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REVIEW ARTICLE

A Review of David Gottlieb's Work on the Resolution of the Gibbs Phenomenon

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To the memory of David Gottlieb

Abstract. Given a piecewise smooth function, it is possible to construct a global expansion in some complete orthogonal basis, such as the Fourier basis. However, the local discontinuities of the function will destroy the convergence of global approximations, even in regions for which the underlying function is analytic. The global expansions are contaminated by the presence of a local discontinuity, and the result is that the partial sums are oscillatory and feature non-uniform convergence. This characteristic behavior is called the Gibbs phenomenon. However, David Gottlieb and Chi-Wang Shu showed that these slowly and non-uniformly convergent global approximations retain within them high order information which can be recovered with suitable post-processing. In this paper we review the history of the Gibbs phenomenon and the story of its resolution.

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Key words: Gibbs phenomenon, post-processing, Galerkin approximation, collocation approximation, spectral methods, exponential accuracy.

Contents

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1 Introduction

The purpose of this paper is to review the history of the Gibbs phenomenon and the groundbreaking work of David Gottlieb, Chi-Wang Shu, and their co-workers, [16,25–30] on the resolution of the Gibbs phenomenon, for this special issue in memory of David Gottlieb.

To understand the Gibbs phenomenon, we begin with a classical problem: the square wave function,

$$f(x)=\begin{cases} -1, & -1\leq x<0,\\ 1, & 0\leq x\leq 1,\end{cases}$$

which can be written as a Fourier sine series

$$f(x)=\frac{4}{\pi}\sum_{j=odd}^{\infty}\frac{1}{j}\sin(j\pi x)=\frac{4}{\pi}\Big(\sin(\pi x)+\frac{1}{3}\sin(3\pi x)+\frac{1}{5}\sin(5\pi x)+\frac{1}{7}\sin(7\pi x)+\cdots\Big).$$

However, when we look at a Fourier partial sum

$$f_N(x)=\frac{4}{\pi}\sum_{j=odd}^{N}\frac{1}{j}\sin(j\pi x),$$

we observe that it is oscillatory, and that there is an overshoot and undershoot near the discontinuity and the boundaries (Fig. 1). As more terms are used, the overshoot and undershoot get closer to the discontinuity $x=0$ and boundaries $x=\pm 1$, but do not diminish. This indicates that the convergence of the series is not uniform, i.e., even though for each fixed x, the sequence of Fourier partial sums converges as $N\to\infty$ (pointwise convergence), the sequence does not converge as $x\to 0$ and $N\to\infty$ simultaneously. Furthermore, even the pointwise convergence is slow, due to the oscillations.

The convergence of a Fourier series to a discontinuous (or, equivalently, a non-periodic) function is non-uniform, the partial sums are oscillatory and the pointwise convergence is slow, even when we are looking at a point x for which the function is continuous. The oscillatory behavior of the Fourier finite sums was first remarked upon by Wilbraham in 1848, and later, inspired by Josiah Willard Gibbs' spirited correspondence in NATURE in 1898 and 1899, called the Gibbs phenomenon. The Gibbs phenomenon is due to the fact that the local behavior of the function (i.e., a discontinuity

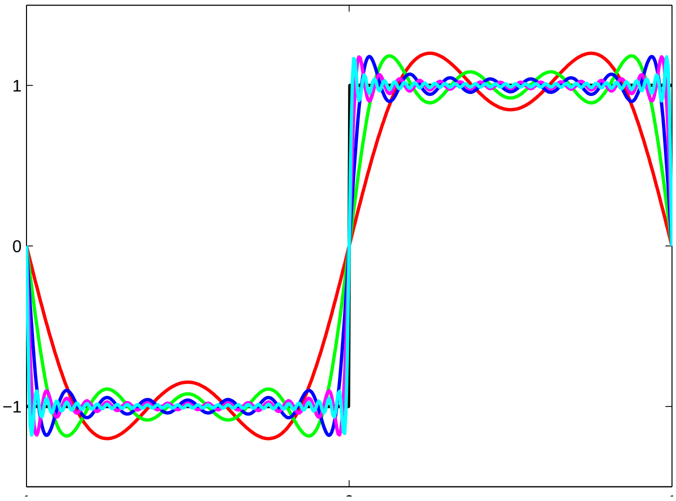


Figure 1: Squarewave function (in black) and its Fourier partial sums for $N=4$ (red), $N=8$ (green), $N=16$ (blue), $N=32$ (magenta), and $N=64$ (cyan).

or lack of periodicity) pollutes the expansion coefficients which are used to construct a global approximation to the function. The Gibbs phenomenon occurs in all other global expansions as well, and has been studied as early as the 1920's in Bessel and Schlömich functions [12, 13, 46, 47].

In the 1990's D. Gottlieb, together with C.-W. Shu and other co-workers, showed that it is possible to completely remove the Gibbs phenomenon by post-processing the Fourier expansion in regions in which the function is analytic, using a re-expansion of the partial sums $f_N(x)$ in a different ("Gibbs complementary") basis [25]. This subject formed the basis of David Gottlieb's last public lecture [31], the John von Neumann lecture titled "The effect of local features on global expansions" given at the SIAM Annual Meeting in San Diego on July 8, 2008. This review paper was inspired by this lecture, which contained a gentle introduction and a historical overview of the Gibbs phenomenon, and the theory behind the resolution of the Gibbs phenomenon. It is our hope that this paper retains the flavor of this lecture, which can be listened to online [31].

2 A history of the Gibbs phenomenon

The story of the Gibbs phenomenon is an interesting episode in the history of mathematics, and has been reviewed in [35] and [30]. The first appearance of a Fourier series was in the middle of the 18th century, when Euler observed that a linear function can be written as an infinite summation of waves, as in

$$\sum_{k=1}^{\infty}\frac{\sin(kx)}{k}=\frac{1}{2}(\pi-x), \qquad 0<x<2\pi.$$

This idea was later used by Fourier to model a complicated heat source as a linear combination of simple sine and cosine waves, which enabled the solution of heat equations as a superposition of the corresponding waves. However, the first study of the overshoots and undershoots which characterize the Gibbs phenomenon (as it later came to be called) was published by Henry Wilbraham in 1848 [45]. A later paper in 1874 by Du Bois-Reymond [14] published an analysis of the Fourier series near the points of discontinuity, but missed identifying the Gibbs phenomenon. In 1898 Michelson and Stratton built a harmonic analyzer (later pictured in the Encyclopedia Brittanica [8]) which, due to Hooke's law, stored up to 80 Fourier coefficients in its springs. A description of the harmonic analyzer was published [39] and featured graphs of functions reconstructed from the Fourier coefficients, including the square wave function (similar to those in Section 1). However, the overshoots and undershoots were not mentioned.

Apparently, though, Michelson was troubled by the behavior he observed in the Fourier partial sums, and worried that the sequence of partial sums did not seem to converge. In October 6, 1898 his letter appeared in NATURE [38] which pointed out the difficulty of constructing $f(x)=x$ from its Fourier coefficients.

> In all expositions of Fourier's series which have come to my notice, it is expressly stated that the series can represent a discontinuous function. The idea that a real discontinuity can replace a sum of continuous curves is so utterly at variance with the physicist's notions of quantity, that is seems to me to be worth while giving a very elementary statement of the problem in such a simple form that the mathematicians can at once point to the inconsistency if any there be. Consider the series
>
> $$y=2\Big[\sin x-\frac{1}{2}\sin 2x+\frac{1}{3}\sin 3x-\cdots\Big].$$
>
> If for x in the given series we substitute $\pi+\epsilon$ we have, omitting the factor 2,
>
> $$-y=\sin\epsilon+\frac{1}{2}\sin 2\epsilon+\frac{1}{3}\sin 3\epsilon+\cdots+\frac{1}{n}\sin n\epsilon\cdots.$$
>
> This series increases with n until $n\epsilon=\pi$. Suppose, therefore, $\epsilon=k\pi/n$, where k is a small fraction. The series will now be nearly equal to $n\epsilon=k\pi$, a finite quantity even if $n=\infty$. Hence the value of y in the immediate vicinity of $x=\pi$ is not an isolated point $y=0$, but a straight line $-y=nx$. [38]

Michelson went on to explain that this problem also plagues the derivative computed by the Fourier series.

At least some mathematicians were happy to respond to the invitation to "point to the inconsistency if any there be". A. E. H. Love replied in the next issue of Nature, one week later (October 13, 1898).

> In a letter to NATURE of October 6, Prof. Michelson, referring to the statement that a Fourier series can represent a discontinuous function, describes "the idea that a real discontinuity can replace a sum of continuous curves" as "utterly at variance with the physicist's notions of quantity." If, as this seems to imply, there are physicists who hold

> "notions of quantity" opposed to the mathematical result that the sum of an infinite series of continuous functions may itself be discontinuous, they would be likely to profit by reading some standard treatise dealing with the theory of infinite series, such, for example, as Hobson's "trigonometry". [37]

After this insulting introduction, Love goes on to restate the problem and then explains the mathematical weakness in Michelson's argument.

> The processes employed are invalid. It is not the case that the sum of an infinite series is the same as the sum of the first n terms, however great n is taken. It is not legitimate to sum an infinite series by stopping at some convenient nth term. It is not legitimate to evaluate an expression for a particular value of x, e.g., $x=\pi$, by putting $x=\pi+\epsilon$ and passing to a limit; to do so is to assume that the expression represents a continuous function. [37]

However, this (correct) statement of the impermissibility of Michelson's argument does not explain what Michelson was observing, and did not satisfy Michelson, who responded with the remark that

> If it is inadmissible to stop at "any convenient nth term" it is quite as illogical to stop at the equally "convenient" value π/n.

In other words, Michelson believed that convergence should happen at any neighborhood of the discontinuity. In the same issue of NATURE, there appeared a letter by Gibbs [23], which explained Michelson's concerns, pointed out that Love ignored them, and described the oscillations which have come to be called "the Gibbs phenomenon". However, in this letter, Gibbs implied that these oscillations decay with N, which is incorrect.

Love responded to Gibbs' letter by expounding on the notion of nonuniform convergence and commenting that "The matter $\cdots$ is perhaps that referred to by Prof. Michelson $\cdots$ but I did not understand his letter so.". Finally, in an April 12, 1899 letter to NATURE (published April 27, 1899), Gibbs corrected his analysis.

> I should like to correct a careless error which I made (Nature, December 29, 1898) in describing the limiting form of the family of curves represented by the equation $\cdots$ whatever differences of opinion have been expressed on this subject seem due, for the most part, to the fact that some writers have had in mind *the limit of the graphs*, and others *the graphs of the limit* of the sum. A misunderstanding on this point is a natural consequence of the usage which allows us to omit the word *limit* in certain connections, as when we speak of the sums of an infinite series. In terms thus abbreviated, either of the things which I have sought to distinguish may be called the graph of the sum of the infinite series. [24]

A follow-up consists of a note from Poincare defending Michelson (forwarded by Michelson and published in the May 18, 1899 issue), and a later letter by Love explaining Fourier's theorem and reiterating the distinction between the limit of the sum and the sum of the limits. However, while the issues of convergence, and the difference between pointwise and uniform convergence were clearly identified in this correspondence, it did not yield an thorough analysis which was needed for understanding the behavior of the finite sum to reconstructing the function, and in particular the need to study those oscillations which we now refer to as the Gibbs phenomenon. This analysis, including a proof, appeared in a long and careful paper by Böcher [6] published in 1906. It was in this paper that the behavior of the Fourier partial sums was given the name "Gibbs phenomenon".

3 Global approximations

The Gibbs phenomenon is a feature of all global approximations, and is not limited to the Fourier series. Thus, we begin with some results about global expansions of a smooth function. Given a function square integrable $f(x)\in L^2_w[-1,1]$, (i.e., where $w(x)$ is some weight, to be described below), we can represent it in an infinite series

$$f(x)=\sum_k \hat{f}_k \Psi_k(x) \tag{3.1}$$

in a basis $\{\Psi_k(x)\}$ which is *orthonormal* under some weight $w(x)$,

$$\int_{-1}^{1} w(x)\Psi_k(x)\Psi_j(x)dx=\delta_{kj}$$

and *complete* in $L^2_w[-1,1]$. The *expansion coefficients* are given by

$$\hat{f}_k=(f,\Psi_k)_w=\int_{-1}^{1} w(x)f(x)\Psi_k(x)dx.$$

Some well-known examples of complete orthogonal bases are the Fourier, Legendre, and Chebyshev bases, which will be used in the remainder of the paper. We will also use the family of Gegenbauer polynomials [5], which is a generalization of the Chebyshev and Legendre bases. The Gegenbauer polynomials $G^\lambda_k(x)$ are defined by the recurrence relation

$$G^\lambda_{k+1}(x)=\frac{2(k+\lambda)}{k+1}xG^\lambda_k(x)-\frac{k+2\lambda-1}{k+1}G^\lambda_{k-1}(x), \qquad k\geq 2.$$

The first two terms are $G^\lambda_0(x)=1$ and $G^\lambda_1(x)=2\lambda x$. They are orthogonal under the weight function

$$w(x)=(1-x^2)^{\lambda-\frac{1}{2}},$$

and can be normalized recognizing that

$$\left(h^\lambda_k\right)^2=\int_{-1}^{1}(1-x^2)^{\lambda-\frac{1}{2}}\left(G^\lambda_k(x)\right)^2dx=\sqrt{\pi}G^\lambda_k(1)\frac{\Gamma(\lambda+\frac{1}{2})}{\Gamma(\lambda)(k+\lambda)},$$

where

$$G_k^\lambda(1)=\frac{\Gamma(k+2\lambda)}{k!\Gamma(2\lambda)}.$$

The special cases $\lambda=0$ and $\lambda=1/2$ give the Chebyshev and Legendre polynomials.

When we deal with approximations of the function $f(x)$ based on global expansions in these bases, we have two typical situations:

Approximation from a finite number of expansion coefficients

Given $N+1$ expansion coefficients $\hat{f}_k$, of the unknown function $f(x)$ which is defined on $-1\le x\le 1$, we would like to construct an approximation which will give us accurate point values of the function.

An approximation can be obtained by simply truncating the series in (3.1)

$$f_N(x)=\sum_{k=0}^{N}\hat{f}_k\Psi_k(x). \tag{3.2}$$

These Gegenbauer polynomial bases are all solutions of a singular Sturm-Liouville problem with weight $w(x)$, and so are orthogonal and complete in $L^2_w[-1,1]$. For this reason, when these basis functions are used to approximate $f(x)\in C^\infty[-1,1]$, the expansion coefficients decay exponentially and the sequence of partial sums is exponentially convergent. To make this more precise, if the function $f(x)\in C^\infty[-1,1]$, then the partial sum $f_N(x)$ given by (3.2), where $\Psi_k(x)$ are eigenfunctions of a singular Sturm-Liouville problem which form a complete orthonormal basis, converges exponentially. If the function $f(x)\in C^K[-1,1]$, then we get convergence of order K. In other words, a discontinuity in the function or in any of its derivative will result in reduced order of convergence.

For the Fourier case, we can write

$$f_N(x)=\sum_{k=-N/2}^{N/2}\hat{f}_k\Psi_k(x)$$

instead of (3.2). The Fourier basis is a solution of a regular Sturm-Liouville problems, and it too produces exponentially decaying coefficients and approximations, but only if the function $f(x)$ and all its derivatives are not only smooth but also periodic.

Approximation from a finite number of point values

Alternatively, we are given $N+1$ point values of the function $f(x_k)$ at some set of points x_k, $k=0,\cdots,N$, and wish to construct an approximation which will give us accurate point values of the function at any point x.

In this case, the usual procedure is to approximate the expansion coefficients by collocation: we require that the approximation match the function values. The approximation is now given by

$$\tilde{f}_N(x)=\sum_{k=0}^{N} a_k \Psi_k(x), \tag{3.3}$$

where the collocation coefficients a_k are evaluated by the requirement that

$$\sum_{k=0}^{N} a_k \Psi_k(x_j)=f(x_j), \qquad j=0,\cdots,N+1.$$

This procedure suffers from two types of errors: that of truncating the infinite series, and that of approximating the exact expansion coefficients $\hat{f}_k$ by the collocation coefficients a_k. The collocation coefficients do not equal to the exact coefficients, and so the collocation approximation $\tilde{f}_N(x)$ differs from the Galerkin approximation $f_N(x)$. This second source of errors decays with the number of collocation points, but is also sensitive to the location of the collocation points.

The choice of interpolation points is critical: each basis $\Psi_k(x)$ has an associated set of interpolation points. For example, the $(N+1)$ Gauss-Lobatto quadrature points for a given polynomial basis are computed by finding the zeroes of the derivative of the degree N basis polynomial, and the endpoints. The $(N+1)$ Gauss points, on the other hand, are computed by finding the zeroes of the degree $(N+1)$ basis polynomial.

For these reasons, the approximation theory for collocation approximations is more complicated, However, in the case where the basis functions $\Psi_k(x)$ are the Fourier, Legendre, Chebyshev, or any of the Gegenbauer polynomials, and where the interpolation nodes are the appropriate Gauss or the Gauss Lobatto points, there are results which prove that in these cases the collocation approximation converges exponentially when the function is analytic [10, 15]. In the following lemma, we state the version of these results which appeared in [29].

Lemma 3.1. ([29]) *Let*

$$\tilde{f}_N(x)=\sum_{k=0}^{N} a_k \Psi_k(x)$$

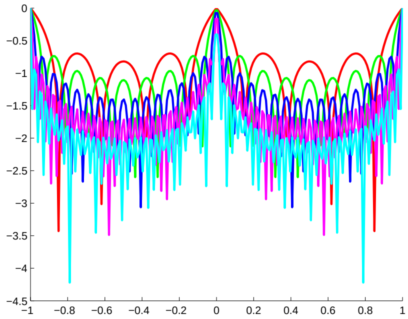
be the collocation approximation with the basis $\{\Psi_k(x)\}$ being the trigonometric polynomials $e^{ik\pi x}$ or the Gegenbauer polynomials $G_k^\lambda(x)$ for $\lambda>-1/2$ with weight $w(x)$, and where the collocation coefficients are computed by interpolation of the function $f(x)$ on the Gauss or Gauss-Lobatto points associated with the basis. If $f(x)$ has K continuous derivatives on $[-1,1]$, then the collocation approximation converges exponentially in the sense that

$$\|f-\tilde{f}\|_{L^2_w} \le \frac{A}{N^K}\|f^{(K)}\|_{L^\infty},$$

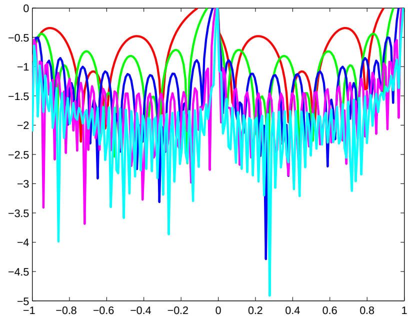
where the weighted L^2 norm is defined by

$$\|f\|^2_{L^2_w}=\int_{-1}^{1} w(x)|f(x)|^2 dx,$$

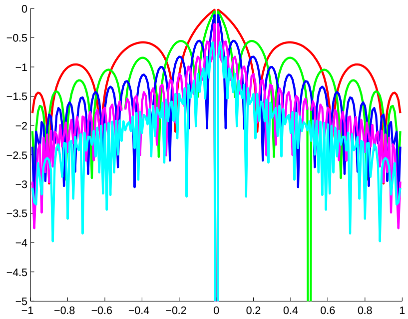
and A is a constant independent of N and K.



(a)



(b)



(c)

Figure 2: Pointwise errors of the Fourier partial sums (a), Fourier collocation (b) and Chebyshev (chebfun) collocation (c) of the square wave function for $N=4$ (red), $N=8$ (green), $N=16$ (blue), $N=32$ (magenta), and $N=64$ (cyan).

Example 3.1. To better understand the Gibbs phenomenon, let's take a closer look at the square wave we used as the motivating example in Section 1. We compute the Fourier Galerkin approximation using the exact coefficients and the collocation approximation, and the Chebyshev approximation (using Trefethen's CHEBFUN [44]), and examine the pointwise errors using both approaches. As expected, the errors are oscillatory everywhere, and are particularly large at the boundaries for the Fourier approximation and at the point of discontinuity $x=0$ for both the Fourier and Chebyshev approximations (Fig. 2). Worse yet, at those points the error does not decay even as more points are taken.

The Gibbs phenomenon happens when we use information from the domain $(-1,1)$, on which $f(x)$ is not analytic, to construct an approximation to $f(x)$. Even when the function is smooth enough that the Gibbs phenomenon is not obvious (i.e., no overshoots and undershoots), it causes slowed convergence and therefore a poor approximation. Of course, if we could use only data from an interval where $f(x)$ is analytic our approximations would not suffer from the Gibbs phenomenon. Unfortunately, we typically have no choice in the matter, as we are usually given the expansion coefficients which were computed this way, for example as a result of some natural Fourier transform (as in satellite images or CT scan or NMR data), or point values which were computed as part of a pseudo-spectral approximation to a partial differential equation. The problem facing us is that of recovering high order local information in a region of smoothness from global information which is contaminated by the presence of discontinuities. In [16,25–30] it was shown that starting with the approximations $f_N(x)$ or $\tilde{f}_N(x)$ it is possible to construct high order approximations in smooth regions which eliminate the Gibbs phenomenon. In the next two sections we will discuss how this is done.

4 Post-processing the Galerkin approximation using Gibbs complementary functions

In this section, we will focus on the case where we begin with the knowledge of the first $N+1$ exact expansion coefficients. The usual approximation to $f(x)$ is then given by

$$f_N(x)=\sum_{k=0}^{N}\hat{f}_k\Psi_k(x). \tag{4.1}$$

This approximation is *global* because the expansion coefficients $\hat{f}_k$ depend on the value of the function over the entire domain

$$\hat{f}_k=(f,\Psi_k)_w=\int_{-1}^{1}w(x)f(x)\Psi_k(x)dx.$$

The problem is that if the function $f(x)$ is only piecewise continuous, the expansion coefficients $\hat{f}_k$ are all affected by this, and the series (4.1) does not converge uniformly to $f(x)$. Furthermore, the pointwise convergence of (4.1) away from the discontinuity is no longer exponential. This means that even if we only care about the approximation $f_N(x)$ to the function $f(x)$ at points $x\in[a,b]$ where the function is very smooth, the approximation is contaminated by the fact that the expansion coefficients are defined on a domain $-1\le x\le 1$ on which the function is not smooth.

In [16,25–30] it was shown that even though the sequence of partial sums $f_N(x)$ converges slowly and non-uniformly, it still contains enough information so that we are able to recover exponential accuracy in the regions in which $f(x)$ is smooth by re-expanding these in an appropriate two-parameter family $\{\Phi_l^\lambda(\xi)\}$.

To transform between the domain $\xi\in[-1,1]$ and $x\in[a,b]$, we define

$$x=\left(\frac{b-a}{2}\right)\xi+\left(\frac{b+a}{2}\right)=\epsilon\xi+\delta.$$

The new approximation, defined on $a\le x\le b$, is

$$\sum_{k=0}^{m}\left\langle f_N,\Phi_l^\lambda\right\rangle_\lambda\Phi_l^\lambda(\xi(x)), \tag{4.2}$$

where

$$\langle f_N, \Phi_l^\lambda \rangle_\lambda = \int_{-1}^{1} (1-\xi^2)^{\lambda-\frac{1}{2}} f_N(x(\xi)) \Phi_l(\xi) d\xi.$$

Note that this new approximation does not depend on the original (exact) expansion coefficients directly, but only on $f_N(x)$, and only from the interval over which $f(x)$ is analytic, $x \in [a,b]$. For this reason, the new approximation (4.2) is referred to as the post-processed approximation.

We will show in Theorem 4.2 that, for appropriate choices of parameters λ and m, (chosen, for simplicity, to be $\lambda = m$), this new approximation (4.2) converges exponentially to $f(x)$ on the interval $x \in [a,b]$ as long as this new basis family $\{\Phi_l^\lambda(\xi)\}$ satisfies the following conditions [34] :

(a) **Orthonormality** For each λ, the basis family $\{\Phi_l^\lambda(\xi)\}$ is orthonormal under the weighted inner product

$$\langle \Phi_l^\lambda(\xi), \Phi_{l'}^\lambda(\xi) \rangle_\lambda = \int_{-1}^{1} (1-\xi^2)^{\lambda-\frac{1}{2}} \Phi_l^\lambda(\xi) \Phi_{l'}^\lambda(\xi) d\xi = \delta_{ll'}. \tag{4.3}$$

(b) **Spectral Convergence** The expansion of an function $g(\xi)$, which is analytic in $-1 \le \xi \le 1$, in the bases $\Phi_k^\lambda(\xi)$ converges uniformly exponentially fast with $\lambda = m$,

$$\max_{-1\le\xi\le1} \left| g(\xi) - \sum_{l=0}^{m} \langle g, \Phi_l^\lambda \rangle_\lambda \Phi_l^\lambda(\xi) \right| \le e^{-q_1 \lambda}, \qquad q_1 > 0. \tag{4.4}$$

(c) **The Gibbs Condition** There exists a number $\beta < 1$ such that if $\lambda = \beta N$ then

$$\left| \langle \Phi_l^\lambda(\xi), \Psi_k(x(\xi)) \rangle_\lambda \right| \max_{-1\le\xi\le1} |\Phi_l^\lambda(\xi)| \le \left(\frac{\alpha N}{k} \right)^\lambda, \tag{4.5}$$

where $k > N$, $l \le \lambda$, $\alpha < 1$.

The first two conditions are properties of the re-projection basis $\Phi_l^\lambda(x)$ only, while the third condition interrelates the two basis, requiring that the projection of the high modes of the basis $\{\Psi_k\}$ (large k) on the low modes of $\Phi_l^\lambda(\xi)$ (small l) is exponentially small in the interval $-1 \le \xi \le 1$ for λ proportional to N.

Using these conditions on the post-processing basis, we can show that the new approximation indeed converges exponentially.

Theorem 4.1. ([34]) *Let $f(x) \in L^2[-1,1]$ be analytic in the subinterval $[a,b] \subset [-1,1]$. Suppose that $\Psi_k(x)$ is an orthonormal family under the inner product $(\cdot,\cdot)_w$ such that*

$$|(f, \Psi_k)_w| \le C$$

for some constant C independent of k, and

$$\lim_{N\to\infty} |f(x) - f_N(x)| = 0$$

almost everywhere in $x\in[-1,1]$. *Let* $\{\Phi_l^\lambda(\xi)\}$ *be a Gibbs complementary basis to* $\{\Psi_k(x)\}$, *with* $\lambda=\beta N$. *Furthermore, assume that the approximation error can be expressed as the tail of the series*

$$\langle f-f_N,\Phi_l^m\rangle_\lambda=\sum_{k=N+1}^{\infty}(f,\Psi_k)_w\langle\Phi_l^\lambda,\Psi_k\rangle_\lambda. \tag{4.6}$$

Then the new approximation converges uniformly and exponentially

$$\max_{a\le x\le b}\Big|f(x)-\sum_{l=0}^{m}\langle f_N,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi(x))\Big|\le e^{-qN},\quad q>0. \tag{4.7}$$

Proof. We begin with the observation that

$$\begin{aligned}&\max_{a\le x\le b}\Big|f(x)-\sum_{l=0}^{m}\langle f_N,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi(x))\Big|\\ \le&\max_{a\le x\le b}\Big|f(x)-\sum_{l=0}^{m}\langle f,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi(x))\Big|+\max_{a\le x\le b}\Big|\sum_{l=0}^{m}\langle f-f_N,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi(x))\Big|.\end{aligned}$$

We wish to show that this converges exponentially and uniformly in $[a,b]$.

To approximate the maximum of first term on the interval $[a,b]$, we note that because $f(x)$ analytic for $x\in[a,b]$, the Spectral Convergence Condition (b) implies that

$$\max_{a\le x\le b}\Big|f(x)-\sum_{l=0}^{m}\langle f,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi)\Big|\le e^{-q_2m},\quad q_2>0.$$

The second term can be estimated by rewriting it as the tail of the series

$$\max_{a\le x\le b}\Big|\sum_{l=0}^{m}\langle f-f_N,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi(x))\Big|\le\max_{a\le x\le b}\sum_{l=0}^{m}\sum_{k=N+1}^{\infty}\Big|(f,\Psi_k)_u\langle\Phi_l^\lambda,\Psi_k\rangle_\lambda\Phi_l^\lambda(\xi)\Big|.$$

Recalling that $|(f,\Psi_k)_w|\le C$ and that there exists some $\beta<1$ so that for $\lambda=\beta N$

$$\Big|\langle\Phi_l^\lambda,\Psi_k\rangle_\lambda\Big|\max_{-1\le\xi\le1}|\Phi_l^\lambda(\xi)|\le\Big(\frac{\alpha N}{k}\Big)^\lambda,$$

for $k>N$, $l<\lambda$, $\alpha<1$, we conclude

$$\max_{a\le x\le b}\Big|\sum_{l=0}^{m}\langle f-f_N,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi(x))\Big|\le C\sum_{l=0}^{m}\sum_{k=N+1}^{\infty}\Big(\frac{\alpha N}{k}\Big)^\lambda\le e^{-qN},\quad q>0.$$

The proof is complete. □

The post-processing procedure discussed here requires knowledge of the interval of analyticity $[a,b]$. Many methods have been proposed to find the edges, based on knowledge of the Fourier, Chebyshev, or Legendre coefficients, or on the point values of a function [1,9,11,20–22].

The natural question to ask is if there actually exist any Gibbs complementary families for the types of bases commonly in use. This is indeed the case: an orthonormal basis based on the Gegenbauer polynomials can be shown to be Gibbs complementary to the Fourier, Legendre, and Chebyshev bases, and more generally to the Gegenbauer polynomials [30].

Theorem 4.2. ([30]) *Assume that $f(x)$ is an analytic function on $[a,b]\subset[-1,1]$. Given the first $(N+1)$ coefficients of a Fourier series or a polynomial expansion based on the Gegenbauer polynomial basis $\{G_k^\mu\}$, define the Fourier or Gegenbauer approximation $f_N(x)$ as above, and use it to compute the first $m+1$ Gegenbauer coefficients*

$$\hat{g}_l^\lambda=\frac{1}{h_l^\lambda}\int_{-1}^{1}(1-\xi^2)^{\lambda-\frac{1}{2}}f_N(x(\xi))G_l^\lambda(\xi)d\xi, \qquad l=0,\cdots,m.$$

Then for $\lambda=m=\beta\epsilon N$ where $\beta<2\pi e/27$ for the Fourier case, or $\beta<2/27$ for any Gegenbauer basis, we have

$$\max_{-1\le x\le 1}\left|f(\xi)-\frac{1}{h_l^\lambda}\sum_{k=0}^{m}\hat{g}_l^\lambda G_l^\lambda(\xi)\right|\le Aq^{-\epsilon N},$$

for some $q<1$, and a constant A.

Remark 4.1. These results, suitably modified, work even if $f(x)$ is not analytic on $[a,b]$, but only has some number of continuous derivatives. In this case, however, the post-processed solution will not converge exponentially, but will recover the order of convergence expected in the function $f(x)$ on the interval $[a,b]$. In the case where $f(x)$ is not analytic, but only has K continuous derivatives, this process can still be followed and will yield a uniformly convergent approximation of order $(1/N)^K$.

Example 4.1. Once again, we look at the square wave function computed by the first $2N+1$ exact Fourier coefficients. The errors of the partial sums are large and do not decay at all at the points $x=0,-1,1$. After post-processing with Gegenbauer polynomials on the domains $[-1,0]$ and $[0,1]$, the errors are significantly reduced and decay rapidly (Fig. 3). However, our implementation of the Gegenbauer method is sensitive to roundoff errors at the boundaries, which accounts for the larger errors at the points $x=-1,0,1$.

Example 4.2. We repeat this experiment on the sawtooth function computed by the first $2N+1$ exact Fourier coefficients. The errors of the partial sums are large and do not decay at all at the boundaries. After post-processing with Gegenbauer polynomials, the errors are significantly reduced and decay rapidly (Fig. 4).

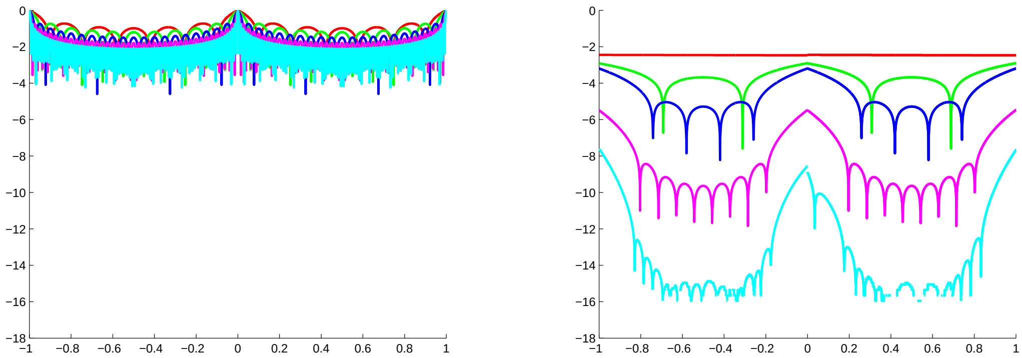


Figure 3: Fourier Galerkin approximation of the squarewave function before and after post-processing with $\lambda=0.4N$ and $m=0.2N$ and their pointwise errors for $N=5$ (red), $N=10$ (green), $N=20$ (blue), $N=40$ (magenta), and $N=80$ (cyan).

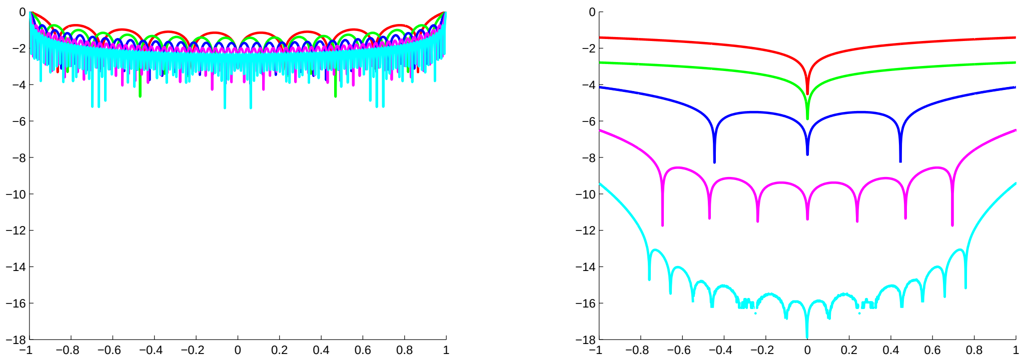


Figure 4: Fourier Galerkin approximation of the sawtooth function before and after post-processing with $\lambda=m=N/4$ and their pointwise errors for $N=4$ (red), $N=8$ (green), $N=16$ (blue), $N=32$ (magenta), and $N=64$ (cyan).

In practice, the use of Gegenbauer polynomials is not robust. Gegenbauer polynomials suffer from roundoff errors [7,17], and the choice of parameters λ and m has a detailed theory of its own, analyzed in [17, 18]. Furthermore, singularities in the complex plane can ruin the convergence of the Gegenbauer method unless β is below some threshold [7]. A more robust Gibbs complementary basis was proposed by [19], in which it was shown that for an analytic function the expansion of the function in the new basis converges exponentially, that the projection of high modes in the original basis on the low modes in the new basis is exponentially small. This new basis is also a two-parameter family for which, as the order of the original expansion increases, the weight function of the new basis converges to a weight whose associate basis satisfies the spectral convergence condition.

5 Post-processing the collocation approximation

When beginning with a Galerkin approximation $f_N(x)$ the error has one source: the truncation of the infinite series. However, the collocation approximation $\tilde{f}_N(x)$ has two sources of errors: the truncation of the infinite series and the approximation of the expansion coefficients by interpolation. For the Galerkin approximation post-processing with a Gibbs complementary basis eliminates the Gibbs phenomenon, which is caused by truncation of the infinite series for a function which is not smooth, but in the case of a collocation approximation there are other problems which may come into play: the aliasing error and the Runge phenomenon. Aliasing error is a phenomenon that is caused by the fact that the data may be sampled at points which are too far away, so that higher modes may be indistinguishable from ("aliased to") lower modes. The Runge phenomenon is a problem commonly seen in polynomial interpolation of functions on equidistant points, and is characterized by oscillations near the boundary; The Runge phenomenon depends on the distribution of interpolation points, and is not eliminated by post-processing.

In Section 3, we discussed the collocation approximation

$$\tilde{f}_N(x)=\sum_{k=0}^{N}a_k\Psi_k(x),$$

where the coefficients are given by the interpolation requirement

$$\sum_{k=0}^{N}a_k\Psi_k(x_j)=f(x_j),\qquad j=0,\cdots,N+1,$$

where $\{x_j\}$ are the Gauss or Gauss-Lobatto points associated with the basis $\Psi_k(x)$, which are trigonometric polynomials or Gegenbauer polynomials. In Lemma (3.1), we saw that if the function $f(x)$ and its derivatives are smooth on $x\in[-1,1]$ then the collocation approximation converges uniformly and rapidly. Of course, the problem we face is that the function $f(x)$ is not continuous on $[-1,1]$, and so the Gibbs phenomenon occurs and we have slow convergence away from the discontinuity and non-uniform convergence.

Our question is: given a finite number of point values (conveniently located on the Gauss or Gauss-Lobatto points of the trigonometric polynomials or of any of the Gegenbauer polynomials) is it possible to get a high order approximation to the function $f(x)$ on a subinterval $[a,b]$ on which $f(x)$ is very smooth?

A simple approach would be to repeat the process used in Section 4, but instead of starting with the Galerkin approximation $f_N(x)$ we use the collocation approximation $\tilde{f}_N(x)$, so that the new approximation, defined on the region of analyticity of $f(x)$, $a\le x\le b$, is

$$\sum_{k=0}^{m}\langle\tilde{f}_N,\Phi_l^\lambda\rangle_\lambda\Phi_l^\lambda(\xi(x)),\tag{5.1}$$

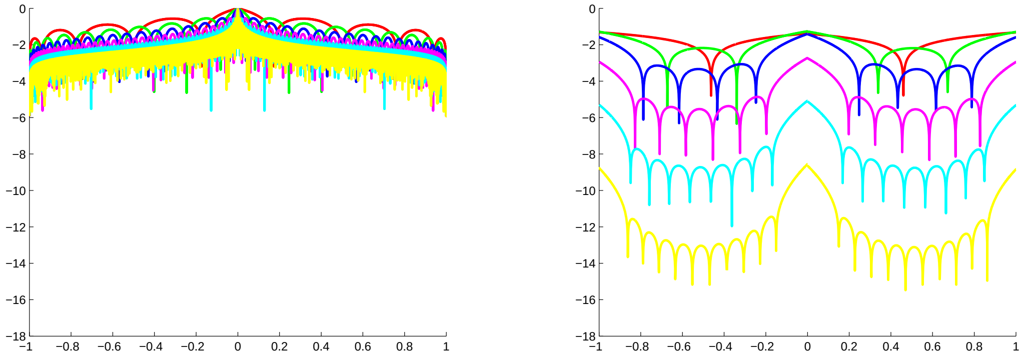


Figure 5: Pointwise errors of Chebyshev interpolation of the square wave function without (left) and with (right) post-processing with $N=10$ (red), $N=20$ (green), $N=40$ (blue), $N=80$ (magenta), $N=160$ (cyan), and $N=320$ (yellow) and parameters as listed in the text.

where

$$\langle \tilde{f}_N,\Phi_l^\lambda\rangle_\lambda=\int_{-1}^{1}(1-\xi^2)^{\lambda-\frac{1}{2}}\tilde{f}_N(x(\xi))\Phi_l(\xi)d\xi.$$

Example 5.1. The square wave function is computed using the Chebyshev collocation method, using Trefethen's CHEBFUN [44] with $N+1$ Chebyshev points $x_j=-\cos\big(j\pi/N\big)$, $j=0,\cdots,N$, for $N=8,16,32,48,64$. The errors before post-processing (Fig. 5, left) exhibit evidence of the Gibbs phenomenon, while the errors of the post-processed approximation (5.1) show significant improvement (Fig. 5, right). the post-processing parameters are given in the following table:

N	m	λ	N	m	λ
10	1	1	80	6	8
20	2	4	160	8	10
40	4	6	320	10	12

In this numerical example we observe that Gegenbauer post-processing recovers order of accuracy of the collocation approximation. Many other numerical examples [29] demonstrate that this approach seems to work well in general. However, from a theoretical point of view, we cannot show that this process is convergent.

However, there is an alternative process that can be justified theoretically [29]: rather than interpolating the function $f(x)$ at the point values $f(x_j)$, we interpolate a new function, $f_\lambda^\alpha(x)$, when this function is postprocessed using normalized Gegenbauer polynomials $\Phi_l^\lambda(x)$, the result will be exponentially convergent. The process is described below:

Given point values $f(x_j)$, $j=0,\cdots,N$ where x_j are the Gauss or Gauss-Lobatto points of the trigonometric polynomials or of any of the Gegenbauer polynomials G_k^λ with $\lambda>$

$-1/2$, define the function

$$\alpha_\lambda(x)=\begin{cases}(1-\xi(x)^2)^{\lambda-\frac{1}{2}}, & a\le x\le b,\\ 0, & \text{otherwise},\end{cases}$$

where λ is a suitably chosen number which linearly depends on N. The effect of the multiplying a function which is smooth on $a\le x\le b$ by α_λ is that the resulting function is smooth on the domain $-1\le x\le 1$.

Now we define the interpolating function $I_N(\alpha_\lambda\cdot f)(x)$, an expansion in the Fourier, Chebyshev or Legendre basis $\Psi_k(x)$ which satisfies the condition

$$I_N(\alpha_\lambda\cdot f)(x_j)=\alpha_\lambda(x_j)f(x_j),\qquad j=0,\cdots,N.$$

Which basis is chosen is, of course, dependent on which points x_j are given. The Gegenbauer coefficients are computed based on $I_N(\alpha_\lambda\cdot f)(x)$, instead of $\tilde{f}_N(x)$:

$$\hat{\gamma}_l^\lambda=\int_{-1}^1 I_N(\alpha\cdot f)(x(\xi))\Phi_l^\lambda(\xi)d\xi,$$

and the Gegenbauer approximation is

$$\tilde{g}_N(x)=\sum_{l=0}^m \hat{\gamma}_l^\lambda\Phi_l^\lambda(x). \tag{5.2}$$

The theorem below states that, following such a procedure, for an appropriated choice of λ, $\tilde{g}_N(x)$ converges exponentially to $f(x)$ in the interval $a\le x\le b$, for a wide variety of bases.

Theorem 5.1. ([29]) *Let $f(x)$ be an analytic function on $[a,b]$, which satisfies*

$$\max_{a\le x\le b}\left|f^{(k)}(x)\right|\le C(\rho)\frac{k!}{\rho^k},\quad \textit{for any}\ \ k\ge 0,\ \ \textit{with some}\ \ \rho\ge 1.$$

Given a set of point values $\{f(x_j)\}_{j=0}^N$ on a set of Gauss or Gauss-Lobatto points $\{x_j\}_{j=0}^N$ associated with the orthogonal basis $\Psi_k(x)$ consisting of the trigonometric polynomials $e^{ik\pi x}$ or the Gegenbauer polynomials $G_k^\mu(x)$ for $-1/2<\mu<3/2$, then the approximation (5.2) *converges uniformly and exponentially on $[a,b]$ for $\lambda=m=\beta\epsilon N$ with $\beta<2e/\left[27(1+\frac{1}{2\rho})\right]$*

$$\max_{a\le x\le b}\left|f(x)-\tilde{g}_N(x)\right|\le A\left(q_T^{\epsilon N}+q_R^{\epsilon N}\right),$$

where

$$q_T=\left[\frac{27\beta}{2e}\left(1+\frac{1}{2\rho}\right)\right]^\beta<1,\qquad q_R=\left(\frac{27\epsilon}{32\rho}\right)^\beta<1,$$

and A grows at most as $N^{(5+\mu)/2}$.

The result in this theorem is also true when we use higher order Gegenbauer bases, $\Psi_k(x) = G_k^{\mu}(x)$ for $\mu \geq 3/2$, but in that case we need to define

$$\tilde{\alpha}_\lambda(x) = \begin{cases} \frac{\left(1-\xi(x)^2\right)^{\lambda-\frac{1}{2}}}{(1-x^2)^{\frac{\mu}{2}-\frac{1}{4}}}, & a \leq x \leq b, \\ 0, & \text{otherwise,} \end{cases}$$

and

$$\hat{\gamma}_l^\lambda = \int_{-1}^{1} \left(1 - x(\xi)^2\right)^{\frac{\mu}{2}-\frac{1}{4}} I_N(\tilde{\alpha}_\lambda \cdot f)(x(\xi)) \Phi_l^\lambda(\xi) d\xi.$$

We have here two approaches to the interpolation. The first approach is simple and seems to work well in practice, but is not guaranteed by any theory. In fact, it is very possible that aliasing error can ruin its convergence. On the other hand, we have a non-standard process that has a theoretical guarantee, but is more cumbersome and may in practice increase the Gegenbauer method's sensitivity to roundoff errors. Fortunately, the results in [29] show that in a variety of examples the standard interpolation, when post-processed in the usual way (i.e., replacing $f_N(x)$ in the previous section by $\tilde{f}_N(x)$), gives equivalent results.

6 Extension to spectral and pseudo-spectral approximations of partial differential equations

Up to now we have discussed the post-processing of a Galerkin or collocation approximation of a function $f(x)$ which is analytic on the subinterval $a \leq x \leq b$. This post-processing procedure builds a new function which converges quickly to $f(x)$. In this section we show that these results can be useful for spectral approximations of linear and nonlinear hyperbolic partial differential equations.

The case of a Galerkin approximation has very clear and complete results, and these can be extended to the spectral methods solutions of linear hyperbolic partial differential equations (PDEs). However, the situation for pseudo-spectral (collocation) approximations of a linear hyperbolic PDE is quite different because the convergence result that we do have is not for the interpolation of $f(x)$, but rather when we interpolate $\alpha \cdot f$, as we discussed above. Nevertheless, numerical evidence demonstrates that not only is the post-processed collocation approximation rapidly converging, but that even after stepping forward in time, high order accuracy can be recovered by post-processing. Finally, we want to consider the case for a nonlinear hyperbolic partial differential equation. Spectral (and pseudo-spectral) approximations of scalar nonlinear hyperbolic PDEs are stable if we filter the solution appropriately [34, 42]. When the solution is discontinuous, we can still stabilize the method using filtering, but the high order information seems lost. Numerical evidence demonstrates that this high order information is retained and can be recovered by post-processing. In the following example we present the discontinuous solutions of a Burgers' equation by spectral and pseudo-spectral methods, post-processed to recover order of accuracy.

Example 6.1. Taken from [41]: Given Burgers' equation

$$u_t + \left(\frac{u^2}{2}\right)_x = 0, \qquad x \in [-1,1], \quad t > 0,$$
$$u(x,0) = 0.3 + 0.7\sin(\pi x).$$

The solution develops a shock at $t = 1/0.7\pi$ and we compute the solution up to $t = 1$. The initial condition is chosen such that the shock is moving with time. Using a Fourier spectral method with filtering to stabilize the method, to approximate the solution to this equation, the pointwise errors before post-processing (Fig. 6 (left)) show slow convergence, while the pointwise errors of the post-processed solution 6 (right) show good accuracy everywhere including at the discontinuity $x = \pm 1 + 0.3$.

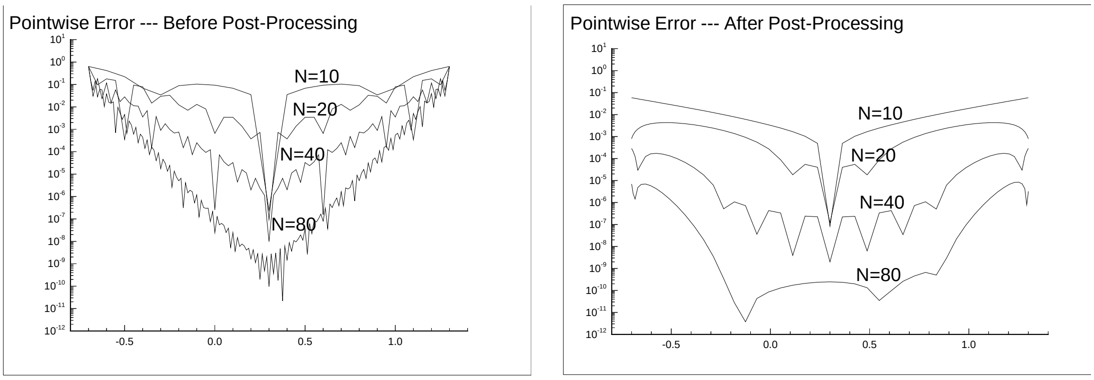


Figure 6: Pointwise errors in log scale, Burgers equation. Fourier Galerkin using $2N+1$ modes with exponential solution filters of order r. $r=4$ for $N=10$; $r=6$ for $N=20$; $r=8$ for $N=40$ and $r=12$ for $N=80$. Figures taken from [41]. Left: before post-processing. Right: after post-processing with parameters $\lambda=2, m=1$ for $N=10$; $\lambda=3, m=3$ for $N=20$; $\lambda=12, m=7$ for $N=40$ and $\lambda=62, m=15$, for $N=80$.

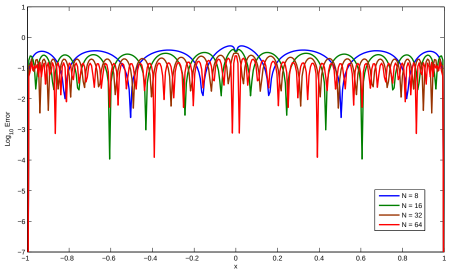
Example 6.2. We solve the Burgers' equation

$$u_t + \left(\frac{u^2}{2}\right)_x = 0, \quad x \in [-1,1], \quad t > 0,$$

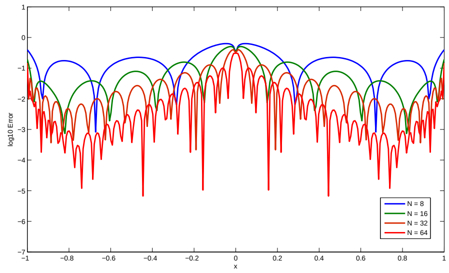
with the initial condition

$$u(x,0) = -\sin(\pi x).$$

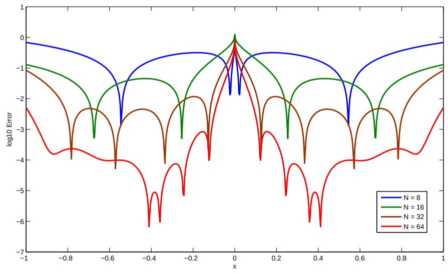
With this initial condition the shock forms at $t = t_s = 1/\pi$ at $x = 0$. We use the Chebyshev collocation (pseudo-spectral) method with $N+1$ Gauss Lobatto collocation points.



(a)



(b)



(c)

Figure 7: Pointwise error for (a) solution with $N=8,16,32,64$; (b) filtered solution with the filtering order $p=16$ (without Gegenbauer reconstruction); (c) Gegenbauer post-processed solution of unfiltered solutions.

Fig. 7(a) shows the pointwise errors with $N=8,16,32,64$, Fig. 7(b) shows the pointwise errors with exponential filtering with $p=16$. Filtering is included here because it is needed for stabilizing the method. Fig. 7(c) the Gegenbauer reconstruction with $\lambda=N/8$, $m=N/8$. For the Gegenbauer reconstruction we use the fact that the shock location is at $x=0$ for $\forall t \geq t_s$. Once again, we observe that the Gegenbauer post-processing of the Chebyshev collocation is sensitive to roundoff errors at the boundary.

7 Conclusions

Although local discontinuities destroy the convergence of global approximations even on regions which feature smooth solutions, these global approximations still contain within them high order information which can be recovered with suitable post-processing. For the Galerkin approximation, there is a complete theory that guarantees that convergent approximations can be obtained by post-processing with a *Gibbs complementary* basis. For the collocation approximation, the situation is more delicate: in this case, the theory requires interpolation on a specialized set of nodes, and an interpolation procedure on a new function, rather than the original set of points. However, in many cases, no difference is observed if the post-processing is performed on the original or the modified interpolation.

A significant use of the post-processing method is in the numerical solution of partial differential equations with shocks. Theoretical justification exists for the case of linear hyperbolic PDEs solved with a Galerkin method, and for the collocation method and for nonlinear equations there is numerical evidence which shows that this approach is applicable. These methods have been used to simulate sophisticated problems, such as the Richtmyer Meshkov instability calculated by W. S. Don [32], and have also been successfully applied to the field of image reconstruction by Archibald and Gelb [2–4]. Surprisingly, the Gegenbauer basis has also been successful in recovering order of accuracy lost in other types of approximations, such as weighted essentially non-oscillatory (WENO) solutions of hyperbolic PDEs [33], and in radial basis functions approximations of linear and nonlinear hyperbolic PDEs [36].

While the Gegenbauer basis has been used often and successfully, it suffers from practical drawbacks including difficulties in the choice of parameters. Other bases have been considered, with greater success [19]. While the practical aspects of post-processing continue to be developed, the underlying message of the work reviewed here is that global expansions which are contaminated by local discontinuities still retain within them high order information, and the Gibbs phenomenon can be removed by post-processing.

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