Introduction

The purpose of this book is to collect, in one volume, all the ingredients necessary for the understanding of spectral methods for time-dependent problems, and, in particular, hyperbolic partial differential equations. It is intended as a graduate-level text, covering not only the basic concepts in spectral methods, but some of the modern developments as well. There are already several excellent books on spectral methods by authors who are well-known and active researchers in this field. This book is distinguished by the exclusive treatment of time-dependent problems, and so the derivation of spectral methods is influenced primarily by the research on finite-difference schemes, and less so by the finite-element methodology. Furthermore, this book is unique in its focus on the stability analysis of spectral methods, both for the semi-discrete and fully discrete cases. In the book we address advanced topics such as spectral methods for discontinuous problems and spectral methods on arbitrary grids, which are necessary for the implementation of pseudo-spectral methods on complex multi-dimensional domains.

In Chapter 1, we demonstrate the benefits of high order methods using phase error analysis. Typical finite difference methods use a local stencil to compute the derivative at a given point; higher order methods are then obtained by using a wider stencil, i.e., more points. The Fourier spectral method is obtained by using all the points in the domain. In Chapter 2, we discuss the trigonometric polynomial approximations to smooth functions, and the associated approximation theory for both the continuous and the discrete case. In Chapter 3, we present Fourier spectral methods, using both the Galerkin and collocation approaches, and discuss their stability for both hyperbolic and parabolic equations. We also present ways of stabilizing these methods, through super viscosity or filtering.

Chapter 4 features a discussion of families of orthogonal polynomials which are eigensolutions of a Sturm–Liouville problem. We focus on the Legendre and Chebyshev polynomials, which are suitable for representing functions on finite

domains. In this chapter, we present the properties of Jacobi polynomials, and their associated recursion relations. Many useful formulas can be found in this chapter. In Chapter 5, we discuss the continuous and discrete polynomial expansions based on Jacobi polynomials; in particular, the Legendre and Chebyshev polynomials. We present the Gauss-type quadrature formulas, and the different points on which each is accurate. Finally, we discuss the connections between Lagrange interpolation and electrostatics. Chapter 6 presents the approximation theory for polynomial expansions of smooth functions using the ultraspherical polynomials. Both the continuous and discrete expansions are discussed. This discussion sets the stage for Chapter 7, in which we introduce polynomial spectral methods, useful for problems with non-periodic boundary conditions. We present the Galerkin, tau, and collocation approaches and give examples of the formulation of Chebyshev and Legendre spectral methods for a variety of problems. We also introduce the penalty method approach for dealing with boundary conditions. In Chapter 8 we analyze the stability properties of the methods discussed in Chapter 7.

In the final chapters, we introduce some more advanced topics. In Chapter 9 we discuss the spectral approximations of non-smooth problems. We address the Gibbs phenomenon and its effect on the convergence rate of these approximations, and present methods which can, partially or completely, overcome the Gibbs phenomenon. We present a variety of filters, both for Fourier and polynomial methods, and an approximation theory for filters. Finally, we discuss the resolution of the Gibbs phenomenon using spectral reprojection methods. In Chapter 10, we turn to the issues of time discretization and fully discrete stability. We discuss the eigenvalue spectrum of each of the spectral spatial discretizations, which provides a necessary, but not sufficient, condition for stability. We proceed to the fully discrete analysis of the stability of the forward Euler time discretization for the Legendre collocation method. We then present some of the standard time integration methods, especially the Runge–Kutta methods. At the end of the chapter, we introduce the class of strong stability preserving methods and present some of the optimal schemes. In Chapter 11, we turn to the computational issues which arise when using spectral methods, such as the use of the fast Fourier transform for interpolation and differentiation, the efficient computation of the Gauss quadrature points and weights, and the effect of round-off errors on spectral methods. Finally, we address the use of mappings for treatment of non-standard intervals and for improving accuracy in the computation of higher order derivatives. In Chapter 12, we talk about the implementation of spectral methods on general grids. We discuss how the penalty method formulation enables the use of spectral methods on general grids in one dimension, and in complex domains in multiple dimensions, and illustrate this

using both the Galerkin and collocation approaches. We also show how penalty methods allow us to easily generalize to complicated boundary conditions and on triangular meshes. The discontinuous Galerkin method is an alternative way of deriving these schemes, and penalty methods can thus be used to construct methods based on multiple spectral elements.

Chapters 1, 2, 3, 5, 6, 7, 8 of the book comprise a complete first course in spectral methods, covering the motivation, derivation, approximation theory and stability analysis of both Fourier and polynomial spectral methods. Chapters 1, 2, and 3 can be used to introduce Fourier methods within a course on numerical solution of partial differential equations. Chapters 9, 10, 11, and 12 address advanced topics and are thus suitable for an advanced course in spectral methods. However, depending on the focus of the course, many other combinations are possible.

A good resource for use with this book is PseudoPack. PseudoPack Rio and PseudoPack 2000 are software libraries in Fortran 77 and Fortran 90 (respectively) for numerical differentiation by pseudospectral methods, created by Wai Sun Don and Bruno Costa. More information can be found at http://www.labma.ufrj.br/bcosta/pseudopack/main.html and http://www.labma.ufrj.br/bcosta/pseudopack2000/main.html.

As the oldest author of this book, I (David Gottlieb) would like to take a paragraph or so to tell you my personal story of involvement in spectral methods. This is a personal narrative, and therefore may not be an accurate history of spectral methods. In 1973 I was an instructor at MIT, where I met Steve Orszag, who presented me with the problem of stability of polynomial methods for hyperbolic equations. Working on this, I became aware of the pioneering work of Orszag and his co-authors and of Kreiss and his co-authors on Fourier spectral methods. The work on polynomial spectral methods led to the book *Numerical Analysis of Spectral Methods: Theory and Applications* by Steve Orszag and myself, published by SIAM in 1977. At this stage, spectral methods enjoyed popularity among the practitioners, particularly in the meteorology and turbulence community. However, there were few theoretical results on these methods. The situation changed after the summer course I gave in 1979 in France. P. A. Raviart was a participant in this course, and his interest in spectral methods was sparked. When he returned to Paris he introduced his postdoctoral researchers, Claudio Canuto and Alfio Quarteroni, and his students, Yvon Maday and Christine Bernardi, to these methods. The work of this European group led to an explosion of spectral methods, both in theory and applications. After this point, the field became too extensive to further review it. Nowadays, I particularly enjoy the experience of receiving a paper on spectral methods which I do not understand. This is an indication of the maturity of the field.

The following excellent books can be used to deepen one's understanding of many aspects of spectral methods. For a treatment of spectral methods for incompressible flows, the interested reader is referred to the classical book by C. Canuto, M. Y. Hussaini, A. Quarteroni and T. A. Zang, *Spectral Methods: Fundamentals in single domains* (2006), the more recent *Spectral Methods for Incompressible Viscous Flow* (2002) by R. Peyret and the modern text *High-Order Methods in Incompressible Fluid Flows* (2002) by M. Deville, P. F. Fischer, and E. Mund (2002). The book *Spectral/hp Methods in Computational Fluid Dynamics*, by G. E. Karniadakis and S. J. Sherwin (2005), deals with many important practical aspects of spectral methods computations for large scale fluid dynamics application. A comprehensive discussion of approximation theory may be found in *Approximations Spectrales De Problemes Aux Limites Elliptiques* (1992) by C. Bernardi and Y. Maday and in *Polynomial Approximation of Differential Equations* (1992) by D. Funaro. Many interesting results can be found in the book by B. -Y. Guo, *Spectral Methods and their Applications* (1998). For those wishing to implement spectral methods in Matlab, a good supplement to this book is *Spectral Methods in Matlab* (2000), by L. N. Trefethen.

For the treatment of spectral methods as a limit of high order finite difference methods, see *A Practical Guide to Pseudospectral Methods* (1996) by B. Fornberg. For a discussion of spectral methods to solve boundary value and eigenvalue problems, as well as Hermite, Laguerre, rational Chebyshev, sinc, and spherical harmonic functions, see *Chebyshev and Fourier Spectral Methods* (2000) by J. P. Boyd.

This text has as its foundation the work of many researchers who make up the vibrant spectral methods community. A complete bibliography of spectral methods is a book in and of itself. In our list of references we present only a partial list of those papers which have direct relevance to the text. This necessary process of selection meant that many excellent papers and books were excluded. For this, we apologize.

1

From local to global approximation

Spectral methods are global methods, where the computation at any given point depends not only on information at neighboring points, but on information from the entire domain. To understand the idea of a global method, we begin by considering local methods, and present the global Fourier method as a limit of local finite difference approximations of increasing orders of accuracy. We will introduce phase error analysis, and using this tool we will show the merits of high-order methods, and in particular, their limit: the Fourier method. The phase error analysis leads to the conclusion that high-order methods are beneficial for problems requiring well resolved fine details of the solution or long time integrations.

Finite difference methods are obtained by approximating a function $u(x)$ by a local polynomial interpolant. The derivatives of $u(x)$ are then approximated by differentiating this local polynomial. In this context, *local* refers to the use of nearby grid points to approximate the function or its derivative at a given point.

For slowly varying functions, the use of local polynomial interpolants based on a small number of interpolating grid points is very reasonable. Indeed, it seems to make little sense to include function values far away from the point of interest in approximating the derivative. However, using low-degree local polynomials to approximate solutions containing very significant spatial or temporal variation requires a very fine grid in order to accurately resolve the function. Clearly, the use of fine grids requires significant computational resources in simulations of interest to science and engineering. In the face of such limitations we seek alternative schemes that will allow coarser grids, and therefore fewer computational resources. Spectral methods are such methods; they use *all* available function values to construct the necessary approximations. Thus, they are *global* methods.

Example 1.1 Consider the wave equation

$$\frac{\partial u}{\partial t} = -2\pi \frac{\partial u}{\partial x} \quad 0 \le x \le 2\pi, \tag{1.1}$$
$$u(x,0) = e^{\sin(x)},$$

with periodic boundary conditions.

The exact solution to Equation (1.1) is a right-moving wave of the form

$$u(x,t) = e^{\sin(x-2\pi t)},$$

i.e., the initial condition is propagating with a speed 2π.

In the following, we compare three schemes, each of different order of accuracy, for the solution of Equation (1.1) using the uniform grid

$$x_j = j\Delta x = \frac{2\pi j}{N+1}, \quad j \in [0, \ldots, N]$$

(where N is an even integer).

Second-order finite difference scheme A quadratic local polynomial interpolant to $u(x)$ in the neighborhood of x_j is given by

$$u(x) = \frac{1}{2\Delta x^2}(x - x_j)(x - x_{j+1})u_{j-1} - \frac{1}{\Delta x^2}(x - x_{j-1})(x - x_{j+1})u_j + \frac{1}{2\Delta x^2}(x - x_{j-1})(x - x_j)u_{j+1}. \tag{1.2}$$

Differentiating this formula yields a second-order centered-difference approximation to the derivative du/dx at the grid point x_j:

$$\left.\frac{du}{dx}\right|_{x_j} = \frac{u_{j+1} - u_{j-1}}{2\Delta x}.$$

High-order finite difference scheme Similarly, differentiating the interpolant based on the points $\{x_{j-2}, x_{j-1}, x_j, x_{j+1}, x_{j+2}\}$ yields the fourth-order centered-difference scheme

$$\left.\frac{du}{dx}\right|_{x_j} = \frac{1}{12\Delta x}(u_{j-2} - 8u_{j-1} + 8u_{j+1} - u_{j+2}).$$

Global scheme Using all the available grid points, we obtain a global scheme. For each point x_j we use the interpolating polynomial based on the points $\{x_{j-k}, \ldots, x_{j+k}\}$ where $k = N/2$. The periodicity of the problem furnishes us with the needed information at any grid point. The derivative at the grid points is calculated using a matrix-vector product

$$\left.\frac{du}{dx}\right|_{x_j} = \sum_{i=0}^{N} \tilde{D}_{ji} u_i,$$

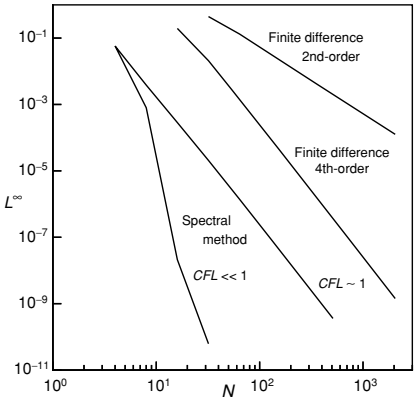

Figure 1.1 The maximum pointwise (L^∞) error of the numerical solution of Example 1.1, measured at $t = \pi$, obtained using second-order, fourth-order and global spectral schemes as a function of the total number of points, N. Here the Courant–Friedrichs–Lewy coefficient, CFL $= \Delta t/\Delta x$.

where the entries of the matrix is $\tilde{\mathrm{D}}$ are

$$\tilde{\mathrm{D}}_{ji} = \begin{cases} \frac{(-1)^{j+i}}{2}\left[\sin\left(\frac{(j-i)\pi}{N+1}\right)\right]^{-1} & i \neq j, \\ 0 & i = j. \end{cases}$$

The formal proof of this will be given in Section 1.1.3. This approach is equivalent to an infinite-order finite difference method as well as a Fourier spectral method.

To advance Equation (1.1) in time, we use the classical fourth-order Runge–Kutta method with a sufficiently small time-step, Δt, to ensure stability.

Now, let's consider the dependence of the maximum pointwise error (the L^∞-error) on the number of grid points N. In Figure 1.1 we plot the L^∞-error at $t = \pi$ for an increasing number of grid points. It is clear that the higher the order of the method used for approximating the spatial derivative, the more accurate it is. Indeed, the error obtained with $N = 2048$ using the second-order finite difference scheme is the same as that computed using the fourth-order method with $N = 128$, or the global method with only $N = 12$. It is also evident that by lowering Δt for the global method one can obtain even more accurate results, i.e., the error in the global scheme is dominated by time-stepping errors rather than errors in the spatial discretization.

Figure 1.2 shows a comparison between the local second-order finite difference scheme and the global method following a long time integration. Again, we clearly observe that the global scheme is superior in accuracy to the local scheme, even though the latter scheme employs 20 times as many grid points and is significantly slower.

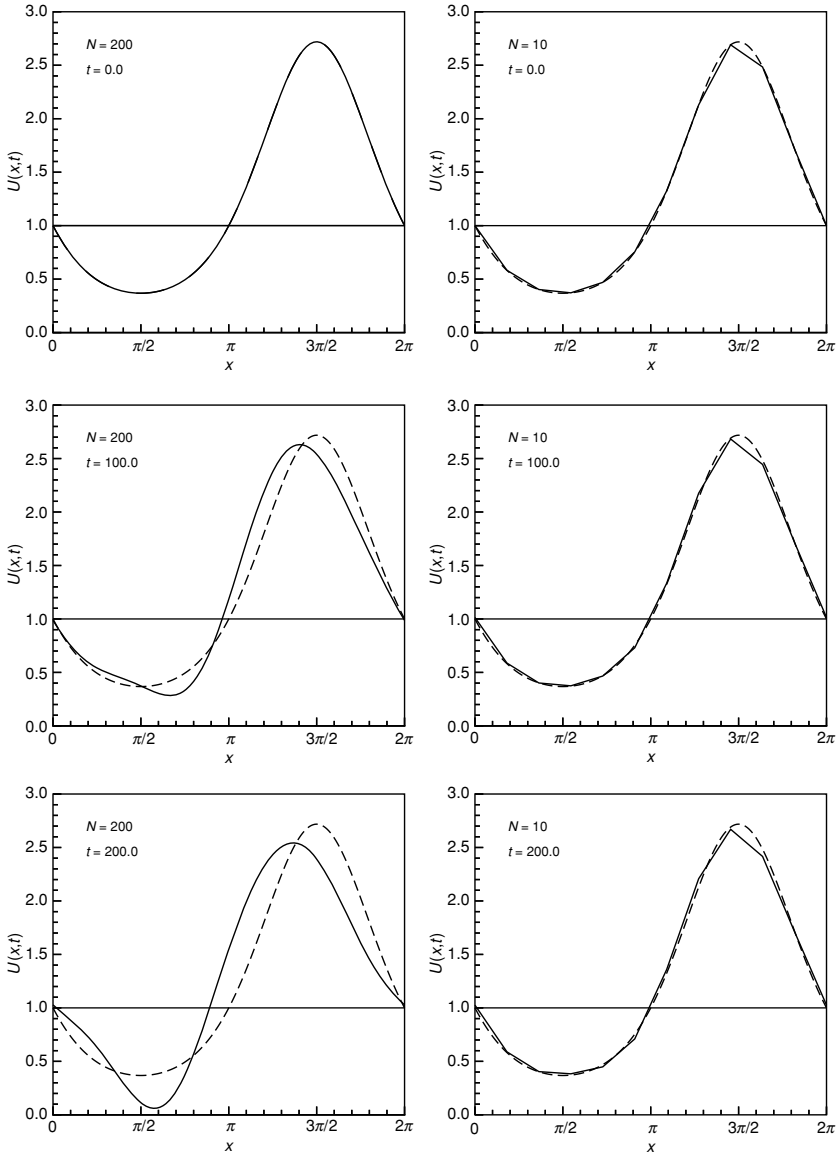

Figure 1.2 An illustration of the impact of using a global method for problems requiring long time integration. On the left we show the solution of Equation (1.1) computed using a second-order centered-difference scheme. On the right we show the same problem solved using a global method. The full line represents the computed solution, while the dashed line represents the exact solution.

1.1 Comparisons of finite difference schemes

The previous example illustrates that global methods are superior in performance to local methods, not only when very high spatial resolution is required but also when long time integration is important. In this section, we shall introduce the concept of phase error analysis in an attempt to clarify the observations made in the previous section. The analysis confirms that high-order and/or global methods are a better choice when very accurate solutions or long time integrations on coarse grids are required. It is clear that the computing needs of the future require both.

1.1.1 Phase error analysis

To analyze the phase error associated with a particular spatial approximation scheme, let's consider, once again, the linear wave problem

$$\begin{aligned} \frac{\partial u}{\partial t} &= -c\frac{\partial u}{\partial x} \quad 0 \le x \le 2\pi, \\ u(x,0) &= e^{ikx}, \end{aligned} \tag{1.3}$$

with periodic boundary conditions, where $i = \sqrt{-1}$ and k is the wave number. The solution to Equation (1.3) is a travelling wave

$$u(x,t) = e^{ik(x-ct)}, \tag{1.4}$$

with phase speed c.

Once again, we use the equidistant grid

$$x_j = j\Delta x = \frac{2\pi j}{N+1}, \quad j \in [0,\ldots,N].$$

The $2m$-order approximation of the derivative of a function $f(x)$ is

$$\left.\frac{df}{dx}\right|_{x_j} = \sum_{n=1}^{m} \alpha_n^m \mathcal{D}_n f(x_j), \tag{1.5}$$

where

$$\mathcal{D}_n f(x_j) = \frac{f(x_j + n\Delta x) - f(x_j - n\Delta x)}{2n\Delta x} = \frac{f_{j+n} - f_{j-n}}{2n\Delta x}, \tag{1.6}$$

and the weights, α_n^m, are

$$\alpha_n^m = -2(-1)^n \frac{(m!)^2}{(m-n)!(m+n)!}. \tag{1.7}$$

In the semi-discrete version of Equation (1.3) we seek a vector $\boldsymbol{v} = (v_0(t), \ldots, v_N(t))$ which satisfies

$$\frac{dv_j}{dt} = -c \sum_{n=1}^{m} \alpha_n^m \mathcal{D}_n v_j, \tag{1.8}$$
$$v_j(0) = e^{ikx_j}.$$

We may interpret the grid vector, $\boldsymbol{v}$, as a vector of grid point values of a trigonometric polynomial, $v(x,t)$, with $v(x_j,t) = \boldsymbol{v}_j(t)$, such that

$$\frac{\partial v}{\partial t} = -c \sum_{n=1}^{m} \alpha_n^m \mathcal{D}_n v(x,t), \tag{1.9}$$
$$v(x,0) = e^{ikx}.$$

If $v(x,t)$ satisfies Equation (1.9), the solution to Equation (1.8) is given by $v(x_j,t)$. The solution to Equation (1.9) is

$$v(x,t) = e^{ik(x - c_m(k)t)}, \tag{1.10}$$

where $c_m(k)$ is the numerical wave speed. The dependence of c_m on the wave number k is known as the dispersion relation.

The phase error $e_m(k)$, is defined as the leading term in the relative error between the actual solution $u(x,t)$ and the approximate solution $v(x,t)$:

$$\left| \frac{u(x,t) - v(x,t)}{u(x,t)} \right| = \left| 1 - e^{ik(c - c_m(k))t} \right| \simeq |k(c - c_m(k))t| = e_m(k).$$

As there is no difference in the amplitude of the two solutions, the phase error is the dominant error, as is clearly seen in Figure 1.2.

In the next section we will compare the phase errors of the schemes in Example 1.1. In particular, this analysis allows us to identify the most efficient scheme satisfying the phase accuracy requirement over a specified period of time.

1.1.2 Finite-order finite difference schemes

Applying phase error analysis to the second-order finite difference scheme introduced in Example 1.1, i.e.,

$$\frac{\partial v(x,t)}{\partial t} = -c \frac{v(x + \Delta x, t) - v(x - \Delta x, t)}{2\Delta x},$$
$$v(x,0) = e^{ikx},$$