Rigorous A-Posteriori Analysis Using Numerical Eigenvalue Bounds in a Surface Growth Model

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Abstract
In order to prove numerically the global existence and uniqueness of smooth solutions of a fourth order, nonlinear PDE, we derive rigorous a-posteriori upper bounds on the supremum of the numerical range of the linearized operator. These bounds also have to be easily computable in order to be applicable to our rigorous a-posteriori methods, as we use them in each time-step of the numerical discretization. The final goal is to establish global bounds on smooth local solutions, which then establish global uniqueness.

Keywords Eigenvalue estimate · Rigorous numerics · Nonlinear parabolic PDEs · Regularity of PDEs

1 Introduction
This paper deals with the rigorous numerical verification of global existence and uniqueness of smooth solutions to the surface growth equation

$$u_t = -u_{xxxx} - (u_x^2)_{xx}$$

for $x \in [0, 2\pi]$ and $t > 0$ subject to periodic boundary conditions and moving frame

$$\int_0^{2\pi} u(t, x) dx = 0.$$

This equation, usually formulated with additional lower order terms and noise, was introduced as a phenomenological model for the growth of vapor deposited amorphous surfaces [22,23]. It was also used to describe ion-sputtering processes, where a surface is eroded by an ion-beam [5]. The one dimensional equation appears as a model for the boundaries of terraces in the epitaxy of silicon [8]. A more detailed list of references can be found in the review article [2].

Analytically, this PDE was studied by Blömker and Romito in several papers which are reviewed in [2], including the existence of smooth local solutions in the largest critical space
and an example for a blowup in the case of the complex valued equation, which rules out the possibility that standard energy estimates alone might be sufficient to prove global uniqueness. The existence of these smooth and unique local solutions, which we will heavily rely on, is given by the following theorem

Theorem 1 (Local Existence and Uniqueness, Theorem 3.1 of [3]) Let $u_0 \in H^1$, then there exists a time $\tau(u_0) > 0$ such that there is a unique solution $u \in C^0([0, \tau(u_0)), H^1)$ satisfying

1. If $\tau(u_0) < \infty$, then $\limsup_{t \to \tau(u_0)} \|u(t)\|_{H^1} = \infty$.
2. $u$ is $C^\infty$ in both, space and time, for all $(t, x) \in (0, \tau(u_0)) \times [0, 2\pi]$.

Except for small initial data, there are no analytic methods to prove the existence of smooth global solutions known so far. The equation only has uniform in time bounds on the spatial $L^2$-norm of solutions, and global existence of solutions for all initial conditions in $L^2$. But in contrast to that uniqueness only holds for initial conditions of higher regularity like continuous functions in $C^0$, Sobolev functions in $H^{1/2}$, or some suitable Besov-space. See [2] for details. The result for small initial data is given by

Theorem 2 (Smallness Condition, Theorem 2 of [1]) If for some $t \in [0, T]$ one has that $\|u_x\|$ is finite on $[0, t]$ and

$$\|u_x(t)\| < \frac{1}{2},$$

then we have global regularity (and thus uniqueness) of the solution $u$ on $[0, \infty)$. Based on this smallness condition, we can further determine a time $T^*$, only depending on the initial value $u_0$, such that $\|u_x(T^*)\| < \varepsilon_0$.

Theorem 3 (Time Condition, Theorem 3 of [1]) If a solution $u$ is regular up to time

$$T^*(u_0) := 2\|u_0\|^2,$$

then we have global regularity of the solution $u$.

A simple proof for both these theorems can be found in [1].

For problems where analytic methods are not yet able to produce results, the application of rigorous computational methods is a steadily increasing field over the recent years. The used methods vary as much as the problems they are applied to. For proving numerically the existence of solutions for PDEs, in addition to our approach, there are methods based on topological arguments like the Conley index, see [6,16], for example. For solutions of elliptic PDEs there are methods using Banach’s fixed-point theorem, as discussed in the review article [21] and the references therein. Analytic bounds based on an approximate pair of eigenvalues and eigenvectors are classical. See [12] and [13]. Finite element methods to obtain explicitly computable lower bounds on eigenvalues were still studied in recent years. See e.g. [9–11,15]. For periodic solutions or invariant manifolds for dissipative PDE see for example [26] and [25]. A nice introductory overview is [24].

1.1 The General Approach and the Previous Worst Case Method

Our method for establishing rigorous a-posteriori bounds is based on [4] which is formulated for the 3D Navier-Stokes equation, and related ideas can be found in [17], although no
numerical experiments are present in all of these papers. A different approach to the problem is studied by [14], which is more in the direction of the methods cited in the previous section.

The key idea of [4] is to establish a scalar ODE that bounds the difference $d$ between a unique smooth local solution $u$ and an arbitrary approximation $\varphi$, which is provided by a numerical method, for instance. As the existence and uniqueness of solutions $u$ for the surface growth equation, for example in $H^1$, is known as cited before, we obtain the following result: As long as we can bound the $H^1$-norm $\|d_x\|$, we obtain a bound on $\|u_x\|$ that enables us to use the unique continuation of the smooth local solution (see Theorem 1) and obtain a unique smooth solution up to the blow up time of our error bound on $\|d_x\|$.

As for any initial value $u_0 \in H^1$ there is a time $T^*(u_0)$ (see Theorem 3) with the property that if there was no blow up until time $T^*$, there can not occur one afterwards. Thus one can also obtain global existence and uniqueness by controlling the $H^1$-norm of the error up to that time. Similar properties are also well known for the 3D Navier-Stokes equation.

Let us comment in more detail on the result of [1], which is based on to [4]. The key analytic result of that paper is the following differential inequality for the error

$$\partial_t \|d_x\|^2 \leq \frac{77}{2} \|d_x\|^{10} + \left(18 \|\varphi_{xx}\|_{\infty} + 1\right)\|d_x\|^{2} + 2 \|\text{Res}\|_1^2,$$

where $\text{Res} := \varphi_t + \varphi_{xxxx} + (\varphi_x^2)_{xx}$ is the residual of the approximation $\varphi$ that measures how close $\varphi$ is to being a solution of (1).

As the coefficients of the right hand side of (2) depend only on the numerical data, using the time discretization of the numerical solution $\varphi$ this ODE could be evaluated rigorously.

Remark 4 For the numerical method we are based on the code used in [1]. There we evaluated numerically an analytically derived upper bound for an ODE of the type (2). This error estimate is then iterated on every time-intervall of the numerical computation.

As this is quite technical, we refer for further details to [1]. Our key aim is to improve the terms in (2), and then evaluate it with the existing numerical method in order to compare the results.

As we were mainly interested in performing a case study whether the approach is working at all, we did not yet implement interval arithmetic in our numeric simulations, but this is just a technical issue in programming.

Further, in [1] we showed that this approach could give global existence for initial conditions larger than the analytic smallness result, which is limited to solutions of $H^1$-norm smaller than $1/2$ (see Theorem 2). In the numerical simulations we could easily treat larger initial conditions like $u_0 = \sin(x)$. On the other hand, the method based on (2) still fails for even moderately increased frequencies in the initial value (without dampening by the amplitude) like $u_0 = \sin(2x) + \cos(3x)$, as the $H^1$-norm gets too large. The aim of this paper is to improve this result, and we will see later in the numerical results that this is possible.

Let us finally remark that due to the scaling properties of the equation, once we have one global solution we can always treat some initial conditions that are arbitrarily large in $H^1$. If $u(t,x)$ is any spatially $2\pi$-periodic solution of (1), then for any $k \in \mathbb{N}$ the rescaled solution $u_k(t,x) = u(k^4t, kx)$ is also a $2\pi$-periodic solution. But now it is easy to see that for the initial condition $\|u_k(0, \cdot)\|_{H^1} \to \infty$ if $k \to \infty$. 

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1.2 Improvement Based on Numerical Eigenvalues

It turned out in our numerical experiments of [1], that the most sensitive part for our rigorous method based on (2) is the $18 \| \varphi_{xx} \|_\infty^2$ term that leads to a strong exponential growth. In contrast to that the residual Res seems to be always extremely small, indicating a fast convergence of the numerical method which we use to obtain $\varphi$. But we are analytically far from proving any convergence of the numerical method.

As the quintic nonlinearity in our ODE for the error (2) immediately leads to a blow up in finite time, once the error is sufficiently large, we were looking for a way to improve our error estimate, by replacing our previous “worst case” estimates leading to the term $18 \| \varphi_{xx} \|_\infty^2$. This estimate was purely analytic and largely relied on general interpolation inequalities, bounding the respective quadratic form of the linearized operator. Hereby, we are following the idea of [18,19], where the spectrum of the linearized operator is analyzed. A related idea is [7] that is currently in preparation. In our case we consider the non-symmetric operator

$$L_{\varphi}u = -\partial_x^4 u - 2\partial_x^2 (\varphi_x u_x),$$

where $\varphi$ is some given numerical data, and thus $L_{\varphi}u$ is just the linearization of the full nonlinear SPDE (1) along the numerical approximation $\varphi$.

The bound is based on a rigorous numerical method for the largest eigenvalue, which in the case of an unstable linear operator yields substantially better results, at the price of a significantly higher computational time.

Let us comment in more detail on this. In order to derive an improvement of (2), we are interested in the supremum of the numerical range of $L_{\varphi}$, which means we want to bound the quadratic form

$$\lambda(\varphi) = \sup_{\|u_x\| = 1} \langle \partial_x L_{\varphi}u, \partial_x u \rangle$$

in order to finally obtain a bound

$$\langle \partial_x L_{\varphi}u, \partial_x u \rangle \leq \lambda(\varphi) \|u_x\|^2.$$

This is equivalent to bounding the largest eigenvalue of the symmetrized operator $\frac{1}{2} (L_{\varphi} + L_{\varphi}^*)$. Although there are already results for upper bounds on the largest eigenvalue of self-adjoint operators, we have the requirement that our estimate is also (relatively) easy and fast to compute in order to be applicable to our a-posteriori method as it has to be calculated in every time step of the discretization.

1.3 Structure of the Paper

In Sect. 2, we state the basic notation used throughout the paper. The main result for the numerical eigenvalue is stated in Sect. 3, and proven in Sect. 4. In Sect. 5 we compare the new estimate with the previous worst case estimate and demonstrate in a simple example how much better the verification for global existence and uniqueness works with the new estimate based on the numerical eigenvalue.
2 Setting & Problem

As solutions to our surface growth equation (1) are subject to periodic boundary conditions on \([0, 2\pi]\) with mean average zero, we are working on the Hilbert space

\[ H = \{ u : \mathbb{R} \rightarrow \mathbb{R} : 2\pi \text{-periodic, } \int_0^{2\pi} u(x) \, dx = 0, \int_0^{2\pi} |u(x)|^2 \, dx < \infty \} \]

with standard \(L^2\)-scalar product \(\langle \cdot , \cdot \rangle\) and corresponding \(L^2\)-norm

\[ \|u\| = \left( \int_0^{2\pi} |u(x)|^2 \, dx \right)^{1/2}. \]

We further define the Sobolev-spaces

\[ H^k = \{ u \in H : \partial^\ell_x u \in H, \forall \ell \in \{1, \ldots, k\} \}. \]

Note, that by periodicity \(u \in H^1\) implies \(u_x \in H\) and similarly for higher derivatives. Moreover, we have Poincaré inequality with optimal constant 1

\[ \|u\| \leq \|u_x\| \text{ for all } u \in H^1 \]

and thus

\[ \|u\|_{H^1} := \|u_x\| \]

is a norm on \(H^1\), which is equivalent to the standard \(H^1\)-Sobolev norm, and we always refer to it as the \(H^1\)-norm.

Furthermore, interpolation inequality holds also with constant 1

\[ \|u_x\|^2 \leq \|u_{xx}\| \|u\| \text{ for all } u \in H^2. \]

In both cases the value of the optimal constants are easy to verify. For details see [20].

Let us recall in more detail the results of [1]. There, in order to control the \(H^1\)-norm of a unique smooth local solution \(u\) to the surface growth equation (1), we derived a differential inequality to bound the \(H^1\)-norm of the difference

\[ d(x, t) := u(x, t) - \varphi(x, t), \]

where \(\varphi\) is any arbitrary, but sufficiently smooth approximation, that satisfies periodic boundary conditions. In the numerical examples we always use a spectral Galerkin method in space and a semi-implicit Euler scheme in time, which we then extend by piece-wise linear interpolation of the numerical data in time. Thus \(\varphi\) is arbitrarily smooth in space (i.e., \(C^\infty\)) and Lipschitz in time (i.e., \(W^{1,\infty}\)).

Using a standard a-priori type estimate, the differential inequality for the error is given by

\[
\frac{1}{2} \partial_t \|d_x\|^2 = \langle d_{xx}, d_{xxxx} + 2(d_x \varphi)_x \rangle + \langle d_{xx}, (d_x^2)_x \rangle + \langle d_{xx}, \text{Res} \rangle \]

\[ \leq \frac{7}{4} \|d_x\|^2 + \left(9 \|\varphi_{xx}\|_\infty^2 - \frac{1}{4}\right) \|d_x\|^2 + \|\text{Res}\|^2_{H^{-1}}, \]

with residual \(\text{Res} := \varphi_t + \varphi_{xxxx} + (\varphi_x^2)_xx\). The estimate above is based on a crude “worst case” estimate for A+B and was established in [1].

Our aim of this paper is to improve this estimate specifically for the term A+B, by using a numerical calculation that computes a more problem specific estimate.

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Therefore consider the following linearized operator, as \( \phi \) is sufficiently smooth,

\[
L_\phi u = -\partial_\chi^4 u - 2\partial_\chi^2 (\phi_x u_x).
\]

This is for smooth \( \phi \) a bounded linear operator from \( \mathcal{H}^k \) to \( \mathcal{H}^{k-4} \) for \( k \geq 1 \). We are interested in bounding the quadratic form

\[
\lambda = \sup_{\|u_x\|=1, \ u \in \mathcal{H}^2} \langle \partial_x L_\phi u, \partial_x u \rangle
\]

in order to finally obtain a bound

\[
A + B = \langle \partial_x L_\phi d, \partial_x d \rangle \leq \lambda \|d_x\|^2.
\]

Note that we neglect the explicit dependence of \( \lambda \) on \( \phi \) and thus on time in the notation. Moreover, although the quadratic form is directly defined for \( u \in \mathcal{H}^5 \) only, we can easily extend it by continuity and using dual pairings to \( u \in \mathcal{H}^3 \). We extend it to \( u \in \mathcal{H}^2 \) by setting it \(-\infty\) for \( u \notin \mathcal{H}^3 \).

In order to transform this to an eigenvalue problem with \( L^2 \)-scalar product, we substitute \( v = u_x \) in (4) and immediately get

\[
\lambda = \sup_{\|v\|=1} \langle A_\phi v, v \rangle.
\]

with non-symmetric operator

\[
A_\phi u = -\partial_\chi^4 u - 2\partial_\chi^3 (\phi_x u_x).
\]

This is a bounded linear operator from \( \mathcal{H}^k \) to \( \mathcal{H}^{k-4} \) for \( k \geq 0 \).

For the numerical computation of \( \lambda \) we also use a spectral Galerkin method. Define \( H_n \) as the \( 2^n \)-dimensional subspace spanned by \( e^{ix}, \ldots, e^{inx} \) and its complex conjugates \( e^{-ix}, \ldots, e^{-inx} \). Note that we can omit the constant mode due to our solution space \( \mathcal{H} \). Denote by \( P_n \) the orthogonal projection onto \( H_n \).

Finally, we set the numerical approximation of \( \lambda \) as

\[
\lambda_n := \sup_{\|u\|=1, u \in \mathcal{H}} \langle P_n A_\phi P_n u, u \rangle = \sup_{\|u\|=1, u \in H_n} \langle A_\phi u, u \rangle
\]

which is just the largest eigenvalue of a symmetric \( 2n \times 2n \) matrix given by the symmetrized matrix \( \frac{1}{2}(P_n A_\phi P_n + P_n A_\phi^* P_n) \).

Obviously, as the supremum is over a larger set, it immediately holds for all \( n \in \mathbb{N} \) that

\[
\lambda_n \leq \lambda.
\]

and moreover, the sequence \( (\lambda_n)_{n \in \mathbb{N}} \) is monotone and thus convergent.

In the following sections we want to bound \( \lambda \) from above by \( \lambda_n \) plus an explicit error term that we can evaluate using the numerical data, which is the difficult task.

### 3 Main Theorem

We will now prove a bound on the quadratic form of the linearized operator. First, let us recall the “worst case” estimate from [1]. This is not a very sophisticated estimate that we are going to improve later.
Proposition 5 Consider $A_{\varphi}$ as defined in (5) with $\varphi \in W^{2,\infty}$, then it holds that
\[(A_{\varphi} u, u) \leq -\frac{1}{2} \| u_{xx} \|^2 + \frac{9}{2} \| \varphi_{xx} \|_{\infty}^2 \| u \|^2 \leq \left[ -\frac{1}{2} + \frac{9}{2} \| \varphi_{xx} \|_{\infty}^2 \right] \cdot \| u \|^2 \]
f for all $u \in H^2$.

Note that we are working with smooth local solutions or finite Fourier series, so this estimate will only be applied to sufficiently smooth $u$. We will show the proof for completeness as parts of it will be reused later.

Proof The estimate is first proven for sufficiently smooth $u \in H^4$, as the quadratic form needs a fourth derivative, and then the estimate is easily extended by continuity of the quadratic form to $u \in H^2$.

First using integration by parts
\[
(A_{\varphi} u, u) = -\| u_{xx} \|^2 + 2 \int \varphi_{xx} u_{xxx} \, dx = -\| u_{xx} \|^2 - 2 \int \varphi_{xx} u_{xx} \, dx + \int \varphi_{xx} u_x^2 \, dx.
\]

Now, Hölder, interpolation, and Poincaré inequalities are used to obtain
\[
\leq -\| u_{xx} \|^2 + 2 \| \varphi_{xx} \|_{\infty} \| u \| \| u_{xx} \| + \| \varphi_{xx} \|_{\infty} \| u_x \|^2 \\
\leq -\| u_{xx} \|^2 + 3 \| \varphi_{xx} \|_{\infty} \| u \| \| u_{xx} \| \\
\leq -\frac{1}{2} \| u_{xx} \|^2 + \frac{9}{2} \| \varphi_{xx} \|_{\infty}^2 \| u \|^2 \\
\leq -\frac{1}{2} \| u \|^2 + \frac{9}{2} \| \varphi_{xx} \|_{\infty}^2 \| u \|^2.
\]

Thus we obtain for the supremum of the quadratic form defined in (5)
\[
\lambda \leq -\frac{1}{2} + \frac{9}{2} \| \varphi_{xx} \|_{\infty}^2.
\] (7)

This is the worst case estimate used in [1] to obtain the differential inequality stated in (3).

Instead, the following theorem shows an improved estimate by analyzing the quadratic form (4) separately for different mode ranges.

Theorem 6 Let $u$ be a smooth local solution to our surface growth equation (1) with initial condition $u(0) \in H^1$, $\varphi$ an arbitrary $H_n$-valued approximation and $H_n$, $\lambda$ and $\lambda_n$ be defined as in Sect. 2. Then, for
\[
n \geq \sqrt{2} C_{\varphi} = \sqrt{2} (2 \| \varphi_{xxx} \|_{\infty} + 6 \| \varphi_{xx} \|_{\infty} + 4 \| \varphi_x \|_{\infty})
\]
it holds that
\[
\lambda_n \leq \lambda \leq \lambda_n + \frac{1}{2} \max \left\{ 2 C_{\varphi}^2 \frac{9 \| \varphi_{xx} \|_{\infty}^2}{n^2} - 2 \lambda_n, 9 \| \varphi_{xx} \|_{\infty}^2 - 2 \lambda_n - \frac{1}{2} n^4 \right\} =: \bar{\lambda}.
\]

Remark 7 We want to emphasize that the $H_n$ spaces are nested and grow monotonically for $n \to \infty$. Thus once we pick $\varphi$ as a fixed $H_N$-valued function, we can send $n$ to infinity without changing $\varphi$. In the numerics, we implement this by appending zeros to the increasing Fourier representation of $\varphi$. 

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Remark 8 Note that due to monotonicity $\lambda_n$ converges, and thus the previous result shows the convergence of $\lambda_n$ to $\lambda$. Moreover, we obtain the asymptotic rate of convergence

$$\lambda = \lambda_n + O(1/n^2) .$$

On the other hand, for a given $n$ and a given $\varphi$, we can calculate $\lambda_n$ and the error given by the previous theorem fairly quickly.

4 Proof of the Main Theorem

As a preparation, we split $u = p + q$, where $p \in H_n$ and $q \perp H_n$. Thus

$$\lambda = \sup_{\|u\| = 1} \langle A_\varphi u, u \rangle = \sup_{\|p\|^2 + \|q\|^2 = 1} \left\{ \langle A_\varphi p, p \rangle + \langle A_\varphi p, q \rangle + \langle A_\varphi q, p \rangle + \langle A_\varphi q, q \rangle \right\} .$$

Now, we will treat these scalar products separately, where we will denote with “low modes” the parts only depending on $p$ and with “high modes” everything solely depending on $q$.

Note that $A_\varphi$ is not symmetric and thus $\langle A_\varphi p, q \rangle \neq \langle A_\varphi q, p \rangle$, in general.

Low Modes

First, notice that by the brute force estimate of Proposition 5 we have

$$\langle A_\varphi p, p \rangle \leq -\frac{1}{2} \| p_{xx} \|^2 + \frac{9}{2} \| \varphi_{xx} \|_{\infty} \| p \|^2 .$$

Second, it holds by the definition of $\lambda_n$, as $p \in H_n$

$$\langle A_\varphi p, p \rangle \leq \lambda_n \| p \|^2 .$$

In summary, we get for some $\eta_n \in [0, 1]$, that we will fix later,

$$\langle A_\varphi p, p \rangle \leq (1 - \eta_n) \lambda_n \| p \|^2 - \frac{1}{2} \eta_n \| p_{xx} \|^2 + \frac{9}{2} \eta_n \| \varphi_{xx} \|_{\infty} \| p \|^2 .$$

We do not use only the numerical eigenvalue to bound the quadratic form, as we also need to control terms involving $\| p_{xx} \|$ arising in the estimate of the mixed terms.

Mixed Terms

For the mixed terms we use the elementary estimates

$$\| p \| \leq \| p_x \| \leq \| p_{xx} \| \quad \text{and} \quad \| q \| \leq \frac{1}{n} \| q_x \| \leq \frac{1}{n^2} \| q_{xx} \| . \quad (8)$$

Note that any derivatives of $p$ and $q$ are still orthogonal in $\mathcal{H}$, so in the mixed terms the only terms that are non-zero are the ones that contain $\varphi$.

We obtain first

$$\langle A_\varphi p, q \rangle = -2 \int (\varphi_x p)_{xxx} q \, dx = 2 \int (\varphi_x p)_{xx} q_x \, dx$$
\[ = 2 \int (\varphi_{xxx} p + 2 \varphi_{xx} p_x + \varphi_x p_{xx}) q_x \, dx \]
\[ \leq 2 \| q_x \| \cdot (\| \varphi_{xxx} \| \| p_x \| + 2 \| \varphi_{xx} \| \| p \| + \| \varphi_x \| \| p_{xx} \|) \]
\[ \leq C^{(1)}_\varphi \frac{1}{n} \| q_{xx} \| \| p_{xx} \| \]

with
\[ C^{(1)}_\varphi = 2 \| \varphi_{xxx} \|_\infty + 4 \| \varphi_{xx} \|_\infty + 2 \| \varphi_x \|_\infty. \]

For the second mixed term we derive similarly
\[ \langle A \varphi q, p \rangle = 2 \int (\varphi_x q) p_{xxx} \, dx = -2 \int (\varphi_x q_x) p_{xx} \, dx \]
\[ \leq 2 \| p_{xx} \| \cdot (\| \varphi_{xx} \|_\infty \| q_x \| + \| \varphi_x \|_\infty \| q \|) \]
\[ \leq C^{(2)}_\varphi \frac{1}{n} \| q_{xx} \| \| p_{xx} \| \]

with
\[ C^{(2)}_\varphi = 2 \| \varphi_{xx} \|_\infty + 2 \| \varphi_x \|_\infty. \]

Further, we define
\[ C_\varphi = C^{(1)}_\varphi + C^{(2)}_\varphi = 2 \| \varphi_{xxx} \|_\infty + 6 \| \varphi_{xx} \|_\infty + 4 \| \varphi_x \|_\infty. \]

**High Modes**

Finally, for the high modes we have no other option, but to use the rough "worst case" estimate of Proposition 5 which yields
\[ \langle A \varphi q, q \rangle \leq -\frac{1}{2} \| q_{xx} \|^2 + \frac{9}{2} \| \varphi_{xx} \|_\infty^2 \| q \|^2. \]

We will apply the improved Poincaré inequality (8) which is valid on the high modes in a later step.

**Summary**

Combining all estimates, we obtain (using Young inequality \( ab \leq \frac{1}{2} a^2 + \frac{1}{2} b^2 \) and eliminating \( p_{xx} \) terms)
\[ \langle A \varphi u, u \rangle = \langle A \varphi p, p \rangle + \langle A \varphi p, q \rangle + \langle A \varphi q, p \rangle + \langle A \varphi q, q \rangle \]
\[ \leq (1 - \eta_n) \lambda_n \| p \|^2 - \frac{1}{2} \eta_n \| p_{xx} \|^2 + \frac{9}{2} \eta_n \| \varphi_{xx} \|_\infty^2 \| p \|^2 \]
\[ + C_\varphi \frac{1}{n} \| q_{xx} \| \| p_{xx} \| \]
\[ - \frac{1}{2} \| q_{xx} \|^2 + \frac{9}{2} \| \varphi_{xx} \|_\infty^2 \| q \|^2 \]
\[ \leq (1 - \eta_n) \lambda_n \| p \|^2 + \frac{9}{2} \eta_n \| \varphi_{xx} \|_\infty^2 \| p \|^2 \]
\[ + \frac{1}{2} \left( C^2_\varphi \eta_n - 1 \right) \| q_{xx} \|^2 + \frac{9}{2} \| \varphi_{xx} \|_\infty^2 \| q \|^2. \]
In order to apply the improved Poincaré inequality (8) for $q$, we define

$$\eta_n := \frac{2C^2}{n^2}$$

and thus we need $n \geq \sqrt{2C\varphi}$ to assert $\eta_n \leq 1$.

We obtain

$$\langle A\varphi u, u \rangle \leq \left[ (1 - \eta_n)\lambda_n + \frac{9}{2}\eta_n\|\varphi_{xx}\|_\infty^2 \right]\|p\|^2 + \frac{1}{2}\left[ 9\|\varphi_{xx}\|_\infty^2 - \frac{1}{2}n^4 \right]\|q\|^2$$

which proves our main theorem

$$\lambda = \sup\limits_{\|u\|=1} \langle A\varphi u, u \rangle = \sup\limits_{\|p\|^2 + \|q\|^2=1} \langle A\varphi u, u \rangle \leq \max \left\{ \left[ (1 - \eta_n)\lambda_n + \frac{9}{2}\eta_n\|\varphi_{xx}\|_\infty^2 \right], \frac{1}{2}\left[ 9\|\varphi_{xx}\|_\infty^2 - \frac{1}{2}n^4 \right] \right\}$$

$$= \lambda_n + \frac{1}{2} \max \left\{ \eta_n[9\|\varphi_{xx}\|_\infty^2 - 2\lambda_n], 9\|\varphi_{xx}\|_\infty^2 - 2\lambda_n - \frac{1}{2}n^4 \right\}.$$

\[ \square \]

5 Simulations

Before we come to the results of the simulations, let us first explain the numerical methods and necessary preparations that we use to calculate $\varphi$ and the upper bounds on $\|d_k\|^2$.

Calculating the Approximation $\varphi$

To compute our arbitrary approximation $\varphi$, we use a spectral Galerkin method to convert the PDE to a system of ODEs. Note that we only need any approximation, so no interval arithmetic is necessary in this step. The basis of eigenfunctions is in our case the standard Fourier basis $e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx)$. As a welcome side effect this allows us to compute quantities like $L^2$ scalar products and norms very efficiently and accurately.

With $u := \sum_k a_k(t)e_k$ our surface growth equation (1) turns into the following infinite system of coupled (through the nonlinearity) ODEs

$$a_k'(t) = -(ik)^4 a_k(t) - (ik)^2 \left( \sum_{s+l=k} (is) a_s(t) \times (il) a_l(t) \right) \forall k.$$

For the spectral Galerkin approximation, we truncate the sum for $b_k$ to a finite range of modes. To solve this system, we now use a semi-implicit Euler scheme, i.e. we use time $t_{j+1} = t_j + h$ in the linear part, and $t_j$ inside the nonlinearity

$$\frac{1}{h} (a_k(t_{j+1}) - a_k(t_j)) = -(ik)^4 a_k(t_{j+1}) - (ik)^2 b_k(t_j)$$

and thus

$$a_k(t_{j+1}) = (1 + h(k)^4)^{-1} (a_k(t_j) + hk^2 b_k(t_j))$$

for all $k$ in the finite range.
Applying the Eigenvalue Estimate

Before we define how to calculate the bound on $\|d_s\|^2$, we have to incorporate the eigenvalue estimate from Theorem 6 into the bounding ODE (3), which is given by

$$\frac{1}{2} \partial_t \|d_s\|^2 = \langle d_{xx}, d_{xxxx} + 2(d_x \varphi_x)_{xx} \rangle + \langle d_{xx}, (d_x^2)_{xx} \rangle + \langle d_{xx}, \text{Res} \rangle$$

$$\leq \frac{7}{4} \|d_s\|^2 + (\frac{9}{2} \|\varphi_{xx}\|_{L^\infty}^2 - \frac{1}{4}) \|d_x\|^2 + \|\text{Res}\|^2_{H^{-1}}.$$  

Let us denote the eigenvalue bound from Theorem 6 with $\lambda$. If we want to apply this result to our framework, we have to consider, that in order to control the (C) and (D) terms, we need some part of the (A) term of

$$\frac{1}{2} \partial_t \|d_s\|^2 = \langle d_{xx}, d_{xxxx} + 2(d_x \varphi_x)_{xx} \rangle + \langle d_{xx}, (d_x^2)_{xx} + \text{Res} \rangle.$$  

Therefore, we split the first term into two parts ($\delta \in (0, 1)$)

$$\frac{1}{2} \partial_t \|d_s\|^2 = (1 - \delta) \langle d_{xx}, d_{xxxx} + 2(d_x \varphi_x)_{xx} \rangle + \delta \langle d_{xx}, d_{xxxx} + 2(d_x \varphi_x)_{xx} \rangle$$

$$+ \langle d_{xx}, (d_x^2)_{xx} + \text{Res} \rangle.$$  

Now, we can bound the first term with our new method and the remaining parts like before in (3). If we do not fix the constants used in the Young inequalities, we have after a short calculation (for details see [1] or [20])

$$A = - \|d_{xxxx}\|^2$$

$$|B| \leq \varepsilon_B \|d_{xxxx}\|^2 + \frac{9}{4\varepsilon_B} \|d_x\|^2 \|\varphi_{xx}\|_{L^\infty}^2$$

$$|C| \leq \varepsilon_C \|d_{xxxx}\|^2 + \frac{(\frac{4}{10})^7}{4} \|d_x\|^2$$

$$|D| \leq \varepsilon_D \|d_{xxxx}\|^2 + \frac{1}{4\varepsilon_D} \|\text{Res}\|^2_{-1},$$

where we can set all $\varepsilon_{[B,C,D]} > 0$ arbitrarily small.

In this case, our differential inequality is

$$\frac{1}{2} \partial_t \|d_s\|^2 \leq (1 - \delta) \tilde{\lambda} \|d_x\|^2 + \frac{9}{4\varepsilon_B} \delta \|d_x\|^2 \|\varphi_{xx}\|_{L^\infty}^2 + \frac{(\frac{4}{10})^7}{4} \|d_x\|^2$$

$$+ \frac{1}{4\varepsilon_D} \|\text{Res}\|^2_{-1} + (\delta \varepsilon_B + \varepsilon_C + \varepsilon_D - \delta) \|d_{xxxx}\|^2,$$

where $\varepsilon_{[B,C,D]} > 0$, $\delta \in (0, 1)$ and $\tilde{\lambda}$ is our rigorous upper bound from Theorem 6. By substituting $\varepsilon_{[C,D]} \mapsto \delta \varepsilon_{[C,D]}$, this is equivalent to

$$\frac{1}{2} \partial_t \|d_s\|^2 \leq (1 - \delta) \tilde{\lambda} \|d_x\|^2 + \frac{9}{4\varepsilon_B} \delta \|d_x\|^2 \|\varphi_{xx}\|_{L^\infty}^2 + \frac{(\frac{4}{10})^7}{4} \|d_x\|^2$$

$$+ \frac{1}{4\delta \varepsilon_D} \|\text{Res}\|^2_{-1} + \delta (\varepsilon_B + \varepsilon_C + \varepsilon_D - 1) \|d_{xxxx}\|^2,$$
where $\varepsilon_{(B,C,D)} > 0$ and $\delta \in (0,1)$. Next, we set $\varepsilon_B + \varepsilon_C + \varepsilon_D = 1$ to remove the last term, and therefore, our final ODE is given by

$$\frac{1}{2} \frac{\partial}{\partial t} \| dx \|^2 \leq (1 - \delta) \tilde{\lambda} \| dx \|^2 + \frac{9 \delta}{4 \varepsilon_B} \| dx \|^2 \| \varphi_{xx} \|_\infty + \frac{7^7}{4^8 (\delta \varepsilon_C)^7} \| dx \|^{10}$$

(9)

under the constraints $\varepsilon_{(B,C,D)} > 0$, $\sum_{k \in \{B,C,D\}} \varepsilon_k = 1$, $\delta \in (0,1)$. Unfortunately, there is no easy to determine global minimum in regard of the constraints. We could rewrite this problem and finally solve it using Ferrari’s method for quartic equations, but sadly this approach has a very bad cost-benefit ratio as the involved calculations are too complex. Luckily, we can not do anything wrong here that breaks the rigorosity of our calculations, as valid parameter combinations just might not be optimal. Therefore, we just use MATLAB’s nonlinear optimization solver to find an approximate local minimum and update it after a given time interval. We could do this in every step, but given that the step-size is quite small and the data is continuous, this is not necessary and would just cost us lots of computational time. See [20] for details.

**Numerical Comparison**

We will now investigate the improvement of the new estimate from Theorem 6 compared to the previous “worst case” estimate (7) in numerical simulations of our rigorous a-posteriori method. Again, please note that interval arithmetic was not used for these simulations, and the results are therefore not yet rigorous.

**Remark 9** We use the rigorous analytic bound for an ODE of the type (3) or (9) based on restarting the estimate on every time step of the numerical discretization. First the methods for bounding the solution of the ODE by a numerically computable upper bound are defined in detail and proven in [1]. This is based on Gronwall-type arguments but taking also into account higher order nonlinear terms. This both applies to the old ODE (3) as well as to the improved estimate (9). As the upper bound is lengthy and technical, we refer the reader to [1] for details.

Further, the precise implementation of the computable upper bound and all necessary technical steps to rigorously calculate the bounds are carried out in [20]. Again, we will not repeat it here as it is a quite lengthy and not very insightful exercise in calculus.

Figure 1 shows the comparison for four different initial values. The solid red line indicates the value of the “worst case” estimate, the dash-dotted blue line our new eigenvalue estimate and the dashed orange line the value of the finite dimensional eigenvalue $\lambda_n$. The dotted green line indicates the “number of modes needed” for our eigenvalue estimate to be valid. Please consider the difference between $n$, the number used in Theorem 6, and $N$ the number of Fourier modes used for a simulation. (e.g the condition $n \geq \sqrt{2C\varphi}$ where $2\sqrt{2C\varphi} + 1$ is the minimal number of Fourier modes needed).

The first two images (a) and (b) show for both our methods easy to handle initial values, whereas (c) and (d) are only treatable with the new eigenvalue estimate. The reason can be seen in the magnitude of the “worst case” estimate which amounts to around 800 in the latter examples, whereas the new estimate stays below 200. Recall that these values are an exponential growth-rate in our ODEs. Therefore, an improvement of about 600 is a huge benefit.
Although it is a major improvement, this new estimate does not resolve the problem connected to higher frequencies in the initial value for the rigorous a-posteriori method. This is not a huge surprise as it does not remove the exponential growth of the error itself, it just significantly reduces its exponent.

In Fig. 2 we can see how the rigorous eigenvalue bound from Theorem 6 converges to the finite dimensional eigenvalue $\lambda_n$ for increasing $n$. Note, that the axes are using a logarithmic scaling. The results show, that there is room for improvement if one is willing and able to use more modes in the eigenvalue estimate which on the other hand increases calculation time drastically. Also, the finite dimensional numerical eigenvalue stays basically constant after a certain number of modes is reached (i.e. that $\phi^2$ can be represented).

Finally, in Fig. 3 we show our methods as described above, where Method 1 uses the former “worst case” estimate and Method 2 the new eigenvalue estimate from Theorem 6. The “Smallness Method X” plots will show the $H^1$-norm of the approximation $\phi$ surrounded by the gray area in which the smooth solution lies (the borders are given by the respective method). The red dotted line in these plots represents the threshold for the smallness criterion. If the upper bound of the gray area falls below this threshold, we have global regularity. The simulations show that whereas Method 1 reaches a blowup relatively fast, Method 2 stays small enough to reach both, the smallness and the time criterion, due to the new eigenvalue estimate. The corresponding plot of the eigenvalue estimate can be found in Fig. 1b (truncated in time, but the interesting part is there).
Fig. 2 Convergence of the rigorous eigenvalue bound to the finite dimensional eigenvalue for increasing $n$. The values for $n$ are 8, 16, 32, 64, 128, 256, 512, 1024. Please note the logarithmic scale of the x- and y-axis.

Fig. 3 $u_0 = 2 \sin(x)$, $N = 256$ and $h = 10^{-6}$. $N$ is larger than the maximum for modes needed, so that Method 2 (with eigenvalue estimate) is valid. Method 1 (without eigenvalue estimate) fails relatively fast whereas Method 2 succeeds in both the smallness and time criterion.

6 Conclusion

We presented a rigorous eigenvalue estimate based on numerical calculations to improve our previous estimates which relied heavily on general interpolation inequalities for numerical verification of global uniqueness for solutions of the surface growth equation. Our simulations show that this eigenvalue estimate is a significant improvement to the previous results of [1], which improved the analytic results given by Theorem 2, and suggest that the eigenvalue bound converges to the true eigenvalue for $n \to \infty$. Please keep in mind that in order to speed up the calculations our simulations are not fully rigorous as interval arithmetic was not used, although every mathematical preparation was carried out. We only wanted to establish a proof of concept that the methods have the potential to actually establish a proof.

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