Progress in Scientific Computing
Vol. 6

Birkhäuser
Boston · Basel · Stuttgart

Progress and Supercomputing in Computational Fluid Dynamics

Proceedings of U.S.-Israel Workshop, 1984

Earll M. Murman
Saul S. Abarbanel
editors

1985

Birkhäuser
Boston · Basel · Stuttgart

Progress in Scientific Computing, Vol. 6
Proceedings of U.S.-Israel Workshop, 1984

RECOVERING POINTWISE VALUES OF DISCONTINUOUS DATA WITHIN SPECTRAL ACCURACY

David Gottlieb and Eitan Tadmor

1. INTRODUCTION

Let $f(x)$ be a bounded 2π-periodic function whose Fourier coefficients are given by

$$\hat{f}(k) = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(y)e^{-ik\cdot y}dy\ , \qquad -\infty < k < \infty\ . \tag{1.1}$$

It is well-known that whenever f is a smooth function, then its spectral approximation - consisting of the partial sums

$$S_N f(x) \equiv \hat{f}_N(x) = \sum_{|k|\leq N} \hat{f}(k)e^{ik\cdot x}\ , \tag{1.2}$$

converges pointwise to $f(x)$. A typical error estimate in this case, asserts that for any x in the domain we have

$$|f(x) - \hat{f}_N(x)| \leq C_s||f||_{(s)}\cdot N^{-s+1}\ , \qquad s > 1\ . \tag{1.3}$$

Here and below, C_s stands for (possibly different) generic constant bounds, and $||f||_{(s)}$ denotes the largest maximum norm of f and its first s derivatives, the maximum taken over the whole domain.

We thus see that the decay rate of the truncation error on the left of (1.3), is restricted only by the degree of smoothness of the function f. In this sense, the spectral approximation is termed to be spectrally accurate. If, in particular, f is a C^∞-function, the truncation error is rapidly decaying, faster than any fixed ($\equiv$ independent of N) polynomial rate. Thus, the spectral approximation of C^∞-functions, enjoys the so called infinite order of accuracy; this is in constrast to the usually slower convergence rate due to a fixed degree polynomial accuracy.

Next, assume only the gridvalues $f_\nu = f(y_\nu)$ are known, at the $2N$ equidistant gridpoints $y_\nu = -\pi + \nu h$, $h = 2\pi/2N$, $\nu = 0,1,\ldots,2N-1$. Invoking the trapezoidal rule, the (exact) Fourier coefficients in (1.1) are approximated by discrete sums of these known gridvalues

$$\tilde{f}(k) = \frac{1}{2N} \sum_{\nu=0}^{2N-1} f_\nu e^{-ik \cdot y_\nu}, \quad -N \leq k \leq N . \tag{1.4}$$

The difference between the exact Fourier coefficients and their discrete approximation is also known to be spectrally small

$$|\hat{f}(k) - \tilde{f}(k)| \leq C_s ||f||_{(s)} N^{-s}, \quad s > 1 . \tag{1.5}$$

As a substitute to the (exact) Fourier coefficients appearing in the spectral approximation (1.2), $\hat{f}(k)$, let us use their discrete counterpart, $\tilde{f}(k)$. The resulting new approximation is found to be exact at the gridpoints $x = y_\nu$. In other words, we arrive at the trigonometric interpolant[(1)].

$$I_N f(x) \equiv \tilde{f}_N(x) = \sum_{|k| \leq N}{}'' \tilde{f}(k) e^{ik \cdot x} . \tag{1.6}$$

The two type of errors committed in this case - the original truncation error in (1.3) padded with the aliasing errors in (1.5) - both are spectrally small. Hence, if f is smooth over the whole domain, then its pseudo-spectral approximation (1.6) is spectrally accurate even in between the gridpoints

$$|f(x) - \tilde{f}_N(x)| \leq C_s ||f||_{(s)} N^{-s+1}, \quad s > 1 . \tag{1.7}$$

We also note that as in the spectral and pseudo-spectral cases (1.3) and (1.7), similar error decay is obtained with higher derivatives and in more space variables; the norm on the right hand-side of (1.3), (1.5) and (1.7) should be "raised" accordingly. Moreover, if the function is in particular analytic, then the spectral accuracy is further improved to be exponential: let $2\eta > 0$ be the width of analyticity strip with maximum modulus $||f||_\eta$ then an error bound of the form $C_\eta ||f||_\eta e^{-N\eta}$ follows, e.g. [7].

Unfortunately, the pointwise errors associated with the spectral or pseudospectral approximations, suffer from the limitation of being dependent on the smoothness of the function f over the whole domain (real or complex), and not just on its local behavior in the neighborhood of the point of interest. This dependence of the local convergence rate on the global smoothness, which is reflected by (though not a consequence of) the error estimates (1.3) and (1.7), is indeed inherent in both approximations. That is, the roughness of the function in one part of its domain, decelerates the convergence rate in the smoother part of it. Most notably is the case of piecewise smooth functions: not only that Gibbs phenomenon is recorded at points of discontinuity, but in addition, the spectral accuracy is lost at regions where the function is smooth.

In this paper we show how pointwise values of the function $f(x)$ can be recovered from the information contained in either its spectral or pseudo-spectral approximations, so that the accuracy solely depends on the local smoothness of f, that is, its smoothness in the neighborhood of the point of interest x. If, in particular, f is infinitely smooth in that neighborhood, then the value $f(x)$ is approximated within infinite order of accuracy. Most notably, we rocover pointwise values within spectral accuracy, despite the possible presence of discontinuities scattered in the domain.

For such pointwise recovery, we should dismantle the above local-global coupling limitation, associated with the (pseudo-) spectral approximations. To this end, we employ a regularization kernel which is convoluted against the (pseudo-) spectral approximation in the usual fashion. Our regularization kernel consists of the product of two terms: first we introduce a cut-off function to localize the kernel in the spirit advocated above; secondly, it is multiplied by the spectral approximation of the delta function (≡ Dirichlet kernel), so that spectral accuracy is guaranteed. Convolution with the resulting kernel has then the effect of (locally) smoothing the spectral and pseudo-spectral approximations.

The paper is organized as follows: in Section 2 we briefly discuss those fundamentals of Fourier summation which will be later needed. Smoothing of the spectral approximation is described in Section 3. In Section 4, we similarily treat the pseudo-spectral approximation. It should be emphasized that the latter case, directly involves only neighboring gridvalues, so that the construction of the pseudo-spectral approximation can be avoided altogether. In other words, (intermediate) pointvalues are recovered here, via a locally supported yet spectrally accurate interpolation recipe. We remark that more general orthogonal families - other than the treated above trigonometric one - can be used as well, to yield spectral smoothing: the notable examples of Legendre and Tchebyshev are brielfy sketched in Section 5. We conclude with numerical evidence which back up on theoretical considerations.

In [6], Mock and Lax have shown how to recover within polynomial accuracy, pointwise values of discontinuous solutions to linear hyperbolic equations. They have employed a locally supported unit mass post-processing kernel with a finite number of vanishing higher moments. Our spectral smoothing is motivated by Mock and Lax discussion- indeed, our regularization kernel based on the Legendre spectral approximation is intimately related to their kernel. Majda and McDonough and Osher [5] on the other hand, extending their previous study [4] with regard to the same problem, have employed a spectrally accurate smoothing procedure by operating directly in the Fourier space. Our smoothing in the real space rather than in the transformed one seems to offer more robustness, resulting from the use of physical space localization; the latter is in fact the key element which enables us to apply our smoothing procedure to pseudo-spectral approximations. Moreover, it is also applicable in conjunction with orthogonal families other than the trigonometric one.

This work has been motivated by the numerical studies of (pseudo-) spectral simulation of shock waves. However, in this paper we restrict our attention to the level of approximation only; applications to P.D.E. will be discussed elsewhere.

2. PRELIMINARIES ON FOURIER SUMMATION

Given a 2π-periodic function Φ with Fourier coefficient $\hat{\Phi}(k) = (2\pi)^{-1}\int_{-\pi}^{\pi}\Phi(y)e^{-ik\cdot y}dy$, its spectral approximation $\hat{\Phi}_p(x)$ is

$$\hat{\Phi}_p(x) \equiv \sum_{|k|\leq p}\frac{1}{2\pi}\int_{-\pi}^{\pi}\Phi(y)e^{-ik\cdot y}dy\,e^{ik\cdot x} = \int_{-\pi}^{\pi}\Phi(x-y)D_p(y)dy\ ; \tag{2.1a}$$

here $D_p(y)$ stands for the Dirichlet kernel

$$D_p(y) = \frac{1}{2\pi}\sum_{|k|\leq p}e^{ik\cdot y} = \frac{1}{2\pi}\frac{\sin(p+1/2)y}{\sin y/2} \tag{2.1b}$$

normalized so that it has a unit mass

$$\int_{-\pi}^{\pi} D_p(y)dy = 1\ . \tag{2.1c}$$

An (a' postriori) bound on the truncation error is given by

$$\Big|\sum_{|k|>p}\hat{\Phi}(k)e^{ik\cdot x}\Big| \leq \sum_{|k|>p}|k|^s|\hat{\Phi}(k)||k|^{-s} \leq ||\Phi||_{(s)}\sum_{|k|>p}|k|^{-s} \leq$$

$$\leq ||\Phi||_{(s)}p^{-s+1} \qquad s > 1\ , \tag{2.2}$$

in agreement with (1.3), taking $(\Phi,p) = (f,N)$. Thus we have

$$\Big|\int_{-\pi}^{\pi}\Phi(y)D_p(x-y)dy-\Phi(x)\Big| \leq C_s||\Phi||_{(s)}p^{-s+1}\ , \qquad s > 1\ ; \tag{2.3a}$$

for later purpose, we quote here the special case $x = 0$,

$$\Big|\int_{-\pi}^{\pi}\Phi(y)D_p(y)dy - \Phi(0)\Big| \leq C_s||\Phi||_{(s)}p^{-s+1}\ , \qquad s > 1\ . \tag{2.3b}$$

The above error bound is not the sharpest bound possible: let $\omega(\ ;\ )$ denotes the function's modulus of continuity, then Kolmogorov's result yields an asymptotrially exact bound[2]

$$\Big|\int_{-\pi}^{\pi}\Phi(y)D_p(x-y)dy-\Phi(x)\Big| \leq \frac{2\ln p}{\pi^2 p^s}\int_0^{\pi/2}\omega\Big(\frac{2\xi}{p};D^s\Phi\Big)\sin\xi d\xi + O\Big(p^{-s}\omega\Big(\frac{1}{p}\Big)\Big). \tag{2.4}$$

Turning to the pseudo-spectral approximation, we have encountered the additional source of aliasing errors, due to discretization of the (exact) Fourier coefficients' integral. Invoking the aliasing relations, e.g. [3],

$$\tilde{\Phi}(k) = \sum_{j=-\infty}^{\infty}\hat{\Phi}(k+2jp)\ , \qquad -p \leq k \leq p\ , \tag{2.5}$$

(2p equidistant point's interpolant is assumed). The aliasing errors do not exceed

$$|\hat{\Phi}(k)-\tilde{\Phi}(k)| \leq \sum_{j\neq 0}|\hat{\Phi}(k+2jp)| \leq ||\Phi||_{(s)}\cdot\sum_{j\neq 0}|k+2jp|^{-s} \leq$$

$$\leq C_s||\Phi||_{(s)}p^{-s}\ , \qquad s > 1\ , \tag{2.6}$$

in agreement with (1.5), taking $(\Phi,p) = (f,N)$. Hence, the aliasing error $|\hat{\Phi}(k) - \tilde{\Phi}(k)|$, $k = -p,\dots,p$, adds up to a contribution similar to that of the truncation error, yielding in view of (2.5)

$$|\tilde{\Phi}_p(x)-\Phi(x)| \leq |\sum_{|k|>p} \hat{\Phi}(k)e^{ik\cdot x}| + \sum_{|k|\leq p} |\hat{\Phi}(k)| + \frac{1}{2}|\tilde{\Phi}(-p)+\tilde{\Phi}(p)| \leq$$

$$\leq C_s||\Phi||_{(s)}p^{-s+1}, \qquad s \geq 1, \tag{2.7}$$

in agreement with (1.7), taking $(\Phi,p) = (f,N)$. It should be noted, (e.g. [3]), that there is no qualitative difference between the spectral and pseudo-spectral approximations.

3. RECOVERING POINTWISE VALUES FROM THE SPECTRAL APPROXIMATION

In this section, we show how to extract highly accurate approximation to the point values of a discontinuous function from its first N Fourier coefficients in regions where the function is smooth. The basic idea is that these coefficients are moments of the functions and consequently, integral of any smooth function against the spectral approximation is highly accurate with that against the function itself. We therefore construct an auxilliary function such that when the spectral approximation is integrated against it, the desired original point value at a given point is recovered.

To do that, let $\rho(y)$ be a C^s-function vanishing outside the interval $(-\pi,\pi)$ and normalized to take the value one at the origin

$$\rho(y=0) = 1\ . \tag{3.1}$$

We recall that the Dirichlet kernel in (2.1b) is given by

$$D_p(y) \equiv \frac{1}{2\pi} \sum_{|k|\leq p} e^{ik\cdot y} = \frac{1}{2\pi}\frac{\sin\,(p+1/2)y}{\sin\,(y/2)}\ ; \tag{3.2}$$

multiplying the two we obtain

$$\psi^{1,p}(y) = \rho(y)D_p(y)\ . \tag{3.3}$$

We now set as our regularization kernel

$$\psi^{\theta,p}(y) \equiv \theta^{-1}\psi^{1,p}(\theta^{-1}y) = \theta^{-1}\rho(\theta^{-1}y)D_p(\theta^{-1}y)\ , \tag{3.4}$$

depending on a yet to be determined free parameter θ, $0 \leq \theta \leq 1$.

Given the spectral approximation, $\hat{f}_N$, we smooth its value via convolution with the above regularization kernel, computing

$$\hat{f}_N * \psi^{\theta,p}(x) = \int_{-\pi}^{\pi} \hat{f}_N(y')\psi^{\theta,p}(x-y')dy'\ . \tag{3.5}$$

In order to estimate the error, we decompose

$$\hat{f}_N * \psi^{\theta,p} - f = (\hat{f}_N-f) * \hat{\psi}_N^{\theta,p} + (\hat{f}_N-f) * (\psi^{\theta,p} - \hat{\psi}_N^{\theta,p}) +$$

$$+ (f * \psi^{\theta,p} - f). \tag{3.6}$$

The first term on the right vanishes in view of the orthogonality between the N-degree (trigonometric) polynomial $\hat{\psi}_N^{\theta,p}$ and the truncated sum $\hat{f}_N - f$,

$$(\hat{f}_N-f) * \hat{\psi}_N^{\theta,p} = 0\ . \tag{3.7a}$$

Thus we are left with two sources of error in this case: the truncation error in the second term

$$T_N^{\theta,p} \equiv (\hat{f}_N-f) * (\psi^{\theta,p} - \hat{\psi}_N^{\theta,p}) \tag{3.7b}$$

and the regularization error in the third term,

$$R^{\theta,p} \equiv f * \psi^{\theta,p} - f\ . \tag{3.7c}$$

With regard to the truncation error $T_N^{\theta,p}$, Young inequality implies

$$||(\hat{f}_N-f) * (\psi^{\theta,p} - \hat{\psi}_N^{\theta,p})|| \leq ||\hat{f}_N-f||_{L^1}||\psi^{\theta,p}- \hat{\psi}_N^{\theta,p}||\ , \tag{3.8a}$$

and in the view of (1.3) we conclude that this term is spectrally small

$$||T_N^{\theta,p}|| \equiv ||(\hat{f}_N-f) * (\psi^{\theta,p} - \hat{\psi}_N^{\theta,p})|| \leq$$

$$\leq C_s||\hat{f}_N-f||_{L^1}||\psi^{\theta,p}||_{(s)}N^{-s+1}\ . \tag{3.8b}$$

Turning to the regularization error, $R^{\theta,p}$, we compute at a given fixed point x

$$R^{\theta,p}_{(x)} \equiv f * \psi^{\theta,p}(x) - f(x) = \int_{x-\theta\pi}^{x+\theta\pi} f(y')\theta^{-1}\rho(\frac{x-y'}{\theta})D_p(\frac{x-y'}{\theta})dy' - f(x). \tag{3.9a}$$

Changing variables $y = \frac{x-y'}{\theta}$ and making use of (2.1c), the regularization error is simplified into

$$R^{\theta,p}_{(x)} \equiv f * \psi^{\theta,p}(x) - f(x) = \int_{-\pi}^{\pi} \Phi^{\theta,x}(y)D_p(y)dy \tag{3.9b}$$

where the auxiliary function $\Phi^{\theta,x}(y)$ is given by

$$\Phi^{\theta,x}(y) \equiv f(x-\theta y)\rho(y) - f(x) . \tag{3.9c}$$

In view of the normalization (3.1), $\Phi^{\theta,x}(y)$ vanishes at $y = 0$, and by appealing to the truncation error estimate quoted in (2.3b), we end up with

$$|R^{\theta,p}_{(x)}| \equiv |\int_{-\pi}^{\pi} \Phi^{\theta,x}(y)D_p(y)dy| \leq C_s||\Phi^{\theta,x}||_{(s)}p^{-s+1} . \tag{3.9d}$$

Added together, we have shown in (3.6) - (3.9) the following:

Proposition 3.1 (Main Error Estimate)

Let $\psi^{\theta,p}$ be the regularization kernel (3.4). Fix a point x in the domain, and set $\Phi^{\theta,x}$ to be the auxiliary function in (3.9c). Then, the following error estimate holds

$$|\hat{f}_N * \psi^{\theta,p}(x) - f(x)| \leq C_s||f||\cdot||\psi^{\theta,p}||_{(s)}N^{-s+1} + C_s||\Phi^{\theta,x}||_{(s)}p^{-s+1} . \tag{3.10}$$

The following two lemmas whose technical proofs are postponed to the end of this section, provide us with the necessary explicit bounds on the two terms appearing on the right of (3.10).

Lemma 3.2

Let $\psi^{\theta,p}$ denote the regularization kernel in (3.4). The following estimate holds

$$||\psi^{\theta,p}||_{(s)} \leq \theta^{-s-1}\cdot||\rho||_{(s)}\cdot(1+p)^{s+1} . \tag{3.11}$$

Lemma 3.3

Let $\Phi^{\theta,x}$ denote the auxiliary function in (3.9c). The following estimate holds

$$||\Phi^{\theta,x}||_{(s)} \leq (1+\theta)^s\cdot||\rho||_{(s)}\cdot \max_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq s}} |D^k f(y)| . \tag{3.12}$$

Choosing $p = N^\beta$, $0 < \beta \leq 1$, we conclude from (3.6), (3.8b), (3.9d) and the last two lemmas, the main result of this section, stating

THEOREM 3.4

Let f be a bounded 2π-periodic function with a given N-degree spectral approximation $\hat{f}_N$. Setting the regularization kernel

$$\psi^{\theta,N^\beta}(y) = \frac{1}{2\pi\theta}\rho(\theta^{-1}y)\frac{\sin (N^\beta + 1/2)y/\theta}{\sin (y/2\theta)} , \tag{3.13}$$

then for any x in the domain, we have the pointwise error estimate

$$|\hat{f}_N * \psi^{\theta,N^\beta}(x) - f(x)| \leq C_s||\rho||_{(s)}\cdot N^\beta[N\cdot\theta^{-s}||\hat{f}_N - f||_{L^1}\cdot N^{-(1-\beta)s} + \max_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq s}} |D^k f(y)|\cdot N^{-\beta s}] . \tag{3.14}$$

Choosing $\theta = \beta = 1$ brings us back to the exactly same global error estimate we had in (1.3). Taking $\beta = 1/2$ on the other hand, the truncation and aliasing errors' contributions in (3.14) are balanced, and we are led to the following:

Corollary 3.5 (Spectral Smoothing)

Let $\rho(y)$ be a C^{2s}-function, supported in $[-\pi,\pi]$ and satisfying (2.1). Then, for any x in the domain, the value $f(x)$ can be recovered via the spectral smoothing of $\hat{f}_N$, which obeys the following error estimate

$$|\hat{f}_N * \psi^{\theta,\sqrt{N}}(x) - f(x)| \leq C_s\cdot||\rho||_{(2s)}\cdot[N\cdot\theta^{-2s}\cdot||f|| + \max_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq 2s}} |D^k f(y)|]\cdot N^{-s+1} , \quad s > 1. \tag{3.15}$$

In general, of course, the choices of the cut-off function, ρ , and the β-exponent, $0 < \beta < 1$, provide us with a whole variety of admissible kernels, for which we have:

Corollary 3.6 (Infinite Order of Accuracy)

Let $\rho(y)$ be a C^∞-function, supported in $[-\pi,\pi]$ and taking the value one at the origin. Assume the function f is C^∞ in the ε-neighborhood of a point x in the domain. Then the spectral smoothing

$$\hat{f}_N * \psi^{\theta=\varepsilon/\pi,N^\beta}(x) = \frac{1}{2\varepsilon}\int_{y=x-\varepsilon}^{x+\varepsilon} \hat{f}_N(y)\rho\left(\frac{\pi(x-y)}{\varepsilon}\right)\frac{\sin(N^\beta+\frac{1}{2})\frac{\pi(x-y)}{\varepsilon}}{\sin\frac{\pi(x-y)}{2\varepsilon}}\,dy\ , \quad 0<\beta<1\ , \tag{3.16}$$

recovers the function value $f(x)$ within infinite order of accuracy.

Remarks

(i) Suppose f is known to be smooth in the asymmetric neighborhood of x , $(x-\varepsilon_L\ ,\ x+\varepsilon_R)$, $0<\varepsilon_L,\ \varepsilon_R \le \pi$. Let ρ be a C^∞-function supported in the interval $[-\theta^{-1}\varepsilon_L,\ \theta^{-1}\varepsilon_R]$ inside of $[-\pi,\pi]$, such that $\rho(y=0) = 1$. Then a nonsymmetric version of the above spectral smoothing reads

$$\hat{f}_N * \psi^{\theta,N^\beta}(x) = \frac{1}{2\pi\theta}\int_{x-\varepsilon_L}^{x+\varepsilon_R} \hat{f}_N(y)\rho\left(\frac{x-y}{\theta}\right)\frac{\sin(N^\beta+\frac{1}{2})\left(\frac{x-y}{\theta}\right)}{\sin\frac{x-y}{2\theta}}\,dy\ , \tag{3.17}$$

recovering $f(x)$ within spectral accuracy. The case $\varepsilon_L = \varepsilon_R = \varepsilon = \pi\theta$ coincides with Corollary 3.6.

(ii) The above error estimates concerning the spectral smoothing $\hat{f}_N * \psi^{\theta,p}$ still enjoy the further flexibility in choosing different s-orders in (3.10). This provides us with even further richness so as to tune the different free parameters to yield accurate results.

As promised, we conclude this section with the following:

Proof of Lemma 3.2

With the regularization kernel $\psi^{\theta,p}$ in (3.4), Liebnitz's rule gives us

$$||\psi^{\theta,p}||_{(s)} \le \theta^{-s-1}||\rho(y)D_p(y)||_{(s)} \le$$

$$\le \theta^{-s-1}\sum_{j=0}^{s}\binom{s}{j}||\rho||_{(s-j)}||D_p||_{(j)}\ ; \tag{3.18}$$

complemented by the maximum norm estimate

$$||D_p||_{(j)} \le \frac{1}{2\pi}\sum_{|k|\le p}|k|^j \le \frac{1}{\pi(j+1)}p^{j+1}\ , \tag{3.19}$$

the desired result follows

$$||\psi^{\theta,p}||_{(s)} \le \frac{1}{\pi}\theta^{-s-1}\sum_{j=0}^{s+1}\binom{s+1}{j}||\rho||_{(s)}p^j \le \theta^{-s-1}||\rho||_{(s)}(1+p)^{s+1}. \tag{3.20}$$

Proof of Lemma 3.3

Let $\phi^{\theta,x}(y) = f(x-\theta y)\rho(y) - f(x)$ be the auxiliary function in (3.9c) with $\rho(y)$ supported in $[-\pi,\pi]$. We observe that the only f-values participating in the definition of $\phi^{\theta,x}$ are those from the $\theta\cdot\pi$ neighborhood of x , $|y-x| \le \theta\cdot\pi$. Applying Liebnitz's rule restricted to that neighborhood, we find

$$||\phi^{\theta,x}||_{(s)} \le \sum_{j=0}^{s}\binom{s}{j}||\rho||_{(j)}\theta^{s-j}\cdot \max_{\substack{|y-x|\le\theta\pi\\ 0\le k\le s-j}}|D^k f| \le$$

$$\le (1+\theta)^s||\rho||_{(s)}\cdot \max_{\substack{|y-x|\le\theta\pi\\ 0\le k\le s}}|D^k f(y)| \tag{3.21}$$

as asserted.

4. RECOVERING POINTWISE VALUES FROM THE PSEUDOSPECTRAL APPROXIMATION

In this section we treat the case where the discrete gridvalues $f_\nu = f(y_\nu)$ are given, so that a peudo-spectral approximation $\tilde{f}_N$ collocating these gridvalues is uniquely determined, see (1.6). The key observation here is that the integrand $\hat{f}_N(y')\psi^{\theta,p}(x-y')$ in (3.5) is smooth over the whole domain, due to the kernel localization in the neighborhood of the point of interest, x . Hence, replacing the convolution integral with an appropriate trapezoidal sum, only an additional spectrally small aliasing error is committed. Thus, in analogy with (3.5), we smooth the pseudo-spectral approximation via the convolution sum

$$\frac{2\pi}{2N}\sum_{\nu=0}^{2N-1}\tilde{f}_N(y_\nu)\psi^{\theta,p}(x-y_\nu) \equiv \frac{2\pi}{2N}\sum_{\nu=0}^{2N-1}f_\nu\psi^{\theta,p}(x-y_\nu)\ . \tag{4.1}$$

Observe that since $\psi^{\theta,p}$ is supported in the neighborhood of x , only those neighboring gridvalues are taking part in the pseudo-spectral smoothing.

The computed error at a fixed point x , amounts to

$$\frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu\psi^{\theta,p}(x-y_\nu) - f(x) =$$

$$= \left(\frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu\psi^{\theta,p}(x-y_\nu) - f * \psi^{\theta,p}(x)\right) + \left(f * \psi^{\theta,p}(x) - f(x)\right). \tag{4.2a}$$

There are two sources of errors in this case: the aliasing error due to the use of the trapezoidal rule in the first difference

$$A_N^{\theta,p} \equiv \frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu\psi^{\theta,p}(x-y_\nu) - f * \psi^{\theta,p}(x), \tag{4.2b}$$

and as before, the regularization error in the second difference

$$R^{\theta,p} = f * \psi^{\theta,p} - f. \tag{4.2c}$$

The aliasing error estimate in $(1.5)_0$ and the regularization error estimate in (3.9d) yield:

Proposition 4.1 (Main Error Estimate)

Let $\psi^{\theta,p}$ be the regularization kernel (3.4). Fix a point x in the domain and denote

$$\chi^{\theta,p,x}(y) = f(y)\cdot\psi^{\theta,p}(x-y). \tag{4.3}$$

Also, let $\Phi^{\theta,x}$ be the auxiliary function in (3.9c). Then, the following error estimate holds

$$\left|\frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu\psi^{\theta,p}(x-y_\nu) - f(x)\right| \leq C_s\|\chi^{\theta,p,x}\|_{(s)}N^{-s} +$$

$$+ C_s\|\Phi^{\theta,x}\|_{(s)}p^{-s+1}. \tag{4.4}$$

We observe that the newly introduced auxiliary function $\chi^{\theta,p,x}(y)$ is supported in the $\theta\cdot\pi$-neighborhood of x, where Liebnitz's rule yields

$$\|\chi^{\theta,p,x}\|_{(s)} \leq \sum_{j=0}^{s}\binom{s}{j}\|\psi^{\theta,p}\|_{(j)}\cdot \operatorname*{Max}_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq s-j}} |D^k f(y)|; \tag{4.5a}$$

invoking (3.11), the following bound is found

$$\|\chi^{\theta,p,x}\|_{(s)} \leq \sum_{j=0}^{s}\binom{s}{j}\theta^{-j+1}\|\rho\|_{(j)}(1+p)^{j+1}\cdot \operatorname*{Max}_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq s}} |D^k f(y)| \leq$$

$$\leq \theta(1+p)\|\rho\|_{(s)}\cdot \operatorname*{Max}_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq s}} |D^k f(y)|\left(\frac{1+\theta+p}{\theta}\right)^s. \tag{4.5b}$$

The last estimate on the aliasing part of the error, augmented with the previously derived estimate on the regularization error in Lemma 3.3, lead us to the main result of this section, stating:

THEOREM 4.2

Let f be a bounded 2π-periodic function with given gridvalues $f_\nu = f(y_\nu)$. Setting the regularization kernel

$$\psi^{\theta,N^\beta}(y) = \frac{1}{2\pi\theta}\rho(\theta^{-1}y)\frac{\sin(N^\beta+1/2)y/\theta}{\sin y/2\theta}, \tag{4.6}$$

then for any x in the domain, we have the pointwise error estimate

$$\left|\frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu\psi^{\theta,N^\beta}(x-y_\nu) - f(x)\right| \leq$$

$$\leq C_s\|\rho\|_s\cdot \operatorname*{Max}_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq s}} |D^k f(y)|\cdot[N^{-\beta s+1} + \theta^{-s}\cdot N^\beta\cdot N^{-(1-\beta)s}]. \tag{4.7}$$

Taking $\beta = 1/2$ to balance the two error's contributions, we find:

Corollary 4.3 (Pseudo-Spectral Smoothing)

Let $\rho(y)$ be a C^{2s}-function, supported in $[-\pi,\pi]$ and satisfying (2.1). Then for any x in the domain, the value $f(x)$ can be recovered via the pseudo-spectral smoothing of the neighboring gridvalues, f_ν, which obeys the following error estimate

$$\left|\frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu\psi^{\theta,\sqrt{N}}(x-y_\nu) - f(x)\right| \leq$$

$$\leq C_s\|\rho\|_{(2s)}\cdot \operatorname*{Max}_{\substack{|y-x|\leq\theta\pi \\ 0\leq k\leq 2s}} |D^k f(y)|(1+\theta^{-2s})\cdot N^{-s+1}, \quad s > 1. \tag{4.8}$$

In analogy with Corollary 3.6, we also have:

Corollary 4.4 (Infinite Order of Accuracy)

Let $\rho(y)$ be a C^∞-function, supported in $[-\pi,\pi]$ and taking the value one at the origin. Assume the function f is C^∞ in the ε-neighborhood of a point x in the domain. Then the pseudo-spectral smoothing

$$\frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu \psi^{\theta=\varepsilon/\pi,N^\beta}(x-y_\nu) = \frac{\pi}{2\varepsilon N}\sum_{y_\nu \geq x-\varepsilon}^{y_\nu \leq x+\varepsilon} f_\nu \rho\left(\frac{\pi(x-y_\nu)}{\varepsilon}\right)\frac{\sin(N^\beta+\frac{1}{2})\frac{\pi(x-y_\nu)}{\varepsilon}}{\sin\frac{\pi(x-y_\nu)}{2\varepsilon}},$$

$$0 < \beta < 1 \qquad (4.9)$$

recovers the function value $f(x)$ within infinite order of accuracy.

In closing this section, we would like to emphasize another, slightly more global variant of the pseudo-spectral smoothing, based on integral convolution of the pseudo-spectral interpolant against the regularization kernel

$$\tilde{f}_N * \psi^{\theta,N^\beta} - f = \tilde{f}_N * \left(\psi^{\theta,N^\beta} - \tilde{\psi}_N^{\theta,N^\beta}\right) +$$
$$+ \left(\tilde{f}_N * \tilde{\psi}_N^{\theta,N^\beta} - f * \psi^{\theta,N^\beta}\right) + \left(f * \psi^{\theta,N^\beta} - f\right). \qquad (4.10)$$

The first term is spectrally small due to the interpolation error associated with the smooth regularization kernel as argued in Section 2; by the exactness of the trapezoidal rule applied to (trigonometric) polynomials of degree $\leq 2N$, we have

$$\tilde{f}_N * \tilde{\psi}_N^{\theta,N^\beta} = \frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} f_\nu \psi^{\theta,N^\beta}(x-y_\nu) \qquad (4.11)$$

and consequently, the second difference is spectrally small as argued above in relation to the aliasing errors. Finally the third difference is the spectrally small regularization error.

5. CONCLUDING REMARKS

The above arguments also apply to other orthogonal families. In conjunction with Legendre polynomials, we set as our regularization kernel

$$\psi^{\theta,p}(y) \equiv \theta^{-1}\rho(\theta^{-1}y)K_p(\theta^{-1}y) \; ; \qquad (5.1a)$$

here $\rho(y)$ is C^s-function supported in the interval $[-1,1]$ such that $\rho(y=0) = 1$, and $K_p(y)$ stands for Legendre spectral approximation of the delta function

$$K_p(y) = \sum_{k=0}^{p} (k+\tfrac{1}{2})P_k(y)P_k(0) \qquad (5.1b)$$

normalized to have a unit mass

$$\int_{-1}^{1} K_p(y)dy = 1 \; . \qquad (5.1c)$$

In view of the Christoffel-Durboux identity, we can rewrite

$$K_p(y) = \frac{p+1}{2}\,\frac{P_{p+1}(0)P_p(y) - P_p(0)P_{p+1}(y)}{y} \; . \qquad (5.1d)$$

The resulting spectral smoothing via the above Legendre-type regularization kernel was introduced in [1], and is intimately related to Mock and Lax [6] post processing: indeed, $\psi^{\theta,p}$ serves as a locally supported kernel with vanishing higher moments and unit mass - modulo a negligble spectral error.

Similarily, we can use Tchebyshev orthogonal expansion where $K_p(y)$ in (5.1a) is replaced by

$$K_p(y) = \frac{2}{\pi}\sum_{k=0}^{p}{}' \, T_k(y)T_k(0) = \frac{(1-y^2)}{p\pi}\,\frac{T_p'(y)}{} \qquad (5.2)$$

We note that the (pseudo-) spectral smoothing done with the Tchebyshev kernel is not translated to the usual cut-off in the transformed space.

6. NUMERICAL EXAMPLES

In this section we demonstrate the efficacy of the smoothing procedure outlined above. As a test function we have chosen the piecewise C^∞-function

$$f(x) = \begin{cases} \sin\frac{x}{2} & 0 \leq x \leq \pi \\ -\sin\frac{x}{2} & \pi \leq x \leq 2\pi \; . \end{cases} \qquad (6.1)$$

As before, denote its spectral approximation by $\hat{f}_N(x)$, and let $\tilde{f}_N(x)$ be the pseudo-spectral approximation to $f(x)$. It is evident from the first column of Tables I and III that $\hat{f}_N(y_\nu)$ - the spectral approximation sampled at $y_\nu = \nu\pi/N$ - do not approximate $f(y_\nu)$ within spectral accuracy. In fact, the error committed by $\hat{f}_{128}(y_\nu)$ is only half of that committed by $\hat{f}_{64}(y_\nu)$; this is in accordance with a suitably sharpened error estimate of type (1.3) - consult e.g. (3.4). Regarding the pseudo-spectral approximation, $\tilde{f}_N(x)$, it of course collocates the exact values at the sampling gridpoints, $\tilde{f}_N(y_\nu) = f(y_\nu)$; yet, in between these gridpoints, $\tilde{f}_N(y_{\nu+1/2} = (\nu + 1/2)\pi/N)$ approximate $f(y_{\nu+1/2})$ within first order accuracy only, as shown in the first column of Tables II and IV.

In order to construct our regularization kernel, we define the cut-off function $\rho(\xi) = \rho_\alpha(\xi)$ to be

$$\rho_\alpha(\xi) = \begin{cases} \exp \dfrac{\alpha\xi^2}{\xi^2-1} & |\xi| < 1 \\ 0 & \text{otherwise} \end{cases} \tag{6.2}$$

namely $\rho_\alpha(\xi)$ is a C^∞-function whose support is the interval $|\xi| < 1$. Our regularization kernel is now of the form (see (3.4))

$$\psi^{\theta,p}(y) = \frac{1}{2\pi\theta}\,\rho_\alpha(\theta^{-1}y)\,\frac{\sin\,(p+1/2)y/\theta}{\sin\,y/2\theta} \tag{6.3}$$

The post processing procedure of the spectral approximation $\hat{f}_N$ involves convoluting $\hat{f}_N$ against $\psi^{\theta,p}$, namely

$$f(x) \sim \frac{1}{2\pi\theta}\int_0^{2\pi} \hat{f}_N(y)\rho\left(\frac{x-y}{\theta}\right)\frac{\sin\,(p+1/2)(x-y)/\theta}{\sin\,(x-y)/2\theta}\,dy \tag{6.4}$$

where x is a fixed point of interest. (In practice we use the trapezoidal rule to evaluate the right-hand-side of (6.4) taking a large number of quaderture points.)

The parameter θ was chosen as

$$\theta = \;|x - \pi| \;; \tag{6.5}$$

this guarantees that ψ is so localized that it does not interact with regions of discontinuity.

It should be noted, in this stage, that if θ was so chosen to be the same for each x , (and not as in (6.5)), the formula (6.4) admits a simpler form; that is, if

$$\psi^{\theta,p}(y) = \sum_{k=-\infty}^{\infty} \sigma_k e^{iky} \tag{6.6}$$

then

$$f(x) \sim \sum_{k=-N}^{N} \hat{f}(k)\sigma_k e^{ikx} . \tag{6.7}$$

This procedure can be carried out efficiently in the Fourier space.

Next, we turn to the post-processing for the pseudo-spectral approximation $\hat{f}_N(x)$ which is simpler than (6.4). In fact, in this case

$$f(x) \sim \frac{2\pi}{2N}\sum_{\nu=0}^{2N-1} \tilde{f}(y_\nu)\psi^{\theta,p}(x-y_\nu) \tag{6.8}$$

Note that carrying out the smoothing procedure defined in (6.8) does not involve any extra evaluation of $\tilde{f}(y)$ in points other than y_ν , in contrast to spectral smoothing procedure in (6.4). As before, the parameter θ was chosen according to (6.5). We have yet to determine the parameters p and α . The parameter p must be equal to N^β for $0 < \beta < 1$ in view of (3.14), in order to assure infinite accuracy. (In our computations $\beta \approx .8$). Finally we feel that α is problem dependent and we chose $\alpha = 10$. We have not tuned the parameters to get optimal results; further tuning may improve the quality of our filtering procedure.

In Tables I, II, III, and IV we give the results of the smoothing procedure at several points in the domain. The pointwise values are now recovered with high accuracy. The first column in each table indicates the points in which the procedure was performed. We limited ourselves to four points in the interval $(0,\pi)$ because of the symmetry of of the function $f(x)$.

The second column gives either the spectral approximation $\hat{f}_N(x)$ or the pseudo-spectral approximation $\tilde{f}_N(x)$, $N = 128$ in Table I and II and $N = 64$ in Tables III and IV. The third column gives the smoothed results, when filtered by (6.4) on (6.8), at the same points as in column I.

The results indicate the dramatic improvement obtained by the smoothing procedure. Moreover, note that the error committed by $\tilde{f}_{128}$ (or $\hat{f}_{128}$) is better than the one committed by $\tilde{f}_{64}$ (or $\hat{f}_{64}$) only by a factor of 2 , whereas after the post-processing the error improves by a factor of 10^4.

Table I.

Results of smoothing of the spectral approximation of $f(x)$, $N = 128$.

$x_\nu = \frac{\pi\nu}{8}$ ν equals	$\lvert f(x_\nu) - \hat{f}_N(x_\nu)\rvert$	$\lvert f - \hat{f}_N * \psi\rvert$ at $x = x_\nu$
2	3.2 (-3)	5.8 (-10)
3	5.2 (-3)	7.9 (-10)
4	7.8 (-3)	6.3 (-10)
5	1.1 (-2)	1.1 (-10)

Table II.

Same as Table I for the pseudo-spectral approximation $\tilde{f}_N(x)$.

$x_{\nu+\frac{1}{2}} = \frac{\pi}{8}(\nu+\frac{1}{2})$ ν equals	$\lvert f(x_{\nu+\frac{1}{2}}) - \tilde{f}_N(x_{\nu+\frac{1}{2}})\rvert$	$\lvert f - \tilde{f}_N * \psi\rvert$ at $x = x_{\nu+\frac{1}{2}}$
2	5 (-3)	7 (-10)
3	8.1 (-3)	7.9 (-10)
4	1.2 (-2)	6.4 (-10)
5	1.8 (-2)	1.2 (-10)

Table III.

Results of smoothing of the spectral approximation of $f(x)$, $N = 64$.

$x_\nu = \frac{\pi\nu}{8}$ ν equals	$\lvert f(x_\nu) - \hat{f}_N(x_\nu)\rvert$	$\lvert f - \hat{f}_N * \psi\rvert$ at $x = x_\nu$
2	6.4 (-3)	4.8 (-6)
3	1 (-2)	5.9 (-6)
4	1.5 (-2)	7.7 (-6)
5	2.3 (-2)	8.9 (-6)

Table IV.

Same as Table III for the pseudospectral approximation, $\tilde{f}_N(x)$.

$x_{\nu+\frac{1}{2}} = \frac{\pi}{8}(\nu+\frac{1}{2})$ ν equals	$\lvert f(x_{\nu+\frac{1}{2}}) - \tilde{f}_N(x_{\nu+\frac{1}{2}})\rvert$	$\lvert f - \tilde{f}_N * \psi\rvert$ at $x = x_{\nu+\frac{1}{2}}$
2	1 (-2)	4.1 (-6)
3	1.6 (-2)	6 (-6)
4	2.4 (-2)	7.8 (-6)
5	3.6 (-2)	8.9 (-6)

7. ENDNOTES

[1] The single and double primed summations indicate halving the first and the last terms, respectively. It is used in this case to compensate for the use of even number of gridpoints.

[2] Referring to the convex case.

8. REFERENCES

[1] Gottlieb, D., "Spectral Methods for Compressible Flow Problems", ICASE Report No. 84-29.

[2] Gottlieb, D. and Orszag, S.A., "Numerical Analysis of Spectral Methods: Theory and Applications", CBMS, No. 26, SIAM, 1977.

[3] Kreiss, H.O. and Oliger, J., "Methods for the Approximate Solution of Time Dependent Problems", GARP Publications Series No. 10, 1973.

[4] Majda, A. and Osher, S., "Propagation of Error into Regions of Smoothness for Accurate Difference Approximations to Hyperbolic Equations", Comm. Pure Appl. Math., V. 30, 1977, p. 671-705.

[5] Majda, A. and Osher, S., "The Fourier Method for Nonsmooth Initial Data", Math. Comp., V. 32, 1978, p. 1041-1081.

[6] Mock, M.S. and Lax, P.D., "The Computation of Discontinuous Solutions of Linear Hyperbolic Equations", Comm. Pure Appl. Math., V. 31, 1978, p. 423-430.

[7] Tadmor, E., "The Exponential Accuracy of Fourier and Tchebyshev Differencing Methods", ICASE Report No. 84-40.

School of Mathematical Sciences
Raymond and Beverly Sackler Faculty of Exact Sciences
Tel Aviv University, Tel Aviv, Israel.

Both authors were supported in part by the National Aeronautical and Space Administration under NASA contract No. NAS1-17070 while the authors were in residence at ICASE, NASA LANGLEY Research Center, Hampton, Va. 23665. The first author was also supported in part by the Air-Force Office of Scientific Research under Contract No. AFOSR 83-0089.