unwanted finite oscillations into the numerical solution. Such oscillations die away only very slowly with increasing j, and usually occur in the x-neighbourhood of points of discontinuity in the initial values or between initial values and boundary values.

Solution of the equations by Gauss's elimination method (without pivoting)

When there are $N-1$ internal mesh points along each time row the Crank–Nicolson equations (2.10) can be written very generally as

$$
\begin{aligned}
&+b_1u_1-c_1u_2 &&= d_1,\\
&-a_2u_1+b_2u_2-c_2u_3 &&= d_2,\\
&\quad\cdot\quad\cdot\quad\cdot &&\\
&\qquad\quad\cdot\quad\cdot\quad\cdot &&\\
&\qquad\qquad -a_iu_{i-1}+b_iu_i-c_iu_{i+1} &&= d_i,\\
&\qquad\qquad\qquad\quad\cdot\quad\cdot\quad\cdot &&\\
&\qquad\qquad\qquad\qquad -a_{N-1}u_{N-2}+b_{N-1}u_{N-1} &&= d_{N-1},
\end{aligned}
$$

where the a's, b's, c's, and d's are known. The first equation can be used to eliminate u_1 from the second equation, the new second equation used to eliminate u_2 from the third equation and so on, until finally, the new last but one equation can be used to eliminate u_{N-2} from the last equation, giving one equation with only one unknown, u_{N-1}. The unknowns u_{N-2}, $u_{N-3}, \ldots u_2$, u_1 can then be found in turn by back-substitution. Noting that the coefficient c in each new equation is the same as in the corresponding old equation, assume that the following stage of the eliminations has been reached,

$$\alpha_{i-1}u_{i-1}-c_{i-1}u_i=S_{i-1},$$

$$-a_iu_{i-1}+b_iu_i-c_iu_{i+1}=d_i,$$

where $\alpha_1=b_1$, $S_1=d_1$.

Eliminating u_{i-1} leads to

$$\left(b_i-\frac{a_ic_{i-1}}{\alpha_{i-1}}\right)u_i-c_iu_{i+1}=d_i+\frac{a_iS_{i-1}}{\alpha_{i-1}},$$

i.e.

$$\alpha_iu_i-c_iu_{i+1}=S_i, \tag{2.12}$$

where
$$\alpha_i = b_i - \frac{a_i c_{i-1}}{\alpha_{i-1}} \quad \text{and} \quad S_i = d_i + \frac{a_i S_{i-1}}{\alpha_{i-1}} \quad (i = 2, 3, \ldots).$$

The last pair of simultaneous equations are

$$\alpha_{N-2} u_{N-2} - c_{N-2} u_{N-1} = S_{N-2}$$

and

$$-a_{N-1} u_{N-2} + b_{N-1} u_{N-1} = d_{N-1}.$$

Elimination of u_{N-2} gives

$$\left(b_{N-1} - \frac{a_{N-1} c_{N-2}}{\alpha_{N-2}}\right) u_{N-1} = d_{N-1} + \frac{a_{N-1} S_{N-2}}{\alpha_{N-2}},$$

i.e.

$$\alpha_{N-1} u_{N-1} = S_{N-1}, \tag{2.13}$$

Equations (2.12) and (2.13) show that the solution can be calculated from

$$u_{N-1} = \frac{S_{N-1}}{\alpha_{N-1}},$$

$$u_i = \frac{1}{\alpha_i}(S_i + c_i u_{i+1}) \quad (i = N-2, N-3, \ldots, 1),$$

where the α's and S's are given recursively by

$$\alpha_1 = b_1; \quad \alpha_i = b_i - \frac{a_i}{\alpha_{i-1}} c_{i-1},$$

$$S_1 = d_1; \quad S_i = d_i + \frac{a_i}{\alpha_{i-1}} S_{i-1} \quad (i = 2, 3, \ldots, N-1).$$

In many problems α_i and a_i/α_{i-1} are independent of time and need only be calculated once, irrespective of the number of time-steps.

As an illustration consider the last worked example for which the equations were

$$4u_1 - u_2 = 0.4,$$

$$-u_1 + 4u_2 - u_3 = 0.8,$$

$$-u_2 + 4u_3 - u_4 = 1.2,$$

$$-u_3 + 4u_4 - u_5 = 1.6,$$

$$-2u_4 + 4u_5 = 1.6.$$

Hence

$$a_2=a_3=a_4=1,\ a_5=2,\ b_1=b_2=b_3=b_4=b_5=4;$$

$$c_1=c_2=c_3=c_4=1;\ d_1=0.4,\ d_2=0.8,\ d_3=1.2,\ d_4=d_5=1.6,$$

so

$$\alpha_1=b_1=4; \quad \alpha_i=b_i-\frac{a_i}{\alpha_{i-1}}c_{i-1}=4-\frac{a_i}{\alpha_{i-1}} \quad (i=2, 3, 4, 5),$$

giving the following coefficients which are invariant for every time-step.

$$\alpha_1=4,$$

$$\frac{a_2}{\alpha_1}=\frac{1}{4}=0.25, \qquad \alpha_2=4-\frac{a_2}{\alpha_1}=3.75,$$

$$\frac{a_3}{\alpha_2}=\frac{1}{3.75}=0.2667, \qquad \alpha_3=4-\frac{a_3}{\alpha_2}=3.7333,$$

$$\frac{a_4}{\alpha_3}=\frac{1}{3.7333}=0.2679, \qquad \alpha_4=4-\frac{a_4}{\alpha_3}=3.7321,$$

$$\frac{a_5}{\alpha_4}=\frac{2}{3.7321}=0.5359, \qquad \alpha_5=4-\frac{a_5}{\alpha_4}=3.4641.$$

As

$$S_1=d_1=0.4 \quad \text{and} \quad S_i=d_i+\frac{a_i}{\alpha_{i-1}}S_{i-1} \quad (i=2, 3, 4, 5),$$

$$S_1=0.4,$$

$$S_2=0.8+\frac{a_2}{\alpha_1}S_1=0.8+(0.25)(0.4)=0.9,$$

$$S_3=1.2+\frac{a_3}{\alpha_2}S_2=1.4400,$$

$$S_4=1.6+\frac{a_4}{\alpha_3}S_3=1.9858,$$

$$S_5=1.6+\frac{a_5}{\alpha_4}S_4=2.6642,$$

and the solution for the first time-step is

$$u_5 = \frac{S_5}{\alpha_5} = 0.7691,$$

$$u_4 = \frac{1}{\alpha_4}(S_4 + c_4 u_5) = 0.7381,$$

$$u_3 = \frac{1}{\alpha_3}(S_3 + c_3 u_4) = 0.5834,$$

$$u_2 = \frac{1}{\alpha_2}(S_2 + c_2 u_3) = 0.3956,$$

$$u_1 = \frac{1}{\alpha_1}(S_1 + c_1 u_2) = 0.1989.$$

A comment on the stability of the elimination method

The non-pivoting elimination method previously described for solving the set of linear equations $\mathbf{Au} = \mathbf{d}$, with a tridiagonal matrix $\mathbf{A}$, is always stable, that is, with no growth of rounding errors, if

(i) $a_i > 0$, $b_i > 0$ and $c_i > 0$,

(ii) $b_i > a_{i+1} + c_{i-1}$ for $i = 1, 2, \ldots, N-1$, defining $c_0 = a_N = 0$, and

(iii) $b_i > a_i + c_i$ for $i = 1, 2, \ldots, N-1$, defining $a_1 = c_{N-1} = 0$.

Conditions (i) and (ii), which ensure that the forward elimination is stable, state that the diagonal element must exceed the sum of the moduli of the other elements in the same column of the matrix $\mathbf{A}$ of coefficients. Conditions (i) and (iii), which ensure that the back substitution is stable, state that the diagonal element must exceed the sum of the moduli of the other elements in the same row. When these conditions are satisfied the algorithm is a very efficient one for programming on a digital computer, using a minimum of storage space.

Proof

To prove that the forward elimination procedure is stable it is necessary to show that the moduli of the multipliers $m_i = a_i/\alpha_{i-1}$

used to eliminate $u_1, u_2, \ldots,$ are $\leqslant 1$. By p. 25.

$$\alpha_i = b_i - \frac{a_i c_{i-1}}{\alpha_{i-1}} = b_i - m_i c_{i-1},$$

Therefore,

$$m_{i+1} = \frac{a_{i+1}}{\alpha_i} = \frac{a_{i+1}}{b_i - m_i c_{i-1}}.$$

Hence,

$$0 < m_2 < \frac{a_2}{b_1} < 1 \quad \text{since} \quad b_1 > a_2 > 0 = c_0.$$

Similarly,

$$\begin{aligned} 0 < m_3 &= \frac{a_3}{b_2 - m_2 c_1} \quad \text{since} \quad a_3 > 0, b_2 > c_1 \text{ and } 0 < m_2 < 1, \\ &< \frac{a_3}{b_2 - c_1} \quad \text{since} \quad c_1 > 0, \\ &< \frac{a_3}{(a_3 + c_1) - c_1} = 1 \quad \text{since} \quad b_2 > a_3 + c_1. \end{aligned}$$

In this way, $0 < m_4, m_5, \ldots, m_{N-1} < 1$. The stability of the back substitution is proved in Exercise 4, Chapter 2.

A weighted average approximation

A more general finite-difference approximation to $\partial U/\partial t = \partial^2 U/\partial x^2$ than those considered is given by

$$\frac{u_{i,j+1} - u_{i,j}}{\delta t} = \frac{1}{(\delta x)^2}\{\theta(u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}) + (1-\theta) \\ \times (u_{i+1,j} - 2u_{i,j} + u_{i-1,j})\},$$

where, in practice, $0 \leqslant \theta \leqslant 1$. For readers familiar with finite-difference notation this replacement approximates the partial differential equation at the point $\{i\delta x, (j+\frac{1}{2})\delta t\}$ by the difference equation

$$\frac{1}{\delta t}\,\delta_t u_{i,j+\frac{1}{2}} = \frac{1}{(\delta x)^2}\{\theta \delta_x^2 u_{i,j+1} + (1-\theta)\delta_x^2 u_{i,j}\},$$

where the subscripts t and x denote differencing in the t- and x-directions respectively. $\theta=0$ gives the explicit scheme, $\theta=\frac{1}{2}$ the Crank–Nicolson, and $\theta=1$ a fully implicit backward time-difference method. The equations are unconditionally valid, i.e. stable and convergent for $\frac{1}{2}\leqslant\theta\leqslant 1$, but for $0\leqslant\theta<\frac{1}{2}$ we must have

$$r=\frac{\delta t}{(\delta x)^2}\leqslant\frac{1}{2(1-2\theta)}. \quad \text{(See Exercise 20, Chapter 2.)}$$

Derivative boundary conditions

Boundary conditions expressed in terms of derivatives occur very frequently in practice. When, for example, the surface of a heat-conducting material is thermally insulated, there is no heat flow normal to the surface and the corresponding boundary condition is $\partial U/\partial n=0$ at every point of the insulated surface, where the differentiation of the temperature U is in the direction of the normal to the surface. Similarly, the rate at which heat is transferred by radiation from an external surface at temperature U into a surrounding medium at temperature v is often assumed to be proportional to $(U-v)$. As the fundamental assumption of heat-conduction theory is that the rate of flow across any surface is equal to $-K\partial U/\partial n$ units of heat per unit time in the direction of the outward normal, the corresponding boundary condition for surface radiation is

$$-K\frac{\partial U}{\partial n}=H(U-v).$$

The constant K is the thermal conductivity of the material and the constant H its coefficient of surface heat transfer. The negative sign indicates that heat is assumed to flow in the opposite direction to that in which U increases algebraically. This equation can be written as

$$\frac{\partial U}{\partial n}=-h(U-v),$$

where h is a positive constant.

Consider a thin rod that is thermally insulated along its length and which radiates heat from the end $x=0$. The temperature at this end at time t is now unknown and its determination requires an extra equation. This equation can be the boundary condition itself when a forward difference is used for $\partial U/\partial x$, because the boundary condition at $x=0$, the left-hand end, namely,

$$-\frac{\partial U}{\partial x}=-h(U-v),$$

will be represented by

$$\frac{u_{1,j}-u_{0,j}}{\delta x}=h(u_{0,j}-v),$$

giving one extra equation for the temperature $u_{0,j}$. A negative sign must be associated with $\partial U/\partial x$ because the outward normal to the rod at this end is in the negative direction of the x-axis. Alternatively, in the heat-flow law, $-K\partial U/\partial n$ implies that when the positive direction of the x-axis (and of U) is to the *right*, then the quantity of heat flowing from *right to left* across unit area per unit time is $+K\partial U/\partial x$, and this is proportional to the excess temperature at $x=0$.

If we wish to represent $\partial U/\partial x$ more accurately at $x=0$ by a central difference formula it is necessary to introduce the 'fictitious' temperature $u_{-1,j}$ at the external mesh point $(-\delta x, j\delta t)$ (Fig. 2.7), by imagining the rod to be extended a distance δx at this end. The boundary condition can then be represented by

$$\frac{u_{1,j}-u_{-1,j}}{2\delta x}=h(u_{0,j}-v).$$

The temperature $u_{-1,j}$ is unknown and necessitates another equation. This is obtained by assuming that the heat conduction

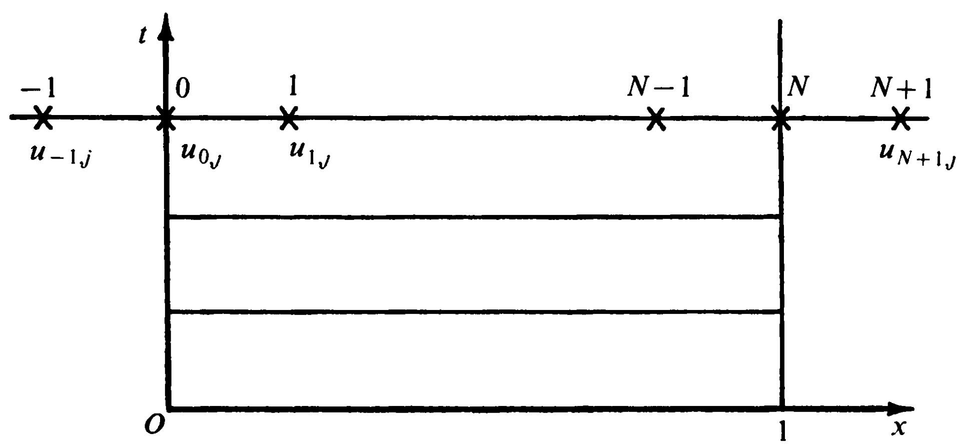

Fig. 2.7

equation is satisfied at the end $x=0$ of the rod. The unknown $u_{-1,j}$ can then be eliminated between these equations. Similar equations can be written down for radiation from the other end of the rod.

These methods are applied below to the problem of the cooling of a homogeneous rod by radiation from its ends into air at a constant temperature, the rod being at a different constant temperature initially.

Example 2.3

Solve the equation

$$\frac{\partial U}{\partial t}=\frac{\partial^2 U}{\partial x^2}, \tag{2.14}$$

satisfying the initial condition,

$$U=1 \text{ for } 0\leqslant x\leqslant 1 \text{ when } t=0,$$

and the boundary conditions,

$$\frac{\partial U}{\partial x}=U \text{ at } x=0, \text{ for all } t,$$

$$\frac{\partial U}{\partial x}=-U \text{ at } x=1, \text{ for all } t,$$

using an explicit method and employing central-differences for the boundary conditions.

One explicit finite-difference representation of eqn (2.14) is

$$\frac{u_{i,j+1}-u_{i,j}}{\delta t}=\frac{u_{i-1,j}-2u_{i,j}+u_{i+1,j}}{(\delta x)^2},$$

i.e.

$$u_{i,j+1}=u_{i,j}+r(u_{i-1,j}-2u_{i,j}+u_{i+1,j}), \tag{2.15}$$

where $r=\delta t/(\delta x)^2$.

At $x=0$,

$$u_{0,j+1}=u_{0,j}+r(u_{-1,j}-2u_{0,j}+u_{1,j}). \tag{2.16}$$

The boundary condition at $x=0$, in terms of central-differences, can be written as

$$\frac{u_{1,j}-u_{-1,j}}{2\delta x}=u_{0,j}. \tag{2.17}$$

Eliminating $u_{-1,j}$ between (2.16) and (2.17) gives

$$u_{0,j+1} = u_{0,j} + 2r\{u_{1,j} - (1+\delta x)u_{0,j}\}. \tag{2.18}$$

Let $\delta x = 0.1$. Then at $x = 1$, eqn (2.15) becomes

$$u_{10,j+1} = u_{10,j} + r(u_{9,j} - 2u_{10,j} + u_{11,j}), \tag{2.19}$$

and the boundary condition is

$$\frac{u_{11,j} - u_{9,j}}{2\delta x} = -u_{10,j}. \tag{2.20}$$

Elimination of the 'fictitious' value $u_{11,j}$ between (2.19) and (2.20) yields

$$u_{10,j+1} = u_{10,j} + 2r\{u_{9,j} - (1+\delta x)u_{10,j}\}. \tag{2.21}$$

This result could have been deduced from the corresponding equation at $x = 0$ because of the symmetry with respect to $x = \frac{1}{2}$.

Later in this chapter this scheme is proved to be valid for $r \leqslant 1/(2 + h\delta x)$, i.e. $r \leqslant 1/2.1$ in this example.

Choose $r = \frac{1}{4}$. The difference equations (2.18), (2.15), then become

$$u_{0,j+1} = \tfrac{1}{2}(0.9u_{0,j} + u_{1,j}),$$

$$u_{i,j+1} = \tfrac{1}{4}(u_{i-1,j} + 2u_{i,j} + u_{i+1,j}) \quad (i = 1, 2, 3, 4),$$

and the use of symmetry rather than eqn (2.21) gives

$$u_{5,j+1} = \tfrac{1}{4}(2u_{4,j} + 2u_{5,j}).$$

As the initial temperature is $u = 1$, the values of u at the end of the first time-step when $t = r(\delta x)^2 = \frac{1}{400}$, are

$$u_{0,1} = \tfrac{1}{2}(0.9 + 1) = 0.95,$$

$$u_{1,1} = \tfrac{1}{4}(1 + 2 + 1) = 1 = u_{2,1} = u_{3,1} = u_{4,1} = u_{5,1},$$

and the values at the end of the second time-step are

$$u_{0,2} = \tfrac{1}{2}(0.9 \times 0.95 + 1) = 0.9275,$$

$$u_{1,2} = \tfrac{1}{4}(0.95 + 2 + 1) = 0.9875,$$

$$u_{2,2} = \tfrac{1}{4}(1 + 2 + 1) = 1 = u_{3,2} = u_{4,2} = u_{5,2}.$$

Similarly for subsequent time-steps. The values for several steps are recorded in Table 2.10.

The analytical solution of the partial differential equation satis-

TABLE 2.10

	$i=0$	1	2	3	4	5
	$x=0$	0.1	0.2	0.3	0.4	0.5
$t=0.0000$	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.0025	0.9500	1.0000	1.0000	1.0000	1.0000	1.0000
$t=0.005$	0.9275	0.9875	1.0000	1.0000	1.0000	1.0000
0.0075	0.9111	0.9756	0.9969	1.0000	1.0000	1.0000
0.0100	0.8978	0.9648	0.9923	0.9992	1.0000	1.0000
0.0125	0.8864	0.9549	0.9872	0.9977	0.9998	1.0000
0.0150	0.8764	0.9459	0.9818	0.9956	0.9993	0.9999
0.0175	0.8673	0.9375	0.9762	0.9931	0.9985	0.9996
0.0200	0.8590	0.9296	0.9708	0.9902	0.9974	0.9991
....						
....						
0.1000	0.7175	0.7829	0.8345	0.8718	0.8942	0.9017
0.2500	0.5542	0.6048	0.6452	0.6745	0.6923	0.6983
0.5000	0.3612	0.3942	0.4205	0.4396	0.4512	0.4551
1.0000	0.1534	0.1674	0.1786	0.1867	0.1917	0.1933

fying these boundary and initial conditions is

$$U=4\sum_{n=1}^{\infty}\left\{\frac{\sec\alpha_n}{(3+4\alpha_n^2)}e^{-4\alpha_n{}^2t}\cos 2\alpha_n(x-\tfrac{1}{2})\right\}\quad(0<x<1),$$

where α_n are the positive roots of

$$\alpha\tan\alpha=\tfrac{1}{2}.$$

Values of U calculated from this analytical solution are recorded in Table 2.11.

The two solutions are compared at $x=0{\cdot}2$ in Table 2.12.

The finite-difference solution is clearly very accurate for this small value of r.

Because of the symmetry with respect to $x=\frac{1}{2}$ the solution above is the same for a rod of length $\frac{1}{2}$, thermally insulated along its length and at $x=\frac{1}{2}$, and which cools by radiation from $x=0$ into a medium at zero temperature.

Example 2.4

Re-solve the Worked Example 2.3 using an explicit method and employing a forward-difference for the boundary condition at $x=0$.