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

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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

A Model Problem - Kuramoto-Sivashinsky PDE

Consider the Kuramoto-Sivashinsky (KS) eq.

$$u_t = -\nu u_{xxxx} - u_{xx} + 2uu_x$$

where $(t,x) \in [0,\infty) \times \mathbf{R}$ subject to periodic and odd boundary conditions

$$\begin{aligned} u(t,0) &= u(t,2\pi) \\ u(t,-x) &= -u(t,x) \end{aligned}$$

For various values of ν 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 ν
- proof an existence of attractive fixed points for various values of ν

Soon (hopefully):

- rigorous steady states bifurcation diagram for KS PDE
- a proof of an existence of chaotic dynamics for KS $\nu \approx 0.03$

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 $k >> \frac{1}{\sqrt{\nu}}$ should be irrelevant for the dynamics

The method of self-consistent bounds

H - Hilbert space,
$e_1, e_2, \dots$ - an orthogonal basis in H
The corresponding projections are

$$\begin{aligned} p_m = P_m a &:= (a_1, a_2, \dots, a_m) \\ q_m = Q_m a &:= (a_{m+1}, a_{m+2}, \dots) \end{aligned}$$

The problem:

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

F is not continuous, with dense domain in H.

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

Later $F(a) = L(a) + N(a)$, L - linear, N- non-linear
$e_1, e_2, \dots$ - 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* $\{a_k^{\pm} \in \mathbf{R} \mid a_k^- < a_k^+,\ k \in \mathbf{Z}^+\}$ *form self-consistent a-priori bounds if:*

C1 *For* $k > M$*,* $a_k^- < 0 < a_k^+$*.*

C2 *Let* $\hat{a}_k := \max |a_k^{\pm}|$ *and set* $\hat{u} = \sum_{k=0}^{\infty} \hat{a}_k e_k$*. Then,* $\hat{u} \in H$*, (*$\{\hat{a}_k\} \in l_2$*)*

C3 *The function* $u \mapsto F(u)$ *is continuous on*

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

Moreover, if we define $\hat{f}_k = \max_{u \in W \oplus \prod_{k=m+1}^{\infty} [a_k^-, a_k^+]} |A_k F(u)|$ *and set* $\hat{f} = \sum \hat{f}_k e_k$*, 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

$$\begin{aligned} a_k = a_k^+ \qquad &\Rightarrow \quad \dot{a}_k < 0 \\ a_k = a_k^- \qquad &\Rightarrow \quad \dot{a}_k > 0 \end{aligned}$$

2. Finite dimensional rigorous computations in m first variables

Basic Differential Inclusion:

$$\dot{p} \in P_m F(p) + R_m, \qquad p \in \mathbf{R}^m, \tag{2}$$

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

$$p(t) \in p_I(t), \qquad q(t) \in T, \qquad \text{for } t \in [0, t_1]$$

3. Extracting dynamics of PDE from topological information about the Galerkin projections

$N \oplus \Pi_{j=m+1}^{k}[a_j^-, a_j^+]$ 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

$$u_t = F(u) = Lu + N(u) \quad (*)$$

L-linear, N-nonlinear.
$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \dots$ - eigenvalues of L
$e_1, e_2, \dots$ - eigenvectors

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

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

$$\begin{aligned} a_k = a_k^+ \quad &\Rightarrow \quad \dot{a}_k < 0 \\ a_k = a_k^- \quad &\Rightarrow \quad \dot{a}_k > 0 \end{aligned}$$

Data. $T = \Pi_{k=m+1}^{\infty}[a_k^-, a_k^+]$. $Iso[k]$, $i = m + 1, \ldots,$

$Iso[k] = true$ 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 $k = m + 1, n + 2, \dots, M$,
- table $Iso[k]$ $m < k \leq M$
- constants $C \in \mathbf{R}^{+}$ and $s \in Z^{+}$ 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 ρ_0, ρ_1, and $T = T(u_0)$ such that for all $t > T$

$$||u(t)||_2 \le \rho_0 \quad \text{and} \quad ||u_x(t)||_2 \le \rho_1.$$

Furthermore, if $m^4 > \frac{1}{\nu^2}$ then

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

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

Lohner-type algorithm for differential inclusion

$$x'(t) = f(x(t), y(t)) \tag{3}$$

$x \in \mathbf{R}^{n_1}$, $y(t) \in \mathbf{R}^{n_2}$ (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 $y_c \in \mathbf{R}^{n_2}$ we compare the solutions of two ODEs

$$\begin{aligned} x_1' &= f(x_1, y_c), \qquad (4)\\ x_2' &= f(x_2, y_c) + (f(x_2, y(t)) - f(x_2, y_c)) \qquad (5)\\ &x_1(t_0) = x_2(t_0) = x_0 \qquad (6) \end{aligned}$$

where $y(t)$ is given (but unknown) function.

Lohner-type algorithm for differential inclusion - Fundamental Lemma

Lemma: Let:
$[W_y] \subset \mathbf{R}^{n_2}$, convex, $y([t_0, t_0 + h]) \subset [W_y]$.
$[W_1] \subset [W_2] \subset \mathbf{R}^{n_1}$ - convex and compact.
$x_1([t_0, t_0+h]) \subset [W_1]$, $x_2([t_0, t_0+h]) \subset [W_2]$ for any continuous function $y : [t_0, t_0 + h] \to [W_y]$.

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

$$|x_{1,i}(t) - x_{2,i}(t)| \leq \left(\int_{t_0}^{t} e^{J(t-s)} C \, ds \right)_i , \qquad (7)$$

where

$$\begin{aligned} [\delta] &= \{ f(x, y_c) - f(x, y) \mid x \in [W_1], y \in [W_y] \}, \\ C_i &\geq \text{sup} \left| [\delta_i] \right| , \qquad i = 1, \ldots, n_1 \\ J_{ij} &\geq \text{sup} \frac{\partial f_i}{\partial x_j}([W_2], [W_y]) \text{if } i = j, \\ J_{ij} &\geq \text{sup} \left| \frac{\partial f_i}{\partial x_j}([W_2], [W_y]) \right| \text{if } i \neq j. \end{aligned}$$

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 $y(0) = y_0$.
$\overline{\varphi}(t, x_0, y_0)$ - a solution of $x' = f(x, y)$, $y' = 0$, $x(0) = x_0$ and $y(0) = y_0$.
Let $\pi_x : \mathbf{R}^{n_1} \times \mathbf{R}^{n_2}$ be a projection onto $\mathbf{R}^{n_1}$, i.e. $\pi_x(x, y) = x$.

Input data:
t_k, h_k - a time step,
$[x_k] \subset \mathbf{R}^{n_1}$, such that $\pi_x \varphi(t_k, [x_0], [y_0]) \subset [x_k]$,
$[y_k]$ - bounds for $y(t_k)$.

Output data:
$t_{k+1} = t_k + h_k$,
$[x_{k+1}] \subset \mathbf{R}^{n_1}$, 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 φ.
Find a convex and compact set $[W_2] \subset \mathbf{R}^{n_1}$ and a convex set $[W_y] \subset \mathbf{R}^{n_2}$, such that

$$\varphi([0, h_k], [x_k], [y_k]) \subset [W_2] \times [W_y]. \qquad (8)$$

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

3. Computation of $\overline{\varphi}$. We use Lohner algorithm to obtain $[\overline{x}_{k+1}] \subset \mathbf{R}^{n_1}$ and a convex and compact set $[W_1] \subset \mathbf{R}^{n_1}$, such that

$$\begin{aligned} \pi_x\overline{\varphi}(h_k, [x_k], y_c) &\subset [\overline{x}_{k+1}] \\ \pi_x\overline{\varphi}([0, h_k], [x_k], y_c) &\subset [W_1] \end{aligned}$$

Lohner-type algorithm for differential inclusion - one step - details continued

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

$$\pi_x \varphi(t_{k+1}, [x_0], [y_0]) \subset \pi_x \overline{\varphi}(h_k, [x_k], y_c) + [\Delta]. \tag{9}$$

Hence

$$\pi_x \varphi(t_{k+1}, [x_0], [y_0]) \subset [x_{k+1}] = [\overline{x}_{k+1}] + [\Delta] \tag{10}$$

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

$$[W_2] \subset W. \tag{11}$$

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

$$\begin{aligned}
[\delta] &= [\{f(x,y_c) - f(x,y) \mid x \in [W_1], y \in [W_y]\}]_I \\
C_i &= \text{right}\left(|[\delta_i]|\right), \quad i = 1,\dots,n_1 \\
J_{ij} &= \text{right}\left(\frac{\partial f_i}{\partial x_i}([W_2],[W_y])\right) \text{ if } i = j, \\
J_{ij} &= \text{right}\left(\left|\frac{\partial f_i}{\partial x_j}([W_2],[W_y])\right|\right), \text{if } i \neq j.
\end{aligned}$$

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

3. $[\Delta_i] = [-D_i, D_i]$, for $i = 1,\dots,n_1$

Lohner-type .. - Computation of $\int_0^t e^{A(t-s)} C\, ds$.

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

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

$$\tilde{A} = At, \qquad A_n = \frac{\tilde{A}^n}{(n+1)!},$$

$$\sum_{n=0}^{\infty} \frac{(At)^n}{(n+1)!} = \sum_{n=0}^{\infty} A_n$$

$$A_0 = \mathrm{Id}, \qquad A_{n+1} = A_n \cdot \frac{\tilde{A}}{n+2}$$

Remainder: $\|A_{N+k}\| \le \|A_N\| \cdot \left\| \frac{\tilde{A}}{N+2} \right\|^k$. If $\left\| \frac{\tilde{A}}{N+2} \right\| < 1$, then

$$\left\| \sum_{n>N} A_n \right\| \le \|A_N\| \cdot \left\| \frac{\tilde{A}}{N+2} \right\| \cdot \left(1 - \left\| \frac{\tilde{A}}{N+2} \right\| \right)^{-1}$$

Lohner-type .. - Representation of sets and rearrangement.

Lohner's approach.

In part 4:

$$[x_{k+1}] = [\overline{x}_{k+1}] + [\Delta] \tag{13}$$

Evaluations 2 and 3. In this representation

$$[x_k] = x_k + [B_k][\tilde{r}_k]. \tag{14}$$

In the context of our algorithm in part 3 we obtain

$$[\overline{x}_{k+1}] = \overline{x}_{k+1} + [B_{k+1}][\overline{r}_{k+1}]. \tag{15}$$

We set

$$x_{k+1} = \mathrm{m}(\overline{x}_{k+1} + [\Delta]) \tag{16}$$

$$[\tilde{r}_{k+1}] = [\overline{r}_{k+1}] + [B_{k+1}^{-1}]\left(\overline{x}_{k+1} + [\Delta] - x_{k+1}\right). \tag{17}$$

Lohner-type .. - Representation of sets and rearrangement II

Evaluation 4. In this representation

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

In the context of our algorithm in part 3 we obtain

$$[\overline{x}_{k+1}] = \overline{x}_{k+1} + C_{k+1}[r_0] + [B_{k+1}][\overline{r}_{k+1}]. \tag{19}$$

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,
$[x_k] \subset \mathbf{R}^{n_1}$, $\pi_x \varphi(t_k, [x_0], [y_0]) \subset [x_k]$,
$[x_{k+1}] \subset \mathbf{R}^{n_1}$, $\pi_x \varphi(t_k + h_k, [x_0], [y_0]) \subset [x_{k+1}]$,
a convex and compact set $[W_2] \subset \mathbf{R}^{n_1}$ and a convex set $[W_y] \subset \mathbf{R}^{n_2}$, such that

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

$y_c \in [W_y]$,
$[\overline{x}_{k+1}] \subset \mathbf{R}^{n_1}$, such that $\pi_x \overline{\varphi}(h_k, [x_k], y_c) \subset [\overline{x}_{k+1}]$,
$[W_1] \subset \mathbf{R}^{n_1}$ compact and convex, such that $\pi_x \overline{\varphi}([0, h_k], [x_k], y_c) \subset [W_1]$.

Output:
We compute $[E_k] \subset \mathbf{R}^{n_1}$ such that

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

Algorithm:

- if $0 \notin f_i([W_2],[W_y])_i$, 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 $[\overline{E}_k] \subset \mathbf{R}^{n_1}$, such that

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

  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 Δ is added twice.

Lohner-type algorithm for differential inclusion - some remarks and problems

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

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

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 $\lambda_n \to \infty$ for $n \to \infty$. 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.

$a_1 = 2.012106e-01$	$a_2 = 1.289980$
$a_3 = 2.012109e-01$	$a_4 = -3.778662e-01$
$a_5 = -4.230950e-02$	$a_6 = 4.316159e-02$
$a_7 = 6.940217e-03$	$a_8 = -4.156484e-03$
$a_9 = -7.944907e-04$	$a_{10} = 3.316061e-04$
$a_{11} = 7.939456e-05$	$a_{12} = -2.390962e-05$
$a_{13} = -7.087251e-06$	$a_{14} = 1.568377e-06$

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