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5 Boundary Value Problems and Partial Differential Equations

Recall the following difference equations:

Backward Difference

	f_{n-4}	f_{n-3}	f_{n-2}	f_{n-1}	f_n
$h\ f_n'$				-1	1
$h^2 f_n''$			1	-2	1
$h^3 f_n'''$		-1	3	-3	1
$h^4 f_n^{iv}$	1	-4	6	-4	1

Forward difference

	f_n	f_{n+1}	f_{n+2}	f_{n+3}	f_{n+4}
$h\ f_n'$	-1	1			
$h^2 f_n''$	1	-2	1		
$h^3 f_n'''$	-1	3	-3	1	
$h^4 f_n^{iv}$	1	-4	6	-4	1

(5.1)

Central difference

	f_{n-2}	f_{n-1}	f_n	f_{n+1}	f_{n+2}
$h\ f_n'$		-0.5	0	0.5	
$h^2 f_n''$		1	-2	1	
$h^3 f_n'''$	-0.5	1	0	-1	0.5
$h^4 f_n^{iv}$	1	-4	6	-4	1

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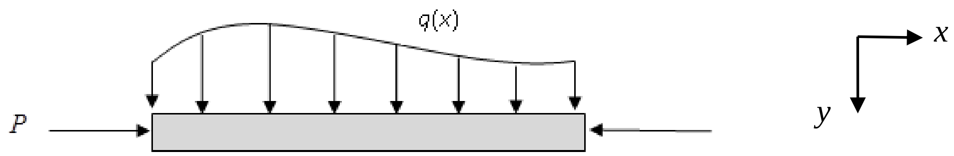
5.1 Finite Difference for ODEs

Recall from Chapter 1 that the governing equation for a beam of constant *EI* is given as



$$EI\frac{d^4y}{dx^4}+P\frac{d^2y}{dx^2}=q \tag{5.2}$$

with the following boundary conditions

- Fixed end

$$y=0 \quad , \quad \theta=\frac{dy}{dx}=0$$

- Free end

$$V=0 \Rightarrow \frac{d^3y}{dx^3}=0 \quad , \quad M=0 \Rightarrow \frac{d^2y}{dx^2}=0$$

- Simply supported (pinned)

$$y=0 \quad , \quad M=0 \Rightarrow \frac{d^2y}{dx^2}=0$$

Consider the beam bending problem in Fig 5.1,

$$\frac{d^4y}{dx^4}=\frac{q}{EI} \tag{5.3}$$

where one end is fixed, and the other end is pinned.

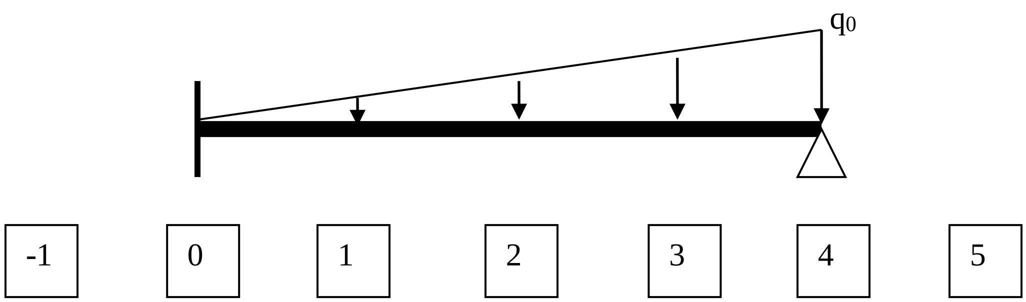


Fig 5.1

Divide the beam into 4 equal segments. We are interested in the beam deflection at nodes 1, 2 and 3. Suppose that we would like to solve the problem using the central difference method. Referring to the coefficient table in (5.1), the numerical approximation for a 4th order differential term, at a given point, involves two neighboring points to the left and right of the said point. Accordingly, we introduce two imaginary points to the problem.

The nodal deflections are given by

Node 1: $y_{-1} - 4y_0 + 6y_1 - 4y_2 + y_3 = 0.25 q_0 h^4 / EI$

Node 2: $y_0 - 4y_1 + 6y_2 - 4y_3 + y_4 = 0.5 q_0 h^4 / EI$ (5.4)

Node 3: $y_1 - 4y_2 + 6y_3 - 4y_4 + y_5 = 0.75 q_0 h^4 / EI$

Note that we have 3 equations in (5.4), for 5 unknowns. To solve the problem, make use of the boundary conditions to 'generate' more equations.

At node 0, apply the central difference approximation in (5.1) to the fixed end boundary condition to give

$$y_0' = \frac{1}{2h}\left[y_1 - y_{-1}\right] = 0 \quad \Rightarrow \quad y_{-1} = y_1 \tag{5.5}$$

The other boundary condition gives $y_0 = 0$.

Similarly, apply the central difference approximation to node 4 where the curvature is zero,

$$y_4'' = [y_5 - 2y_4 + y_3]/h^2 = 0 \quad \Rightarrow \quad y_5 = -y_3 \tag{5.6}$$

where we have make use of the second boundary condition $y_4 = 0$.

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The equations in (5.4), together with the boundary conditions, are arranged in the matrix form.

$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 6 & -4 & 1 & 0 \\ 0 & -4 & 6 & -4 & 0 \\ 0 & 1 & -4 & 6 & 1 \end{bmatrix} \begin{Bmatrix} y_{-1} \\ y_1 \\ y_2 \\ y_3 \\ y_5 \end{Bmatrix} = \frac{q_0 h^4}{EI} \begin{Bmatrix} 0 \\ 0 \\ 0.25 \\ 0.5 \\ 0.75 \end{Bmatrix} \tag{5.7}$$

which can be solved easily for the unknown displacements.

5.2 Beam buckling

As illustrated in the previous section, beams under static loads can be solved easily by FDM. The same method can be used to solve buckling problems in beam.

Fig 5.2

For the beam shown in Fig 5.2, the bending moment at any point is given by

$$M = Py \tag{5.8}$$

Substituting $M = -EI\dfrac{d^2y}{dx^2}$, the governing equation is thus

$$y'' = -\frac{Py}{EI} \tag{5.9}$$

with boundary conditions $y(0) = y(L) = 0$.

Solve the problem using central difference method.

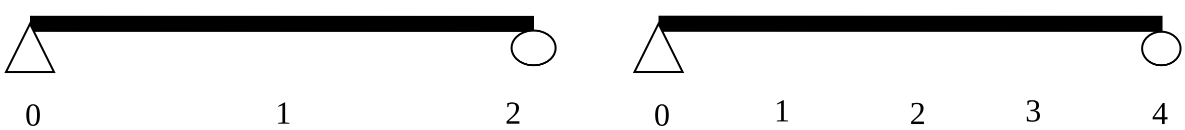


Fig 5.3

i. Beam divided into 2 segments in Fig 5.3a ($h = L/2$)

$$\frac{y_2 - 2y_1 + y_0}{(L/2)^2} + \frac{P}{EI} y_1 = 0 \tag{5.10}$$

Solving (5.10) with the BCs $y_0 = y_2 = 0$ gives $y_1\left(PL^2/4EI - 2\right) = 0$. Hence, the critical load is obtained as $P_{cr} = 8EI/L^2$. Note that the exact solution is $P_{cr} = \pi^2 EI/L^2 = 9.87EI/L^2$.

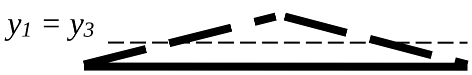
ii. Beam divided into 4 segments in Fig 5.3b ($h = L/4$)

$$\begin{aligned} &\text{Node}\,1: y_2 + (\lambda-2)y_1 = 0 \\ &\text{Node}\,2: y_3 + (\lambda-2)y_2 + y_1 = 0 \\ &\text{Node}\,3: (\lambda-2)y_3 + y_2 = 0 \end{aligned} \tag{5.11}$$

where $\lambda = PL^2/16EI$. Note that we have utilized the BCs $y_0 = y_4 = 0$.

Consider the possible buckling modes:

- Symmetric mode: $y_1 = y_3$

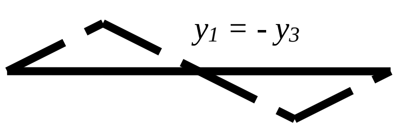


Hence (5.11a) = (5.11c). Arranging the equations in the matrix form,

$$\begin{bmatrix} (\lambda-2) & 1 \\ 2 & (\lambda-2) \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \tag{5.12}$$

For non-trivial solution, $(\lambda-2)^2 - 2 = 0$, resulting in a critical load of $P_{cr} = 9.4EI/L^2$.

- Anti-symmetric mode: $y_1 = -y_3$



This results in $(\lambda-2) = 0$ and the critical load is obtained as $P_{cr} = 32EI/L^2$ (exact solution = $4\pi^2 EI/L^2$).

- Question: Can we solve the problem in (5.11) as a 3x3 matrix instead of a 2x2 matrix?

$$\begin{bmatrix} \lambda-2 & 1 & 0 \\ 1 & \lambda-2 & 1 \\ 0 & 1 & \lambda-2 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \end{Bmatrix}$$

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5.3 FD approximations of partial derivatives

Taylor series expansion in two variables: first in the *x* direction,

$$
\begin{aligned}
u(x+h,y) &= u(x,y) + u_x(x,y)h + u_{xx}(x,y)\frac{h^2}{2!} + \ldots \\
u(x-h,y) &= u(x,y) - u_x(x,y)h + u_{xx}(x,y)\frac{h^2}{2!} - \ldots
\end{aligned}
\tag{5.13}
$$

where h is the grid spacing (or size).

Note the conventions used: subscripts i and j designate the location of pivotal points as shown in Fig 5.4.

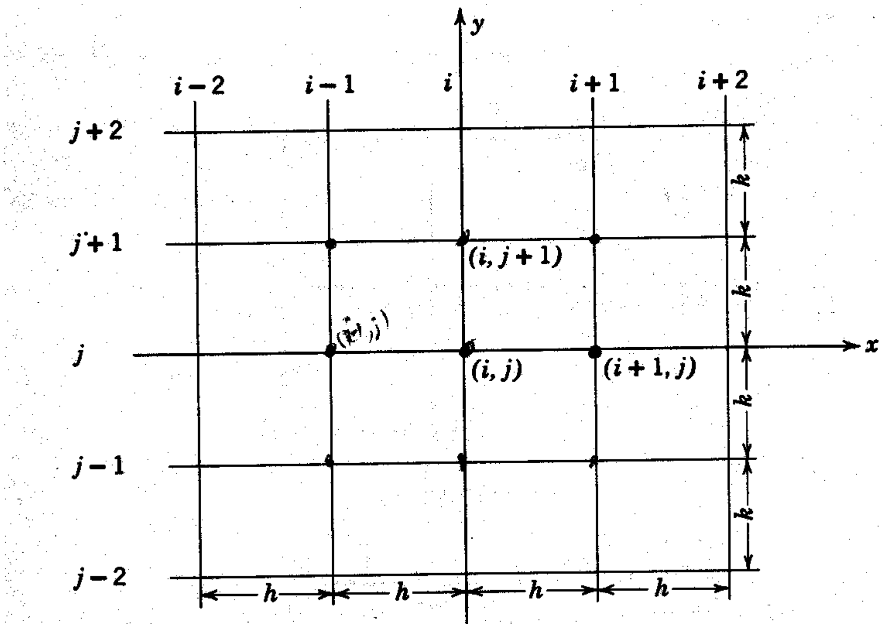

Fig 5.4

Eq (5.13) becomes

$$
\begin{aligned}
u_{i+1,j} &= u_{i,j} + h\frac{\partial u_{i,j}}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 u_{i,j}}{\partial x^2} + \frac{h^3}{3!}\frac{\partial^3 u_{i,j}}{\partial x^3} + \ldots \\
u_{i-1,j} &= u_{i,j} - h\frac{\partial u_{i,j}}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 u_{i,j}}{\partial x^2} - \frac{h^3}{3!}\frac{\partial^3 u_{i,j}}{\partial x^3} + \ldots
\end{aligned}
\tag{5.14}
$$

The gradients can be approximated from (5.14) to give

$$
\begin{aligned}
&\text{Forward difference:} \quad \frac{\partial u_{i,j}}{\partial x} = \frac{u_{i+1,j} - u_{i,j}}{h} + O(h) \qquad \textit{by rearranging (5.14a)} \\
&\text{Backward difference:} \quad \frac{\partial u_{i,j}}{\partial x} = \frac{u_{i,j} - u_{i-1,j}}{h} + O(h) \qquad \textit{by rearranging (5.14b)}
\end{aligned}
\tag{5.15}
$$

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Central difference: $\dfrac{\partial u_{i,j}}{\partial x} = \dfrac{u_{i+1,j} - u_{i-1,j}}{2h} + O(h^2)$ *from (5.14a) - (5.14b)*

$\dfrac{\partial^2 u_{i,j}}{\partial x^2} = \dfrac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + O(h^2)$ *from (5.14a) + (5.14b)*

Similarly for the *y* direction,

Forward difference: $\dfrac{\partial u_{i,j}}{\partial y} = \dfrac{u_{i,j+1} - u_{i,j}}{k} + O(k)$

Backward difference: $\dfrac{\partial u_{i,j}}{\partial y} = \dfrac{u_{i,j} - u_{i,j-1}}{k} + O(k)$ (5.16)

Central difference: $\dfrac{\partial u_{i,j}}{\partial y} = \dfrac{u_{i,j+1} - u_{i,j-1}}{2k} + O(k^2)$

$\dfrac{\partial^2 u_{i,j}}{\partial y^2} = \dfrac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} + O(k^2)$

In engineering applications, mixed second-order derivatives $\partial^2 u / \partial x \partial y$ are often required. From Taylor series expansion

$$u(x+h, y+k) = u(x,y) + \left(h\frac{\partial u(x,y)}{\partial x} + k\frac{\partial u(x,y)}{\partial y} \right) + \left(\frac{h^2}{2!}\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{2hk}{2!}\frac{\partial^2 u(x,y)}{\partial x \partial y} + \frac{k^2}{2!}\frac{\partial^2 u(x,y)}{\partial y^2} \right) + \ldots \tag{5.17}$$

It can be shown that

$$u(x+h, y+k) - u(x+h, y-k) - u(x-h, y+k) + u(x-h, y-k) = 4hk\frac{\partial^2 u(x,y)}{\partial x \partial y} + O\left((h+k)^4\right) \tag{5.18}$$

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Hence the second-order central difference approximation can be written as

$$\frac{\partial^2 u_{i,j}}{\partial x \partial y} = \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4hk} + O\left(\frac{(h+k)^4}{hk}\right)$$

or (5.19)

$$\frac{\partial^2 u_{i,j}}{\partial x \partial y} = \frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4h^2} + O\left(h^2\right) \quad \text{for } h = k.$$

The coefficients at the pivotal points for (5.19) are shown below.

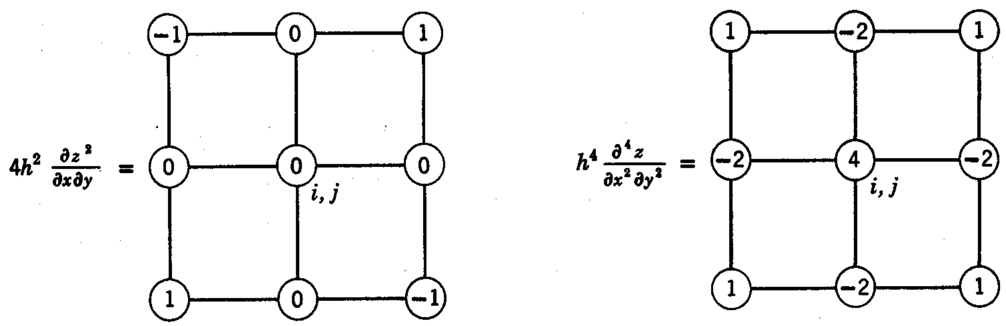

Fig 5.5

Similarly, it can be shown that

$$\frac{\partial^4 u(x,y)}{\partial y^2 \partial x^2} = \frac{\partial^2}{\partial y^2}\left(\frac{\partial^2 u(x,y)}{\partial x^2}\right)$$

(5.20)

$$= \frac{1}{k^2}\left[\left\{\left.\frac{\partial^2 u(x,y)}{\partial x^2}\right|_{i,j+1} - 2\left.\frac{\partial^2 u(x,y)}{\partial x^2}\right|_{i,j} + \left.\frac{\partial^2 u(x,y)}{\partial x^2}\right|_{i,j-1}\right\}\right]$$

$$= \frac{1}{k^2}\left[\frac{1}{h^2}\left(u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}\right) - \frac{2}{h^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right) + \frac{1}{h^2}\left(u_{i+1,j-1} - 2u_{i,j-1} + u_{i-1,j-1}\right)\right]$$

$$= \frac{1}{h^2 k^2}\left(u_{i+1,j+1} - 2u_{i+1,j} + u_{i+1,j-1} - 2u_{i,j+1} + 4u_{i,j} - 2u_{i,j-1} + u_{i-1,j+1} - 2u_{i-1,j} + u_{i-1,j-1}\right)$$

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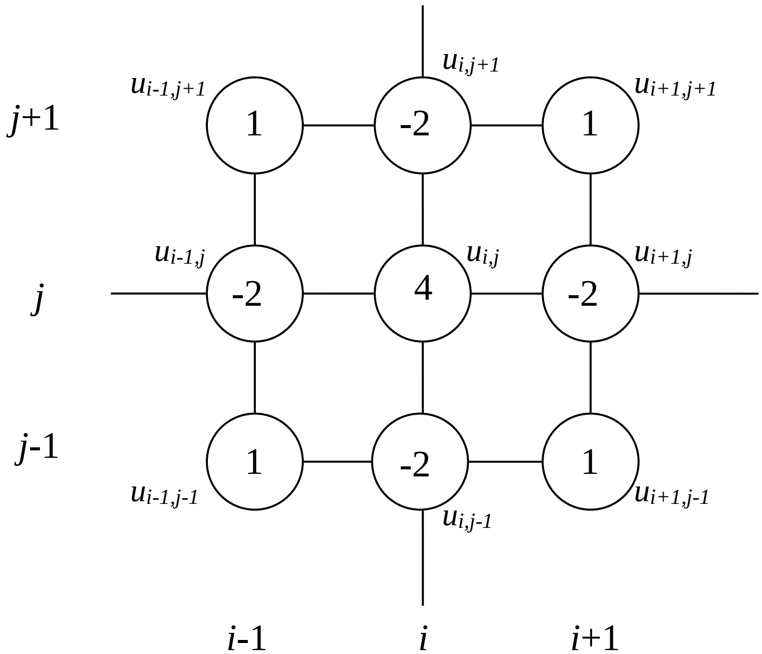

$$h^2 k^2 \frac{\partial^4 u}{\partial^2 x\, \partial^2 y}$$

5.4 Solution of plate problems by FDM

5.4.1 Deflection of Thin Membrane by FDM

Deflection of thin square membrane set at the boundary by tensile forces s per unit length and under uniform load q is governed by Poisson's equation

$$\frac{\partial^2 z}{\partial x^2} + \frac{\partial^2 z}{\partial y^2} = \nabla^2 z = -\frac{q}{s} \tag{5.21}$$

with Dirichlet BCs $z = 0$.

Using Central difference approximation in (5.1),

$$\begin{aligned} &\left(z_{i+1,j} - 2z_{i,j} + z_{i-1,j}\right) + \left(z_{i,j+1} - 2z_{i,j} + z_{i,j-1}\right) = -qh^2 / s \\ &\Rightarrow z_{i+1,j} + z_{i-1,j} + z_{i,j+1} + z_{i,j-1} - 4z_{i,j} = -qh^2 / s \end{aligned} \tag{5.22}$$

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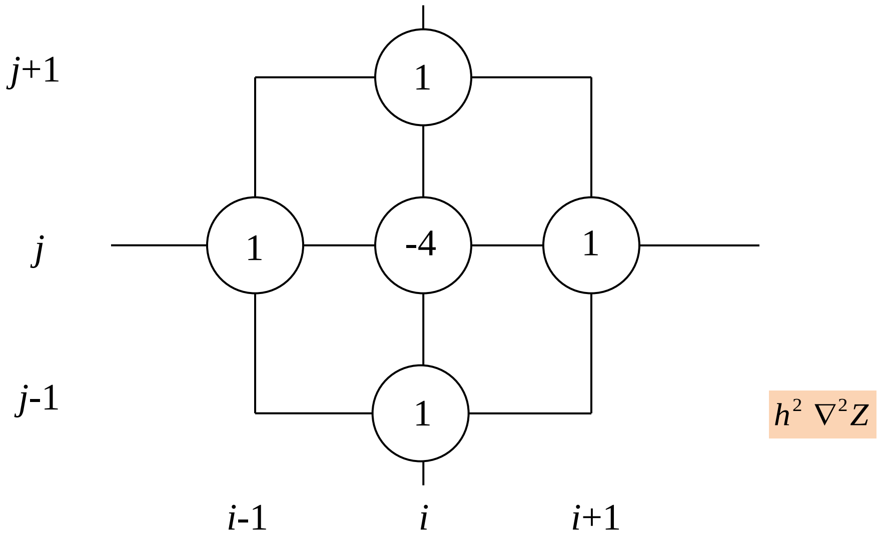

Fig 5.6

Consider a square membrane of width b. Only quarter of membrane is needed to formulate the systems of equations due to symmetry about centerlines and diagonal lines. The 6 pivotal points considered are shown in Fig 5.7. Note that the boundary displacements are zero.

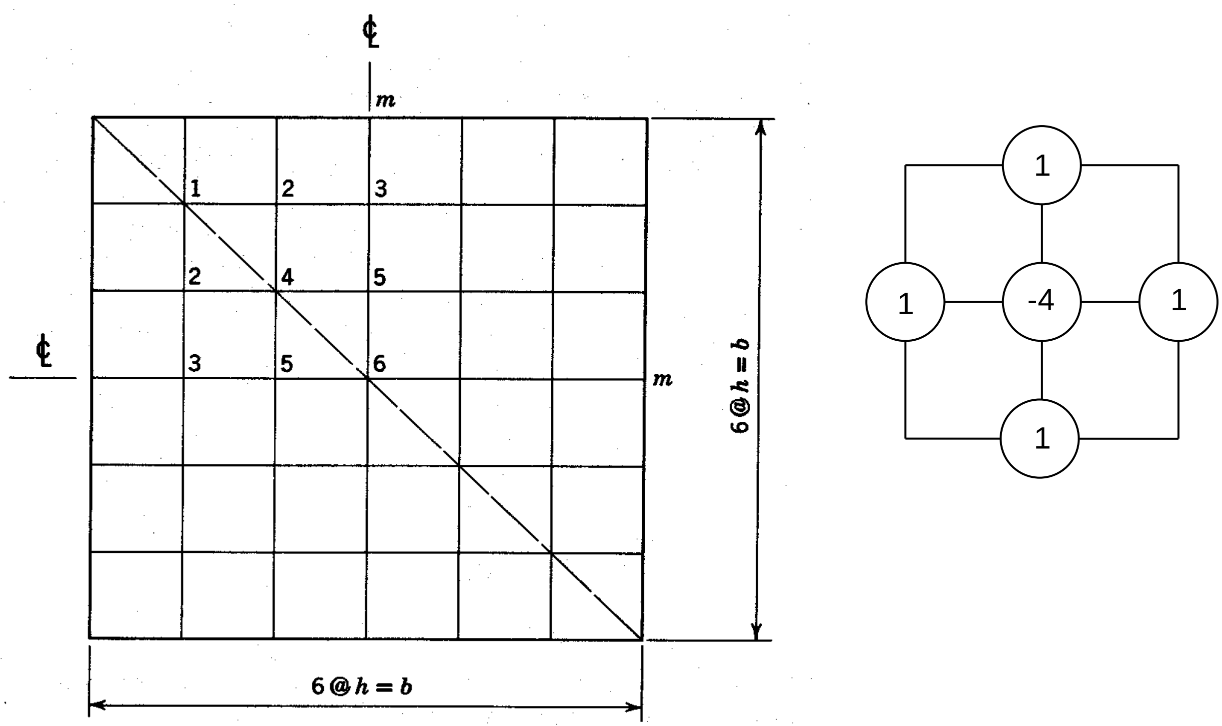

Fig 5.7

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From (5.22), we have the following system of equations,

$$
\begin{aligned}
&\text{Node 1: } -4z_1 + 2z_2 = -h^2 q/s \\
&\text{Node 2: } z_1 - 4z_2 + z_3 + z_4 = -h^2 q/s \\
&\text{Node 3: } 2z_2 - 4z_3 + z_5 = -h^2 q/s \\
&\text{Node 4: } 2z_2 - 4z_4 + 2z_5 = -h^2 q/s \\
&\text{Node 5: } z_3 + 2z_4 - 4z_5 + z_6 = -h^2 q/s \\
&\text{Node 6: } 4z_5 - 4z_6 = -h^2 q/s
\end{aligned}
\tag{5.23}
$$

The equations in (5.23) can be solved easily in the matrix form to give $z_1 = 0.952h^2 \dfrac{q}{s}$, $z_2 = 1.404h^2 \dfrac{q}{s}$, $z_3 = 1.539h^2 \dfrac{q}{s}$, $z_4 = 2.125h^2 \dfrac{q}{s}$, $z_5 = 2.346h^2 \dfrac{q}{s}$ and $z_6 = 2.596h^2 \dfrac{q}{s}$.

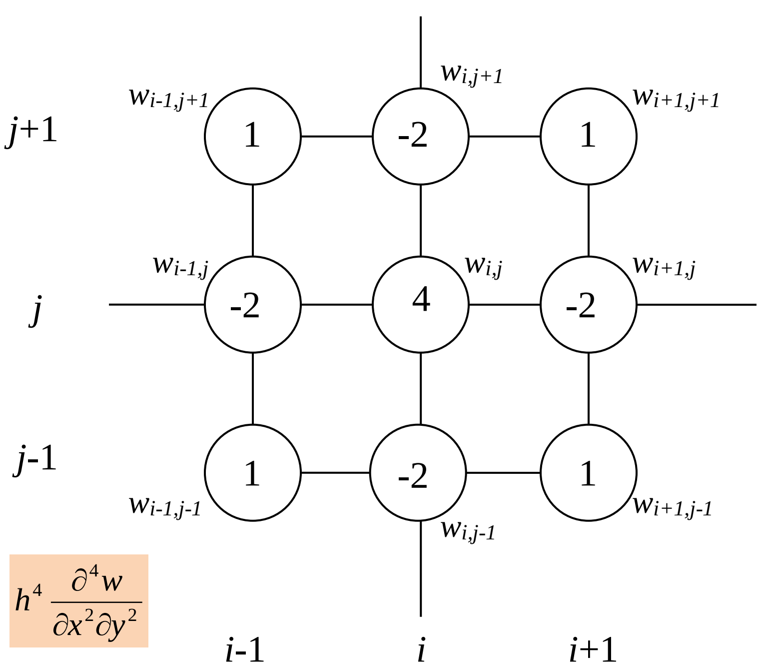
5.4.2 Deflection of Plates by FDM

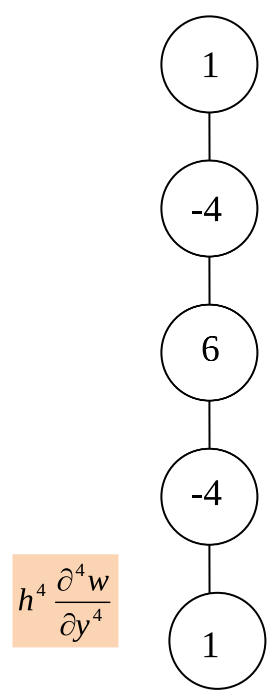
Governing equation for plate is

$$
\frac{\partial^4 w}{\partial x^4} + 2\frac{\partial^4 w}{\partial x^2 \partial y^2} + \frac{\partial^4 w}{\partial y^4} = \nabla^4 w = \nabla^2 \nabla^2 w = q/D \tag{5.24}
$$

where $D = Et^3/12(1-\upsilon^2)$ is the stiffness.

Recall from (5.1) and (5.20) that





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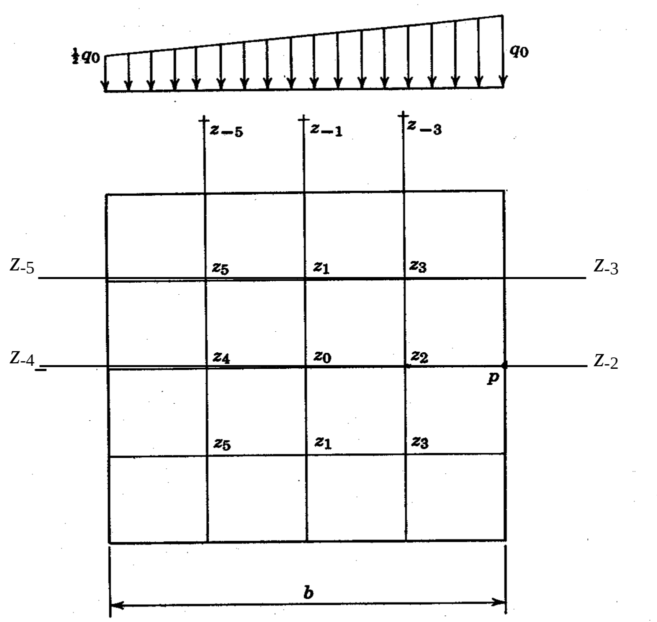
Coefficients of the finite difference equation at (i,j) for (5.24) can be derived as

	i-2		*i-1*		*i*		*i+1*		*i+2*
j-2					**1**				
j-1			2(1)	-----	-4+2(-2)	-----	2(1)		
j	*1*	-----	-4+2(-2)	-----	6+6+2(4)	-----	-4+2(-2)	-----	*1*
j+1			2(1)	-----	-4+2(-2)	-----	2(1)		
j+2					**1**				



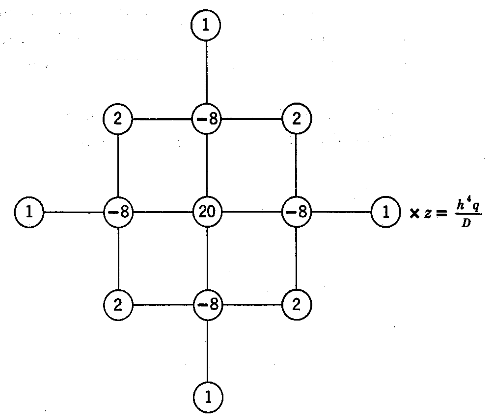


Fig 5.8

Consider a plate which is simply supported at the four edges. Using Fig 5.8, the system of finite difference equations for (5.24) is

$$
\begin{aligned}
20z_0 - 16z_1 - 8z_2 + 4z_3 - 8z_4 + 4z_5 &= 0.750 q_0 h^4 / D \quad &&(\text{at point } z_0)\\
-8z_0 + 20z_1 + 2z_2 - 8z_3 + 2z_4 - 8z_5 &= 0.750 q_0 h^4 / D \quad &&(\text{at point } z_1)\\
-8z_0 + 4z_1 + 19z_2 - 16z_3 + z_4 &= 0.875 q_0 h^4 / D \quad &&(\text{at point } z_2)\\
2z_0 - 8z_1 - 8z_2 + 19z_3 + z_5 &= 0.875 q_0 h^4 / D \quad &&(\text{at point } z_3)\\
-8z_0 + 4z_1 + z_2 + 19z_4 - 16z_5 &= 0.625 q_0 h^4 / D \quad &&(\text{at point } z_4)\\
2z_0 - 8z_1 + z_3 - 8z_4 + 19z_5 &= 0.625 q_0 h^4 / D \quad &&(\text{at point } z_5)
\end{aligned}
\qquad (5.25)
$$

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The solution is given by

$$z_0 = 0.774\frac{q_0 h^4}{D}, \; z_1 = 0.562\frac{q_0 h^4}{D}, \; z_2 = 0.584\frac{q_0 h^4}{D},$$

$$z_3 = 0.427\frac{q_0 h^4}{D}, \; z_4 = 0.541\frac{q_0 h^4}{D}, \; z_5 = 0.394\frac{q_0 h^4}{D}.$$

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5.5 Parabolic PDE by FDM

Unlike elliptic PDE, hyperbolic and parabolic PDE involves time in addition to space. The idea behind the solution technique is that the solution at $t = 0$ is known and the solution for subsequent times, namely $t = \Delta t, 2\Delta t, 3\Delta t$ ... are found by a marching process.

If the solution for $u_{i,j}$ can be expressed in difference equation form explicitly in terms of the solution at earlier times, then it is known as an explicit formulation or explicit marching process.

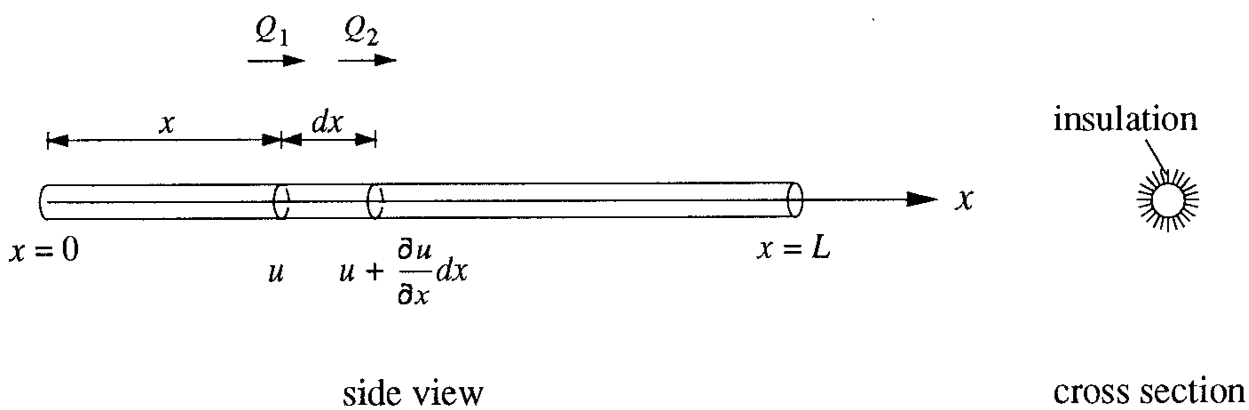

Fig 5.9

As an illustration, consider the heat flow along a rod insulated along its length as shown in Fig 5.9. The governing equation in terms of the temperature distribution $u(x,t)$ is given by

$$\frac{\partial u}{\partial t} = \frac{k}{\rho\sigma}\frac{\partial^2 u}{\partial x^2} \qquad \text{or} \qquad u_t = c^2 u_{xx} \tag{5.26}$$

where c^2= thermal diffusivity, k = thermal conductivity, σ = specific heat and ρ = density of the medium. (*Compare to consolidation equation in soil → diffusion equation*)

Eq (5.26) is 1st order in time and 2nd order in space, requiring one IC and two BC to solve the problem. The marching scheme thus starts from IC $u(x,0)$ as shown in Fig 5.10.

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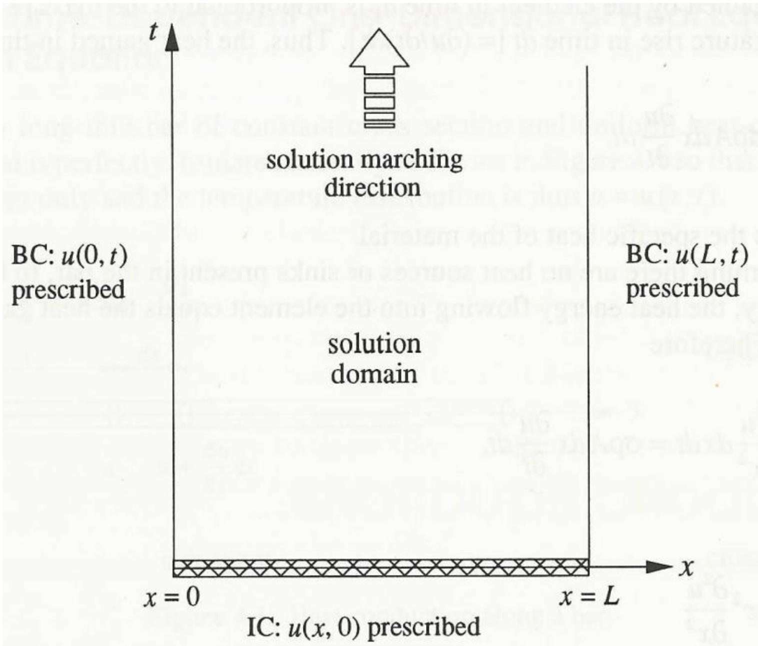
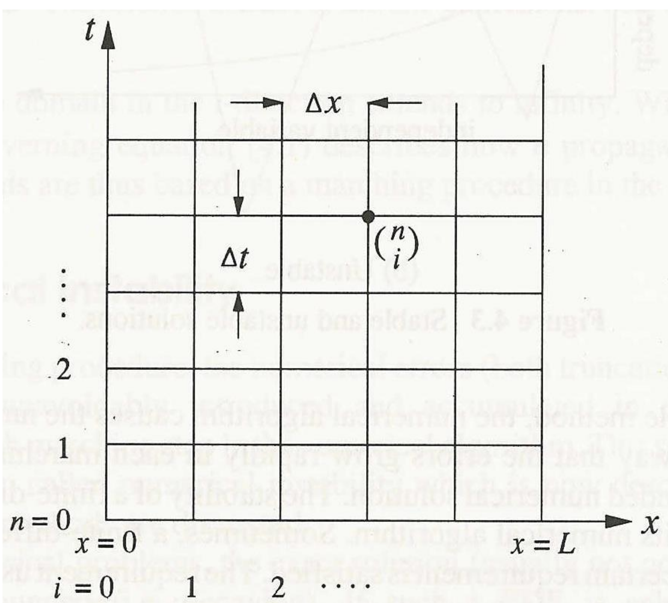


Fig 5.10

Eq (5.26) can be replaced by FD approximation, for example, by forward difference for the LHS and central difference for the RHS.



$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = c^2 \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right] \quad \Rightarrow \quad u_i^{n+1} = F u_{i+1}^n + (1-2F) u_i^n + F u_{i-1}^n \tag{5.27}$$

where $F = c^2 \Delta t / (\Delta x)^2$.

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From (5.27), the $(n+1)^{\text{th}}$ step can be found from values at the n^{th} step explicitly. This method is known as the explicit Euler method or forward time central space method. This method is stable iff $F \leq 0.5$.

As an illustration, consider the heat flow problem with F=0.25. Eq (5.27) becomes $u_i^{n+1} = \left(u_{i+1}^n + 2u_i^n + u_{i-1}^n\right)/4$

Assume the BCs are $u(0,t)=u(L,t)=0$ and IC is $u(x,0)=\sin(\pi x/L)$. Dividing the rod into 5 segments, the BCs become $u_0^n = u_5^n = 0$. The IC is thus $u_0^0 = u_5^0 = 0$, $u_1^0 = u_4^0 = \sin 0.2\pi = 0.5878$, $u_2^0 = u_3^0 = \sin 0.4\pi = 0.9511$.

i =	0	1	2	3	4	5
n = 0:	0	0.5878	0.9511	0.9511	0.5878	0
n = 1:	0	$u_1^1 = ?$	$u_2^1 = ?$	$u_3^1 = ?$	$u_4^1 = ?$	0

Note that a single equation is used to solve for each point without the need for iteration. Hence, it can be solved explicitly.

Solve for u_i^1:

$$u_1^1 = (u_2^0 + 2u_1^0 + u_0^0)/4 = (0.9511 + 2*0.5878 + 0)/4 = 0.5317$$
$$u_2^1 = (u_3^0 + 2u_2^0 + u_1^0)/4 = (0.9511 + 2*0.9511 + 0.5878)/4 = 0.8603$$
$$u_3^1 = (u_4^0 + 2u_3^0 + u_2^0)/4 = (0.5878 + 2*0.9511 + 0.9511)/4 = 0.8603$$
$$u_4^1 = (u_5^0 + 2u_4^0 + u_3^0)/4 = (0 + 2*0.5878 + 0.9511)/4 = 0.5317$$

i =	0	1	2	3	4	5
n = 0:	0	0.5878	0.9511	0.9511	0.5878	0
n = 1:	0	0.5317	0.8603	0.8603	0.5317	0
n = 2:	0	$u_1^2 = ?$	$u_2^2 = ?$	$u_3^2 = ?$	$u_4^2 = ?$	0

Proceed next with u_i^2,

$$u_1^2 = (u_2^1 + 2u_1^1 + u_0^1)/4 = (0.8603 + 2*0.5317 + 0)/4 = 0.4809$$
$$u_2^2 = (u_3^1 + 2u_2^1 + u_1^1)/4 = (0.8603 + 2*0.8603 + 0.5317)/4 = 0.7782$$

……….

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Program: Forward difference method for heat diffusion equation

```
function U = FDM_Heat(U0, c, L, F, T, ss, bc1, bc2)
% Forward Difference Method for heat diffusion equation Ut=c^2Uxx

% U0 = initial condition U(x,0)entered as a string
% c = thermal diffusivity
% L = length of rod
% F = c^2*dt/dx^2
% T = total time
% ss = number of spatial steps
% bc1 = boundary condition at x=0
% bc2 = boundary condition at x=L

dx = L/(ss-1);     % delta x
dt = F*dx^2/c^2;   % delta t
ts = round(T/dt); % number of temporal steps

U = zeros(ts,ss); % initialization
U(:, 1) = bc1;
U(:, ss) = bc2;

% Initial condition along bar
U(1, 2:ss-1) = feval(U0, dx:dx:(L-dx), L);

% at time step i, compute temperature profile as U(n,:)
for n=2:ts
    for i=2:ss-1
        U(n,i) = F*U(n-1,i+1) + (1-2*F)*U(n-1,i) + F*U(n-1,i-1);
    end
end

% plottng U(x,t)
x=0:dx:L;
t=zeros(size(x));
clf
for i=1:ts
    plot3(x,t,U(i,:));
    hold on
    t=t+dt;
end
grid on
xlabel('x-axis'), ylabel('time'), zlabel('U(t)')
```

```
function U0 = U0(x,L)
% Initial condition for heat diffusion example
% x = spatial grid points
% L = length of rod

U0 = sin(pi*x)/L;
```

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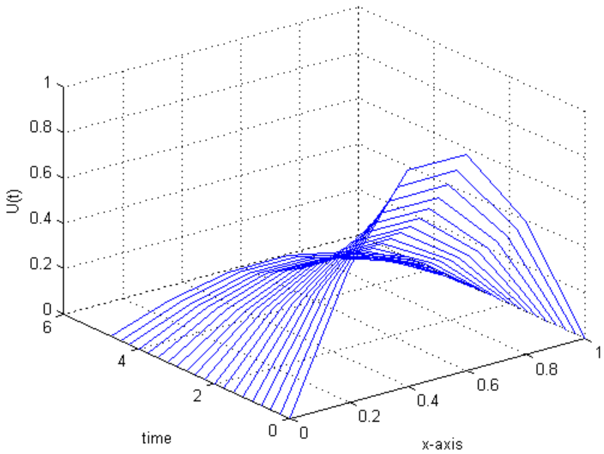
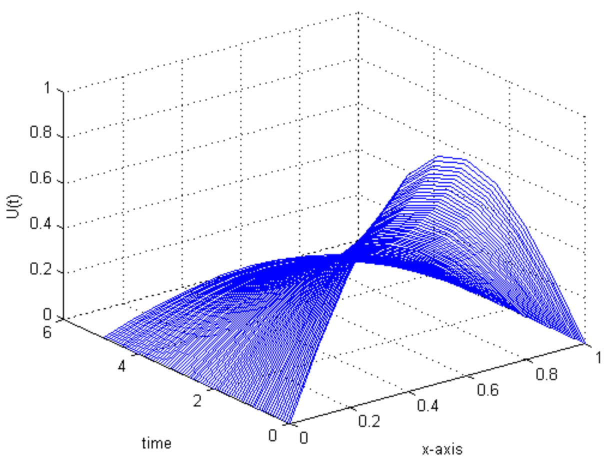
```
>> U = FDM_Heat('U0', 0.2, 1, 0.25, 5, 6, 0, 0);
```



$\Delta x = 0.2$, $\Delta t = 0.25$, $F = 0.25$ (20 time-steps to *T*=5)

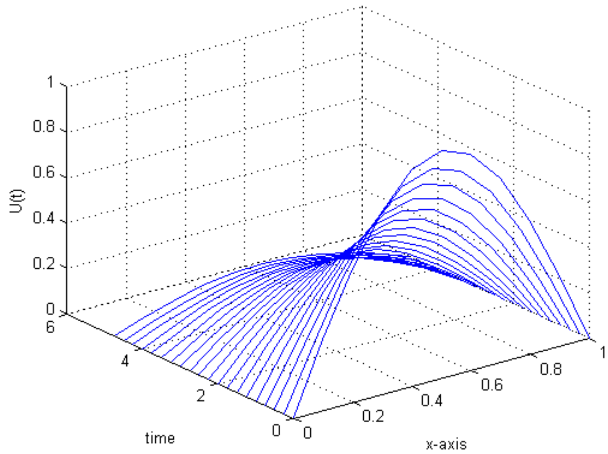
```
>> U = FDM_Heat('U0', 0.2, 1, 0.25, 5, 11, 0, 0);
```



$\Delta x = 0.1$, $\Delta t = 0.0625$, $F = 0.25$ (80 time-steps to *T*=5)

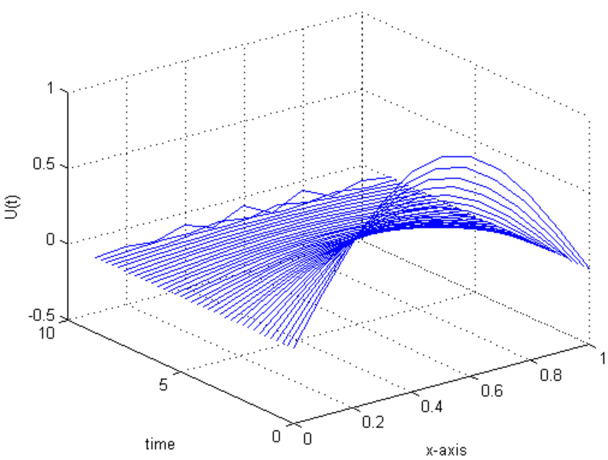
Note: with a small *F*, a refinement in the spatial grid size leads to a significant increase of time-steps required for a given time *T*, hence higher computational cost.

```
>> U = FDM_Heat('U0', 0.2, 1, 1, 5, 11, 0, 0);
```



$\Delta x = 0.1$, $\Delta t = 0.25$, $F = 1$ (20 time-steps to T=5)

```
>> U = FDM_Heat('U0', 0.2, 1, 1, 9, 11, 0, 0);
```



Note: with F=1, for the same spatial grid size, the number of time-steps required for a given T is much smaller than the previous example (F=0.25). However, numerical instabilities set in at some point in time.

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Can we use central difference in time for this problem?

Using $(u_t)_i^n = \dfrac{u_i^{n+1} - u_i^{n-1}}{2\Delta t}$, the equivalent of (5.27) is

$$u_i^{n+1} = 2Fu_{i+1}^n - 4Fu_i^n + 2Fu_{i-1}^n + u_i^{n-1} \tag{5.28}$$

5.6 Hyperbolic PDE by FDM

One of the most famous hyperbolic PDE is the wave equation

$$\frac{\partial^2 u}{\partial t^2} = k^2 \frac{\partial^2 u}{\partial x^2} \qquad \text{or} \qquad u_{tt} = k^2 u_{xx} \tag{5.29}$$

An example described by the above PDE is the transverse displacement $u(x,t)$ of an initially tightly stretched string (compared to gravitational force) released to vibrate freely. The slope of the string is assumed to be small (small displacement).

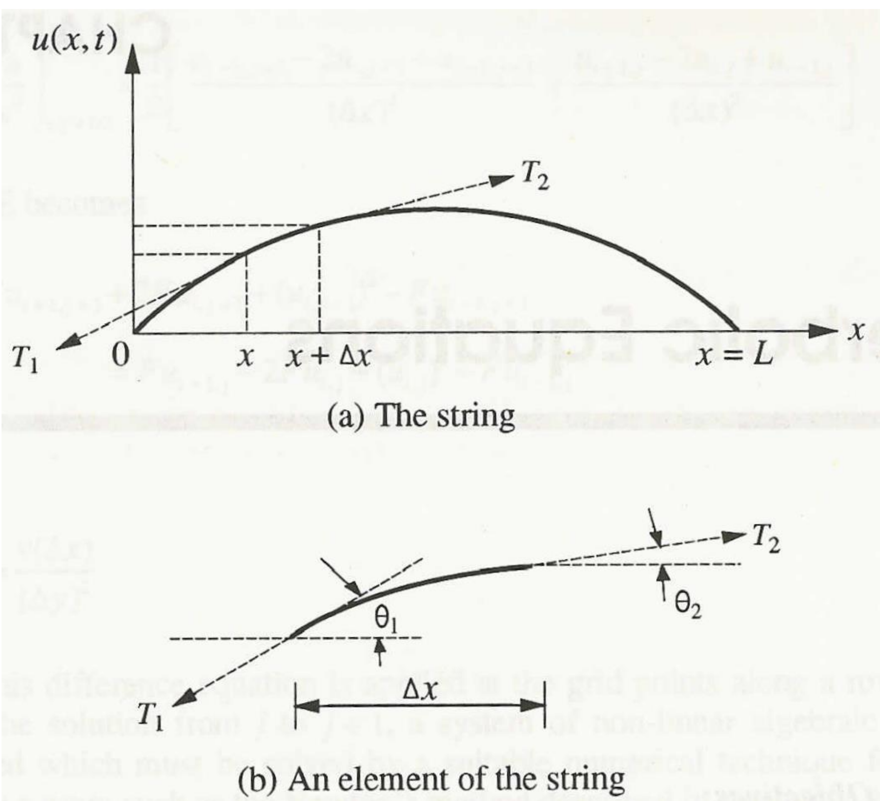

Fig 5.11

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$$\frac{\partial^2 u}{\partial t^2} = k^2 \frac{\partial^2 u}{\partial x^2} \qquad \text{or} \qquad u_{tt} = k^2 u_{xx}$$

Solution of (5.29) requires two BCs and two ICs.

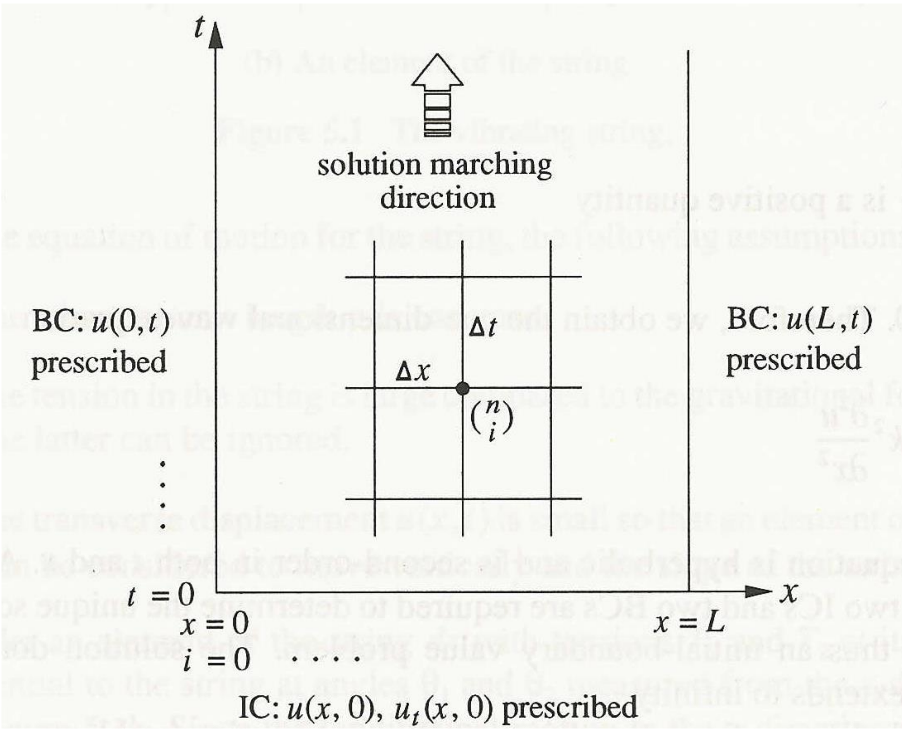

Fig 5.12

Using central difference approximation, (5.29) can be written as

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\Delta t)^2} = k^2 \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right]$$

Rearranging the terms,

$$u_i^{n+1} = R^2 u_{i+1}^n + 2(1 - R^2) u_i^n + R^2 u_{i-1}^n - u_i^{n-1} \tag{5.30}$$

where $R = k\Delta t / \Delta x$.

The computation starts with time $n = 0$

$$u_i^1 = R^2 u_{i+1}^0 + 2(1 - R^2) u_i^0 + R^2 u_{i-1}^0 - u_i^{-1} \tag{5.31}$$

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The initial conditions are

a) displacement: $u_i^0 = f(x_i) = f(i\Delta x) = f_i$

b) velocity: $(u_t)_i^0 = \left(\dfrac{\partial u}{\partial t}\right)_i^0 = \dfrac{u_i^1 - u_i^{-1}}{2\Delta t} = g_i \;\Rightarrow\; u_i^{-1} = u_i^1 - 2(\Delta t)g_i$ (5.32)

Substituting (5.32b) into (5.31) yields

$$u_i^1 = \frac{R^2}{2}u_{i+1}^0 + (1-R^2)u_i^0 + \frac{R^2}{2}u_{i-1}^0 + (\Delta t)g_i \tag{5.33}$$

Stability of results requires that the Courant condition $R \le 1$ be satisfied, i.e. $k\Delta t \le \Delta x$.

5.7 Implicit FDM for Hyperbolic and Parabolic PDE

In the explicit FDM, the step sizes Δt and Δx to use is a very important consideration affecting the accuracy of the results. For example with parabolic FDM, $F = c^2\Delta t/(\Delta x)^2 \le 0.5$ must be satisfied for stability. This implies that <u>Δt and Δx cannot be drastically different</u> since $\Delta t \le (\Delta x/c)^2/2$. Even if this condition is satisfied, the individual <u>absolute value for Δt and Δx cannot be too large</u> – we are approximating the differential in time with a difference equation and a coarse Δt will yield poor results. Same argument goes for the displacement shape.

As the step sizes Δt and Δx decreases, the <u>truncation error</u> caused by approximating the derivatives using finite difference decreases. However, with smaller grid sizes, more computations are needed to arrive at a particular time step. This causes an accumulation of <u>round-off errors</u>. Thus the total error may decrease with step size when the grid size is decreased from a coarse grid until a certain threshold, after which it will increase with the decrease of step size, as shown in Fig 5.13.

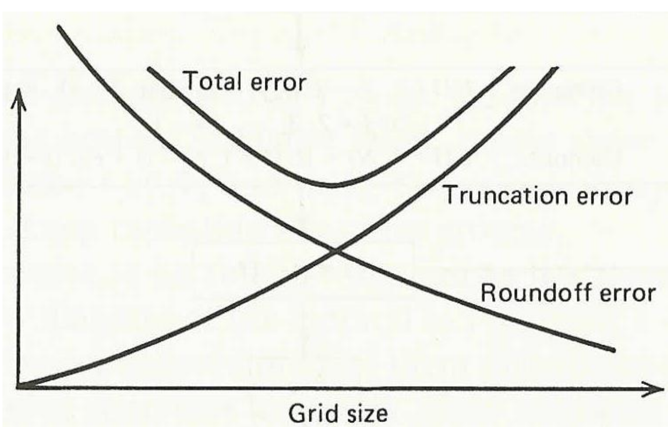

Fig 5.13

Implicit FDM removes the restriction of $F \leq 0.5$ for stability. To overcome the build-up of round-off errors, an implicit FDM formulation may be employed where larger step size can be used without loss of accuracy. However, such formulation results in a system of equation to be solved instead of a single propagating equation.

As an illustration of an implicit FDM formulation, consider the parabolic PDE in Section 5.5 involving the heat flow problem. Eqs (5.26) and (5.27) are reproduced below for convenience.

$$u_t = c^2 u_{xx} \quad , \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} = c^2 \left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right]$$

For the implicit formulation, (5.27) is written as a weighted average of the central difference of u_{xx} at time n+1 and n

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = c^2 \left[\lambda \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} + (1-\lambda) \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right] \tag{5.34}$$

Rearranging the terms,

$$-\lambda F u_{i+1}^{n+1} + (1 + 2\lambda F) u_i^{n+1} - \lambda F u_{i-1}^{n+1} = (1-\lambda) F u_{i+1}^n + [1 - 2(1-\lambda)F] u_i^n + (1-\lambda) F u_{i-1}^n \tag{5.35}$$

where $F = c^2 \Delta t / (\Delta x)^2$.

To proceed with the solution, a value of λ has to be specified. If $\lambda=1/2$, then we have the Crank Nicholson Method. For purpose of illustration, set $F=2$ and $\lambda=1/2$ giving $\lambda F=1$. Eq (5.35) becomes

$$-u_{i+1}^{n+1} + 3u_i^{n+1} - u_{i-1}^{n+1} = u_{i+1}^n - u_i^n + u_{i-1}^n \tag{5.36}$$

Assume BCs are $u(0,t)=u(L,t)=0$ and IC is $u(x,0)=\sin(\pi x/L)$. Divide the rod into 5 segments to give

i =	0	1	2	3	4	5
n = 0:	0	0.5878	0.9511	0.9511	0.5878	0
n = 1:	0	$u_1^1 = ?$	$u_2^1 = ?$	$u_3^1 = ?$	$u_4^1 = ?$	0

Starting with n = 0 in (5.36),

$$\begin{aligned}
i = 1: &\quad -u_2^1 + 3u_1^1 - u_0^1 = u_2^0 - u_1^0 + u_0^0 = 0.3633 \\
i = 2: &\quad -u_3^1 + 3u_2^1 - u_1^1 = u_3^0 - u_2^0 + u_1^0 = 0.5878 \\
i = 3: &\quad -u_4^1 + 3u_3^1 - u_2^1 = u_4^0 - u_3^0 + u_2^0 = 0.5878 \\
i = 4: &\quad -u_5^1 + 3u_4^1 - u_3^1 = u_5^0 - u_4^0 + u_3^0 = 0.3633
\end{aligned} \tag{5.37}$$

Note that instead of a single equation to solve explicitly for each point as shown in Section 5.5, the system of equations in (5.37) have to be solved implicitly, i.e.

$$\begin{bmatrix} 3 & -1 & 0 & 0 \\ -1 & 3 & -1 & 0 \\ 0 & -1 & 3 & -1 \\ 0 & 0 & -1 & 3 \end{bmatrix} \begin{Bmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \\ u_4^1 \end{Bmatrix} = \begin{Bmatrix} 0.3633 \\ 0.5878 \\ 0.5878 \\ 0.3633 \end{Bmatrix} \tag{5.38}$$

which results in $u_1^1 = 0.2629$, $u_2^1 = 0.4253$, $u_3^1 = 0.4253$ and $u_4^1 = 0.2629$.

These values for n = 0 are then used to proceed for the next time step (n = 1), where another set of equations similar to (3.63) need to be solved.

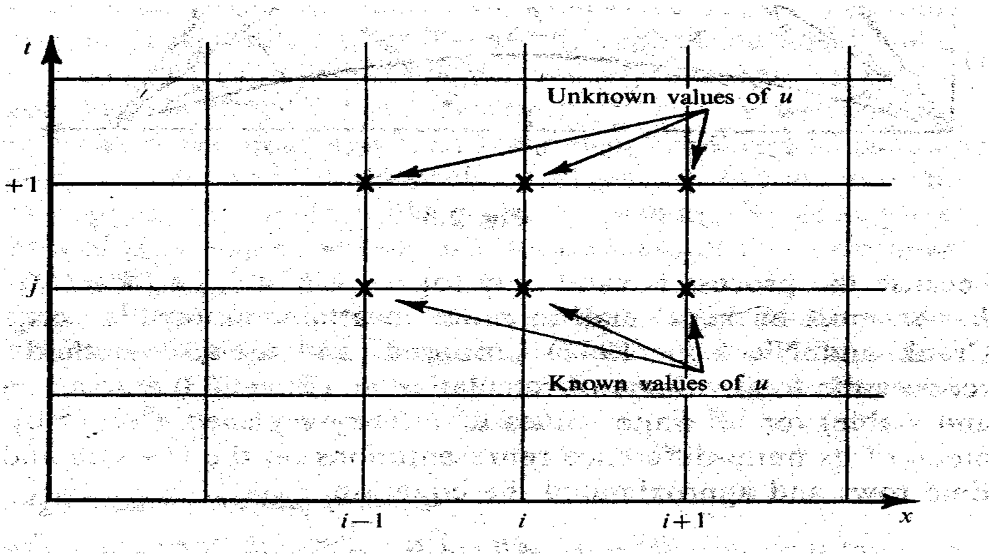

Fig 5.14

Note that (3.63) has a special tri-diagonal form,

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 \\ a_1 & b_2 & c_2 & \vdots \\ 0 & \dots & ... & c_{n-1} \\ 0 & \dots & a_{n-1} & b_n \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} = \begin{Bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{Bmatrix}$$

For such tri-diagonal matrices, we can perform a special transformation to simplify the numerical computation for large size problems, i.e.

$$\begin{bmatrix} 1 & c_1^* & 0 & 0 \\ 0 & 1 & c_2^* & \vdots \\ 0 & \dots & \dots & c_{n-1}^* \\ 0 & \dots & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} = \begin{Bmatrix} d_1^* \\ d_2^* \\ \vdots \\ d_n^* \end{Bmatrix} \tag{5.39}$$

where

$$c_1^* = c_1 / b_1$$
$$d_1^* = d_1 / b_1$$
$$c_{i+1}^* = c_{i+1} / (b_{i+1} - a_i c_i^*) \quad , \quad i = 1, 2, \cdots, n-2$$
$$d_{i+1}^* = (d_{i+1} - a_i d_i^*) / (b_{i+1} - a_i c_i^*) \quad , \quad i = 1, 2, \cdots, n-1$$

The solution is then given by

$$x_n = d_n^*$$
$$x_i = d_i^* - c_i^* x_{i+1} \quad , \quad i = n-1,\ n-2,\ \cdots, 1$$

The above facilitates hand computation or just a few lines of MATLAB or Fortran code if the problem is large.

5.8 Consistency, Convergence and Stability

This section gives a very brief treatment of consistency, convergence and stability in FDM. For detailed treatment, interested students should refer to FD textbooks or papers. FD is a numerical model to approximate the differential equations and IC & BCs. This results in <u>truncation</u> errors which can be deduced from the Taylor series expansion.

For example, from (5.15),

$$\frac{\partial u_{i,j}}{\partial x} = \frac{u_{i+1,j} - u_{i,j}}{h} + O(h)$$
$$\frac{\partial^2 u_{i,j}}{\partial x^2} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + O(h^2)\,.$$

The truncation error for parabolic PDE based on (5.27) at point i and time n is thus

$$T_i^n = \left(\frac{\partial u}{\partial t} - c^2 \frac{\partial^2 u}{\partial x^2} \right)_i^n - \left[\frac{u_i^{n+1} - u_i^n}{k} - c^2 \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2} \right] = O(k) + c^2 O(h^2) \tag{5.40}$$

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T_i is the local error arising from (a) discretization size of h and k and (b) truncating the Taylor series.

Consider point (i, n). Note that the local error decreases with the step size ($T_i^n \to 0$ as $h \to 0$ and $k \to 0$). This implies that the FD formulation is consistent.

Convergence of a model requires that across all points in space and time, the norm of the differences between the exact and FD solution approaches 0. Hence this is a global truncation error which results from the accumulation of local truncation error.

Convergence is usually difficult to investigate as illustrated below for the case of parabolic PDE in Section 5.5. Consider the heat diffusion equation $u_t = c^2 u_{xx}$. From (5.27),

$$u_i^{n+1} = Fu_{i+1}^n + (1-2F)u_i^n + Fu_{i-1}^n$$

where $F = c^2 \Delta t / (\Delta x)^2 = c^2 k / h^2$.

Let U_i^n be the exact solution and the error given by $e_i^n = U_i^n - u_i^n$. (5.27) can thus be re-written as

$$\begin{aligned} U_i^{n+1} - e_i^{n+1} &= F\left(U_{i+1}^n - e_{i+1}^n\right) + (1-2F)\left(U_i^n - e_i^n\right) + F\left(U_{i-1}^n - e_{i-1}^n\right) \\ e_i^{n+1} &= Fe_{i+1}^n + (1-2F)e_i^n + Fe_{i-1}^n + \left[U_i^{n+1} - FU_{i+1}^n - (1-2F)U_i^n - FU_{i-1}^n\right] \end{aligned} \tag{5.41}$$

Since U is the exact solution, the limiting value of the term in square bracket should approach zero ($h \to 0$, $k = Fh^2/c^2 \to 0$). If the coefficients of the terms on the RHS are positive ($F \geq 0$ and $(1-2F) \geq 0 \Rightarrow 0 \leq F \leq 0.5$), then one can deduce from (5.41) that

$$e_i^{n+1} \leq \left|e_i^{n+1}\right| \leq F\left|e_{i+1}^n\right| + (1-2F)\left|e_i^n\right| + F\left|e_{i-1}^n\right| \tag{5.42}$$

Let $E^n = \max\left|e_i^n\right|$ for all i. Then substituting into the above,

$$E^{n+1} \leq E^n \tag{5.43}$$

From the IC, $E^0 = 0$. Hence, in the limit $h \to 0$ and $k = Fh^2/c^2 \to 0$, then $E^n \to 0$. Since $\left|U_i^n - u_i^n\right| \leq E^n$, it implies that u converges to U as $h \to 0$ and $k = Fh^2/c^2 \to 0$, provided $0 \leq F \leq ½$.

Stability of an approximation refers to the condition when the propagation of the total error remains small as t increases.

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5.8.1 Lax equivalent theorem

For a consistent finite difference approximation to a well-posed, linear, initial-boundary-value problem (satisfying the condition of existence, uniqueness and continuity), then stability is a necessary and sufficient condition for convergence (equivalently, if an approximation is consistent, then it is convergent if and only if it is stable).

The stability conditions for parabolic and hyperbolic PDEs have been given earlier, though not proven, for explicit formulation. The formulation is thus said to be conditionally stable. If the method is stable without conditions, such as in the implicit formulation of which the Crank-Nicholson Method is one variation, then it is said to be unconditionally stable.

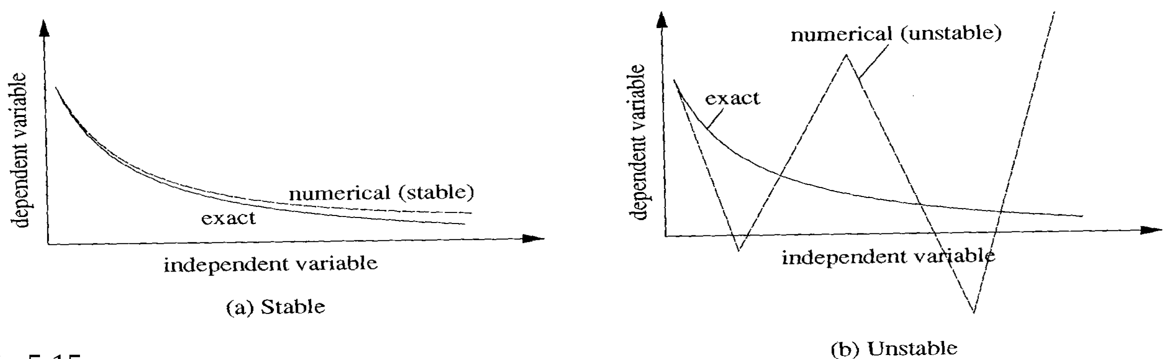

Fig 5.15

There are various methods for stability analysis of FDM. These include the perturbation method, the matrix method and the von Neumann analysis. The latter is described in "Numerical Recipes in Fortran" by W.H. Press et al, Second Edition, Cambridge.

5.8.2 von Neumann Stability Analysis

Consider the separable function

$$u(x,t) = \xi(t)\exp(ikx) = \xi(t)[\cos x + i\sin x] \tag{5.44}$$

The term in the square bracket is oscillatory between -1 and 1 with amplitude $\cos^2 x + \sin^2 x = 1$. The coefficient $\xi(t)$ is therefore amplitude of $u(x, t)$ with respect to t variation (in other words, how u changes with t).

If $\xi(t) < 1$ for all t, then the amplitude of the function $u(x, t)$ will always be inside the unit circle in the complex plane plot.

Also note that $\sin\theta = (e^{i\theta} - e^{-i\theta})/2i$ and $\cos\theta = (e^{i\theta} + e^{-i\theta})/2$.

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Now consider the FTCS for the parabolic PDE in (5.27)

$$u_j^{n+1} = Fu_{j+1}^n + (1-2F)u_j^n + Fu_{j-1}^n \quad , \quad F = c^2 \Delta t \big/ (\Delta x)^2 \ .$$

For the case where the coefficients are constant, one can express the solution in separable form. The total displacement at time n for point j is written as

$$u_j^n = \sum_{k=1}^{N} \xi_k(t)^n \exp(ikj\Delta x)$$

where k is a real spatial wave number.

For simplicity, consider only the displacement for a particular mode k,

$$u_j^n = \xi_k(t)^n \exp(ikj\Delta x) \tag{5.45}$$

which is similar to (5.44).

Note that

$$\begin{aligned} u_{j+1}^n &= \xi_k(t)^n \exp(ik(j+1)\Delta x) = \xi_k(t)^n \exp(ikj\Delta x)\exp(ik\Delta x) \\ u_{j-1}^n &= \xi_k(t)^n \exp(ik(j-1)\Delta x) = \xi_k(t)^n \exp(ikj\Delta x)\exp(-ik\Delta x) \\ u_j^{n+1} &= \xi_k(t)^{n+1} \exp(ikj\Delta x) \end{aligned} \tag{5.46}$$

$$u_i^{n+1} = Fu_{i+1}^n + (1-2F)u_i^n + Fu_{i-1}^n$$

Substituting (5.46) into (5.27) gives

$$\begin{aligned} \xi_k(t)^{n+1} \exp(ikj\Delta x) = F\ &\xi_k(t)^n \exp(ikj\Delta x)\exp(ik\Delta x) \\ &+ (1-2F)\xi_k(t)^n \exp(ikj\Delta x) \\ &+ F\ \xi_k(t)^n \exp(ikj\Delta x)\exp(-ik\Delta x) \\ \zeta(k) &= \xi_k(t)^{n+1} / \xi_k(t)^n \\ &= F\exp(ik\Delta x) + (1-2F) + F\exp(-ik\Delta x) \\ &= 1 - 2F(1-\cos k\Delta x) \end{aligned} \tag{5.47}$$

Stability condition requires that $|\zeta| \le 1$ (no component in the eigenvector expansion of u grows without bound). The maximum value for $\cos k\Delta x$ = 1, which satisfies the stability condition. Hence, the critical point is governed by $\cos k\Delta x$ = -1, which results in the condition $F \le 0.5$.

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5.8.3 Stability Analysis for Backward Time Central Difference Scheme

The BTCS for the PDE in (5.26) is given by

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

Rearranging the terms,

$$-u_j^{n-1} = F u_{j+1}^n - (1+2F) u_j^n + F u_{j-1}^n \tag{5.48}$$

where $F = c^2 \Delta t / (\Delta x)^2$

From (5.45),

$$\begin{aligned} u_{j+1}^n &= \xi_k(t)^n \exp(ikj\Delta x) \exp(ik\Delta x) \\ u_{j-1}^n &= \xi_k(t)^n \exp(ikj\Delta x) \exp(-ik\Delta x) \\ u_j^{n-1} &= \xi_k(t)^{n-1} \exp(ikj\Delta x) \end{aligned} \tag{5.49}$$

Substituting (5.49) into (5.48),

$$\begin{aligned} \zeta(k) &= \xi_k(t)^n / \xi_k(t)^{n-1} \\ &= -1/[F\exp(ik\Delta x) - (1+2F) + F\exp(-ik\Delta x)] \\ &= 1/[1+2F(1-\cos(k\Delta x)] \end{aligned} \tag{5.50}$$

Since $1-\cos(k\Delta x) \geq 0$, the denominator in (5.50) is always greater than 1. Hence, stability is guaranteed.