Efficient rigorous numerics for high-dimensional PDEs via one-dimensional estimates

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Abstract
Computing numerical approximations of solutions of high-dimensional PDEs is inevitably affected by the so-called curse of dimensionality. In order to address this fundamental issue, we introduce a computational method that not only produces rigorous mathematical theorems regarding the correctness of the numerical output, but also has the important property that most of the extra computational cost involved in the proofs is not affected by the curse of dimensionality. The idea is to prove the existence of solutions of high-dimensional nonlinear PDEs by verifying computationally the hypotheses of a contraction mapping theorem and by bounding the nonlinearities via one-dimensional estimates. It is demonstrated that with this new approach it is dramatically cheaper to prove that the numerical output is correct than to recompute at a finer resolution. This claim is illustrated in the context of a pattern formation model defined on a three-dimensional spatial domain.

1 Introduction
Scientists using mathematical models to predict and understand phenomena in fields as broad as physics and finance face the fact that realistic models often need to be defined on high-dimensional spatial domains. For instance, partial differential equations (PDEs) arising in fluids and material science are naturally defined on three-dimensional domains, and mathematical finance models like the Black-Scholes equation can be defined on domains of dimension as large as ten. These models are on the one hand more realistic than lower-dimensional versions, but on the other hand have the disadvantage of being affected by the so-called curse of dimensionality. In other words, given a fixed grid size, the number of spatial discretization points required to realize that size increases exponentially as the dimension of the domain grows. As a result, and motivated by the increasingly important role played by numerical simulations, scientists are constantly developing efficient algorithms in order to reduce the computational cost involved in computing approximate solutions of high-dimensional PDEs. However, when done at the frontiers of computability, it may be very hard to verify the correctness of the numerical output. For instance, in the context of a three-dimensional PDE, the standard approach of assessing the correctness of the numerical result simply based upon its reproducibility at different levels of refinement may be impractical. More explicitly, suppose that a numerical method to solve a three-dimensional model involves an algorithm of computational complexity \(n^3\) (e.g. computing the LU decomposition of an \(n \times n\) matrix). Since the input of the algorithm is a discretization of a function

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defined on a three-dimensional domain, its size is $n = m^3$, where $m$ represents the number of points in the discretization in each dimension. An attempt to reproduce the result by doubling the number of mesh points in each dimension would increase the computational cost by a factor of 512, since then $n = (2m)^3 = 8m^3$ and $n^3 = 512m^9$. Using this standard approach a one week numerical simulation could take about ten years to be verified. In order to address this fundamental issue in the context of high-dimensional PDEs, we propose here a computational method that not only produces rigorous mathematical theorems regarding the correctness of the numerical output, but also has the important property that most of the extra computational cost involved in the proof is not affected by the curse of dimensionality.

It is important to mention that several methods have been developed to address the problem of the curse of dimensionality arising from computing solutions of high-dimensional PDEs. We refer to [1] and the references therein for an extensive review of the methods. Just to give a few examples, sparse tensor product approximations [2, 3] and tensor-product wavelet bases [4] have been developed to compute solutions of parabolic and elliptic PDEs, and the Monte Carlo method [5] is by now a standard tool used in computing numerical solutions of high-dimensional PDEs arising in mathematical finance. However, to the best of our knowledge, none of these novel approaches have been adapted to produce rigorous computer-assisted proofs regarding the correctness of the numerical output.

One of the key ingredient of the proposed approach is to use a computer program with interval arithmetic [6] to generate sharp one-dimensional analytic estimates (see Appendix A) which are then used to produce high-dimensional estimates. The purpose of the high-dimensional estimates is twofold. First, they are used to construct rigorous upper bounds for the convolution terms involved in the nonlinearities of the PDE. Second, they are used to estimate the truncation error terms introduced by computing on a finite dimensional approximation of the original problem. Furthermore, since these high-dimensional estimates are solely based on product of one-dimensional estimates, their rigorous computer-assisted construction does not increase in complexity as the dimension of the domain increases.

It is well known that evaluating nonlinearities of high-dimensional PDEs can be very expensive. Efficient algorithms like the Fast Fourier Transform (FFT) (e.g. see [7] and the references therein) have been successfully applied to speed up such computations, but as mentioned earlier, when done at the frontier of computability, such algorithms can be hard to apply (e.g. see Example 1.2). In order to address this difficulty, the present method proposes using sharp analytic estimates to bound the nonlinearities as opposed to computing them with FFT. As it is discussed in details in Section 2.2, with this new approach,

\[
\text{it is dramatically cheaper to prove that the numerical output is correct than to recompute at a finer resolution.}
\]

Note that this result is similar in spirit to the result of [8], where it was demonstrated that the computational cost of the so-called validated continuation method is less than twice the cost of the standard continuation method alone. It is important to remark however that only one-dimensional examples were presented in [8], and that the method there did not include control of the floating point errors involved in the computations by means of interval arithmetic, meaning that the cost comparison there is a result regarding non-rigorous computations.

The method introduced in the present work is based on the rigorous continuation method of [9], which has been developed to prove existence of equilibrium solutions of parameter
dependent PDEs of the form
\[ u_t = L(u, \lambda) + \sum_{n=2}^{p} q_n u^n, \]  
(1)
in a rectangular domain \( \Omega \subset \mathbb{R}^d \), where \( \lambda \in \mathbb{R} \) is a parameter, \( L(\cdot, \lambda) \) is a linear operator, and \( q_n = q_n(\lambda) \in \mathbb{R} \) are the coefficients of the polynomial nonlinearities. The main differences with the work introduced in [9] and the present work are introduced at the end of this section. It is demonstrated in [9] that under certain regularity conditions on the solutions, finding equilibria of (1) is equivalent to finding solutions of
\[ f(x, \lambda) = 0, \]  
(2)
for \( x = \{x_k\}_{k \in \mathbb{Z}^d} \) in a Banach space \( X^* \) of coefficients decaying algebraically at least as fast as \( \{1/\omega_k^d\}_{k \in \mathbb{Z}^d} \), where \( \{\omega_k^d\}_{k \in \mathbb{Z}^d} \) are weights with decay rate \( s \). The map \( f := \{f_k\}_{k \in \mathbb{Z}^d} \) is given component-wise by
\[ f_k(x, \lambda) := \mu_k(\lambda) x_k + \sum_{n=2}^{p} q_n \sum_{\substack{k_1, \ldots, k_n \in \mathbb{Z}^d \text{ such that } k_1 + \cdots + k_n = k}} x_{k_1} \cdots x_{k_n}, \quad k \in \mathbb{Z}^d. \]  
(3)

At the parameter value \( \lambda = \lambda_0 \), the rigorous continuation is based on a contraction mapping argument applied to a Newton-like operator \( T \), which depends on an approximation of the inverse of \( Df(\bar{x}, \lambda_0) \), where \( \bar{x} \) is a numerical approximation of a finite dimensional Galerkin approximation of (2), for \( \lambda = \lambda_0 \). The method focuses on efficiently determining balls \( B(\bar{x}, r) := \bar{x} + B(r) \) centered at \( \bar{x} \) and of positive radius \( r \) in \( X^* \) on which \( T \) is a contraction mapping. In the end, the proof of existence of solutions of (2) is obtained by verifying a finite number of polynomial inequalities, the so-called radii polynomials \( \{p_k(r)\}_{k \in \mathbb{Z}^d} \), which provide sufficient conditions to have that \( T : B(\bar{x}, r) \to B(\bar{x}, r) \) is a contraction.

Since the extra cost of the proof of the rigorous continuation method of [9] is the construction of the coefficients of these polynomials, the strategy here is to reduce the cost involved in their computation. In order to present this strategy, we briefly review the philosophy and the ingredients involved in the construction of the radii polynomials. For more details, we refer to [9]. The radii polynomials \( \{p_k(r)\}_{k \in \mathbb{Z}^d} \) are upper bounds satisfying
\[ \left| T(\bar{x}) - \bar{x} \right|_k + \sup_{b \in B(r)} \left| \left[ DT(\bar{x} + b) c \right]_k \right| - \frac{r}{\omega_k^d} \leq p_k(r), \quad \text{for every } k \in \mathbb{Z}^d. \]  
(4)
Assuming that one can find a radius \( r > 0 \) such that \( p_k(r) < 0 \) for all \( k \in \mathbb{Z}^d \), then by the Banach Fixed Point Theorem, the operator \( T \) has a unique fixed point within the set \( B(\bar{x}, r) \subset X^* \). In order to avoid having to verify an infinite number of polynomial inequalities, one can construct a polynomial \( \tilde{p}_M(r) \), independent of \( k \), such that
\[ p_k(r) = \tilde{p}_M(r) \frac{r}{\omega_k^d}, \quad \text{for } k \notin F_M, \]  
(5)
where \( M = (M_1, \ldots, M_d) \in \mathbb{N}^d \) is a computational parameter referred to as the verification dimension and \( F_M := \{k \in \mathbb{Z}^d \mid |k| < M \} \), where \( k < M \) and \( |k| \) denote component-wise inequalities and absolute values, respectively. Note that the verification dimension \( M \) provides the size of the finite dimensional system on which the hypotheses of the contraction mapping theorem will be verified. More explicitly, if \( N \) is the cardinality of \( F_M \), one computes \( N \) finite radii polynomials \( \{p_k(r)\}_{k \in F_M} \) satisfying (4) and one tail radii polynomial satisfying (5). To prove existence of steady states of the PDE (1), it is sufficient to verify the hypotheses of the following Lemma.
Lemma 1.1. [9] Consider the finite radii polynomials \( \{p_k\}_{k \in F_M} \) satisfying (4) and the tail radii polynomial \( \tilde{p}_M \) satisfying (5). If there exists an \( r > 0 \) such that \( p_k(r) < 0 \) for all \( k \in F_M \) and \( \tilde{p}_M(r) < 0 \), then there exists a unique \( \hat{x} \in B(\tilde{x}, r) \) such that \( f(\hat{x}, \lambda_0) = 0 \).

Before proceeding further, it is worth mentioning that the idea of the radii polynomials were introduced in [8] with the goal of providing, in the context of equilibria of one-dimensional PDEs, an efficient means of determining a domain on which the contraction mapping theorem is applicable. Since then, they have been extended to prove existence of equilibria of high-dimensional PDEs [9, 10], of connecting orbits of ODEs [13], of time periodic solutions of PDEs [14] and of fundamental matrix solutions arising in Floquet theory [15]. We refer to [16] for a more general discussion of the radii polynomials.

Since the finite radii polynomials \( \{p_k\}_{k \in F_M} \) and the tail radii polynomial \( \tilde{p}_M \) encode the upper bounds (4), one has a certain freedom in how to construct them. There are however two fundamental constraints to be satisfied in their construction. First, the verification dimension \( M \) has to be chosen large enough so that the tail radii polynomial satisfies \( \tilde{p}_M(r) < 0 \) for some \( r > 0 \). Second, the finite radii polynomials have to be efficiently constructed so that their evaluation is not too computationally expensive. In the way that the radii polynomials are constructed in [9], these two constraints compete against each other. Indeed, the nonlinearities of \( f_k \) given by (3) are split as follows

\[
\sum_{\substack{k_1 + \cdots + k^n = k \in \mathbb{Z}^d \atop k_i \in F_M}} x_{k_1} \cdots x_{k^n} = \sum_{\substack{k_1 + \cdots + k^n = k \in F_M}} x_{k_1} \cdots x_{k^n} + \sum_{\substack{k_1 + \cdots + k^n = k \not\in F_M}} x_{k_1} \cdots x_{k^n}, \tag{6}
\]

and the first finite sum is evaluated using the FFT algorithm while the second infinite sum is bounded using analytic estimates. Since the dimension of the FFT computations is larger than the verification dimension \( M \), this approach is very expensive as the dimension \( d \) of the spatial domain \( \Omega \) increases. One of the reasons comes from the aliasing errors that need to be eliminated in order to get rigorous bounds using the FFT [17]. In order to make that important point clear, we give an explicit example.

Example 1.2. Consider \( d = 3, M = (M, M, M) \) and a vector \( x = \{x_k\}_{k \in F_M} \in \mathbb{R}^{(2M-1)^3} \). In order to compute a rigorous upper bound for the sum

\[
\sum_{\substack{k_1 + k_2 + k_3 = k \in F_M}} x_{k_1} x_{k_2} x_{k_3}, \tag{7}
\]

using FFT, one needs to enlarge the vector \( x \) to control the aliasing error (e.g. see [17]). Consider \( M^* \) to be the smallest power of 2 such that \( M^* \geq 2\delta M - 1 \), where \( \delta = 2 \) in this case. Define \( M^* = (M^*, M^*, M^*) \) and consider a new vector \( \tilde{x} = \{\tilde{x}_k\}_{k \in F_{M^*}} \in \mathbb{R}^{(M^*)^3} \) such that

\[
\tilde{x}_k := \begin{cases} 
    x_k, & \text{if } k \in F_M \\
    0, & \text{if } k \in F_{M^*} \setminus F_M.
\end{cases}
\]

An upper bound for (7) can be obtained by computing the Fourier transform of \( \tilde{x} \in \mathbb{R}^{(M^*)^3} \). This computational task can be done using the FFT algorithm, which is a powerful way to compute high-dimensional convolutions (see [7]). However, in the case of three-dimensional PDEs, this algorithm may be hard to apply, since the actual value of \( (M^*)^3 \) can be very large. For example, in [9], in order to prove existence of non trivial equilibria for the 3D Cahn-Hilliard equation, the authors computed a cubic convolution of the form (7) with
$M = 218$, where $M$ was chosen to be the smallest integer so that the tail radii polynomial (5) could be successfully solved (see Figure 4 in [9]). In this case $\delta = 2$ and then $M^* = 2^{10} = 1024 \geq 2\delta M - 1 = 871$. Obtaining a rigorous upper bound for (7) therefore involved computing a FFT of the vector $\tilde{x} \in \mathbb{R}^{(M^*)^3} \approx \mathbb{R}^{10^9}$. This is a serious computational task.

Based on the previous example, we now underline three important differences between the work of [9] and the present work. The first and most significant improvement is a strategy to fight the curse of dimensionality involved in the computation of high-dimensional convolution sums using the FFT. In the present work, a new construction of the polynomials is presented where the nonlinearities of the form (7) are bounded by products of one-dimensional estimates as opposed to using the FFT with large inputs. Second, we introduce an explicit construction of the radii polynomials for general polynomials nonlinearities. In [9], the explicit presentation was done only for cubic nonlinearities. Finally, since this new approach depends heavily on sharp estimates, we improve significantly in Appendix A the one-dimensional estimates presented in [9] (see Figure 7 for a comparison). In order to demonstrate the sharpness of the new estimates in a simple context, we present in Section 3.2 a result about the existence of several equilibria of the one-dimensional Allen-Cahn equation. We refer to Figure 6 for a result which improves dramatically a result of [17].

The paper is organized as follows. In Section 2, the new proposed efficient rigorous numerical method for PDEs via one-dimensional estimates is introduced. The section begins by reviewing some recent methods that combine rigorous computations and efficient numerics. In Section 2.1, the general formulae of the radii polynomials are introduced, where the derivation and the justification is left out for later. In Section 2.2, an analysis of the computational cost involved in the evaluation of the radii polynomials is presented. In Section 3, applications are presented. First, the method is applied in Section 3.1 to prove existence (and local uniqueness) of several equilibrium solutions of a pattern formation model defined on a three-dimensional domain, where it is demonstrated that it is about two hundred times cheaper to prove that the numerical output is correct than to recompute at a finer resolution. Second it is shown in Section 3.2 that the present method provides a significant improvement over the method introduced in [17]. The mathematical justification of the radii polynomials is finally presented in Section 4. The Appendix contains the derivation of the one-dimensional convolution estimates, which are an improvement over the ones presented in [9].

## 2 Efficient rigorous numerics via one-dimensional estimates

Mathematicians are often inclined to emphasize the importance of rigorous mathematical proofs and thus marginalize the computational cost of the verification methods. On the other hand, scientists are often more interested in investigating numerically a wide variety of models rather than answering a particular question about a specific problem. This is a strong motivation to develop numerically efficient rigorous methods. In an attempt to reduce the computational cost and hence make rigorous methods more amenable to large scale computations, efficient algorithms from numerical analysis and scientific computing have been recently incorporated within rigorous computations. For instance, in order to study global solution curves of steady states, path-following algorithms have been used to handle parameter dependent equations more efficiently [8, 18, 19, 20, 10, 21, 22]. Similarly, in order to speed up the computations and to obtain rigorous bounds for the evaluation of the nonlinearities of the PDEs, the fast Fourier transform (FFT) algorithm has been combined
with interval arithmetic [17, 23]. However, like many other numerical methods, the cost of the rigorous computational techniques increases dramatically as the dimension of the spatial domain of the PDE under study increases (e.g. see Example 1.2). Hence, one has to find ways to decrease the number of variables used in the computations while still producing a reliable rigorous numerical output. As mentioned earlier, the goal of the present work is to address the curse of dimensionality in the context of the rigorous continuation method for equilibria of higher-dimensional PDEs introduced in [9]. As mentioned in Section 1, the extra computational cost required to prove the correctness of the numerical output of the Newton method applied on a finite dimensional Galerkin projection is the construction of the radii polynomials satisfying the hypotheses of Lemma 1.1. The general formulae of the radii polynomials are now presented, while their derivation is done in Section 4.

2.1 General formulae for the radii polynomials

In order to perform the necessary computations one needs a finite dimensional approximation to (2). Fix a computational parameter \( m = (m_1, \ldots, m_d) \), which is referred as the Galerkin projection dimension. Denote \( F_m := \{ k \in \mathbb{Z}^d \mid |k| < m \} \), where for \( k = (k_1, \ldots, k_d) \in \mathbb{Z}^d \) and \( |k| = (|k_1|, \ldots, |k_d|) \). The \( m \)-dimensional Galerkin projection \( f^m := \{ f^m_k \}_{k \in F_m} \), with \( f^m_k : \mathbb{R}^{m_1 \cdots m_d} \times \mathbb{R} \to \mathbb{R}^{m_1 \cdots m_d} \) is given by

\[
 f^m_k(x_{F_m}, \lambda) := f_k((x_{F_m}, 0 I_m), \lambda) = \mu_k c_k + \sum_{n=2}^{p} q_n \sum_{k^1, \ldots, k^n = k} c_{k^1} \cdots c_{k^n}, \tag{8}
\]

where \( x_{F_m} := \{ x_k \}_{k \in F_m} \) and \( x_{I_m} := \{ x_k \}_{k \not\in F_m} \) denote, respectively, the finite part of size \( m = (m_1, \ldots, m_d) \in \mathbb{N}^d \) and the corresponding infinite part of \( x = \{ x_k \}_{k \in \mathbb{Z}^d} \).

Assume that one computed a numerical zero for \( f^m \) at a given parameter value \( \lambda_0 \), that is, \( \bar{x}_{F_m} \) such that \( f^m(\bar{x}_{F_m}, \lambda_0) \approx 0 \). Let \( J_m^{-1} \) be a numerical approximation for the inverse of the Jacobian matrix \( Df^m(\bar{x}_{F_m}, \lambda_0) \), which is assumed to be invertible. Fix a computational parameter \( M = (M_1, \ldots, M_d) \), which is referred as the verification dimension. More explicitly, the parameter \( M \) determines the size of the finite radii polynomials, that is there are \( M_1 M_2 \cdots M_d \) finite radii polynomials. Recalling the value \( \mu_k \) in (3), define

\[
 Y_k := \begin{cases} 
 [J_m^{-1} f^m(\bar{x}_{F_m}, \lambda_0)]_k, & \text{if } k \in F_m \\
 \mu_k^{-1} f_k(\bar{x}, \lambda_0), & \text{if } k \in F_m \setminus F_m \\
 0, & \text{if } k \not\in F_m. 
\end{cases} \tag{9}
\]

The one-dimensional weights

\[
 \omega_k^s := \begin{cases} 
 1, & \text{if } k = 0 \\
 |k|^s, & \text{if } k \neq 0,
\end{cases}
\]

are used to define the \( d \)-dimensional weights

\[
 \omega_k^s := \prod_{j=1}^{d} \omega_{k_j}^{s_j} > 0, \tag{10}
\]

where \( s = (s_1, \ldots, s_d) \) is the decay rate. The \( d \)-dimensional weights are used to define the norm

\[
 \|x\|_s := \sup_{k \in \mathbb{Z}^d} \omega_k^s |x_k|. \tag{11}
\]
Using (10), define \( \omega^{-s} := \{1/\omega_k^s\}_{k \in \mathbb{Z}^d} \) and \( \omega^{-s}_{F_m} := \{1/\omega_k^s\}_{k \in F_m} \) and
\[
\tilde{Z}_k^{(1)} := \left[ I - J^{-1} m D f^{(m)}(\bar{x}_{F_m}, \lambda_0) \right] \omega^{-s}_{F_m},
\]
(12)
where \( |·| \) denotes component-wise absolute value and \( I \) denotes the identity operator. Using the definition of the one-dimensional estimates \( \alpha^{(n)}_{k} \) given by (32) and (33) in Section A.2 we define the high-dimensional estimates by
\[
\alpha^{(n)}_{k} = \alpha^{(n)}_{k}(s, M) := \prod_{j=1}^{d} \alpha^{(n)}_{k_j}(s_j, M_j) > 0.
\]
(13)
The usefulness of the estimates (13) is that convolution sums of the form (6) can be bounded by terms of the form \( \alpha^{(n)}_{k}/\omega_k^s \), assuming that the vector \( \bar{x} = \{x_k\}_{k \in \mathbb{Z}^d} \) in (6) decays to zero at least as fast as \( 1/\omega_k^s \). We refer to Figure 1 for an example of the geometrical interpretation of the decay of the high-dimensional estimates (13).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig1.png}
\caption{The case \( d = 2 \): two dimensional estimates \( \alpha^{(3)}_{k} = \alpha^{(3)}_{k_1, k_2} \) as product of one-dimensional estimates for \( M = (50, 50) \) and \( s = (s, s) \). The cases \( s = 2 \) (top–left), \( s = 3 \) (top-right), \( s = 4 \) (bottom-left) and \( s = 5 \) (bottom-right) are depicted.}
\end{figure}

Using the definition of the one-dimensional estimates \( \varepsilon^{(n)}_{k} \) given by (36) in Section A.2 one defines another set of high-dimensional estimates by
\[
\varepsilon^{(n)}_{k} = \varepsilon^{(n)}_{k}(s, M) := \frac{\alpha^{(n)}_{k}}{\omega_k^s} \max_{j=1, \ldots, d} \left\{ \frac{\omega_k^s}{\alpha^{(n)}_{k_j}(s_j, M_j)} \varepsilon^{(n)}_{k_j}(s_j, M_j) \right\}.
\]
(14)
Consider now a computational parameter
\[
\bar{M} := (\bar{M}_1, \ldots, \bar{M}_d), \quad \text{such that} \quad m \leq \bar{M} \leq M,
\]
(15)
which is referred to as the FFT computation dimension. Using (13) and (14) we define

$$Z_k^{(1)} := \begin{cases} \sum_{n=2}^p n |q_n| \left( |x|^n \cdot \left( \text{\omega}_n^s \cdot \text{i}_m^s \right) \right) + \sum_{n=2}^p n |q_n| \|x\|^n \varepsilon_{(n)}^{(1)} & \text{for } k \in F_m \\
\sum_{n=2}^p n |q_n| \left( |x|^n \cdot \left( \text{\omega}_n^s \cdot \text{i}_m^s \right) \right) + \sum_{n=2}^p n |q_n| \|x\|^n \varepsilon_{(n)}^{(1)} & \text{for } k \in F_m \setminus F_m \\
\sum_{n=2}^p n |q_n| \|x\|^n \varepsilon_{(n)}^{(1)} & \text{for } k \not\in F_M \end{cases}$$

and for $\ell \in \{1, \ldots, p - 1\}$

$$Z_k^{(\ell+1)} := \begin{cases} \sum_{n=\ell+1}^p n |q_n| \left( \left( |x|^n \cdot \left( \text{\omega}_n^s \cdot \text{i}_m^s \right) \right) + \|x\|^n \varepsilon_{(n)}^{(\ell+1)} \right) & \text{for } k \in F_m \\
\sum_{n=\ell+1}^p n |q_n| \|x\|^n \varepsilon_{(n)}^{(\ell+1)} & \text{for } k \in F_m \setminus F_m \end{cases}$$

where for the sake of simplicity of the presentation, we identify $x_{F_m}$ with $(x_{F_m}, 0_{I_M})$, $x_{I_M}$ with $(0_{F_M}, x_{I_M})$ and $x_{F_m}$ with $(x_{F_m}, 0_{I_m})$, and we use the discrete convolution notation

$$(x^n)_k = (x \ast \cdots \ast x)_k = \sum_{k_1 + \cdots + k_n = k} x_{k_1} \cdots x_{k_n}.$$

Combining (12), (16) and (17), we define

$$Z_k(r) := \begin{cases} \sum_{\ell=0}^{r-1} \left( |J_m| \cdot Z_k^{(\ell+1)} \right)_k \cdot r^{\ell+1} + Z_k^{(1)}_r & \text{for } k \in F_m \\
\sum_{\ell=0}^{r-1} |\mu| \cdot Z_k^{(\ell+1)}_k \cdot r^{\ell+1} & \text{for } k \in F_m \setminus F_m. \end{cases}$$

Assume that we can find $\tilde{\mu}_M$, independent of $k$, such that

$$\tilde{\mu}_M \leq |\mu|, \quad \text{for all } k \not\in F_M. \quad (19)$$

As in [9], for $M \in \mathbb{N}$, with $M \geq 6$ and $s \geq 2$ we define the one-dimensional asymptotic estimate

$$\alpha_{(n)}^M = \alpha_{(n)}(s, M) := \max \left\{ \alpha_{k_{(n)}}(s, M) \mid k = 0, \ldots, M \right\},$$

which is used to define the high-dimensional asymptotic estimate

$$\alpha_{(n)}^M = \alpha_{(n)}(s, M) := \max_{j_0=1, \ldots, d} \left\{ \alpha_{M_j_0}^n(s_0, M_0) \prod_{j=1}^d \alpha_{M_j}^n(s_j, M_j) \right\}. \quad (20)$$

Define

$$\tilde{Z}_M(r) := \frac{1}{\tilde{\mu}_M} \sum_{\ell=0}^{r-1} \sum_{n=\max\{\ell+1, 2\}}^p n |q_n| \|x\|^n \varepsilon_{(n)}^{(\ell+1)} \left( \frac{n-1}{\ell} \right) \alpha_{(n)}^{\ell}. \quad (21)$$
Definition 2.1. Recall the definition of $Y_k$ and $Z_k(r)$ given respectively in (9) and (18). The finite radii polynomials $\{p_k\}_{k \in F_M}$ are given by

$$p_k(r) = Y_k + Z_k(r) - \frac{r}{\omega_k}, \quad \text{for } k \in F_M. \quad (22)$$

Recall $\tilde{Z}_M(r)$ given by (21). The tail radii polynomial is given defined by

$$\tilde{p}_M(r) = \tilde{Z}_M(r) - 1. \quad (23)$$

2.2 Computational cost involved in computing the polynomials

The FFT computation dimension $\bar{M}$ such that $m \leq \bar{M} \leq M$ is precisely the parameter that governs the computational cost involved in the construction of the finite radii polynomials defined in (22). More precisely, since the convolution sums in (16) and (17) are evaluated using the FFT algorithm with inputs of size $\bar{M}$, the closer $\bar{M}$ is to the Galerkin projection dimension $m$, the more efficient the computation of the polynomials are. The smallest possible “distance” between $\bar{M}$ and $m$ so that the hypotheses of Lemma 1.1 are satisfied is determined by the sharpness of the estimates $\varepsilon_k^{(n)}$ given by (14). Hence, the sharper the one-dimensional estimates $\alpha_k^{(n)}$ and $\varepsilon_k^{(n)}$ from Section A.2 are, the sharper the high-dimensional estimates $\varepsilon_k^{(n)}$ are, the smaller the FFT computation dimension $\bar{M}$ is and therefore the more efficient the computation of the finite radii polynomials are. This fundamental importance of the one-dimensional estimates is the reason why we had to improve the estimates from [9] and present a new improved version in Appendix A. We refer to Figure 7 for an explicit and direct comparison.

It is also important to note that the construction of $Z_k^{(1)}, \ldots, Z_k^{(d)}$ in (16) and (17) corresponding to the cases $k \notin F_{\bar{M}}$ is not affected by the curse of dimensionality, because their computation only involves evaluating the estimates $\alpha_k^{(n)}$, which are mere products of the one-dimensional estimates $\alpha_k^{(n)}$ computed in Section A.2. Therefore, in case we can set $\bar{M} = m$, we have that most of the extra computational cost involved in the proofs is not affected by the curse of dimensionality. As a consequence, in Section 3.1, we demonstrate that in the context of a three-dimensional PDE, we can set $\bar{M} = m$ and it is about two hundred times cheaper to prove that the numerical output is accurate than to recompute at a finer resolution.

3 Applications

3.1 Cost comparison for Swift-Hohenberg in 3D

In this section we consider a pattern formation model defined on a three-dimensional spatial domain and present a cost comparison between the numerical computation of the equilibria and the verification method to prove that the numerical solution represents a true solution of the PDE.

We consider the Swift-Hohenberg equation

$$u_t = \nu u - (1 + \Delta)^2 u - u^3 \quad (24)$$

with even periodic boundary conditions on a rectangular bounded domain $\Omega \subset \mathbb{R}^3$, that is, we are interested in periodic solutions that satisfies the symmetry conditions $u(y,t) = u(|y|,t)$, where $|y| := (|y_1|, |y_3|, |y_3|)$. Equation (24) describes the onset of Rayleigh-Bénard
convection, and is widely used as a model for pattern formation. The parameter \( \nu > 0 \) is the reduced Rayleigh number.

Notice that this equation was considered in [9], where computations in 3D could be performed only for relatively small ranges of parameters due to high computational costs for larger values of the parameter. Figure 2 shows the diagram of the computed solutions of (24). Notice that the range of parameters presented in Figure 2 is much larger than the one considered in [9]. A plot of the level surfaces of the last point on the branch in Figure 2 is presented in Figure 3.

![Figure 2](image_url)

Figure 2: Branch of equilibria for the Swift-Hohenberg equation in the 3D rectangle \( \Omega = [0, 2\pi] \times [0, 2\pi/1.1] \times [0, 2\pi/1.2] \). For all the points on the plot the verification method was successful in proving the existence of a unique equilibria of (24) near the numerically computed solution. For the computations we used \( m = (m, m, m) \) and \( s = (2, 2, 2) \). The projection dimension is \( m = 8 \) for the first point on the branch and it increases as needed along the branch to \( m = 12 \) for the last point.

In Figure 4 and in Table 1, we show a cost comparison between the numerical computation (Numerics) of the equilibria and the verification method (Verification). The verification time measures the cost involved in computing the radii polynomials and verifying the hypotheses of Lemma 1.1. In other words, it represents the extra computational cost involved in performing a computer-assisted proof of existence and local uniqueness of equilibria of (24). The running times in the plot correspond to a single solution on the branch of Figure 2 at \( \nu = 7.4093499072734623 \), which corresponds to the fourth non trivial point rigorously computed on the branch. We recomputed the same solution for several values of \( m \) and ran the verification algorithm on that solution for each value of \( m \). As we can see from Figure 4 the cost of proving the existence of a solution near the numerical result is comparable to the cost of computing the numerical solution itself. Hence it is dramatically cheaper to prove the correctness of the output than to recompute the solution at a finer grid resolution, since the computational cost increases dramatically with \( m \). Let us give a more quantitative description of that claim.

Consider the case \( m = 9 \) in Table 1. It took about 5.84624 seconds to compute a numerical approximation of an equilibrium solution of (24). As mentioned in Section 1, a standard approach of assessing the correctness of a numerical result is based upon its reproducibility at a finer level of refinement. In that case, such a standard approach would
Figure 3: Level surfaces for the solution corresponding to the last point on the branch of Figure 2, corresponding to $\nu = 53.824306721432478$. This solution was computed using $m = (12, 12, 12)$ and the proof was performed using $M = (58, 58, 58)$.

Figure 4: Running times for the numerics and the verification method for a solution in Figure 2. The horizontal axis represent the projection dimension $m$ and the vertical axis refers to the time in seconds needed for the computations. The times shown refer to the same solution that was recomputed for several values of $m$. This demonstrates that it is dramatically cheaper to verify the correctness of the solution than to recompute it with a larger value of $m$. 
require taking \( m = 18 \) to assess the correctness of the output, meaning that in the context of computing equilibria of (24), the extra computational cost to verify the numerical output would be 3084.07 seconds (see Table 1). On the other hand, the extra computational cost of our new proposed rigorous verification method is 15.73299 seconds. This implies that the ratio between the cost of the standard validating method versus our rigorous method is \( 3084.07/15.73299 = 196.025676 \). Therefore, in the context of computing equilibrium solutions of the PDE model (24) in 3D

\[
\text{it is about 200 times cheaper to prove that the numerical output is correct than to recompute at a twice as fine resolution.}
\]

Note that while the above ratio (≈ 196) was computed with a Galerkin projection dimension \( m = (m,m,m) \), where \( m = 9 \), we believe that this ratio should increase as one increases \( m \).

<table>
<thead>
<tr>
<th>( m )</th>
<th>Numerics</th>
<th>Verification</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1.78967</td>
<td>11.94395</td>
</tr>
<tr>
<td>9</td>
<td>5.84624</td>
<td>15.73299</td>
</tr>
<tr>
<td>11</td>
<td>37.8836</td>
<td>35.01097</td>
</tr>
<tr>
<td>14</td>
<td>323.518</td>
<td>317.60105</td>
</tr>
<tr>
<td>18</td>
<td>3084.07</td>
<td>2539.81061</td>
</tr>
</tbody>
</table>

Table 1: Running times in seconds.

### 3.2 A dramatic improvement for Allen-Cahn 1D

As mentioned in Section 1, in order to demonstrate the efficiency of the new proposed method and the sharpness of the new estimates of Appendix A, we now present a comparison with the rigorous computational method introduced in [17]. There, the construction of the radii polynomials is done with different estimates. In particular, the method is applied to the one-dimensional Allen-Cahn equation

\[
\begin{aligned}
&\frac{u_t}{\epsilon^2} = u_{xx} + u - u^3, \quad \text{in } \Omega = [0,1] \\
&u_x = 0, \quad \text{on } \partial\Omega,
\end{aligned}
\]

(25)

where \( \lambda = \pi^2/\epsilon^2 \) is used as the continuation parameter. For (25) the Fourier basis \( \{\cos(k\pi x) \mid k = 0,1,2,\ldots\} \) is used and then the solutions of (25) are represented using the expansion

\[
\begin{aligned}
u(x,t) &= u_0(t) + 2\sum_{k=1}^{\infty} u_k(t) \cos(k\pi x).
\end{aligned}
\]

So (25) takes the form

\[
\begin{aligned}
\mu_k u_k - \sum_{k_1+k_2+k_3 = k} u_{k_1} u_{k_2} u_{k_3}.
\end{aligned}
\]

(26)

where \( \mu_k = 1 - \pi^2k^2/\lambda \) are the eigenvalues of the linear operator in (25). The radii polynomials introduced in Definition 2.1 were constructed in the context of (26) and several equilibria of (25) were proved to exist by verifying the hypotheses of Lemma 1.1. In Figure 5, we present a comparison of the branches computed with the construction of [17] and
the branches computed using the new method introduced in this paper. Note that using
the present method, we did not encounter any failure for the method. This is a significant
improvement compared to the result of [17], where all computations eventually failed at fairly
small parameter values.

Figure 5: Branches from [17] (left) and the ones computed using the new method presented
in this paper (right).

Another improvement of the method can be seen by comparing the minimal Galerkin
projection dimension $m$ that is required to verify the hypotheses of Lemma 1.1 using the
construction of the radii polynomials from [17] and the construction of the radii polynomials
done in this paper. Notice that using the present method, the finite dimensional Galerkin
projection can be taken $10^5$ times smaller than in [17] while still producing a proof. This is
a dramatic improvement.

Figure 6: The minimal required dimension of the Galerkin projection $m$ as a function of the
continuation parameter $\lambda$ along: (a) the black dotted branch of equilibria of Allen-Cahn
from Figure 5 (left) which was proved using the method from [17]; (b) the branch (3) of
equilibria of Allen-Cahn from Figure 5 (right) which was proved using the present method.
4 Justification of the formulae of the radii polynomials

In this section, we justify and describe the construction of the radii polynomials that are defined in Section 2.1. The first ingredient in the construction of the radii polynomials is to find a numerical zero for \( f^{(m)} \) at a given parameter value \( \lambda_0 \), that is, one finds \( \bar{x}_{F_m} \) such that \( f^{(m)}(\bar{x}_{F_m}, \lambda_0) \approx 0 \). Defining \( \bar{x} := (\bar{x}_{F_m}, 0) \) one expects that \( f(\bar{x}, \lambda_0) \approx 0 \) provided \( \bar{x}_{F_m} \) is computed using a sufficiently large Galerkin projection dimension \( m \). This assumption is mathematically justified by the fact that since equilibria of parabolic PDEs are solutions which exist globally in time, the linear term \( L \) in (1) regularizes the solutions and hence equilibria are very smooth (e.g. see [24]). This implies that the coefficients of the Fourier expansion should decay very fast (exponentially) and so by increasing the dimension of the Galerkin projection, one expects to approximate a true solution of the infinite dimensional PDE.

Using the numerical solution \( \bar{x} \), the equation \( f(x, \lambda_0) = 0 \), where \( f \) is given component-wise by (3), is now transformed into an equivalent fixed point problem for a Newton-like operator about \( \bar{x} \). For this purpose, let \( J^{-1}_m \) be a numerical approximation for the inverse of the Jacobian matrix \( Df^{(m)}(\bar{x}_{F_m}, \lambda_0) \), which is assumed to be invertible. Recalling the definition of the high-dimensional weights in (10), we define the Banach space

\[
X^s = \{ x \mid \|x\|_s < \infty \},
\]

consisting of sequences with algebraically decaying tails according to the rate \( s \). The linear operator \( J^{-1} \) on \( X^s \) is defined by

\[
J^{-1}(x)_k := \begin{cases} J^{-1}_m(x_{F_m})_k, & \text{if } k \in F_m \\ \mu_k^{-1} x_k, & \text{if } k \not\in F_m. \end{cases}
\]

Notice that \( J^{-1} \) is an approximation for the inverse of \( Df(\bar{x}, \lambda_0) \). Defining

\[
T(x) := x - J^{-1}f(x, \lambda_0)
\]

one can readily see that finding zeros of \( f \) is equivalent to finding fixed points of \( T \) (see [9]). The idea is to uniquely enclose fixed points of \( T \) into closed balls \( B(\bar{x}, r) \) in \( X^s \) centered at \( \bar{x} \). One can easily check that the closed ball of radius \( r \) in \( X^s \), centered at the origin, is given by

\[
B(r) := B(0, r) = \prod_{k \in \mathbb{Z}^d} \left[ -\frac{r}{\omega_k}, \frac{r}{\omega_k} \right].
\]

The closed ball of radius \( r \) centered at \( \bar{x} \) is

\[
B(\bar{x}, r) = \bar{x} + B(r).
\]

As proved in Lemma 3.3 in [9], to show that \( T : B(\bar{x}, r) \to B(\bar{x}, r) \) is a contraction mapping in \( X^s \), one needs bounds \( Y_k \) and \( Z_k \) satisfying

\[
|T(\bar{x}) - \bar{x}|_k \leq Y_k, \quad \text{for every } k \in \mathbb{Z}^d.
\]

\[
\sup_{b \in B(r)} |DT(\bar{x} + b)c|_k \leq Z_k(r), \quad \text{for every } k \in \mathbb{Z}^d.
\]

Recalling that the radii polynomials must satisfy (4), it is sufficient to compute \( Y_k \) and \( Z_k \) satisfying (28) and (29) to construct them.
4.1 Computation of $Y_k$

In order to compute the upper bounds $Y_k$, it is important to note that, since $\bar{x}$ is such that $\bar{x}_k = 0$ for $k \notin F_m$, we have $(\bar{x}^n)_k = 0$ for every $n \geq 1$ and $k \in \mathbb{Z}^d$ such that $k_j \geq n(m_j - 1) + 1$ for some $1 \leq j \leq d$. Hence, choosing $M$ such that $M_j \geq p(m_j - 1) + 1$ for all $1 \leq j \leq d$, we have that $f_k(\bar{x}, \lambda_0) = 0$ for every $k \geq M$. Therefore, since $T(\bar{x}) - \bar{x} = -J^{-1}f(\bar{x}, \lambda_0)$, we can define $Y = \{Y_k\}_{k \in \mathbb{Z}^d}$ as

$$Y_k := \begin{cases} 
\lfloor J^{-1}f(m)(\bar{x}_{F_m}, \lambda_0) \rfloor_k, & \text{if } k \in F_m \\
\mu_k^{-1}f_k(\bar{x}, \lambda_0), & \text{if } k \in F_M \setminus F_m \\
0, & \text{if } k \notin F_M.
\end{cases}$$

4.2 Computation of $Z_k$

In order to compute $Z_k$ we denote $\bar{J}_m := Df(m)(\bar{x}_{F_m}, \lambda_0)$ and introduce the linear operator on $X^*$

$$\bar{J}(x)_k := \begin{cases} 
\bar{J}_m(x_{F_m})_k, & \text{if } k \in F_m \\
\mu_k x_k, & \text{if } k \notin F_m,
\end{cases}$$

which is an approximate inverse to $J^{-1}$. Define $\omega^- := \{1/\omega_k^m\}_{k \in \mathbb{Z}^d}$ and $\omega^{m} := \{1/\omega_k^m\}_{k \in F_m}$. We write

$$DT(\bar{x} + b)c = (I - J^{-1}\bar{J})c - J^{-1}(Df(\bar{x} + b, \lambda_0) - \bar{J})c,$$

and notice that the first term on the right hand side of (30) is zero for $k \notin F_m$, and is very small for $k \in F_m$ admitting the following upper bound

$$\left| (I - J^{-1}\bar{J})c \right|_k \leq r \left| (I - J^{-1}Df(m)(\bar{x}_{F_m}, \lambda_0) | \omega^{m}_{F_m} \right|_k := r \bar{Z}^{(1)}_k,$$

where $\cdot | \cdot$ denotes component-wise absolute value. Notice that

$$\left[Df(\bar{x} + b, \lambda_0)c\right]_k = \mu_k c_k + \sum_{n=2}^{p} nq_n \sum_{\ell=0}^{n-1} \binom{n - 1}{\ell} (\bar{x}^{n-1-\ell} * b^\ell + c)_k$$

and

$$\left[\bar{J}c\right]_k := \begin{cases} 
\mu_k c_k + \sum_{n=2}^{p} nq_n (\bar{x}^{n-1} * c_{F_m})_k, & \text{for } k \in F_m \\
\mu_k c_k, & \text{for } k \notin F_m.
\end{cases}$$

Set $b = ru$ and $c = rv$, with $u, v \in B(1)$. Now, for the sake of simplicity of presentation, we identify $u_{F_M}$ with $(u_{F_M}, 0_{I_M})$ and $u_{I_M}$ with $(0_{F_M}, u_{I_M})$, for $u \in X^*$. Hence, we have

$$\left[(Df(\bar{x} + b, \lambda_0) - \bar{J})c\right]_k = \sum_{j=1}^{p} C^{(j)}_k v^j,$$

where

$$C^{(1)}_k := \begin{cases} 
\sum_{n=2}^{p} nq_n (\bar{x}^{n-1} * v_{I_m})_k, & \text{for } k \in F_m \\
\sum_{n=2}^{p} nq_n (\bar{x}^{n-1} + v)_k, & \text{for } k \notin F_m.
\end{cases}$$
and for \( \ell \in \{1, \ldots, p-1\} \),

\[
C^{(\ell+1)}_k := \sum_{n=\ell+1}^p n q_n \binom{n-1}{\ell} \left( \bar{x}^{n-\ell} * u^\ell * v \right)_k, \quad \text{for } \ell = 1, \ldots, p-1.
\]

Next upper bounds \( Z^{(j)}_k \) so that \( |C^{(j)}_k| \leq Z^{(j)}_k \), for \( j = 1, \ldots, p \), are constructed. For the cases \( k \in F_M \), we split the sums involved in the \( C^{(1)}_k, \ldots, C^{(p)}_k \). Recalling that \( \bar{x}_{k^j} = 0 \) for \( k^j \not\in F_m \) we can write

\[
C^{(1)}_k = \begin{cases}
\sum_{n=2}^p n q_n (\bar{x}^{n-1} * (v_{I_m} - v_{I_{5\alpha}}))_k + \sum_{n=2}^p n q_n (\bar{x}^{n-1} * v_{I_{5\alpha}})_k, & \text{for } k \in F_m \\
\sum_{n=2}^p n q_n (\bar{x}^{n-1} * v_{F_{5\alpha}})_k + \sum_{n=2}^p n q_n (\bar{x}^{n-1} * v_{I_{5\alpha}})_k, & \text{for } k \in F_M \setminus F_m.
\end{cases}
\]

Now, for a given \( \ell \in \{1, \ldots, p-1\} \) and \( k \in F_M \), consider the splitting

\[
C^{(\ell+1)}_k = \sum_{n=\ell+1}^p n q_n \binom{n-1}{\ell} \left( \bar{x}^{n-\ell} * u^\ell * v_{F_{5\alpha}} \right)_k
\]

Hence, for general \( k \in \mathbb{Z}^d \), one has the following component-wise upper bounds

\[
C^{(1)}_k \leq \begin{cases}
\sum_{n=2}^p n |q_n| \left| \left( \bar{x}^{n-1} * (\omega_{I_m} - \omega_{I_{5\alpha}}) \right)_k \right| + \sum_{n=2}^p n |q_n| ||\bar{x}||_s^{n-1} \left( (\omega^{-s})^{n-1} * \omega_{I_{5\alpha}} \right)_k, & \text{for } k \in F_m \\
\sum_{n=2}^p n |q_n| \left| \left( \bar{x}^{n-1} * \omega_{F_{5\alpha}} \right)_k \right| + \sum_{n=2}^p n |q_n| ||\bar{x}||_s^{n-1} \left( (\omega^{-s})^{n-1} * \omega_{I_{5\alpha}} \right)_k, & \text{for } k \in F_M \setminus F_m \\
\sum_{n=2}^p n |q_n| ||\bar{x}||_s^{n-1} (\omega^{-s})^n_k, & \text{for } k \not\in F_M
\end{cases}
\]

and for \( \ell \in \{1, \ldots, p-1\} \),

\[
C^{(\ell+1)}_k \leq \begin{cases}
\sum_{n=\ell+1}^p n |q_n| \binom{n-1}{\ell} \left| \left( \bar{x}^{n-\ell} * (\omega_{F_{5\alpha}})^{\ell+1} \right)_k \right|
\end{cases}
\]

The fundamental step required to finalize the construction of the radii polynomials is to find efficient ways to bound the nonlinear convolutions. This is precisely where the sharp one-dimensional estimates presented in Appendix A become fundamental. Fix \( \ell \in \)
\{0, \ldots, p\}, n \in \{\max\{\ell + 1, 2\}, \ldots, p\} \text{ and } k \in F_{\overline{M}}. \text{ Using the definition of the one-dimensional estimates } \alpha_{k}^{(n)} \text{ from Section A.2 we define the high-dimensional estimates}

\[ \alpha_{k}^{(n)} = \alpha_{k}^{(n)}(s, M) := \prod_{j=1}^{d} \alpha_{kj}^{(n)}(s_j, M_j). \]

Using the definition of the one-dimensional estimates \( \varepsilon_{k}^{(n)} \) given by (36) in Section A.2 we define another set of high-dimensional estimates

\[ \varepsilon_{k}^{(n)} = \varepsilon_{k}^{(n)}(s, M) := \max_{j=1, \ldots, d} \left\{ \frac{\omega_{kj}^{s}}{\alpha_{kj}^{(n)}(s_j, M_j)} \varepsilon_{kj}^{(n)}(s_j, M_j) \right\}. \]

From Lemma 2.2 in [9], we have that

\[ \left( (\omega^{-s})^{n-1-\ell} \right) \left( (\omega^{-s})_{F}^{\ell+1} \right) \right) \alpha_{k}^{(n)} \text{ for } \alpha_{k}^{(n)} \leq (\ell + 1)\varepsilon_{k}^{(n)}. \]

Similarly, given \( n \in \{2, \ldots, p\} \text{ and } k \notin F_{\overline{M}}, \text{ we can use the Lemma 2.1 from [9] to get that}

\[ \left( (\omega^{-s})^{n} \right) \alpha_{k}^{(n)} \leq \omega_{k}^{s}. \]

As defined in (16) and (17), letting

\[ Z_{k}^{(1)} := \begin{cases} \sum_{n=2}^{p} n |q_{n}| \left( |x|^{n-1} \ast (\omega_{m}^{-s} - \omega_{F}^{-s}) \right)_{k} + \sum_{n=2}^{p} n |q_{n}| \|x\|_{s}^{n-1} \varepsilon_{k}^{(n)}, & \text{for } k \in F_{m} \\
\sum_{n=2}^{p} n |q_{n}| \left( |x|^{n-1} \ast (\omega_{m}^{-s}) \right)_{k} + \sum_{n=2}^{p} n |q_{n}| \|x\|_{s}^{n-1} \varepsilon_{k}^{(n)}, & \text{for } k \notin F_{m} \end{cases} \]

and, for \( \ell \in \{1, \ldots, p - 1\} \),

\[ Z_{k}^{(\ell+1)} := \begin{cases} \sum_{n=\ell+1}^{p} n |q_{n}| \left( \frac{n-1}{\ell} \right) \left( |x|^{n-1-\ell} \ast (\omega_{F}^{-s})^{\ell+1} \right)_{k} + \|x\|_{s}^{n-1-\ell} (\ell + 1) \varepsilon_{k}^{(n)}, & \text{for } k \in F_{\overline{M}} \\
\sum_{n=\ell+1}^{p} n |q_{n}| \|x\|_{s}^{n-1-\ell} \left( \frac{n-1}{\ell} \right) \alpha_{k}^{(n)}, & \text{for } k \notin F_{\overline{M}} \end{cases} \]

we recall the definition of \( Z_{k}(r) \) in (18) to obtain

\[ \sup_{b, c \in B(r)} \left[ DT(\bar{x} + b)c \right]_{k} \leq \begin{cases} Z_{k}(r) = \sum_{\ell=0}^{p-1} \left( J_{m}^{1-\ell} \right) Z_{k}^{(\ell+1)}_{m} r^{\ell+1} + \bar{Z}_{k}^{(1)} r, & \text{for } k \in F_{m} \\
Z_{k}(r) = \sum_{\ell=0}^{p-1} \mu_{k}^{-1} Z_{k}^{(\ell+1)} m^{\ell+1}, & \text{for } k \notin F_{m} \end{cases} \]

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Now assume that we can find $\tilde{\mu}_M$, independent of $k$, such that

$$\tilde{\mu}_M \leq |\mu_k|, \text{ for all } k \notin F_M.$$ 

Then, for $k \notin F_M$, we have

$$\sup_{b,c \in B(r)} \left| \left[ DT(\bar{x} + b)c \right]_k \right| \leq \sum_{\ell=0}^{p-1} |\mu_k|^{\ell+1} \omega_k^{\ell+1} \leq \sum_{\ell=0}^{p-1} \frac{\mu_k}{n=\max\{\ell+1,2\}} n|q_n||\bar{x}|_s^{n-1-\ell} \left( \frac{n-1}{\ell} \right) \alpha_k^{(n)} r^{\ell+1}$$

$$\leq \frac{r}{\omega_k^s} \tilde{Z}_M(r)$$

$$= \frac{r}{\omega_k^s} \left[ \frac{1}{\tilde{\mu}_M} \sum_{\ell=0}^{p-1} \sum_{n=\max\{\ell+1,2\}} n|q_n||\bar{x}|_s^{n-1-\ell} \left( \frac{n-1}{\ell} \right) \alpha_k^{(n)} r^{\ell} \right].$$

We now have all the bounds required to define the radii polynomials given by (22) and (23).

## A Appendix: sharper one-dimensional estimates

In this section some improvements of the one-dimensional estimates of [9] are introduced. The reason for presenting these estimates is because the one-dimensional estimates need to be as sharp as possible since they play a fundamental role in the construction of the radii polynomials. Consider a decay rate $s \geq 2$, a computational parameter $M \geq 6$ and define, for $k \geq 3$,

$$\gamma_k = \gamma_k(s) := 2 \left[ \frac{k}{k-1} \right]^s + \frac{4 \ln(k-2)}{k} + \frac{\pi^2 - 6}{3} \left[ \frac{2}{k} + \frac{1}{2} \right]^{s-2}. \quad (31)$$

**Lemma A.1.** For $s \geq 2$ and $k \geq M \geq 6$ we have

$$\sum_{k_1=1}^{k-1} \frac{\omega_k^s}{\omega_k^s \omega_{k-k_1}} = \sum_{k_1=1}^{k-1} \frac{k^s}{k_1^s(k-k_1)^s} \leq \gamma_k \leq \gamma_M.$$

### A.1 Sharper quadratic estimates

For $k \in \mathbb{Z}$, we define $\alpha_k^{(2)} = \alpha_k^{(2)}(s, M)$ by

$$\alpha_k^{(2)} := \begin{cases} 
1 + 2 \sum_{k_1=1}^{M} \frac{1}{\omega_k^{2k_1}} + \frac{2}{M^{2s-1}(2s-1)}, & \text{for } k = 0 \\
M \sum_{k_1=1}^{M} \frac{2\omega_k^s}{\omega_k^s \omega_{k+k_1}^s} + \frac{2\omega_k^s}{(k+M+1)^s M^{s-1}(s-1)} + 2 + \sum_{k_1=1}^{k-1} \frac{\omega_k^s}{\omega_k^s \omega_{k-k_1}^s}, & \text{for } 1 \leq k \leq M-1 \\
2 + 2 \sum_{k_1=1}^{M} \frac{1}{\omega_k^{s-1}(s-1)} + \frac{2}{M^{s-1}(s-1)} + \gamma_M, & \text{for } k \geq M,
\end{cases} \quad (32)$$
and for $k<0$,

$$\alpha_k^{(2)} := \alpha_{|k|}^{(2)}.$$

**Lemma A.2 (Quadratic estimates).** Given $s \geq 2$ and $M \geq 6$. Then, for any $k \in \mathbb{Z}$, we have that

$$\sum_{k_1+k_2=k \atop k_j \in \mathbb{Z}} \frac{1}{\omega_k \omega_{k_1} \omega_{k_2}} \leq \frac{\alpha_k^{(2)}}{\omega_k^s}.$$

**Proof.** For $k = 0$ we have

$$\sum_{k_1+k_2=k \atop k_j \in \mathbb{Z}} \frac{1}{\omega_k \omega_{k_1} \omega_{k_2}} = 1 + 2 \sum_{k_1=1}^{\infty} \frac{1}{\omega_{2k_1}^s} \leq 1 + 2 \sum_{k_1=1}^{M} \frac{1}{\omega_{2k_1}^s} + \frac{2}{M^{2s-1}(2s-1)} = \frac{\alpha_0^{(2)}}{\omega_0^s}.$$

For $1 \leq k \leq M-1$ we have

$$\sum_{k_1+k_2=k \atop k_j \in \mathbb{Z}} \frac{1}{\omega_k \omega_{k_1} \omega_{k_2}} = \frac{1}{\omega_k^s} \left[ 2 \sum_{k_1=1}^{\infty} \frac{\omega_k^s}{\omega_{k_1} \omega_{k+k_1}^s} + \frac{2}{\omega_0} + \sum_{k_1=1}^{k-1} \frac{\omega_k^s}{\omega_{k_1} \omega_{k-k_1}^s} \right]$$

$$\leq \frac{1}{\omega_k^s} \left[ \sum_{k_1=1}^{M} \frac{2\omega_k^s}{\omega_{k_1} \omega_{k+k_1}^s} + \frac{2\omega_k^s}{(k+M+1)^s} M^{s-1}(s-1) + 2 + \sum_{k_1=1}^{k-1} \frac{\omega_k^s}{\omega_{k_1} \omega_{k-k_1}^s} \right]$$

$$= \alpha_k^{(2)} \frac{\omega_k^s}{\omega_k^s}.$$

Finally, for $k \geq M$,

$$\sum_{k_1+k_2=k \atop k_j \in \mathbb{Z}} \frac{1}{\omega_k \omega_{k_1} \omega_{k_2}} = \frac{1}{\omega_k^s} \left[ 2 \sum_{k_1=1}^{\infty} \frac{\omega_k^s}{\omega_{k_1} \omega_{k+k_1}^s} + \frac{2}{\omega_0} + \sum_{k_1=1}^{k-1} \frac{\omega_k^s}{\omega_{k_1} \omega_{k-k_1}^s} \right]$$

$$\leq \frac{1}{\omega_k^s} \left[ \sum_{k_1=1}^{M} \frac{2\omega_k^s}{\omega_{k_1} \omega_{k+k_1}^s} + \frac{2}{M^{s-1}(s-1)} + 2 + \gamma_M \right] = \alpha_k^{(2)} \frac{\omega_k^s}{\omega_k^s}.$$

In the two inequalities above we used integral estimates to bound the infinite sums. Using these inequalities and the upper bound $\gamma_k$ from Lemma A.1 we have the result. $\blacksquare$
A.2 Shaper general estimates

We also define \( \alpha_k^{(n)} = \alpha_k^{(n)}(s, M) \), for \( n \geq 3 \), by

\[
\alpha_k^{(n)} := \begin{cases} 
\alpha_0^{(n-1)} + 2 \sum_{k_1=1}^{M-1} \frac{\alpha_{k_1}^{(n-1)}}{\omega_{k_1}^s} + \frac{2\alpha_M^{(n-1)}}{(M-1)^{2s-1}(2s-1)}, & \text{for } k = 0 \\
\sum_{k_1=1}^{M-k} \frac{\alpha_{k+k_1}^{(n-1)} \omega_{k_1}^s}{\omega_{k_1}^s} + \frac{\alpha_M^{(n-1)} \omega_k^s}{\omega_{k}^s} + \sum_{k_1=1}^{k-1} \frac{\alpha_{k_1}^{(n-1)} \omega_{k_k-k_1}^s}{\omega_{k_k-k_1}^s} + \alpha_k^{(n-1)} + \alpha_0^{(n-1)}, & \text{for } 1 \leq k \leq M-1 \\
\alpha_M^{(n-1)} \sum_{k_1=1}^{M} \frac{1}{\omega_{k_1}^s} + \frac{2\alpha_M^{(n-1)}}{(M-1)^{s-1}(s-1) + \Sigma^s} + \sum_{k_1=1}^{M} \frac{\alpha_{k_1}^{(n-1)}}{\omega_{k_1}^s} + \alpha_M^{(n-1)} + \alpha_0^{(n-1)}, & \text{for } k \geq M 
\end{cases}
\]

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and for \( k < 0 \),

\[
\alpha_k^{(n)} := \alpha_{|k|}^{(n)}.
\]

Lemma A.3 (General estimates). Given \( s \geq 2 \) and \( M \geq 6 \). Then, for any \( k \in \mathbb{Z} \), we have that

\[
\sum_{k_1 + \ldots + k_n = k, \ k_j \in \mathbb{Z}} \frac{1}{\omega_{k_1}^s \ldots \omega_{k_n}^s} \leq \frac{\alpha_k^{(n)}}{\omega_k^s}.
\]

Proof. For \( k = 0 \) we have

\[
\sum_{k_1 + \ldots + k_n = 0, \ k_j \in \mathbb{Z}} \frac{1}{\omega_{k_1}^s \ldots \omega_{k_n}^s} \leq \alpha_0^{(n-1)} + 2 \sum_{k_1=1}^{M-1} \frac{\alpha_{k_1}^{(n-1)}}{\omega_{k_1}^s} + \frac{2\alpha_M^{(n-1)}}{(M-1)^{2s-1}(2s-1)} = \alpha_0^{(n)}.
\]

For \( k > 0 \) we have

\[
\sum_{k_1 + \ldots + k_n = k, \ k_j \in \mathbb{Z}} \frac{1}{\omega_{k_1}^s \ldots \omega_{k_n}^s} \leq \sum_{k_1=1}^{\infty} \frac{1}{\omega_{k_1}^s \omega_{k+k_1}^s} + \sum_{k_1=1}^{k-1} \frac{1}{\omega_{k_1}^s \omega_{k-k_1}^s} + \sum_{k_1=1}^{\infty} \frac{1}{\omega_{k+k_1}^s \omega_{k_1}^s} + \frac{1}{\omega_0^s} + \frac{1}{\omega_k^s}.
\]

Consider \( k \in \{1, \ldots, M-1\} \). Since \( \alpha_k^{(n-1)} \leq \alpha_M^{(n-1)} \), for all \( k \geq M \), we have

\[
\sum_{k_1=1}^{\infty} \frac{\alpha_{k+k_1}^{(n-1)}}{\omega_{k_1}^s \omega_{k+k_1}^s} \leq \frac{1}{\omega_k^s} \sum_{k_1=1}^{M-k} \frac{\alpha_{k+k_1}^{(n-1)} \omega_{k_1}^s}{\omega_{k_1}^s} + \frac{\alpha_M^{(n-1)} \omega_k^s}{(M+1)^s(M-k)^{s-1}(s-1)}.
\]

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Similarly,
\[
\sum_{k_1=1}^{\infty} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k^{\omega_{k_1}^{s} k^{n-k_1}}} \leq \frac{1}{\omega_k^{s}} \left[ \sum_{k_1=1}^{M} \frac{\alpha_{k_1}^{(n-1)} \omega_k^{s}}{\omega_k^{s} k^{\omega_{k_1}^{s} k_1} + \alpha_M^{(n-1)} \omega_k^{s}} \right].
\]

From the definition of $\alpha_k^{(n)}$ for $k \in \{1, \ldots, M-1\}$, it follows that
\[
\sum_{k_1+\ldots+k_n=k, k \in \mathbb{Z}} \frac{1}{\omega_k^{s} \omega_{k_1}^{s} \ldots \omega_{k_n}^{s}} \leq \frac{\alpha_k^{(n)}}{\omega_k^{s}}.
\]

Consider now $k \geq M$, then
\[
\sum_{k_1=1}^{\infty} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k^{\omega_{k_1}^{s} k_1}} \leq \frac{1}{\omega_k^{s}} \left[ \alpha_M^{(n)} \sum_{k_1=1}^{M} \frac{1}{\omega_k^{s} k_1} + \alpha_M^{(n-1)} M^{\omega_{k_1}^{s} (s-1)} \right].
\]

Using Lemma A.1, we get that
\[
\sum_{k_1=1}^{k-1} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k^{\omega_{k_1}^{s} k_1}} = \sum_{k_1=1}^{M-1} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k^{\omega_{k_1}^{s} k_1}} + \frac{1}{\omega_k^{s}} \sum_{k_1=M}^{k-1} \omega_k^{s} \sum_{k_1=M}^{k-1} \alpha_{k_1}^{(n-1)} \omega_k^{s} k^{\omega_{k_1}^{s} k_1} - \sum_{k_1=1}^{M-1} \frac{\alpha_M^{(n-1)} \omega_k^{s} k^{\omega_{k_1}^{s} k_1}}{\omega_k^{s}} - \sum_{k_1=1}^{M-1} \frac{\alpha_M^{(n-1)} \omega_k^{s} k^{\omega_{k_1}^{s} k_1}}{\omega_k^{s}} \leq \frac{1}{\omega_k^{s}} \sum_{k_1=1}^{M-1} \omega_k^{s} \left( \frac{M^{\omega_{k_1}^{s} (s-1)}}{1 - \frac{k_1}{M}} \right) \leq \frac{1}{\omega_k^{s}} \sum_{k_1=1}^{M-1} \omega_k^{s} \left( \frac{M^{\omega_{k_1}^{s} (s-1)}}{1 - \frac{k_1}{M}} \right) \leq \frac{1}{\omega_k^{s}} \sum_{k_1=1}^{M-1} \omega_k^{s} \left( \frac{M^{\omega_{k_1}^{s} (s-1)}}{1 - \frac{k_1}{M}} \right) \leq \frac{1}{\omega_k^{s}} \sum_{k_1=1}^{M-1} \omega_k^{s} \left( \frac{M^{\omega_{k_1}^{s} (s-1)}}{1 - \frac{k_1}{M}} \right) \leq \frac{1}{\omega_k^{s}} \sum_{k_1=1}^{M-1} \omega_k^{s} \left( \frac{M^{\omega_{k_1}^{s} (s-1)}}{1 - \frac{k_1}{M}} \right)
\]

Note that we can also (as defined in [9]) let
\[
\tilde{\alpha}_M^{(n)} = \max \left\{ \alpha_k^{(n-1)}(s, M) \mid k = 0, \ldots, M \right\},
\]
and get that
\[
\sum_{k_1=1}^{k-1} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k^{\omega_{k_1}^{s} k_1}} \leq \tilde{\alpha}_M^{(n)} M^{\omega_{k_1}^{s} (s-1)} =: \frac{1}{\omega_k^{s}} \Sigma^*,
\]
Hence, defining
\[
\Sigma^* = \min \{ \Sigma^a, \Sigma^b \},
\]
we have that
\[
\sum_{k_1=1}^{k-1} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k^{\omega_{k_1}^{s} k_1}} \leq \frac{1}{\omega_k^{s}} \Sigma^*.
\]
Also,
\[
\sum_{k_1=1}^{\infty} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k^{\omega_{k_1}^{s} k_1}} \leq \frac{1}{\omega_k^{s}} \left[ \sum_{k_1=1}^{M} \frac{\alpha_{k_1}^{(n-1)}}{\omega_k^{s} k_1} + \alpha_M^{(n-1)} M^{\omega_{k_1}^{s} (s-1)} \right].
\]
Combining the above inequalities, we get, for the case \( k \geq M \),
\[
\sum_{k_1, \ldots, k_n = -k \atop k_j \in \mathbb{Z}} \frac{1}{\omega_{k_1}^s \cdots \omega_{k_n}^s} \leq \frac{1}{\omega_k^s} \left[ \sum_{k_1 = 1}^M \frac{1}{\omega_{k_1}^s} + \frac{2\alpha_{M}^{(n-1)}}{M^{s-1}(s-1)} + \sum_{k_1 = 1}^M \frac{\alpha_{k_1}}{\omega_{k_1}^s} + \alpha_{M}^{(n-1)} + \alpha_{0}^{(n-1)} \right] = \frac{\alpha_{k}^{(n)}}{\omega_k^s}. \quad \blacksquare
\]

Figure 7: Comparison of the \( \alpha_k^{(3)} \) (in red) defined in the present paper and the \( \alpha_k^{(3)} \) (in blue) presented in [9] with \( M = 200 \). The cases \( s = 2 \) (left) and \( s = 3 \) (right) are depicted.

A.3 New formulas for \( \varepsilon_k^{(n)} \)

Given \( s \geq 2 \) and \( M \geq \bar{M} \geq 6 \) we define, for \( 0 \leq k \leq \bar{M} - 1 \),
\[
\varepsilon_k^{(n)} = \varepsilon_k^{(n)}(s, \bar{M}, M) := \sum_{k_1 = \bar{M}}^{M-k} \frac{\alpha_{k_1}^{(n-1)}}{\omega_{k_1}^s \omega_{k+k_1}^s} + \sum_{k_1 = \bar{M}}^{M+k} \frac{\alpha_{k_1}^{(n-1)}}{\omega_{k_1}^s \omega_{k-k_1}^s} + \frac{\alpha_{M}^{(n-1)}}{(M+1)^s(s-1)} \left[ \frac{1}{(M-k)^{s-1}} + \frac{1}{(M+k)^{s-1}} \right]
\]
and for \( k < 0 \)
\[
\varepsilon_k^{(n)}(s, \bar{M}, M) := \varepsilon_{|k|}^{(n)}(s, \bar{M}, M).
\]

Lemma A.4. Given \( s \geq 2 \) and \( M \geq \bar{M} \geq 6 \), for \( n \geq 3 \) and \( 0 \leq |k| \leq \bar{M} - 1 \) we have that
\[
\left| \sum_{k_1 + \cdots + k_n = k \atop \max\{|k_1|, \ldots, |k_n|\} \geq \bar{M}} c_{k_1}^{(1)} \cdots c_{k_n}^{(n)} \right| \leq \ell \left( \prod_{i=1}^{n} A_i \right) \varepsilon_k^{(n)}.
\]

Proof. We have that
\[
\sum_{k_1 + \cdots + k_n = k \atop \max\{|k_1|, \ldots, |k_n|\} \geq \bar{M}} \frac{1}{\omega_{k_1}^s \cdots \omega_{k_n}^s} \leq \ell \sum_{k_1 + \cdots + k_n = k \atop |k_1| \geq \bar{M}} \frac{1}{\omega_{k_1}^s \cdots \omega_{k_n}^s},
\]
and
\[
\sum_{k_1 + \cdots + k_n = k} \frac{1}{\omega_{k_1} \cdots \omega_{k_n}} = \sum_{k_1 = -\infty}^{-M} \frac{1}{\omega_{k_1}} \sum_{k_2 + \cdots + k_n = k - k_1} \frac{1}{\omega_{k_2} \cdots \omega_{k_n}} + \sum_{k_1 = M}^{\infty} \frac{1}{\omega_{k_1}} \sum_{k_2 + \cdots + k_n = k - k_1} \frac{1}{\omega_{k_2} \cdots \omega_{k_n}}.
\]

The result then follows from the definition of \( \varepsilon_k^{(n)} \).

**References**


[16] Roberto Castelli, Marcio Gameiro, and Jean-Philippe Lessard. The radii polynomials: a rigorous computational tool to study differential equations. *In preparation*.


