Rigorous numerics and computer assisted proofs for dissipative PDEs. Validated PDE solver, and what is needed to improve it

P. Zgliczyński
Jagiellonian University, Kraków, Poland
http://www.im.uj.edu.pl/~zgliczyn
Outline of this talk

1. Model problem - Kuramoto-Sivashinsky Eq.

2. Method of self-consistent bounds

3. Algorithm for generation of self-consistent bounds

4. Lohner-type algorithm for integration of differential inclusion

5. Some data from the proofs

6. Conclusions
Consider the Kuramoto-Sivashinsky (KS) eq. \( u_t = -\nu u_{xxxx} - u_{xx} + 2uu_x \)
where \((t, x) \in [0, \infty) \times \mathbb{R}\) subject to periodic and odd boundary conditions
\[
\begin{align*}
  u(t, 0) &= u(t, 2\pi) \\
  u(t, -x) &= -u(t, x)
\end{align*}
\]

For various values of \( \nu \) a variety of dynamics, fixed points, periodic orbits, heteroclinic orbits, chaotic dynamics, have been observed numerically.

**Goal:** A rigorous means of proving these numerical results.
A Model Problem - Kuramoto-Sivashinsky PDE, known results

Known results:

• an existence of global attractor, the functions from attractor are analytic - Fourier series converge at geometric rate

• an existence of finite dimensional inertial manifold

No results on dynamics more complicated than fixed points
Our rigorous results for Kuramoto-Sivashinsky PDE

• proof of an existence of a nontrivial periodic orbit for $\nu = 0.127$

• proof an existence of multiple fixed points for various values of $\nu$

• proof an existence of attractive fixed points for various values of $\nu$

Soon (hopefully):

• rigorous steady states bifurcation diagram for KS PDE

• a proof of an existence of chaotic dynamics for $\nu \approx 0.03$
About the method

- self-consistent bounds - a kind of approximate inertial manifold approach

- finite dimensional tools from dynamics

- computer assisted

An existence and uniqueness theorems are not required to apply the method

could be applied to other dissipative PDEs: Ginzburg-Landau, Navier-Stokes in 2D and 3D
A Model Problem - Kuramoto-Sivashinsky
PDE, Fourier expansion

Fourier expansion is: \( u(t, x) = \sum_{k=-\infty}^{\infty} b_k(t) e^{ikx} \)

Substituting in KS and applying boundary conditions gives:

\[
\dot{a}_k = k^2(1-\nu k^2)a_k - k \sum_{n=1}^{k-1} a_n a_{k-n} + 2k \sum_{n=1}^{\infty} a_n a_{n+k}
\]

where \( b_k = i a_k \) and \( k = 1, 2, 3, \ldots \).

Linearization: \( \dot{a}_k = k^2(1 - \nu k^2)a_k \)

- \( k \)-th mode is unstable for \( k < \frac{1}{\sqrt{\nu}} \)
- \( k \)-th mode is stable for \( k > \frac{1}{\sqrt{\nu}} \)
- the modes with \( k \gg \frac{1}{\sqrt{\nu}} \) should be irrelevant for the dynamics
The method of self-consistent bounds

$H$ - Hilbert space,
$e_1, e_2, \ldots$ - an orthogonal basis in $H$

The corresponding projections are

$$p_m = P_{ma} := (a_1, a_2, \ldots, a_m)$$
$$q_m = Q_{ma} := (a_{m+1}, a_{m+2}, \ldots)$$

The problem:

$$\dot{a} = F(a)$$  (1)

$F$ is not continuous, with dense domain in $H$.

$F_k \circ P_n$ is a $C^1$-function for $n, k \in \mathbb{N}$

Later $F(a) = L(a) + N(a)$, $L$ - linear, $N$ - non-linear

$e_1, e_2, \ldots$ - eigenvectors of $L$ - very helpful
The method:

1. Find self-consistent a-priori bounds. Fix \( m, M \) (\( m \leq M \)). A compact set \( W \subset P_m(H) \) and a sequence of pairs \( \{a_k^\pm \in \mathbb{R} | a_k^- < a_k^+, k \in \mathbb{Z}^+ \} \) form self-consistent a-priori bounds if:

\[ \text{C1} \quad \text{For } k > M, a_k^- < 0 < a_k^+. \]

\[ \text{C2} \quad \text{Let } \hat{a}_k := \max |a_k^\pm| \text{ and set } \hat{u} = \sum_{k=0}^\infty \hat{a}_k e_k. \text{ Then, } \hat{u} \in H, \{\hat{a}_k\} \in l_2. \]

\[ \text{C3} \quad \text{The function } u \mapsto F(u) \text{ is continuous on } \]

\[ W \oplus \prod_{k=m+1}^\infty [a_k^-, a_k^+] \subset H. \]

Moreover, if we define

\[ \hat{f}_k = \max_{u \in W \oplus \prod_{k=m+1}^\infty [a_k^-, a_k^+]} |A_k F(u)| \quad \text{and} \]

set \( \hat{f} = \sum \hat{f}_k e_k, \text{ then } \hat{f} \in H. \{\hat{f}_k\} \in l_2. \)

Notation: \( T = \prod_{k=m+1}^\infty [a_k^-, a_k^+] \) - Tail
ISOLATION for \( n > m \)

For \( a \in W \oplus T \) and \( k > m \) holds

\[
\begin{align*}
    a_k &= a_k^+ \quad \Rightarrow \quad \dot{a}_k < 0 \\
    a_k &= a_k^- \quad \Rightarrow \quad \dot{a}_k > 0
\end{align*}
\]
2. Finite dimensional rigorous computations in $m$ first variables

Basic Differential Inclusion:

$$\dot{p} \in P_m F(p) + R_m, \quad p \in \mathbb{R}^m,$$

(2)

where $R_m = \{P_m F(p) - P_m F(p + q) \mid q \in T\}$

Theorem: If $p_I : [0, t_1] \to X_m = P_m(H)$ is a solution of (2), such that $p_I([0, t_1]) \subset W$.

Then for any $p_0 \in p_I(t)$ and $q_0 \in T$, the problem $u' = F(u)$ (and all its Galerkin projects $u' = P_n(u)$, $n \geq m$) has a solution $u(t) = (p(t), q(t))$ for $t \in [0, t_1]$, such that

$$p(t) \in p_I(t), \quad q(t) \in T, \quad \text{for } t \in [0, t_1]$$
3. Extracting dynamics of PDE from topological information about the Galerkin projections

\[ N \oplus \prod_{j=m+1}^{k} [a_j^-, a_j^+] \] is an isolating block for \( k \)-dimensional projection of \( \dot{u} = F(u) \) and the same index (a kind of topological information)

If an index is nontrivial, then we have an existence of fixed point (periodic orbit, etc) for each \( k \)-dimensional Galerkin projection.

In the limit \( k \to \infty \) we obtain a fixed point for \( \dot{u} = F(u) \) (periodic orbit or other phenomena we looking for and which survive the passage to the limit).
The method - comments

• \( m \) and \( W \subset P_m(H) \) - chosen so that, the interesting dynamics is in \( W \) for \( n \)-dimensional Galerkin projections \( n \geq m \)

• conditions \( C1, C2, C3 \) have nothing to do with the dynamics, \( a_{k}^{\pm} \) have to decay fast enough

• \( \max_{a \in W \oplus T} |F(a) - F(P_n(a))| \to 0, \ n \to \infty \)

• \( (I - P_n)W \oplus T \to 0, \ n \to \infty \)

• satisfying \( C1, C2, C3 \) and an isolation for \( k > m \) is relatively easy - we have an efficient algorithm

• Finding an isolation in first \( m \) variables is a difficult part of the problem
The method - getting more than $C^0$-properties

What other dynamical phenomena can be treated with this method?

We may need new assumptions.

• the stability (instability) of fixed points, periodic orbits

• bifurcations for fixed points, periodic orbits

• …*take any theorem from dynamical system theory and try to embed it into this framework*
Algorithm for generation of self-consistent a-priori bounds

\[ u_t = F(u) = Lu + N(u) \]  

\( L \)-linear, \( N \)-nonlinear.
\( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \) - eigenvalues of \( L \)
\( e_1, e_2, \ldots \) - eigenvectors

Fix \( m \), \( W \subset \mathbb{R}^m \) (\( m \)-big enough to reproduce dynamics of (*) ).
\( \lambda_{m+1} < 0 \)

Goal: Find \( T(tail) = \prod_{k=m+1}^{\infty} [a_k^-, a_k^+] \), such that C1, C2, C3 hold on \( W \oplus T \) and for each \( a \in W \oplus T \) and \( k > m \) we have isolation

\[ a_k = a_k^+ \quad \Rightarrow \quad \dot{a}_k < 0 \]
\[ a_k = a_k^- \quad \Rightarrow \quad \dot{a}_k > 0 \]
Data. \( T = \prod_{k=m+1}^{\infty} [a_k^-, a_k^+] \). \( Iso[k] \), \( i = m + 1, \ldots \),
\( Iso[k] = true \) iff isolation holds for \( k \)
\( Iso[k] = false \), otherwise.
Initialization. We choose \( T \), such that \( C1, C2, C3 \) are satisfied for \( W \oplus T \)
\( Iso[k] = false \), for all \( k > m \)
Iteration step. For each \( k \) we find
\[
c_k < N_k(u) < C_k, \quad \text{for all } u \in W \oplus T
\]
Hence
\[
\lambda_k(a_k + \frac{c_k}{\lambda_k}) < \frac{da_k}{dt} < \lambda_k(a_k + \frac{C_k}{\lambda_k})
\]
\[
 u_k = -\frac{C_k}{\lambda_k}, \quad d_k = -\frac{c_k}{\lambda_k}
\]
If \( u_k \leq a_k^+ \) and \( a_k^- \leq d_k \), then update:
\( Iso[k] = true \), \( [a_k^-, a_k^+] = [d_k, u_k] \).
Ending condition: \( Iso[k] = true \) for all \( k > m \).
In the actual implementation of the algorithm we cannot work with an infinite tail $T$ or an infinite table $Iso$. Instead we introduce another dimension cut-off $M$, $M > m$. The whole structure is represented as follows:

- tables $T^{\pm}[k]$, for $k = m + 1, n + 2, \ldots, M$,

- table $Iso[k]$ $m < k \leq M$

- constants $C \in \mathbb{R}^+$ and $s \in \mathbb{Z}^+$ describing $[a_k^-, a_k^+]$ for $k > m$ as follows
  \[ a_k^+ = -a_k^- = \frac{C}{k^s} \]

- a variable $IsoTail$, which is set to true if during iteration the isolation conditions are true for all $k > M$
Two Initial Estimates: (These are standard types of estimates for KS)

Theorem A: (There exists a compact global attractor) There exist constants $\rho_0$, $\rho_1$, and $T = T(u_0)$ such that for all $t > T$

$$\| u(t) \|_2 \leq \rho_0 \quad \text{and} \quad \| u_x(t) \|_2 \leq \rho_1.$$  
Furthermore, if $m^4 > \frac{1}{\nu^2}$ then

$$\limsup_{t \to \infty} \| q_m(t) \|_2 \leq \frac{4 \sqrt{2\pi \rho_0 \rho_1^3}}{(m + 1)^4 (\nu - (m + 1)^{-2})}$$

Theorem B: (Solutions on the attractor are smooth) $\forall s \in \mathbb{Z}^+$ there exists a constant $C_s$ such that $|a_k| \leq \frac{C_s}{k^s}$. 


Lohner-type algorithm for differential inclusion

\[ x'(t) = f(x(t), y(t)) \quad (3) \]

\( x \in \mathbb{R}^{n_1}, \ y(t) \in \mathbb{R}^{n_2} \) (we allow for \( n_2 = \infty \)).
Assume some knowledge about \( y(t) \), for example \( |y(t)| < \epsilon \) for \( 0 \leq t \leq T \).
Find a rigorous enclosure for \( x(t) \).

For a fixed \( y_c \in \mathbb{R}^{n_2} \) we compare the solutions of two ODEs

\[ x_1' = f(x_1, y_c), \quad (4) \]
\[ x_2' = f(x_2, y_c) + (f(x_2, y(t)) - f(x_2, y_c)), \quad (5) \]
\[ x_1(t_0) = x_2(t_0) = x_0 \quad (6) \]

where \( y(t) \) is given (but unknown) function.
Lohner-type algorithm for differential inclusion - Fundamental Lemma

**Lemma:** Let:

\[ W_y \subset \mathbb{R}^{n_2}, \text{ convex, } y([t_0, t_0 + h]) \subset [W_y]. \]

\[ W_1 \subset [W_2] \subset \mathbb{R}^{n_1} - \text{ convex and compact.} \]

\[ x_1([t_0, t_0 + h]) \subset [W_1], \ x_2([t_0, t_0 + h]) \subset [W_2] \text{ for any continuous function } y : [t_0, t_0 + h] \rightarrow [W_y]. \]

Then the following inequality holds for \( t \in [t_0, t_0 + h] \) and for \( i = 1, \ldots, n_1 \)

\[
|x_{1,i}(t) - x_{2,i}(t)| \leq \left( \int_{t_0}^{t} e^{J(t-s)} C \, ds \right)_i,
\]

where

\[
[\delta] = \{ f(x, y_c) - f(x, y) \mid x \in [W_1], y \in [W_y] \},
\]

\[ C_i \geq \sup |[\delta_i]|, \quad i = 1, \ldots, n_1 \]

\[ J_{ij} \geq \sup \frac{\partial f_i}{\partial x_j}([W_2], [W_y]) \text{ if } i = j, \]

\[ J_{ij} \geq \sup \left| \frac{\partial f_i}{\partial x_j}([W_2], [W_y]) \right| \text{ if } i \neq j. \]
Lohner-type algorithm for differential inclusion - one step

\( \varphi(t, x_0, y_0) \) - a solution of \( x' = f(x, y) \), \( x(0) = x_0 \) and \( y(0) = y_0 \).

\( \bar{\varphi}(t, x_0, y_0) \) - a solution of \( x' = f(x, y) \), \( y' = 0 \), \( x(0) = x_0 \) and \( y(0) = y_0 \).

Let \( \pi_x : \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \) be a projection onto \( \mathbb{R}^{n_1} \), i.e. \( \pi_x(x, y) = x \).

**Input data:**

\( t_k, h_k \) - a time step,

\([x_k] \subset \mathbb{R}^{n_1}\), such that \( \pi_x \varphi(t_k, [x_0], [y_0]) \subset [x_k] \),

\([y_k] \) - bounds for \( y(t_k) \).

**Output data:**

\( t_{k+1} = t_k + h_k \),

\([x_{k+1}] \subset \mathbb{R}^{n_1}\), such that \( \pi_x \varphi(t_{k+1}, [x_0], [y_0]) \subset [x_{k+1}] \),

\([y_{k+1}] \) - bounds for \( y(t_{k+1}) \).
Lohner-type algorithm for differential inclusion - one step - details

1. Generation of a priori bounds for $\varphi$.
   Find a convex and compact set $[W_2] \subset \mathbb{R}^{n_1}$ and a convex set $[W_y] \subset \mathbb{R}^{n_2}$, such that
   \[
   \varphi([0, h_k], [x_k], [y_k]) \subset [W_2] \times [W_y]. \quad (8)
   \]

2. We fix $y_c \in [W_y]$.

3. Computation of $\overline{\varphi}$. We use Lohner algorithm to obtain $[\overline{x}_{k+1}] \subset \mathbb{R}^{n_1}$ and a convex and compact set $[W_1] \subset \mathbb{R}^{n_1}$, such that
   \[
   \pi_x \overline{\varphi}(h_k, [x_k], y_c) \subset [\overline{x}_{k+1}]
   \]
   \[
   \pi_x \overline{\varphi}([0, h_k], [x_k], y_c) \subset [W_1]
   \]
Lohner-type algorithm for differential inclusion - one step - details continued

4. Computation of perturbation. Using Fundamental Lemma we find a set $[\Delta] \subset \mathbb{R}^{n_1}$, such that

$$\pi_x \varphi(t_{k+1}, [x_0], [y_0]) \subset \pi_x \varphi(h_k, [x_k], y_c) + [\Delta].$$

Hence

$$\pi_x \varphi(t_{k+1}, [x_0], [y_0]) \subset [x_{k+1}] = [\bar{x}_{k+1}] + [\Delta]$$

(9)

5. Computation of $[y_{k+1}]$. This part is not necessary in the bounds for $y$ are known and fixed in advance.
Lohner-type..-details and comments

For dissipative PDE and self-consistent bounds \( W \oplus V, [W_y] = V \) and we have to satisfy the following

\[
[W_2] \subset W. \quad (11)
\]

The last condition is a consistency condition required by Basic Differential Inclusion, namely \([\delta]\) is computed under this assumption.

Part 4 - details

1. We set

\[
[\delta] = \{ f(x, y_c) - f(x, y) \mid x \in [W_1], y \in [W_y] \}\]

\( C_i = \text{right} (|[\delta_i]|), \quad i = 1, \ldots, n_1 \)

\( J_{ij} = \text{right} \left( \frac{\partial f_i}{\partial x_j} ([W_2], [W_y]) \right) \) if \( i = j \),

\( J_{ij} = \text{right} \left( \left| \frac{\partial f_i}{\partial x_j} ([W_2], [W_y]) \right| \right) \), if \( i \neq j \).

2. \( D = \int_0^h e^{J(h-s)} C \, ds \)

3. \([\Delta_i] = [-D_i, D_i] , \text{ for } i = 1, \ldots, n_1\)
Lohner-type - Computation of 
\[ \int_0^t e^{A(t-s)}C \, ds. \]

\[ \int_0^t e^{A(t-s)}C \, ds = t \left( \sum_{n=0}^{\infty} \frac{(At)^n}{(n+1)!} \right) \cdot C. \] (12)

We fix any norm \( \| \cdot \| \), preferably the \( L^\infty \)-norm, \((\|x\|_\infty = \max_i |x_i|)\).

\[ \tilde{A} = At, \quad A_n = \frac{\tilde{A}^n}{(n + 1)!}, \]
\[ \sum_{n=0}^{\infty} \frac{(At)^n}{(n + 1)!} = \sum_{n=0}^{\infty} A_n \]
\[ A_0 = \text{Id}, \quad A_{n+1} = A_n \cdot \frac{\tilde{A}}{n + 2} \]

Remainder: \( \|A_{N+k}\| \leq \|A_N\| \cdot \left\| \frac{\tilde{A}}{N+2} \right\|^k \cdot \left(1 - \| \frac{\tilde{A}}{N+2} \| \right)^{-1} \)
Lohner-type .. - Representation of sets and rearrangement.

Lohner’s approach.

In part 4:

\[ [x_{k+1}] = [\bar{x}_{k+1}] + [\Delta] \]  \hspace{1cm} (13)

**Evaluations 2 and 3.** In this representation

\[ [x_k] = x_k + [B_k][\tilde{r}_k]. \]  \hspace{1cm} (14)

In the context of our algorithm in part 3 we obtain

\[ [\bar{x}_{k+1}] = \bar{x}_{k+1} + [B_{k+1}][\tilde{r}_{k+1}]. \]  \hspace{1cm} (15)

We set

\[ x_{k+1} = m(\bar{x}_{k+1} + [\Delta]) \]  \hspace{1cm} (16)

\[ [\tilde{r}_{k+1}] = [\bar{r}_{k+1}] + [B_{k+1}^{-1}](\bar{x}_{k+1} + [\Delta] - x_{k+1}). \]
Lohner-type .. - Representation of sets and rearrangement II

**Evaluation 4.** In this representation

\[ [x_k] = x_k + C_k [r_0] + [B_k] [\tilde{r}_k]. \] (18)

In the context of our algorithm in part 3 we obtain

\[ [\bar{x}_{k+1}] = \bar{x}_{k+1} + C_{k+1} [r_0] + [B_{k+1}] [\tilde{r}_{k+1}]. \] (19)

Equation (13) is taken into account exactly in the same way as in previous evaluations, i.e. we use equations (16) and (17).
Computation of the Poincaré map

One needs a procedure which gives a rigorous estimates between time step for \( x \)-variable for perturbed ODE.

**Input parameters:** \( h_k \),

\([x_k] \subset \mathbb{R}^{n_1}, \pi_x \varphi(t_k, [x_0], [y_0]) \subset [x_k], \]

\([x_{k+1}] \subset \mathbb{R}^{n_1}, \pi_x \varphi(t_k + h_k, [x_0], [y_0]) \subset [x_{k+1}], \)

a convex and compact set \([W_2] \subset \mathbb{R}^{n_1} \) and a convex set \([W_y] \subset \mathbb{R}^{n_2} \), such that

\[
\varphi([t_k, t_k + h_k], [x_0], [y_0]) \subset [W_2] \times [W_y], \quad (20)
\]

\( y_c \in [W_y], \)

\([x_{k+1}] \subset \mathbb{R}^{n_1}, \) such that \( \pi_x \varphi(h_k, [x_k], y_c) \subset [x_{k+1}], \)

\([W_1] \subset \mathbb{R}^{n_1} \) compact and convex, such that \( \pi_x \varphi([0, h_k], [x_k], y_c) \subset [W_1]. \)

**Output:**

We compute \([E_k] \subset \mathbb{R}^{n_1} \) such that

\[
\pi_x \varphi(t_k + [0, h_k], [x_0], [y_0]) \subset [E_k],
\]
Algorithm:

- if $0 \notin f_i([W_2], [W_y])$, then $i$-th coordinate is strictly monotone on $[W_2] \times [W_y]$, hence we set

$$[E_k]_i = \text{hull}([x_k]_i, [x_{k+1}]_i)$$

- if $0 \in f_i([W_2], [W_y])$, then we compute $[\overline{E}_k] \subset \mathbb{R}^{n_1}$, such that

$$\pi_{x\varphi}([0, h_k], [x_k], y_c) \subset [\overline{E}_k]$$

using a procedure for an ODE. This procedure requires as input data: $h_k$, $[x_k]$, $[\overline{x}_{k+1}]$ and $[W_1]$.

$$\pi_{x\varphi}(t_k + [0, h_k], [x_0], [y_0])_i \subset [E_k]_i = [\overline{E}_k]_i + [\Delta]_i.$$

A drawback of this approach: if we have to perform several time steps during which computed enclosure for the trajectory has a nonempty intersection with the section, then $\Delta$ is added twice.
Lohner-type algorithm for differential inclusion - some remarks and problems

very good message - For $m \rightarrow \infty$ the error of Galerkin projection for $i-th$ coordinate

$$\max_{p \in W, q \in T} |F_i(p) - F_i(p + q)| \rightarrow 0$$

bad message - for $m$ large the time step is small due to presence of terms of the form $x'_n = -\lambda_n x_n$, where $\lambda_n \rightarrow \infty$ for $n \rightarrow \infty$. The coordinates inessential for the dynamics force very small time steps and large computation times.
Periodic point for KS-equation

**Theorem:** Let \( u_0(x) = \sum_{k=1}^{14} -2a_k \sin(kx) \), where \( a_k \) are given in table below. There exists a function \( u^*(t,x) \) a classical solution of KS for \( \nu = 0.127 \), such that

\[
\|u_0 - u^*(0,\cdot)\|_{L^2} < 5 \cdot 10^{-5}, \\
\|u_0 - u^*(0,\cdot)\|_{C^0} < 7 \cdot 10^{-5}
\]

such that \( u^* \) is periodic with respect to \( t \).

| \( a_1 \) | 2.012106e-01 |
| \( a_3 \) | 2.012109e-01 |
| \( a_5 \) | -4.230950e-02 |
| \( a_7 \) | 6.940217e-03 |
| \( a_9 \) | -7.944079e-04 |
| \( a_{11} \) | 7.939456e-05 |
| \( a_{13} \) | -7.087251e-06 |
| \( a_2 \) | 1.289980 |
| \( a_4 \) | -3.778662e-01 |
| \( a_6 \) | 4.316159e-02 |
| \( a_8 \) | -4.156484e-03 |
| \( a_{10} \) | 3.316061e-04 |
| \( a_{12} \) | -2.390962e-05 |
| \( a_{14} \) | 1.568377e-06 |
Conclusions

• a lot of dynamical system theory should be possible to be applied to dissipative PDEs within this framework

• rigorous numerics for dissipative PDEs is possible

• rigorous numerical finite time shadowing algorithms should be possible

• a global existence and uniqueness theorems are not required to apply the method, interesting solutions are constructed

• could be applied to (hopefully): Ginzburg-Landau, Navier-Stokes in 2D and 3D