5

Difference Methods for Parabolic Partial Differential Equations

5.1 INTRODUCTION

A number of mathematical models describing the physical systems are the special cases of the general second order partial differential equation

$$L[u] = A\frac{\partial^2 u}{\partial x^2}+2B\frac{\partial^2 u}{\partial x\,\partial y}+C\frac{\partial^2 u}{\partial y^2}-H\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = 0 \qquad (5.1)$$

Equation (5.1) is called *semilinear* if A, B and C are functions of the independent variables x and y only. If A, B and C are functions of x, y, u, $\partial u/\partial x$ and $\partial u/\partial y$, then (5.1) is termed as *quasilinear*.

When A, B and C are functions of x and y, and H is a linear function of u, $\partial u/\partial x$ and $\partial u/\partial y$ then (5.1) is called linear. The most general second order linear partial differential equation in two independent variables x and y can be expressed as

$$A(x, y)\frac{\partial^2 u}{\partial x^2}+2B(x, y)\frac{\partial^2 u}{\partial x\partial y}+C(x, y)\frac{\partial^2 u}{\partial y^2}+D(x, y)\frac{\partial u}{\partial x}$$
$$+E(x, y)\frac{\partial u}{\partial y}+F(x, y)u+G(x, y) = 0 \qquad (5.2)$$

If $G = 0$, the partial differentia! quation is termed as homogeneous, otherwise it is called inhomogeneous.

A solution of (5.1) or (5.2) will be of the form

$$u = u(x, y)$$

which represents a surface in (x, y, u) space called the *integral surface*. If on the integral surfaces there exist curves across which the partial derivatives $\partial^2 u/\partial x^2$, $\partial^2 u/\partial x\partial y$ and $\partial^2 u/\partial y^2$ are discontinuous or indeterminate, the curves are called as *characteristics*. Let us assume that the solution to (5.1) is to pass through a curve Γ whose parameteric equations are

$$x = x(s),\ y = y(s),\ u = u(s) \qquad (5.3)$$

We also assume that at each point (x, y, u) of Γ the partial derivatives $\partial u/\partial x$ and $\partial u/\partial y$ are known. Since the solution will be of the form $u = u(x, y)$, at each point x and y of Γ we have

$$\frac{du}{ds} = \frac{\partial u}{\partial x}\frac{dx}{ds}+\frac{\partial u}{\partial y}\frac{dy}{ds} \tag{5.4}$$

For $\partial u/\partial x = p = p(x, y)$ and $\partial u/\partial y = q = q(x, y)$, we have

$$\frac{dp}{ds} = \frac{\partial p}{\partial x}\frac{dx}{ds}+\frac{\partial p}{\partial y}\frac{dy}{ds} \tag{5.5}$$

$$\frac{dq}{ds} = \frac{\partial q}{\partial x}\frac{dx}{ds}+\frac{\partial q}{\partial y}\frac{dy}{ds} \tag{5.6}$$

Keeping in view the fact that in Equations (5.1), (5.5) and (5.6), the quantities A, B, C, H, dx/ds, dy/ds, p, q, dp/ds and dq/ds at each point of Γ are known, these equations can be treated as three simultaneous equations for the unknowns $\partial^2u/\partial x^2$, $\partial^2u/\partial x\partial y$ and $\partial^2u/\partial y^2$ at each point of Γ. The solution of these equations exists and is unique, unless the determinant

$$\begin{vmatrix} A & 2B & C \\ \frac{dx}{ds} & \frac{dy}{ds} & 0 \\ 0 & \frac{dx}{ds} & \frac{dy}{ds} \end{vmatrix} = 0 \tag{5.7}$$

which may be simplified to give

$$A\left(\frac{dy}{ds}\right)^2-2B\frac{dx}{ds}\frac{dy}{ds}+C\left(\frac{dx}{ds}\right)^2 = 0 \tag{5.8}$$

or

$$\frac{dy}{dx} = \frac{1}{A}[B\pm\sqrt{B^2-AC}] \tag{5.9}$$

Equation (5.9) can be separated into two equations

$$A\,dy-(B+\sqrt{B^2-AC})\,dx = 0 \tag{5.10}$$
$$A\,dy-(B-\sqrt{B^2-AC})\,dx = 0$$

whose solution can be represented as

$$V_1(x, y) = \text{constant},\; V_2(x, y) = \text{constant} \tag{5.11}$$

Thus, there are two families of curves given by (5.11) along which the second order partial derivatives will not be determined in a definite and finite manner. The curves are called the characteristics and they are either real and distinct or real and coincident or imaginary according as

$$B^2-AC > 0,\; B^2-AC = 0 \text{ and } B^2-AC < 0 \tag{5.12}$$

The partial differential equation (5.1) or (5.2) is said to be of *hyperbolic* type at a point in the xy plane if two real distinct families of characteristics exist at that point or $B^2 - AC > 0$; to be of *parabolic* type, if one real and coincident family of characteristics exist or $B^2 - AC = 0$; and to be of *elliptic* type if no real characteristics exist or $B^2 - AC < 0$.

In the general linear case, the coefficients A, B and C may depend upon position, then the type of the equation may also depend upon position. In the quasilinear case, the type of the equation may not only depend upon the position but also upon the behaviour of the solution at that position. However, if A, B and C are constants then the equation is of one type throughout the xy plane.

The well known examples of the three types are:

Heat flow equation

$$\frac{\partial u}{\partial y} = \frac{\partial^2 u}{\partial x^2} \tag{5.13}$$

which is of parabolic type.

Wave equation

$$\frac{\partial^2 u}{\partial y^2} = \frac{\partial^2 u}{\partial x^2} \tag{5.14}$$

which is of hyperbolic type.

Laplace equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{5.15}$$

which is of elliptic type.

The parabolic and hyperbolic type of equations are either initial value problems or initial boundary value problems whereas the elliptic type equation is always a boundary value problem. The boundary conditions can be one of the following three types.

(i) *The Dirichlet or first boundary condition.* Here, the solution is prescribed along the boundary. If the solution takes on zero value along the boundary, the condition is called homogeneous Dirichlet otherwise it is inhomogeneous *Dirichlet* condition.

(ii) *The Neumann or second boundary condition.* Here, the derivative of the solution is specified along the boundary. We may also have homogeneous or inhomogeneous *Neumann* boundary conditions.

(iii) *The third or mixed boundary condition.* Here, the solution and its derivative are prescribed along the boundary. We may also have homogeneous or inhomogeneous mixed boundary conditions.

We assume throughout our discussion that our mathematical problem is *well posed*, i.e. if its solution exists, is unique, and depends continuously on the given data. The most common method of solution of partial differential equations is the finite difference method. We superimpose on the region of interest a network which is generally of the rectangular (square) form. The

partial derivatives in the equ $\sum_j A_j \xi^n(j) \exp(\sqrt{-1}\beta_j mh)$ (5.22)
converting the different
difference equation any real or complex number.
the intersections (equations, the sum of independent solutions is a solution,
we consider a single term

$$\bar{\epsilon}^n_m = A\,\xi^n\, e^{i\beta mh} \tag{5.23}$$

where $i = \sqrt{-1}$, β is any real number and A is an arbitrary constant. In order that the original error $e^{i\beta mh}$ shall not grow as n increases, it is necessary and sufficient that

$$|\,\xi\,| \leqslant 1 \tag{5.24}$$

The equation (5.24) gives the required condition for the stability of the difference scheme.

This method of stability analysis is known as the *von Neumann method* or the finite *Fourier series method.* Substituting (5.23) into (5.20) and simplifying, we obtain

$$\xi - 1 = r(e^{i\beta h} - 2 + e^{-i\beta h})$$

$$= 2r(\cos\beta h - 1) = -4r\sin^2\left(\frac{\beta h}{2}\right)$$

The conditions (5.24) yield

$$-1 \leqslant 1 - 4r\sin^2\left(\frac{\beta h}{2}\right) \leqslant 1$$

The right inequality is satisfied trivially; the left inequality will be satisfied for all β if, and only if,

$$r \leqslant 1/2$$

Thus $r = 1/2$ separates the region of stability, where errors decay, from the region of instability, where some errors grow.

Next we consider the difference schemes for the general heat flow equation of the form

$$\frac{\partial u}{\partial t} = L^* u \tag{5.25}$$

where L^*u is a differential operator in u, which contains only partial derivatives with respect to the space coordinates $x_1, x_2, \ldots, x_s$ and coefficients which may either be constants or functions of both space and time variables. We will only be interested in (5.25) when, together with appropriate initial and boundary conditions, it consitutes a *well posed* problem.

In general, the unknown $u(\mathbf{x}, t) = u(x_1, x_2, \ldots, x_s, t)$ may be either a scalar or a vector function. The solution of (5.25) is required in an arbitrary region $\mathcal{R} \times [0, T]$ with suitable boundary conditions on $\partial\mathcal{R} \times [0, T]$ where $\mathcal{R}$ is normally a closed region in $x_1, x_2, \ldots, x_s$, space, $\partial\mathcal{R}$ is the boundary of $\mathcal{R}$, and

[0, T] is the time interval $0 \leqslant t \leqslant T$. Now, we ·d by u_m^n. An implicit dif-
rectilinear grid with grid lines parallel to coordine grid point at time grid
k in space and time directions, respectively. 1) for (5.33) becomes

The grid times are given by $t = nk$, $n = 0, 1, 2, \ldots$
The set of mesh points on $\partial\mathcal{R}$ (i.e. those points which a (5.36)
tersection of the grid lines with the boundary $\partial\mathcal{R}$) will be
The mesh points in the region $\mathcal{R}$ form the set $\mathcal{R}_h$. The space n
nth time grid constitute the nth layer or level. Let $u(x_1, x_2, \ldots, x_s, t_{n+1})$ de
the solution to (5.25) at the $(n+1)$th layer. Then, since

$$\frac{\partial}{\partial t} = -k^{-1} \log(1 - \nabla_t)$$

it follows that (5.25) becomes

$$-k^{-1} \log(1 - \nabla_t) u(x, t_{n+1}) = L^* u(x, t_{n+1}) \tag{5.26}$$

where ∇_t is the backward difference operator.

This is a discrete analogue of (5.25) and our difference schemes will be approximations of (5.26). The construction of our difference schemes will involve two distinct parts. First, we approximate in the time direction, i.e. a function $F(\nabla_t)$ is constructed such that

$$\begin{aligned} k^{-1}[-\log(1-\nabla_t) - F(\nabla_t)] &= (k^{-1} \nabla_t^{\sigma_1+1}) \\ &= 0(k^{\sigma_1}) \end{aligned} \tag{5.27}$$

where $\sigma_1 \geqslant 1$. Next, approximation in the space direction, L_h^* is obtained such that

$$[L^* - h^{-\sigma_2} L_h^*]\, u(x, t_{n+1}) \mp 0(h^{\sigma_3}) \tag{5.28}$$

where σ_2 is some integer and $\sigma_3 \geqslant 1$. Substituting (5.27) and (5.28) into (5.26), we obtain

$$k^{-1}F(\nabla_t)u(x, t_{n+1}) - h^{-\sigma_2} L_h^* u(x, t_{n+1}) + 0(k^{\sigma_1} + h^{\sigma_3}) = 0 \tag{5.29}$$

or

$$\begin{aligned} F(\nabla_t)\, u(x, t_{n+1}) - \frac{k}{h^{\sigma_2}} L_h^*\, u(x, t_{n+1}) \\ = 0(k^{\sigma_1+1} + k\, h^{\sigma_3}) \end{aligned} \tag{5.30}$$

The first nonzero term on the right side of (5.30) is called the *principal part* of the local truncation error. Neglecting the trunction error in (5.30), we obtain the difference scheme at a nodal point (x, t_{n+1}) as

$$F(\nabla_t)u^{n+1} - rL_h^* u^{n+1} = 0 \tag{5.31}$$

where u^{n+1} is an approximate value of $u(x, t)$ at $t = t_{n+1}$. The difference scheme (5.31) will have a truncation error of $0(k^{\sigma_1} + h^{\sigma_3})$. The quantity $r = k/h^{\sigma_2}$ for some integer σ_2 is known as the mesh ratio. If we write (5.31) as a difference scheme which involves only one grid point at time grid $t = (n+1)k$,

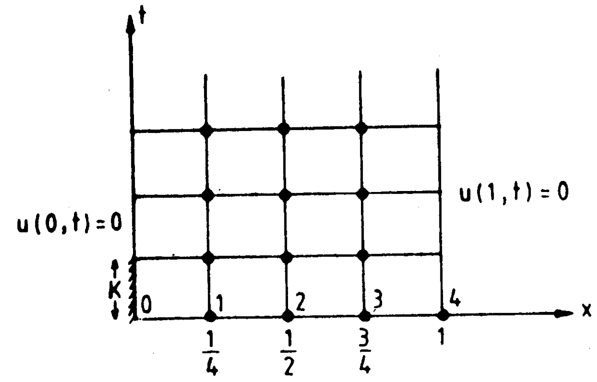

Fig. 5.1(a) Representation of nodal points

Now we obtain,

for $n = 0, m = 1, 2, 3;$

$$u_1^1 = \frac{1}{6}(u_0^0+4u_1^0+u_2^0) = \frac{1}{6}\left(0+4\sin\frac{\pi}{4}+\sin\frac{\pi}{2}\right)$$

$$u_1^1 = .6380711$$

$$u_2^1 = \frac{1}{6}(u_1^0+4u_2^0+u_3^0) = \frac{1}{6}\left(\sin\frac{\pi}{4}+4\sin\frac{\pi}{2}+\sin\frac{3\pi}{4}\right)$$

$$u_2^1 = .9023689$$

$$u_3^1 = \frac{1}{6}(u_2^0+4u_3^0+u_4^0) = \frac{1}{6}\left(\sin\frac{\pi}{2}+4\sin\frac{3\pi}{4}\right)$$

$$u_3^1 = .6380711$$

for $n = 1, m = 1, 2, 3;$

$$u_1^2 = \frac{1}{6}(u_0^1+4u_1^1+u_2^1) = \frac{1}{6}(4(.6380711)+.9023689)$$

$$u_1^2 = .5757755$$

$$u_2^2 = \frac{1}{6}(u_1^1+4u_2^1+u_3^1) = \frac{1}{6}(.6380711+4(.9023689)+.6380711)$$

$$u_2^2 = .8142696$$

$$u_3^2 = \frac{1}{6}(u_2^1+4u_3^1+u_4^1) = \frac{1}{6}(.9023689+4(.6380711))+0)$$

$$u_3^2 = .5757755$$

The solution $u(x, t)$ is symmetric about the line $x = 1/2$.

5.3.2 Multilevel explicit difference schemes

The general three level explicit difference scheme for (5.33) will involve seven points (see Figure 5.1b) and may be written as

$$(1-\gamma_1^*\nabla_t)^{-1}(\nabla_t+\tau_1^*\nabla_t^2)\,u_m^{n+1} = r\delta_x^2 u_m^n \qquad (5.39)$$

or $$(1+\tau_1^*)u_m^{n+1} = [1+2\tau_1^*+r(1-\gamma_1^*)\delta_x^2]u_m^n-(\tau_1^*-r\gamma_1^*\delta_x^2)u_m^{n-1} \tag{5.40}$$

where τ_1^* and γ_1^* are arbitrary parameters. The truncation error of (5.40) is given by

$$T_m^{*n} = (\nabla_t+\tau_1^*\nabla_t^2)u(x_m, t_{n+1})-r\delta_x^2(1-\gamma_1^*\nabla_t)u(x_m, t_n) \tag{5.41}$$

where $u(x_m, t_n)$ satisfies (5.33)

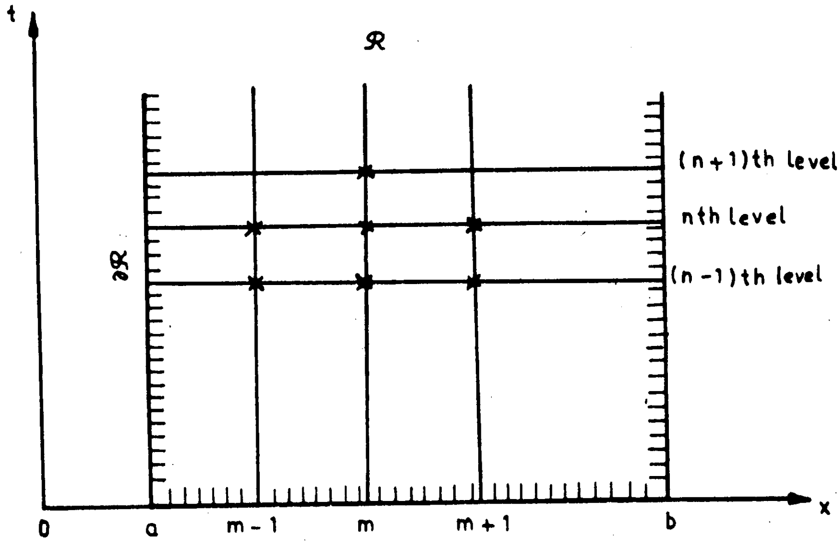

Fig. 5.1(b) Grid points of the three level explicit methods

Expanding (5.41) in the Taylor series in terms of $u(x_m, t_n)$ and its derivatives and replacing the derivatives involving t by the relation

$$\frac{\partial^{p+q}u(x, t)}{\partial x^p\,\partial t^q} = \frac{\partial^{p+2q}u(x, t)}{\partial x^{p+2q}} \tag{5.42}$$

we obtain $$T_m^{*n} = k\left[\left(\tau_1^*+\gamma_1^*+\frac{1}{2}\right)k-\frac{1}{12}h^2\right]\left(\frac{\partial^4 u}{\partial x^4}\right)_m^n + k\left[\frac{1}{2}\left(-\gamma_1^*+\frac{1}{3}\right)k^2+\frac{1}{12}\gamma_1^*kh^2-\frac{1}{360}h^4\right]\left(\frac{\partial^6 u}{\partial x^6}\right)_m^n+\cdots \tag{5.43}$$

Thus, we find that the difference scheme (5.40) has the truncation error of order

(i) $(k+h^2)$ if γ_1^* and τ_1^* are arbitrary,

(ii) (k^2+h^2) if $\tau_1^*+\gamma_1^*+\frac{1}{2} = 0$ and either γ_1^* or τ_1^* is arbitrary,

(iii) (h^4) if $\tau_1^*+\gamma_1^*+\frac{1}{2}-\frac{1}{12r} = 0$ and either γ_1^* or τ_1^* is arbitrary. (5.44)

Alternatively, we may write (5.56) as

$$\frac{1}{2}\left(1+\frac{1}{6r}\right)u_m^{n+1} = r(u_{m-1}^n+u_{m+1}^n)-\left(2r-\frac{1}{6r}\right)u_m^n+\frac{1}{2}\left(1-\frac{1}{6r}\right)u_m^{n-1}$$

For the values $\tau_1^* = 0$ and $\gamma_1^* = -1/2+1/12r$, we get the difference formula

$$\nabla_t u_m^{n+1} = r\delta_x^2\left[1-\left(-\frac{1}{2}+\frac{1}{12r}\right)\nabla_t\right]u_m^n \tag{5.57}$$

or

$$u_m^{n+1} = \left(\frac{7}{6}-3r\right)u_m^n+\frac{1}{2}\left(3r-\frac{1}{6}\right)(u_{m-1}^n+u_{m+1}^n) - \frac{1}{2}\left(r-\frac{1}{6}\right)(u_{m-1}^{n-1}-2u_m^{n-1}+u_{m+1}^{n-1})$$

which is stable if $0 < r \leqslant 1/3$. The truncation error becomes $0(h^6)$ if $r = 1/10$.

Further, we choose

$$G(\nabla_t) = (1+\sum_{p=1}^{s}(-1)^p\gamma_p^*\nabla_t^p)^{-1}[\nabla_t+\sum_{p=1}^{q}\tau_p^*\nabla_t^{p+1}] \tag{5.58}$$

in (5.34) where τ_p^* and γ_p^* are arbitrary parameters. Thus our difference scheme (5.34) subject to (5.58) is a $(q+2)$-level scheme for $(q \geqslant s)$ with truncation error of $0(k+h^2)$. Table 5.1 presents the Padé approximations of $[-(1-\nabla_t)\log(1-\nabla_t)]$ through $q = 3$ and $s = 2$.

From Theorem 3.1, we know that the accuracy of the stable $(q+1)$-level explicit difference scheme (5.34) cannot exceed q in the time direction. The values $\tau_1^* = -5/6$, $\gamma_1^* = 1/3$ give a three level explicit difference scheme

$$\left(\nabla_t-\frac{5}{6}\nabla_t^2\right)u_m^{n+1} = r\delta_x^2\left(1-\frac{1}{3}\nabla_t\right)u_m^n$$

which has truncation error of order (k^3+h^2), and it is an unstable scheme. We now give a few $(q+2)$-level schemes of order $(k^{q+1}+h^2)$. The values $\tau_p^* = 0$, $1 \leqslant p \leqslant q$, give the Adams-Bashforth type difference schemes

$$\nabla_t u_m^{n+1} = r\delta_x^2\left(1+\frac{1}{2}\nabla_t+\frac{5}{12}\nabla_t^2+\frac{3}{8}\nabla_t^3+\cdots\right)u_m^n \tag{5.59}$$

A four level difference scheme is given by

$$\nabla_t u_m^{n+1} = r\delta_x^2\left(1+\frac{1}{2}\nabla_t+\frac{5}{12}\nabla_t^2\right)u_m^n = \frac{1}{12}r\delta_x^2(23u_m^n-16u_m^{n-1}+5u_m^{n-2})$$

If we choose the parameters $\tau_p^* = 0$, $2 \leqslant p \leqslant q$ and $\gamma_1^* = 0$, we obtain multilevel difference scheme of the Adams-Nystrom type

$$\left(\nabla_t-\frac{1}{2}\nabla_t^2\right)u_m^{n+1} = r\delta_x^2\left[1+0\nabla_t+\frac{1}{6}\nabla_t^2+\frac{1}{6}\nabla_t^3+\frac{29}{180}\nabla_t^4\cdots\right]u_m^n$$

TABLE 5.1 PADE' APPROXIMATION TO $[-(1-\nabla_t)\log(1-\nabla_t)]$

$s \backslash q$	0	1	2	3
0	∇_t	$\nabla_t-\frac{1}{2}\nabla_t^2$	$\nabla_t-\frac{1}{2}\nabla_t^2-\frac{1}{6}\nabla_t^3$	$\nabla_t-\frac{1}{2}\nabla_t^2-\frac{1}{6}\nabla_t^3-\frac{1}{12}\nabla_t^4$
1	$\dfrac{\nabla_t}{1+\frac{1}{2}\nabla_t}$	$\dfrac{\nabla_t-\frac{5}{6}\nabla_t^2}{1-\frac{1}{3}\nabla_t}$	$\dfrac{\nabla_t-\nabla_t^2+\frac{1}{12}\nabla_t^2}{1-\frac{1}{2}\nabla_t}$	$\dfrac{\nabla_t-\frac{11}{10}\nabla_t^2+\frac{2}{5}\nabla_t^3+\frac{1}{60}\nabla_t^4}{1-\frac{3}{5}\nabla_t}$
2	$\dfrac{\nabla_t}{1+\frac{1}{2}\nabla_t+\frac{5}{12}\nabla_t^2}$	$\dfrac{\nabla_t-\frac{9}{10}\nabla_t^2}{1-\frac{2}{5}\nabla_t-\frac{1}{30}\nabla_t^2}$	$\dfrac{\nabla_t-\frac{13}{10}\nabla_t^2+\frac{1}{3}\nabla_t^3}{1+\frac{4}{5}\nabla_t+\frac{1}{10}\nabla_t^2}$	$\dfrac{\nabla_t-\frac{3}{2}\nabla_t^2+\frac{8}{15}\nabla_t^3-\frac{1}{60}\nabla_t^4}{1-\nabla_t+\frac{1}{5}\nabla_t^2}$

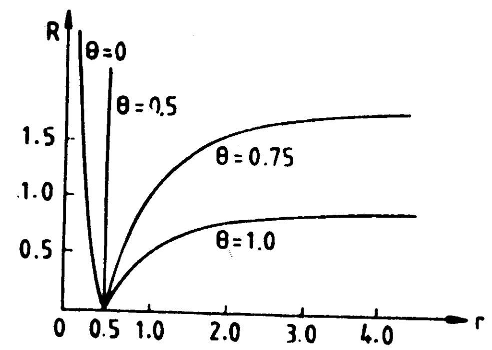

Fig. 5.2 Stability region to the left of the boundary line of the explicit method (5.66)

5.3.4 Two level implicit difference schemes

A general two level implicit difference scheme involving six points (Figure 5.3) is obtained if we write (5.36) as

$$(1-\gamma_1\nabla_t)^{-1}\nabla_t u_m^{n+1} = r[(1+\sigma\delta_x^2)^{-1}\delta_x^2]\, u_m^{n+1} \tag{5.71}$$

which on simplification becomes

$$[1+(\sigma-r(1-\gamma_1))\delta_x^2]\, u_m^{n+1} = [1+(\sigma+r\gamma_1)\,\delta_x^2]\, u_m^n \tag{5.72}$$

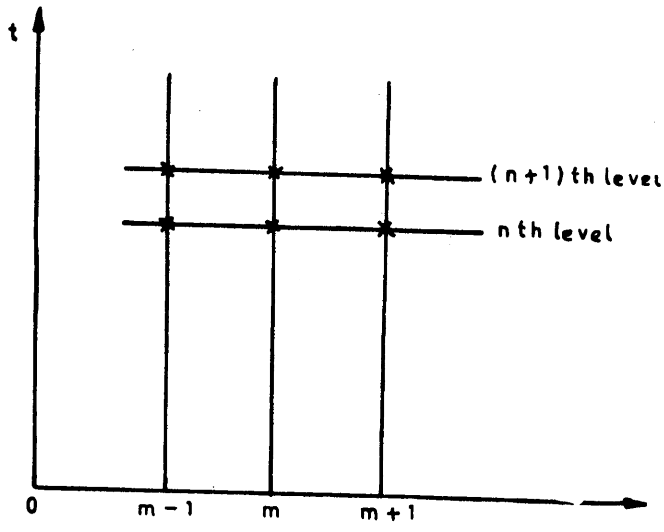

Fig. 5.3 Grid points of the two level implicit methods

where γ_1 and σ are arbitrary parameters. The truncation error of formula (5.72) is given by

$$T_m^n = [1+(\sigma-r(1-\gamma_1))\,\delta_x^2]\,u(x_m, t_{n+1})-[1+(\sigma+r\gamma_1)\,\delta_x^2]\,u(x_m, t_n)$$
$$= k\left[k\left(\gamma_1-\frac{1}{2}\right)+\left(\sigma-\frac{1}{12}\right)h^2\right]\left(\frac{\partial^4 u}{\partial x^4}\right)_m^n+k\left[\frac{1}{2}\left(\gamma_1-\frac{2}{3}\right)r^2\right.$$
$$\left.+\frac{1}{2}\left(\sigma-\frac{1}{6}+\frac{1}{6}\gamma_1\right)r+\frac{1}{12}\left(\sigma-\frac{1}{30}\right)\right]h^4\left(\frac{\partial^6 u}{\partial x^6}\right)_m^n+\cdots \quad (5.73)$$

We find that the truncation error is of

(i) $0(k+h^2)$, for γ_1 and σ arbitrary,

(ii) $0(k^2+h^2)$, for $\gamma_1 = \frac{1}{2}$ and $\sigma \neq \frac{1}{12}$

(iii) $0(k^2+h^4)$, for $\gamma_1 = \frac{1}{2}$ and $\sigma = \frac{1}{12}$ or $\sigma = 0$, and $\gamma_1 = \frac{1}{2}+\frac{1}{12r}$

(iv) $0(h^6)$ for $\gamma_1 = \frac{1}{2}$, $\sigma = \frac{1}{12}$ and $r = \frac{1}{2\sqrt{5}}$

The characteristic equation of (5.72) after substituting $\xi = (1+z)/(1-z)$ becomes

$$\left[1-4\sigma\sin^2\frac{\beta h}{2}+2r(1-2\gamma_1)\sin^2\frac{\beta h}{2}\right]z+2r\sin^2\frac{\beta h}{2} = 0 \quad (5.74)$$

From the Routh-Hurwitz criterion (1.43), we get

$$1-4\sigma\sin^2\frac{\beta h}{2}+2r(1-2\gamma_1)\sin^2\frac{\beta h}{2} > 0$$

and

$$2r\sin^2\frac{\beta h}{2} > 0$$

Since $0 \leqslant \sin^2 \beta h/2 \leqslant 1$, the above conditions will be satisfied if

$$1-4\sigma+2r(1-2\gamma_1) > 0 \quad (5.75)$$

The stability region is shown in Figure 5.4. The shaded part $\sigma < 1/4$ and $\gamma_1 \leqslant 1/2$ represents the region of stability for all values $r > 0$ (unconditional stability). The unshaded region $\sigma \leqslant 1/4$, $\gamma_1 > 1/2$ gives the region of stability for $0 < r \leqslant (1-4\sigma)/2(2\gamma_1-1)$ (conditional stability).

For various values of σ and γ_1, we get the following unconditionally stable methods:

(i) The values $\sigma = 0$, $\gamma_1 = 0$ give the formula

$$\nabla_t u_m^{n+1} = r\delta_x^2 u_m^{n+1} \quad (5.76)$$

which is called the *Laasonen* formula.

(ii) The values $\sigma = 0$, $\gamma_1 = 1/2$ give the *Crank-Nicolson* formula

$$\nabla_t u_m^{n+1} = \frac{r}{2}\delta_x^2\left(u_m^{n+1}+u_m^n\right) \quad (5.77)$$

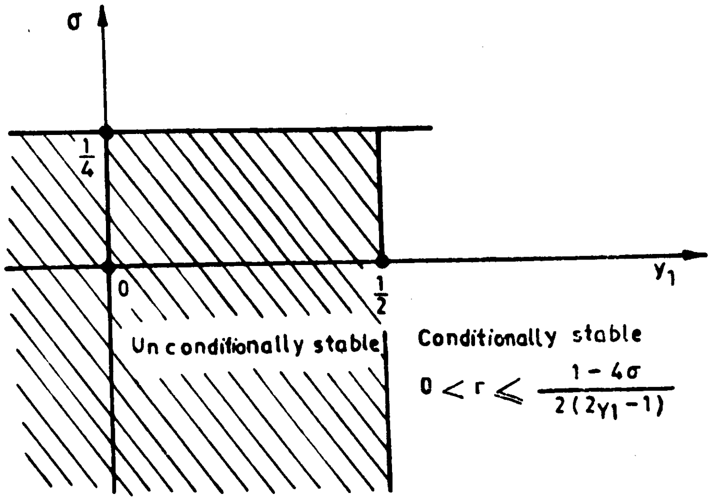

Fig. 5.4 Stability region for two level implicit methods

(iii) The values $\sigma = \frac{1}{12}$, $\gamma_1 = \frac{1}{2}$ give the *Crandall* formula

$$\left(1+\frac{1}{12}\delta_x^2\right)\nabla_t u_m^{n+1} = \frac{r}{2}\delta_x^2\left(u_m^{n+1}+u_m^n\right) \tag{5.78}$$

Example 5.2 Use the Crank-Nicolson method to determine the numerical solution of the initial boundary value problem

$$u_t = u_{xx}$$
$$u(x, 0) = \sin \pi x, \qquad 0 < x < 1$$
$$u(0, t) = u(1, t) = 0, \qquad t \geqslant 0$$

The Crank-Nicolson method is given by

$$-r\, u_{m-1}^{n+1}+2(1+r)u_m^{n+1}-r\, u_{m+1}^{n+1} = r\, u_{m-1}^n+2(1-r)u_m^n+r\, u_{m+1}^n$$

where $r = k/h^2$ and, k and h are step lengths in t and x directions respectively. We choose, $h = 1/4$ and $r = 1/6$. The nodal points are shown in Figure 5.1(a).

The boundary conditions give

$$u_0^n = u_4^n = 0, \quad n = 0, 1, 2\ldots,$$

We obtain,

for $n = 0$, $m = 1, 2, 3$;

$$-\frac{1}{6}u_0^1+\frac{14}{6}u_1^1-\frac{1}{6}u_2^1 = \frac{1}{6}u_0^0+\frac{10}{6}u_1^0+\frac{1}{6}u_2^0$$

$$-\frac{1}{6}u_1^1+\frac{14}{6}u_2^1-\frac{1}{6}u_3^1 = \frac{1}{6}u_1^0+\frac{10}{6}u_2^0+\frac{1}{6}u_3^0$$

$$-\frac{1}{6}u_2^1+\frac{14}{6}u_3^1-\frac{1}{6}u_4^1 = \frac{1}{6}u_2^0+\frac{10}{6}u_3^0+\frac{1}{6}u_4^0$$

which may be written as

$$\mathbf{A}\mathbf{u}^1 = \mathbf{b}^1,$$

where

$$\mathbf{A} = \begin{bmatrix} \frac{14}{6} & -\frac{1}{6} & 0 \\ -\frac{1}{6} & \frac{14}{6} & -\frac{1}{6} \\ 0 & -\frac{1}{6} & \frac{14}{6} \end{bmatrix}, \quad \mathbf{u}^1 = \begin{bmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \end{bmatrix},$$

$$\mathbf{b}^1 = \begin{bmatrix} \frac{1}{6\sqrt{2}}(10+\sqrt{2}) \\ \frac{1}{6\sqrt{2}}(2+10\sqrt{2}) \\ \frac{1}{6\sqrt{2}}(\sqrt{2}+10) \end{bmatrix}$$

Solving, we get

$$\mathbf{u}^1 = \mathbf{A}^{-1}\mathbf{b}^1$$

where

$$\mathbf{A}^{-1} = \frac{3}{1358}\begin{bmatrix} 195 & 14 & 1 \\ 14 & 196 & 14 \\ 1 & 14 & 195 \end{bmatrix}$$

or

$$u_1^1 = .6412843$$
$$u_2^1 = .9069129$$
$$u_3^1 = .6412843$$

The matrix **A** does not depend upon n and we determine the column vector $\mathbf{b}^n$, $n = 1, 2, \ldots$ to find the corresponding solution vector $\mathbf{u}^n$, $n = 1, 2, \ldots$.

5.3 5 Multilevel implicit difference schemes

We choose

$$F(\nabla_t) = (1-\gamma_1\nabla_t+\gamma_2\nabla_t^2)^{-1}(\nabla_t+\tau_1\nabla_t^2)$$

(i) The values $\gamma_1 = 0$ and $\gamma_2 = 0$ give the formula

$$\left(\nabla_t + \frac{1}{2}\nabla_t^2\right)u_m^{n+1} = r\delta_x^2 u_m^{n+1}$$

which may be called the *Richtmyer* formula.

(ii) For $\gamma_1 = 0$, $\gamma_2 = -1/4$, we get the formula

$$\left(\nabla_t + \frac{1}{2}\nabla_t^2\right)u_m^{n+1} = r\delta_x^2\left(1 - \frac{1}{4}\nabla_t^2\right)u_m^{n+1}$$

(iii) Substituting the values $\gamma_1 = 1$ and $\gamma_2 \geqslant 1/4$ in (5.80), we get the formula

$$\left(\nabla_t - \frac{1}{2}\nabla_t^2\right)u_m^{n+1} = r\delta_x^2\left(\gamma_2 u_m^{n+1} + (1-2\gamma_2)u_m^n + \gamma_2 u_m^{n-1}\right)$$

which for $\gamma_2 = 1/3$ may be called the *Douglas-Gunn* formula.

(iv) The values $\gamma_2 = \gamma_1/2$ and $\gamma_1 < 1$ give an unconditionally stable method.

(a)
$$\left[\frac{3}{2} - \gamma_1 - r\left(1 - \frac{1}{2}\gamma_1\right)\delta_x^2\right]u_m^{n+1} = 2(1-\gamma_1)u_m^n - \left[\left(\frac{1}{2} - \gamma_1\right) - \frac{1}{2}r\gamma_1\right]\delta_x^2 u_m^{n-1}$$

(b) For $\gamma_1 = 1 - 1/2r$, we get the formula

$$\left[1 + \frac{1}{r} - r\left(1 + \frac{1}{2r}\right)\delta_x^2\right]u_m^{n+1} = \frac{2}{r}u_m^n + \left[1 - \frac{1}{r} + r\left(1 - \frac{1}{2r}\right)\delta_x^2\right]u_m^{n-1} \quad (5.84)$$

(v) The values $\sigma = 1/12$, $\gamma_2 = (1/2)\gamma_1$, $\gamma_1 = 1 - 1/2r$ give high accuracy formula of $0(k^2+h^4)$

$$\left[\left(\frac{1}{2} + \frac{1}{2r}\right) + \left(\frac{1}{12}\left(\frac{1}{2} + \frac{1}{2r}\right) - r\left(\frac{1}{2} + \frac{1}{4r}\right)\right)\delta_x^2\right]u_m^{n+1}$$
$$= \frac{1}{r}\left(1 + \frac{1}{12}\delta_x^2\right)u_m^n - \left[\left(-\frac{1}{2} + \frac{1}{2r}\right) + \left(\frac{1}{12}\left(-\frac{1}{2} + \frac{1}{2r}\right) - r\left(\frac{1}{2} - \frac{1}{4r}\right)\right)\delta_x^2\right]u_m^{n-1}$$

(vi) The values $\gamma_1 = 1/2$, $\gamma_2 = -1/12$ give the conditionally stable formula $(0 < r \leqslant 3/2)$ which is the Adams-Moulton type method

$$\nabla_t u_m^{n+1} = r\delta_x^2\left(1 - \frac{1}{2}\nabla_t - \frac{1}{12}\nabla_t^2\right)u_m^{n+1}$$

(vii) For $\gamma_1 = 1$ and $\gamma_2 = 1/6$, we obtain the *Milne* type method

$$\left(\nabla_t - \frac{1}{2}\nabla_t^2\right)u_m^{n+1} = r\delta_x^2\left(1-\nabla_t+\frac{1}{6}\nabla_t^2\right)u_m^{n+1}$$

of order of accuracy (k^4+h^2) which is unstable.

Further, we choose

$$F(\nabla_t) = \left(1+\sum_{p=1}^{s}(-1)^p\gamma_p\nabla_t^p\right)^{-1}\left(\nabla_t+\sum_{p=1}^{q}\tau_p\nabla_t^{p+1}\right) \tag{5.85}$$

with τ_p and γ_p arbitrary.

The difference scheme (5.36) with $F(\nabla_t)$ given by (5.85) has the truncation error of $0(k+h^2)$ for arbitrary τ_p, γ_p and σ. Substituting $\nabla_t = (1-E_t^{-1})$, we find that (5.36) represents $(q+2)$-level difference scheme if $q \geqslant s$ and $(s+1)$-level scheme if $q+1 < s$. There are $q+s$ arbitrary parameters on the left hand side of (5.36) and we expect to be able to choose τ_p's and γ_p's so that the scheme (5.36) has order of accuracy $0(k^{q+s})$ in time variable. The Padé approximations to $[-\log(1-\nabla_t)]$ for $0 \leqslant q \leqslant 3$ and $0 \leqslant s \leqslant 2$ are given in Table 5.2.

For example the values $q=2$, $s=0$ give four level implicit unconditionally stable scheme

$$\left(\nabla_t+\frac{1}{2}\nabla_t^2+\frac{1}{3}\nabla_t^3\right)u_m^{n+1} = r\delta_x^2u_m^{n+1}$$

The conditionally stable difference schemes of the Adams-Moulton type can also be obtained if we put $\tau_p = 0$, $1 \leqslant p \leqslant q$. We find

$$(1+\sigma\delta_x^2)\nabla_t u_m^{n+1} = r\delta_x^2\left(1-\frac{1}{2}\nabla_t-\frac{1}{12}\nabla_t^2-\frac{1}{24}\nabla_t^3-\ldots\right)u_m^{n+1}$$

where $\sigma < \frac{1}{4}$.

5.3.6 Implicit difference schemes for the diffusion convection equation

The general two level implicit difference scheme when the first order spatial derivative in (5.60) is approximated by the mean-central differences may be written as

$$\nabla_t u_m^{n+1} = \frac{k\nu}{h^2}\delta_x^2\left(\theta_1 u_m^{n+1}+(1-\theta_1)u_m^n\right)-\frac{\bar{u}k}{h}\mu_x\delta_x\left(\theta u_m^{n+1}+(1-\theta)u_m^n\right) \tag{5.86}$$

where $0 \leqslant \theta_1, \theta \leqslant 1$.

The values $\theta = \theta_1 = 1$ give the fully implicit difference scheme which on simplification becomes

$$u_m^{n+1} = u_m^n+r(u_{m+1}^{n+1}-2u_m^{n+1}+u_{m-1}^{n+1})-rR(u_{m+1}^{n+1}-u_{m-1}^{n+1}) \tag{5.87}$$

where $r = \frac{k\nu}{h^2}$ and $R = \frac{\bar{u}h}{2\nu}$.

where $\mathcal{R} = [-\infty < x < \infty] \times [t > 0]$ and $f(x)$ is a known function.

(ii) initial and Dirichlet conditions

$$u(x, 0) = f(x),\ a \leqslant x \leqslant b$$
$$u(a, t) = g(t),\ t > 0$$
$$u(b, t) = h(t),\ t > 0 \tag{5.94}$$

where $\mathcal{R} = [a \leqslant x \leqslant b] \times [0, T]$ and $f(x)$, $g(t)$ and $h(t)$ are known functions.

(iii) initial and the mixed boundary conditions

$$u(x, 0) = f(x),\ a \leqslant x \leqslant b$$
$$\frac{\partial u}{\partial x} - pu = \phi_1(t),\ x = a,\ t > 0$$
$$\frac{\partial u}{\partial x} + qu = \phi_2(t),\ x = b,\ t > 0 \tag{5.95}$$

where $\mathcal{R} = [a \leqslant x \leqslant b] \times [0, T]$, p and q are assumed as constants. The functions $\phi_1(t)$, $\phi_2(t)$ are continuous and bounded as $t \to \infty$ and there are no discontinuities in the initial or boundary conditions, or at the corners of $\mathcal{R}$. For the values $p = q = 0$, we get the *Neumann* conditions.

We now illustrate the application of the explicit and the implicit difference schemes in solving the heat flow equation (5.33) together with the appropriate initial and boundary conditions.

5.4.1 The initial value problem

The nodal points are formed by the points of intersection between the two families of parallel lines

$$x_m = mh,\ m = 0, \pm 1, \pm 2, \ldots$$
$$t_n = nk,\ \ n = 0, 1, 2, \ldots \tag{5.96}$$

The initial condition (5.93) can be replaced by the conditions

$$u(x_m, 0) = u_m^0 = f(mh) = f_m,\ m = 0, \pm 1, \pm 2, \ldots \tag{5.97}$$

The use of the two level explicit difference scheme (5.38) involves the solution of the following difference equations:

$$u_m^{n+1} = (1-2r)u_m^n + r(u_{m-1}^n + u_{m+1}^n) \tag{5.98}$$
$$u_m^0 = f_m, \qquad m = 0, \pm 1, \pm 2, \ldots,$$
$$n = 0, 1, 2, \ldots$$

Choosing r, $0 < r \leqslant 1/2$, the values of the solution at the nodes on the first level, i.e. u_m^1, $(m = 0, \pm 1, \pm 2, \ldots)$ are known from the initial conditions and it is easy to calculate u_m^2 from the first level and so on. If we know the values $u_m^1 (m = 0, \pm 1, \pm 2, \ldots)$ then the application of a three level explicit difference scheme is straightforward like the two level explicit difference scheme. The application of the implicit method to (5.33) subject to (5.93) will involve the solution of the infinite set of equations.

5.4.2 The initial Dirichlet boundary value problem

The nodal points (m, n) of the region $\mathcal{R}$ are given by

$$x_m = a+mh,\ m = 0, 1, 2, \ldots, M,\ Mh = b-a, \qquad (5.99)$$
$$t_n = nk, \qquad k = 0, 1, 2, \ldots, N,\ Nk = T$$

Firstly, if we use (5.38), we arrive at the following difference equations:

$$u_m^{n+1} = (1-2r)u_m^n+r(u_{m-1}^n+u_{m+1}^n),\ 1 \leqslant m \leqslant M-1$$
$$n = 0, 1, 2, \ldots N, \qquad (5.100)$$

$$u(x_m, 0) = u_m^0 = f(x_m) = f_m,\ 0 \leqslant m \leqslant M$$
$$u(a, t_n) = u_0^n = g(t_n) = g^n,\ n > 0$$
$$u(b, t_n) = u_M^n = h(t_n) = h^n,\ n > 0 \qquad (5.101)$$

Substituting $n = 0$ in (5.100), we obtain

$$u_m^1 = (1-2r)u_m^0+r(u_{m-1}^0+u_{m+1}^0) \qquad (5.102)$$

Since the values $u_m^0 (0 \leqslant m \leqslant M)$ are known from the initial condition in (5.101), we can use (5.102) to compute the values $u_m^1 (1 \leqslant m \leqslant M-1)$ in any order and the values u_0^1 and u_M^1 are known from the boundary conditions in (5.101). For $n = 1$ in (5.100) we get

$$u_m^2 = (1-2r)u_m^1+r(u_{m-1}^1+u_{m+1}^1) \qquad (5.103)$$

From the values $u_m^1 (1 \leqslant m \leqslant M-1)$ we compute $u_m^2 (1 \leqslant m \leqslant M-1)$ from (5.103). The values u_0^2 and u_M^2 are given by (5.101). Thus we repeat the steps to advance in the time direction by taking $n = 2$ and so forth.

The difference equations (5.100) may also be written as

$$\begin{aligned}
u_1^{n+1} &= ru_0^n + (1-2r)u_1^n + ru_2^n \\
u_2^{n+1} &= ru_1^n + (1-2r)u_2^n + ru_3^n \\
&\vdots \\
u_{M-2}^{n+1} &= ru_{M-3}^n + (1-2r)u_{M-2}^n + ru_{M-1}^n \\
u_{M-1}^{n+1} &= ru_{M-2}^n + (1-2r)u_{M-1}^n + ru_M^n
\end{aligned} \qquad (5.104)$$

which in matrix notation becomes

$$\mathbf{u}^{n+1} = [\mathbf{I}+r\mathbf{C}]\mathbf{u}^n+r\mathbf{b}^n, \qquad n = 0, 1, 2, \ldots \qquad (5.105)$$

where $\mathbf{u}^s = [u_1^s u_2^s \cdots u_{M-1}^s]^T, \qquad s = n, n+1$

$$\mathbf{b}^n = \begin{bmatrix} g^n \\ 0 \\ \vdots \\ 0 \\ h^n \end{bmatrix} \text{ and } \mathbf{C} = \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \qquad (5.106)$$

$$m = 1,\ u_1^1 = \frac{1}{3}(u_0^0+u_1^0+u_2^0)$$

$$= \frac{1}{3}\left(1+\frac{\sqrt{3}}{2}+\frac{1}{2}\right) = 0.7887$$

$$m = 2,\ u_2^1 = \frac{1}{3}\ (u_1^0+u_2^0+u_3^0)$$

$$= \frac{1}{3}\left(\frac{\sqrt{3}}{2}+\frac{1}{2}\right) = 0.4553$$

$$n = 1,\ u_m^2 = \frac{1}{3}\ (u_{m-1}^1+u_m^1+u_{m+1}^1)\quad 0 \leqslant m \leqslant 2$$

$$m = 0,\ u_0^2 = \frac{1}{3}\ (u_{-1}^1+u_0^1+u_1^1) = \frac{1}{3}\ (u_0^1+2u_1^1)$$

$$= \frac{1}{3}\ (0.9107+2\times 0.7887) = 0.8294$$

$$m = 1,\ u_1^2 = \frac{1}{3}\ (u_0^1+u_1^1+u_2^1)$$

$$= \frac{1}{3}(0.9107+0.7887+0.4553) = 0.7182$$

$$m = 2,\ u_2^2 = \frac{1}{3}\ (u_1^1+u_2^1+u_3^1)$$

$$= \frac{1}{3}\ (0.7887+0.4553) = 0.4147$$

The DuFort-Frankel method, for $r = 1/3$ becomes

$$u_m^{n+1} = \frac{1}{5}u_m^{n-1}+\frac{2}{5}\ (u_{m-1}^n+u_{m+1}^n),\ 0 \leqslant m \leqslant 2$$

$$n = 1, 2, \ldots$$

Here we need another method to start the computation. The Schmidt method is used for the first time step.
We have,

$$n = 1,\ u_m^2 = \frac{1}{5}(u_m^0+2(u_{m-1}^1+u_{m+1}^1)),\ 0 \leqslant m \leqslant 2$$

$$m = 0,\ u_0^2 = \frac{1}{5}(u_0^0+2(u_{-1}^1+u_1^1)) = \frac{1}{5}(u_0^0+4u_1^1)$$

$$= \frac{1}{5}(1+4\times 0.7887) = 0.8310$$

$$m = 1,\ u_1^2 = \frac{1}{5}(u_1^0+2(u_0^1+u_2^1))$$

$$= \frac{1}{5}\left(\frac{\sqrt{3}}{2}+2(0.9107+0.4553)\right) = 0.7196$$

$$m = 2,\ u_2^2 = \frac{1}{5}(u_2^0+2(u_1^1+u_3^1)) = \frac{1}{5}(u_2^0 + 2u_1^1)$$

$$= \frac{1}{5}\left(\frac{1}{2}+2\times 0.7887\right) = 0.4155$$

The Crank-Nicolson method, for $r = \frac{1}{3}$ becomes

$$-u_{m-1}^{n+1}+8u_m^{n+1}-u_{m+1}^{n+1} = u_{m-1}^n+4u_m^n+u_{m+1}^n,\ 0 \leqslant m \leqslant 2$$
$$n = 0, 1, 2, \ldots$$

We have;

$$n = 0,\ -u_{m-1}^1+8u_m^1-u_{m+1}^1 = u_{m-1}^0+4u_m^0+u_{m+1}^0$$
$$m = 0,\ -u_{-1}^1+8u_0^1-u_1^1 = u_{-1}^0+4u_0^0+u_1^0$$
$$m = 1,\ -u_0^1+8u_1^1-u_2^1 = u_0^0+4u_1^0+u_2^0$$
$$m = 2,\ -u_1^1+8u_2^1-u_3^1 = u_1^0+4u_2^0+u_3^0$$

which may be written as

$$\begin{bmatrix} 8 & -2 & 0 \\ -1 & 8 & -1 \\ 0 & -1 & 8 \end{bmatrix} \begin{bmatrix} u_0^1 \\ u_1^1 \\ u_2^1 \end{bmatrix} = \begin{bmatrix} 5.7311 \\ 4.9641 \\ 2.3660 \end{bmatrix}$$

or $\quad u_0^1 = 0.9125 \quad u_1^1 = 0.7838 \quad u_2^1 = 0.3937$

$$n = 1,\ -u_{m-1}^2+8u_m^2-u_{m+1}^2 = u_{m-1}^1+4u_m^1+u_{m+1}^1$$
$$m = 0 \quad -u_{-1}^2+8u_0^2-u_1^2 = u_{-1}^1+4u_0^1+u_1^1$$
$$m = 1 \quad -u_0^2+8u_1^2-u_2^2 = u_0^1+4u_1^1+u_2^1$$
$$m = 2 \quad -u_1^2+8u_2^2-u_3^2 = u_1^1+4u_2^1+u_3^1$$

which may be written as

$$\begin{bmatrix} 8 & -2 & 0 \\ -1 & 8 & -1 \\ 0 & -1 & 8 \end{bmatrix} \begin{bmatrix} u_0^2 \\ u_1^2 \\ u_2^2 \end{bmatrix} = \begin{bmatrix} 5.2176 \\ 4.4414 \\ 2.3586 \end{bmatrix}$$

or

$$u_0^2 = 0.8579 \quad u_1^2 = 0.7067 \quad u_2^2 = 0.3832$$

5.4.3 The initial mixed boundary value problem

The difference scheme used to solve this problem is the Crank-Nicolson formula

$$-ru_{m-1}^{n+1}+2(1+r)u_m^{n+1}-ru_{m+1}^{n+1} = ru_{m-1}^n+2(1-r)u_m^n+ru_{m+1}^n,$$
$$m = 0, 1, 2, \ldots, M,$$
$$n = 0, 1, 2, \ldots, N \qquad (5.112)$$

In the equation (5.112) when $n = 0$, the values of u_m^0, $0 \leqslant m \leqslant M$ are obtained from the initial conditions. When $m = 0, M$, the values u_{-1}^s and u_{M+1}^s, $(s = n, n+1)$ which occur in (5.112) are eliminated using the boundary conditions (5.95).

The derivatives in the boundary conditions (5.95) are approximated by the equation

$$\left(\frac{\partial u}{\partial x}\right)_m^s = \frac{1}{2h}(u_{m+1}^s - u_{m-1}^s),\ m = 0,\ M$$

where $s = n, n+1$.

On simplification, we obtain the discrete analogue of the boundary conditions as

$$\begin{aligned} u_{-1}^s &= u_1^s - 2hpu_0^s - 2h\phi_1^s \\ u_{M+1}^s &= u_{M-1}^s - 2hqu_M^s + 2h\phi_2^s \end{aligned} \tag{5.113}$$

If we use (5.113) into (5.112) when $m = 0$ and M, we may write the totality of difference equations in the form

$$\left(\mathbf{I} + \frac{r}{2}\mathbf{Q}\right)\mathbf{u}^{n+1} = \left(\mathbf{I} - \frac{r}{2}\mathbf{Q}\right)\mathbf{u}^n + rh\boldsymbol{\phi} \tag{5.114}$$

where Q is a $M+1 \times M+1$ matrix

$$\mathbf{Q} = \begin{bmatrix} 2+2hp & -2 & & & \\ -1 & 2 & -1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & \cdot & \cdot & \cdot \\ & & -1 & 2 & -1 \\ & & & -2 & 2+2hq \end{bmatrix}$$

and

$$\mathbf{u}^s = [u_0^s\ u_1^s \cdots u_{M-1}^s u_M^s]^T$$

$$\boldsymbol{\phi} = [-(\phi_1^{n+1} + \phi_1^n)\ 0 \ \dots\ (\phi_2^{n+1} + \phi_2^n)]^T$$

The tridiagonal system (5.114) can again be solved by the method discussed in Section 4.3.3.

5.4.4 Results from computation

We have solved the differential equation (5.33) subject to the initial and boundary conditions

$$\begin{aligned} u &= \cos\frac{\pi}{2}x,\ -1 \leqslant x \leqslant 1,\ t = 0 \\ u &= 0, \qquad x = \pm 1, \qquad t > 0 \end{aligned} \tag{5.115}$$

The theoretical solution is given by

$$u(x, t) = \exp(-\pi^2 t/4)\cos\frac{\pi}{2}x$$

For the purpose of comparison we have solved this problem with the help of a number of explicit and implicit methods. The values of the maximum absolute error $E = \max_m |u_m^n - u(x_m, t_n)|$ at $t = \frac{8}{25}$ have been determined for various values of r and these are listed in Tables 5.3-5.5.

TABLE 5.3 THE VALUES OF $10^3 \times E$ AT $t = 0.32$ FOR THE PROBLEM (5.33) WITH INITIAL BOUNDARY CONDITIONS (5.115) AND METHOD (5.84 iv a)

r	h/γ_1	$\frac{3}{4}$	$\frac{2}{3}$	$\frac{1}{2}$	0
$\frac{1}{8}$	$\frac{1}{10}$	0.7375	0.7372	0.7370	0.7368
	$\frac{1}{20}$	0.1843	0.1843	0.1843	0.1843
$\frac{1}{6}$	$\frac{1}{10}$	0.7389	0.7384	0.7379	0.7374
	$\frac{1}{20}$	0.1844	0.1844	0.1843	0.1843
$\frac{1}{4}$	$\frac{1}{10}$	0.7447	0.7430	0.7413	0.7396
	$\frac{1}{20}$	0.1848	0.1847	0.1845	0.1844
$\frac{1}{3}$	$\frac{1}{10}$	0.7559	0.7519	0.7479	0.7439
	$\frac{1}{20}$	0.1855	0.1852	0.1850	0.1847
$\frac{1}{2}$	$\frac{1}{10}$	0.7999	0.7866	0.7732	0.7597
	$\frac{1}{20}$	0.1882	0.1874	0.1866	0.1857

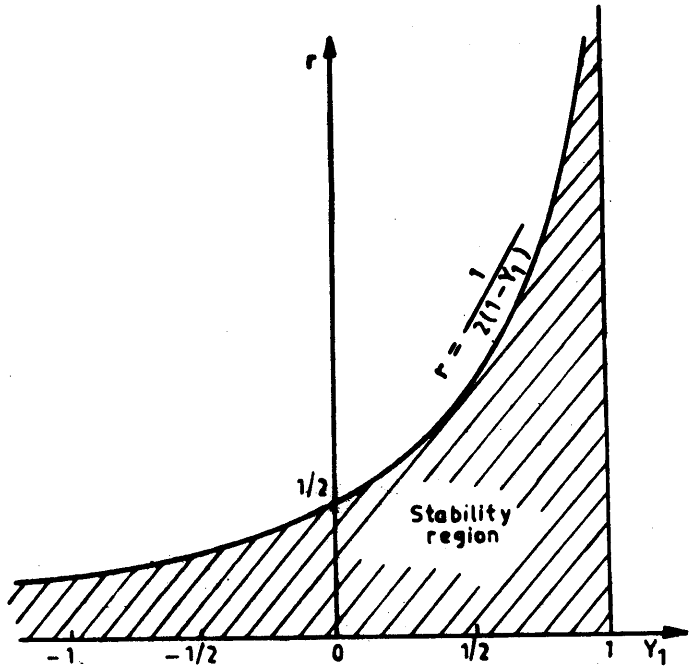

Fig. 5.6 Stability and accuracy region for the implicit methods (5.84 iv a)

The comparison of the explicit methods is given in Table 5.5. If $r < 1/2$ and if $\eta = 1/12$ belongs to the interval $r/2 \leqslant \eta \leqslant 1/4$, then the Hadjidimos method gives better results in comparison to the Schmidt method and the DuFort-Frankel method. For $r = 1/6$, the Schmidt method gives best results as it is then equivalent to the Crandall method of $O(h^4)$.

In conclusion, we may summarize as follows:

(i) The implicit method (5.84a, b) gives more accurate results as compared to the other implicit methods of $O(k+h^2)$ or (k^2+h^2).

(ii) It is found that the accuracy with respect to time variable is of secondary importance while the accuracy with respect to the space variable is essential. Thus, the Crandall method produces the best results among all the implicit methods.

5.5 STABILITY ANALYSIS AND CONVERGENCE OF DIFFERENCE SCHEMES

The analytical solution $u(x_m, t_n)$ of the differential equation, the difference solution u_m^n of the difference equation and the numerical solution $\bar{u}_m^n$ can be related by a relation of the form

$$| u(x_m, t_n) - \bar{u}_m^n | \leqslant | u(x_m, t_n) - u_m^n | + | u_m^n - \bar{u}_m^n | \tag{5.116}$$

In practice we would like the difference between the analytical and the numerical solution to be small. From (5.116), we find that this difference depends on the values $| u(x_m, t_n)-u_m^n |$ and $| u_m^n-\bar{u}_m^n |$. The value $| u(x_m, t_n)-u_m^n |$ is the truncation error which arises because the differential equation is replaced by the difference equation. For a convergent difference scheme the truncation error converges to zero as h and k both approach zero. The numerical error $| u_m^n-\bar{u}_m^n |$ arises because in actual computation we cannot construct the difference solution exactly as we are faced with the round-off errors. In fact, in some cases the numerical solution may differ considerably from the difference solution. If the difference equation is stable, the second term in (5.116) practically equals zero. Thus, the results of the convergent and stable method are very close to the analytical values.

5.5.1 Matrix stability analysis

Assuming periodic initial data and neglecting the boundary conditions, we have used the von Neumann method to determine the stability of the difference schemes. We now apply the matrix method which automatically takes into account the boundary conditions of the problem, to difference schemes for the stability analysis.

From equation (5.111), the two level difference scheme may be written as

$$\mathbf{A}_0\mathbf{u}^{n+1} = \mathbf{A}_1\mathbf{u}^n+\mathbf{b}^n \tag{5.117}$$

where $\mathbf{b}^n$ contains boundary conditions and $| \mathbf{A}_0 | \neq \mathbf{0}$. For $A_0 = \mathbf{I}$, the difference scheme (5.117) will be an explicit scheme otherwise an implicit scheme. We now assume that an error is introduced by round-off or some other source into the solution $\mathbf{u}^q$ and call it $\bar{\mathbf{u}}^q$. Then, we calculate further using (5.117) to determine $\bar{\mathbf{u}}^{q+1}, \ldots, \bar{\mathbf{u}}^{n+1}$. The resulting equations become

$$\begin{aligned}
\mathbf{A}_0\bar{\mathbf{u}}^{q+1} &= \mathbf{A}_1\bar{\mathbf{u}}^q+\mathbf{b}^q \\
\mathbf{A}_0\bar{\mathbf{u}}^{q+2} &= \mathbf{A}_1\bar{\mathbf{u}}^{q+1}+\mathbf{b}^{q+1} \\
&\vdots \\
\mathbf{A}_0\bar{\mathbf{u}}^{n+1} &= \mathbf{A}_1\bar{\mathbf{u}}^n+\mathbf{b}^n \quad n \geqslant q
\end{aligned} \tag{5.118}$$

Subtracting (5.117) from the last equation in (5.118), we get

$$\mathbf{A}_0\bar{\boldsymbol{\epsilon}}^{n+1} = A_1\bar{\boldsymbol{\epsilon}}^n \tag{5.119}$$

where $\bar{\mathbf{u}}^n-\mathbf{u}^n = \bar{\boldsymbol{\epsilon}}^n$ is the numerical error vector. We note that (5.119) is nothing more than the homogeneous equation corresponding to (5.117). We take $q = 0$ which amounts to assuming the introduction of the error in the initial data.

In the stability anylysis by the matrix method, we determine the conditions under which the value of the numerical error vector

$$\| \bar{\boldsymbol{\epsilon}}^n \| = \| \bar{\mathbf{u}}^n-\mathbf{u}^n \| \tag{5.120}$$

where $\| \cdot \|$ denotes a suitable norm, remains bounded as n increases indefinitely, with k remaining fixed.

$$\bar{\epsilon}^{n+1} = \alpha G \bar{\epsilon}^{n} + (1-2\alpha)\bar{\epsilon}^{n-1} \tag{5.129}$$

where $$G = 2I + C,$$

which can be rewritten as

$$\bar{E}^{n+1} = H\,\bar{E}^{n} \tag{5.130}$$

where $\bar{E}^n$ is the $2M-2$-dimensional vector $[\bar{\epsilon}^{n+1}\ \bar{\epsilon}^{n}]$ and H is the $2M-2 \times 2M-2$ matrix

$$H = \begin{bmatrix} \alpha G & (1-2\alpha) I \\ I & 0 \end{bmatrix}$$

The eigenvalues of H are those of

$$\begin{bmatrix} \alpha \gamma_s^* & 1-2\alpha \\ 1 & 0 \end{bmatrix},$$

i.e., the roots of the quadratic equation

$$\lambda^2 - \alpha \gamma_s^* \lambda - (1-2\alpha) = 0 \tag{5.131}$$

where γ_s^* is the eigenvalue of G and

$$\gamma_s^* = 2\cos\frac{s\pi}{M},\ 1 \leqslant s \leqslant M-1$$

We consider

$$\lambda^2 - 2\alpha\lambda\cos\phi - 1 + 2\alpha = 0,\ 0 < \phi < \pi$$

and for stability we have

$$|\lambda_1| \leqslant 1 \text{ and } |\lambda_2| \leqslant 1$$

If the roots are complex then they are equal in magnitude and

$$|\lambda_i| = \sqrt{[(1-2r)/(1+2r)]} < 1$$

For real roots, we obtain

$$\lambda_i = \alpha\cos\phi \pm \sqrt{(\alpha^2\cos^2\phi + 1 - 2\alpha)}$$

Since, $$0 < \phi < \pi,\ \alpha > 0$$

$$\sqrt{(\alpha^2\cos^2\phi + 1 - 2\alpha)} = [(1-\alpha\cos\phi)^2 - 2\alpha(1-\cos\phi)]^{1/2} < (1-\alpha\cos\phi),$$

it follows that $|\lambda_i| < 1$.

Hence the DuFort-Frankel scheme is unconditionally stable. In a similar manner, the error equation corresponding to the Richardson scheme (5.108) can be expressed as

$$\bar{\epsilon}^{n+1} = 2r\,C\,\bar{\epsilon}^{n} + \bar{\epsilon}^{n-1}$$

or as (5.130) where H is given by

$$H = \begin{bmatrix} 2r\,C & I \\ I & 0 \end{bmatrix}$$