Connections in Infinite Dimensional Dynamics (20w5145)

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1. Description the area

Understanding dramatic changes in the dynamics of physical systems is a critical part of describing real world phenomena like stock market fluctuations, the formation of hurricanes, and even the progression of global pandemics. Mathematically such dynamic transitions are modeled by connections in nonlinear dynamical systems, mainly in the form of ordinary differential equations, partial differential equations and delay differential equations. This workshop focused on combining computational techniques with abstract mathematics to improve our fundamental understanding of transitions in dynamical systems.

The participants of the workshop were experts in dynamical systems theory, computational mathematics, algebraic topology, and functional analysis. Discussions focused on mathematically rigorous arguments where the digital computer plays a substantial role. The goal of the workshop was not to share new results. Rather participants were encouraged to share problems at the boundary of our understanding, discuss possible methods for moving forward, and help to set the agenda of the field for the coming years. Participants hailed from three continents and represented the full spectrum of professional development: from graduate students to postdoctoral scholars, to senior researchers. In spite of the major obstacles presented by the world wide Covid 19 crisis, the workshop was extremely productive and led to a number of important new lines of research.

2. Meeting Overview

The meeting was moved to an online, zoom enabled workshop in response to travel restrictions. Nevertheless, the organizers tried to come up with a format that would lead to as much discussion of new unsolved problems as possible. Since participants were dispersed through multiple time zones we decided to have a very small number of short talks, leaving as much time for open discussion as possible and making the best use of the roughly 5 hours per day work window.

The idea of the organizers was to start the meeting with four short 15 minutes talks on major open problems in the area, each followed by 15 minutes of conversation. The slogan for the talks was "don't tell us what you know how to do, tell us what you don't know how to do". Volunteers were solicited by correspondence before the meeting. The Monday morning talks were:

- **Connecting orbits for strongly indefinite problems/ill posed PDEs** (Jonathan Jaquette)
- **DSGRN and Hill Function Continuation** (Konstantin Mischaikow)
- **Stability of nonlinear waves for delayed PDEs** (Blake Barker)
- **Forcing and topology from partial information in infinite dimensions** (Jan Bouwe van den Berg)

On Monday afternoon (after lunch) participants broke into two working groups to discuss two of the problems of Mischaikow and Jaquette. On Tuesday morning participants broke into two working groups to discuss the problems of Barker and van den Berg. Tuesday afternoon was dedicated to pursue discussions in smaller groups on the four projects. On Wednesday two new problems were proposed using the same 15 min format.

- **Hopf bifurcations in the FitzHugh-Nagumo PDE** (Elana Queirolo)
- **Traveling waves for a fourth order problem with exponential nonlinearity** (Michael Plum)

On Wednesday afternoon these talks were discussed in working groups. Already on Thursday, nontrivial progress toward some of the project had been made and people divided in sub-groups to pursue the work. Friday morning was dedicated to writing the report. Each person who proposed a project was assigned the task to write a short description of the problems and the progress made. All participants were assigned to a group and separate break-out rooms on zoom were created to facilitate this task. Friday afternoon was used to wrap things up and for goodbyes.

Positive outcomes: It was fantastic and extremely valuable to have this opportunity to focus on open problems and meet with collaborators during the Covid 19 pandemic when travel is impossible. We made substantial progress on a number of problems that would not have otherwise been possible, as discussed below.

Shortcomings: What we missed in this online format, as opposed to an in person meeting was all the side conversations and new contacts that develop naturally in a typical Banff meeting. It was harder to forge new relationships. People ended up working largely with collaborators they already knew fairly well. The level of novelty was somewhat lower than in previous in person meetings, and multiple time zones made it impossible to work the long hours we typically devote to an in person meeting. Being isolated together in a common physical location definitely has positive aspects.

Small logistical issues: we struggled with learning curve on breakout rooms, and never came up with an easy way for people to be able to move more freely between rooms. Also, it would have been helpful to be able to save chat threads.

That being said, the BIRS staff were incredibly helpful and the meeting would not have worked at all without their diligent support. The organizers thank them sincerely for all of their hard work.

In the next six Sections, we discuss each of the six projects we worked on during the week.

3. ill-posed problems

Growing out of the ample literature on computer assisted proofs for connecting orbits in finite dimensional flows and maps, development of rigorous numerics to study similar problem in infinite dimensional dynamical systems is blossoming. Along this vein, an aspirational goal is the study of strongly indefinite problems – where critical points have an infinite number of both stable and unstable eigenvalues, and dynamics in the classical sense is ill posed – which now been brought within reach.

During the conference, an approach was proposed to computing the connecting orbits between critical points which comprise the boundary operator in Hamiltonian Floer homology. While a semiflow in this problem cannot be defined, there is a well defined notion of stable and unstable eigenvectors about a critical point. By using a variation of constants formula, a solution to the connecting orbit problem may be defined as the fixed point of an integral equation which integrates forward along the stable eigendirections, and backwards along the unstable eigendirections. This approach could be applied to extend recent work on stable manifolds in parabolic PDEs by [v/d Berg, Jaquette, Mireles James] (a topic of discussion at the BIRS 14w5098 workshop) to the strongly indefinite case. Again, by integrating forward along stable directions and backwards along unstable directions, the infinite length connecting orbit problem may be formulated as a finite length boundary value problem, imposing Dirichlet boundary conditions to connect the infinite dimensional (un)stable manifolds at either ends. During the conference, the feasibility of this approach was discussed.

It turns out that recently developed techniques for rigorously integrating parabolic PDEs, some of which were discussed at another previous BIRS workshop, namely 17w5141, are exactly the tools we need to rigorously carry out those forward and backward integrations between the manifolds.

Numerical experiments of the Floer equation related to Hamiltonian Floer Homology were conducted to explore the feasibility of rigorous numerics for the ill-posed PDE. MATLAB's boundary value problem solver (bvp4c/bvp5c) makes it possible to compute boundary value problems of a certain size numerically. However, as expected, the effect of the numerical instability that is caused by the ill-posedness of problem is strong. That is, the larger the domain of the boundary value problem to be considered, the more the numerical solution becomes unstable. We expect this problem to be resolved by incorporating a precise approximation of the manifolds at both ends of the orbit, and by employing a multi-step method using domain decomposition. To develop this technique for time-dependent PDEs is an ongoing project for this community.

Additionally, extensions of the technique to study multi-dimensional traveling waves were also discussed. This prompted an investigation of a different approach, namely directly treating the problem as an elliptic one. While this point of view seems at first fundamentally different, it turns out that a reformulation of the boundary value problem using Greens functions yields a somewhat similar set of equations, which could be handled with the above mentioned tools in an even more efficient way, by taking advantage of the elliptic regularization.

To put this problem into a broader context, we note that being able to rigorously validate connecting orbits in ill-posed problems has both direct and indirect benefits. An example of the former is that one will be able to prove the existence of traveling waves in the suspension bridge problem on domains with "cylindrical" shape $\mathbb{R} \times [0, L]$, an open problem raised in Section 8. Moreover, since explicit error bounds are provided by the computational method, the stability problem is then within reach.

An instance of the indirect type is that any connecting orbit found between equilibria with index difference one will contribute to the partial information in the Morse-Conley-Floer forcing theory which is the topic of Section 6, potentially leading to stronger forcing results. Similarly, connecting orbit found between equilibria with index difference zero (a parameter needs to be varied, as this is a co-dimension one phenomenon) can indicate where structural changes in the global dynamics on the attractor occur.

4. DSGRN and Hill function continuation

Though there are a few heavily exploited exceptions, understanding the dynamics of a given nonlinear system can only be done using numerical methods. Work over the past few decades has shown that it is possible to efficiently perform numerical computations with rigorous bounds so that there are mathematical guarantees that the results that are obtained are correct. To be more specific consider a differential equation

$$\frac{dx}{dt} = f(x, \lambda). \tag{1}$$

Assume that the parameter value is fixed, i.e. $\lambda = c \in \mathbb{R}$. Without downplaying the wide range of extremely challenging problems that still remain, it is safe to say that for large classes of problems, where (1) is an ODE, PDE, or DDE, there are standard techniques for identifying fixed points, periodic orbits, homoclinic and heteroclinic orbits, invariant tori, and chaotic dynamics.

A more challenging set of problems involves understanding the dynamics for all $\lambda \in \Lambda \subset \mathbb{R}$. This requires the ability to rigorously identify bifurcations. Again, considerable progress has been made. We understand saddle-node and Hopf bifurcations which implies that we can follow fixed points and to a large extent periodic orbits. Keeping track of heteroclinic and homoclinic orbits and invariant tori is harder, but there are tools. With respect to chaotic dynamics there are isolated results. Again these comments are applicable to a broad range of ODEs, PDEs, or DDEs.

However, if we move to the setting where we want to understand the dynamics of all $\lambda \in \Lambda \subset \mathbb{R}^d$ for $d >> 2$, then we know of only isolated results in the context of fixed points of ODEs and these depend crucially on the form of the equation. With this in mind we have been developing a software tool DSGRN (Dynamic Signatures Generated by Regulatory Networks) that is capable of taking as input a regulatory network (a directed graph capturing interactions and whether they are activating or inhibiting) and efficiently producing a database that describes the global dynamics over all of parameter space. It is useful to think of this database as providing a readily accessible map of dynamics as a function of parameters, i.e. a **Mapquest** of nonlinear dynamics. There is, of course, a cost to this capability. The description of the dynamics comes in the language of combinatorics and algebraic topology. Furthermore, for a natural class of differential equations the DSGRN description of the dynamics is only valid if some parameters are extremely large. To emphasize: DSGRN is only providing a map of the dynamics, not classical descriptions in the language of invariant sets or explicit analytic solutions.

The general question is: can we use the output of DSGRN, e.g. the map of the dynamics, as input to the tools that we have for finding invariant sets and bifurcations to understand the structure of invariant sets over large regions of parameters and in particular away from the constraint of some parameters being extremely large?

4.1. **Work during the conference.**

4.1.1. *Extract High Level Information from DSGRN.* DSGRN divides and organizes the parameter space into regions (called parameter nodes) where the global dynamics obtained is constant. For each parameter node, there is a decomposition of the phase space into a set of cells $\mathcal{X}$ with a multivalued map $\mathcal{F} : \mathcal{X} \rightrightarrows \mathcal{X}$ that describes the dynamics combinatorially (see for instance the right image in Figure 2 where $\mathcal{F}$ is represented by the black arrows). This combinatorial characterization is expressed by a graph called the state transition graph. Such a graph can be reduced into a compact representation of the global dynamics called the Conley-Morse graph which identifies recurrent versus nonrecurrent dynamics (see the left image of Figure 2). Algebraic topological techniques such as the Conley index are used to obtain information about the local and global structures of invariant sets associated with smooth dynamics that is compatible with the combinatorial dynamics.

Consider two adjacent parameter regions in the parameter graph. A specific example involves regions 712 (see Figure 2) and 1512 (see Figure 1) that arise from a specific two node network (the details of the network are not important for this discussion). When going from parameter region 712 to its adjacent region 1512, there is a significant change in the combinatorial and algebraic description of the dynamics.

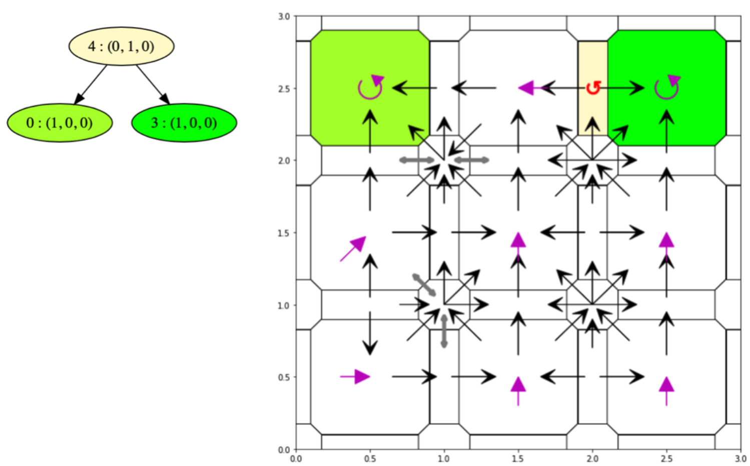

FIGURE 1. Conley-Morse graph and combinatorial dynamics at parameter region 1512.

In both cases, dynamics over a parameter region or dynamics as one changes parameter regions, we are interested in efficient and rigorous extraction of dynamics for associated differential equations.

A natural question that arises from this approach is how to define $\mathcal{F}$ in such a way that the derived algebraic topology captures the optimal global dynamics of the associated differential equations. We spent considerable time this week discussing different approaches to addressing this problem.

4.1.2. *Hill Model Continuation Platform.* As indicated above the DSGRN software provides a coarse overview of the parameter landscape, thus a natural goal is to extract finer scale descriptions of the dynamics. This motivates some of our recent work which has been to develop the "HillCont" software library for numerically exploring the dynamics of gene regulatory networks within and across combinatorial parameter nodes using ODE models based on Hill functions.

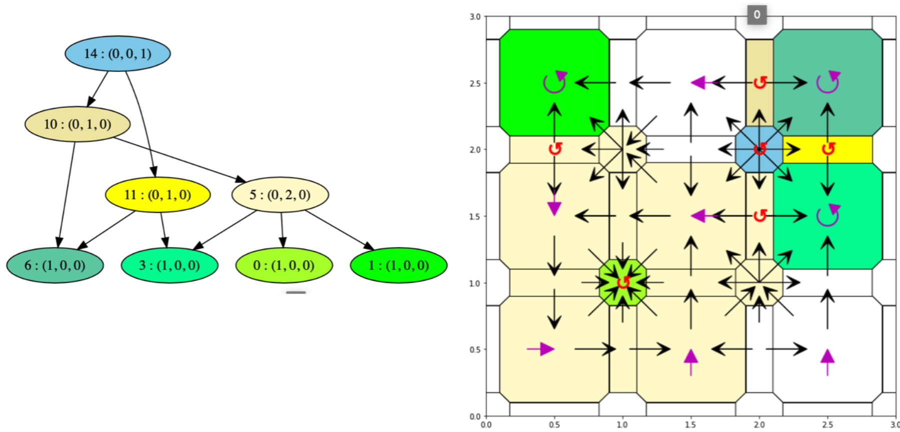

FIGURE 2. Conley-Morse graph and combinatorial dynamics at parameter region 712.

The core function of this library allows one to build an ODE model by specifying only the network topology of the GRN. The modeling assumption is that the differential equations take the form $\dot{x}_i = -\gamma_i x_i + f_i(x)$ where each f_i takes the form

$$f_i(x) = p\left(H_1(x_1), \ldots, H_K(x_K)\right).$$

and p is a polynomial of the form

$$p(z) = \prod_{m=1}^{q} p_m(z) \qquad p_m = \sum_{j \in I_m} z_j$$

where $\{I_1, \ldots, I_q\}$ is a partition of the integers, $\{1, \ldots, K\}$. Each H_k is a Hill function given by one of the following formulas

$$H^+\left(x; \ell, \delta, \theta, n\right) := \ell + \delta \frac{x^n}{\theta^n + x^n}$$

$$H^-\left(x; \ell, \delta, \theta, n\right) := \ell + \delta \frac{\theta^n}{\theta^n + x^n}$$

depending on whether or not x_k has a positive or negative interaction with x_i.

Hill models are widely used in biological modeling and the models used by DSGRN can be thought of as a Hill Model in which each $n = \infty$ for each H. This makes these models obvious candidates to combine with DSGRN. The goal of the HillCont library is to look closer at the dynamics for specific parameter values in the regions distinguished by DSGRN.

As a concrete example, we have considered the problem of finding saddle-node bifurcations. Using techniques largely developed by the rigorous numerics community, this can be transformed into a zero finding problem as follows. If $\dot{x} = f(x, \lambda)$ is the Hill model ODE, then for fixed parameter λ, a saddle-node bifurcation is a zero of an expanded map of the form

$$g_\lambda(x, v, n) = \begin{pmatrix} f_\lambda(x, n) \\ Df_\lambda(x, n)v \\ \|v\| - 1 \end{pmatrix}.$$

While the dynamics in a high dimensional Hill Model may be intractable to analyze numerically, zero-finding problems such as this are feasible to solve. In fact, one may do continuation with respect to parameters to follow surfaces of saddle-node bifurcations and ask other interesting questions.

This week our discussion has focused on how to apply this tool to optimization problems. The simplest such example is identify all of the "n" parameters in Hill function as a single scalar parameter and consider the problem of minimizing the value of this parameter for which a saddle-node bifurcation occurs at a given equilibrium. This amounts to doing continuation in the $\ell, \delta, \theta, \gamma$ parameters.

Other examples of work which may be of interest were discussed throughout the week and we worked on adding necessary functionality to the HillCont library to carry out these computations. These discussions and subsequent example implementations have already lead to some interesting discoveries, such as existence of local minima for n which do not occur at pitchfork bifurcations. This was discovered this week and was quite surprising.

5. Stability of traveling waves for PDEs with delays

A great deal of work has been done studying the existence, uniqueness, and stability of traveling wave solutions to delay PDEs. However, there are many open problems concerning traveling wave solutions with larger delay, or concerning stability. In recent years, rigorous numerics have been used to prove existence and uniqueness of solutions to boundary value problems in DDEs, and also to prove stability of traveling waves in non-delay PDEs with a single spatial dimension. To prove stability of traveling waves with one spatial dimension, the Evans function is a very useful tool because zeros of the Evans function correspond to eigenvalues of the linearized PDE problem. Samaey and Sandstede developed a strategy for determining stability of pulses for partial differential equations with time delays using the Evans function. However, relatively little has been done using the Evans function for delay PDEs.

During the BIRS workshop, it was proposed to use rigorous numerics and the Evans function as described by Samaey and Sandstede to prove stability of traveling wave solutions to delay PDEs. Through discussions at this workshop, a group of five participants began working and making significant progress on this problem. By the end of the workshop, they already had four pages of the eventual paper written up and several steps of the numerical proof completed or in progress.

Every member of the group working on this project has one or more new collaborators as a result of this workshop. The combined expertise of the participants is what makes the fast progress on this problem possible. Without the workshop, this team would not have come together.

6. Forcing connecting orbits from partial information about equilibria

To set the scene, consider gradient-like systems. We assume there are sufficient compactness and genericity-transversality results available so that a Morse-Floer homology theory exists.

We are interested in the situation where, through continuation to a "trivial" system, the Morse-Floer homology is known, with the Betti numbers denoted by $\{b_k\}_{k\in\mathbb{Z}}$. The rigorous validated numerics techniques from the past decades often allow us to find a finite number of equilibria together with their (relative) index. To fix ideas, say we have found c_k equilibria with index k. In particular, it follows from the proof method that these equilibria are hyperbolic. Usually, we do not know whether we have found all equilibria, so the $\{c_k\}_{k\in\mathbb{Z}}$ provide a lower bound only. In addition, we can get a very good bound on the energy of each of the equilibria.

How many connecting orbits are forced to exist based on this information? At the moment, the state-of-the-art seems to be a "crude" ad-hoc construction which leads to a lower bound of the type

$$\frac{1}{2}\sum_{k\in\mathbb{Z}}\max\{c_k-b_k,0\}. \tag{2}$$

This is found by relatively naive arguments which essentially only consider the short exact sequence $C_{k+1}\to C_k\to C_{k-1}$, the C_k being the chain groups in the homology construction. No aspects of a more global nature, such as energy ordering, Morse decompositions or connection matrices, are being exploited.

The main open question is whether one can do better by developing properly a Morse-Conley-Floer *forcing theory of connecting orbits* in the face of *partial information.*

The hope is that one obtains stronger forcing results, but also that moving from ad-hoc arguments to ones based on a proper theory will make it easier to deal with situations where we add partial information about existence of connecting orbits (e.g. once again coming from validated numerics) into the mix. Similarly, symmetries could perhaps be incorporated naturally into such a theory.

Discussions during the week led to an additional side path of investigation. Namely, it seems that in "most" systems one can find, with enough effort, a set of equilibria where the number of connecting orbits forced by the naive lower bound (2) is very natural. This may be due to the strong ability of the community to find equilibrium solutions, and the general observation that any system can be reached by continuation starting from a trivial one and encountering only nondegenerate saddle-node bifurcations along the way, at least when restricting attention to equilibria only. This refocusses attention on exploring whether we can find model equations where the connecting orbits undergo interesting bifurcations, i.e., the system does not always have the Morse-Smale property when all equilibria are hyperbolic. One natural place to start looking is in the enormous database of annotated dynamics provided by DSGRN, see Section 4.

7. Validated Hopf bifurcation curves in the FitzHugh-Nagumo PDE

When discussing dynamical behavior, bifurcation curves are fundamental information to discuss qualitative changes in dynamics. In the case of Hopf bifurcations, the system is moving from a time independent solution to a periodic solution. In this conference, we have studied the FitzHugh-Nagumo equation,

$$\begin{cases} u_t = \Delta u + \varepsilon^{-1}(u - \frac{1}{3}u^3 - v), \\ v_t = \delta\Delta v + \varepsilon(u + \beta - \gamma v), \end{cases} \tag{3}$$

as a PDE describing neuron firing patterns in the human heart. The parameters δ and γ are set to 0 and 0.5 respectively, while ε and β might vary.[1]

In this equation, varying the two parameters ε and β can generate qualitatively different solutions. Numerical results have given a first understanding of the bifurcation curves in this system, as presented in Figure 3. While numerical understanding is necessary, a validated version of this graph would be of interest, not only for the information it would carry but also because it would allow us to develop new methods for bifurcation validation in the infinite dimensional context.

[1]from: D. Barkley and I. Kevrekidis. A dynamical systems approach to spiral wave dynamics. Chaos, 4(3):453460, 1994.

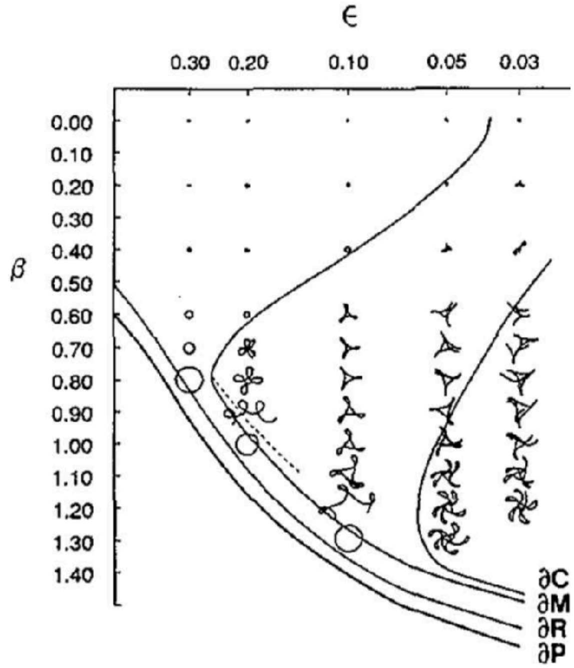

FIGURE 3. Bifurcation curves in the $\varepsilon - \beta$ plane

For this reason, our goal is to validate one of the bifurcation curves in Figure 3, the one denoted by $\partial\mathbf{R}$, representing a curve of Hopf bifurcations. This undertaking require us to have extensive understanding of the eigenvalues of the derivative operator associated to (3)

In particular, the derivative operator should have a simple eigenvalue crossing the imaginary axes, should satisfy a shifted Fredholm operator index condition and a non-resonance condition. Those were the main topic of discussion during BIRS.

Many inputs were given by the participants to rigorously verify these conditions and many approaches were proposed. The ones that seem the most promising for each element are

(1) **eigenvalue simplicity -** *eigenvalue counting*: having precise information on the eigenvalues of an approximation of the derivative operator, interpret them as approximations of the eigenvalues of the derivative operator and have analytic bounds on the error,
(2) **Fredholm index condition -** *adjoint operator validation*: deduce the operator's Fredholm index from the adjoint operator's properties, or possibly *compact perturbation*: using the continuation properties of the Fredholm indices, continue the Fredholm index along bounded perturbations,
(3) **Non-resonance condition -** *broad eigenvalue enclosure*: construct broad analytic bounds for the position of the eigenvalues and rigorously verify the non-resonance condition only within these bounds. This should transform the non-resonance condition into a finite set of conditions that can be rigorously verified.

8. Traveling waves for a fourth order problem with exponential nonlinearity

We consider the fourth-order wave equation (often used as a suspension bridge model)

$$\varphi_{tt} + \varphi_{xxxx} + e^{\varphi} - 1 = 0, \ (x,t) \in \mathbb{R} \times \mathbb{R}. \tag{4}$$

Traveling waves $\varphi(x,t) = u(x-ct)$ satisfy the ODE

$$u'''' + c^2 u'' + e^u - 1 = 0 \text{ on } \mathbb{R}, \quad u \to 0 \text{ as } |x| \to \infty. \tag{5}$$

Smets and van den Berg have proved existence of at least one solution for almost all wave speeds $c \in (0, \sqrt{2})$. Santra and Wei proved existence for all c in some subinterval of $(0, \sqrt{2})$, and this interval was further extended by van den Berg, Breden, Lessard, and Murray using computer assistance. For $c = 1.3$ the existence of at least 36 solitary travelling waves was proved by Breuer, Horak, McKenna, Plum by computer assisted means.

Nagatou, Plum, McKenna investigated the orbital stability of these solutions via computation of their Morse indices and using criteria by Grillakis, Strauss, Shatah. Stability could be proved for one of the 36 solutions, and instability for 15 of them. For the remaining 20 solutions, the criteria by Grillakis, Strauss, Shatah turned out not to be applicable.

QUESTION: Can we prove stability or instability of (some of) these remaining solutions by other means, e.g. via the Evans function?

Next we consider a higher dimensional analogue

$$\varphi_{tt} + \Delta^2 \varphi + e^{\varphi} - 1 = 0, \ (x,t) \in \mathbb{R}^n \times \mathbb{R}. \tag{6}$$

Traveling wave solutions of the form $\varphi(x,t) = u(x_1 - ct, x_2, ..., x_n)$ satisfy the equation

$$\Delta^2 u + c^2 \frac{\partial^2 u}{\partial x_1^2} + e^u - 1 = 0, \quad u \to 0 \text{ as } |x| \to \infty. \tag{7}$$

Some plots and videos of numerical approximations have been created by Horak and can be found on his webpage under

`http://www.mi.uni-koeln.de/\%7Ejhorak/waves/`

But so far there is no existence proof for any of these traveling waves.

QUESTION: Can we prove existence of such traveling waves? If yes, can we prove stability or instability? A possible simplification would be the same differential equation on a 2D strip domain (which is unbounded in x_1- and bounded in x_2- direction), or on a bounded rectangle with periodic boundary conditions, instead of the whole of $\mathbb{R}^2$. Then, not a solitary traveling wave profile, but a periodically repeated one would be the object of investigation.

When considering the problem on a rectangle with periodic boundary conditions (or Neumann boundary conditions on the sides perpendicular to the direction of propagation) one may be able to find periodic traveling profiles with long period, thus approximating solitary waves. The advantage is that here Fourier theory can be used. This could also enable a rigorous analysis of the spectrum, leading to linear (in)stability results. Two nonstandard technical matters are the interpolation estimates needed to deal with the exponential nonlinearity, as well as the two zero eigenvalues due to shift invariance (of course these do not appear if one is happy to restrict the symmetric perturbations). Neither of these issues seems insurmountable.