Chapter 4

THE SEMI-DISCRETE APPROACH

One strategy for obtaining finite-difference approximations to a PDE is to start by differencing the space derivatives only, without approximating the time derivative. In the following chapters, we proceed with an analysis making considerable use of this concept, which we refer to as the *semi-discrete* approach. Differencing the space derivatives converts the basic PDE into a set of coupled ODE's. In the most general notation, these ODE's would be expressed in the form

$$\frac{d\vec{u}}{dt} = \vec{F}(\vec{u}, t) \tag{4.1}$$

which includes all manner of nonlinear and time-dependent possibilities. On occasion, we use this form, but the rest of this chapter is devoted to a more specialized matrix notation described below.

Another strategy for constructing a finite-difference approximation to a PDE is to approximate all the partial derivatives at once. This generally leads to a point difference operator (see Section 3.3.1) which, in turn, can be used for the time advance of the solution at any given point in the mesh. As an example let us consider the model equation for diffusion

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}$$

Using three-point central-differencing schemes for both the time and space derivatives, we find

$$\frac{u_j^{(n+1)} - u_j^{(n-1)}}{2h} = \nu \left[\frac{u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)}}{\Delta x^2} \right]$$

or

$$u_j^{(n+1)} = u_j^{(n-1)} + \frac{2h\nu}{\Delta x^2} \left[u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)} \right] \tag{4.2}$$

Clearly Eq. 4.2 is a difference equation which can be used at the space point j to advance the value of u from the previous time levels n and $n-1$ to the level $n+1$. It is a full discretization of the PDE. Note, however, that the spatial and temporal discretizations are separable. Thus, this method has an intermediate semi-discrete form and can be analyzed by the methods discussed in the next few chapters.

Another possibility is to replace the value of $u_j^{(n)}$ in the right hand side of Eq. 4.2 with the time average of u at that point, namely $(u_j^{(n+1)} + u_j^{(n-1)})/2$. This results in the formula

$$u_j^{(n+1)} = u_j^{(n-1)} + \frac{2h\nu}{\Delta x^2}\left[u_{j+1}^{(n)} - 2\left(\frac{u_j^{(n+1)} + u_j^{(n-1)}}{2}\right) + u_{j-1}^{(n)}\right] \tag{4.3}$$

which can be solved for $u^{(n+1)}$ and time advanced at the point j. In this case, the spatial and temporal discretizations are not separable, and no semi-discrete form exists.

Equation 4.2 is sometimes called Richardson's method of overlapping steps and Eq. 4.3 is referred to as the DuFort-Frankel method. As we shall see later on, there are subtle points to be made about using these methods to find a numerical solution to the diffusion equation. There are a number of issues concerning the accuracy, stability, and convergence of Eqs. 4.2 and 4.3 which we cannot comment on until we develop a framework for such investigations. We introduce these methods here only to distinguish between methods in which the temporal and spatial terms are discretized separately and those for which no such separation is possible. For the time being, we shall separate the space difference approximations from the time differencing. In this approach, we reduce the governing PDE's to ODE's by discretizing the spatial terms and use the well-developed theory of ODE solutions to aid us in the development of an analysis of accuracy and stability.

4.1 Reduction of PDE's to ODE's

4.1.1 The Model ODE's

First let us consider the model PDE's for diffusion and biconvection described in Chapter 2. In these simple cases, we can approximate the space derivatives with difference operators and express the resulting ODE's with a matrix formulation. This is a simple and natural formulation when the ODE's are linear.

Model ODE for Diffusion

For example, using the 3-point central-differencing scheme to represent the second derivative in the scalar PDE governing diffusion leads to the following ODE diffusion model

$$\frac{d\vec{u}}{dt} = \frac{\nu}{\Delta x^2} B(1, -2, 1)\vec{u} + (\vec{bc}) \tag{4.4}$$

with Dirichlet boundary conditions folded into the $(\vec{bc})$ vector.

Model ODE for Biconvection

The term biconvection was introduced in Section 2.3. It is used for the scalar convection model when the boundary conditions are periodic. In this case, the 3-point central-differencing approximation produces the ODE model given by

$$\frac{d\vec{u}}{dt} = -\frac{a}{2\Delta x} B_p(-1, 0, 1)\vec{u} \tag{4.5}$$

where the boundary condition vector is absent because the flow is periodic.

Eqs. 4.4 and 4.5 are the model ODE's for diffusion and biconvection of a scalar in one dimension. They are linear with coefficient matrices which are independent of x and t.

4.1.2 The Generic Matrix Form

The generic matrix form of a semi-discrete approximation is expressed by the equation

$$\boxed{\frac{d\vec{u}}{dt} = A\vec{u} - \vec{f}(t)} \tag{4.6}$$

Note that the elements in the matrix A depend upon both the PDE and the type of differencing scheme chosen for the space terms. The vector $\vec{f}(t)$ is usually determined by the boundary conditions and possibly source terms. In general, even the Euler and Navier-Stokes equations can be expressed in the form of Eq. 4.6. In such cases the equations are nonlinear, that is, the elements of A depend on the solution $\vec{u}$ and are usually derived by finding the Jacobian of a flux vector. Although the equations are nonlinear, the linear analysis presented in this book leads to diagnostics that are surprisingly accurate when used to evaluate many aspects of numerical methods as they apply to the Euler and Navier-Stokes equations.

4.2 Exact Solutions of Linear ODE's

In order to advance Eq. 4.1 in time, the system of ODE's must be integrated using a time-marching method. In order to analyze time-marching methods, we will make use of exact solutions of coupled systems of ODE's, which exist under certain conditions. The ODE's represented by Eq. 4.1 are said to be *linear* if F is linearly dependent on u (i.e., if $\partial F/\partial u = A$ where A is independent of u). As we have already pointed out, when the ODE's are linear they can be expressed in a matrix notation as Eq. 4.6 in which the coefficient matrix, A, is independent of u. If A *does* depend explicitly on t, the general solution *cannot* be written; whereas, if A *does not* depend explicitly on t, the general solution to Eq. 4.6 *can* be written. This holds regardless of whether or not the forcing function, $\vec{f}$, depends explicitly on t.

As we shall soon see, the exact solution of Eq. 4.6 can be written in terms of the eigenvalues and eigenvectors of A. This will lead us to a representative scalar equation for use in analyzing time-marching methods. These ideas are developed in the following sections.

4.2.1 Eigensystems of Semi-Discrete Linear Forms

Complete Systems

An $M \times M$ matrix is represented by a *complete eigensystem* if it has a complete set of linearly independent eigenvectors (see Appendix A) . An eigenvector, $\vec{x}_m$, and its corresponding eigenvalue, λ_m, have the property that

$$\begin{aligned} A\vec{x}_m &= \lambda_m \vec{x}_m \qquad \text{or} \\ [\mathrm{A} - \lambda_m \mathrm{I}]\vec{x}_m &= 0 \end{aligned} \tag{4.7}$$

The eigenvalues are the roots of the equation

$$\det[\mathrm{A} - \lambda \mathrm{I}] = 0$$

We form the right-hand eigenvector matrix of a complete system by filling its columns with the eigenvectors $\vec{x}_m$:

$$X = \left[\vec{x}_1\ ,\ \vec{x}_2\ \dots\ ,\vec{x}_M\right]$$

The inverse is the left-hand eigenvector matrix, and together they have the property that

$$X^{-1}AX = \Lambda \tag{4.8}$$

where Λ is a diagonal matrix whose elements are the eigenvalues of A.

Defective Systems

If an $M \times M$ matrix does *not* have a complete set of linearly independent eigenvectors, it cannot be transformed to a diagonal matrix of scalars, and it is said to be defective. It can, however, be transformed to a diagonal set of *blocks*, some of which may be scalars (see Appendix A). In general, there exists some S which transforms any matrix A such that

$$S^{-1}AS = J$$

where

$$J = \begin{bmatrix} J_1 & & & & \\ & J_2 & & & \\ & & \ddots & & \\ & & & J_m & \\ & & & & \ddots \end{bmatrix}$$

and

$$J_m^{(n)} = \begin{array}{c} \begin{bmatrix} \lambda_m & 1 & & \\ & \lambda_m & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_m \end{bmatrix} \end{array} \begin{array}{c} 1 \\ \vdots \\ \vdots \\ n \end{array}$$

The matrix J is said to be in *Jordan canonical form*, and an eigenvalue with multiplicity n within a Jordan block is said to be a defective eigenvalue. Defective systems play a role in numerical stability analysis.

4.2.2 Single ODE's of First- and Second-Order

First-Order Equations

The simplest nonhomogeneous ODE of interest is given by the single, first-order equation

$$\frac{du}{dt} = \lambda u + ae^{\mu t} \tag{4.9}$$

where λ, a, and μ are scalars, all of which can be complex numbers. The equation is linear because λ does not depend on u, and has a general solution because λ does not depend on t. It has a steady-state solution if the right-hand side is independent of t, i.e., if $\mu = 0$, and is homogeneous if the forcing function is zero, i.e., if $a = 0$. Although it is quite simple, the numerical analysis of Eq. 4.9 displays many of the fundamental properties and issues involved in the construction and study of most popular time-marching methods. This theme will be developed as we proceed.

The exact solution of Eq. 4.9 is, for $\mu \neq \lambda$,

$$u(t) = c_1 e^{\lambda t} + \frac{a e^{\mu t}}{\mu - \lambda}$$

where c_1 is a constant determined by the initial conditions. In terms of the initial value of u, it can be written

$$u(t) = u(0)e^{\lambda t} + a\frac{e^{\mu t} - e^{\lambda t}}{\mu - \lambda}$$

The interesting question can arise: What happens to the solution of Eq. 4.9 when $\mu = \lambda$? This is easily found by setting $\mu = \lambda + \epsilon$, solving, and then taking the limit as $\epsilon \to 0$. Using this limiting device, we find that the solution to

$$\frac{du}{dt} = \lambda u + a e^{\lambda t} \tag{4.10}$$

is given by

$$u(t) = [u(0) + at]e^{\lambda t}$$

As we shall soon see, this solution is required for the analysis of defective systems.

Second-Order Equations

The homogeneous form of a second-order equation is given by

$$\frac{d^2 u}{dt^2} + a_1 \frac{du}{dt} + a_0 u = 0 \tag{4.11}$$

where a_1 and a_0 are complex constants. Now we introduce the differential operator D such that

$$\boxed{D \equiv \frac{d}{dt}}$$

and factor $u(t)$ out of Eq. 4.11, giving

$$(D^2 + a_1 D + a_0)\, u(t) = 0$$

The polynomial in D is referred to as a *characteristic polynomial* and designated $P(D)$. Characteristic polynomials are fundamental to the analysis of both ODE's and OΔE's, since the roots of these polynomials determine the solutions of the equations. For ODE's, we often label these roots in order of increasing modulus as λ_1, λ_2, $\cdots$, λ_m,

$\cdots$, λ_M. They are found by solving the equation $P(\lambda) = 0$. In our simple example, there would be two roots, λ_1 and λ_2, determined from

$$P(\lambda) = \lambda^2 + a_1\lambda + a_0 = 0 \tag{4.12}$$

and the solution to Eq. 4.11 is given by

$$u(t) = c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t} \tag{4.13}$$

where c_1 and c_2 are constants determined from initial conditions. The proof of this is simple and is found by substituting Eq. 4.13 into Eq. 4.11. One finds the result

$$c_1 e^{\lambda_1 t}(\lambda_1^2 + a_1\lambda_1 + a_0) + c_2 e^{\lambda_2 t}(\lambda_2^2 + a_1\lambda_2 + a_0)$$

which is identically zero for all c_1, c_2, and t if and only if the λ's satisfy Eq. 4.12.

4.2.3 Coupled First-Order ODE's

A Complete System

A set of coupled, first-order, homogeneous equations is given by

$$\begin{aligned} u_1' &= a_{11}\,u_1 + a_{12}\,u_2 \\ u_2' &= a_{21}\,u_1 + a_{22}\,u_2 \end{aligned} \tag{4.14}$$

which can be written

$$\vec{u}' = A\vec{u} \quad , \quad \vec{u} = [u_1, u_2]^T \quad , \quad A = (a_{ij}) = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

Consider the possibility that a solution is represented by

$$\begin{aligned} u_1 &= c_1\,x_{11}e^{\lambda_1 t} + c_2\,x_{12}e^{\lambda_2 t} \\ u_2 &= c_1\,x_{21}e^{\lambda_1 t} + c_2\,x_{22}e^{\lambda_2 t} \end{aligned} \tag{4.15}$$

By substitution, these are indeed solutions to Eq. 4.14 if and only if

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\begin{bmatrix} x_{11} \\ x_{21} \end{bmatrix} = \lambda_1 \begin{bmatrix} x_{11} \\ x_{21} \end{bmatrix} \quad , \quad \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\begin{bmatrix} x_{12} \\ x_{22} \end{bmatrix} = \lambda_2 \begin{bmatrix} x_{12} \\ x_{22} \end{bmatrix} \tag{4.16}$$

Notice that a higher-order equation can be reduced to a coupled set of first-order equations by introducing a new set of dependent variables. Thus, by setting

$$u_1 = u' \quad , \quad u_2 = u \quad ,$$

we find Eq. 4.11 can be written

$$\begin{aligned} u_1' &= -a_1 u_1 - a_0 u_2 \\ u_2' &= u_1 \end{aligned} \tag{4.17}$$

which is a subset of Eq. 4.14.

A Derogatory System

Eq. 4.15 is still a solution to Eq. 4.14 if $\lambda_1 = \lambda_2 = \lambda$, provided two linearly independent vectors exist to satisfy Eq. 4.16 with $A = \Lambda$. In this case

$$\begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \lambda \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \text{and} \qquad \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \lambda \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

provide such a solution. This is the case where A has a complete set of eigenvectors and is not defective.

A Defective System

If A is defective, then it can be represented by the *Jordan canonical form*

$$\begin{bmatrix} u_1' \\ u_2' \end{bmatrix} = \begin{bmatrix} \lambda & 0 \\ 1 & \lambda \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \tag{4.18}$$

whose solution is not obvious. However, in this case, one can solve the top equation first, giving $u_1(t) = u_1(0)e^{\lambda t}$. Then, substituting this result into the second equation, one finds

$$\frac{du_2}{dt} = \lambda u_2 + u_1(0)e^{\lambda t}$$

which is identical in form to Eq. 4.10 and has the solution

$$u_2(t) = [u_2(0) + u_1(0)t]e^{\lambda t}$$

From this the reader should be able to verify that

$$u_3(t) = \left(a + bt + ct^2\right)e^{\lambda t}$$

is a solution to

$$\begin{bmatrix} u_1' \\ u_2' \\ u_3' \end{bmatrix} = \begin{bmatrix} \lambda & & \\ 1 & \lambda & \\ & 1 & \lambda \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

if

$$a = u_3(0) \quad , \quad b = u_2(0) \quad , \quad c = \frac{1}{2}u_1(0) \tag{4.19}$$

The general solution to such defective systems is left as an exercise.

4.2.4 General Solution of Coupled ODE's with Complete Eigensystems

Let us consider a set of coupled, nonhomogeneous, linear, first-order ODE's with constant coefficients which might have been derived by space differencing a set of PDE's. Represent them by the equation

$$\frac{d\vec{u}}{dt} = A\vec{u} - \vec{f}(t) \tag{4.20}$$

Our assumption is that the $M \times M$ matrix A has a complete eigensystem[1] and can be transformed by the left and right eigenvector matrices, X^{-1} and X, to a diagonal matrix Λ having diagonal elements which are the eigenvalues of A, see Section 4.2.1. Now let us multiply Eq. 4.20 from the left by X^{-1} and insert the identity combination $XX^{-1} = I$ between A and $\vec{u}$. There results

$$X^{-1}\frac{d\vec{u}}{dt} = X^{-1}AX \cdot X^{-1}\vec{u} - X^{-1}\vec{f}(t) \tag{4.21}$$

Since A is independent of both $\vec{u}$ and t, the elements in X^{-1} and X are also independent of both $\vec{u}$ and t, and Eq. 4.21 can be modified to

$$\frac{d}{dt}X^{-1}\vec{u} = \Lambda X^{-1}\vec{u} - X^{-1}\vec{f}(t)$$

Finally, by introducing the new variables $\vec{w}$ and $\vec{g}$ such that

$$\vec{w} = X^{-1}\vec{u} \quad , \quad \vec{g}(t) = X^{-1}\vec{f}(t) \tag{4.22}$$

we reduce Eq. 4.20 to a new algebraic form

$$\frac{d\vec{w}}{dt} = \Lambda\vec{w} - \vec{g}(t) \tag{4.23}$$

It is important at this point to review the results of the previous paragraph. Notice that Eqs. 4.20 and 4.23 are expressing exactly the same equality. The only difference between them was brought about by algebraic manipulations which regrouped the variables. However, this regrouping is crucial for the solution process because Eqs.

[1]In the following, we exclude defective systems, not because they cannot be analyzed (the example at the conclusion of the previous section proves otherwise), but because they are only of limited interest in the general development of our theory.

4.23 are no longer coupled. They can be written line by line as a set of independent, single, first-order equations, thus

$$\begin{aligned}
w_1' &= \lambda_1 w_1 - g_1(t) \\
&\vdots \\
w_m' &= \lambda_m w_m - g_m(t) \\
&\vdots \\
w_M' &= \lambda_M w_M - g_M(t)
\end{aligned} \tag{4.24}$$

For any given set of $g_m(t)$ each of these equations can be solved separately and then recoupled, using the inverse of the relations given in Eqs. 4.22:

$$\begin{aligned}
\vec{u}(t) &= X\vec{w}(t) \\
&= \sum_{m=1}^{M} w_m(t)\vec{x}_m
\end{aligned} \tag{4.25}$$

where $\vec{x}_m$ is the m'th column of X, i.e., the eigenvector corresponding to λ_m.

We next focus on the very important subset of Eq. 4.20 when neither A nor $\vec{f}$ has any explicit dependence on t. In such a case, the g_m in Eqs. 4.23 and 4.24 are also time invariant and the solution to any line in Eq. 4.24 is

$$w_m(t) = c_m e^{\lambda_m t} + \frac{1}{\lambda_m} g_m$$

where the c_m are constants that depend on the initial conditions. Transforming back to the u-system gives

$$\begin{aligned}
\vec{u}(t) &= X\vec{w}(t) \\
&= \sum_{m=1}^{M} w_m(t)\vec{x}_m \\
&= \sum_{m=1}^{M} c_m e^{\lambda_m t}\,\vec{x}_m + \sum_{m=1}^{M} \frac{1}{\lambda_m} g_m \vec{x}_m \\
&= \sum_{m=1}^{M} c_m e^{\lambda_m t}\,\vec{x}_m + X\Lambda^{-1}X^{-1}\vec{f} \\
&= \underbrace{\sum_{m=1}^{M} c_m e^{\lambda_m t}\,\vec{x}_m}_{\text{Transient}} + \underbrace{A^{-1}\vec{f}}_{\text{Steady-state}}
\end{aligned} \tag{4.26}$$

Note that the steady-state solution is $A^{-1}\vec{f}$, as might be expected.

The first group of terms on the right side of this equation is referred to classically as the *complementary solution* or the solution of the homogeneous equations. The second group is referred to classically as the *particular solution* or the particular integral. In our application to fluid dynamics, it is more instructive to refer to these groups as the *transient* and *steady-state* solutions, respectively. An alternative, but entirely equivalent, form of the solution is

$$\vec{u}(t) = c_1 e^{\lambda_1 t}\,\vec{x}_1 + \cdots + c_m e^{\lambda_m t}\,\vec{x}_m + \cdots + c_M e^{\lambda_M t}\,\vec{x}_M \;+\; A^{-1}\vec{f} \tag{4.27}$$

4.3 Real Space and Eigenspace

4.3.1 Definition

Following the semi-discrete approach discussed in Section 4.1, we reduce the partial differential equations to a set of ordinary differential equations represented by the generic form

$$\frac{d\vec{u}}{dt} = A\vec{u} - \vec{f} \tag{4.28}$$

The dependent variable $\vec{u}$ represents some physical quantity or quantities which relate to the problem of interest. For the model problems on which we are focusing most of our attention, the elements of A are independent of both u and t. This permits us to say a great deal about such problems and serves as the basis for this section. In particular, we can develop some very important and fundamental concepts that underly the *global* properties of the numerical solutions to the model problems. How these relate to the numerical solutions of more practical problems depends upon the problem and, to a much greater extent, on the cleverness of the relator.

We begin by developing the concept of “spaces”. That is, we identify different mathematical reference frames (spaces) and view our solutions from within each. In this way, we get different perspectives of the same solution, and this can add significantly to our understanding.

The most natural reference frame is the physical one. We say

> If a solution is expressed in terms of $\vec{u}$, it is said to be in *real space*.

There is, however, another very useful frame. We saw in Sections 4.2.1 and 4.2 that pre- and post-multiplication of A by the appropriate similarity matrices transforms A into a diagonal matrix, composed, in the most general case, of Jordan blocks or, in the simplest nondefective case, of scalars. Following Section 4.2 and, for simplicity, using only complete systems for our examples, we found that Eq. 4.28 had the alternative form

$$\frac{d\vec{w}}{dt} = \Lambda\vec{w} - \vec{g}$$

which is an uncoupled set of first-order ODE's that can be solved independently for the dependent variable vector $\vec{w}$. We say

If a solution is expressed in terms of $\vec{w}$, it is said to be in *eigenspace* (often referred to as wave space).

The relations that transfer from one space to the other are:

$$\begin{array}{|lclclcl|} \vec{w} & = & X^{-1}\vec{u} & \qquad & \vec{u} & = & X\vec{w} \\ \vec{g} & = & X^{-1}\vec{f} & \qquad & \vec{f} & = & X\vec{g} \end{array}$$

The elements of $\vec{u}$ relate directly to the local physics of the problem. However, the elements of $\vec{w}$ are linear combinations of all of the elements of $\vec{u}$, and individually they have no direct local physical interpretation.

When the forcing function $\vec{f}$ is independent of t, the solutions in the two spaces are represented by

$$\vec{u}(t) = \sum c_m e^{\lambda_m t}\,\vec{x}_m + X\Lambda^{-1}X^{-1}\vec{f}$$

and

$$w_m(t) = c_m e^{\lambda_m t} + \frac{1}{\lambda_m} g_m \quad ; \quad m = 1, 2, \cdots, M$$

for real space and eigenspace, respectively. At this point we make two observations:

1. the transient portion of the solution in real space consists of a linear combination of contributions from each eigenvector, and

2. the transient portion of the solution in eigenspace provides the weighting of each eigenvector component of the transient solution in real space.

4.3.2 Eigenvalue Spectrums for Model ODE's

It is instructive to consider the eigenvalue spectrums of the ODE's formulated by central differencing the model equations for diffusion and biconvection. These model ODE's are presented in Section 4.1. Equations for the eigenvalues of the simple tridiagonals, $B(M : a, b, c)$ and $B_p(M : a, b, c)$, are given in Appendix B. From Section B.1, we find for the model diffusion equation with Dirichlet boundary conditions

$$\begin{aligned}\lambda_m &= \frac{\nu}{\Delta x^2}\left[-2 + 2\cos\left(\frac{m\pi}{M+1}\right)\right] \\ &= \frac{-4\nu}{\Delta x^2}\sin^2\left(\frac{m\pi}{2(M+1)}\right) \quad ; \quad m = 1, 2, \cdots, M \end{aligned} \tag{4.29}$$

and, from Section B.4, for the model biconvection equation

$$\begin{aligned}\lambda_m &= \frac{-ia}{\Delta x}\sin\left(\frac{2m\pi}{M}\right) \qquad m = 0, 1, \cdots, M-1 \\ &= -i\kappa_m^* a \qquad m = 0, 1, \cdots, M-1 \end{aligned} \tag{4.30}$$

where

$$\kappa_m^* = \frac{\sin \kappa_m \Delta x}{\Delta x} \qquad m = 0, 1, \cdots, M-1 \tag{4.31}$$

is the modified wavenumber from Section 3.5, $\kappa_m = m$, and $\Delta x = 2\pi/M$. Notice that the diffusion eigenvalues are real and negative while those representing periodic convection are all pure imaginary. The interpretation of this result plays a very important role later in our stability analysis.

4.3.3 Eigenvectors of the Model Equations

Next we consider the eigenvectors of the two model equations. These follow as special cases from the results given in Appendix B.

The Diffusion Model

Consider Eq. 4.4, the model ODE's for diffusion. First, to help visualize the matrix structure, we present results for a simple 4-point mesh and then we give the general case. The right-hand eigenvector matrix X is given by

$$\begin{bmatrix} \sin(x_1) & \sin(2x_1) & \sin(3x_1) & \sin(4x_1) \\ \sin(x_2) & \sin(2x_2) & \sin(3x_2) & \sin(4x_2) \\ \sin(x_3) & \sin(2x_3) & \sin(3x_3) & \sin(4x_3) \\ \sin(x_4) & \sin(2x_4) & \sin(3x_4) & \sin(4x_4) \end{bmatrix}$$

The columns of the matrix are proportional to the eigenvectors. Recall that $x_j = j\Delta x = j\pi/(M+1)$, so in general the relation $\vec{u} = X\vec{w}$ can be written as

$$u_j = \sum_{m=1}^{M} w_m \sin m x_j \quad ; \quad j = 1, 2, \cdots, M \tag{4.32}$$

For the inverse, or left-hand eigenvector matrix X^{-1}, we find

$$\begin{bmatrix} \sin(x_1) & \sin(x_2) & \sin(x_3) & \sin(x_4) \\ \sin(2x_1) & \sin(2x_2) & \sin(2x_3) & \sin(2x_4) \\ \sin(3x_1) & \sin(3x_2) & \sin(3x_3) & \sin(3x_4) \\ \sin(4x_1) & \sin(4x_2) & \sin(4x_3) & \sin(4x_4) \end{bmatrix}$$

The rows of the matrix are proportional to the eigenvectors. In general $\vec{w} = X^{-1}\vec{u}$ gives

$$w_m = \sum_{j=1}^{M} u_j \sin m x_j \quad ; \quad m = 1, 2, \cdots, M \tag{4.33}$$

In the field of harmonic analysis, Eq. 4.33 represents a sine transform of the function $u(x)$ for an M-point sample between the boundaries $x = 0$ and $x = \pi$ with the condition $u(0) = u(\pi) = 0$. Similarly, Eq. 4.32 represents the sine synthesis that companions the sine transform given by Eq. 4.33. In summary,

For the model diffusion equation:

$\vec{w} = X^{-1}\vec{u}$ is a sine transform from real space to (sine) wave space.

$\vec{u} = X\vec{w}$ is a sine synthesis from wave space back to real space.

The Biconvection Model

Next consider the model ODE's for periodic convection, Eq. 4.5. The coefficient matrices for these ODE's are always circulant. For our model ODE, the right-hand eigenvectors are given by

$$\vec{x}_m = e^{i\,j\,(2\pi m/M)}, \quad \begin{array}{ll} j & = 0, 1, \cdots, M-1 \\ m & = 0, 1, \cdots, M-1 \end{array}$$

With $x_j = j \cdot \Delta x = j \cdot 2\pi/M$, we can write $\vec{u} = X\vec{w}$ as

$$u_j = \sum_{m=0}^{M-1} w_m e^{i m x_j} \quad ; \quad j = 0, 1, \cdots, M-1 \tag{4.34}$$

For a 4-point periodic mesh, we find the following left-hand eigenvector matrix from Appendix B.4:

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & e^{-2i\pi/4} & e^{-4i\pi/4} & e^{-6i\pi/4} \\ 1 & e^{-4i\pi/4} & e^{-8i\pi/4} & e^{-12i\pi/4} \\ 1 & e^{-6i\pi/4} & e^{-12i\pi/4} & e^{-18i\pi/4} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = X^{-1}\vec{u}$$

In general

$$w_m = \frac{1}{M} \sum_{j=0}^{M-1} u_j e^{-imx_j} \quad ; \quad m = 0, 1, \cdots, M-1$$

This equation is identical to a discrete Fourier transform of the periodic dependent variable $\vec{u}$ using an M-point sample between and including $x = 0$ and $x = 2\pi - \Delta x$.

For circulant matrices, it is straightforward to establish the fact that the relation $\vec{u} = X\vec{w}$ represents the Fourier synthesis of the variable $\vec{w}$ back to $\vec{u}$. In summary,

For any circulant system:

$\vec{w} = X^{-1}\vec{u}$ is a complex Fourier transform from real space to wave space.

$\vec{u} = X\vec{w}$ is a complex Fourier synthesis from wave space back to real space.

4.3.4 Solutions of the Model ODE's

We can now combine the results of the previous sections to write the solutions of our model ODE's.

The Diffusion Equation

For the diffusion equation, Eq. 4.27 becomes

$$u_j(t) = \sum_{m=1}^{M} c_m e^{\lambda_m t} \sin m x_j + (A^{-1}f)_j, \qquad j = 1, 2, \cdots, M \tag{4.35}$$

where

$$\lambda_m = \frac{-4\nu}{\Delta x^2} \sin^2\left(\frac{m\pi}{2(M+1)}\right) \tag{4.36}$$

With the modified wavenumber defined as

$$\kappa_m^* = \frac{2}{\Delta x}\sin\left(\frac{\kappa_m \Delta x}{2}\right) \tag{4.37}$$

and using $\kappa_m = m$, we can write the ODE solution as

$$u_j(t) = \sum_{m=1}^{M} c_m e^{-\nu {\kappa_m^*}^2 t}\sin\kappa_m x_j + (A^{-1}f)_j, \qquad j = 1, 2, \cdots, M \tag{4.38}$$

This can be compared with the exact solution to the PDE, Eq. 2.37, evaluated at the nodes of the grid:

$$u_j(t) = \sum_{m=1}^{M} c_m e^{-\nu {\kappa_m}^2 t}\sin\kappa_m x_j + h(x_j), \qquad j = 1, 2, \cdots, M \tag{4.39}$$

We see that the solutions are identical except for the steady solution and the modified wavenumber in the transient term. The modified wavenumber is an approximation to the actual wavenumber. The difference between the modified wavenumber and the actual wavenumber depends on the differencing scheme and the grid resolution. This difference causes the various modes (or eigenvector components) to decay at rates which differ from the exact solution. With conventional differencing schemes, low wavenumber modes are accurately represented, while high wavenumber modes (if they have significant amplitudes) can have large errors.

The Convection Equation

For the biconvection equation, we obtain

$$u_j(t) = \sum_{m=0}^{M-1} c_m e^{\lambda_m t} e^{i\kappa_m x_j}, \qquad j = 0, 1, \cdots, M-1 \tag{4.40}$$

where

$$\lambda_m \quad = \quad -i\kappa_m^* a \tag{4.41}$$

with the modified wavenumber defined in Eq. 4.31. We can write this ODE solution as

$$u_j(t) = \sum_{m=0}^{M-1} c_m e^{-i\kappa_m^* a t} e^{i\kappa_m x_j}, \qquad j = 0, 1, \cdots, M-1 \tag{4.42}$$

and compare it to the exact solution of the PDE, Eq. 2.26, evaluated at the nodes of the grid:

$$u_j(t) = \sum_{m=0}^{M-1} f_m(0) e^{-i\kappa_m a t} e^{i\kappa_m x_j}, \qquad j = 0, 1, \cdots, M-1 \tag{4.43}$$

Once again the difference appears through the modified wavenumber contained in λ_m. As discussed in Section 3.5, this leads to an error in the speed with which various modes are convected, since κ^* is real. Since the error in the phase speed depends on the wavenumber, while the actual phase speed is independent of the wavenumber, the result is erroneous numerical dispersion. In the case of non-centered differencing, discussed in Chapter 11, the modified wavenumber is complex. The form of Eq. 4.42 shows that the imaginary portion of the modified wavenumber produces nonphysical decay or growth in the numerical solution.

4.4 The Representative Equation

In Section 4.3, we pointed out that Eqs. 4.20 and 4.23 express identical results but in terms of different groupings of the dependent variables, which are related by algebraic manipulation. This leads to the following important concept:

> The numerical solution to a set of linear ODE's (in which A is *not* a function of t) is entirely equivalent to the solution obtained if the equations are transformed to eigenspace, solved there in their uncoupled form, and then returned as a coupled set to real space.

The importance of this concept resides in its message that we can analyze time-marching methods by applying them to a single, uncoupled equation and our conclusions will apply in general. This is helpful both in analyzing the accuracy of time-marching methods and in studying their stability, topics which are covered in Chapters 6 and 7.

Our next objective is to find a "typical" single ODE to analyze. We found the uncoupled solution to a set of ODE's in Section 4.2. A typical member of the family is

$$\frac{dw_m}{dt} = \lambda_m w_m - g_m(t) \tag{4.44}$$

The goal in our analysis is to study typical behavior of general situations, not particular problems. For such a purpose Eq. 4.44 is not quite satisfactory. The role of λ_m is clear; it stands for some representative eigenvalue in the original A matrix. However, the question is: What should we use for $g_m(t)$ when the time dependence cannot be ignored? To answer this question, we note that, in principle, one can express any one of the forcing terms $g_m(t)$ as a finite Fourier series. For example

$$-g(t) = \sum_k a_k e^{ikt}$$

for which Eq. 4.44 has the exact solution:

$$w(t) = ce^{\lambda t} + \sum_k \frac{a_k e^{ikt}}{ik - \lambda}$$

From this we can extract the k'th term and replace ik with μ. This leads to

$$\boxed{\begin{array}{c}\text{The Representative ODE}\\[1em] \dfrac{dw}{dt} = \lambda w + ae^{\mu t}\end{array}} \tag{4.45}$$

which can be used to evaluate all manner of time-marching methods. In such evaluations the parameters λ and μ must be allowed to take the worst possible combination of values that might occur in the ODE eigensystem. The exact solution of the representative ODE is (for $\mu \neq \lambda$):

$$w(t) = ce^{\lambda t} + \frac{ae^{\mu t}}{\mu - \lambda} \tag{4.46}$$

4.5 Problems

1. Consider the finite-difference operator derived in question 1 of Chapter 3. Using this operator to approximate the spatial derivative in the linear convection equation, write the semi-discrete form obtained with periodic boundary conditions on a 5-point grid ($M = 5$).

2. Consider the application of the operator given in Eq. 3.52 to the 1-D diffusion equation with Dirichlet boundary conditions. Write the resulting semi-discrete ODE form. Find the entries in the boundary-condition vector.

3. Write the semi-discrete form resulting from the application of second-order centered differences to the following equation on the domain $0 \leq x \leq 1$ with boundary conditions $u(0) = 0$, $u(1) = 1$:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - 6x$$

4. Consider a grid with 10 interior points spanning the domain $0 \leq x \leq \pi$. For initial conditions $u(x,0) = \sin(mx)$ and boundary conditions $u(0,t) = u(\pi,t) = 0$, plot the exact solution of the diffusion equation with $\nu = 1$ at $t = 1$ with $m = 1$ and $m = 3$. (Plot the solution at the grid nodes only.) Calculate the corresponding modified wavenumbers for the second-order centered operator from Eq. 4.37. Calculate and plot the corresponding ODE solutions.

5. Consider the matrix

$$A = -B_p(10, -1, 0, 1)/(2\Delta x)$$

corresponding to the ODE form of the biconvection equation resulting from the application of second-order central differencing on a 10-point grid. Note that the domain is $0 \leq x \leq 2\pi$ and $\Delta x = 2\pi/10$. The grid nodes are given by $x_j = j\Delta x,\ \ j = 0, 1, \ldots 9$. The eigenvalues of the above matrix A, as well as the matrices X and X^{-1}, can be found from Appendix B.4. Using these, compute and plot the ODE solution at $t = 2\pi$ for the initial condition $u(x,0) = \sin x$. Compare with the exact solution of the PDE. Calculate the numerical phase speed from the modified wavenumber corresponding to this initial condition and show that it is consistent with the ODE solution. Repeat for the initial condition $u(x,0) = \sin 2x$.