temperature at zero time. Put

$$x=\frac{X}{L}\quad\text{and}\quad u=\frac{U}{U_0}.$$

Then

$$\frac{\partial U}{\partial X}=\frac{\partial U}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}X}=\frac{\partial U}{\partial x}\frac{1}{L}$$

and

$$\frac{\partial^2 U}{\partial X^2}=\frac{\partial}{\partial X}\left(\frac{\partial U}{\partial X}\right)=\frac{\partial}{\partial x}\left(\frac{1}{L}\frac{\partial U}{\partial X}\right)\frac{\mathrm{d}x}{\mathrm{d}X}=\frac{1}{L^2}\frac{\partial^2 U}{\partial x^2},$$

so eqn (2.1) transforms to

$$\frac{\partial(uU_0)}{\partial T}=\frac{\kappa}{L^2}\frac{\partial^2(uU_0)}{\partial x^2},$$

i.e.

$$\frac{1}{\kappa L^{-2}}\frac{\partial u}{\partial T}=\frac{\partial^2 u}{\partial x^2}.$$

Writing $t=\kappa T/L^2$ and applying the function of a function rule to the left side yields

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}\tag{2.2}$$

as the non-dimensional form of (2.1).

It should be noted that the number representing the length of the rod is 1.

An explicit method of solution

By eqns (1.10) and (1.8) one finite-difference approximation to

$$\frac{\partial U}{\partial t}=\frac{\partial^2 U}{\partial x^2}\tag{2.3}$$

is

$$\frac{u_{i,j+1}-u_{i,j}}{k}=\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h^2},$$

where u is the exact solution of the approximating difference equations,

$$x_i = ih, \quad (i = 0, 1, 2, \ldots),$$

and

$$t_j = jk, \quad (j = 0, 1, 2, \ldots).$$

This can be written as

$$u_{i,j+1} = ru_{i-1,j} + (1-2r)u_{i,j} + ru_{i+1,j}, \tag{2.4}$$

where $r = \delta t/(\delta x)^2 = k/h^2$, and gives a formula for the unknown 'temperature' $u_{i,j+1}$ at the $(i, j+1)$th mesh point in terms of known 'temperatures' along the jth time-row (Fig. 2.1). Hence we can calculate the unknown pivotal values of u along the first time-row, $t = k$, in terms of known boundary and initial values along $t = 0$, then the unknown pivotal values along the second time-row in terms of the calculated pivotal values along the first, and so on. A formula such as this which expresses *one* unknown pivotal value directly in terms of known pivotal values is called an explicit formula.

Example 2.1

As a numerical example let us solve (2.4) given that the ends of the rod are kept in contact with blocks of melting ice and that the

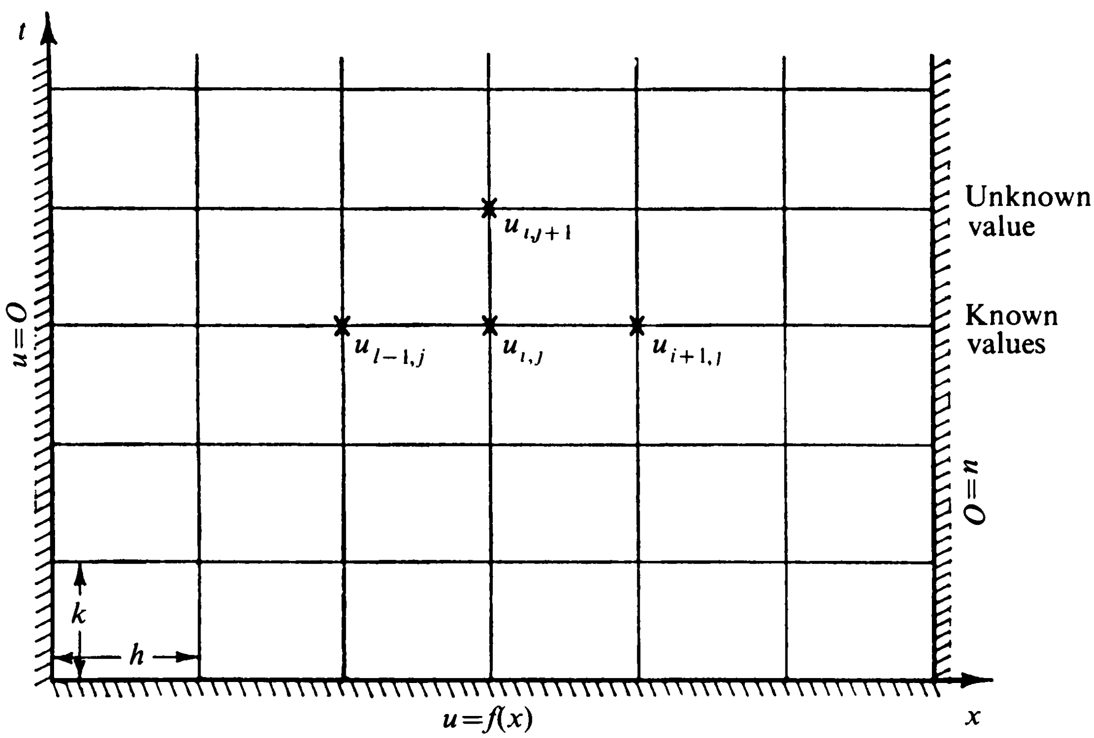

Fig. 2.1

initial temperature distribution in non-dimensional form is

$$\begin{aligned}&\text{(a)}\ U=2x \qquad 0\leqslant x\leqslant\tfrac{1}{2},\\&\text{(b)}\ U=2(1-x),\ \tfrac{1}{2}\leqslant x\leqslant 1.\end{aligned} \tag{2.5}$$

In other words, we are seeking a numerical solution of $\partial U/\partial t = \partial^2 U/\partial x^2$ which satisfies

(i) $U=0$ at $x=0$ and 1 for all $t>0$. (The boundary condition.)

(ii) $U=2x$ for $0\leqslant x\leqslant\frac{1}{2}$ and $U=2(1-x)$ for $\frac{1}{2}\leqslant x\leqslant 1$. $\Big\}$ $t=0$. (The initial condition.)

(This initial temperature distribution could be obtained by heating the centre of the rod for a long time and keeping the ends in contact with the ice.)

For $\delta x = h = \frac{1}{10}$, the initial values and boundary values are as shown in Table 2.1. The problem is symmetric with respect to $x=\frac{1}{2}$ so we need the solution only for $0\leqslant x\leqslant\frac{1}{2}$.

Case 1

Take $\delta x = h = \frac{1}{10}$, $\delta t = k = \frac{1}{1000}$, so $r = k/h^2 = \frac{1}{10}$. Equation (2.4) then reads as

$$u_{i,j+1} = \tfrac{1}{10}(u_{i-1,j} + 8u_{i,j} + u_{i+1,j}). \tag{2.6}$$

For pencil and paper calculations the relationship between these four function values is represented very conveniently by the 'molecule' in Fig. 2.2. The numbers in the 'atoms' are the multipliers of the function values at the corresponding mesh points.

Application of eqn (2.6) to the data of Table 2.1 is shown in Table 2.2, and readers are recommended to check some of the

TABLE 2.1

t \ x	$x=0$	0.1	0.2	0.3	0.4	0.5	0.6
$j=0$	0	0.2	0.4	0.6	0.8	1.0	0.8
$j=1$	0						
$j=2$	0						
$j=3$	0						
$j=4$	0						

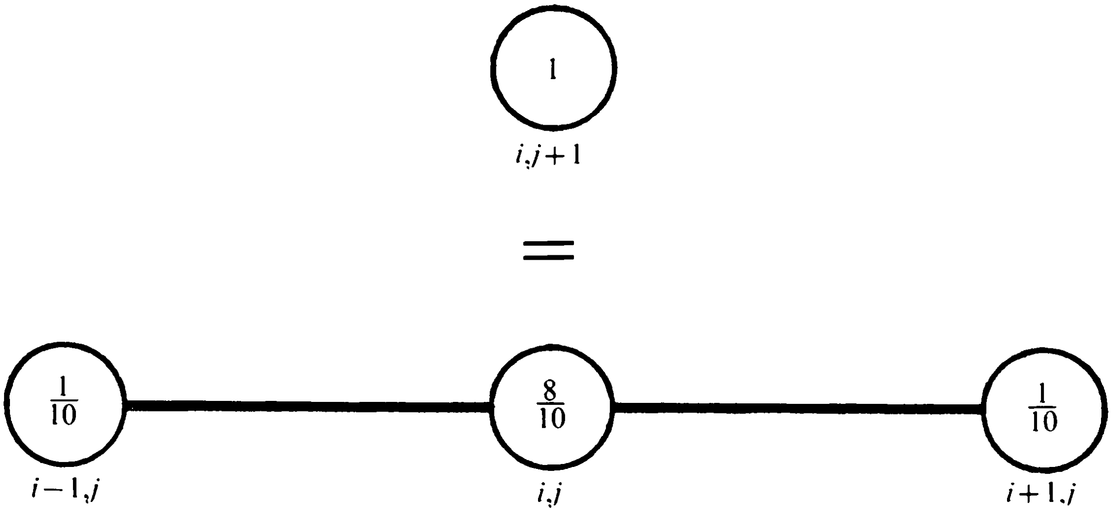

Fig. 2.2

calculations, remembering that the values of U at $x = \frac{4}{10}$ and $\frac{6}{10}$ are equal because of symmetry. (Increasing values of t, i.e. of j, are shown moving downwards for convenience of calculation.) As examples,

$$u_{5,1} = \tfrac{1}{10}\{0.8 + (8 \times 1) + 0.8\} = 0.9600.$$

$$u_{4,2} = \tfrac{1}{10}\{0.6 + (8 \times 0.8) + 0.96\} = 0.7960.$$

The analytical solution of the partial differential equation satisfying these conditions is

$$U = \frac{8}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} (\sin \tfrac{1}{2} n\pi)(\sin n\pi x) \exp(-n^2\pi^2 t).$$

TABLE 2.2

	$i=0$ $x=0$	$i=1$ 0.1	$i=2$ 0.2	$i=3$ 0.3	$i=4$ 0.4	$i=5$ 0.5	$i=6$ 0.6
$(j=0)\,t=0.000$	0	0.2000	0.4000	0.6000	0.8000	1.0000	0.8000
$(j=1)$ 0.001	0	0.2000	0.4000	0.6000	0.8000	0.9600	0.8000
$(j=2)$ 0.002	0	0.2000	0.4000	0.6000	0.7960	0.9280	0.7960
$(j=3)$ 0.003	0	0.2000	0.4000	0.5996	0.7896	0.9016	0.7896
$(j=4)$ 0.004	0	0.2000	0.4000	0.5986	0.7818	0.8792	0.7818
$(j=5)$ 0.005	0	0.2000	0.3999	0.5971	0.7732	0.8597	0.7732
⋮							
$(j=10)$ 0.01	0	0.1996	0.3968	0.5822	0.7281	0.7867	0.7281
⋮							
$(j=20)$ 0.02	0	0.1938	0.3781	0.5373	0.6486	0.6891	0.6486

TABLE 2.3

	Finite-difference solution ($x=0.3$)	Analytical solution ($x=0.3$)	Difference	Percentage error
$t=0.005$	0.5971	0.5966	0.0005	0.08
$t=0.01$	0.5822	0.5799	0.0023	0.4
$t=0.02$	0.5373	0.5334	0.0039	0.7
$t=0.10$	0.2472	0.2444	0.0028	1.1

Comparison of this solution with the finite-difference one at $x=0.3$, as given above, shows that the finite-difference solution is reasonably accurate. The percentage error is the difference of the solutions expressed as a percentage of the analytical solution of the partial differential equation.

The comparison at $x=0.5$ is not quite so good because of the discontinuity in the initial value of $\partial U/\partial x$, from $+2$ to -2, at this point (eqn 2.5). Inspection of Table 2.4 shows, however, that the effect of this discontinuity dies away as t increases.

It can be proved analytically that when the boundary values are constant the effect of discontinuities in initial values and initial derivatives upon the solution of a parabolic equation decreases as t increases.

An examination of Tables 2.19 and 2.21 given in Exercise 1 at the end of this chapter shows that the same finite-difference solution for a problem in which the initial function and all its derivatives are continuous is very close indeed to the solution of the partial differential equation.

Richtmyer, reference 25, has shown for this particular finite-difference scheme that when the initial function and its first $(p-1)$ derivatives are continuous and the pth derivative ordinar-

TABLE 2.4

	Finite-difference solution ($x=0.5$)	Analytical solution ($x=0.5$)	Difference	Percentage error
$t=0.005$	0.8597	0.8404	0.0193	2.3
$t=0.01$	0.7867	0.7743	0.0124	1.6
$t=0.02$	0.6891	0.6809	0.0082	1.2
$t=0.10$	0.3056	0.3021	0.0035	1.2

TABLE 2.5

	$i=0$	1	2	3	4	5	6
	$x=0$	0.1	0.2	0.3	0.4	0.5	0.6
$T=0.000$	0	0.2000	0.4000	0.6000	0.8000	1.0000	0.8000
0.005	0	0.2000	0.4000	0.6000	0.8000	0.8000	0.8000
0.010	0	0.2000	0.4000	0.6000	0.7000	0.8000	0.7000
0.015	0	0.2000	0.4000	0.5500	0.7000	0.7000	0.7000
0.020	0	0.2000	0.3750	0.5500	0.6250	0.7000	0.6250
⋮							
0.100	0	0.0949	0.1717	0.2484	0.2778	0.3071	0.2778

ily discontinuous (i.e. changes by finite jumps), then the difference between the solution of the partial differential equation and a convergent solution of the difference equation is of order $(\delta t)^{(p+2)/(p+4)}$, for small δt.

In this example, $p=1$, so the difference is of order $(\delta t)^{\frac{3}{5}}$. As $(0.001)^{\frac{3}{5}}=0.016$, it is seen that the finite-difference solution is actually better than the estimate indicates, a feature common to most error estimates. When all the derivatives are continuous, $p\to\infty$, and the error is of order δt.

Case 2

Take $\delta x=h=\frac{1}{10}$, $\delta t=k=\frac{5}{1000}$, so $r=k/h^2=0.5$. Then eqn (2.4) gives

$$u_{i,j+1}=\tfrac{1}{2}(u_{i-1,j}+u_{i+1,j}), \tag{2.7}$$

and the solution obtained by applying this finite-difference equation to the boundary and initial values is recorded in Table 2.5.

TABLE 2.6

	Finite-difference solution ($x=0.3$)	Analytical solution ($x=0.3$)	Difference	Percentage error
$t=0.005$	0.6000	0.5966	0.0034	0.57
$t=0.01$	0.6000	0.5799	0.0201	3.5
$t=0.02$	0.5500	0.5334	0.0166	3.1
$t=0.1$	0.2484	0.2444	0.0040	1.6

It is seen that this finite-difference solution is not quite as good an approximation to the solution of the partial differential equation as the previous one; nevertheless it would be adequate for most technical purposes.

Case 3

Take $\delta x = \frac{1}{10}$, $\delta t = \frac{1}{100}$, so $r = \delta t/(\delta x)^2 = 1$. Then eqn (2.4) gives

$$u_{i,j+1} = u_{i-1,j} - u_{i,j} + u_{i+1,j}, \tag{2.9}$$

and the solution of this finite-difference scheme is as below.

TABLE 2.7

	$i=0$	1	2	3	4	5	6
	$x=0$	0.1	0.2	0.3	0.4	0.5	0.6
$t=0.00$	0	0.2	0.4	0.6	0.8	1.0	0.8
0.01	0	0.2	0.4	0.6	0.8	0.6	0.8
0.02	0	0.2	0.4	0.6	0.4	1.0	0.4
0.03	0	0.2	0.4	0.2	1.2	−0.2	1.2
0.04	0	0.2	0.0	1.4	−1.2	2.6	−1.2

Considered as a solution of the partial differential equation this is obviously meaningless, although it is, of course, the correct solution of eqn (2.9) with respect to the initial values and boundary values given.

These three cases clearly indicate that the value of r is important and it will be proved later that this explicit method is valid only for $0 < r \leqslant \frac{1}{2}$. The conditions that must be satisfied for a valid solution are dealt with both descriptively and analytically later in this chapter under the headings of convergence, stability, and consistency. Any reader who would prefer to have an introduction to these concepts at this stage could do so by reading the descriptive treatments of these topics as they are independent of the remainder of this chapter.

The graphs opposite compare the analytical solution of the partial differential equation (shown as continuous curves) with the finite-difference solution (shown by dots) for values of r just below and above $\frac{1}{2}$, and the same number of time-steps.

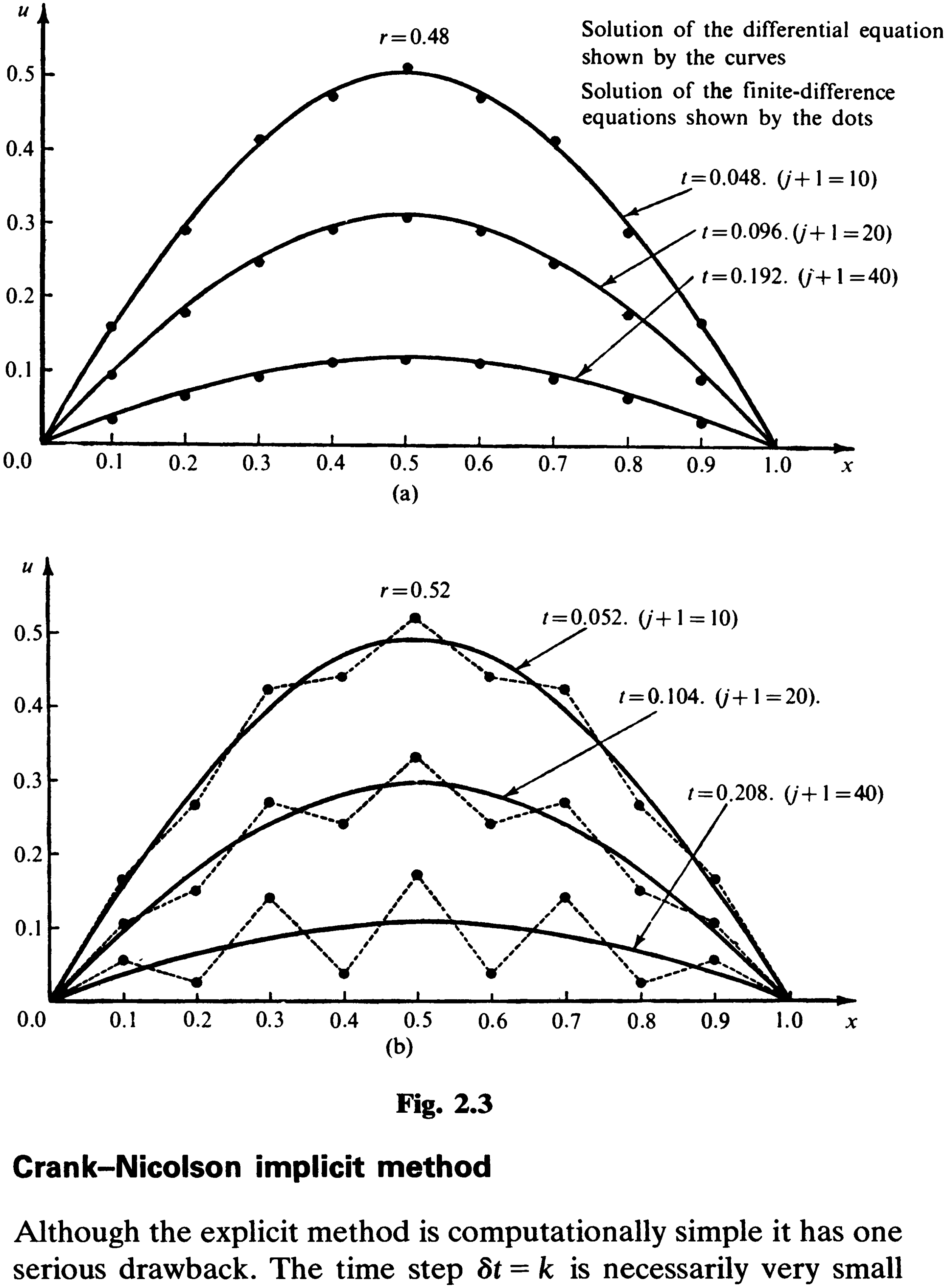

Fig. 2.3

Crank–Nicolson implicit method

Although the explicit method is computationally simple it has one serious drawback. The time step $\delta t = k$ is necessarily very small because the process is valid only for $0 < k/h^2 \leqslant \frac{1}{2}$, i.e. $k \leqslant \frac{1}{2}h^2$, and $h = \delta x$ must be kept small in order to attain reasonable accuracy. Crank and Nicolson (1947) proposed, and used, a method that reduces the total volume of calculation and is valid (i.e., convergent and stable) for all finite values of r. They considered the