1

Introduction

The partial differential equations (PDEs) that arise in applications can only rarely be solved in closed form. Even when they can be, the solutions are often impractical to work with and to visualize. Numerical techniques, on the other hand, can be applied successfully to virtually all well-posed PDEs. Broadly applicable techniques include finite element (FE), finite volume (FV), finite difference (FD), and, more recently, spectral methods. The complexity of the domain and the required levels of accuracy are often the key factors in selecting among these approaches.

Finite-element methods are particularly well suited to problems in very complex geometries (e.g. 3-D engineering structures), whereas spectral methods can offer superior accuracies (and cost efficiencies) mainly in simple geometries such as boxes and spheres (which can, however, be combined into more complex shapes). FD methods perform well over a broad range of accuracy requirements and (moderately complex) domains.

Both FE and FV methods are closely related to FD methods. FE methods can frequently be seen as a very convenient way to generate and administer complex FD schemes and to obtain results with relatively sharp error estimates. The connection between spectral methods – in particular the so-called pseudospectral (PS) methods, the topic of this book – and FD methods is closer still. A key theme in this book is to exploit this connection, both to make PS methods more intuitively understandable and to obtain particularly powerful and flexible PS variations.

Finite difference methods approximate derivatives of a function by *local* arguments (such as $du(x)/dx \approx [u(x+h)-u(x-h)]/2h$, where h is a small grid spacing; these methods are typically designed to be exact for polynomials of low order). This approach is very reasonable: because the derivative is a local property of a function (which need not be smooth), it

seems unnecessary (and is certainly costly) to invoke many function values far away from the point of interest.

In contrast, spectral methods are *global*. A common way to introduce them starts by approximating the function we want to differentiate as a sum of very smooth basis functions:

$$u(x) \approx \sum_{k=0}^{N} a_k \phi_k(x),$$

where the $\phi_k(x)$ are for example Chebyshev polynomials or trigonometric functions. We then differentiate these functions exactly. In the context of solving time-dependent PDEs, this approach has notable strengths.

+ For analytic functions, errors typically decay (as N increases) at exponential rather than at (much slower) polynomial rates.
+ The method is virtually free of both dissipative and dispersive errors.

  In the context of solving high–Reynolds number fluid flows, the low physical dissipation will not be overwhelmed by large numerical dissipation. For convection-type problems, sharp gradients in a solution will not turn into wavetrains because of dispersive errors (making different frequency components propagate at different speeds).

+ The approach is surprisingly powerful for many cases in which both solutions and variable coefficients are nonsmooth or even discontinuous.
+ Especially in several space dimensions, the relatively coarse grids that suffice for most accuracy requirements allow very time- and memory-efficient calculations.

However, the following factors can cause difficulties or inefficiencies when using spectral methods:

– certain boundary conditions;
– irregular domains;
– strong shocks;
– variable resolution requirements in different parts of a large domain; and
– partly incomplete theoretical understanding.

In some applications – where these disadvantages are not present or can somehow be overcome – FE, FV, or FD methods do not even come close in efficiency. However, in most areas of application the situation is not so clear-cut. At present, spectral methods are highly successful in several areas: turbulence modeling, weather prediction, nonlinear waves, seismic

modeling, et cetera; the list is growing (see e.g. Boyd 1989 for examples and references).

Spectral representations have been used for analytic studies of differential equations since the days of Fourier (1822). The idea of using them for numerical solutions of ordinary differential equations (ODEs) goes back at least to Lanczos (1938). Some present spectral methods can also be traced back to the "method of weighted residuals" (Finlayson and Scriven 1966). Their current popularity for PDEs dates back to the early 1970s. The major advance at that time was the pseudospectral approach of Kreiss and Oliger (1972), which – like most other spectral methods – benefited greatly from the fast Fourier transform (FFT) algorithm of Cooley and Tukey (1965).

Although PS methods are nowadays often introduced as indicated here (through expansions using smooth global functions, the topic of Chapter 2), there exists a very useful alternative: they can be seen as limiting cases of increasing-order FD methods. The basic idea (in the case of periodic problems) goes back to Kreiss and Oliger (1972), and was developed further by Fornberg (1975, 1987, 1990a,b). The introduction to Chapter 3 lists some of the advantages offered by this FD approach. In the remaining chapters, key properties and variations of PS methods are discussed, using whichever viewpoint is most illuminating. The last chapter briefly discusses some application areas.

2

Introduction to spectral methods via orthogonal functions

Spectral methods are usually described in the way we first indicated – as expansions based on global functions. Given a differential equation with boundary conditions, the idea is to approximate a solution $u(x)$ by a finite sum $v(x) = \sum_{k=0}^{N} a_k \phi_k(x)$; in the case of a time-dependent problem, $u(x,t)$ is approximated by $v(x,t)$ and $a_k(t)$. Two main questions arise: from which function class should $\phi_k(x)$, $k = 0, 1, \ldots$, be chosen; and how should the expansion coefficients a_k be determined. These questions are addressed in Sections 2.1 and 2.2. Section 2.3 introduces cardinal functions and differentiation matrices, important tools both for understanding and for computation. The last section describes Gibbs' phenomenon – the most notable example of how the expansion of a function loses accuracy in the vicinity of an irregularity.

Books that review this approach to spectral methods include Gottlieb and Orszag (1977), Voigt, Gottlieb, and Hussani (1984), Canuto et al. (1988), Boyd (1989), Mercier (1989), and Funaro (1992).

2.1. Function classes

Three requirements need to be met:

(1) the approximations $\sum_{k=0}^{N} a_k \phi_k(x)$ of $v(x)$ must converge rapidly (at least for reasonably smooth functions);

(2) given coefficients a_k, it should be easy to determine b_k such that

$$\frac{d}{dx}\left(\sum_{k=0}^{N} a_k \phi_k(x) \right) = \sum_{k=0}^{N} b_k \phi_k(x), \tag{2.1-1}$$

and

(3) it should be fast to convert between coefficients a_k, $k = 0, \ldots, N$, and the values for the sum $v(x_i)$ at some set of nodes x_i, $i = 0, \ldots, N$.

Periodic problems. The choice here is easy: *trigonometric expansions* satisfy all the three requirements. The first two are immediate; the third became satisfied in 1965 through the FFT algorithm.

Nonperiodic problems. In this case, trigonometric expansions fail to satisfy requirement (1) – an irregularity will arise where the periodicity is artificially imposed. In case of a discontinuity, a Gibbs' phenomenon will occur (see Section 2.4). The coefficients a_k then decrease only like $O(1/N)$ as $N \to \infty$. Truncated *Taylor expansions* $v(x) = \sum_{k=0}^{N} a_k x^k$ will also fail on requirement (1), as convergence over $[-1, 1]$ requires extreme smoothness of $v(x)$ (analyticity throughout the unit circle).

The function class that has proven to be the most successful by far is *orthogonal polynomials* of Jacobi type, with Chebyshev and Legendre polynomials as the most important special cases. These polynomials are discussed in Appendix A. They arise in many contexts, such as the following.

- *Gaussian integration formulas* achieve a high accuracy by using zeros of orthogonal polynomials as nodes (see Section 4.7).
- *Singular Sturm–Liouville eigensystems* are well known to offer excellent bases for approximation. The Jacobi polynomials are the only polynomials that arise in this way.
- Truncated expansions in *Legendre polynomials* are optimal in the L^2 norm.

  For max-norm approximations of smooth functions, truncated *Chebyshev expansions* are particularly accurate.

- Interpolation at the *Chebyshev nodes* $x_k = -\cos(\pi k/N)$, $k = 0, 1, \ldots, N$, gives polynomials P_N^{Ch} that are always within a very small factor of the optimal polynomial in the max-norm approximation of any function $f(x)$:

$$\|f - P_N^{\text{Ch}}\| \le (1 + \Lambda_N^{\text{Ch}}) \|f - P_N^{\text{opt}}\|.$$

  Here, Λ_N^{Ch} is known as the Lebesgue constant of order N for Chebyshev interpolation. It is a particularly useful quantity since it depends only on N and not on the function that is interpolated. The way in which properties of f affect $\|f - P_N^{\text{opt}}\|$ is described by Jackson's theorems (Cheney 1966, Powell 1981). Λ_N^{Ch} is smaller than the corresponding constant for interpolation using Legendre nodes, and far superior to the disastrous one for equi-spaced interpolation:

$$\Lambda_N^{\text{Ch}} = O(\ln N);$$
$$\Lambda_N^{\text{Leg}} = O(\sqrt{N}); \tag{2.1-2}$$
$$\Lambda_N^{\text{eq}} = O\left(\frac{2^N}{N \ln N}\right).$$

These Lebesgue constants are discussed further in Section 3.3 and Appendix D.

The foregoing remarks confirm that Jacobi polynomials satisfy requirement (1) (to be discussed further in Sections 3.4 and 4.1). Because of the first-derivative recursions and the lack of explicit x-dependence therein (cf. bottom line in Table A-1), requirement (2) is met.

Applying the Chebyshev recursion to (2.1-1) and equating coefficients gives

$$\begin{bmatrix} 1 & 0 & -\frac{1}{2} & & & & & \\ & \frac{1}{4} & 0 & -\frac{1}{4} & & & & \\ & & \frac{1}{6} & 0 & -\frac{1}{6} & & & \\ & & & \frac{1}{8} & 0 & -\frac{1}{8} & & \\ & & & & \ddots & \ddots & \ddots & \\ & & & & & \frac{1}{2N-2} & 0 & \\ & & & & & & \frac{1}{2N} & \end{bmatrix} \times \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{N-2} \\ b_{N-1} \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ \vdots \\ a_{N-1} \\ a_N \end{bmatrix}. \tag{2.1-3}$$

Explicit formulas for $\{b_k\}$ in terms of $\{a_k\}$ are sometimes needed; see Appendix B.

Requirement (3) is satisfied for the Chebyshev case if we choose $x_i = -\cos(\pi i/N)$, $i = 0, \ldots, N$. Conversions between coefficients a_k and node values $v(x_i)$ can then be performed with a cosine version of the FFT algorithm (see Appendix F). As we will see in Sections 4.3 and 6.1 and in Figure F.3-1, the additional cost in the other cases need not be prohibitive. For these reasons, Chebyshev (and, to a lesser extent, Legendre) polynomials have become the almost universally preferred choice for nonperiodic spectral approximations.

Formulas similar to (2.1-3) can be found also when the LHS (left-hand side) of (2.1-1) is generalized to expressions involving rational coefficients and derivatives of many orders (Coutsias, Hagstrom, and Torres 1994):

$$\sum_{r=0}^{R} \frac{p_{m_r}(x)}{q_{n_r}(x)} \frac{d^r}{dx^r}\left(\sum_{k=0}^{N} a_k T_k(x)\right). \tag{2.1-4}$$

Here p_{m_r} and q_{n_r} are polynomials of degrees m_r and n_r respectively, and $r = 0, 1, 2, \ldots, R$. The coefficients $\{a_k\}$ and $\{b_k\}$ can be related through the following steps.

- Multiply by the denominators.
- Re-arrange the LHS into derivatives of products of polynomials by Leibniz's rule.
- Re-arrange all polynomials as expansions in Chebyshev polynomials.
- Express products of Chebyshev polynomials as simple Chebyshev polynomials through use of the relation $2T_m(x)T_n(x) = T_{m+n}(x) + T_{m-n}(x)$, $m \geq n$. If $T_m(x)\sum_{k=0}^{n} a_k T_k(x) = \sum_{k=0}^{m+n} b_k T_k(x)$, the matrix form of this becomes:

$$\begin{array}{lll} \text{row} & 1 & \Rightarrow \\ & \vdots & \\ \text{row} & m & \Rightarrow \\ & \vdots & \\ & & \\ & & \\ & \vdots & \\ \text{row} & m+n & \Rightarrow \end{array} \begin{bmatrix} & & 1 & & & & \\ & 1 & & 1 & & & \\ 2 & & & & \ddots & & \\ & 1 & & & & & 1 \\ & & 1 & & & & \\ & & & 1 & & & \\ & & & & \ddots & & \\ & & & & & & 1 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ \\ \vdots \\ a_n \end{bmatrix} = 2 \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ \\ \\ \vdots \\ b_{m+n} \end{bmatrix},$$

  with more diagonals present in cases of more complex multiplying functions.
- Use (repeatedly) (2.1-3).

A few special cases of (2.1-4) are addressed in the appendix of Gottlieb and Orszag (1977). Relations between expansion coefficients such as these are essential for Galerkin and tau approximations, but not for collocation (PS) approximations; see Section 2.2 and Appendix B.

2.2. Techniques for determining expansion coefficients

The three main techniques used to determine the expansion coefficients a_k are the tau, Galerkin, and collocation (PS) methods. In all cases, we consider the residual $R_n(x)$ (or $R_n(x, t)$) when an expansion is substituted into the governing equation. We want to keep the residual as small as possible across the domain while satisfying the boundary conditions.

Tau. Require that a_k be selected so that the boundary conditions are satisfied, and make the residual *orthogonal* to as many of the basis functions as possible.

Galerkin. Combine the original basis functions into a new set in which all the functions satisfy the boundary conditions. Then require that the residual be orthogonal to as many of these new basis functions as possible.

Collocation (PS). This is similar to the tau method: Require that a_k be selected so that the boundary conditions are satisfied, but make the residual *zero* at as many (suitably chosen) spatial points as possible.

Implementation details for a linear, time-independent model problem are given in Appendix B.

For linear problems, the systems of equations that arise from the tau and Galerkin methods can sometimes be solved rapidly thanks to favorable sparsity patterns. However, variable coefficients and nonlinearities are often difficult to handle. The tau method was first used by Lanczos (1938). The Galerkin procedure is central to FE methods; spectral (global) versions of it have been in use since the mid-1950s. The FFT algorithm and contributions by Orszag (1969 and 1970, on ways to deal with nonlinearities) encouraged the use of these methods.

As illustrated by the example in Appendix B, the collocation (PS) method can be viewed as a method of finding numerical approximations to derivatives at gridpoints. Then, in a finite difference–like manner, the governing equations are satisfied pointwise in physical space. The PS method then becomes particularly easy to apply to equations with variable coefficients and nonlinearities, since these give rise only to products of numbers (rather than to problems of determining the expansion coefficients for products of expansions). This is how the collocation approach was originally presented (for PDEs with periodic solutions) by Kreiss and Oliger (1972). It was referred to as the *pseudospectral* method in Orszag (1972).

The rest of this book will focus on the PS method.

2.3. Cardinal functions: example of a differentiation matrix

The concepts of cardinal functions (CFs) and differentiation matrices (DMs) are both theoretically and numerically useful well beyond the realm of methods derived from orthogonal functions. Therefore, we postpone the main discussion of these until Sections 4.3 and 4.4 (when our background is more general) and consider them here only in the case of the Fourier–PS method.

The interpolating trigonometric polynomial to periodic data can be thought of as a weighted sum of CFs, each with the property of having unit value at one of the data points and zero at the rest. This is much like how Lagrange's interpolation formula works, with the main difference that, in the Fourier case, all CFs are simply translates of each other.

Assume for simplicity that we have an odd number $N = 2m+1$ of gridpoints at locations $x_i = i/(m+\frac{1}{2})$, $i = -m, \ldots, -1, 0, 1, \ldots, m$ in $[-1, 1]$. By inspection,

$$\phi_m(x) = \frac{2}{N}\left\{\frac{1}{2} + \cos \pi x + \cos 2\pi x + \cdots + \cos m\pi x\right\}$$
$$= \frac{\sin(N\pi x/2)}{N \sin(\pi x/2)} \qquad (2.3\text{-}1)$$

is a $[-1, 1]$-periodic trigonometric polynomial that satisfies

$$\phi_m(x_i) = \begin{cases} 1 & \text{if } i = 0 \quad [\pm N, \pm 2N, \ldots \text{ if periodically extended}], \\ 0 & \text{otherwise.} \end{cases}$$

Figure 2.3-1 displays the CF $\phi_8(x)$, shows how translates of it add up to give the trigonometric interpolant to a step function, and graphs the Gibbs' phenomenon – a finite "overshoot" beside a discontinuity.

The cardinal function

$$\text{sinc}(x) = \frac{\sin \pi x}{\pi x} = \lim_{m \to \infty} \phi_m\left(\frac{x}{m}\right) \qquad (2.3\text{-}2)$$

is often convenient to use in analysis. Sir E. T. Whittaker (1915) found this CF quite noteworthy: ". . . a function of royal blood . . . whose distinguished properties separates it from its bourgeois brethren". Additional references on CFs can be found e.g. in J. M. Whittaker (1927) and Stenger (1993).

From (2.3-1) follows

$$\left.\frac{d}{dx}\phi_m(x)\right|_{x=x_i} = \begin{cases} 0 & \text{if } i = 0, \\ \dfrac{(-1)^i \pi}{2 \sin(i\pi/N)} & \text{otherwise.} \end{cases} \qquad (2.3\text{-}3)$$

Given a vector of periodic data values $v(x_j)$, $j = -m, \ldots, m$, the interpolating polynomial can be written

$$v(x) = \sum_{j=-m}^{m} v(x_j)\phi_m(x - x_j).$$

The derivative of this function at $x = x_i$ becomes

$$v'(x_i) = \sum_{j=-m}^{m} v(x_j) \left.\frac{d}{dx}\phi_m(x - x_j)\right|_{x=x_i} = \sum_{j=-m}^{m} v(x_j) \left.\frac{d}{dx}\phi_m(x)\right|_{x=x_{i-j}}.$$

Written in matrix form, this becomes

$$\begin{bmatrix} v'(x_{-m}) \\ \vdots \\ \vdots \\ \vdots \\ v'(x_m) \end{bmatrix} = \begin{bmatrix} & & \\ & D & \\ & & \end{bmatrix} \begin{bmatrix} v(x_{-m}) \\ \vdots \\ \vdots \\ \vdots \\ v(x_m) \end{bmatrix},$$

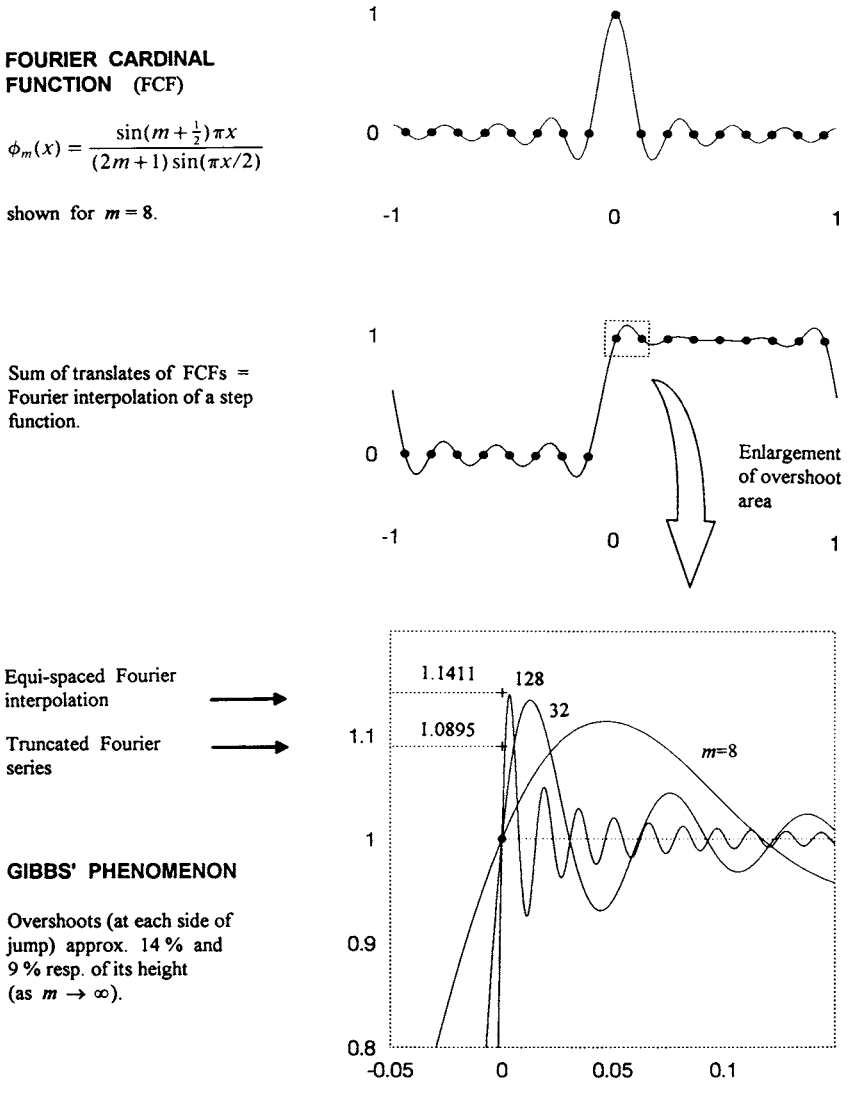

Figure 2.3-1. Fourier cardinal functions and Gibbs' phenomenon.

where the differentiation matrix D has the elements (making use of equation (2.2-3)):

$$D_{i,j} = \frac{d}{dx}\phi_m(x)\Big|_{x=x_{i-j}} = \begin{cases} \dfrac{\pi(-1)^{i-j}}{2\sin(\pi(i-j)/N)} & \text{if } i \neq j, \\ 0 & \text{if } i = j. \end{cases} \tag{2.3-4}$$