Rigorous computation for infinite dimensional nonlinear dynamics

organized by
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Workshop Summary

This workshop focused on extending rigorous computational tools and techniques to infinite dimensional dynamical systems with a particular emphasis on evolutionary partial differential equations. What follows is a brief summary and description of a variety of problems (and in some cases suggestions of techniques that may lead to solutions) that were discussed. The references that are provided are at best a partial collection of those that arose in lectures or discussions. They are by no means complete nor intended to be representative of the variety of topics that were discussed.

1 Computer Assisted Study of Connecting Orbits Between Fixed Points of Renormalization Group Operators

Connecting orbits (transversal intersections of the stable and unstable manifolds of periodic orbits) have been a main-stay of finite dimensional dynamical systems. Since computing a connecting orbit is a non-local problem, doing computer assisted proof of them is a useful tool (when outside of an integrable case). For finite dimensional problems there are a number of methods for doing this. It would be interesting to extend these computations to infinite dimensions.

Infinite dimensions presents a host of problems. A good entry problem could be renormalization group operators, which are indeed infinite dimensional, but which have some properties that make them more tractable. For example, renormalization operators are bounded operators. We also note that there are analytical tools which provide quantitative statements about the universal rescaling constants associated with renormalization operators, provided that one has some quantitative information about the transverse intersections.

Also, in some cases (for example the case of renormalization operators for unimodal maps) there is a good topological theory which says that connecting orbits exist. In addition, there have been already computer assisted proofs of existence of fixed points for renormalization operators and some studies of their invariant manifolds including that they intersect transversally some bifurcation manifolds.

Thus much of the machinery needed in order to set up a computer assisted proof of the transversal connecting orbits is already available for the case of unimodal maps. The goal would be to implement the computer assisted proof first in cases where there is an topological theory. This would provide quantitative results not available through topological methods. Afterwards, the tools developed will be sharpened to tackle other problems for which the topological theory is not available.

2 Computer Assisted Proof methods in KAM

During the AIM sessions there was some discussion about which problems could be of interest in trying to apply CAP methods in KAM. Some of the problems that arose were:

- Siegel disks in complex dynamics.
- 2d twist maps.
- 3 degrees of freedom hamiltonian systems.
- Differences and similarities between 1D and higher dimensional KAM objects.

Then, a discussion of all these problems was done. The relation between KAM theory and renormalization theory was also discussed.

3 Rigorous Finite Elements Methods

In searching for rigorous techniques for problems for which spectral methods are not feasible, we started to look at methods developed by Nakao and others beginning in the 1980s and in some cases even earlier. We focused on the survey article by Nakao [nakao]. The article outlines the general framework as well as a number of applications that are given in more detail in referenced papers.

We also discussed applying Nakao's method to the Kot-Schaffer map in order to compare to the approach and results in [day:kalies] and [day:junge:mischaikow]. In particular, replacing the Fourier basis with finite elements may allow for the study of maps with less smooth dispersal kernels and spatial heterogeneity terms as well as other problems with lower regularity. One could also try to apply this approach to elliptic problems, for example on a disk, that are more challenging for a spectral approach due to a lack of an appropriate choice of basis. Many of the rigorous spectral methods discussed during the workshop are limited by the need to find an appropriate basis for which explicit error estimates of nonlinear terms can be computed and appropriate (essentially diagonal) inverses of the linearization can be found. Therefore lower regularity methods may have an advantage in some problems of interest.

4 Uniqueness of solutions to Navier-Stokes

An important open problem in the theory of the Navier-Stokes equations is the uniqueness of the Leray-Hopf weak solutions with L^2 initial data. In the recent paper [JS], this problem was linked to the following eigenvalue problem. In $\mathbb{R}^3$, consider the equation:

$$\Delta U_\sigma + \frac{x}{2}\cdot\nabla U_\sigma + \frac{1}{2}U_\sigma - U_\sigma\cdot\nabla U_\sigma + \nabla P = 0 \tag{1}$$

with $\operatorname{div} U_\sigma = 0$ and

$$U_\sigma(x) = \sigma u_0(x) + O\left(\frac{1}{|x|^3}\right), \qquad |x|\to\infty. \tag{2}$$

Solutions to this problem are known to exist by [JS]. The associated linear operator is given by

$$\mathcal{L}_\sigma = \Delta\phi + \frac{x}{2}\cdot\nabla\phi + \frac{1}{2}\phi - U_\sigma\cdot\nabla\phi - \phi\cdot\nabla U_\sigma - \phi\cdot\nabla\phi + \nabla\pi\,, \tag{3}$$

for a suitable function π (related to the pressure).

It is known that for small enough σ the whole spectrum of the operator $\mathcal{L}$ is located at the halfplane $\Re\{z\} < 0$. However, it is conjectured that for bigger σ, some eigenvalues can cross the imaginary axis. This would imply non-uniqueness for Leray-Hopf solutions with L^2 initial data.

Issues surrounding the numerical verification of this conjecture were discussed at the meeting. A number of strategies were outlined and possible areas of potential problems with the nonrigorous numerics were identified:

- Using the right parametrization of the space of approximate solutions is crucial. It seems that truncation to a finite region may not be appropriate and working in the Fourier space might be a better option. Even at the level of linear problems, these issues are not completely understood.
- In order to gain better understanding, some simpler problems in lower dimensions were proposed such as Surface Quasi-Geostrophic (SQG) equations, Burgers equation with fractional diffusion. However it is expected that for Burgers with fractional diffusion, the spectrum will not cross.
- Another approach was to work with the space of axisymmetric solutions and use separation of variables. This would reduce the linear problem to a two dimensional calculation, simplifying it by one dimension. In this case the boundary condition u_0 should have a significant angular component.

5 A non-autonomous boundary value problem posed on an infinite domain.

Bjorn Sandstede presented a problem from his research in pattern formation [sandstede]. He can rigorously prove the existence of certain localized solutions to the Swift-Hohenberg equation if there is an existence proof for solutions to

$$\begin{cases} A_{rr} + \frac{1}{r}A_r - \kappa\frac{A}{r^2} = cA - \lambda|A|^2A, \quad \kappa\in\mathbb{R}, c,\lambda\in\mathbb{C}. \\ A:[0,\infty)\to\mathbb{C}, \quad A(0)=0, \quad \lim_{r\to\infty}A(r)=0 \end{cases} \tag{4}$$

The first simplified problem of interest is the real case ($A(r)\in\mathbb{R}$)

$$\begin{cases} w_{rr} + \frac{1}{r}w_r - \frac{w}{4r^2} = w - w^3 \\ w(0)=0 \\ \lim_{r\to\infty} w(r) = 0 \end{cases} \tag{5}$$

Sandstede has done non-rigourous computations only for (5) .

Equation (5) is similar to problems that have been previously been computed rigourously but with two key differences:

- (5) is non-autonomous with potentially singular terms

- (5) is posed on an infinite domain.

Two approaches to overcoming these issues were discussed. The first is to transform the problem to a finite domain and write it as an integral operator. This approach uses the machinery of radii polynomials and contraction mappings on Banach spaces. The second method is classical shooting method, which combines rigourous integration with analysis of the dynamics of the ODE near $r = 0$ and $r = \infty$.

5.1 A solution with integral operators.

To make (5) amenable to existing techniques various transformations of both the dependent and independent variables are required. This leaves us with

$$v(t) = -\frac{1}{2}\frac{1-t^2}{t^2}\int_0^t \frac{s^3 v(s)^3}{\ln s}\, ds - \frac{1}{2}\int_t^1 s(1-s^2)\frac{v(s)^3}{\ln s}\, ds. \tag{6}$$

Once (6) is solved for $v(t)$, $w(r)$ can be recovered by substituting $r = -\ln t$ and multiplying by a rational function of r.

At this point there is a numerical solver for (6) but the estimates required to make it rigourous need to be extended to handle the (mildly) singular kernels.

5.2 A solution via shooting method

The software for the rigorous integration for ODEs (for example CAPD) exists, so there is not a problem in obtaining bounds of good quality for behavior of solutions of ODEs on reasonably long, but finite, time intervals. However in the present problem the infinite time interval has to be considered.

Therefore to realize the shooting method for (5) one needs to deal with the following issues

1: the singularity for $r = 0$

2: since the equation is non-autonomous the standard tools for the estimates of the stable manifold of the point $(A, A') = (0, 0)$ does not apply

Issue 1 is dealt with via the change of the independent variable $\rho = \ln r$. The equation (5) becomes

$$w'' - w/4 = e^{2\rho}(w - w^3). \tag{7}$$

Now we seek a solution such that $\lim_{\rho \to -\infty} w(\rho) = 0$, so we need estimates for the unstable set of $(w = 0, w' = 0)$ for $\rho \to -\infty$ for our non-autonomous ODE (7), which is basically issue 2 above.

Rigorous bounds for the stable and unstable manifolds for fixed point for nonautonomous ODEs can be obtained by adapting the methods of cones for ODEs in the present context. The computations by pen and pencil show we can estimate these sets in our problem up to the distance 0.1 from the origin. This is a good news, because the time interval for which we would like to obtain rigorous bounds for the integration will be not to long.

6 Ill posed problems

Ill-posed problems in partial differential equations occur in various areas of mathematics, such a symplectic geometry, Hamiltonian dynamics, traveling wave theory, etc. The objective of this project is to determine the bounded solutions in time of ill-posed partial differential equations.

6.1 Connecting orbits in ill-posed problems and Floer Homology

To best illustrate the questions and problems involved we consider two model problems.

6.1.1 Gradient systems

Consider the equations:

$$\begin{aligned} u_t - v_x - f(u) &= 0 \\ v_t + u_x - v &= 0, \end{aligned} \tag{8}$$

where $(u,v) \in \mathbb{R}^2$, $(t,x) \in \Omega = \mathbb{R}\times[0,1]$ — the infinite strip — and $f(u)$ is a smooth function such that $f(u) \sim u^3$ as $|u| \to \infty$. We use the boundary condition $u(t,0) = u(t,1) = 0$ for all $t \in \mathbb{R}$. These equations can be referred to as the Cauchy-Riemann equations. There is no well-posed initial value problem for these equations — ill-posed. Important to point out is that the equations are the L^2-gradient flow of the action function

$$A = \int_0^1 vu_x - \tfrac{1}{2}v^2 - F(u),$$

where $F(u)$ is the anti-derivative of f. The ill-posedness of the problem can be understood by considering the spectrum of the linearized operators

$$\begin{pmatrix} -f'(\bar{u}) & -\frac{d}{dx} \\ \frac{d}{dx} & \bar{v} \end{pmatrix},$$

where $(\bar{u},\bar{v})$ is a stationary solution of the boundary value problem in x. The spectrum of the self-adjoint operator has infinitely many positive and negative real eigenvalues, unbounded in both directions on the real line!. The latter calls for an alternative of the Morse index: a relative index. The idea is to build a Floer homology theory by using rigorous computations for stationary solutions and indices and use the Floer invariants to prove results about connecting orbits (bounded solutions) of Equation (8).

6.1.2 Traveling waves

A second toy problem comes from the theory of traveling waves. Consider the parabolic equation $u_s = u_{tt} + u_{xx} + f(u)$, with f as above. Seek traveling waves of the form $u = u(t-cs,x)$, $c \neq 0$. Upon substitution into the equation this gives

$$u_{tt} + u_{xx} + cu_t + f(u) = 0, \tag{9}$$

where $u \in$, and $(t,x) \in \Omega = \times[0,1]$. As before we use the boundary condition $u(t,0) = u(t,1) = 0$ for all $t \in$. This is a 'damped' Hamiltonian system with Hamiltionian

$$\mathcal{H} = \int_0^1 \tfrac{1}{2}u_t^2 - \tfrac{1}{2}u_x^2 + F(u),$$

which satisfies the identity

$$\frac{d}{dt}\mathcal{H}(u(t,x)) = -c\int_0^1 u_t^2.$$

For example for $c > 0$ this yields a gradient like system as in Sect. 6.1.1. The only difference is that the linearized operator is no longer self-adjoint, but the spectrum is unbounded in the sense that there are infinitely many eigenvalues with both positive and negative real part and unbounded in both directions. The stationary problems for Equations (8) and (9) are identical. Equation (9) is also appealing because the Floer theory still needs to be developed. Due to the gradient-like structure of the problem this is doable. Another interesting aspect of this is defining a relative index for the damped Hamiltionian problems.

6.1.3 The Theory

Problems (8) and (9) are toy problems. Proof of concept will allow us to extend the ideas to much larger classes of equations such as elliptic systems, forward-backward delay equations, etc.

As we already pointed out in the previous section, the objective is to find connecting orbits. The ingredients for that will be to computationally determine the stationary solutions and there indices. Floer homology theory for both problems produces invariants that can be computed using continuation techniques. The Floer theory for Equation (8) can be found in [MR1703347]. The analogous theory for Equation (9) needs to be developed.

Computing connecting orbits using rigorous computational techniques is also an important, but more difficult question. This could provide additional information that can be combined with the Floer invariants. The latter is of particular interest when Floer theory is not available for particular classes of equations (not gradient-like).

6.1.4 Computing the relative indices

Given a solution u let us denote by A the linearized operator around this solution. When we rigorously compute this solution we use an approximate linearized operator $\tilde{A}$, which has the following form:

$$\tilde{A} = \begin{pmatrix} \tilde{A}_F & & & \\ & \Lambda_m & & \\ & & \Lambda_{m+1} & \\ & & & \ddots \end{pmatrix},$$

where $\tilde{A}_F$ is a finite dimensional operator (Jacobian matrix) numerically computed around a finite dimensional numerical approximation $\tilde{u}_F$. Since $\tilde{A}$ is close to A, if the eigenvalues of $\tilde{A}$ are non-zero, we can conclude that the eigenvalues of A also are non-zero by considering the homotopy path $(1-\lambda)\tilde{A} + \lambda A$. We can rigorously compute the eigenvalues of $\tilde{A}_F$, and hence we have the eigenvalues of $\tilde{A}$.

Now given two solutions u_0 and u_1, to compute their relative index we can consider the path $(1-\lambda)A_0 + \lambda A_1$. Associated with A_0 and A_1 we have the approximate operators $\tilde{A}_0$ and $\tilde{A}_1$ as above. Hence, to compute the relative index of A_0 and A_1 we can consider the path $(1-\lambda)\tilde{A}_0 + \lambda\tilde{A}_1$, and since $\tilde{A}_0$ and $\tilde{A}_1$ have the same tail we just need to count the positive eigenvalues of $\tilde{A}_{0F}$ and $\tilde{A}_{1F}$, which can be rigorously computed.

6.2 Periodic orbits in the Boussinesq equation

The Boussinesq equation arises in the theory of water waves and is given by

$$u_{tt} = u_{xx} + \mu u_{xxxx} + (u^2)_{xx}$$
$$\mu > 0,\ x \in [0,1],\ t \in \mathbb{R}. \tag{10}$$

Equation (10) is not well posed in any reasonable space and it is not hard to find analytic initial conditions for which the solution is not defined (in almost any weak sense) on any interval of time (e.g. see [MR795808,MR668408]). On the other hand existence of traveling waves, periodic orbits and quasi-periodic orbits can be investigated and in principle, the already existing methods of rigorous computations should be applicable to find some of these bounded solutions. Here, we propose to investigate existence of time periodic solutions.

As already mentioned in [MR2538946], the space of spatially symmetric solutions is invariant. Therefore we plan on studying the equation supplemented with the even periodic boundary conditions $u(t,x) = u(t,x+1)$ and $u(t,-x) = u(t,x)$. Expanding time periodic solution using a space-time Fourier expansion and using analytic estimates in higher dimension (e.g. [MR2718657]) to bound the nonlinearities, the plan is to use a Galerkin projection, the radii polynomials and the Banach fixed point theorem to show that near approximate solutions there exist exact time periodic orbits of (10).

7 Dynamics of delay equations

We discussed revisiting several relatively old questions in the field of differential delay equations. The idea is to apply recently improved rigorous computational techniques.

We decided to investigate the possibility of using so-called Wiener-algebras to improve on the existence results, presented in [MR2592879], to the Wright's equation

$$\dot{x}(t) = -\alpha x(t-1)(1+x(t)), \quad \alpha \in \mathbb{R}. \tag{11}$$

Namely, we hope to increase the range of the parameter α for which the existence of (slowly oscillating) periodic solutions to (11) can be proved.

The dynamics of the Mackey-Glass equation

$$\dot{x}(t) = \beta \frac{x(t-\tau)}{1 + x^n(t-\tau)} - \gamma x, \quad \tau, \gamma, \beta, n > 0, \tag{12}$$

poses many intriguing questions. Because of the non-linearity of (12), the above mentioned computational technique cannot be applied here. Thus the development of a rigorous integrator is desirable. This tool cannot only be used to tackle existence questions but also to learn about stability properties of solutions.

The above mentioned techniques can be developed further for computing invariant manifolds to solutions, and thus to establish existence results for connecting orbits observed numerically to various functional differential equations. In particular, existence of connecting orbits between solutions may explain the existence of complex oscillations to

$$\dot{x}(t) = -\alpha \sin(x(t-1)), \quad \alpha \in \mathbb{R}.^1 \tag{13}$$

The above mentioned advances in rigorous computations can provide invaluable insight into the global dynamics of neutral functional differential equation, as well, another class of history-dependent dynamical systems.

[1] Existence of erratic solutions to equations approximating the non-linearity in (13) are established in [MR1827805]

8 2D incompressible Navier-Stokes equations

We plan to carry out rigorous computations for the 2D incompressible Navier-Stokes equations. The strategy is to adapt an existing C++ software package dedicated to rigorous integration of dissipative partial differential equations, which has already been applied to several 1D PDEs: the Burgers equation, the Swift-Hohenberg equation and the Kuramoto-Sivashinsky equation. The rigorous integration process guarantees to include the exact solution in the output set. Whereas in any standard (non-rigorous) integration process, numerical analysis provides only asymptotic justification for the approximation method.

We also plan to explore issues in 2D turbulence. One approach is to carry out non rigorous computations with long time averaging and a stochastic force to see where the statistical steady state lands in the enstrophy,palinstrophy-plane. Another is to develop symbolic dynamics in that plane using differential inequalities that follow from energy-type estimates.

9 Maslov Index

The Maslov Index is a topological invariant that is well-known within the algebraic topology and geometry communities. Recently, it has attracted interest within the dynamical systems community due to its potential utility as a stability index. Being able to determine the stability of a given solution of a PDE is important, because it is typically the stable solutions that attract nearby data, thus determining the long-time evolution of the system. Recently it has been shown that, for certain self-adjoint linear operators obtained by linearizing a PDE about a stationary solution of interest, the number of unstable (positive) eigenvalues can be determined by computing the Maslov index of an appropriately defined path of Lagrangian planes associated with the linearized evolution. Thus, being able to compute the Maslov index enables one to determine the stability of the solution. This is very promising from an abstract point of view, but it does not necessarily provide a way to compute the Maslov index in practice for a given model. Therefore, the idea was to explore whether or not techniques from the theory of rigorous computation might be useful in this context.

Recently, numerical evidence has been obtained suggesting that the Maslov index is connected with singularities of solutions of a matrix Riccati equation that is determined by the linearized evolution. The thinking was that it might be easier compute the Maslov index by computing solutions of this Riccati equation, rather than taking a more direct approach. The reason is that existing numerical techniques for computing the Maslov index involve the exterior algebra, which, for an n-dimensional system, requires a computation involving a number of variables that grows exponentially in n. On the other hand, computing the evolution of the matrix Riccati equation involves only n^2 variables, with the trade-off being that now one must deal with the singularities of solutions.

After discussions during the workshop, the general opinion was that perhaps it was not natural to study an object (solutions to the matrix Riccati equation) that possess singularities that are effectively artificially introduced. Understanding such singularities and the precise way in which they are connected with the Maslov index count seems potentially challenging from both a theoretical and computational point of view. An alternative approach that was suggested was to lift the calculation to an appropriate universal covering space, in which the singularities are absent.

10 Boundary value problems

Our motivation to consider boundary value problems is that we would like to solve

- connecting orbits problems in infinite dimensional systems;
- non-periodic boundary value problems for (elliptic) PDEs.

The first of these problems naturally splits into two parts: parametrizing (or in some other way dealing with) the local stable and unstable manifolds of the equilibria, and the transition between these two (local) invariant manifolds. The latter part thus reduces to a boundary value problem. Notice that the connecting orbits that appear in ill-posed problems also fit into this setting.

As an example, we focus on reaction-diffusion problems of the form

$$\begin{cases} u_t(t,x) = u_{xx}(t,x) + f(u(t,x)) \\ u \text{ periodic in } x \\ B[u(0,x), u(1,x)] = 0. \end{cases}$$

where B represents the boundary conditions (including the special case of the initial value problem $u(t_0,x) = u_0(x)$). From a scientific computing perspective it is natural to try to solve such a problem using a Fourier-Chebyshev expansion. However, it is not straightforward to make that basic idea rigorous.

In order to highlight the obstacles, consider the equivalent problem after Fourier transforming in the spatial variable x:

$$\begin{cases} \frac{da_k}{dt}(t) = -k^2 a_k(t) + N(a(t)) \\ \tilde{B}[a(0), a(1)] = 0. \end{cases}$$

Viewing this as an infinite system of ODEs and trying to deal with the time variable using a Chebyshev expansion, as was very successfully implemented for finite systems of ODEs recently, one runs into difficulties. Roughly speaking, the higher the wave number k, the more Chebyshev modes are needed for the rigorous estimates. On the other hand, it is natural from a PDE perspective to use the dissipativity (or ellipticity) of the problem to somehow deal with the "high" Fourier modes. Hence one is lead to a description in terms of a splitting between low and high Fourier modes. The low modes can then be treated as a finite system of ODEs, weakly influenced by the high modes, while the high modes are controlled via dissipativity, with their small amplitudes being "slaved" by the low modes.

Of course all of this needs to be made precise. To mention just one additional difficulty, the low modes can in fact not be treated as a generic low-dimensional system of ODEs. In a naive implementation, for "intermediate" Fourier modes, the ones that you compute with but have (relatively) high wave number, one would need too many Chebyshev modes to get good estimates. One natural idea to overcome this is to use, for these intermediate modes, a formulation in terms of a variation of constants formula. However, this requires revisiting the Chebyshev convolution estimates, which now no longer follow directly from the "Chebyshev is Fourier in disguise" paradigm, that was so successfully exploited in the ODE setting (as mentioned previously).

We now go into some more details of the above mentioned example equation. As a first step we focus on the initial value problem. Let us write

$$\dot{a}_k = \mu_k a_k + N(a) \quad k \geq 0,$$

where $\lim_{k\to\infty} \mu_k = -\infty$. The idea of the splitting is to divide the set of ODEs into a finite dimensional part and an infinite dimensional tail part to be controlled by using the dissipativity of the equation. More concretely we get for the finite dimensional part $a_F = (a_0, \ldots, a_{m-1})$

$$\dot{a}_F = L_F(a_F) + N_F(a).$$

By rewriting this set of ODEs as an integral equation this part can be tackled by using Chebyshev series in time. Potentially this will have to be revisited to overcome the difficulty stemming from the high wave numbers alluded to above. For the infinite tail part $a_I = (0, \ldots, 0, a_m, \ldots)$

$$\dot{a}_I = L_I a_I + N_I(a)$$

we
aim to use a reformulation geared towards using an argument based on the Picard iteration.

Model ODE As a starting point we consider a 2D ODE system of the form

$$\begin{aligned}\dot{u} &= -k_1 u + h(u, v)\\ \dot{v} &= -k_2 v + g(u, v)\end{aligned}$$

where $k_1, k_2 > 0$ with $k_1 \ll k_2$ as a structural model. The functions h, g encode the nonlinearities. The idea behind this is that the linear part in the higher Fourier modes will dominate the linear part in the lower Fourier modes. Next we reformulate the second component in the following way as fixed point equation:

$$v(t) = e^{-k_2(t+1)} v(-1) + \int_{-1}^{t} e^{k_2(s-t)} g(u(s), v(s)) ds. \tag{14}$$

Using a Chebyshev expansion of $u = \sum_{k\geq 0} a_k T_k(t)$ and $v = \sum_{k\geq 0} b_k T_k(t)$ we get an expansion for

$$u(t) - u(-1) - \int_{-1}^{t} -k_1 u(s) + h(u(s), v(s)) ds$$

of the form

$$\sum_{k\geq 0} f_k(a, b) T_k(t).$$

By construction we then need to solve for a, b such that $f(a, b) = (f_k(a, b))_{k\geq 0} = 0$. Next we set up a fixed point operator T on the space

$$\Omega^s \times C([-1, 1]).$$

The operator T splits into two parts

$$T = T_{\Omega^s} \oplus T_C,$$

where T_{Ω^s} a Newton-like fixed point operator as used before and T_C is given by (14). In order to obtain more regularity for v we can first solve the second fixed point equation treating u as a parameter, and then plug in this solution into the first equation and solve for its fixed point.

11 Dynamics of the Diblock Copolymer Model

Diblock copolymers are formed by the chemical reaction of two linear polymer blocks which contain different monomers. These blocks are often thermodynamically incompatible, which means that following the reaction the blocks may be compelled to separate, despite already being covalently bonded – and these competing effects lead to microphase separation. Ohta and Kawasaki [ohta:kawasaki:86] and Bahiana and Oono [bahiana:oono:90a] proposed the partial differential equation

$$\begin{aligned} u_t &= -\Delta\left(\epsilon^2\Delta u + f(u)\right) - \sigma(u-\mu) \\ &\quad \text{subject to} \quad \mu = \int_\Omega u(x)\,dx\;, \quad \text{and} \quad \frac{\partial u}{\partial\nu} = \frac{\partial\Delta u}{\partial\nu} = 0\;, \quad x\in\partial\Omega\;, \end{aligned}$$

as a model for this separation process. In this model, the function u can be thought of as the difference in concentrations between the two polymer blocks, with the value 1 being interpreted as only block A being present at a point, and the value -1 being interpreted as only block B being present. The nonlinearity f is the negative derivative of a standard double-well potential F, i.e., $f(u) = u - u^3$. Generally, one is interested in results for small values of the dimensionless parameter $\epsilon > 0$ which models interaction length. The equation is a gradient system with respect to the energy functional

$$E_{\epsilon,\sigma}[u] = \int_\Omega \left(\frac{\epsilon^2}{2}|\nabla u|^2 + F(u)\right)dx + \frac{\sigma}{2}\int_\Omega \left|(-\triangle)^{-1/2}(u(x)-\mu)\right|^2 dx\;.$$

For the case of the one-dimensional diblock copolymer model, i.e., for the case $\mu = 0$, $\sigma > 0$, and $\Omega = (0,1)$, Ren and Wei [Ren:2003p16] have shown that the global minimizer of the diblock copolymer energy is in general uniquely determined up to multiplication by -1, and is periodic with minimal period $P^{\epsilon,\sigma}$ satisfying

$$P^{\epsilon,\sigma} = 2\left(3\sqrt{2}A\frac{\epsilon}{\sigma}\right)^{1/3} + O\left(\epsilon^{2/3}\right) \qquad \text{for} \qquad \epsilon\to 0\;,$$

where $A = 4\int_{-1}^{1}\sqrt{F(s)}\,ds = 8/3$. In other words, asymptotically for large integers k, the global energy minimizer has a wave number k (i.e., it is qualitatively like $\cos k\pi x$), if the interaction parameters $\lambda = 1/\epsilon^2$ and σ satisfy

$$\sigma\sqrt{\lambda} \;\approx\; 96\sqrt{2}\cdot\frac{2}{3}\cdot\left(\frac{k}{2}\right)^3 \;=\; 8\sqrt{2}\cdot k^3\;.$$

Thus, for small values of ϵ the global minimizers of the diblock copolymer energy exhibit fine structure, i.e., periodicity with large wave number k. In addition, it was shown [nishiura:ohnishi:98a, nishiura:02a] that in the limit $\epsilon\to 0$ the number of local minimizers of the energy functional $E_{\epsilon,\sigma}$ converges to ∞. These results are in stark contrast to the Cahn-Hilliard case $\sigma = 0$. It is known [grinfeld:novickcohen:95a] that the one-dimensional Cahn-Hilliard model has only two stable equilibrium solutions with exactly one transition layer each. One of these solutions is increasing, while the other one is decreasing.

This discussion raises two natural questions. On the one hand, which mechanism introduces numerous stable solutions into the equilibrium structure of the diblock copolymer equation as σ is increased from zero? On the other hand, how do these changes affect the long-term dynamics of solutions which originate close to the unstable homogeneous equilibrium?

In particular, while generic solutions of the Cahn-Hilliard model always converge to the global energy minimizer, can the same be said for the diblock copolymer model?

While some of these problems were considered in the recent paper [johnson:etal:13a], much of the study in this paper was purely numerical and it was only able to address some of the above questions. During the workshop, progress was made both towards providing computer-assisted proofs to some numerical observations in [johnson:etal:13a] and towards addressing some of the remaining more global questions:

- The numerical results in [johnson:etal:13a] have shown that the first quadrant in the λ-σ-plane ($\lambda = 1/\epsilon^2$) can be divided into clearly delineated regions which give the periodicity of the observed final state if a solution originates close to the homogeneous equilibrium state. These curves have been identified as location curves of certain secondary bifurcation points. During the workshop we could set up extended systems which use ideas from equivariant bifurcations, and which have the potential to lead to rigorous path-following by extending the ideas of [MR2630003].
- The most interesting question is the rigorous determination of connecting orbits from the homogeneous state to the local energy minimizers and their global bifurcations. Two possible avenues have been proposed:
  - As a starting point, one can consider projections of the infinite-dimensional dynamics on finite-dimensional inertial manifolds. Studies during the workshop have shown that for a reasonable parameter range, few dimensions suffice to give a qualitative description of the projected dynamics. The plan is to use the methods in [MR2821596] to study these finite-dimensional reductions rigorously. The long-term challenge to extend these methods to the infinite-dimensional case is the precise description of stable manifolds.
  - The second proposed approach is based on direct simulation using the CAPD library. Due to the low-dimensional projections mentioned before, the contraction in higher Fourier modes should be strong enough to make this possible.

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