Spectral Methods for Discontinuous Problems

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1 Introduction

Spectral methods have emerged as powerful computational techniques for simulation of complex, smooth physical phenomena. Among other applications they have contributed to our understanding of turbulence by successfully simulating incompressible turbulent flows, have been extensively used in meteorology and geophysics, and have been recently applied to time domain electromagnetics. Several issues arise when applying spectral methods to problems which feature sharp gradients and discontinuities. In the presence of such phenomena the accuracy of high order methods deteriorates. This is due to the well known Gibbs phenomenon that states that the pointwise convergence of global approximations of discontinuous functions is at most first order. In the presence of a shock wave global approximations are oscillatory and converge nonuniformly. Recent advances in the theory and application of spectral methods indicate that high order information is retained in stable spectral simulations of discontinuous phenomena and can be recovered by suitable postprocessing techniques.

2 The Gibbs Phenomenon

The partial Fourier sum

$$\sum_{k=-N}^{N} \hat{f}_k e^{\pi i k x}$$

based on the first $2N+1$ Fourier coefficients of a nonsmooth function $f(x)$, converges slowly away from the discontinuity and features non-decaying oscillations. This behavior of all global approximations of nonsmooth functions is known as the classical Gibbs phenomenon (see [20]).

Euler (in 1755) was probably the first to witness the phenomenon in the Fourier expansion of the function $f(x) = x$. Wilbraham (in 1848) analyzed this series and discussed the oscillatory behavior of the approximation. However, the first to address the issue of reconstructing a discontinuous function from its partial series was the eminent physicist

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Albert Michelson. In 1898 Michelson, together with Stratton, built a harmonic analyzer, a mechanical device which stored the Fourier coefficients of a given curve. A detailed description of this device is given in the 1910 edition of the Britannica. In their Philosophical magazine paper (1898) they presented graphs of functions reconstructed from their Fourier coefficients. One of those curves was a square wave that displayed the Gibbs oscillations. Shortly after the appearance of this paper, Michelson, in a letter to the British journal NATURE (October 6 1898), pointed out the difficulty in reconstructing the function $f(x) = x$ from its Fourier coefficients. In particular Michelson claimed that looking at the point $x_0 = 1 - \frac{1}{N}$ no convergence is observed. Michelson states:

> The idea that a real discontinuity can replace a sum of continuous curves is so utterly at variance with the physicists' notion of quantity that it seems to me to be worth while giving a very elementary statement of the problem in such simple form that the mathematicians can at once point to the inconsistency if any there be.

This appeal to mathematicians was answered by the mathematician A.E.H. Love in the next issue of NATURE (December 1898), though probably not in the spirit that Michelson intended. Love claimed that the partial sum does converges pointwise and for this type of convergence, the point has to be unchanged in the limit process. Insultingly, Love recommended to Michelson and his physicist friends some elementary books in mathematics. Love, of course, overlooked the concept of uniform convergence which is at the heart of this issue. This seems to be the gist of Michelson's terse response in the December 29, 1898 issue of Nature that restated his original example. The same issue contains a letter from Gibbs beginning with the observation that in Love's response "the point of view of Professor Michelson is hardly considered" and attempting to analyze the phenomenon. However Gibbs seems to argue that there was indeed uniform convergence. The same issue contains also the (now more respectful) response of Love to Gibbs' letter which now admits the importance of the issue of uniform convergence.

It was not until the April 27, 1899 issue of Nature that Gibbs presented the correct analysis of this phenomenon. It was Poincare's eminence that ultimately decided this issue in a letter (forwarded by Michelson to Nature and published in May 1899) stating the correct behavior of the partial Fourier sums.

Sufficient conditions for the removal of the Gibbs phenomenon were given in [21]. Consider a function $f(x) \in L^2[-1,1]$ and assume that there is a subinterval $[a,b] \subset [-1,1]$ in which $f(x)$ is analytic. (For convenience we define the local variable, $\xi = -1 + 2\frac{x-a}{b-a}$ such that if $a \leq x \leq b$ then $-1 \leq \xi \leq 1$.) Let the family $\{\Psi_k(x)\}$, be orthonormal under a scalar product $(\cdot, \cdot)$, and denote the finite expansion of $f(x)$ in this basis by $f_N(x)$,

$$f_N(x) = \sum_{k=0}^{N} (f, \Psi_k)\Psi_k(x).$$

Let the family $\{\Phi_k^\lambda(\xi)\}$ be Gibbs complementary to the family $\{\Psi_k(x)\}$ (see [21] for its exact definition), then the postprocessed reconstruction given by

$$g_N(x) = \sum_{l=0}^{\lambda} \langle f_N, \Phi_l^\lambda \rangle_\lambda \Phi_l^\lambda(\xi(x))$$

converges exponentially to $f(x)$, i.e.

$$\max_{a \le x \le b} |f(x) - g_N(x)| \ \le \ e^{-qN}, \qquad q > 0.$$

In a series of papers [15]–[19] we showed that the Gegenbauer polynomials

$$\Phi_k^\lambda(\xi) \ = \ \frac{1}{\sqrt{h_k^\lambda}} C_k^\lambda(\xi)$$

which are orthonormal under the inner product $\langle \cdot, \cdot \rangle_\lambda$ defined by

$$\langle f, g \rangle_\lambda \ = \ \int_{-1}^{1} (1-\xi^2)^{\lambda - \frac{1}{2}} f(\xi) g(\xi) \, d\xi$$

are Gibbs complementary to all commonly used spectral approximations.

The theory presented above does not prescribe an optimal way of constructing a Gibbs complementary basis. This is still an open question. The Gegenbauer method is not robust, it is sensitive to roundoff errors and to the choice of the parameters λ and m. A different implementation of the Gegenbauer postprocessing method has been suggested recently by Jung and Shizgal [25]. To explain the differences between the direct Gegenbauer method and the inverse Gegenbauer method suggested in [25], consider the case of the the Fourier expansion of a nonperiodic problem. The Fourier approximation $f_N(x)$ of $f(x)$ is

$$f_N(x) \ = \ \sum_{k=-N}^{N} \hat{f}_k e^{ik\pi x},$$

where $\hat{f}_k = \big(f(x), e^{ik\pi x}\big)$, and we construct

$$f_N^m(x) \ = \ \sum_{l=0}^{m} \hat{g}_l C_l^\lambda(x),$$

where $\hat{g}_l = \langle f_N, C_l^\lambda(x) \rangle_\lambda$. In the Inverse method we use the relationship

$$\hat{f}_k = (f_N^m(x), e^{ik\pi x})$$

and invert to find $\hat{g}_l$.

Thus if we define the matrix $W_{kl} = (C_l^\lambda(x), e^{ik\pi x})_F = \int_{-1}^{1} (1-x^2)^{\lambda-\frac{1}{2}} C_l^\lambda(x) e^{ik\pi x} dx$, and $\hat{f}_k = (f, e^{ik\pi x})$

$$\sum_{l=0}^{m} W_{kl} g_l^\lambda = \hat{f}_k.$$

The method seems to be less sensitive to roundoff errors or to the choice of parameters. In particular if the original function is a polynomial, the inverse method is exact.

3 Recovering Order of Accuracy for Solutions of PDEs

Just as spectral accuracy can be recovered in spectral approximations of nonsmooth functions, it can also be recovered in the case of discontinuous solutions of linear hyperbolic equations.

Consider the hyperbolic system of the form

$$\frac{\partial U}{\partial t} = \mathcal{L}U; \;\; U(t=0) = U_0.$$

Let u be the spectral approximation to U. For smooth solutions we have the classical error estimate:

$$||U-u|| \leq K||U_0||_s \frac{1}{N^{s-1}}.$$

This estimate, obviously, requires the initial condition to be smooth everywhere and does not apply in the case of piecewise smooth initial conditions. However it has been proven in [1] that :

$$|(U(T)-u(T),\phi)| \leq K||\phi||_s \frac{1}{N^s}$$

for any smooth function ϕ provided that the numerical initial conditions are preprocessed. Equation (3) implies that the Fourier coefficients of u approximate those of U with spectral accuracy. It is therefore possible to postprocess to get spectral accuracy for the point values in any interval where the solution U is smooth. In the case of the nonlinear hyperbolic system

$$\frac{\partial U}{\partial t} + \frac{\partial f(U)}{\partial x} = 0,$$

Lax ([23]) argued that high order information is contained in a convergent high resolution scheme.

To stabilize the spectral schemes we use either the Spectral Viscosity (SV) Method or the Super Spectral Viscosity (SSV) Method (see [27],[28],[24]). These methods amount to the addition of viscosity terms for the high modes of the solution. In [10] we demonstrate that this is equivalent to filtering, and in fact, filtering can be seen as an efficient way of applying these methods.

The theory developed by Tadmor and Tadmor and Maday demonstrates that both the SV and SSV methods converge to the correct entropy solution for Fourier and Legendre approximations to scalar nonlinear hyperbolic equations. Carpenter, Gottlieb and Shu [2] proved that even for systems, if the solution converges it converges to the correct entropy solution.

4 Applications

There is extensive literature reporting results of the application of spectral methods to shock wave problems [12],[13],[27],[28][24].

In [4] the authors compared ENO and spectral methods for the numerical simulations of shock- cylinder interactions in the case of reactive flows. The authors demonstrated that spectral methods required fewer resources than the ENO schemes for comparable accuracy. In [3], the author considered interactions of shock waves and entropy waves as well as interactions of shock waves and vortices. The calculations involved solutions of the two dimensional Euler equations and the results compared well with ENO methods. In [10] [9] we presented spectral simulations of the Richtmyer-Meshkov instabilities and showed comparisons with WENO schemes. It has been shown that with increased order of accuracy the WENO results converge to the spectral ones.

A more extensive study of spectral simulations of compressible reactive high Mach number flows has been reported in [6]. In this work the interaction of shock waves and hydrogen jets were studied. This involves the solution of the Navier Stokes equations with chemical interactions. The work gives a clear demonstration of the fact that spectral methods are very suitable for studies of complicated flows that involve shock waves.

Several model problems confirm Lax's argument concerning the information contained in high resolution schemes. Shu and Wang [26] recovered spectral accuracy for the nonlinear Burgers equation where discontinuity develops and moves around the domain. It is interesting to note that the Gegenbauer postprocessing technique recovers the design order accuracy even for finite difference schemes. In [22] the postprocessing recovered design accuracy, in the maximum norm, for the WENO steady state solution of a converging–diverging nozzle.

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