states.

Only an innovative combination of computational methods and topological techniques can provide results that are both sufficiently detailed and robust, validating predictions beyond the scope of simulations. The outcomes are then fully justified, which is vital for our aim of making rock-solid predictions about concrete models. This is the way forward in key evolution problems for finite and infinite dimensional dynamical systems, such as pattern formation phenomena.

1D Keywords

nonlinear dynamics
connecting orbits
computer-assisted calculations
topological techniques
pattern formation

1E Host Institution

VU University Amsterdam

1F NWO Division

EW (Physical sciences)

1G NWO Divisional Discipline

EW 03: Mathematics

1H NWO Domain

Beta
2 RESEARCH PROPOSAL

2A DESCRIPTION OF THE PROPOSED RESEARCH

CONNECTING ORBITS IN NONLINEAR SYSTEMS

I OBJECTIVES

I.1 INTRODUCTION

We recognize patterns everywhere. They appear in myriad shapes with bright contrasts, their structure changes and they occasionally vanish, the fundamental question being: how does one type of behaviour develop into another? The paths along which such changes occur are connecting orbits in an underlying nonlinear dynamical system. In their organizing role in pattern formation, connecting orbits are crucial for our understanding. On the one hand these connections are robust objects, while on the other hand they are very sparse in phase space, making them difficult to pin down.

By their very nature, connections require a global (geometric and topological) approach. Ideally this is coupled with numerical calculations, which offer clear pictures of the dynamics, but the information the numerics provide is local (in phase and parameter space) and non-rigorous. Strikingly, today’s advances in computer speed and algorithm development make it possible to utilize the power and robustness of topological methods to rigorously validate computational results. The current practice in scientific computing is to select a finite dimensional (i.e. approximate) version of the problem, and compute on this prototype. The fundamental novelty of our approach lies in developing topological tools that unequivocally link the outcome of such calculations with the true problem. My goal is to create

Topologically validated computational machinery for finding connecting orbits which are pivotal in global nonlinear dynamics and large amplitude patterns.

Patterns distinctly visualize the complexity of the dynamical systems that describe the evolution of general nonlinear processes. By Conley’s decomposition theorem [21], connecting orbits universally form the backbone of any nonlinear dynamical system. In the special case of gradient (i.e. dissipative) systems, all dynamics consists of connecting orbits going from one equilibrium state to another. General nonlinear dynamical systems are decomposed into “recurrent components” (e.g. periodic orbits, homoclinic loops, chaotic attractors) and “transient dynamics”: the orbits that evolve the system from one recurrent component to another [21]. The connecting orbit structure is thus essential for understanding the dynamics.

The topologically validated computational approach is stable under errors in parameter values, and provides precise information (e.g. about shape). The connections can thus be used as building blocks for understanding complicated dynamics, as ingredients for forcing theorems, and as seeds of topological information in Morse-Conley-Floer complexes. The combination of qualitative global analysis with quantitative information from topologically validated computations will establish a breakthrough. The resulting understanding of connecting orbit structures leads to novel insights in global evolutionary aspects of dynamical systems in general, and pattern formation in particular.

I.2 TOPOLOGY AND COMPUTATION

The state-of-the-art mathematical description of pattern formation is largely restricted to situations where either smallness of the pattern (bifurcation methods, normal forms), or separation of scales, can be exploited, sometimes rigorously (geometric singular perturbation theory, oscillatory integrals, justification of amplitude equations), often formally through matched asymptotic expansions. Those “asymptoteness” assumptions (e.g. separation of scales) are usually made to make the problem mathematically tractable, often without physical justification. Moreover, such an analysis is feasible only if the asymptotic problems are sufficiently simple, limiting its applicability considerably.

The objective of this proposal is to go far beyond the perturbative setting. Two complementary tools
Pattern formation

The transition from normal heartbeat to ventricular fibrillation is a potentially lethal phenomenon. Rather than contracting in a coordinated fashion, electric signals and contraction waves travel through the ventricular muscle in a seemingly chaotic fashion (due to “re-entry” of the waves), and the heart fails to pump blood into the arteries. The crucial issue is: how does the dynamical system (representing the spatio-temporal behaviour of the heart) move from one state (normal heartbeat) to another (re-entry)?

This is a seminal and extremely complicated instance of a transition between spatio-temporal patterns. We see such patterns and transitions everywhere around us in science and daily life, inspiring researchers in a diversity of fields: physics (e.g. crystal growth, turbulent flows), biology (e.g. neural activation patterns, animal skins) medicine (e.g. spiral waves in heart tissue), geology (e.g. curved rock layers, desert formation). The science of pattern formation revolves around finding common principles behind patterns from different contexts that look similar. In all these studies connecting orbits act as important centers of information for three reasons.

First, we often observe very localized patterns, such as light pulses (solitons) and cell walls (lipid bi-layers). In the appropriate dynamical system setting these correspond to connecting orbits; homoclinic if a homogeneous state is the backdrop for a local pattern, heteroclinic when it concerns the boundary between two different states.

Second, when there are localized patterns, one often observes a great variety of combinations of such “simple” patterns (e.g. multiple pulses, polycrystalline materials, many patches of vegetation). Understanding these more complicated patterns thus requires two steps: analyzing the individual building block patterns, as well as understanding the “rules” governing the combinatorics of the building blocks.

Third, many patterns are not static but evolving. Usually a system stays in one configuration for a long time and then transits to another. For example, the heart beats regularly for years until it suddenly transfers to a fibrillating state. More generally, spatial patterns may be invaded by energetically more favorable ones. In particular, the initial emergence of a pattern from a pristine background state is such a transition. These temporal transitions between (spatially) different states are precisely what connecting orbits in dynamical systems describe. When the limiting states are spatially homogeneous (e.g. one species completely eradicating another), then these dynamical systems are relatively gentle ordinary differential equations (ODEs). When the spatio-temporal behaviour concerns transitions between truly spatial patterns (periodic or otherwise), then the dynamical system, usually a partial differential equation (PDE), is set in an infinite dimensional space.

In summary, in pattern formation connections both form the patterns and organize their structure.

assist in extrapolating the results from an asymptotic analysis towards large amplitudes, namely numerical simulations and topological/variational techniques. While the reliability of conclusions based on computer simulations is often hard to judge, topological techniques usually provide little qualitative information besides mere existence of solutions. In the best cases one can determine the fixed points of the vectorfield and their linearization. This local behaviour near equilibria tells us only a very limited part of the story: global dynamics is out of reach of direct analysis except in some special low dimensional cases.

With the computational techniques in this proposal we will be able to probe the global dynamics of the vectorfield to a significantly deeper level, including in particular the connections between equilibria, and more generally between sets with recurrent dynamics (such as periodic orbits). Once we get our hands on these connecting orbits, we can draw refined conclusions about the global dynamics, decide on chaoticity, etc. To achieve this we need topologically validated computations: the vast amount of
calculations necessitates computer assistance, while topological validation rigorously controls the errors due to discretization, truncation and rounding, so that spurious solutions are avoided.

There are two major components to this proposal. First, to develop a flexible topologically validated computational method for rigorously establishing connecting orbits. This gives the global dynamics of specific orbits. While this is often important in its own right, it also raises a second fundamental question: what does this tell us about the global dynamics of the entire system? The answer lies in forcing techniques, either based on (analytical) gluing methods or on (topological) Morse-Conley-Floer theory (see page 6).

The timeliness of this undertaking is not rooted in present-day computer speed alone. The computational approach at the center of this proposal is based on recent ideas in my work with Lessard and Mischaikow on stationary (periodic) patterns [8, 9]. We have developed a computational scheme where the patterns are obtained as zeros of a nonlinear map in some (infinite dimensional) function space. This is then translated into a fixed point problem. In a neighborhood of an approximate fixed point we prove that a Newton-like operator is contracting, and the uniform contraction rate allows us to control rigorously the errors due to computational approximations that we inevitably make. Since the contraction mapping principle is an “analysis-style” fixed point theorem, this requires a major analytic effort. Indeed, the Banach fixed point theorem lies on the crossroads of analysis and topology, and we call this rigorous error control the topological validation step.

The work with Lessard and Mischaikow is just the beginning, showing that the ideas can be effectuated. Now we must combine them with more elaborate tools to address connecting orbits, which are analytically much more elusive. With the novel ideas put forward in this proposal, the time is right for a first full scale topological computational theory for connecting orbit problems, which is applicable to nonlinear systems in pattern formation and beyond.

I.3 Principal Example

To illustrate the computational approach, the associated analytic estimates, and some topological aspects, we present an example related to periodic orbits, which allows us to focus on the main ideas and tie the principal ingredients together. The Swift-Hohenberg PDE

$$\frac{\partial u}{\partial t} = -\left(\frac{\partial^2}{\partial x^2} + 1\right)^2 u + \alpha u - u^3$$

is a paradigm in pattern formation science. When heating from below a fluid between two plates, a finite wavelength instability leads to the occurrence of so-called Rayleigh-Bénard convection rolls. The profile $u$, which depends on space $x$ and time $t$, describes the size of convection rolls, and the parameter $\alpha$ indicates the magnitude of the driving force (the temperature difference between the bottom and top). When considering stationary patterns, this reduces to the ODE

$$u''' + 2u'' + (1 - \alpha)u + u^3 = 0,$$

interpreted as a dynamical system in four dimensional phase space. Below we discuss how computation and topology can be combined to prove that the “spatial” dynamics of (2) is chaotic. Taking advantage of the associated variational framework, we can prove that all these stationary profiles of (1) are dynamically stable under physical perturbations [8, 10]. In particular, we infer that when the temperature difference in a Rayleigh-Bénard cell is sufficiently large, then there are many different attractors, all corresponding to geometrically different velocity profiles.

Our approach only requires proving the existence of a single periodic solution, which then by Morse theory arguments, based on an underlying variational principle that we have developed [10, 35], implies chaoticity of the Swift-Hohenberg ODE, schematically [8]:

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$$\Rightarrow \text{chaos.}$$
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The topological forcing theorem can be viewed as a counterpart for fourth order ODEs of the famous
**Global topology and dynamics: Morse-Conley-Floer theory**

Morse theory relates the topology of a closed manifold $X$ with the critical points of a function $\mathcal{F}$ on $X$. This relation involves the Morse index $\mu(\hat{x})$ of critical points $\hat{x}$, i.e., the dimension of the unstable manifold of $\hat{x}$ (or the number of negative eigenvalues of the Hessian $D^2\mathcal{F}(\hat{x})$) under the gradient flow

$$\frac{dx}{dt} = -\nabla\mathcal{F}(x).$$

Let $b_k$ be the $k$-th Betti number of $X$ (characterizing part of its topology), and let $c_k$ be the number of critical points of $\mathcal{F}$ with Morse index $k$. In the generic case (all critical points being nondegenerate) these sequences $b_k$ and $c_k$ must satisfy the Morse inequalities

$$\sum_{k=0}^{\infty} (-1)^{m-k}b_k \leq \sum_{k=0}^{\infty} (-1)^{m-k}c_k, \quad \text{for any } m = 0, 1, 2, \ldots.$$

This implies, among others, that the number of critical points of any function $\mathcal{F}$ on $X$ is bounded below by the sum of the Betti numbers, at least in the generic case (the general statement is only slightly weaker). Another informative way to describe the Morse inequalities is as follows:

$$\sum_{k=0}^{\infty} b_k t^k = \sum_{k=0}^{\infty} c_k t^k - (1+t) \sum_{k=0}^{\infty} q_k t^k, \quad \text{for all } t \in \mathbb{R},$$

where $q_k \geq 0$ is a lower bound on the number of connecting orbits of the gradient flow between a critical point of index $k+1$ and one of index $k$. We conclude that Morse theory provides information about the number of critical points and connecting orbits of a gradient system. For example, for the depicted (deformed) torus, which has Betti numbers $b_0 = 1$, $b_1 = 2$, $b_2 = 1$, the six critical points force the existence of at least one connecting orbit (this is a minimal scenario; there happen to be more in this particular picture).

The relation between critical points, connecting orbits and the (global) topology becomes even stronger, supplying more detailed information, when we consider the Morse-Floer homology. This algebraic topological invariant can be constructed even for strongly indefinite variational problems, which are characterized by the property that all critical points have infinite Morse index $\mu$. These types of problems are commonplace in pattern formation (cf. §II.3 and §II.4). In essence, Floer’s approach resolves this issue by defining a relative index $\mu_{rel}$.

The Morse-Floer homology intricately encodes information about critical points and connecting orbits for gradient flows. The Conley index is a topological generalization of Morse theory that is applicable to arbitrary (non-gradient-like) dynamics, and it relates the flow on (the boundary of) isolating neighborhoods with the topology of their invariant sets. Morse-Conley-Floer theory forms a set of techniques for unveiling global topological information about invariant sets of the dynamics. The theory is strong on general statements about minimal scenarios, but it comes up short in providing precise data for concrete dynamical systems. In this proposal, computational methods are combined with Morse-Conley-Floer theory to get the best of both worlds.

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“period-3 implies chaos” result for interval maps [49]. The variational nature of the problem causes solutions of (2) to conserve the energy

$$E = u'' u - \frac{1}{2} u u^2 + u^2 - \frac{\alpha - 1}{2} u^2 + \frac{1}{4} u^4 + \frac{(\alpha - 1)^2}{4}.$$  

To force chaos we need to find a single periodic solution with energy $E = 0$ and shape as depicted in (3).

In the remainder of this section we focus on the topologically validated computational approach for finding concrete orbits in dynamical systems, which is at the heart of the current proposal. Since in this example we are looking for a periodic solution, we apply a Fourier transformation. Let $\frac{2\pi}{P}$ be the a priori unknown period of the solution that we want to find. Taking advantage of the left-right symmetry of the
problem, we write $u$ as

$$u(y) = a_0 + 2 \sum_{k=1}^{\infty} a_k \cos(kLy).$$  \hfill(4)

This reduces the ODE (2) to an infinite set of algebraic equations for the Fourier coefficients $\{a_k\}$, where $a_{-k} \equiv a_k$:

$$g_k \overset{\text{def}}{=} \left[ L^4 k^4 - 2L^2 k^2 + (1 - \alpha) \right] a_k + \sum_{k_1 + k_2 + k_3 = k} a_{k_1} a_{k_2} a_{k_3} = 0, \quad \text{for all } k \geq 0.$$

The energy constraint $E = 0$ can be (re)written as

$$e \overset{\text{def}}{=} 2^{3/2} L^2 \sum_{k=1}^{\infty} k^2 a_k + \left[ a_0 + 2 \sum_{k=1}^{\infty} a_k \right]^2 - \alpha + 1 = 0.$$

With the notation $x = (L, a_0, a_1, a_2, \ldots)$ for the unknowns and $f(x) = (e, g_0, g_1, g_2, \ldots)$ for the equations, we are thus looking for a solution of the infinite set of equations $f(x) = 0$, and we have arrived at the stage of the analysis where the specifics of the original problem are no longer visible.

We define the finite dimensional truncations $x_F = (L, a_0, \cdots, a_{m-1}, 0, 0, 0, \ldots)$, and the Galerkin projection

$$f_F(x_F) \overset{\text{def}}{=} \begin{bmatrix} e(x_F) \\ g_F(x_F) \end{bmatrix},$$

where $g_F$ denotes the first $m$ components of $g$. Note that $f_F$ has both a finitely truncated domain and a finitely truncated co-domain. A numerical solution $\bar{x}_F = (\bar{L}, \bar{a}_0, \bar{a}_1, \cdots, \bar{a}_{m-1}, 0, 0, 0, \ldots)$ of $f_F(\bar{x}_F) \approx 0$ is found via standard iteration methods.

Crucially, we now need to add a topological validation step (see [24, 8]) to turn this into a mathematically rigorous proof. We stress that not the interval arithmetic, although necessary and computationally time consuming, but the analytic error estimates due to the finite dimensional reduction, are the crux of the problem.

Let the $(m+1) \times (m+1)$ matrix $J_F$ be the numerically computed inverse of the derivative $Df_F(\bar{x}_F)$. We define the “linear part” of $g_k$ as $\lambda_k(L) = L^4 k^4 - 2L^2 k^2 + (1 - \alpha)$. Using these we define the linear operator on sequence spaces

$$A \overset{\text{def}}{=} \begin{bmatrix} J_F & 0 & 0 & 0 & \cdots \\ 0 & \lambda_m(\bar{L})^{-1} & 0 & 0 & \cdots \\ 0 & 0 & \lambda_{m+1}(\bar{L})^{-1} & 0 & \cdots \\ 0 & 0 & 0 & \lambda_{m+2}(\bar{L})^{-1} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$

which acts as an approximate inverse of the linear operator $Df(\bar{x}_F)$. Finally, to lift the finite dimensional computation to the infinite setting of our original problem, we consider the operator

$$T(x) \overset{\text{def}}{=} x - A \cdot f(x),$$

which is reminiscent of a Newton operator. Via rigorous estimates on the remainder terms we show that $T$ is a contraction map on a small ball $B$ around $\bar{x}_F$ in an appropriate Banach space. The (unique) fixed point of $T$ in $B$ solves $f(x) = 0$.

More precisely, we use a weighted $\ell_\infty$-norm ($s > 1$)

$$\|x\|_s = \sup\{ |L|, |a_0|, |a_1|, 2^s|a_2|, 3^s|a_3|, 4^s|a_4|, \ldots \}.$$ 

The weights ensure that the Fourier coefficients decay algebraically for all sequences in the associated Banach space, in accordance with the smoothness of solutions to (2). The ball of radius $r$ centered at $\bar{x}_F$ is

$$B_{\bar{x}_F}(r) \overset{\text{def}}{=} \bar{x}_F + \prod_{k=-1}^{\infty} \left[ -\frac{r}{|k|^s}, \frac{r}{|k|^s} \right], \quad (0^r \overset{\text{def}}{=} 1).$$

We look for fixed points of $T$ by showing that $T$ is a contraction mapping on these balls. Indeed, the unique fixed point $\bar{x}$, that results from the Banach contraction mapping theorem, satisfies $f(\bar{x}) = 0$ and thus corresponds via (4) to a periodic solution of the ODE (2).
For the operator $T$ to be contracting, the radius of the ball $B_{r_k}(r)$ should not be too small (larger than the distance between the approximate solution $\tilde{x}_F$ and the true solution $\tilde{x}$), but also not too large (otherwise uniqueness is lost and the estimates will fail). Analytically, we need the estimates

$$
\sup_{w;\tilde{w} \in B_r(r)} |T(\tilde{x}_F) - \tilde{x}_F| \leq C_k,
$$

where $C_k \geq 0$ are explicit constants and $\tilde{C}_k(r)$ are explicit (fifth order) polynomials in $r$ (with positive coefficients). It turns out that for sufficiently large $k$, say $k \geq M$,

$$
C_k = 0, \quad \text{and} \quad \tilde{C}_k(r) = \left(\frac{M}{k}\right)^s \tilde{C}_M(r).
$$

This uniform estimate enables us [8] to reduce the problem of showing that $T$ is a contraction to merely checking a finite set of polynomial inequalities of the form

$$
P_k(r) \overset{\text{def}}{=} C_k + \tilde{C}_k(r) - \frac{r}{|k|^s} < 0 \quad \text{for } k = -1, 0, 1, \ldots, M. \quad (6)
$$

Cumbersome if not impractical to check by hand, this is easily done using interval arithmetic on a computer. Applying the forcing result (3) then leads to the results about convection patterns discussed at the start of this section.

I.4 STATE-OF-THE-ART

Equilibria, periodic orbits, connecting orbits and more generally invariant manifolds are the fundamental components through which much of the structure of the dynamics of nonlinear differential equations is explained. There is a vast literature on simulation techniques for approximating these objects. Particularly, the last thirty years have witnessed a strong interest in developing numerical methods for connecting orbits [18, 17, 32, 47]. As mentioned in [26], most algorithms for computing heteroclinic or homoclinic orbits reduce the question to numerically solving a boundary value problem on a finite interval, where the boundary conditions are given in terms of linear or higher order approximations of invariant manifolds near the steady states.

This proposal builds on the continuing progress in scientific computing. On the other hand, the veracity of the numerical results can typically not be faithfully established, and we need to overcome this obstacle. The field of rigorous numerics (using interval arithmetic) has made a lasting impact in dynamical systems, by extracting coarse topological information from the systems, often revealing complicated dynamics. Particularly, the proof that the Lorenz attractor is chaotic [64, 53] was an essential breakthrough. In recent years there has been remarkable progress in computational methods, fueled by both computer speed and the development of novel algorithms. Advances have been most rapid in the analysis of maps, i.e., dynamical systems with discrete time, which by their very nature are more receptive to computational techniques, see e.g. [1, 23]. In parallel, the underlying theory has significantly progressed, especially concerning the combinatorial approach to Conley index computations [42].

In the last years a variety of authors have developed tools, combining interval arithmetic with topological constructions, to prove the existence of homoclinic and heteroclinic solutions for specific ordinary differential equations. One effective approach uses advanced ODE integrators and interval arithmetic to investigate the images of rigorously integrated sets on a collection of Poincaré sections, and derive results from the topological information thus obtained through Conley index arguments (e.g. [65, 46, 2]). Other successful methods are based on the Melnikov function to detect intersections of stable and unstable manifolds [39], and functional analytic arguments combined with spectral estimates [13].

The current proposal selects another strategy, which is most amenable to the problems originating from pattern formation (high or infinite dimensional, dependence on physical parameters), and which most closely matches the developments in scientific computing. Our approach, see §I.3, has been shown to work for periodic solutions in [8, 22, 24], while some of the ideas go back to [68, 56]. Recently, we have refined the analytic estimates considerably, which enables us to solve more delicate problems (see Section I.3.
for an overview and [8] for details), including periodic solutions in multiple dimensions [33] and delay equations [48]. Besides, we have shown how this method can be adapted to encompass rigorous parameter continuation and branch following [9], so that we can track families of solutions. These developments form the ideal platform for taking the next leap and tackling the important and elusive connecting orbits.

The current proposal builds on the state of the art and introduces the following innovative features:

1. Novel rigorous combination of topologically validated computational techniques with (approximate) parametrizations of local stable and unstable manifolds. Since the topologically validated computational machinery is rooted in a functional analytic framework, it is scalable and hence ideally suited for extension to infinite dimensional problems, such as connections in pattern forming PDE models.

2. Focus on pivotal solutions of continuous time dynamical systems, namely ordinary and partial differential equations. This emphasis on continuous time problems is essential, since differential equations are by far the most utilized type of mathematical models in physics, chemistry, biology, medicine and economy.

3. The topologically validated computational approach is robust under errors in physical parameter values, and provides precise quantitative (e.g. the shape) as well as qualitative (e.g. stability) information about the connecting orbits.

4. Since topological validation leads to rigorous existence results, the connecting orbits can be used as new seeds of information in Morse-Conley-Floer theory, leading to forcing theorems and insight in the global structure of the nonlinear dynamics.

II METHODOLOGY

The topologically validated computational technique described in §I.3 for periodic solutions, must be overhauled for the purpose of finding connecting orbits. Let us outline the main issues, focussing on connecting orbits for systems of coupled second order ODEs

\[ \frac{d^2 \tilde{u}}{dx^2} = \Psi(\tilde{u}), \]  

(7)

where \( \tilde{u} \in \mathbb{R}^n \), and \( \Psi : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is a smooth nonlinearity. Such systems are ubiquitous in reaction-diffusion problems in chemistry and biology, and a plethora of patterns is found in such models. Reaction-diffusion processes are connected to morphogenesis in biology, as well as at the basis of animal coats and skin pigmentation [54, 51]. They are thus ideal for pilot studies, and we have implemented successfully the main ideas to demonstrate “proof of concept”, taking several shortcuts available for a test problem.

For the sake of clarity (both for exposition and to avoid technicalities) we assume the symmetry condition \( \tilde{u}(0) = 0 \), i.e., we look for symmetric homoclinic orbits, corresponding to left-right symmetric localized patterns, which satisfy the asymptotic “boundary” conditions

\[ \lim_{x \to \pm \infty} \tilde{u}(x) = \tilde{u}_\infty \in \mathbb{R}^n. \]

Let \( \psi = (\tilde{u}, \Psi(\tilde{u})) \) be the vectorfield in \( 2n \)-dimensional phase space corresponding to (7). We assume that the limit point \( p = (\tilde{u}_\infty, 0) \in \mathbb{R}^{2n} \) is a hyperbolic equilibrium with a stable manifold \( W^s(p) \) of dimension \( n \) (reversal symmetry implies the unstable manifold is also \( n \)-dimensional). Hence, a symmetric connecting orbit corresponds to a solution of the boundary value problem (L large)

\[
\begin{cases}
\tilde{u}''(x) = \Psi(\tilde{u}(x)), & \text{in } [0,L], \\
\tilde{u}(0) = 0, \\
(\tilde{u}(L), \tilde{u}'(L)) \in W^s_{\text{loc}}(p).
\end{cases}
\]  

(8)

Before furnishing a finite dimensional reduction necessary for a computational approach, we consider the description of the stable manifold \( W^s(p) \). One can obtain rigorous approximations of the stable manifold in a variety of ways, such as the topological construction in [70]. We make use of the parameterization method for invariant manifolds, which facilitates efficient, high order approximations of local stable and
unstable manifolds. The theoretical developments of these parametrizations [14, 15, 16] have led to numerics for discrete time maps [41]. In this project we pioneer the computational algorithms for continuous time flows, including rigorous control in the form of explicit and sufficiently sharp error estimates.

Let us assume the linearization $D\Psi$ of the vectorfield at the equilibrium $p$ has $n$ distinct eigenvalues $\{\lambda_i\}_{i=1}^n$ with strictly negative real part, with $\{v_i\}_{i=1}^n$ the associated eigenvectors. Let $\Lambda_0$ be the $n \times n$ diagonal matrix having $\{\lambda_i\}$ on the diagonal, and $A_0$ be the $2n \times n$ matrix whose columns are the stable eigenvectors $\{v_i\}$. The parameterization method provides an injection $\mathcal{P}: B_\delta(0) \subset \mathbb{R}^n \to \mathbb{R}^{2n}$, $\delta > 0$, such that $\mathcal{P}(0) = p$, $D\mathcal{P}(0) = A_0$, and $\mathcal{P}(B_\delta(0)) \subset W^s(p)$, i.e., it parametrizes the $n$-dimensional local stable manifold of $p$. We express $\mathcal{P}$ as a power series

$$\mathcal{P}(\theta) = \sum_{|\kappa| \geq 0} a_\kappa \theta^\kappa,$$

where $\kappa$ is a multi-index, and the coefficients $a_\kappa$ are determined recursively through the requirement that $\mathcal{P}$ satisfies the invariance equation $\Psi(\mathcal{P}(\theta)) = D\mathcal{P}(\theta) \Lambda_0 \theta$.

Writing $\mathcal{P} = (\mathcal{P}^{(0)}, \mathcal{P}^{(1)})$, problem (8) corresponds to finding a solution $(\theta, \bar{u}) \in \mathbb{R}^n \times C^2([0, L])^n$ of

$$\begin{cases}
\bar{u}''(x) = \Psi(\bar{u}(x)), & \text{in } [0, L],
\bar{u}(0) = 0,
\bar{u}(L) = \mathcal{P}^{(0)}(\theta), \quad \bar{u}'(L) = \mathcal{P}^{(1)}(\theta).
\end{cases}$$

Integrating the differential equation once from the left and once from the right we obtain the integral equation

$$\bar{u}(x) = f(\theta, \bar{u})(x) \triangleq \mathcal{P}^{(0)}(\theta) + (x - L) \int_0^x \Psi(\bar{u}(s)) ds + \int_x^L (s - L) \Psi(\bar{u}(s)) ds.$$

Finally, appending the remaining boundary condition, one defines $F: \mathbb{R}^n \times C([0, L])^n \to \mathbb{R}^n \times C([0, L])^n$ by

$$F(\theta, \bar{u}) \triangleq \begin{pmatrix}
\mathcal{P}^{(1)}(\theta) - \int_0^L \Psi(\bar{u}(s)) ds
\hline
f(\theta, \bar{u}) - \bar{u}
\end{pmatrix}.$$

Solutions of $F(\theta, \bar{u}) = 0$ then correspond to symmetric homoclinic solutions of (7).

For the periodic solutions in §3.3 it was suitable to use Fourier transformation and truncation of the series to obtain a finite dimensional reduction. Here we need a different strategy, as the Fourier series converge too slowly, and we select an approach naturally adapted from scientific computing. We begin by choosing a mesh $\{x_i = i h\}_{i=0}^m$ of the interval $[0, L]$ $(h = L/m)$. Consider the subset $S_h \subset C([0, L])$ of piecewise linear continuous functions with nodes at $\{x_i\}$. One can identify $S_h$ and $\mathbb{R}^{m+1}$. Given $v \in C([0, L])$ define $\Pi_h v = (v_0, v_1, \ldots, v_m) \in S_h$ by $v_i = v(x_i)$, for $i = 0, \ldots, m$. We denote by $u_h = (\Pi_h)^n \bar{u}$ the component-wise piecewise linear projection.

Choosing a parameterization order $N \in \mathbb{N}$, we let

$$\mathcal{P}_N(\theta) = \left(\mathcal{P}_N^{(0)}(\theta), \mathcal{P}_N^{(1)}(\theta)\right) \triangleq \sum_{0 \leq |\kappa| \leq N} a_\kappa \theta^\kappa.$$

The finite dimensional projection $F^{(m,N)}: \mathbb{R}^n \times (S_h)^n \to \mathbb{R}^n \times (S_h)^n$ of (10) is

$$F^{(m,N)}(\theta, u_h) = \begin{pmatrix}
\mathcal{P}_N^{(1)}(\theta) - \int_0^L \Psi(u_h(s)) ds
\hline
f^{(m,N)}(\theta, u_h) - u_h
\end{pmatrix},$$

where each $f_i^{(m,N)}(\theta, u_h)$, $i = 1, \ldots, n$, is given by

$$[f_i^{(m,N)}(\theta, u_h)]_j = [\mathcal{P}_N^{(0)}(\theta)]_i + (x_j - L) \int_0^{x_j} \Psi_i(u_h(s)) ds + \int_{x_j}^L (s - L) \Psi_i(u_h(s)) ds.$$

Analogous to the setup for periodic solutions, we have the full infinite dimensional problem $F(\theta, \bar{u}) = 0$ and a finite dimensional approximation $F^{(m,N)}(\theta, u_h) = 0$ side by side. Analytic techniques are needed to estimate the defect between the two. For the integral equation component these estimates turn out to be more tractable than for the truncated Fourier series, whereas the components involving the finite truncation
of the parametrization of the local stable manifold are much more involved, but they can in this setting be accomplished using techniques from complex analysis [7].

With this outline of a topologically validated computational approach to connecting orbits as a basis, we next describe four (interconnected) research problems which form the nuclei of PhD and Postdoc projects. They require a combination of techniques from both ODE and PDE theory, substantial computational implementation and algorithm development, as well as advances in their underlying foundational theory. As such, the subprojects will give ample opportunity for the PhD students and Postdocs involved to develop their skills, learn new techniques, and make seminal contributions to dynamical systems theory and the mathematics of pattern formation.

While the nature of exploratory research implies that one cannot foresee all obstacles or provide a very detailed workplan, we nevertheless outline the main ideas in each project. Furthermore, we indicate applications to pattern formation problems throughout.

II.1 CONNECTIONS IN SYSTEMS OF ODES

The first subproject concerns developing efficient algorithms for topologically validated computations of connecting orbits in general systems of ordinary differential equations. We have implemented the main ideas described above for a test problem [7]. However, the current approach is “quick-and-dirty”, taking full advantage of the specifics of the problem. In the seminal steps towards a general method for systems of ODEs, it is crucial to monitor computational efficiency. We will capitalize on prevalent simulation methods from scientific computing (cf. [27, 59]).

**Goal:** Develop a general framework for topologically validated computations of connecting orbits in systems of nonlinear ODEs.

For the general system \( u' = \varphi(u) \) with \( u \in \mathbb{R}^n \), an integral formulation is readily available: \( u(t) = u(0) + \int_0^t \varphi(u(s)) \, ds \). By approximating \( u \) by piecewise linear functions, we may again discretize. Note that the method is very flexible: higher degree splines and refined grid choices, both standard practice in scientific computing, are painless incorporated. Furthermore, in this integral formulation the errors accumulate disproportionally at the right end of the interval, hence it is better to divide the interval into subintervals and discretize the equivalent system \( u(t) = u(\tau) - \int_\tau^t \varphi(u(s)) \, ds = 0 \) for \( t \in (\tau_i, \tau_{i+1}], \; i = 1, \ldots, \ell \).

The parametrization of general stable and unstable manifolds, as well as the associated required analytic bounds, need careful scrutiny, aiming for estimates that are sufficiently sharp to satisfy computational requirements. There is a foundation of theoretical work to build on here [14, 15, 16]. For high dimensional manifolds it is not practical to parametrize the entire (un)stable manifold. Instead, parametrizations and approximations of lower dimensional slowly invariant manifolds will be needed. Namely, connecting orbits generically enter the equilibrium along the eigendirection corresponding to the leading eigenvalue, or the next-leading one in case of an orbit-flip configuration [40]. The parametrization estimates thus may be restricted to those directions, with special care for the role of resonances between eigenvalues [14, 16].

We aim for a generally applicable (and available) code. Indeed, there are many problems where the question of existence of connecting orbits is an obstacle to the full analysis of the problem, since even in low dimensional normal form systems the relevant solutions are often intractable analytically (e.g. [38]). Our approach will lead to a breakthrough. Transitions described by connecting orbits appear for example in reaction-diffusion models in developmental biology [36], chemical reactions [37] and desert formation [45]. One instance of a seminal application to pattern formation in fluid dynamics is the balance between hexagonal and stripe patterns [28]. For a modified version of the Swift-Hohenberg equation with an up-down symmetry breaking term, an asymptotic analysis was performed for patterns just above the onset of the instability of the trivial state. Transitions between stripes and hexagons were found to be governed by the system of second order equations [28]

\[
\begin{align*}
A'' + &\text{cA}' + A_1 b_1 A_1 - b_2 A_1^2 - 3 A_1^3 - 12 A_1 A_2^2 = 0, \\
A'' + &\text{cA}' + A_1 b_1 A_2 - b_2 A_1 A_2 - 9 A_2^3 - 6 A_1 A_2^2 = 0.
\end{align*}
\]
Here $A_1$ and $A_2$ are the amplitudes of stripe and hexagonal patterns, $c$ is the invasion speed of the pattern, and $b_1$ and $b_2$ are parameters measuring the distance to the onset of instability and the extent of symmetry breaking, respectively. Starting with the case of co-existence ($c = 0$) we will apply the developed methods to prove the existence of (moving) boundary layers between the two patterns.

A supplementary fundamental avenue that needs exploration is to incorporate symmetries inherent to many prototypical pattern forming systems, which requires an adapted strategy to accomplish the necessary topological robustness. For example, in (11) the case with zero propagation speed is Hamiltonian. Such a variational symmetry, shared with many other pattern forming systems (e.g. Equation (2)), causes non-genericity of the dynamics. For periodic solutions it means that they come in families (hence the additional requirement $E = 0$ in §I.3), while for connecting orbits the intersection of stable and unstable manifolds is nontransversal. Our customary method demands transversal intersections, and we will use unfoldings and phase conditions (cf. [18]) to handle the nontransversality caused by the symmetries fundamental to many pattern forming systems.

Another generalization concerns connecting orbits between periodic orbits rather than between equilibria. In the context of differential equations one of the simplest and best understood means of “generating” chaotic dynamics is through solutions that are homoclinic to periodic orbits. There are two fundamental prerequisites to obtain results on connections between periodic orbits. First, one must be able to rigorously and accurately identify periodic orbits. The method presented in §I.3 has proven effective for this task [48, 8]. Second, one must be able to parameterize stable and unstable manifolds for the periodic orbits. In principle there is no obstacle to the parameterization method being employed [16], and we intend to instigate an algorithmic implementation suitable for topological validation.

II.2 FAMILIES OF CONNECTIONS AND BUILDING BLOCKS

Establishing connecting orbits through topologically validated computations is just the first step. In this subproject we examine their dynamically relevant properties.

**Goal:** Use connecting orbits as building blocks for complicated patterns.

The first step is to study the dependence on parameters. Most physical models have parameters and one needs to be able to investigate the dynamics over large ranges of parameter values. Thus, the ability to efficiently and rigorously compute branches of solutions is highly desirable. For example, consider the dependence of the Swift-Hohenberg (2) on the parameter $\alpha$, so that (after Fourier transforming) we need to solve $f(x, \alpha) = 0$ for an interval of parameter values $\alpha$, cf. §I.3. Under the assumption that $D_2f(x, \alpha)$ is nonsingular along the branch of zeros that we are computing, the Implicit Function Theorem implies that the branch of zeros can be viewed globally as the graph of a function of the parameter $\alpha$. In an implementation, when computing on the finite dimensional reduction $f_F(x_F, \alpha) = 0$, we first compute an approximate zero $\overline{x}_F$ at a fixed value $\alpha = \alpha_0$. Next, we compute a vector $\dot{x}_F$ tangent to the solution graph:

$$D_1f(x_F, \alpha_0)\dot{x}_F + D_2f(x_F, \alpha_0) \approx 0.$$  

Using the vectors $x_F$ and $\dot{x}_F$, we define the set of predictors by $x_\alpha = x_F + \Delta_\alpha \dot{x}_F$, where $\Delta_\alpha = \alpha - \alpha_0$ is small. We now look for fixed points of $T_\alpha(x) = x - A \cdot f(\alpha, x)$ in balls $B_{x_\alpha}(r)$ centered at these predictors. After developing the appropriate analytic bounds, the problem reduces to checking a finite number of polynomials inequalities of the form $P_k(r, |\Delta_\alpha|) < 0$, $k = -1, 0, \ldots, M$, cf. (6). The polynomials $P_k$ now depend on both the distance $r$ in Banach space and the distance $|\Delta_\alpha|$ in parameter space to the base point $(x_F, \alpha_0)$.

Repeating this process, we can topologically validate the predictor-corrector algorithm to find parameter dependent families of solutions, which form continuous branches due to a pasting procedure that exploits the convenience of the polynomial inequalities, see [9]. The method is amenable to rigorous pseudo-arclength continuation as well [9, 43]. The main challenge in adapting this method to connecting orbits is constructing algorithms for obtaining parameterized families of (un)stable manifolds. From the theoretical point of view this has been described in [15], and we shall focus on the open question of a topologically validated computational implementation.
The next problem is capitalizing on the connecting orbits as building blocks for more complicated patterns. Namely, there are various results that concatenate connecting orbits to form new patterns. For applying these “gluing” theorems, such as [25, 62, 60], transversality of the unstable and stable manifolds is the vital property. Since the connecting solutions are obtained through a topological contraction principle, they are unique and, crucially, stable under perturbations. Intuitively it is thus clear that they must correspond to transversal intersections of stable and unstable manifolds — otherwise perturbations would easily ruin (uniqueness of) the solution — and due to the contraction mapping at the base, a proof using analytic techniques is within grasp. Such a mathematical proof will be a novel results both for periodic patterns and connecting orbits. Our approach thus puts us in a unique position, enabling the rigorous verification of transversality criteria required in forcing and gluing theorems.

A related fundamental problem concerns the “physical” stability against perturbations when the connection is an equilibrium solution of a PDE. This is important because unstable solutions are unlikely to be observed in experiments or show up in nature. This problem is connected to transversality, since non-transversality of the connecting orbit corresponds to the presence of a zero eigenvalue, the border between stability and instability. For self-adjoint problems this means stability cannot change along continuous branches of transversal connecting orbits. The relation between the stability properties in de PDE and the spectrum of the matrix $Df_M(x_F)$ in the finite dimensional reduction needs to be investigated: the “dominant” part of the linearization (which determines (in)stability) is expected to be captured by the eigenvalues of the finite dimensional reduction, cf. [13].

Finally, it will be interesting to investigate the opposite of continuous branches, namely bifurcations. We will work towards a topologically validated computational technique for bifurcations based on a combination of the contraction mapping ideas summarized in §I.3, together with simultaneously obtained information on the derivatives along the solution curve and with respect to parameters, so that general bifurcation results (cf. [19]) can be invoked with explicit analytic bounds. Such methods would be a breakthrough for periodic patterns of ODEs/PDEs (cf. [69]), while applications to connecting orbits, with their zoo of possible bifurcations [40], are the subsequent natural step.

II.3 CONNECTING ORBITS IN PARTIAL DIFFERENTIAL EQUATIONS

Connecting orbits in PDEs describe transitions between patterns. The main challenge, as compared to ODEs, is the infinite dimensional phase space.

**Goal:** Compute and validate connecting orbits in infinite dimensional systems.

We will focus initially on connecting orbits in a purposefully chosen paradigm, the nonlinear Cauchy-Riemann equations

\[
\begin{align*}
    p_t + (q_x - H_p(p,q,x)) &= 0, \\
    q_t - (p_x + H_q(p,q,x)) &= 0,
\end{align*}
\]

where $H(p,q,x) \in C^2(\mathbb{R}^2 \times S^1)$ is a planar non-autonomous Hamiltonian. The stationary problem reduces the PDE to the Hamilton equations. Equation (12) is a classical strongly indefinite PDE [31], with links to pattern formation, and there remain plenty of open questions. It admits a variational formulation as the (formal) gradient flow of the functional

\[
\mathcal{F}(p,q) = \int_0^1 [pq_x - H(p,q,x)] \, dx,
\]

bringing the possibilities of Morse-Floer homology into play to explore the dynamic and topological consequences of connecting orbits, once they have been found. The strongly indefinite character exemplifies the infinite dimensional challenges. Results will be new already for stationary patterns, to which our ODE methods should be extendable in a relatively direct manner, though the main aim of this subproject is to develop widely applicable topologically validated computational techniques for connecting orbits in PDEs.

First, to find the $t$-independent limit states ($x$-periodic equilibria $(\tilde{p}(x), \tilde{q}(x))$), the method as summarized in §I.3 is pertinent. It should be noted that it would be the first time these techniques [8, 34] are used
for strongly indefinite problems. However, the constructions do not directly use the finiteness of the Morse index and we are confident that our methods will extend to the strongly indefinite setting. Indeed, the contraction rate of operator $T$ in (5) depends on the eigenvalues of $A^{-1} \approx DF(x_F) \approx \nabla^2 \mathcal{F}(\tilde{p}, \tilde{q})$: heuristically, the larger their magnitude is, the stronger the contraction is. Thus, eigenvalues with large magnitude do not adversely effect our rigorous computational methods.

To make use of the critical points, their relative index $\mu_{\text{rel}}$, as defined in the context of Floer theory, must be computed in order to determine the dimension of the intersection of stable and unstable manifolds. Our approach to resolve relative indices is based on two related observations. First, our methods for establishing equilibria are based on a finite dimensional computation, and using regularity of the solutions to bound the errors induced by the truncation. Second, the relative index is equivalent to the Fredholm index of the linearized equation (or, more generally, a homotopy of linear operators), hence there exist a priori bounds on the set of eigenvalues which cross zero as a result of the spectral flow. Combining these arguments suggests that, with appropriate global estimates, the relative index can be determined via an absolute index for the corresponding finite dimensional representation.

Having acquired detailed information on the equilibria, attention turns to the connections between them. To adjust the topologically validated computation method for connecting orbits from the ODE to the PDE setting, one may Fourier transform (12) in the $x$ variable to obtain an infinite set of ODEs. This does not change the main issue of looking for connecting orbits in an infinite dimensional space, but it highlights the analogy with the ODE problem. The infinite set of differential equations needs to be finitely truncated to do computations, and this brings fresh challenges to the PDE setting. First, analytic estimates are needed to control the defect introduced by this truncation. Since the bounds on the truncation errors are closely related to the regularity of solutions, we do not expect insurmountable obstacles, as all solutions of (12) are smooth.

The second pressing problem is the infinite dimensionality of the (un)stable manifold. The parametrization method works in general Banach spaces [14], but under the assumption that the underlying dynamics is a flow, hence it is not directly applicable to indefinite problems. Even when one can overcome this, parametrizing infinite dimensional manifolds is impractical from a computational point of view. However, since orbits enter the equilibria along the leading eigenvalue direction, there is no need to approximate the entire stable manifold: the parametrization techniques should be “localized” along these leading directions. Here we may capitalize on the fact that the theory [14] is applicable to (finite dimensional) invariant submanifolds. Once again, an important aspect will be to bring the theory and computational algorithms together through explicit analytic error estimates.

The prototype problem (12) has a special structure, which enables us to harness the discovered connecting orbits in a remarkable way. Since (12) is the formal gradient flow of (13), we may consider the Floer homology of maximal invariant sets. Therefore, both equilibria and connecting orbits obtained through topologically validated computations, can be used to force the existence of other solutions. The crucial topological forcing structure is expressed by braids: consider the evolving strands

$$
\beta^k(\cdot) \equiv \{(x, q^k(\cdot, x), p^k_1(\cdot, x)) \mid x \in [0, 1]\},
$$

where $\{(q^k(t, x), p^k(t, x))\}_{k=1}^K$ are solutions of (12). As illustrated in Figure 1, these solution form braids with both positive and negative crossings. It turns out that the maximum principle implies that along

![Figure 1: Left: strands of a braid. Right: a positive and a negative crossing.](image_url)
the evolution the braid can only change positive crossings into negative crossings. As a consequence, braid classes are isolating neighborhoods and we may consider the Floer homology of a braid class [6]. Since we have independent methods for calculating this invariant [6], it is possible to combine that global topological information with the local information of rigorously computed equilibria and connections to force a multitude of braided solutions of (12). Somewhat surprisingly, there is a connection with mixing processes of viscous fluids, which are elegantly captured [12] by the \( t \)-independent solutions of the Cauchy-Riemann equation (12). Finding connecting orbits for (12) may thus reveal, through Floer homology, information about those mixing solutions.

Finally, the developed methods will be applicable to more general systems. The first step is to replace the Hamiltonian vectorfield in (12) by a general one. Such equations, although no longer gradient systems, have Poincaré-Bendixson like behaviour [30]. The structure of the invariant set is thus still relatively simple. Nevertheless, it means that \( t \)-periodic orbits come into play, and the resulting connections between these pose new computational and analytic challenges. This has a geometric-algebraic counterpart in the accompanying necessary adaptation of the construction of Floer homology in the spirit of Morse-Bott homology [11].

Other application areas of the developed techniques include connecting orbits in lattice dynamics and delay-differential equations (cf. [50, 48]), as well as spiral waves in reaction diffusion systems, which in suitable coordinates may be described as connecting orbits to periodic stationary patterns (modulated waves) in nonlinear PDEs without well-defined initial value problems [61].

II.4 Modulated travelling waves

The final subproject concerns propagating disturbances in PDEs, a problem which in the last few years has taken central stage in pattern formation [28, 29]. Modulated (non-uniformly) translating structures are observed in a variety of systems, leading to stripes, (hexagonal) spots, and spirals [4, 61]. These appear in fluid dynamics (discussed below) and solid combustion models [3], whereas two-dimensional spiral waves, which can described by a very similar mathematical setting, appear in chemical reactions (e.g. the Belousov-Zhabotinsky reaction) [67], in the oxidation of carbon-monoxide on platinum surfaces [55], and in cardiac tissue [66].

Existence of periodically modulated travelling waves has been proved in perturbative, small amplitude settings [20], but fully nonlinear methods are presently unavailable, and we outline below a novel technique.

**Goal:** Use Morse-Floer homology to investigate the propagation of periodically modulated travelling waves.

Consider, for definiteness (one easily generalizes to higher order equations, systems of equations, different nonlinearities, etc), the fourth order equation (incorporating both Swift-Hohenberg and extended Fisher-Kolmogorov models) [63, 57]

\[
\frac{du}{dt} = -\gamma u_{xxxx} + \beta u_{xx} + u - u^3, \quad \gamma > 0, \beta \in \mathbb{R}.
\]  

(14a)

When one perturbs the unstable homogeneous state \( u = 0 \), travelling structures are observed that leave behind a stationary periodic pattern, see Figure 2. In particular, these are not standard travelling waves (i.e. \( u(x,t) = \bar{u}(x-ct) \)), but rather modulated travelling waves characterized by the shift-periodicity

\[
u(t + T, x) = u(t, x - L) \quad \text{for all } t, x \in \mathbb{R},
\]  

(14b)

\[
u(t, x) \to U_{\pm}(x) \quad \text{as } x \to \pm \infty.
\]  

(14c)

Here \( U_{\pm} \) are \( L \)-periodic stationary solutions, and \( c = \frac{T}{L} \) is the velocity of the connecting front. If \( U_{\pm} \) are not both homogeneous states this is not a uniformly travelling wave.

Introduce new variables \((s, y)\) by \( u(t, x) = v(ct - x, s) = v(s, y) \). Then (14b) is equivalent to the periodicity \( v(s, y + L) = v(s, y) \), while (14c) is equivalent to \( \lim_{x \to \pm \infty} v(s, y) = U_{\pm}(y) \). In the new variables the original PDE (14a) transforms into

\[
\gamma (4v_{ssy} - 4v_{syy} + 6v_{syy} - 4v_{yyy} + v_{yyyy}) - \beta (v_{ss} - 2v_{sy} + v_{yy}) + cv_s = v - v^3.
\]  

(15)
We may thus consider the space of $L$-periodic functions in $y$, and look for a connecting orbit of (15) in the time-variable $s$ between the cycles $U_+$ and $U_-$. The PDE (15) does not have a well-posed initial value problem in $s$. On the other hand, the functional

$$L = \int_0^L \left[ \frac{1}{2} (v_{yy}^2 - 6v_{xy}^2 - 8v_{yxy}v_y + 2v_{xyy}v_y - v_{x}^2) + \frac{\beta}{2} (v_y^2 - v_{x}^2) + \frac{1}{4} (v^2 - 1)^2 \right] dy$$

is a Lyapunov functional: $\frac{dL}{ds} = -c \int_0^L v_y^2 \, dy \leq 0$. The setting is very similar to that of spatial dynamics [44], but with a variational twist.

While the techniques that will emerge from the approach in §II.3 are eventually applicable to this type of modulated travelling wave problem, in this subproject we take a different, original route to understand the connecting orbit structure. It has the advantage of disclosing a collection of connections simultaneously. The approach is based on knowledge of the periodic stationary limit states, which can be assessed using the techniques from §I.3, and the fact that the system is variational, hence the natural domain for Floer homology. Actually, it makes for a nonstandard, innovative application of Floer homology theory, since we intend to formulate results about connecting orbits, using known information about critical points, rather than the usual exclusive focus on equilibria.

The main goal of this subproject is therefore to develop a Floer homology in this setting, to explore the existence of connecting orbits and thus to prove the existence of modulated travelling waves. As in all Floer homology constructions, we need to obtain bounds on solutions, so that we can employ compactness to extract converging sequences (these bounds should descend from standard ones for the original parabolic equation (14a)). Furthermore, as also alluded to in §II.3, we need to understand the spectra of critical points and relate them to the Fredholm index of connecting paths.

Finally, to extract information about connecting orbits corresponding to periodically modulated travelling waves, we need to combine the global topological data bestowed by Floer homology, with an analysis of the critical points (stationary periodic patterns). There are two roughly complementary approaches:

1. Local: when $U_+$ is close to $U_-$ (e.g. they appear in a saddle-node bifurcation, cf. [58]) one can use a bifurcation analysis to calculate the homology (in an isolating neighborhood of $U_{\pm}$) to find connecting orbits.

2. Global: continuation away from bifurcation points can be accomplished using a Floer homology analogue of the Conley index techniques from [52] (cf. [22]), as long as the bifurcation diagram of stationary solutions is known. For example, for $\beta > \sqrt{8g}$ the bifurcation diagram of (14a) is completely understood [5], while in other situations we will use topologically validated continuation computations on the stationary solutions.

As generalizations one should subsequently consider problems in several spatial dimensions, i.e., problems in which a more-dimensional periodic pattern (hexagonal for example) is generated behind the front.
III CONCISE PLAN OF WORK

III.1 RESEARCH PLAN

The research team is envisaged to comprise the PI, two Postdocs and two PhD students. Of the four subprojects listed in §II, the first one, developing the method for general systems of ODEs (§II.1) is suitable for a PhD student: he/she can start by working out several applications (as indicated in the main text) and develop the method in steps, with implementation issues being a major component, and a smaller amount of time spent on theoretical aspects. These will be developed in part in collaboration with the first Postdoc, who will work on adapting the method to connections in infinite dimensional settings (PDEs). This requires more advanced analytic abilities and is therefore most suitable for a Postdoc. While we will initially focus on Cauchy-Riemann equations (§II.3) there are plenty of additional challenging avenues to explore, as presented in the main text. The second PhD student will be working on the development of the topological validation of the quantitative and qualitative information about the computed connecting orbits (§II.2). Theoretical development and implementation for test problems will go hand in hand, making it particularly suitable for a PhD project. The last subproject, described in detail in §II.4, requires a wide perspective, and it is an excellent project for a Postdoc, with concrete initial steps towards subgoals, but also with extensive possibilities for generalizations. While all subprojects have well-defined goals, collaboration between Postdocs and PhD students is important, as expertises, especially regarding algorithmic aspects, should be shared for optimal results.

<table>
<thead>
<tr>
<th>team member</th>
<th>task</th>
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<tbody>
<tr>
<td>PI</td>
<td>Coordination, collaboration, coaching, overall responsibility</td>
</tr>
<tr>
<td>PhD student 1</td>
<td>Connections in systems of ODEs §II.1</td>
</tr>
<tr>
<td>PhD student 2</td>
<td>Families of connections and building blocks §II.2</td>
</tr>
<tr>
<td>Postdoc 1</td>
<td>Connecting orbits in PDEs §II.3</td>
</tr>
<tr>
<td>Postdoc 2</td>
<td>Modulated travelling waves §II.4</td>
</tr>
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</table>

III.2 RESEARCH GROUP

The research team will be hosted by the Department of Mathematics within the Faculty of Sciences of the VU University Amsterdam. Mathematical Analysis is one of the focus areas of the Department of Mathematics, illustrating its capacity to support this research project. The members of the nonlinear dynamics group relevant to the project are

<table>
<thead>
<tr>
<th>area of expertise</th>
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<tbody>
<tr>
<td>prof. J.B. van den Berg</td>
<td>dynamical systems &amp; applications</td>
</tr>
<tr>
<td>prof. R.C. van der Vorst</td>
<td>topological and geometric methods</td>
</tr>
<tr>
<td>prof. J. Hulshof</td>
<td>partial differential equations</td>
</tr>
<tr>
<td>dr. B. Rink</td>
<td>lattice dynamics</td>
</tr>
<tr>
<td>dr. R. Planqué</td>
<td>variational methods, mathematical biology</td>
</tr>
<tr>
<td>dr. F. Pasquotto</td>
<td>symplectic geometry, Hamiltonian dynamics</td>
</tr>
</tbody>
</table>

with five PhD students currently working in the group.

The research fits in well with the national mathematics cluster on Nonlinear Dynamics of Natural Systems (NDNS+), the NWO-funded nationwide collaboration in dynamical systems, of which the PI is the director and in which the nonlinear dynamics group plays an important role. Interaction with the groups of Doelman (Leiden; reaction-diffusion systems), Peletier (Eindhoven; variational techniques), Stevenson/Homburg (University of Amsterdam; numerics/bifurcations) and Frank (CWI; scientific computing) is expected to benefit the project. Internationally, collaborations will be continued and extended with S.B. Angenent (Wisconsin), S. Day (William & Mary), R. Ghrist (Pennsylvania), K. Mischaikow (Rutgers), J.-P. Lessard (BCAM, Bilbao) and J.F. Williams (SFU, Vancouver). The latter two collaborators specialize in numerical algorithms and scientific computing, while the others have valuable expertise in theoretical aspects of the proposal.
2B  RESEARCH IMPACT – OPTIONAL, BUT WHEN FILLED OUT THE RESULTS OF THE ASSESSMENT OF THE RESEARCH IMPACT, WHETHER POSITIVE OR NEGATIVE, WILL BE TAKEN INTO ACCOUNT IN THE OVERALL RATING OF THE APPLICATION. Direct societal, technological or industrial implications are not part of the proposal.

2C  NUMBER OF WORDS USED

7990 words in Section 2A.
12 words in Section 2B.

2D  ANY OTHER IMPORTANT REMARKS WITH REGARD TO THIS APPLICATION

2E  LITERATURE REFERENCES


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