Rigorous Numerics and Computer Assisted Proofs for Dynamical Systems

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Applications of Formal Methods to Control Theory and Dynamical Systems
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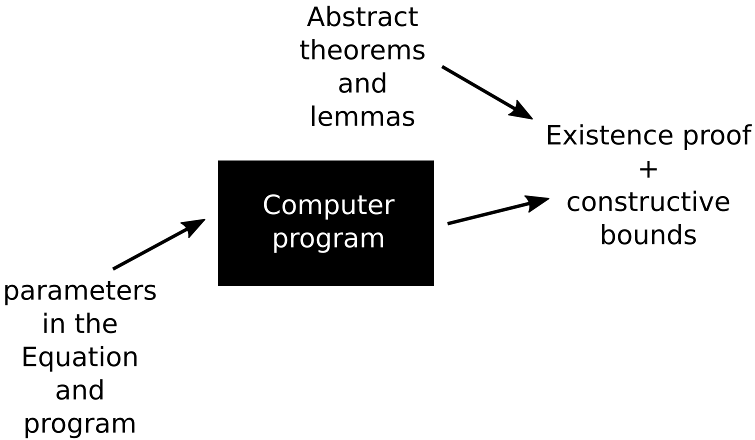
Abstract theorems and lemmas
Computer program
Existence proof + constructive bounds
parameters in the Equation and program

Why we do this?

+ Achieve proofs of existence of some particular solutions, that are hard/impossible using known analytical techniques,
− Proofs are usually obtained only for a set (compact) of parameter values in the equation.

We base our Rigorous Methods on existing standard numerical methods

- Runge-Kutta methods,
- Taylor method,
- Fourier spectral method,
- Chebyshev polynomials.

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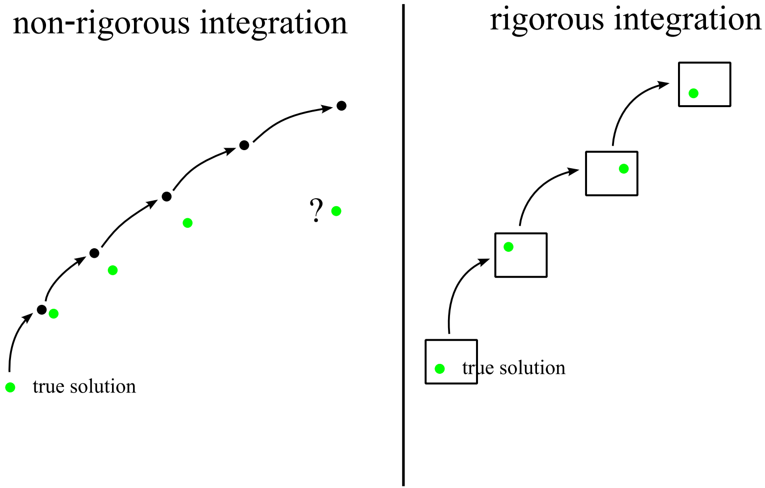
Rigorous integration



Simplest rigorous integration procedure due to *Gronwall lemma*

$$u'(t) = F(u(t)),$$

Assume there exists $L > 0$ – global *Lipshitz constant* of F

$$u'(t) \leq \beta(t)u(t) \leq L \cdot u(t),$$

then we have

$$u(t+h)^+ \leq u(t)^+ \cdot e^{\int_t^{t+h} \beta(s)u(s)\,ds} \leq u(t)^+ \cdot e^{Lh},$$

and

$$e^{Lh} > 1,$$

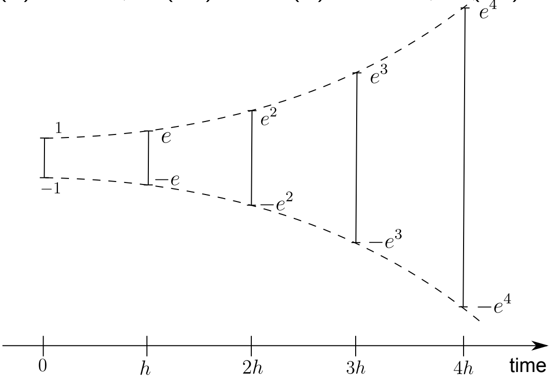
We get exponential explosion of bounds.

But exponential explosion $\neq$ the true solution is unbounded.

$$x = -1000 \cdot x, \quad x(0) = [-1, 1], \quad h = 0.001, \quad L = 1000,$$

hence

$$u(h)^+ \leq u(0)^+ e = e, \;\; u(2h)^+ \leq u(h)^+ e = e^2, \;\; u(3h)^+ \leq u(2h)^+ e = e^3,$$



Classical Taylor method of solving ODEs

The system of ODEs

$$x'(t) = F(x(t)).$$

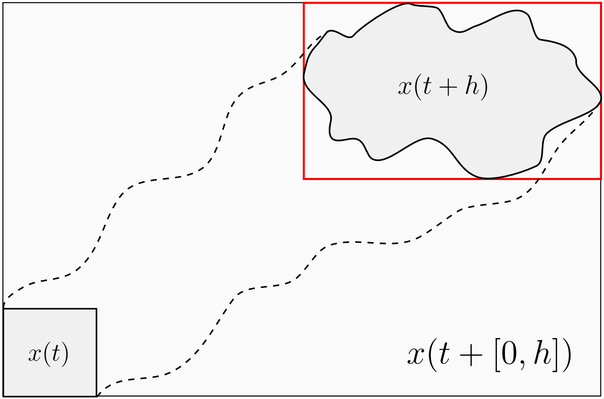
Can be solved using the classic Taylor method, the solution is given by the finite polynomial

$$x(t+h) = x(t)+x'(t)h+\frac{x''(t)}{2!}h^2+\cdots+\frac{x^{(p)}(t)}{p!}h^{(p)}+\underbrace{\frac{x^{(p+1)}(\xi)}{(p+1)!}h^{(p+1)}}_{\text{Remainder term}},$$

where $\xi \in [t, t+h]$.

In our case $[x(t)]$ is a vector of intervals, we define interval Taylor method, but do not evaluate it directly

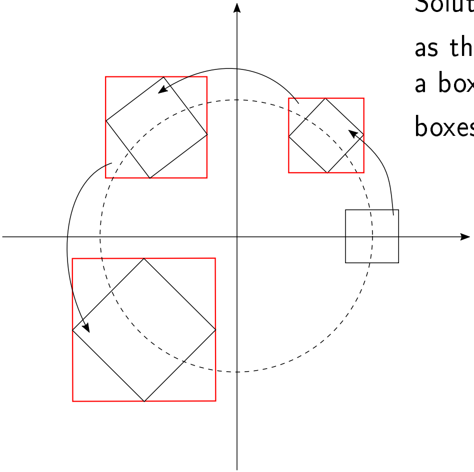
$$\Phi_p([x(t)], h) = [x(t)] + [x'(t)]h + \frac{[x''(t)]}{2!}h^2 + \cdots + \underbrace{\frac{[x^{(p+1)}([t, t+h])]}{(p+1)!}h^{(p+1)}}_{\text{Remainder term}}$$



Wrapping effect

Consider 2D ODEs

$$x' = -y,$$
$$y' = x.$$



Solution trajectories are circles,

as the initial condition we set use a box,

boxes get rotated.

Lohner algorithm – Avoiding the wrapping effect by proper representation

R.J. Lohner. *Computation of Guaranteed Enclosures for the Solutions of Ordinary Initial and Boundary Value Problems*, Computational Ordinary Differential Equations, J.R. Cash, I. Gladwell Eds., Clarendon Press, Oxford, 1992.

$$\begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} * \begin{bmatrix} [-1,1] \\ [0,1] \\ [-1,0] \end{bmatrix} = \begin{bmatrix} [-1,1] \\ [-1,2] \\ [-2,1] \end{bmatrix}$$

(Taylor models) – Taylor series expansion in time and space

M. Berz and K. Makino. *Verified integration of odes and flows using differential algebraic methods on high-order Taylor models*. Reliable Computing, 4(4):361–369, 1998.

Yet another way of reducing the wrapping effect

Julien Alexandre Dit Sandretto, Alexandre Chapoutot, *Validated Explicit and Implicit Runge-Kutta Methods*, Reliable Computing electronic edition, 2016.

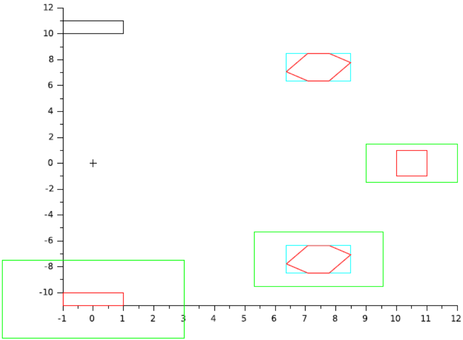


Figure 5.1: Wrapping effect comparison (black: initial, green: interval, blue: interval from QR, red: zonotope from affine)

Affine form $\hat{x}$ (also called a *zonotope*) $\hat{x} = \alpha_0 + \sum_{i=1}^{n} \alpha_i \varepsilon_i$.

Lagrangian reachability

Jacek Cyranka, Md. Ariful Islam, Scott A. Smolka, Sicun Gao, Radu Grosu, *Tight Continuous-Time Reachtubes for Lagrangian Reachability*, submitted 2018.

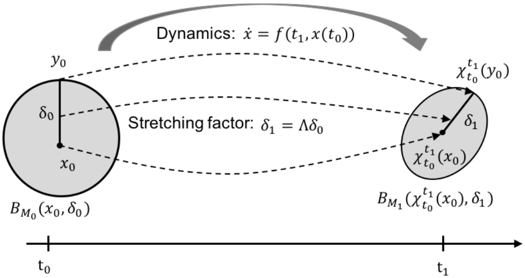


Figure 1: Illustration of LRT algorithm – construction of discrete tube

In LRT the wrapping effect is avoided by computing the optimal metric minimizing the *stretching factor* (denoted $\hat{A}_1$).

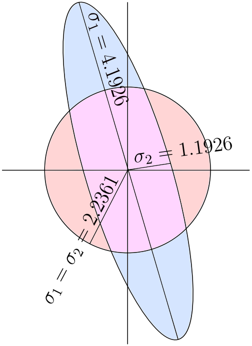


Figure 2: SF $\equiv$ σ_1 (the largest singular value).
Illustration for $F = \begin{bmatrix} 1 & 1 \\ -4 & 1 \end{bmatrix}$. SVD decomposition of F reveals it rotates and transforms unit disc into blue ellipse ($\sigma_1 = 4.1926$, $\sigma_2 = 1.1926$), resp.
SVD of $\hat{A}_1 F \hat{A}_1^{-1}$ reveals $\sigma_1 = \sigma_2 = 2.2361$.

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Example 1. Proof of the heteroclinic connections in the 1D Ohta-Kawasaki (diblock copolymers) model, *joint with Thomas Wanner*

J. Cyranka, T. Wanner. *Computer-assisted proof of heteroclinic connections in the one-dimensional Ohta-Kawasaki model*. SIAM Journal on Applied Dynamical Systems (SIADS), 2018, 17(1), 694 -731.

Motivation I

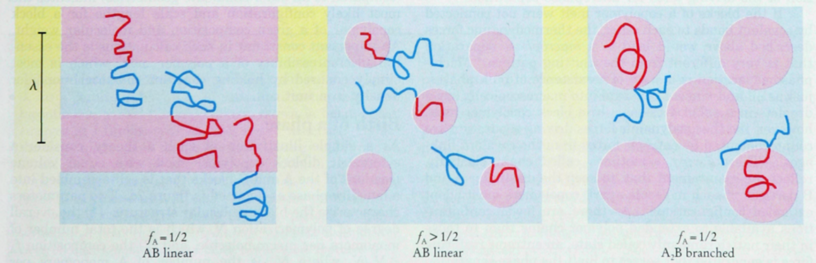


FIGURE 2. DIBLOCK MORPHOLOGY depends on block composition. Interfacial curvature of block copolymers can be controlled by adjusting the composition f or changing the molecular architecture. Shaded regions are block-segregated microdomains colored according to monomer type, with blue for type A and red for type B monomers. **a:** Self-assembly of symmetric ($f_A = f_B = 1/2$) linear AB diblocks leads to a lamellar morphology. **b:** Increasing the volume fraction of one block (in this case, $f_A > 1/2$) induces interfacial curvature, resulting in a nonlamellar morphology, such as cylindrical or spherical. **c:** A branched A_2B architecture can result in a nonlamellar morphology even in a compositionally symmetric molecule, due to asymmetric interfacial crowding.

Case study – a heteroclinic connection

Ohta-Kawasaki diblock copolymer model

$$u_t = -\Delta(\Delta u + \lambda f(u)) - \lambda\sigma(u - \mu),$$
$$\mu = \int_\Omega u(x)\, dx,$$
$$\frac{\partial u}{\partial n} = \frac{\partial \Delta u}{\partial n} = 0, \quad x \in \partial\Omega.$$

there are two *monomers* A,B.
$u(x) \in [-1, 1]$ – *monomer* ratio at $x \in \Omega$, where
$u(x) == 1$ only A(B), and $u(x) == -1$ only B(A),
$u(x) == 0$ the perfect mixture of A and B.

Fix $\mu = 0$ means constant in time, equal total amount of A and B.

Some related works

Introduction of the model

T. Ohta and K. Kawasaki. *Equilibrium morphology of block copolymer melts.* Macromolecules, 19:2621–2632, 1986.

M. Bahiana and Y. Oono. *Cell dynamical system approach to block copolymers.* Physical Review A, 41:6763–6771, 1990.

Numerical study

Ian Johnson, Evelyn Sander, and Thomas Wanner. *Branch interactions and long-term dynamics for the diblock copolymer model in one dimension*. Discrete and Continuous Dynamical Systems, 33(8):3671–3705, 2013.

Our methods

P. Zgliczyński, *Covering relations, cone conditions and stable manifold theorem* , J. of Diff. Equations 246 (2009) 1774–1819.

J. Cyranka, *Efficient and generic algorithm for rigorous integration forward in time of dPDEs: Part I*. Journal of Scientific Computing, 59(1):28–52, 2014.

The studied problem

We study equation on interval in 1D The domain is

$$\Omega = [0, L].$$

and Neumann's boundary condition

$$u_x = u_{xxx} = 0, \quad x = 0, L.$$

And we use the cosine Fourier basis

$$u(t,x) = a_0(t) + 2\sum_{k>0} a_k(t)\cos\frac{\pi}{L}kx$$

The equation becomes the infinite system of equations

$$\frac{da_k}{dt} = \left[-k^2\left(\frac{\pi}{L}\right)^2\left(k^2\left(\frac{\pi}{L}\right)^2 - \lambda\right) - \lambda\sigma\right]a_k - \lambda k^2\left(\frac{\pi}{L}\right)^2 \sum_{\substack{l,m,n\in\mathbb{Z}\\ l+m+n=k}} a_l a_m a_n$$

all coefficients $\{a_k\}$ are real due to the boundary condition, and $a_k = \overline{a_{-k}}$ due to the reality constraint.

Main result

We prove

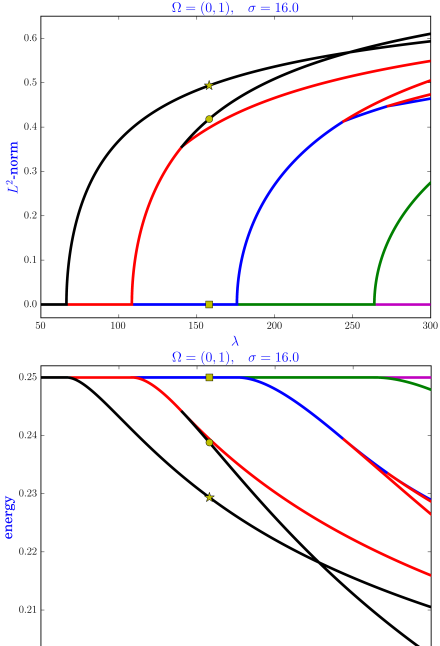
Theorem (Existence of heteroclinic connections)

Consider the diblock copolymer equation on the one-dimensional domain $\Omega = (0, 1)$*, for interaction lengths* $\lambda = 1/\epsilon^2 = 16\pi^2$ *and* $\sigma = 16$*, and for total mass* $\mu = 0$*. Then there exist*

- *heteroclinic connections between the unstable homogeneous stationary state* $u \equiv 0$ *and each of the two local energy minimizers,*
- *heteroclinic connections between the unstable homogeneous stationary state and each of the two suspected global energy minimizers.*

In other words, for the above parameter values the diblock copolymer equation exhibits multistability in the sense that all local or global energy minimizers can be reached from the homogeneous state.

Bifurcation diagram



Functional space

Definition (Sequence space with algebraic coefficient decay)

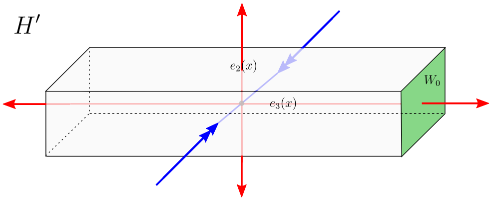
Let H denote the space $\ell^2(\mathbb{Z},\mathbb{R})$. In addition, let $\widetilde{H} \subset H$ denote the subspace of H which is defined by

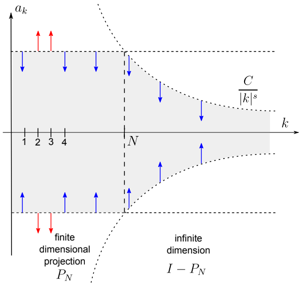
$$\widetilde{H} := \left\{ \{a_k\} \in H \colon \; \text{there exists a } C \geq 0 \text{ such that } |a_k| \leq \frac{C}{\nmid k \nmid^6} \right\} ,$$

where $\nmid x \nmid = |x|$ for $x \neq 0$ and $\nmid 0 \nmid = 1$.

Structure of the proof. Step 1

1. Construct $\mathcal{W}_\mathsf{u}$ – an isolating block about zero (the unstable homogenous state). Additionally verify a *cone condition*





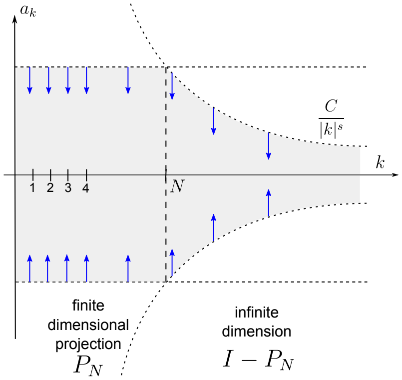
$$\mathcal{W}_{\mathbf{u}} \subset H'$$

k	$\mathbf{a_k}$ interval in the form center + radius
1	$0 + [-2.365, 2.365]10^{-16}$
2	$0 + [-1, 1]10^{-12}$
3	$[-\mathbf{0.075}, \mathbf{0.075}]$
$\ldots$	$\ldots$
$4 - 75$	small intervals of width $\leq 10^{-15}$
≥ 76	$< 1.393 \cdot 10^{-46}/k^6$

The infinite-dimensional cone condition is satisfied with $\varepsilon = 0.08478$.

Step 2

2. Construct $\mathcal{W}_s$ – an isolating block about the stable steady state. Additionally verify the *negativeness of logarithmic norm*.

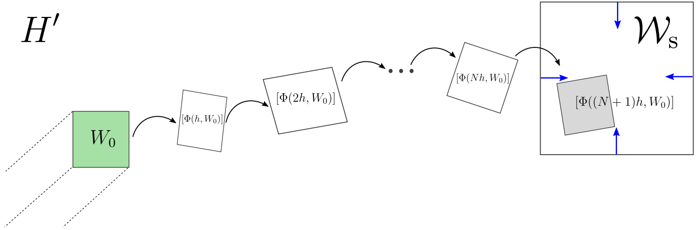


k	a_k
1	$3.321 \cdot 10^{-18} + [-6.895, 6.895]10^{-6}$
2	$8.18 \cdot 10^{-17} + [-1.691, 1.691]10^{-4}$
3	$\mathbf{0.2956 + [-1.031, 1.031]10^{-5}}$
...	...
$4 - 250$	intervals of small width
≥ 251	$< 6.947 \cdot 10^{-38}/k^6$

The infinite-dimensional cone condition is satisfied with $\varepsilon = 0.03816$,

Step 3

3. Rigorously integrate forward in time the face of $\mathcal{W}_\mathrm{u}$, denoted W_0.
If after a finite time the result is mapped into $\mathcal{W}_\mathrm{s}$, the existence of a heteroclinic connection is established.



The infinite-dimensional bounds at time $T = 3.02$ after performing 1510 numerical integration steps (with timestep 0.002) are

k	$\mathbf{a_k}$
1	$-1.014 \cdot 10^{-8} + [-1.49, 1.49]10^{-7}$
2	$1.454 \cdot 10^{-7} + [-2.748, 2.748]10^{-7}$
3	$\mathbf{0.2956 + [-8.522, 8.522]10^{-9}}$
4	$-1.293 \cdot 10^{-7} + [-1.183, 1.183]10^{-7}$
...	...
$5 - 200$	intervals of smaller width
≥ 201	$< 3.295 \cdot 10^{-44}/k^6$

The bounds above are within the set $\mathcal{W}_s$, i.e., within the basin of attraction of the stable fixed point.

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Possible applications of formal methods.

1. The numerical program performing the computations is very long and complicated, the resulting bounds should be checked for correctness a-posteriori using formal methods,
2. Formalize a proof that the outputted bounds contain an approximate solution of the equation with any precision,
3. Formalize a proof that the bounds contains the nonconstructive solution of the true PDE, realized by picking a convergent subsequence in a Banach space.