

TIME DEPENDENT PROBLEMS AND DIFFERENCE METHODS

SECOND EDITION

BERTIL GUSTAFSSON • HEINZ-OTTO KREISS • JOSEPH OLIGER

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TIME-DEPENDENT
PROBLEMS AND
DIFFERENCE METHODS

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TIME-DEPENDENT PROBLEMS AND DIFFERENCE METHODS

Second Edition

Bertil Gustafsson

Department of Information Technology

Uppsala Universitet

Uppsala, Sweden

Heinz-Otto Kreiss

Department of Mathematics

University of California

Los Angeles, California

Joseph Oliger

WILEY

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PREFACE

In the first edition of this book, it was assumed that the partial differential equations (PDEs) are of the form $\partial u/\partial t = P(\partial/\partial x)$, where P is a differential operator of any order in space. Particular emphasis was given to hyperbolic first-order systems. Wave propagation problems most often come in the form $\partial^2 u/\partial t^2 = P(\partial/\partial x)$, where P is a differential operator of second order. Such differential equations can be rewritten as first-order systems, which is then used for discretization and computation. However, the original second-order form might be more convenient for computation and is often used. When it comes to initial-boundary value problems, it turns out that there are new properties to take into account when analyzing stability for second-order systems. This is discussed in Chapter 10.

A short section on staggered grids in Chapter 5 is also new, as well as an extension of SBP (summation by parts) operators in Section 11.4, including second-order derivatives and SAT (simultaneous approximation term) methods for implementation. There is also a new Appendix D containing the explicit form of a number of SBP operators.

Even if new parts have been included, this second edition is shorter than the original one. The reason is that we have tried to simplify certain parts. For example, in the discussion of difference methods in Chapter 4, we have emphasized explicit one-step methods to avoid the more complicated notation that comes with general multistep methods. We have also left out some of the detailed derivations and proofs in Chapters 5, 6, and 12. Furthermore, the Laplace transform methods for analysis of initial-boundary value problems is now limited to hyperbolic problem, where its strength is more pronounced.

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PREFACE TO THE FIRST EDITION

In this preface, we discuss the material to be covered, the point of view we take, and our emphases. Our primary goal is to discuss material relevant to the derivation and analysis of numerical methods for computing approximate solutions to partial differential equations for time-dependent problems arising in the sciences and engineering. It is our intention that this book should be useful for graduate students interested in applied mathematics and scientific computation as well as physical scientists and engineers whose primary interests are in carrying out numerical experiments to investigate physical behavior and test designs.

We carry out a parallel development of material for differential equations and numerical methods. Our motivation for this approach is twofold: the usual treatment of partial differential equations does not follow the lines that are most useful for the analysis of numerical methods, and the derivation of numerical methods is increasingly utilizing and benefiting from following the detailed development for the differential equations.

Most of our development and analysis is for linear equations, whereas most of the calculations done in practice are for nonlinear problems. However, this is not so fruitless as it may sound. If the nonlinear problem of interest has a smooth solution, then it can be linearized about this solution and the solution of the nonlinear problem will be a solution of the linearized problem with a perturbed forcing function. Errors of numerical approximations for the nonlinear problem can thus be estimated locally, and justified in terms of the linearized equations. A problem often arises in this scenario; the mathematical properties required to guarantee that the solution is smooth a priori may not be known or verifiable. So we often perform calculations whose results we cannot justify a priori. In this situation, we can proceed rationally, if not rigorously, by using a method that we could justify for the corresponding linearized problems and can be justified a posteriori, at least in principle, if the obtained solution satisfies certain smoothness properties. The smoothness properties of our computed solutions can be observed to experimentally verify the needed smoothness requirements and justify our computed results a posteriori. However, this procedure is not without

its limitations. There are many problems that do not have smooth solutions. There are genuinely nonlinear phenomena, such as shocks, rarefaction waves, and nonlinear instability, that we must study in a nonlinear framework, and we discuss such issues separately. There are a few general results for nonlinear problems that generally are justifications of the linearization procedure mentioned above and that we include when available.

The material covered in this book emphasizes our own interests and work. In particular, our development of hyperbolic equations is more complete and detailed than our development of parabolic equations and equations of other types. Similarly, we emphasize the construction and analysis of finite difference methods, although we do discuss Fourier methods. We devote a considerable portion of this book to initial boundary value problems and numerical methods for them. This is the first book to contain much of this material and quite a lot of it has been redone for this presentation. We also tend to emphasize the sufficient results needed to justify methods used in applications rather than necessary results, and to stress error bounds and estimates which are valid for finite values of the discretization parameters rather than statements about limits.

We have organized this book in two parts: Part I discusses problems with periodic solutions and Part II discusses initial-boundary-value problems. It is simpler and more clear to develop the general concepts and to analyze problems and methods for the periodic boundary problems where the boundaries can essentially be ignored and Fourier series or trigonometric interpolants can be used. This same development is often carried out elsewhere for the Cauchy, or pure initial-value, problem. These two treatments are dual to each other, one relying upon Fourier series and the other upon Fourier integrals. We have chosen periodic boundary problems, because we are, in this context, dealing with a finite, computable method without any complications arising from the infinite domains of the corresponding Cauchy problems. Periodic boundary problems do arise naturally in many physical situations such as flows in toroids or on the surface of spheres; for example, the separation of periodic boundary and initial-boundary-value problems is also natural, because the results for initial-boundary-value problems often take the following form: If the problem or method is good for the periodic boundary problem and if some additional conditions are satisfied, then the problem or method is good for a corresponding initial-boundary-value problem. So an analysis and understanding of the corresponding periodic boundary problem is often a necessary condition for results for more general problems.

In Part I, we begin with a discussion in Chapter 1 of Fourier series and trigonometric interpolation, which is central to this part of the book. In Chapter 2, we discuss model equations for convection and diffusion. Throughout the book, we often rely upon a model equation approach to our material. Equations typifying various phenomena, such as convection, diffusion, and dispersion, that distinguish the difficulties inherent in approximating equations of different types are central to our analysis and development. Difference methods are first introduced in this chapter and discussed in terms of the model equations. In Chapter 3, we consider the efficiencies of using higher order accurate methods, which, in

a natural limit, lead to the Fourier or pseudospectral method. The concept of a well-posed problem is introduced in Chapter 4 for general linear and nonlinear problems for partial differential equations. The general stability and convergence theory for difference methods is presented in Chapter 5. Sections are devoted to the tools and techniques needed to establish stability for methods for linear problems with constant coefficients and then for those with variable coefficients. Splitting methods are introduced, and their analysis is carried out. These methods are very useful for problems in several space dimensions and to take advantage of special solution techniques for particular operators. The chapter closes with a discussion of stability for nonlinear problems. Chapters 6 and 7 are devoted to specific results and methods for hyperbolic and parabolic equations, respectively. Nonlinear problems with discontinuous solutions, in particular, hyperbolic conservation laws with shocks and numerical methods for them are discussed in Chapter 8, which concludes Part I of the book and our basic treatment of partial differential equations and methods in the periodic boundary setting.

Part II is devoted to the discussion of the initial boundary value problem for partial differential equations and numerical methods for these problems. Chapter 9 discusses the energy method for initial-boundary-value problem for hyperbolic and parabolic equations. Chapter 10 discusses Laplace transform techniques for these problems. Chapter 11 treats stability for difference approximations using the energy method and follows the treatment of the differential equations in Chapter 9. Chapter 12 follows from Chapter 10 in terms of development—here the Laplace transform is used for difference approximations. This treatment is carried out for the semidiscretized problem: Only the spacial part of the operator is discretized. Finally, the fully discretized problem is treated in Chapter 13 using the Laplace transform. The so-called “normal mode analysis” technique is used and developed in these last two chapters. In particular, sufficient stability conditions for the fully discretized problem are obtained in terms of stability results for the semidiscretized problem, which are much easier to obtain.

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Finally, we acknowledge the Office of Naval Research and the National Aeronautics and Space Administration for their support of our work.

I

PROBLEMS WITH PERIODIC SOLUTIONS

1

MODEL EQUATIONS

In this chapter, we examine several model equations to introduce some basic properties of differential equations and difference approximations by example. Generalizations of these ideas are discussed throughout the remainder of this book.

1.1. PERIODIC GRIDFUNCTIONS AND DIFFERENCE OPERATORS

Let $h = 2\pi/(N + 1)$, where N is a natural number, denote a grid interval. A grid on the x -axis is defined to be the set of gridpoints

$$x_j = jh, \quad j = 0, \pm 1, \pm 2, \dots$$

A discrete, possibly complex valued, function u defined on the grid is called a *gridfunction* (see Figure 1.1.1). Here, we are only interested in 2π -periodic gridfunctions, that is,

$$u_j = u(x_j) = u(x_j + 2\pi) = u_{j+N+1}.$$

Clearly, the product and sum of gridfunctions are again gridfunctions. Their gridvalues are

$$(uv)_j = u_j v_j, \quad (u + v)_j = u_j + v_j.$$

We denote the set of all 2π -periodic gridfunctions by P_h . If $u, v \in P_h$, then $uv, u + v \in P_h$.

We now introduce difference operators. They play a fundamental role throughout the book. We start with the translation operator E . It is defined by

$$(Ev)_j = v_{j+1}.$$

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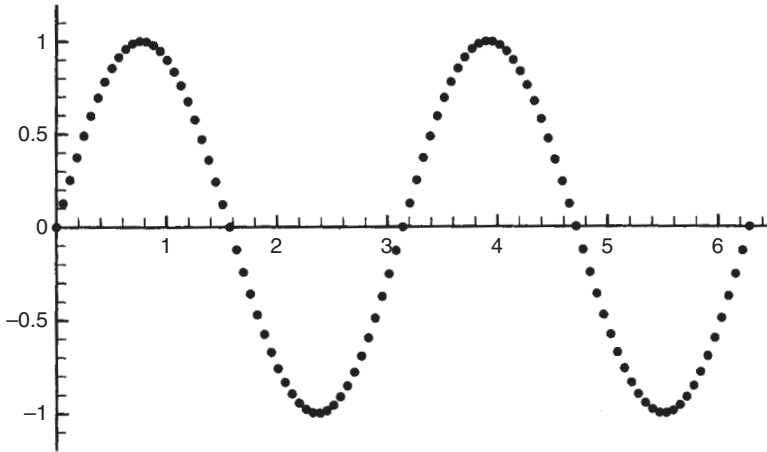


Figure 1.1.1. A gridfunction.

If $v \in P_h$, then $Ev \in P_h$. Powers of E are defined recursively,

$$E^p v = E^{p-1}(Ev).$$

Thus,

$$(E^p v)_j = v_{j+p}. \quad (1.1.1)$$

The inverse also exists and

$$(E^{-1}v)_j = v_{j-1}.$$

If we define E^0 by $E^0 v = v$, then Eq. (1.1.1) holds for all integers p . E is a linear operator and

$$(aE^p + bE^q)v = aE^p v + bE^q v.$$

The forward, backward, and central difference operators are defined by

$$\begin{aligned} D_+ &= (E - E^0)/h, \\ D_- &= (E^0 - E^{-1})/h = E^{-1}D_+, \\ D_0 &= (E - E^{-1})/(2h) = \frac{1}{2}(D_+ + D_-), \end{aligned} \quad (1.1.2)$$

respectively. In particular, consider these operators acting on the functions $e^{i\omega x}$. Then, we have for all $x = x_j$

$$\begin{aligned} hD_+e^{i\omega x} &= (e^{i\omega h} - 1)e^{i\omega x} = (i\omega h + \mathcal{O}(\omega^2 h^2))e^{i\omega x}, \\ hD_-e^{i\omega x} &= (1 - e^{-i\omega h})e^{i\omega x} = (i\omega h + \mathcal{O}(\omega^2 h^2))e^{i\omega x}, \\ hD_0e^{i\omega x} &= i \sin(\omega h)e^{i\omega x} = (i\omega h + \mathcal{O}(\omega^3 h^3))e^{i\omega x}. \end{aligned} \quad (1.1.3)$$

Thus,

$$\begin{aligned} \left| \left(D_+ - \frac{\partial}{\partial x} \right) e^{i\omega x} \right| &= \mathcal{O}(\omega^2 h), \\ \left| \left(D_- - \frac{\partial}{\partial x} \right) e^{i\omega x} \right| &= \mathcal{O}(\omega^2 h), \\ \left| \left(D_0 - \frac{\partial}{\partial x} \right) e^{i\omega x} \right| &= \mathcal{O}(\omega^3 h^2). \end{aligned} \quad (1.1.4)$$

Consequently, one says that D_+ and D_- are first-order accurate approximations of $\partial/\partial x$ because the error is proportional to h . D_0 is second-order accurate.

Higher derivatives are approximated by products of the above operators. For example,

$$(D_+D_-v)_j = (D_-D_+v)_j = h^{-2}((E - 2E^0 + E^{-1})v)_j = h^{-2}(v_{j+1} - 2v_j + v_{j-1}).$$

In particular,

$$\begin{aligned} h^2D_+D_-e^{i\omega x} &= (e^{i\omega h} - 2 + e^{-i\omega h})e^{i\omega x} = -4 \sin^2\left(\frac{\omega h}{2}\right)e^{i\omega x} \\ &= (-\omega^2 h^2 + \mathcal{O}(\omega^4 h^4))e^{i\omega x}. \end{aligned} \quad (1.1.5)$$

Therefore,

$$\left| \left(D_+D_- - \frac{\partial^2}{\partial x^2} \right) e^{i\omega x} \right| = \mathcal{O}(\omega^4 h^2),$$

and D_+D_- is a second-order accurate approximation of $\partial^2/\partial x^2$. Note that all of the above operators commute, because they are all defined in terms of powers of E .

We need to define norms for finite-dimensional vector spaces and discuss some of their properties. We begin with the usual Euclidean inner product and norm. Consider the m -dimensional vector space consisting of all $u = (u^{(1)}, \dots, u^{(m)})^T$

where $u^{(j)}$, $j = 1, \dots, m$, are complex numbers. We denote the conjugate transpose of u by u^* ($u^* = u^T$ if u is real). The inner product and norm are defined by

$$\langle u, v \rangle = u * v = \sum_{j=1}^m \bar{u}^{(j)} v^{(j)}, \quad \text{and} \quad |u| = \langle u, u \rangle^{1/2}, \quad (1.1.6)$$

respectively. The inner product is a bilinear form that satisfies the following equalities:

$$\begin{aligned} \langle u, v \rangle &= \overline{\langle v, u \rangle}, \\ \langle u + w, v \rangle &= \langle u, v \rangle + \langle w, v \rangle, \\ \langle u, \lambda v \rangle &= \lambda \langle u, v \rangle, \quad \lambda \text{ a complex number,} \\ \langle \lambda u, v \rangle &= \bar{\lambda} \langle u, v \rangle. \end{aligned} \quad (1.1.7)$$

The following inequalities hold:

$$\begin{aligned} |\langle u, v \rangle| &\leq |u| |v|, \\ |u + v| &\leq |u| + |v|, \\ \| |u| - |v| \| &\leq |u - v|, \\ \langle u, v \rangle &\leq |u| \cdot |v| \leq \delta |u|^2 + \frac{1}{4\delta} |v|^2 \quad \text{for any } \delta > 0. \end{aligned} \quad (1.1.8)$$

Let $A = (a_{ij})$ be a complex $m \times m$ matrix. Then, its transpose is denoted by $A^T = (a_{ji})$ and its conjugate transpose by $A^* = (\bar{a}_{ji})$. The Euclidean norm of the matrix A is defined by

$$|A| = \max_{|u|=1} |Au|,$$

where the norm on the right-hand side is the vector norm defined above. If A and B are matrices, then

$$\begin{aligned} |Au| &\leq |A| |u|, \\ |A + B| &\leq |A| + |B|, \\ |AB| &\leq |A| |B|. \end{aligned} \quad (1.1.9)$$

If the scalar λ and vector $u \neq 0$ satisfy $Au = \lambda u$, then λ is an eigenvalue of A and u is the corresponding eigenvector. The spectral radius, $\rho(A)$, of a matrix A is defined by

$$\rho(A) = \max_j |\lambda_j|,$$

where the λ_j are the eigenvalues of A . The spectral radius satisfies the inequality

$$\rho(A) \leq |A|. \quad (1.1.10)$$

We next define a scalar product and norm for our periodic gridfunctions of length $N + 1$. For fixed h and $N + 1$, these functions form a vector space. However, we are interested in these functions as $h \rightarrow 0$ and $N(h) + 1 \rightarrow \infty$. The Euclidean inner product and norm defined above would not necessarily be finite in this limit, so we must use a different definition.

We define a discrete scalar product and norm for periodic gridfunctions by

$$(u, v)_h = \sum_{j=0}^N \bar{u}_j v_j h \quad \text{and} \quad \|u\|_h = \sqrt{(u, u)_h}, \quad (1.1.11)$$

respectively.

The scalar product is also a bilinear form and satisfies the same equalities as the Euclidean inner product for vectors in Eq. (1.1.7):

$$\begin{aligned} (u, v)_h &= \overline{(v, u)_h}, \\ (u + w, v)_h &= (u, v)_h + (w, v)_h, \\ (u, \lambda v)_h &= \lambda (u, v)_h, \quad \lambda \text{ a complex number,} \\ (\lambda u, v)_h &= \bar{\lambda} (u, v)_h. \end{aligned} \quad (1.1.12)$$

The following inequalities also hold in analogy with Eq. (1.1.8):

$$\begin{aligned} |(u, v)_h| &\leq \|u\|_h \|v\|_h, \\ |(u, av)_h| &\leq \|a\|_\infty \|u\|_h \|v\|_h, \quad \|a\|_\infty = \max_j |a_j|, \\ \|u + v\|_h &\leq \|u\|_h + \|v\|_h, \\ \left| \|u\|_h - \|v\|_h \right| &\leq \|u - v\|_h. \end{aligned} \quad (1.1.13)$$

For periodic functions $f(x)$, $g(x)$ defined everywhere, the L_2 scalar product and norm are defined by

$$(f, g) = \int_0^{2\pi} \bar{u}(x)v(x) dx, \quad \|f\| = \sqrt{(f, f)}.$$

A function $f(x)$ with finite norm $\|f\|$ is called an L_2 function.

If u, v are the projections of continuous functions onto the grid, then

$$\lim_{h \rightarrow 0} (u, v)_h = (u, v), \quad \lim_{h \rightarrow 0} \|u\|_h^2 = \|u\|^2,$$

converge to the L_2 scalar product and norm. Therefore, the above-mentioned inequalities are also valid for the L_2 scalar product and norm applied to C^1 functions. Because any function $\in L_2$ can be approximated arbitrarily well by a C^1 function, they are valid for all L_2 functions as well.

The norm of an operator is defined in the usual way,

$$\|Q\|_h = \sup_{u \neq 0} \frac{\|Qu\|_h}{\|u\|_h} = \sup_{\|u\|_h=1} \|Qu\|_h.$$

From this definition, it follows that $\|Qu\|_h \leq \|Q\|_h \|u\|_h$. Thus,

$$\|E^p u\|_h^2 = \sum_{j=0}^N |u_{j+p}|^2 h = \sum_{j=0}^N |u_j|^2 h = \|u\|_h^2$$

implies

$$\|E^p\|_h = 1, \quad p = 0, \pm 1, \pm 2, \dots \quad (1.1.14)$$

Also,

$$\|D_+ u\|_h = \frac{1}{h} \|(E - E^0)u\|_h \leq \frac{2}{h} \|u\|_h,$$

that is,

$$\|D_+\|_h \leq 2/h.$$

The general inequalities

$$\|P + Q\|_h \leq \|P\|_h + \|Q\|_h, \quad \|PQ\|_h \leq \|P\|_h \|Q\|_h \quad (1.1.15)$$

give us

$$\|D_-\|_h = \|E^{-1}D_+\|_h \leq \frac{2}{h}, \quad \|D_0\|_h = \frac{1}{2h} \|E - E^{-1}\|_h \leq \frac{1}{h}.$$

Actually, these inequalities for the norms of D_+ , D_- , and D_0 can be replaced by equalities. For D_+ , we define $u_j = (-1)^j$ and obtain

$$\begin{aligned} \|u\|_h^2 &= (N+1)h, \\ \|D_+ u\|_h^2 &= \sum_{j=0}^N ((-1)^{j+1} - (-1)^j)^2 h^{-1} = 4(N+1)h^{-1} = \frac{4}{h^2} \|u\|_h^2, \end{aligned}$$

which yields

$$\|D_+\|_h = 2/h. \quad (1.1.16)$$

Using the same gridfunction u_j again, we get

$$\|D_-\|_h = 2/h. \quad (1.1.17)$$

For D_0 , we choose $u_j = i^j$ (where $i = \sqrt{-1}$) and obtain

$$\begin{aligned} \|u\|_h^2 &= (N + 1)h, \\ \|D_0 u\|_h^2 &= \sum_{j=0}^N \frac{1}{4h} ((-1)^{j+1} - (-i)^{j-1}) (i^{j+1} - i^{j-1}) = \frac{N + 1}{h} = \frac{1}{h^2} \|u\|_h^2, \end{aligned}$$

so

$$\|D_0\|_h = 1/h. \tag{1.1.18}$$

We now consider systems of partial differential equations and consequently need to define a norm and scalar product for vector-valued gridfunctions $u = (u^{(1)}, \dots, u^{(m)})^T$. Let u and v be two such vector-valued gridfunctions, then we define

$$(u, v)_h = \sum_{j=0}^N \langle u_j, v_j \rangle h, \quad \|u\|_h = \sqrt{(u, u)_h}. \tag{1.1.19}$$

The properties shown in Eqs. (1.1.12) and (1.1.13) are still valid. We can also generalize the second inequality in Eq. (1.1.13) when a is replaced by an $(m \times m)$ matrix A . If A is a constant matrix, we have

$$|(Au, v)_h| \leq |A| \|u\|_h \|v\|_h, \tag{1.1.20}$$

If $A = A_j$ is a matrix-valued gridfunction, then

$$|(Au, v)_h| \leq \max_j |A_j| \|u\|_h \|v\|_h. \tag{1.1.21}$$

EXERCISES

1.1.1. Derive estimates for

$$\left| \left(D - \frac{\partial^3}{\partial x^3} \right) e^{i\omega x} \right|,$$

where $D = D_+^3, D_- D_+^2, D_-^2 D_+, D_-^3, D_0 D_+ D_-$.

1.1.2. Both the difference operators D_+ and D_0 approximate $\partial/\partial x$, but they have different norms. Explain why this is not a contradiction.

1.1.3. Compute $\|D_+ D_- \|_h$.

1.2. FIRST-ORDER WAVE EQUATION, CONVERGENCE, AND STABILITY

The equation $u_t = u_x$ is the simplest *hyperbolic* equation; the general definition of the class of hyperbolic equations is given in Section 3.3. We consider the initial value problem

$$\begin{aligned} u_t &= u_x, & -\infty < x < \infty, & t \geq 0, \\ u(x, 0) &= f(x), & -\infty < x < \infty, \end{aligned} \quad (1.2.1)$$

where $f(x) = f(x + 2\pi)$ is a smooth 2π -periodic function. To begin, we assume that the initial function

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{i\omega x} \hat{f}(\omega)$$

consists of one wave. The integer ω is called the *wave number* or the *frequency*. We try to find a solution of the same type

$$u(x, t) = \frac{1}{\sqrt{2\pi}} e^{i\omega x} \hat{u}(\omega, t) \quad (1.2.2)$$

with $\hat{u}(\omega, 0) = \hat{f}(\omega)$. Substituting Eq. (1.2.2) into Eq. (1.2.1) yields an initial value problem for the ordinary differential equation

$$\begin{aligned} \frac{d\hat{u}}{dt} &= i\omega\hat{u}, \\ \hat{u}(\omega, 0) &= \hat{f}(\omega), \end{aligned}$$

which is called the *Fourier transform* of Eq. (1.2.1). Therefore,

$$\hat{u}(\omega, t) = e^{i\omega t} \hat{u}(\omega, 0) = e^{i\omega t} \hat{f}(\omega).$$

It follows that

$$u(x, t) = \frac{1}{\sqrt{2\pi}} e^{i\omega(x+t)} \hat{f}(\omega) = f(x+t) \quad (1.2.3)$$

is a solution to our problem.

Now consider the general case

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{\omega=-\infty}^{\infty} e^{i\omega x} \hat{f}(\omega), \quad (1.2.4)$$

which is the Fourier series representation as described in Section A.1. By the superposition principle,

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \sum_{\omega=-\infty}^{\infty} e^{i\omega(x+t)} \hat{f}(\omega) = f(x+t) \quad (1.2.5)$$

is a solution to our problem. For every fixed t , Parseval's relation (A.1.9) yields

$$\|u(\cdot, t)\|^2 = \sum_{\omega=-\infty}^{\infty} |e^{i\omega t} \hat{f}(\omega)|^2 = \sum_{\omega=-\infty}^{\infty} |\hat{f}(\omega)|^2 = \|f(\cdot)\|^2. \quad (1.2.6)$$

The squared norm $\|u\|^2$ is often called the energy of u . Therefore, the differential equation in Eq. (1.2.1) is said to be energy conserving; the obvious phrase norm conserving is often used in this context as well. Clearly, any method of approximation must be nearly norm conserving to be useful. We also note that there is a *finite speed of propagation* associated with this problem. The expression (1.2.5) shows that the solution is constant along the lines $x+t = \text{const}$, which are called *characteristics* (see Figure 1.2.1).

Any particular feature of the initial data, such as a wave crest, is propagated along these characteristics. In our case, the speed of propagation (or wave speed) is $dx/dt = -1$. For general hyperbolic systems, there may be many families of characteristics corresponding to different wave speeds of different components. The important thing is that these speeds are always finite.

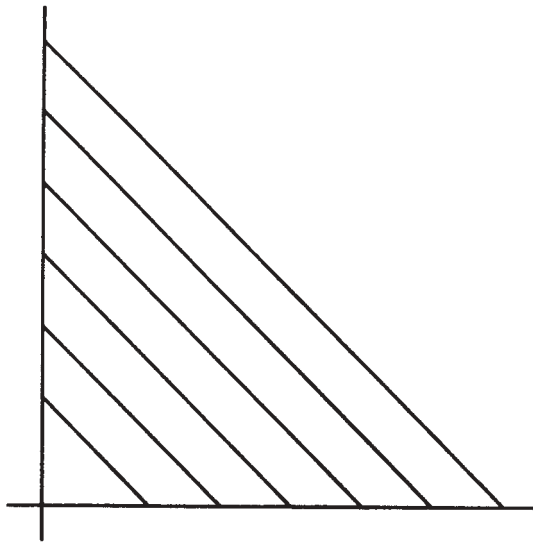


Figure 1.2.1. Characteristics.

We now solve the problem using a difference approximation. We introduce a space step $h = 2\pi/(N + 1)$, with N a natural number, and a time step $k > 0$. The space and time steps h, k define a grid in x, t space, consisting of the gridpoints $(x_j, t_n) := (jh, nk)$. Gridfunctions will be denoted by $u_j^n = u(x_j, t_n)$. A simple approximation based on forward differences in time and centered differences in space is

$$\begin{aligned} v_j^{n+1} &= (I + kD_0)v_j^n =: Qv_j^n, & j = 0, \pm 1, \pm 2, \dots \\ v_j^0 &= f_j. \end{aligned} \quad (1.2.7)$$

If v^n is known at time $t_n = nk$, then we can use Eq. (1.2.7) to calculate v_j^{n+1} for all j . Thus, the initial data determine a unique solution, and we call such a method a *one-step method*. Also, if v^n is 2π -periodic, then v^{n+1} is too. Therefore, we can restrict the calculation to $j = 0, 1, 2, \dots, N$ and use periodicity conditions to extend the solution and provide the extra needed values for Eq. (1.2.7) at $j = 0, N$, that is, $v_{-1}^n = v_N^n$, $v_{N+1}^n = v_0^n$.

We will now calculate the solution analytically. First, consider the case where f consists of one single wave, that is,

$$f_j = \frac{1}{\sqrt{2\pi}} e^{i\omega x_j} \hat{f}(\omega), \quad j = 0, 1, 2, \dots, N.$$

As in the continuous case, we make the ansatz

$$v_j^n = \frac{1}{\sqrt{2\pi}} \hat{v}^n(\omega) e^{i\omega x_j}, \quad (1.2.8)$$

that is, we assume that the solution can also be expressed in terms of one single Fourier component. Substituting Eq. (1.2.8) into Eq. (1.2.7) yields

$$e^{i\omega x_j} \hat{v}^{n+1}(\omega) = \left(e^{i\omega x_j} + \frac{\lambda}{2} (e^{i\omega x_{j+1}} - e^{i\omega x_{j-1}}) \right) \hat{v}^n(\omega),$$

where $\lambda = k/h$. This equation can be rewritten as

$$e^{i\omega x_j} \hat{v}^{n+1}(\omega) = (1 + i\lambda \sin \xi) e^{i\omega x_j} \hat{v}^n(\omega),$$

where $\xi = \omega h$, and we get

$$\hat{v}^{n+1}(\omega) = \hat{Q} \hat{v}^n(\omega), \quad \hat{Q} = 1 + i\lambda \sin \xi. \quad (1.2.9)$$

The complex number \hat{Q} is the *Fourier transform* of $(I + kD_0)$, and Eq. (1.2.9) is the Fourier transform of Eq. (1.2.7). We also call \hat{Q} the *symbol*, or the *amplification factor*. Actually, it is the *discrete* Fourier transform which is further discussed in Appendix A. The solution of Eq. (1.2.9) is

$$\hat{v}^n(\omega) = \hat{Q}^n \hat{v}^0(\omega) = \hat{Q}^n \hat{f}(\omega),$$

and it is clear that

$$v_j^n = \frac{1}{\sqrt{2\pi}} \hat{Q}^n e^{i\omega x_j} \hat{f}(\omega) = \frac{1}{\sqrt{2\pi}} \left(1 + i \frac{k}{h} \sin(\omega h) \right)^n e^{i\omega x_j} \hat{f}(\omega)$$

solves our problem.

Now, we consider a sequence of grid intervals $k, h \rightarrow 0$. We want to show that v_j^n converges to the corresponding solution of the differential equation. We have

$$\begin{aligned} \left(1 + i \frac{k}{h} \sin(\omega h) \right)^n &= (1 + i\omega k + \mathcal{O}(kh^2\omega^3))^n = (e^{i\omega k} + \mathcal{O}(k^2\omega^2 + kh^2\omega^3))^n \\ &= (1 + \mathcal{O}((k\omega^2 + h^2\omega^3)t_n)) e^{i\omega t_n}. \end{aligned}$$

Therefore,

$$v_j^n = \frac{1}{\sqrt{2\pi}} (1 + \mathcal{O}((k\omega^2 + h^2\omega^3)t_n)) e^{i\omega(x_j + t_n)} \hat{f}(\omega).$$

Thus, for every fixed ω , we obtain

$$\lim_{k, h \rightarrow 0} v_j^n = u(x_j, t_n)$$

in any finite interval $0 \leq t \leq T$.

Now assume that the initial data are represented by a trigonometric polynomial

$$u(x, 0) = \frac{1}{\sqrt{2\pi}} \sum_{\omega=-M}^M e^{i\omega x} \hat{f}(\omega).$$

By the superposition principle, the above result implies that the solution of the difference approximation will converge to the solution of the differential equation as $k, h \rightarrow 0$. Thus, one might think that the approximation could be useful in practice. However, consider the problem (1.2.1) with initial data $f(x) \equiv 0$ which has the trivial solution $u(x, t) \equiv 0$. Now consider the problem with perturbed data

$$\hat{f}(\omega) = \begin{cases} \varepsilon, & \text{for } \omega = N/4, \\ 0, & \text{otherwise.} \end{cases}$$

The corresponding solution of the transformed difference approximation is

$$\hat{v}^n(N/4) = \left(1 + i \frac{k}{h} \sin\left(\frac{2\pi}{N+1} \frac{N}{4}\right) \right)^n \varepsilon \sim \left(1 + i \frac{k}{h} \right)^n \varepsilon,$$

that is,

$$|\hat{v}^{t_n/k}(N/4)|^2 \sim \left(1 + \frac{k^2}{h^2}\right)^{t_n/k} \varepsilon^2.$$

For $t_n = 1$, that is, $n = 1/k$

$$|\hat{v}^{1/k}(N/4)|^2 \sim \left(1 + \frac{k^2}{h^2}\right)^{1/k} \varepsilon^2.$$

Now consider any sequence $k, h \rightarrow 0$ with $k/h = \lambda > 0$ fixed. Then,

$$\lim_{k \rightarrow 0} |\hat{v}^{1/k}(N/4)| = \infty.$$

This “explosion,” or growth, can be arbitrarily fast. For example, if we consider $\lambda = 10, k = 10^{-5}$, then

$$|\hat{v}^{1/k}(N/4)|^2 \sim 100^{10^5} \varepsilon^2.$$

The numerical calculation is therefore worthless. In Figure 1.2.2, we have calculated the maximum of the solutions of the difference approximation (1.2.7) with initial data

$$f_j = \begin{cases} x_j, & \text{for } 0 \leq x_j \leq \pi, \\ 2\pi - x_j, & \text{for } \pi \leq x_j \leq 2\pi, \end{cases}$$

and stepsizes $h = 0.01, k = 0.01$ and $h = 0.01, k = 0.1$, respectively.

The analytic results lead us to expect that the solutions will grow like $2^{n/2}$ and $101^{n/2}$, respectively. The numerical results confirm that prediction.

In realistic computations, one must always expect perturbations, either from measurement errors in the data or from rounding errors due to the finite representation of numbers in the computer. Therefore, we must require that $|\hat{Q}^n|$ is bounded independently of h and k , and we call such methods *stable*. (We make the formal definition of this concept later.)

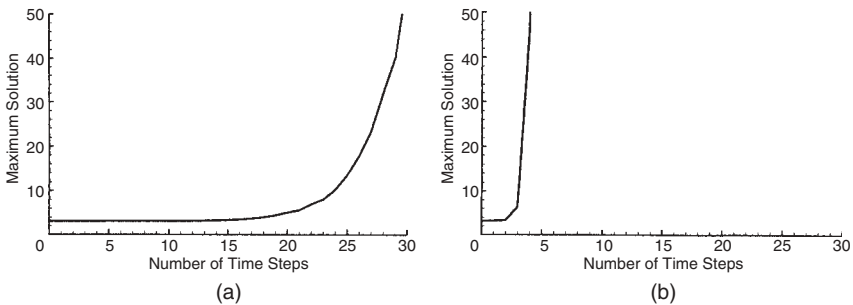


Figure 1.2.2. $\max_j |v_j^n|, v_j^n$ solution of Eq. (1.2.7). (a) $h = 0.01; k = 0.01$ and (b) $h = 0.01; k = 0.1$.