Rigorous Integration Forward in Time of PDEs Using Chebyshev Basis

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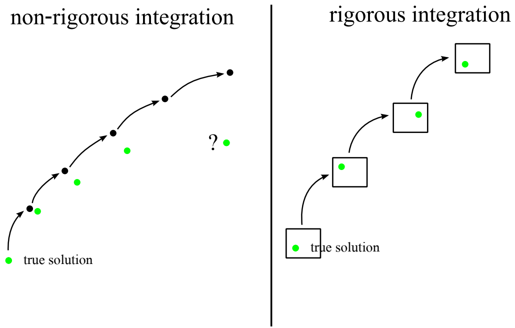
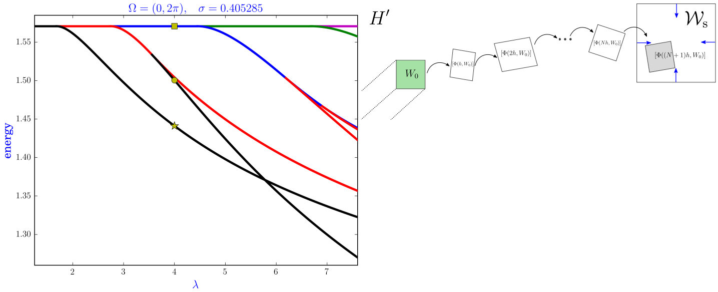
Rigorous integration forward in time

Validated time-stepping routine

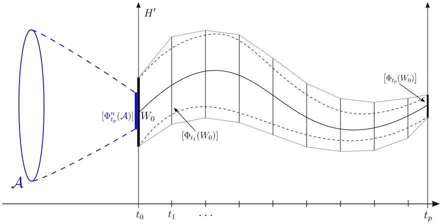


Rigorous numerics results for time-dependent PDEs

- P. Zgliczyński, Existence of periodic orbits for Kuramoto-Sivashinsky PDE, 2004
- S. Day, Y. Hiraoka, K. Mischaikow, T. Ogawa, Proofs of connecting orbits using Conley index, 2005
- S. Maier-Paape, K. Mischaikow, T. Wanner, Connection matrices approach for the Cahn-Hillard equation on a square, 2006
- G. Arioli, H. Koch, dissipative PDEs integration algorithm, periodic orbits for KS equation + stability, 2010
- T. Kinoshita, T. Kimura, M. T. Nakao, Numerical enclosure of solutions of parabolic PDEs using Finite Elements, 2012
- J. Mireles-James, C. Reinhardt, Parametrization of invariant manifolds of parabolic PDEs, 2016
- D. Wilczak, P. Zgliczyński, Computer assisted proof of chaos in Kuramoto-Sivashinsky equation, 2017
- M. Breden, J.-P. Lessard, R. Sheombarsing, work in progress on applying Chebyshev interpolation



J.C. and T. Wanner 2017, Computer assisted proof of heteroclinic connections in 1d Ohta-Kawasaki diblock copolymers model



J.C. and P. Zgliczyński 2015, Computer assisted proof of globally attracting solutions of the forced viscous Burgers equation – a generalization of a result by H. R. Jauslin, J. Moser, H.O. Kreiss

Let us consider a *1D PDE Cauchy problem*

$$
\begin{aligned}
u_t(t,x) &= L(u(t,x)) + N(u(t,x), u_x(t,x), \dots), \\
u(0,x) &= u_0(x), \\
\Omega &= [0,1], \\
&+ \text{bd. condition (periodic / Neumann / Dirichlet)} .
\end{aligned}
$$

Use the Fourier expansion

$$u(t,x) = \sum_{k\in\mathbb{Z}} \tilde{a}_k(t) e^{ikx}$$

Obtain system of equations for the Fourier coefficients $\{\tilde{a}_k\}_{k\in\mathbb{Z}}$

$$\begin{aligned} \tilde{a}_k'(t) &= f_k(\tilde{a}(t)), \\ \tilde{a}_k(0) &= b_k. \end{aligned}$$

Most of the approaches are based on the *Taylor expansion* in time.

$$\tilde{a}(t) = \tilde{a}(0) + \tilde{a}^{[1]}(0)t + \tilde{a}^{[2]}(0)t^2 + \cdots + \tilde{a}^{[p]}(0)t^p + \tilde{a}^{[p+1]}([0,t])t^{p+1} + \ldots.$$

Our goal is to apply the Chebyshev expansion instead.

$$a_k(\tau) = a_{k,0} + 2\sum_{j\geq 1} a_{k,j}T_j(\tau) = a_{k,0} + 2\sum_{j\geq 1} a_{k,j}\cos(j\theta) = \sum_{j\in\mathbb{Z}} a_{k,j}e^{ij\theta},$$

where $\tau = \cos(\theta)$.

Rescale time, integrate the equations in time

$$a_k(\tau) = h\int_{-1}^{h} f_k(a(s)+b)\,ds, \quad k \geq 0,\ \tau \in [-1,1].$$

We also expand $f_k(a(\tau))$ using the Chebyshev series

$$f_k(a(\tau)+b) = \phi_{k,0}(a,b) + 2\sum_{j\geq 1}\phi_{k,j}(a,b)\cos(j\theta) = \sum_{j\in\mathbb{Z}}\phi_{k,j}(a,b)e^{ij\theta},$$

This results in solving $F(a)=0$, where $F(a) = \left(F_{k,j}(a)\right)_{k,j\geq 0}$ is given component-wise by

$$F_{k,j}(a,b) = \begin{cases} a_{k,0} + 2\sum_{\ell=1}^{\infty}(-1)^{\ell}a_{k,\ell}, & j=0, k\geq 0 \\ 2ja_{k,j} + h(\phi_{k,j+1}(a,b) - \phi_{k,j-1}(a,b)), & j>0, k\geq 0. \end{cases} \tag{1}$$

It is tridiagonal in j.

We can write the operator F as

$$F(a,b) = \mathcal{L}a + \mathcal{N}(a,b).$$

The problem is to solve

$$F(a,b) = \mathcal{L}a + \mathcal{N}(a,b) = 0 \iff \mathcal{L}a = -\mathcal{N}(a,b). \tag{2}$$

We interpret the *zero-finding problem* as the *fixed point problem*

$$T(a) = \mathcal{L}^{-1}\left(-\mathcal{N}(a,b)\right) = a.$$

Define the linear operator $\mathcal{L}$ by

$$\mathcal{L}_{k,j}(a) = \begin{cases} a_{k,0} + 2\sum_{\ell=1}^{\infty}(-1)^{\ell} a_{k,\ell}, & j=0,\ k\geq 0 \\ \mu_k a_{k,j-1} + 2j a_{k,j} - \mu_k a_{k,j+1}, & j>0,\ \ k\geq 0, \end{cases}$$

We use stability of the norm of the inverse of $\widetilde{\mathcal{L}}$ (projected operator) with respect to its projection size $\mathbf{N}$.

$$\widetilde{\mathcal{L}} = \begin{bmatrix} \widetilde{\mathcal{L}}_1 & 0 & \dots & 0 \\ 0 & \widetilde{\mathcal{L}}_2 & 0 & \dots \\ & \ddots & \ddots & \\ 0 & \dots & 0 & \widetilde{\mathcal{L}}_N \end{bmatrix} \quad \widetilde{\mathcal{L}}_k = \begin{bmatrix} 1 & -2 & 2 & -2 & 2 & \cdots \\ \mu_k & 2 & -\mu_k & 0 & \cdots & \\ 0 & \mu_k & 4 & -\mu_k & 0 & \cdots \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & \dots & 0 & \mu_k & 2(N-1) & -\mu_k \\ & & \dots & 0 & \mu_k & 2N \end{bmatrix}$$

We use the *Radii polynomial* approach.

Sarah Day, Jean-Philippe Lessard, and Konstantin Mischaikow. Validated continuation for equilibria of PDEs. SIAM J. Numer. Anal., 45(4):1398–1424 (electronic), 2007.

We compute:

- The *residual norm*

$$\|T(\overline{a}) - \overline{a}\| \leq \|\mathcal{L}^{-1}\|\|F(\overline{a})\| =: Y,$$

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- The *residual norm*

$$\|T(\overline{a}) - \overline{a}\| \leq \|\mathcal{L}^{-1}\|\|F(\overline{a})\| =: Y,$$

- and the 'Z' bound in a neighborhood – ball of radius r centered at $\overline{a}$

$$\sup_{a \in B_r(\overline{a})} \|DT(a,b)\| \leq Z(r)$$

we can bound it using

$$Z(r) := \|\mathcal{L}^{-1}\|\|G(\|\overline{a}+b\|, r)\|h,$$

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- Finally, we use local version of *Banach's contraction principle*, which holds under the assumption that r satisfies

$$P(r) := Y + Z(r)r - r < 0.$$

A bound for the inverse of the *infinite dimensional* linear operator

$$\|\mathcal{L}^{-1}\|$$

is essential.

We work in the following *Banach space*

$$X_{\nu,1}^{(M)} \stackrel{\text{def}}{=} \left\{ a = (a_{k,j})_{\substack{k=0,\ldots,M \\ j\geq 0}} \ : \ a_{k,j} \in \mathbb{R}, \quad \sum_{k=0}^{M} \sum_{j\geq 0} |a_{k,j}| \nu^k < \infty \right\}$$

Stability of the norm

$$\|\widetilde{\mathcal{L}}\|_{1,\nu} = \sup_{\substack{1\le k\le M\\ 1\le j\le N}} \nu^k \|\widetilde{\mathcal{L}}_{k,\cdot,j}\|_{l^1} \frac{1}{\nu^k} = \sup_k \|\widetilde{\mathcal{L}}_k\|_{l^1}.$$

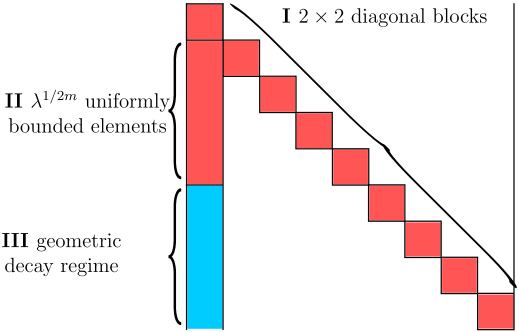
We exploit the tridiagonal + rank one form of blocks

$$\widetilde{\mathcal{L}}_k = A_k + U_k = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ \mu_k & & & \\ 0 & & T_k & \\ \vdots & & & \end{bmatrix} + \begin{bmatrix} 0 & -2 & 2 & \dots \\ & & & \\ & & 0 & \\ & & & \end{bmatrix}.$$

Lemma

For any $\mu_k \in \mathbb{R}$. *For all* k *and* N $\|T_k{}^{-1}\|_{l^1}$ *satisfies the following bound*

$$\|T_k{}^{-1}\|_{l^1} \leq 4.$$



J. Cyranka, P. Mucha, *A construction of two different solutions to an elliptic system*, (2015) arXiv:1502.03363 preprint.

Compute the bound for the inverse of $\mathcal{L}_k$ as a rank-one perturbation of A_k, related with *Sherman-Morrison formula*.

$$\widetilde{\mathcal{L}}_k^{-1} = A_k^{-1} - \frac{A_k^{-1} U_k A_k^{-1}}{1 + v^T A_k^{-1} u}.$$

Theorem

For all k such that $\mu_k \geq 0$ (k sufficiently large for a dissipative PDEs) and for all N it holds that

$$\|\widetilde{\mathcal{L}}_k^{-1}\|_{l^1} \leq 2\|T_k^{-1}\|_{l^1} \leq 8.$$

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Lemma (Passage to the limit)

We have that

$$(\widehat{\mathcal{L}}_{M,N})^{-1} \to (\widehat{\mathcal{L}}_{M,\infty})^{-1}, \text{ as } N \to \infty \text{ in } l^1.$$

Moreover, the limit $(\widehat{\mathcal{L}}_{M,\infty})^{-1}$ satisfies the bound

$$\|(\widehat{\mathcal{L}}_{M,\infty})^{-1}\|_{l^1} \leq 8.$$

Final step

We obtain a solution, which is only l^1 in time.
We do a 'bruteforce' bootstrap of the regularity in time, to verify that we have in fact a solution to a PDE involving a time derivative.

Assume that
$$\alpha_{j-1} \le C_{j-1}\mu, \tag{9}$$
for
$$C_{j-1} \ge 1,$$
then
$$\alpha_j \le (\mu-j)^{\varepsilon} + \frac{d_{N-2j+2}+\mu}{d_{N-2j+1}d_{N-2j+2}+d_{N-2j+1}\mu+\mu^2}\cdot C_{j-1}\mu^2, \tag{10}$$
ineq
$$\alpha_j \le \left(\frac{(\mu-j)^{\varepsilon}}{\mu} + \frac{d_{N-2j+2}+\mu}{d_{N-2j+1}d_{N-2j+2}+d_{N-2j+1}\mu+\mu^2}\cdot\mu\right)C_{j-1}\mu, \tag{11}$$

a_{j-1} dissapeared in the formula (10), in the formula for α_j we used the trivial bound (3) $a_{j-1} \le 1/\mu$, and monotonicity w.r.t. a_{j-1}.

Let
$$f(x) := g(x) + h(x),$$
$$g(x) = (\mu - x)^{\varepsilon}/\mu,$$
$$h(x) = \frac{2(2\mu-2x+2)+\mu}{4(2\mu-2x+1)(2\mu-2x+2)+2(2\mu-2x+1)\mu+\mu^2}\mu.$$

Therefore, for $j = 2, \ldots, \mu-1$ it holds that
$$\alpha_j \le f(j)C_{j-1}\mu, \tag{12}$$
Cjm1

Iterative application of (12) shows that
$$\alpha_j \le f(j)f(j-1)\cdots f(2)C_1\mu, \tag{13}$$
Cjm2

Using substitution $y = \mu - x$ We write $f(x)$ as
$$\hat{f}(y) = \frac{y^{\varepsilon}}{\mu} + \frac{2(2y+2)+\mu}{4(2y+1)(2y+2)+2(2y+1)\mu+\mu^2}\mu. \tag{14}$$
fy

Using the change of variables (12) becomes
$$\alpha_j \le \hat{f}(\mu-j)C_{j-1}\mu,$$
and (15) becomes
$$\alpha_j \le \hat{f}(\mu-j)\hat{f}(\mu-j+1)\cdots\hat{f}(\mu-2)C_1\mu, \tag{15}$$
Cjm2

The derivative of $\hat{f}$ is
$$\hat{f}'(y) = \frac{\varepsilon y^{\varepsilon-1}}{\mu} - \frac{\mu(\mu+2(2y+2))(4\mu+8(2y+1)+8(2y+2))}{(\mu^2+2\mu(2y+1)+4(2y+1)(2y+2))^2} + \frac{4\mu}{\mu^2+2\mu(2y+1)+4(2y+1)(2y+2)} \tag{16}$$
der

Let us pick the following constants
$$C_1 = 0.01,$$
$$C_2 = 0.1,$$
$$C_3 = 0.2.$$

Using the Mathematica notebook *bootstrapping.nb* we prove several facts about $\hat{f}$, we list them below.

Fact I $\hat{f}$ decreasing for $y \ge C_3\mu^{2/3}$.
$$\hat{f}'(y) < 0 \text{ for } y \ge C_3\mu^{2/3} \text{ and } \mu \text{ sufficiently large } (\mu > 1000). \tag{17}$$
fact1

see a proof in *bootstrapping.nb*.

Fact II $\hat{f}(C_3\mu^{2/3})$ is less than 1.
It holds that
$$\hat{f}(C_3\mu^{2/3}) < 1. \tag{18}$$
fact2

From (17) and (18) it follows that
$$\hat{f}(y) < 1, \text{ for } y \ge C_3\mu^{2/3}. \tag{19}$$
fct1and2

Fact III $\hat{f}$ has at least one local max in the interval $[C_1\mu^{2/3}, C_2\mu^{2/3}]$.
$$\hat{f}'(C_1\mu^{2/3}) > 0 \text{ and } \hat{f}'(C_2\mu^{2/3}) < 0. \tag{20}$$

Fact IV $\hat{f}$ is concave down in the interval $[0, C_2\mu^{2/3}]$. The second derivative of $\hat{f}(y)$ is
$$\hat{f}''(y) = \frac{\begin{array}{l} -\mu^6 - 128\mu^5y^{3/2} - 12\mu^5y - 6\mu^5 + 256\mu^4y^{3/2} - 96\mu^4y^2 - 120\mu^4y - 36\mu^4 + 6144\mu^3y^{3/2} \\ +12288\mu^3y^{5/2} + 6144\mu^3y^{7/2} - 448\mu^3y^3 - 864\mu^3y^2 - 528\mu^3y - 104\mu^3 + 8192\mu^2y^{3/2} + 24576\mu^2y^{5/2} \\ +24576\mu^2y^{7/2} + 8192\mu^2y^{9/2} - 1536\mu^2y^4 - 4224\mu^2y^3 - 4224\mu^2y^2 - 1824\mu^2y - 288\mu^2 - 3072\mu y^5 - 10752\mu y^4 - 14592\mu y^3 \\ -9600\mu y^2 - 3072\mu y - 384\mu - 4096y^6 - 18432y^5 - 33792y^4 - 32256y^3 - 16896y^2 - 4608y - 512 \end{array}}{4\mu y^{3/2}\left(\mu^2 + 4\mu y + 2\mu + 16y^2 + 24y + 8\right)^3} \tag{21}$$

By plugging in $y = C\mu^{2/3}$ for any possible value of the constant $C \in [0, 0.2]$. From Mathematica computation using interval arithmetic with $y = [0, 0.2]\mu^{2/3}$ we obtain (see *bootstrapping.nb* file)
$$\hat{f}''([0,0.2]\mu^{2/3}) = \frac{\begin{array}{l} \mu^{2/3}[-921.6, 0] + \mu^{4/3}[-675.84, 0] + \mu^{5/3}[-614.4, 0] + \mu^{7/3}[-384., 0] + \mu^{8/3}[-364.8, 0] + \mu^{10/3}[-168.96, 0] + \mu^{11/3}[-105.6, 0] \\ +\mu^{8/3}[-54.0672, 0] + \mu^{13/3}[-34.56, 0] + \mu^{14/3}[-24., 0] + \mu^{11/3}[-17.2032, 0] + \mu^{10/3}[-5.89824, 0] + \mu^{16/3}[-3.84, 0] \\ +\mu^{14/3}[-2.4576, 0] + \mu^{17/3}[-2.4, 0] + \mu^{13/3}[-0.98304, 0] + \mu^5[-3.584, 0] + \mu^4[-33.792, 0] + \mu^4[-0.262144, 0] + \mu^3[-116.736, 0] \\ +\mu^2[-258.048, 0] - 128\mu^5\left(\mu^{2/3}[0, 0.2]\right)^{3/2} + 256\mu^4\left(\mu^{2/3}[0, 0.2]\right)^{3/2} + 6144\mu^3\left(\mu^{2/3}[0, 0.2]\right)^{3/2} + 12288\mu^3\left(\mu^{2/3}[0, 0.2]\right)^{5/2} \\ +6144\mu^3\left(\mu^{2/3}[0, 0.2]\right)^{7/2} + 8192\mu^2\left(\mu^{2/3}[0, 0.2]\right)^{3/2} + 24576\mu^2\left(\mu^{2/3}[0, 0.2]\right)^{5/2} + 24576\mu^2\left(\mu^{2/3}[0, 0.2]\right)^{7/2} \\ +8192\mu^2\left(\mu^{2/3}[0, 0.2]\right)^{9/2} - \mu^6 - 6\mu^5 - 36\mu^4 - 104\mu^3 - 288\mu^2 - 384\mu - 512 \end{array}}{4\mu\left(\mu^{2/3}[0, 0.2]\right)^{3/2}\left(\mu^{2/3}[0, 4.8] + \mu^{4/3}[0, 0.64] + \mu^{5/3}[0, 0.8] + \mu^2 + 2\mu + 8\right)^3} \tag{22}$$

We take right-end of the intervals for all of the terms with $+$ sign in front of them, and left-end for the terms with $-$ sign and obtain
$$f''([0,0.2]\mu^{2/3}) = \frac{\begin{array}{l} +256\mu^4\left(\mu^{2/3}0.2\right)^{3/2} + 6144\mu^3\left(\mu^{2/3}0.2\right)^{3/2} + 12288\mu^3\left(\mu^{2/3}0.2\right)^{5/2} \\ +6144\mu^3\left(\mu^{2/3}0.2\right)^{7/2} + 8192\mu^2\left(\mu^{2/3}0.2\right)^{3/2} + 24576\mu^2\left(\mu^{2/3}0.2\right)^{5/2} + 24576\mu^2\left(\mu^{2/3}0.2\right)^{7/2} \\ +8192\mu^2\left(\mu^{2/3}0.2\right)^{9/2} - \mu^6 - 6\mu^5 - 36\mu^4 - 104\mu^3 - 288\mu^2 - 384\mu - 512 \end{array}}{4\mu\left(\mu^{2/3}[0, 0.2]\right)^{3/2}\left(\mu^{2/3}[0, 4.8] + \mu^{4/3}[0, 0.64] + \mu^{5/3}[0, 0.8] + \mu^2 + 2\mu + 8\right)^3} \tag{23}$$

The term $-\mu^6$ dominates in the numerator. Now it is clearly seen that $\hat{f}''([0,0.2]\mu^{2/3}) < 0$ for sufficiently large μ.

Fact V $\hat{f}$ has at the global max in the interval $[C_1\mu^{2/3}, C_2\mu^{2/3}]$.
Follows from Fact III and Fact IV.

Numerical tests

A numerical comparison test using some Galerkin approximations of the Fisher equation.

$$\begin{aligned} \frac{\partial}{\partial t}u(t,x) &= \frac{\partial^2}{\partial x^2}u(t,x) + \lambda u(t,x)(1-u(t,x)), \qquad t\in[0,2h],\quad x\in[0,\pi] \\ u(0,x) &= u_0(x), \quad x\in[0,\pi], \\ \frac{\partial}{\partial x}u(t,0) &= \frac{\partial}{\partial x}u(t,\pi) = 0, \qquad \text{for all } t\geq 0. \end{aligned}$$

We have for this equation

$$\mu_k = \lambda - k^2.$$

We compared performing one time-step using our prototype implementation of a Chebyshev method, and a solver based on the Taylor method + Lohner algorithm.

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.

Numerical tests 2

As the initial condition we take

$$\{C(k+1)^{-4}\}_{k=0}^{m},$$

Fixed Taylor method order 15, # Chebyshev modes 25
(it is much cheaper to compute Chebyshev expansion)

			time step/error/remainder	
λ	# Fourier modes m	i.c. ∞ norm C	Taylor	Chebyshev
20	200	10	1e-05/2e-8/1e-28	1.2e-04/1e-09/1e-11
20	200	1	1e-04/2e-9/1e-13	1e-03/1e-06/1e-13
20	200	0.1	1e-04/2e-12/1e-14	2e-03/1e-06/6e-11
20	50	10	1e-04/5e-10/1e-27	same as for $m = 200$
20	50	1	1e-03/5e-11/1e-14	same as for $m = 200$
20	50	0.1	1e-03/5e-14/1e-15	same as for $m = 200$
2	200	10	1e-04/4e-8/1e-12	1e-03/1e-07/1e-11
2	200	1	1e-04/4e-9/1e-13	8e-03/1e-05/3e-10
2	200	0.1	1e-04/2e-12/1e-14	2e-02/3e-05/2e-10
2	50	10	1e-04/1e-07/3e-27	same as for $m = 200$
2	50	1	1e-03/2e-8/2e-14	same as for $m = 200$
2	50	0.1	1e-03/5e-14/1e-15	same as for $m = 200$