

8

Parabolic Partial-Differential Equations

8.0 CONTENTS OF THIS CHAPTER

The previous chapter discussed the solution of partial-differential equations that were time-independent. Such steady-state problems were described by elliptic equations. Unsteady-state problems in which the function is dependent on time are of great importance. We study these in this chapter.

The method of finite-difference equations will be further developed in this and the following chapter, since it is very important in solving parabolic and hyperbolic partial-differential equations. In the realm of available software, one can use PDECOL, distributed by IMSL, for solving a system of parabolic or hyperbolic partial-differential equations as well as boundary-value problems. Finite-element programs can also solve these.

The problem of unsteady-state flow of heat is a physical situation that can be represented by a parabolic partial-differential equation. The simplest situation is for flow of heat in one direction. Imagine a rod that is uniform in cross section and insulated around its perimeter so that heat flows only longitudinally. Consider a differential portion of the rod, dx in length with cross-sectional area A (see Fig. 8.1).

We let u represent the temperature at any point in the rod, whose distance from the left end is x . Heat is flowing from left to right under the influence of the temperature gradient $\partial u / \partial x$. Make a balance of the rate of heat flow into and

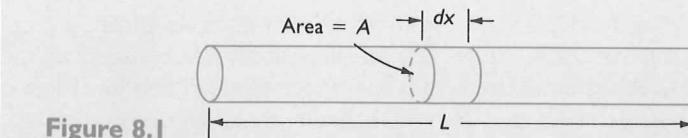


Figure 8.1

out of the element. Use k for thermal conductivity, $\text{cal/g} \cdot \text{cm}^2 \cdot {}^\circ\text{C}/\text{cm}$, which we assume is constant.

$$\text{Rate of flow of heat in: } -kA \frac{\partial u}{\partial x};$$

$$\text{Rate of flow of heat out: } -kA \left(\frac{\partial u}{\partial x} + \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) dx \right).$$

The difference between the rate of flow in and the rate of flow out is the rate at which heat is being stored in the element. If c is the heat capacity, $\text{cal/g} \cdot {}^\circ\text{C}$, and ρ is the density, g/cm^3 , we have, with t for time,

$$-kA \frac{\partial u}{\partial x} - \left(-kA \left(\frac{\partial u}{\partial x} + \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) dx \right) \right) = c\rho(A dx) \frac{\partial u}{\partial t}.$$

Simplifying, we have

$$k \frac{\partial^2 u}{\partial x^2} = c\rho \frac{\partial u}{\partial t}.$$

This is the basic mathematical model for unsteady-state flow. We have derived it for heat flow, but it applies equally to diffusion of material, flow of fluids (under conditions of laminar flow), flow of electricity in cables (the telegraph equations), and so on.

The differential equation is classed as parabolic because comparing to the standard form of an equation in two independent variables, x and t ,

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial t} + C \frac{\partial^2 u}{\partial t^2} + D \left(x, t, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t} \right) = 0,$$

we find that $B^2 - 4AC = 0$.

In two or three space dimensions, analogous equations apply:

$$k \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = c\rho \frac{\partial u}{\partial t},$$

$$k \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) = c\rho \frac{\partial u}{\partial t}.$$

The function that we call the solution to the problem not only must obey the differential equation given above, but also must satisfy an initial condition and a set of boundary conditions. For the one-dimensional heat-flow problem that we first consider, the initial condition will be the initial temperatures at all points along the rod,

$$u(x, t)|_{t=0} = u(x, 0) = f(x).$$

The boundary conditions will describe the temperature at each end of the rod as functions of time. Our first examples will consider the case where these temperatures are held constant:

$$u(0, t) = c_1,$$

$$u(L, t) = c_2.$$

More general (and more practical) boundary conditions will involve not only the temperature but the temperature gradients, and these may vary with time:

$$A_1 u(0, t) + B_1 \frac{\partial u(0, t)}{\partial x} = F_1(t),$$

$$A_2 u(L, t) + B_2 \frac{\partial u(L, t)}{\partial x} = F_2(t).$$

In Chapter 8, you will study the application of finite differences to solve parabolic partial-differential equations. We begin with problems of one space dimension.

8.1 THE EXPLICIT METHOD

Divides space and time into discrete uniform subintervals and replaces both time and space derivatives by finite-difference approximations, permitting one to easily compute values of the function at a time Δt after the initial time. These values are then used to compute a second set of values and the process is repeated.

8.2 CRANK-NICOLSON METHOD

Overcomes the limitations that the explicit method places on the size of Δt and gives improved accuracy at the expense of having to solve a set of equations at each time step. Fortunately, the system is tridiagonal for a one-space-dimension problem.

8.3 DERIVATIVE BOUNDARY CONDITIONS

Really impose no new difficulties because we can extend the region artificially and replace the derivatives at the boundaries also by finite differences.

8.4 STABILITY AND CONVERGENCE CRITERIA

Shows you why there were limitations on the size of Δt in the explicit method and none with implicit methods.

8.5 PARABOLIC EQUATIONS IN TWO OR MORE DIMENSIONS

Extends finite-difference methods to regions of more than one dimension; we discover that the number of equations to be solved in implicit methods grows tremendously, and they are not tridiagonal. A modification, the A.D.I. method, really helps the situation.

8.6 FINITE ELEMENTS FOR HEAT FLOW

Demonstrates that this newer procedure readily applies, though it leads into many simple but tedious steps to set up a system of linear equations that give the solution to the problem.

8.7 CHAPTER SUMMARY

Helps you to review your knowledge of the important topics of the chapter.

8.8 COMPUTER PROGRAMS

Illustrates how FORTRAN programs can solve parabolic partial-differential equations by finite differences.

8.1 THE EXPLICIT METHOD

Our approach to solving parabolic partial-differential equations by a numerical method is to replace the partial derivatives by finite-difference approximations. For the one-dimensional heat-flow equation,

$$\frac{\partial^2 u}{\partial x^2} = \frac{c\rho}{k} \frac{\partial u}{\partial t}, \quad (8.1)$$

we can use the relations

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_{t=t_j}^{x=x_i} = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} + O(\Delta x)^2 \quad (8.2)$$

and

$$\left. \frac{\partial u}{\partial t} \right|_{t=t_j}^{x=x_i} = \frac{u_i^{j+1} - u_i^j}{\Delta t} + O(\Delta t). \quad (8.3)$$

We use subscripts to denote position and superscripts for time. Note that the error terms are of different orders since a forward difference is used in Eq. (8.3). This introduces some special limitations, but when this is done, the procedure is simplified.

Substituting Eqs. (8.2) and (8.3) into (8.1) and solving for u_i^{j+1} gives the equation for the forward-difference method:

$$u_i^{j+1} = \frac{k \Delta t}{c\rho(\Delta x)^2} (u_{i+1}^j + u_{i-1}^j) + \left(1 - \frac{2k \Delta t}{c\rho(\Delta x)^2}\right) u_i^j. \quad (8.4)$$

We have solved for u_i^{j+1} in terms of the temperatures at time t_j in Eq. (8.4) in view of the normally known conditions for a parabolic partial-differential equation. We subdivide the length into uniform subintervals and apply our finite-difference approximation to Eq. (8.1) at each point where u is not known. Equation (8.4) then gives the values of u at each interior point at $t = t_1$ since the values at $t = t_0$ are given by the initial conditions. It can then be used to get values at t_2 using the values at t_1 as initial conditions, so we can step the solution forward in time. At the endpoints, the boundary conditions will determine u .

The relative size of the time and distance steps, Δt and Δx , affects Eq. (8.4). If the ratio of $\Delta t/(\Delta x)^2$ is chosen so that $k \Delta t/c\rho(\Delta x)^2 = \frac{1}{2}$, the equation is simplified in that the last term vanishes and we have

$$u_i^{j+1} = \frac{1}{2}(u_{i+1}^j + u_{i-1}^j). \quad (8.5)$$

If the value of $k \Delta t/c\rho(\Delta x)^2$ is chosen as less than one-half, there will be improved accuracy* (limited, of course, by the errors dependent on the size of Δx). If the value is chosen greater than one-half, which would reduce the number of calculations required to advance the solution through a given interval of time, the phenomenon of *instability* sets in. (We show later in this chapter why this ratio affects stability and convergence.)

We illustrate the method with a simple example, varying the value of $k \Delta t/c\rho(\Delta x)^2$ to demonstrate its effect.

EXAMPLE A large flat steel plate is 2 cm thick. If the initial temperatures ($^{\circ}\text{C}$) within the plate are given, as a function of the distance from one face, by the equations

$$\begin{aligned} u &= 100x & \text{for } 0 \leq x \leq 1, \\ u &= 100(2 - x) & \text{for } 1 \leq x \leq 2, \end{aligned}$$

find the temperatures as a function of x and t if both faces are maintained at 0°C .

*It can be shown that choosing the ratio equal to $\frac{1}{6}$ is especially advantageous in minimizing the truncation error.

Since the plate is large, we can neglect lateral flow of heat relative to the flow perpendicular to the faces and hence use Eq. (8.1) for heat flow in one direction. For steel, $k = 0.13 \text{ cal/sec} \cdot \text{cm} \cdot ^{\circ}\text{C}$, $c = 0.11 \text{ cal/g} \cdot ^{\circ}\text{C}$ and $\rho = 7.8 \text{ g/cm}^3$. In order to use Eq. (8.5) as an approximation to the physical problem, we subdivide the total thickness into an integral number of spaces. Let us use $\Delta x = 0.25$, giving eight subdivisions. If we wish to use Eq. (8.5), we then fix Δt by the relation

$$\frac{k \Delta t}{c\rho(\Delta x)^2} = \frac{1}{2}, \quad \Delta t = \frac{(0.11)(7.8)(0.25)^2}{(2)(0.13)} = 0.206 \text{ sec.}$$

The boundary conditions are

$$u(0, t) = 0, \quad u(2, t) = 0.$$

The initial condition is

$$\begin{aligned} u(x, 0) &= 100x & \text{for } 0 \leq x \leq 1, \\ u(x, 0) &= 100(2 - x) & \text{for } 1 \leq x \leq 2. \end{aligned}$$

Our calculations are conveniently recorded in a table, as in Table 8.1, where each row of figures is at a particular time. We begin by filling in the initial conditions along the first row, at $t = 0.0$. The simple algorithm of Eq. (8.5) tells us that, at each interior point, the temperature at any point at the end of a time step is just the arithmetic average of the temperatures at the adjacent points at the beginning of that time step. The end temperatures are given by the boundary conditions. Because the temperatures are symmetrical on either side of the center line, we compute only for $x \leq 1.0$. The temperature at $x = 1.25$ is the same as at $x = 0.75$.

Table 8.1 Numerical solution to heat-flow example

t	Calculated temperatures at					
	$x = 0$	$x = 0.25$	$x = 0.50$	$x = 0.75$	$x = 1.0$	$x = 1.25$
0.0	0	25.0	50.0	75.0	100.0	75.0
0.206	0	25.0	50.0	75.0	75.0	75.0
0.412	0	25.0	50.0	62.5	75.0	62.5
0.619	0	25.0	43.75	62.5	62.5	62.5
0.825	0	21.88	43.75	53.12	62.5	53.12
1.031	0	21.88	37.5	53.12	53.12	53.12
1.238	0	18.75	37.5	45.31	53.12	45.31
1.444	0	18.75	32.03	45.31	45.31	45.31
1.650	0	16.16	32.03	38.67	45.31	38.67
1.856	0	16.16	27.34	38.67	38.67	38.67
2.062	0	13.67	27.34	33.01	38.67	33.01

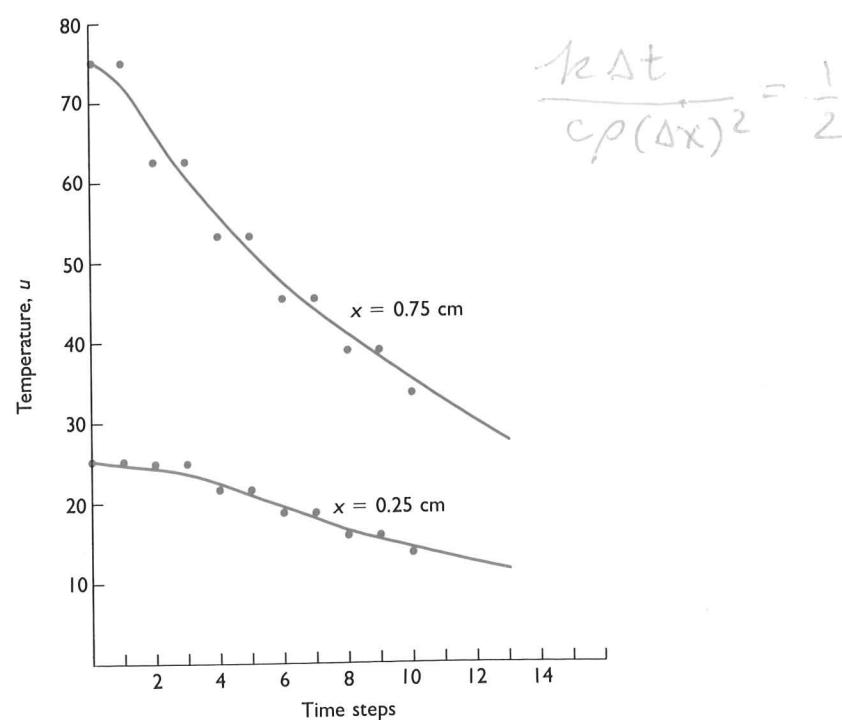


Figure 8.2

In Fig. 8.2, we compare some of the numerical results with the analytical solution, which is

$$u = 800 \sum_{n=0}^{\infty} \frac{1}{\pi^2(2n+1)^2} \cos \frac{(2n+1)\pi(x-1)}{2} e^{-0.3738(2n+1)^2 t}.$$

Note that the numerical values are close to and oscillate about the curves that are drawn to represent the analytical solution. In general the errors of Table 8.1 are less than 4%. If the size of Δx were less, the errors would be smaller. Unfortunately, this easy method is not always so accurate.

When the value for $k \Delta t / cp(\Delta x)^2$ in Eq. (8.4) is other than 0.5, the resulting equation is slightly more complicated, but the related computer program is not significantly slower. The major effect is the size of the time steps; reducing the value requires more successive calculations to reach a given time after the start of heat flow. Increasing the ratio to a value greater than 0.5 would decrease the number of successive calculations and hence reduce the computer time needed to solve a given problem. An extremely important phenomenon occurs, however, when the ratio is > 0.5 ; as illustrated in Fig. 8.3 where temperature profiles are shown at two different times, $t = 0.99$ sec and $t = 1.98$ sec, very inaccurate results may occur. The curves show the solution from the infinite series.

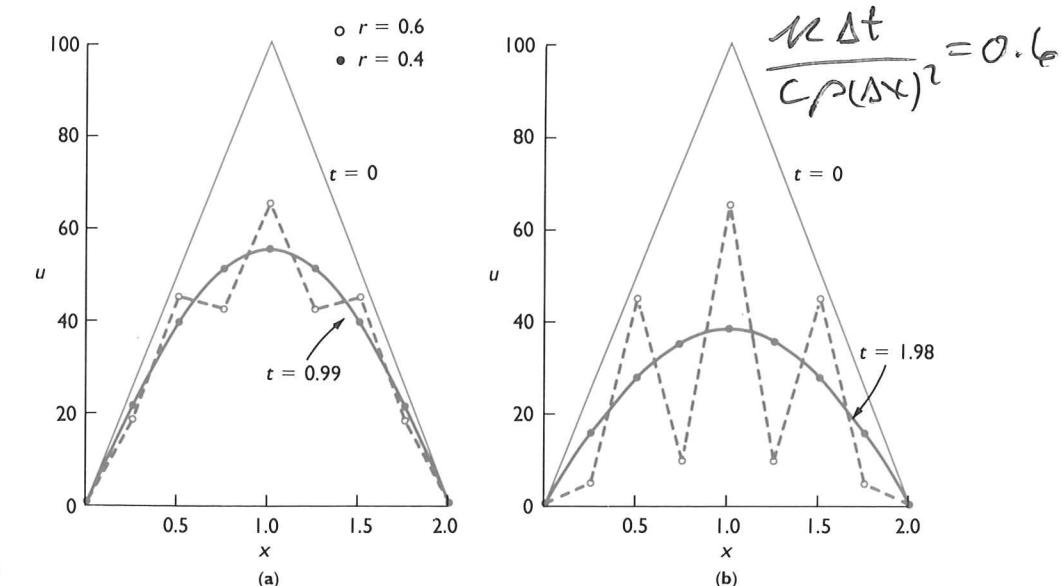


Figure 8.3

The open circles, with $r = 0.6$, show extreme oscillation: The calculated values are very imprecise, and completely impossible behavior is represented. The data for $r = 0.4$ are smooth and almost exactly match the series solution.

The reason for this great difference in behavior is that the choice of the ratio $k \Delta t / cp(\Delta x)^2 = 0.6$ introduces instability in which errors grow at an accelerating rate as time increases. (At values of $t > 2$, negative values of u are computed, a patently impossible situation.) As indicated in Fig. 8.3, when this ratio is taken at 0.4, the results are excellent.

In Fig. 8.2 with $k \Delta t / cp(\Delta x)^2 = 0.5$, the limiting value to avoid instability was used. Even here, the oscillation of points around the curves indicates its borderline value, and the accuracy is hardly acceptable. The phenomena of stability and convergence, more fully discussed in a later section of this chapter, set a maximum value of 0.5 to the ratio $k \Delta t / cp(\Delta x)^2$. When derivative boundary conditions are involved, the ratio must be less than 0.5. Discontinuities in the initial conditions—even a discontinuity in the gradient, $\partial u / \partial x$, at $t = 0$ —cause the accuracy to be poor at the maximum value. The next example will demonstrate this.

We will now solve a problem in diffusion, which is governed by the same mathematical equation as is heat conduction in a solid.

EXAMPLE

A hollow tube 20 cm long is initially filled with air containing 2% of ethyl alcohol vapors. At the bottom of the tube is a pool of alcohol that evaporates into the stagnant gas above. (Heat transfers to the alcohol from the surroundings to maintain a constant temperature of 30°C, at which temperature the vapor pressure is 0.1 atm.) At the upper end of the tube, the alcohol vapors dissipate to the outside air, so the concentration is essentially zero. Considering only the effects of molecular diffusion, determine the concentration of alcohol as a function of time and the distance x measured from the top of the tube.

Molecular diffusion follows the law

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2},$$

where D is the diffusion coefficient, with units of cm^2/sec in the cgs system. (This is the same as for the ratio $k/c\rho$, which is often termed *thermal diffusivity*.) For ethyl alcohol, $D = 0.119 \text{ cm}^2/\text{sec}$ at 30°C , and the vapor pressure is such that 10 volume percent alcohol in air is present at the surface.

Subdivide the length of the tube into five intervals, so $\Delta x = 4 \text{ cm}$. Using the maximum value permitted for Δt yields

$$D \frac{\Delta t}{(\Delta x)^2} = \frac{1}{2} = 0.119 \frac{\Delta t}{(4)^2}, \quad \Delta t = 67.2 \text{ sec.}$$

Our initial condition is $c(x, 0) = 2.0$. The boundary conditions are

$$c(0, t) = 0.0, \quad c(20, t) = 10.0.$$

The concentrations are measured by the percent of alcohol vapor in the air.

The computations are shown in Table 8.2. Again, using Eq. (8.5), each interior value of c is given by the arithmetic average of concentrations on either side in the line above. A little reflection is required to determine the proper concentrations to be used for $x = 0$ and $x = 20$ at $t = 0$. While these are initially at 2%, we assume they are changed instantaneously to 0% and 10% because the effective concentrations acting during the first time interval are not the initial values but the changed values. We have accordingly rewritten these values as shown in the first row of Table 8.2.

Table 8.2 Diffusion of alcohol vapors in a tube—solution of the equation

$$u_i^{j+1} = \frac{1}{2}(u_{i-1}^j + u_{i+1}^j)$$

Time, sec	Concentration of alcohol at					
	$x = 0$	$x = 4$	$x = 8$	$x = 12$	$x = 16$	$x = 20$
0	0.0	2.0	2.0	2.0	2.0	10.0
67.2	0.0	1.00	2.00	2.00	6.00	10.0
134.4	0.0	1.00	1.50	4.00	6.00	10.0
201.6	0.0	0.75	2.50	3.75	7.00	10.0
268.8	0.0	1.25	2.25	4.75	6.875	10.0
336.0	0.0	1.125	3.00	4.562	7.375	10.0
403.2	0.0	1.500	2.844	5.188	7.281	10.0
470.4	0.0	1.422	3.344	5.062	7.594	10.0
537.6	0.0	1.672	3.242	5.469	7.531	10.0
604.8	0.0	1.621	3.570	5.386	7.734	10.0
Steady state	0.0	2.0	4.0	6.0	8.0	10.0

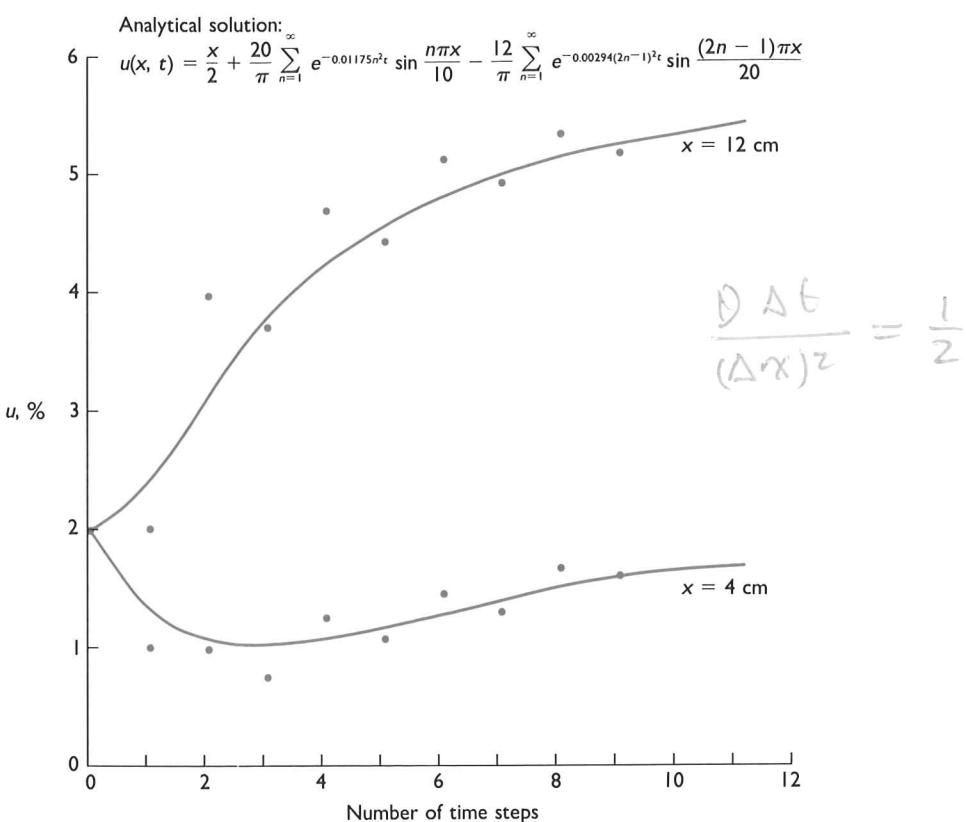


Figure 8.4

As time passes, the concentration will become a linear function of x , from 10% at $x = 20$ to 0% at $x = 0$. The calculated values approach the steady-state concentrations as time passes. However, as Fig. 8.4 shows, the successive calculated values oscillate about the values calculated from the analytical solution.* ■

While the algorithm of Eq. (8.5) is simple to use, the results leave something to be desired in the way of accuracy. The oscillatory nature of the results, when a smooth trend of the concentration is expected, is also of concern. We can improve accuracy by smaller steps, but if we decrease Δx , the time steps must also decrease, because the ratio $D \Delta t / (\Delta x)^2$ cannot exceed $\frac{1}{2}$. Cutting Δx in half will require making Δt one-fourth of its previous value, giving a total of eight times as many calculations. With the mixed order of error terms, it is not obvious what reduction of error this would give, but they should be reduced about fourfold.

*In this instance the analytical solution is given by the infinite series shown in Fig. 8.4.

We can reduce Δt without change in Δx , however, because the method is stable for any value of the ratio less than $\frac{1}{2}$. Suppose we make $D \Delta t / (\Delta x)^2 = \frac{1}{4}$. The basic difference equation, (8.4), now becomes

$$u_i^{j+1} = \frac{1}{4}(u_{i+1}^j + u_{i-1}^j) + \frac{1}{2}u_i^j. \quad (8.6)$$

Table 8.3 summarizes the use of Eq. (8.6) on the same example as before. As shown more clearly by Fig. 8.5, this last calculation causes the calculated concentrations to follow smooth curves, and the error is reduced considerably. The poorest accuracy is near the beginning. The later values are close to the curve.

This initial poor accuracy is a result of the discontinuities in the boundary conditions. The abrupt change of concentrations at the ends of the tube makes the explicit method inaccurate. In a situation with continuity of the initial values of the potential plus continuity of its derivatives and the absence of discontinuities in the boundary conditions, one would get better accuracy throughout.

Table 8.3 Diffusion of alcohol vapors in a tube:

$$u_i^{j+1} = \frac{1}{4}(u_{i-1}^j + u_{i+1}^j) + \frac{1}{2}u_i^j$$

Time, sec	Concentration of alcohol at					
	$x = 0$	$x = 4$	$x = 8$	$x = 12$	$x = 16$	$x = 20$
0.0	0.0	2.0	2.0	2.0	2.0	10.0
33.6	0.0	1.50	2.00	2.00	4.00	10.0
67.2	0.0	1.25	1.875	2.50	5.00	10.0
100.8	0.0	1.094	1.875	2.969	5.625	10.0
134.4	0.0	1.015	1.953	3.360	6.055	10.0
168.0	0.0	0.996	2.070	3.682	6.368	10.0
201.6	0.0	1.015	2.204	3.950	6.604	10.0
235.2	0.0	1.058	2.343	4.177	6.790	10.0
268.8	0.0	1.115	2.480	4.372	6.939	10.0
302.4	0.0	1.177	2.612	4.541	7.062	10.0
336.0	0.0	1.241	2.736	4.689	7.166	10.0
369.6	0.0	1.304	2.850	4.820	7.255	10.0
403.2	0.0	1.364	2.956	4.936	7.332	10.0
436.8	0.0	1.421	3.053	5.040	7.400	10.0
470.4	0.0	1.474	3.142	5.133	7.460	10.0
504.0	0.0	1.522	3.223	5.217	7.513	10.0
537.6	0.0	1.567	3.296	5.292	7.561	10.0
Steady state	0.0	2.0	4.0	6.0	8.0	10.0

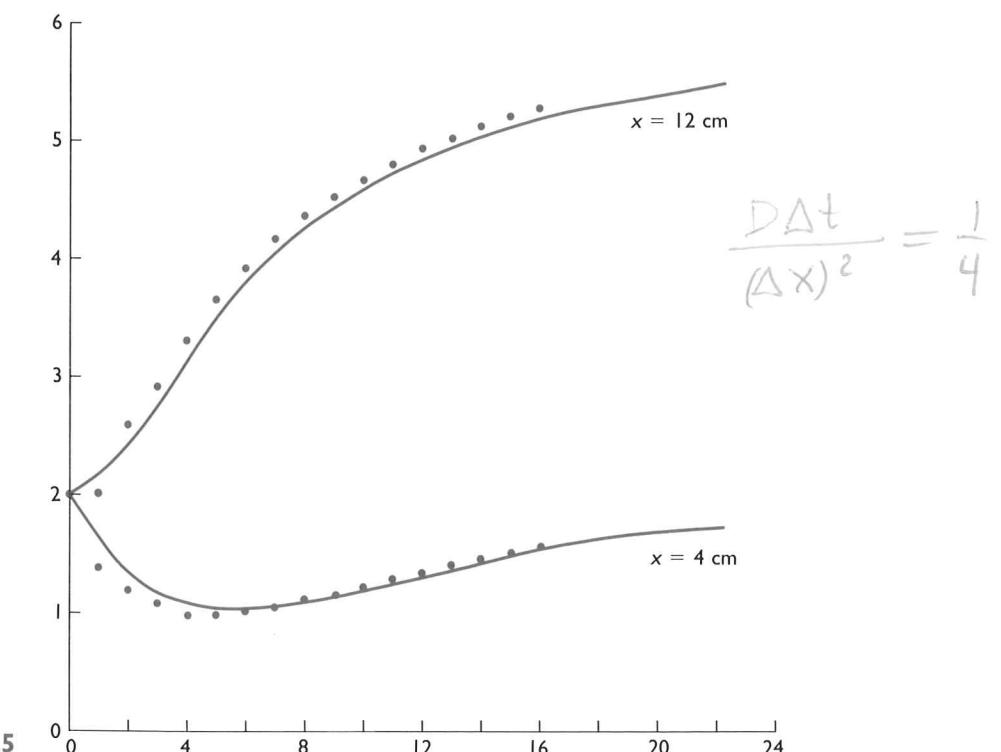


Figure 8.5

The method presented in this section is called the *explicit method* because each new value of the potential can be immediately calculated from quantities that are already known. It is simple and economical of calculation effort but has a severely limited upper value for the ratio $k \Delta t / c\rho(\Delta x)^2$. We can remove this limitation by going to an *implicit method*.

8.2 CRANK-NICOLSON METHOD

When the difference equation, Eq. (8.4), was derived, we noted that a mixed order of error was involved because a forward difference was used to replace the time derivative while a central difference was used for the distance derivative. However, the difference quotient, $(u_i^{j+1} - u_i^j)/\Delta t$, can be considered a central difference if we take it as corresponding to the midpoint of the time interval. Suppose we do consider $(u_i^{j+1} - u_i^j)/\Delta t$ as a central-difference approximation to $\partial u / \partial t$, and equate it to a central-difference quotient for the second derivative with distance, also corresponding to the midpoint in time, by averaging difference quotients at the beginning and end of the time step. Then

$$\frac{\partial^2 u}{\partial x^2} = \frac{c\rho}{k} \frac{\partial u}{\partial t}$$

is approximated by

$$\frac{1}{2} \left(\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} + \frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{(\Delta x)^2} \right) = \frac{cp}{k} \left(\frac{u_i^{j+1} - u_i^j}{\Delta t} \right).$$

Central difference
at t_j

Central difference
at t_{j+1}

Central difference
at $t_{j+1/2}$

When this is rearranged we get the Crank–Nicolson formula, where

$$r = k \Delta t / cp(\Delta x)^2,$$

$$-ru_{i-1}^{j+1} + (2 + 2r)u_i^{j+1} - ru_{i+1}^{j+1} = ru_{i-1}^j + (2 - 2r)u_i^j + ru_{i+1}^j \quad (8.7)$$

Letting $r = 1$, we get some simplification:

$$-u_{i-1}^{j+1} + 4u_i^{j+1} - u_{i+1}^{j+1} = u_{i-1}^j + u_{i+1}^j.$$

As we will discuss in the next section, one advantage of the Crank–Nicolson method is that it is stable for any value of r , although small values are more accurate.

Equation (8.7) is the usual formula for using the Crank–Nicolson method. Note that the new temperature u_i^{j+1} is not given directly in terms of known temperatures one time step earlier, but is a function of unknown temperatures at adjacent positions as well. It is therefore termed an *implicit method* in contrast to the explicit method of the previous section. With implicit methods, the values of u at $t = t_1$ are not just a function of values at $t = t_0$, but also involve the other u values at the same time step. This requires us to solve a set of simultaneous equations at each time step.

E X A M P L E We illustrate the method by solving the problem of diffusion of alcohol vapors, the same as that previously attacked by the explicit method. Again, let us take $\Delta x = 4$ cm and take $r = 1$. Restating the problem, we have

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{D} \frac{\partial u}{\partial t}, \quad u(x, 0) = 2.0, \quad \begin{cases} u(0, t) = 0, \\ u(20, t) = 10.0, \end{cases}$$

$$D = 0.119 \text{ cm}^2/\text{sec.}$$

If $D \Delta t / (\Delta x)^2 = r = 1$ and $\Delta x = 4$ cm, then $\Delta t = 134.4$ sec. For $t = 134.4$, at the end of the first time step, we write the equations at each point whose concentration is unknown. The effective concentrations at the two ends, 0% and 10%, respectively, are again used:

$$\begin{aligned} -0.0 + 4u_1 - u_2 &= 0.0 + 2.0, \\ -u_1 + 4u_2 - u_3 &= 2.0 + 2.0, \\ -u_2 + 4u_3 - u_4 &= 2.0 + 2.0, \\ -u_3 + 4u_4 - 10.0 &= 2.0 + 10.0. \end{aligned}$$

This method requires more work because, at each time step, we must solve a set of equations similar to the above. Fortunately, the system is tridiagonal. Since we will need to repeatedly solve the system with the same coefficient matrix (we transpose the constant values to the right side in the first and last equations), it is desirable to use an *LU* method. We then solve by back-substitution, using the elements of L and U :

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 3.75 & 0 & 0 \\ 0 & -1 & 3.733 & 0 \\ 0 & 0 & -1 & 3.732 \end{bmatrix}, \quad U = \begin{bmatrix} 1 & -0.25 & 0 & 0 \\ 0 & 1 & -0.267 & 0 \\ 0 & 0 & 1 & -0.268 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Remember that, to solve $Ax = b = LUx$, we first solve $Ly = b$ (which requires no reduction of L because it is already triangular) and then we solve $Ux = y$ by back-substitution. Observe that when A is tridiagonal, its zeros are preserved in L and U , and, in fact we need to compute only $2(n - 1)$ new values to get the *LU* equivalent of the $n \times n$ tridiagonal matrix A . Not only is the computational effort minimized, but we can also minimize computer memory space by storing only the three nonzero values in each row. In fact, as discussed in Chapter 2, we can store the elements of both L and U in place of the original values in A .

Table 8.4 Diffusion of alcohol vapors in a tube—Crank–Nicolson method

Time, sec	Calculated concentration values at					
	$x = 0$	$x = 4$	$x = 8$	$x = 12$	$x = 16$	$x = 20$
0.0	0.0	2.0	2.0	2.0	2.0	10.0
134.4	0.0	0.980	2.019	3.072	5.992	10.0
268.8	0.0	1.070	2.363	4.305	6.555	10.0
403.2	0.0	1.276	2.861	4.762	6.962	10.0
537.6	0.0	1.471	3.165	5.115	7.159	10.0

Time, sec	Analytical values	
	$x = 4$	$x = 12$
134.4	1.078	3.191
268.8	1.108	4.272
403.2	1.340	4.873
537.6	1.543	5.248

In Table 8.4 the results of calculations by the Crank–Nicolson method are listed. For the first line of calculations the b -vector has components 2.0, 4.0, 4.0, and 22.0, and the calculated values are the components of $A^{-1}b$. In computing the second line, the components of b are 2.019, 4.052, 8.011, and 23.072. Succeeding lines use the proper sums of values from the line above to determine the b -vector.

When the calculated values are compared to the analytical results, it is observed that the errors of this method, in this example, are about the same as those made in the explicit method with $D \Delta t / (\Delta x)^2 = \frac{1}{4}$. We require only one-fourth as many time steps, however, to reach 537.6 sec. With smaller values of Δx , this freedom of choice in the value of $D \Delta t / (\Delta x)^2$ is especially valuable. ■

8.3 DERIVATIVE BOUNDARY CONDITIONS

In heat-conduction problems, the most usual situation at the endpoints is not that they are held at a constant temperature, but that heat is lost by conduction or radiation at a rate proportional to some power of the temperature difference between the surface of the body and its surroundings. This leads to a relationship involving the space derivative of temperature at the surface. In the analytical solution of heat-flow problems through Fourier series, this adds considerable complication in determining the coefficients, but our numerical technique requires only minor modifications.

The rate of heat loss from the surface of a solid is generally expressed as

$$\text{Rate of heat loss} = hA(u - u_0), \quad (8.8)$$

where A is the surface area, u is the surface temperature, u_0 is the temperature of the surrounding medium, and h is a coefficient of heat transfer; h is increased by motion of the surrounding medium. To facilitate heat flow, the surrounding medium is often caused to flow rapidly by mechanical means (as in some salt evaporators) or by proper design (as in vertical-tube heat exchangers in distillation columns). This situation is called *forced convection*.

In other situations, h is also a function of the surface temperature, as in *natural convection*, in which the motion of surrounding fluid is caused by thermal currents. Another important situation is heat loss by radiation, in which the rate of heat loss is proportional to the fourth power of the temperature difference between the surface and the surrounding surfaces to which heat is being radiated. In both these situations, the rate of heat loss is proportional to some power of the surface temperature. This gives rise to nonlinear equations that are not as readily solved. One usually prefers to force the mathematical model to a linear form even though this is not exactly true. One way to approximate this is to use Eq. (8.8), absorbing the nonlinear aspects into the coefficient h , and to change h appropriately through the progress of the calculations so that it takes on a reasonably correct average value. Our examples will treat only the simpler situations where Eq. (8.8) applies directly.

As we will see, heat loss from the surface by conduction leads to a derivative boundary condition. Our procedure will be to replace the derivatives in both the differential equation and in the boundary conditions by difference quotients. We illustrate with a simple example.

EXAMPLE

An aluminum cube is $4 \times 4 \times 4$ in. ($k = 0.52$, $c = 0.226$, $\rho = 2.70$ in cgs units). All but one face is perfectly insulated, and the cube is initially at 1000°F . Heat is lost from the uninsulated face to a fluid flowing past it according to the equation

$$\text{Rate of heat loss (in Btu per sec)} = hA(u - u_0),$$

where $h = 0.15 \text{ Btu/sec} \cdot \text{ft}^2 \cdot ^{\circ}\text{F}$,

A = surface area in ft^2 ,

u = surface temperature, $^{\circ}\text{F}$,

u_0 = temperature of fluid, $^{\circ}\text{F}$.

If u_0 , the temperature of fluid flowing past the aluminum cube, is constant at 70°F , find the temperatures inside the cube as a function of time. While we could work the problem in cgs units, we elect to use English units, making suitable changes in k , c , and ρ .

Because of the insulation on the lateral faces, again the only direction in which heat will flow is perpendicular to the uninsulated face, and the equation is

$$\frac{\partial u}{\partial t} = \frac{k}{cp} \frac{\partial^2 u}{\partial x^2}.$$

The initial condition, with x representing distance from the uninsulated face, is

$$u(x, 0) = 1000.$$

For boundary conditions, at the open surface we have

$$-kA \frac{\partial u}{\partial x} \Big|_{x=0} = -hA(u - 70),$$

because the rate at which heat leaves the surface must be equal to the rate at which heat flows to the surface. The negative sign on the left is required because heat flows in a direction opposite to a positive gradient; on the right it occurs because heat is being lost in the direction of negative x . At the other side of the cube, the rate of heat flow is zero because of insulation:

$$\frac{\partial u}{\partial x} \Big|_{x=4} = 0.$$

We plan to use the explicit method with

$$r = k \Delta t / cp(\Delta x)^2 = \frac{1}{4}.*$$

*The ratio must be smaller than $\frac{1}{2}$ to give stability with the derivative end conditions.

Suppose we let $\Delta x = 1$ in. To calculate Δt , we need k , c , and ρ expressed in the units of inches, pounds, seconds, and °F. We first convert units:

$$\begin{aligned} k &= \left(0.52 \frac{\text{cal}}{\text{sec} \cdot \text{cm} \cdot ^\circ\text{C}}\right) \left(\frac{1 \text{ Btu}}{252 \text{ cal}}\right) \left(\frac{2.54 \text{ cm}}{1 \text{ in}}\right) \left(\frac{1^\circ\text{C}}{1.8^\circ\text{F}}\right) \\ &= 0.00291 \frac{\text{Btu}}{\text{sec} \cdot \text{in} \cdot ^\circ\text{F}}; \\ c &= \left(0.226 \frac{\text{cal}}{\text{g} \cdot ^\circ\text{C}}\right) \left(\frac{1 \text{ Btu}}{252 \text{ cal}}\right) \left(\frac{454 \text{ g}}{1 \text{ lb}}\right) \left(\frac{1^\circ\text{C}}{1.8^\circ\text{F}}\right) \\ &= 0.226 \frac{\text{Btu}}{\text{lb} \cdot ^\circ\text{F}}; \\ \rho &= \left(2.70 \frac{\text{g}}{\text{cm}^3}\right) \left(\frac{1 \text{ lb}}{454 \text{ g}}\right) \left(\frac{2.54 \text{ cm}}{1 \text{ in}}\right)^3 \\ &= 0.0975 \frac{\text{lb}}{\text{in}^3}; \\ \Delta t &= \frac{c\rho(\Delta x)^2}{4k} = \frac{(0.226)(0.0975)(1)^2}{(4)(0.00291)} = 1.89 \text{ sec.} \end{aligned}$$

For the ratio of values of Δt and Δx that we have chosen, our differential equation becomes

$$u_i^{j+1} = \frac{1}{4}(u_{i+1}^j + u_{i-1}^j) + \frac{1}{2}u_i^j, \quad (8.9)$$

which is to be applied at every point where u is unknown. In this example, this includes the points at $x = 0$ and $x = 4$ as well as the interior points. To enable us to write Eq. (8.9), we extend the domain of u one step on either side of the boundary. Let x_R be a fictitious point to the right of $x = 4$, and let x_L be a fictitious point to the left of $x = 0$. If x_1 signifies $x = 0$, and if x_5 signifies $x = 4$, we have the relations, from Eq. (8.9)

$$u_1^{j+1} = \frac{1}{4}(u_2^j + u_L^j) + \frac{1}{2}u_1^j,$$

$$u_5^{j+1} = \frac{1}{4}(u_R^j + u_4^j) + \frac{1}{2}u_5^j.$$

Now we use the boundary conditions to eliminate the fictitious points, writing them as central-difference quotients:

$$\begin{aligned} -k \frac{\partial u}{\partial x} \Big|_{x=0} &\doteq -(0.00291) \left(\frac{u_2^j - u_L^j}{2(1)} \right) = -\frac{0.15}{144}(u_1^j - 70); \\ -k \frac{\partial u}{\partial x} \Big|_{x=4} &\doteq -(0.00291) \left(\frac{u_R^j - u_4^j}{2(1)} \right) = 0. \end{aligned}$$

The 144 factor in the first equation changes h to a basis of in^2 . Solving for u_L and u_R , we have

$$u_L = u_2 - 0.716u_1 + 50.1,$$

$$u_R = u_4,$$

and the set of equations that give the temperatures becomes

$$\begin{aligned} u_1^{j+1} &= 0.32u_1^j + \frac{1}{2}u_2^j + 12.525, \\ u_2^{j+1} &= \frac{1}{4}(u_1^j + u_3^j) + \frac{1}{2}u_2^j, \\ u_3^{j+1} &= \frac{1}{4}(u_2^j + u_4^j) + \frac{1}{2}u_3^j, \\ u_4^{j+1} &= \frac{1}{4}(u_3^j + u_5^j) + \frac{1}{2}u_4^j, \\ u_5^{j+1} &= \frac{1}{2}u_4^j + \frac{1}{2}u_5^j. \end{aligned} \quad (8.10)$$

A similar treatment of the boundary conditions using the Crank–Nicolson method with $r = k \Delta t / cp(\Delta x)^2 = 1$ leads to the set of simultaneous equations:

$$\begin{aligned} 4.716u_1^{j+1} - 2u_2^{j+1} &= -0.716u_1^j + 2u_2^j + 100.2, \\ -u_1^{j+1} + 4u_2^{j+1} - u_3^{j+1} &= u_1^j + u_3^j, \\ -u_2^{j+1} + 4u_3^{j+1} - u_4^{j+1} &= u_2^j + u_4^j, \\ -u_3^{j+1} + 4u_4^{j+1} - u_5^{j+1} &= u_3^j + u_5^j, \\ -2u_4^{j+1} + 4u_5^{j+1} &= 2u_4^j. \end{aligned} \quad (8.11)$$

For the set of equations in (8.11), Δt will be 7.56 sec. We advance the solution one time step at a time by repeatedly solving either (8.10) or (8.11), using the proper values of u_i^j . ■

8.4 STABILITY AND CONVERGENCE CRITERIA

We have previously stated that in order to ensure stability and convergence in the explicit method, the ratio $r = k \Delta t / c\rho(\Delta x)^2$ must be $\frac{1}{2}$ or less. The implicit Crank–Nicolson method has no such limitation. In this section, these phenomena and criteria will be studied in more detail.

By *convergence*, we mean that the results of the method approach the analytical values as Δt and Δx both approach zero. By *stability*, we mean that errors made at one stage of the calculations do not cause increasingly large errors as the computations are continued, but rather will eventually damp out.

We will first discuss convergence, limiting ourselves to the simple case of the unsteady-state heat-flow equation in one dimension:^{*}

$$\frac{\partial U}{\partial t} = \frac{k}{c\rho} \frac{\partial^2 U}{\partial x^2}. \quad (8.12)$$

Let us use the symbol U to represent the exact solution to Eq. (8.12), and u to represent the numerical solution. At the moment we assume that u is free of round-off errors, so the only difference between U and u is the error made by replacing Eq. (8.12) by the difference equation. Let $e_i^j = U_i^j - u_i^j$, at the point $x = x_i$, $t = t_j$. By the explicit method, Eq. (8.12) becomes

$$u_i^{j+1} = r(u_{i+1}^j + u_{i-1}^j) + (1 - 2r)u_i^j, \quad (8.13)$$

where $r = k \Delta t / c\rho(\Delta x)^2$. Substituting $u = U - e$ into Eq. (8.13), we get

$$e_i^{j+1} = r(e_{i+1}^j + e_{i-1}^j) + (1 - 2r)e_i^j - r(U_{i+1}^j + U_{i-1}^j) - (1 - 2r)U_i^j + U_i^{j+1}. \quad (8.14)$$

By using Taylor-series expansions, we have

$$\begin{aligned} U_{i+1}^j &= U_i^j + \left(\frac{\partial U}{\partial x} \right)_{i,j} \Delta x + \frac{(\Delta x)^2}{2} \frac{\partial^2 U(\xi_1, t_j)}{\partial x^2}, \quad x_i < \xi_1 < x_{i+1}, \\ U_{i-1}^j &= U_i^j - \left(\frac{\partial U}{\partial x} \right)_{i,j} \Delta x + \frac{(\Delta x)^2}{2} \frac{\partial^2 U(\xi_2, t_j)}{\partial x^2}, \quad x_{i-1} < \xi_2 < x_i, \\ U_i^{j+1} &= U_i^j + \Delta t \frac{\partial U(x_i, \eta)}{\partial t}, \quad t_j < \eta < t_{j+1}. \end{aligned}$$

^{*}We could have treated the simpler equation $\partial U / \partial T = \partial^2 U / \partial X^2$ without loss of generality, since with the change of variables $X = \sqrt{c\rho} x$, $T = kt$, the two equations are seen to be identical.

Substituting these into Eq. (8.14) and simplifying, remembering that $r(\Delta x)^2 = k \Delta t / c\rho$, we get

$$e_i^{j+1} = r(e_{i+1}^j + e_{i-1}^j) + (1 - 2r)e_i^j + \Delta t \left[\frac{\partial U(x_i, \eta)}{\partial t} - \frac{k}{c\rho} \frac{\partial^2 U(\xi, t_j)}{\partial x^2} \right], \quad t_j \leq \eta \leq t_{j+1}, \quad x_{i-1} \leq \xi \leq x_{i+1}. \quad (8.15)$$

Let E^j be the magnitude of the maximum error in the row of calculations for $t = t_j$, and let $M > 0$ be an upper bound for the magnitude of the expression in brackets in Eq. (8.15). If $r \leq \frac{1}{2}$, all the coefficients in Eq. (8.15) are positive (or zero) and we may write the inequality

$$|e_i^{j+1}| \leq 2rE^j + (1 - 2r)E^j + M \Delta t = E^j + M \Delta t.$$

This is true for all the e_i^{j+1} at $t = t_{j+1}$, so

$$E^{j+1} \leq E^j + M \Delta t.$$

Since this is true at each time step,

$$\begin{aligned} E^{j+1} &\leq E^j + M \Delta t \leq E^{j-1} + 2M \Delta t \leq \dots \leq E^0 + (j+1)M \Delta t = E^0 + Mt_{j+1} \\ &= Mt_{j+1}, \end{aligned}$$

because E^0 , the errors at $t = 0$, are zero, since U is given by the initial conditions.

Now, as $\Delta x \rightarrow 0$, $\Delta t \rightarrow 0$ if $k \Delta t / c\rho(\Delta x)^2 \leq \frac{1}{2}$, and $M \rightarrow 0$, because, as both Δx and Δt get smaller,

$$\left[\frac{\partial U(x_i, \eta)}{\partial t} - \frac{k}{c\rho} \frac{\partial^2 U(\xi, t_j)}{\partial x^2} \right] \rightarrow \left(\frac{\partial U}{\partial t} - \frac{k}{c\rho} \frac{\partial^2 U}{\partial x^2} \right)_{i,j} = 0.$$

This last is by virtue of Eq. (8.12), of course. Consequently, we have shown that the explicit method is convergent for $r \leq \frac{1}{2}$, because the errors approach zero as Δt and Δx are made smaller.

For the solution to the heat-flow equation by the Crank–Nicolson method, the analysis of convergence may be made by similar methods. The treatment is more complicated, but it can be shown that each E^{j+1} is no greater than a finite multiple of E^j plus a term that vanishes as both Δx and Δt become small, and this is independent of r . Hence, since the initial errors are zero, the finite-difference solution approaches the analytical solution as $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$, requiring only that r stay finite.

Let us begin our discussion of stability with a numerical example. Since the heat-flow equation is linear, if two solutions are known, their sum is also a solution. We are interested in what happens to errors made in one line of the computations as the calculations are continued, and because of the additivity feature, the effect of a succession of errors is just the sum of the effects of the individual errors. We follow, then, a single error,* which most likely occurred due to round-off. If this single error does not grow in magnitude, we will call the method *stable*, since then the cumulative effect of all errors affects the later calculations no more than a linear combination of the previous errors would.

Table 8.5 illustrates the principle. We have calculated for the simple case where the boundary conditions are fixed, so that the errors at the endpoints are zero. We assume that a single error of size e occurs at $t = t_1$ and $x = x_2$. The explicit method, $k \Delta t / cp(\Delta x)^2 = \frac{1}{2}$, was used. The original error quite obviously dies out. As an exercise, it is left to the student to show that with $r > 0.5$, errors have an increasingly large effect on later computations. Table 8.6 shows that errors damp out for the Crank–Nicolson method with $r = 1$ even more rapidly than in the explicit method with $r = 0.5$.

Table 8.5 Propagation of errors—explicit method

t	Endpoint		Endpoint		
	x_1	x_2	x_3	x_4	x_5
t_0	0	0	0	0	0
t_1	0	e	0	0	0
t_2	0	0	$0.50e$	0	0
t_3	0	$0.25e$	0	$0.25e$	0
t_4	0	0	$0.25e$	0	0
t_5	0	$0.125e$	0	$0.125e$	0
t_6	0	0	$0.125e$	0	0
t_7	0	$0.062e$	0	$0.062e$	0
t_8	0	0	$0.062e$	0	0

Table 8.6 Propagation of errors—Crank–Nicolson method

t	x_1	x_2	x_3	x_4	x_5
t_0	0	0	0	0	0
t_1	0	e	0	0	0
t_2	0	$0.071e$	$0.286e$	$0.071e$	0
t_3	0	$0.107e$	$0.143e$	$0.107e$	0
t_4	0	$0.049e$	$0.092e$	$0.049e$	0
t_5	0	$0.036e$	$0.053e$	$0.036e$	0
t_6	0	$0.022e$	$0.033e$	$0.022e$	0
t_7	0	$0.013e$	$0.020e$	$0.013e$	0
t_8	0	$0.008e$	$0.013e$	$0.008e$	0

*A computation made assuming that each of the interior points has an error equal to e at $t = t_1$ demonstrates the effect more rapidly.

In order to discuss stability in a more analytical sense, we need some material from linear algebra. In Chapter 6 we discussed eigenvalues and eigenvectors of a matrix. We recall that for the matrix A and vector x , if

$$Ax = \lambda x,$$

then the scalar λ is an eigenvalue of A and x is the corresponding eigenvector. If the N eigenvalues of the $N \times N$ matrix A are all different, then the corresponding N eigenvectors are linearly independent, and any N -component vector can be written uniquely in terms of them.

Consider the unsteady-state heat-flow problem with fixed boundary conditions. Suppose we subdivide into $N + 1$ subintervals so there are N unknown values of the temperature being calculated at each time step. Think of these N values as the components of a vector. Our algorithm for the explicit method (Eq. (8.4)) can be written as the matrix equation*

$$\begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ \vdots \\ u_N^{j+1} \end{bmatrix} = \begin{bmatrix} (1 - 2r) & r & & & u_1^j \\ r & (1 - 2r) & r & & u_2^j \\ & \ddots & \ddots & \ddots & \vdots \\ & & r & (1 - 2r) & u_N^j \end{bmatrix} \quad (8.16)$$

or

$$u^{j+1} = Au^j,$$

where A represents the coefficient matrix and u^j and u^{j+1} are the vectors whose N components are the successive calculated values of temperature. The components of u^0 are the initial values from which we begin our solution. The successive rows of our calculations are

$$\begin{aligned} u^1 &= Au^0, \\ u^2 &= Au^1 = A^2u^0, \\ &\vdots \\ u^j &= Au^{j-1} = A^2u^{j-2} = \dots = A^ju^0. \end{aligned}$$

(The superscripts on the A are here exponents; on the vectors they indicate time.)

*A change of variable is required to give boundary conditions of $u = 0$ at each end. This can always be done for fixed end conditions.

Suppose that errors are introduced into u^0 , so that it becomes \bar{u}^0 . We will follow the effects of this error through the calculations. The successive lines of calculation are now

$$\bar{u}^j = A\bar{u}^{j-1} = \dots = A^j\bar{u}^0.$$

Let us define the vector e^j as $u^j - \bar{u}^j$ so the e^j represents the errors in u^j caused by the errors in \bar{u}^0 . We have

$$e^j = u^j - \bar{u}^j = A^j u^0 - A^j \bar{u}^0 = A^j e^0. \quad (8.17)$$

This shows that errors are propagated by using the same algorithm as that by which the temperatures are calculated, as was implicitly assumed earlier in this section.

Now the N eigenvalues of A are distinct (see below) so that its N eigenvectors x_1, x_2, \dots, x_N are independent, and

$$Ax_1 = \lambda_1 x_1,$$

$$Ax_2 = \lambda_2 x_2,$$

$$\vdots$$

$$Ax_N = \lambda_N x_N.$$

We now write the error vector e^0 as a linear combination of the x_i :

$$e^0 = c_1 x_1 + c_2 x_2 + \dots + c_N x_N,$$

where the c 's are constants. Then e^1 is, in terms of the x_i ,

$$e^1 = Ae^0 = \sum_{i=1}^N Ac_i x_i = \sum_{i=1}^N c_i Ax_i = \sum_{i=1}^N c_i \lambda_i x_i,$$

and for e^2 ,

$$e^2 = Ae^1 = \sum_{i=1}^N Ac_i \lambda_i x_i = \sum_{i=1}^N c_i \lambda_i^2 x_i.$$

(Again, the superscripts on vectors indicate time; on λ they are exponents.) After j steps, Eq. (8.17) can be written

$$e^j = \sum_{i=1}^N c_i \lambda_i^j x_i.$$

If the magnitudes of all of the eigenvalues are less than or equal to unity, errors will not grow as the computations proceed; that is, the computational scheme is stable. This then is the analytical condition for stability: that the largest eigenvalue of the coefficient matrix for the algorithm be one or less in magnitude.

The eigenvalues of matrix A (Eq. (8.16)) can be shown to be (note they are all distinct):

$$1 - 4r \sin^2 \frac{n\pi}{2(N+1)}, \quad n = 1, 2, \dots, N.$$

We will have stability for the explicit scheme if

$$-1 \leq 1 - 4r \sin^2 \frac{n\pi}{2(N+1)} \leq 1.$$

The limiting value of r is given by

$$\begin{aligned} -1 &\leq 1 - 4r \sin^2 \frac{n\pi}{2(N+1)} \\ r &\leq \frac{1/2}{\sin^2(n\pi/2(N+1))}. \end{aligned}$$

Hence, if $r \leq \frac{1}{2}$, the explicit scheme is stable.

The Crank–Nicolson scheme, in matrix form, is

$$\begin{bmatrix} (2 + 2r) & -r & & & & & u_1^j \\ -r & (2 + 2r) & -r & & & & u_2^j \\ & & \ddots & & & & \vdots \\ & & & \ddots & & & u_N^j \\ & & & & -r & (2 + 2r) & \end{bmatrix} \begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ \vdots \\ u_N^{j+1} \end{bmatrix} = \begin{bmatrix} (2 - 2r) & r & & & & & u_1^j \\ r & (2 - 2r)r & & & & & u_2^j \\ & & \ddots & & & & \vdots \\ & & & \ddots & & & u_N^j \\ & & & & r & (2 - 2r) & \end{bmatrix} \begin{bmatrix} u_1^j \\ u_2^j \\ \vdots \\ u_N^j \end{bmatrix},$$

or

$$Au^{j+1} = Bu^j.$$

We can write

$$u^{j+1} = (A^{-1}B)u^j, \quad (8.18)$$

so that stability is given by the magnitudes of the eigenvalues of $A^{-1}B$. These are

$$\frac{2 - 4r \sin^2(n\pi/2(N-1))}{2 + 4r \sin^2(n\pi/2(N-1))}, \quad n = 1, 2, \dots, N.$$

Clearly all the eigenvalues are no greater than one in magnitude for any positive value of r .

With derivative boundary conditions, a similar analysis shows that the Crank–Nicolson method is stable for any positive value of r . For the explicit scheme, $r = \frac{1}{2}$ leads to instability with a finite surface coefficient. Smith (1978) shows that the limitation on r for stability is

$$r \leq \frac{1}{2 + P \Delta x},$$

where P is the ratio of surface coefficient to conductivity, h/k .

8.5 PARABOLIC EQUATIONS IN TWO OR MORE DIMENSIONS

In principle, we can readily extend the preceding methods to higher space dimensions, especially when the region is rectangular. The heat-flow equation in two directions is

$$\frac{\partial u}{\partial t} = \frac{k}{c\rho} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right).$$

Taking $\Delta x = \Delta y$, and letting $r = k \Delta t / c\rho(\Delta x)^2$, we find that the explicit scheme becomes

$$u_{i,j}^{k+1} - u_{i,j}^k = r(u_{i+1,j}^k - 2u_{i,j}^k + u_{i-1,j}^k + u_{i,j+1}^k - 2u_{i,j}^k + u_{i,j-1}^k)$$

or

$$u_{i,j}^{k+1} = r(u_{i+1,j}^k + u_{i-1,j}^k + u_{i,j+1}^k + u_{i,j-1}^k) + (1 - 4r)u_{i,j}^k.$$

In this scheme, the maximum value permissible for r in the simple case of constant end conditions is $\frac{1}{4}$. (Note that this corresponds again to the numerical value that gives a particularly simple formula.) In the more general case with $\Delta x \neq \Delta y$, the criterion is

$$\frac{k \Delta t}{c\rho[(\Delta x)^2 + (\Delta y)^2]} \leq \frac{1}{8}.$$

The analogous equation in three dimensions, with equal grid spacing each way, has the coefficient $(1 - 6r)$, and $r \leq \frac{1}{6}$ is required for convergence and stability.

The difficulty with the use of the explicit scheme is that the restrictions on Δt require inordinately many rows of calculations. One then looks for a method in which Δt can be made larger without loss of stability. In one dimension, the Crank–Nicolson method was such a method. In the two-dimensional case, using averages of central-difference approximations to give $\partial^2 u / \partial x^2$ and $\partial^2 u / \partial y^2$ at the midvalue of time, we get

$$u_{i,j}^{k+1} - u_{i,j}^k = \frac{r}{2} [u_{i+1,j}^{k+1} - 2u_{i,j}^{k+1} + u_{i-1,j}^{k+1} + u_{i+1,j}^k - 2u_{i,j}^k + u_{i-1,j}^k + u_{i,j+1}^{k+1} - 2u_{i,j}^{k+1} + u_{i,j-1}^{k+1} + u_{i,j+1}^k - 2u_{i,j}^k + u_{i,j-1}^k].$$

The problem now is that a set of $(M)(N)$ simultaneous equations must be solved at each time step, where M is the number of unknown values in the x -direction and N in the y -direction. Furthermore, the coefficient matrix is no longer tridiagonal, so the solution to each set of equations is slower and memory space to store the elements of the matrix becomes exorbitant.

The advantage of a tridiagonal matrix is retained in the alternating-direction-implicit scheme (A.D.I.) proposed by Peaceman and Rachford (1955). It is widely used in modern computer programs for the solution of parabolic partial-differential equations. In this method, we approximate $\nabla^2 u$ by adding a central-difference approximation to $\partial^2 u / \partial x^2$ written at the beginning of the interval to a similar expression for $\partial^2 u / \partial y^2$ written at the end:

$$u_{i,j}^{k+1} - u_{i,j}^k = \underbrace{r[u_{i+1,j}^k - 2u_{i,j}^k + u_{i-1,j}^k]}_{\text{From } \partial^2 u / \partial x^2 \text{ at start}} + \underbrace{u_{i,j+1}^{k+1} - 2u_{i,j}^{k+1} + u_{i,j-1}^{k+1}}_{\text{From } \partial^2 u / \partial y^2 \text{ at end}}. \quad (8.19)$$

The obvious bias in this formula is balanced by reversing the order for the second-derivative approximations in the next time span:

$$u_{i,j}^{k+2} - u_{i,j}^{k+1} = \underbrace{r[u_{i+1,j}^{k+2} - 2u_{i,j}^{k+2} + u_{i-1,j}^{k+2}]}_{\text{From } \partial^2 u / \partial x^2 \text{ at end}} + \underbrace{u_{i,j+1}^{k+1} - 2u_{i,j}^{k+1} + u_{i,j-1}^{k+1}}_{\text{From } \partial^2 u / \partial y^2 \text{ at start}}. \quad (8.20)$$

We illustrate the A.D.I. method with a very simple example.

E X A M P L E A square plate of steel is 15 cm on a side. Initially, all points are at 0°C. Follow the interior temperatures if two adjacent sides are suddenly brought to 100°C and held at that

temperature. The plate is insulated on its flat surfaces, so that heat flows only in the x - and y -directions. We are given that $k = 0.13$, $\rho = 7.8$, $c = 0.11$ in cgs units. Take $\Delta x = \Delta y = 5$ cm, so that there are four interior points. Label the points as shown in Fig. 8.6, with u being used for horizontal traverses, v for vertical traverses.

Equations (8.19) and (8.20) become, with $r = k \Delta t / c \rho (\Delta x)^2$,

$$\begin{bmatrix} (1/r) + 2 & -1 & 0 & 0 \\ -1 & (1/r) + 2 & 0 & 0 \\ 0 & 0 & (1/r) + 2 & -1 \\ 0 & 0 & -1 & (1/r) + 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} 0 + 100 + [(1/r) - 2]v_1 + v_2 \\ 100 + 100 + [(1/r) - 2]v_3 + v_4 \\ 0 + v_1 + [(1/r) - 2]v_2 + 0 \\ 100 + v_3 + [(1/r) - 2]v_4 + 0 \end{bmatrix},$$

$$\begin{bmatrix} (1/r) + 2 & -1 & 0 & 0 \\ -1 & (1/r) + 2 & 0 & 0 \\ 0 & 0 & (1/r) + 2 & -1 \\ 0 & 0 & -1 & (1/r) + 2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} 100 + 0 + [(1/r) - 2]u_1 + u_2 \\ 0 + 0 + [(1/r) - 2]u_3 + u_4 \\ 100 + u_1 + [(1/r) - 2]u_2 + 100 \\ 0 + u_3 + [(1/r) - 2]u_4 + 100 \end{bmatrix}.$$

Table 8.7 Temperature changes in a 15×15 cm steel plate, computed by the A.D.I. method

t , sec	Temperatures at			
	u_1 or v_1	u_2 or v_3	u_3 or v_2	u_4 or v_4
0.0	0.000	0.000	0.000	0.000
16.5*	8.392	17.482	0.699	9.790
33.0	16.529	30.515	2.543	16.529
49.5*	22.306	40.298	4.932	22.923
66.0	27.594	47.741	7.466	27.594
82.5*	31.532	53.444	9.891	31.803
99.0	35.000	57.863	12.138	35.001
115.5*	37.668	61.308	14.148	37.788
132.0	39.959	64.017	15.901	39.959
148.5*	41.758	66.159	17.410	41.811
165.0	43.278	67.864	18.693	43.278
181.5*	44.489	69.225	19.776	44.512
198.0	45.500	70.318	20.683	45.500
214.5*	46.314	71.197	21.440	46.324
231.0	46.988	71.907	22.068	46.988
247.5*	46.533	72.482	22.589	47.538
264.0	46.984	72.948	23.019	47.984
.
.
.
∞	50.00	75.00	25.00	50.00

*Calculations are less accurate at these times.

(Note the similarity to the equations for the A.D.I. method for steady-state temperatures in Section 7.11. This is hardly surprising, since the temperatures for the unsteady-state problem will eventually reach the steady state. One can think of this as the rationale behind the A.D.I. method for elliptic equations.)

We solve for the temperature history by using the above equations in succession. One normally discards the alternate computations, beginning with the first, because they tend to be inaccurate.

Table 8.7 and Fig. 8.7 show the results, with $\Delta t = 16.5$ sec, corresponding to $r = 0.1$.

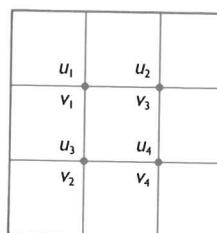


Figure 8.6

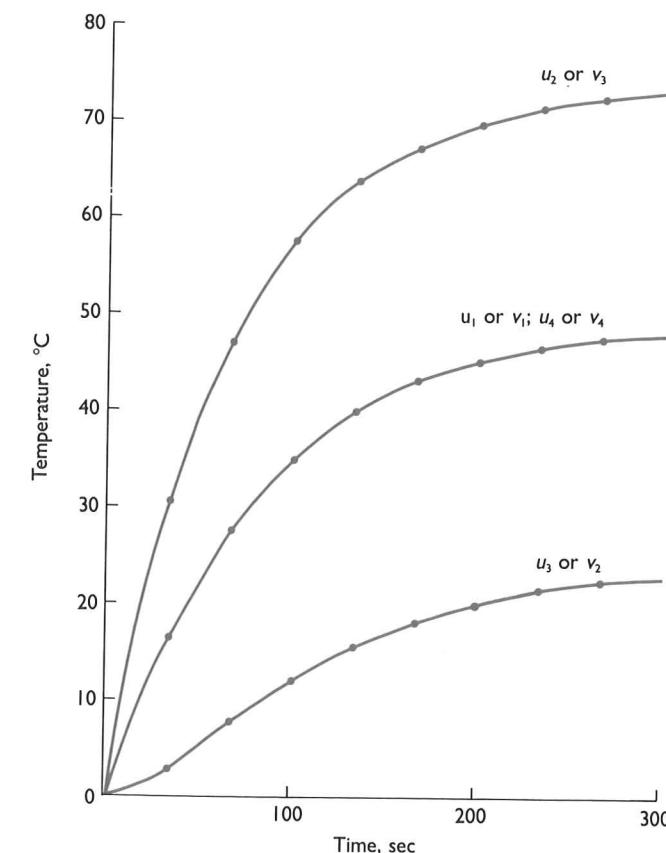


Figure 8.7

The compensation of errors produced by this alternation of direction gives a scheme that is convergent and stable for all values of r , although accuracy requires that r not be too large. The three-dimensional analog alternates three ways, returning to each of the three formulas after every third step. (Unfortunately the three-dimensional case is not stable for all fixed values of $r > 0$. A variant due to Douglas (1962) is unconditionally stable, however.) When the formulas are rearranged, in each case tridiagonal coefficient matrices result.

Note that the equations can be broken up into two independent subsets, each containing only two equations. This is always true in the A.D.I. method; each row gives a set independent of the equations from the other rows. For columns, the same thing occurs. For very large problems, this is important, because it permits the ready overlay of main memory in solving the independent sets.

When the region in which the heat-flow equation is to be satisfied is not rectangular, one may perturb the boundary to make it agree with a square mesh or interpolate from boundary points to estimate u at adjacent mesh points as discussed in Chapter 7 for elliptic equations.

The frequency with which circular or spherical regions occur makes it worthwhile to mention the heat equation in polar and spherical coordinates. The basic equation

$$\frac{\partial u}{\partial t} = \frac{k}{c\rho} \nabla^2 u$$

becomes, in polar coordinates (r, θ) ,

$$\frac{\partial u}{\partial t} = \frac{k}{c\rho} \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} \right),$$

and in spherical coordinates (r, ϕ, θ) ,

$$\frac{\partial u}{\partial t} = \frac{k}{c\rho} \left(\frac{\partial^2 u}{\partial r^2} + \frac{2}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\cot \phi}{r} \frac{\partial u}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 u}{\partial \phi^2} \right).$$

Using finite-difference approximations to convert these to difference equations is straightforward except at the origin where $r = 0$. For this point, consider $\nabla^2 u$ in rectangular coordinates, so that, in two dimensions,

$$\partial^2 u = \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}}{(\Delta r)^2}, \quad u_{ij} \text{ at } r = 0.$$

This is exactly the same as the expression for the Laplacian in Chapter 7, Eq. (7.6a). This expression for $\nabla^2 u$ is obviously independent of the orientation of the axes. We get the best value by using the average value of all points that are a distance Δr from the origin, so that for $r = 0$,

$$\nabla^2 u = \frac{4(u_{av} - u_0)}{(\Delta r)^2} \quad \text{at } r = 0.$$

The corresponding relation for spherical coordinates is

$$\nabla^2 u = \frac{6(u_{av} - u_0)}{(\Delta r)^2} \quad \text{at } r = 0.$$

8.6 FINITE ELEMENTS FOR HEAT FLOW

In Chapters 6 and 7 we observed that the finite-element method often is preferred for obtaining approximate solutions to differential equations whose conditions are specified on the boundaries of a region. They are also an important alternative to finite differences in solving parabolic equations. You should have some exposure to this application of finite elements, but we do not have space enough to give a full treatment.

Consider first the one-dimensional problem that we discussed in Sections 8.1–8.3. The equation for this is

$$\frac{\partial u}{\partial t} = \frac{k}{c\rho} \frac{\partial^2 u}{\partial x^2} \quad \text{over } [x_a, x_b] \quad (8.21)$$

subject to initial conditions that give $u(x, 0)$ and boundary conditions that give $u(x_a, t)$ and $u(x_b, t)$. It is possible to consider this a two-dimensional problem (in x and t) and treat it as in Section 7.12. However, it is customary to apply finite elements only to the x -domain and approximate the time derivative by finite differences. We will adopt this approach, using a forward-difference approximation, so Eq. (8.21) becomes

$$\frac{u^{m+1} - u^m}{\Delta t} - \frac{k}{c\rho} \frac{\partial^2 u}{\partial x^2} = 0. \quad (8.22)$$

Superscripts on u indicate time; subscripts on u in the following indicate position.

We break the region of the problem into discrete contiguous subintervals and approximate u within element (e) , whose endpoints are x_k and x_{k+1} , as a linear interpolation of u_k and u_{k+1} . In other words,

$$u^{(e)} = N_k u_k + N_{k+1} u_{k+1} \quad \text{within } (e).$$

APPLIED NUMERICAL ANALYSIS

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Curtis F. Gerald
Patrick O. Wheatley

California Polytechnic State University
San Luis Obispo



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