# ESO 208A: Computational Methods in Engineering

Partial Differential Equation: Introduction, Parabolic Equation

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### Introduction

### A general 2<sup>nd</sup> Order PDE:

$$\alpha \phi_{xx} + 2\beta \phi_{xy} + \gamma \phi_{yy} + \theta \phi_x + \omega \phi_y + \rho(\phi, x, y) = 0$$

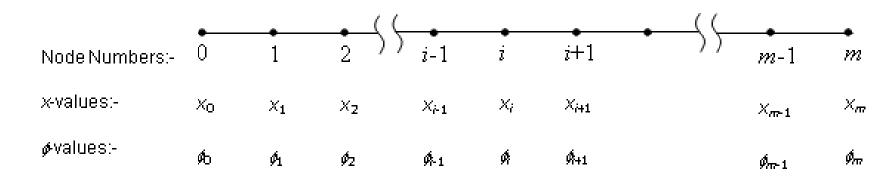
- ✓  $\beta^2 \alpha \gamma = 0$ : Parabolic PDE, *e.g.*, Diffusion and Advection-Diffusion Equation
- $\checkmark \beta^2 \alpha \gamma < 0$ : Elliptic PDE, e.g., Laplace Equation
- $\checkmark \beta^2 \alpha \gamma > 0$ : Hyperbolic PDE, e.g., Wave equation

We will learn a few *Finite Difference* methods for most common PDEs in Engineering Problems!

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \qquad \qquad \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

$$\phi(0,t) = c_0; \ \phi(L,t) = c_L; \ \phi(x,0) = f(x)$$

$$\begin{split} \frac{d\phi_{i}}{dt} &= \alpha_{i} \frac{\phi_{i+1} - 2\phi_{i} + \phi_{i-1}}{\Delta x^{2}} \\ \frac{d\phi_{i}}{dt} &= -u_{i} \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + \alpha_{i} \frac{\phi_{i+1} - 2\phi_{i} + \phi_{i-1}}{\Delta x^{2}} \end{split}$$



Node Numbers:- 
$$0$$
  $1$   $2$   $i-1$   $i$   $i+1$   $m-1$   $m$   $x$ -values:-  $x_0$   $x_1$   $x_2$   $x_{i+1}$   $x_i$   $x_{i+1}$   $x_{m-1}$   $x_m$   $x_m$ 

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \qquad \frac{\partial \phi_i}{\partial t} = \alpha_i \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$
  
$$\phi(0, t) = c_0; \ \phi(L, t) = c_L; \ \phi(x, 0) = f(x); \ m = 4$$

$$\begin{bmatrix} \frac{d\phi_1}{dt} \\ \frac{d\phi_2}{dt} \\ \frac{d\phi_3}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{2\alpha_1}{\Delta x^2} & \frac{\alpha_1}{\Delta x^2} & 0 \\ \frac{\alpha_2}{\Delta x^2} & -\frac{2\alpha_2}{\Delta x^2} & \frac{\alpha_2}{\Delta x^2} \\ 0 & \frac{\alpha_3}{\Delta x^2} & -\frac{2\alpha_3}{\Delta x^2} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} + \begin{bmatrix} \frac{c_0 \alpha_1}{\Delta x^2} \\ \frac{\sigma_2}{\Delta x^2} \\ \frac{\sigma_2}{\Delta x^2} \end{bmatrix}$$

Node Numbers:- 0 1 2 
$$i-1$$
  $i$   $i+1$   $m-1$   $m$   $x$ -values:-  $x_0$   $x_1$   $x_2$   $x_{i+1}$   $x_i$   $x_{i+1}$   $x_{m-1}$   $x_m$   $x_m$ 

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = \alpha \frac{\partial^2 \phi}{\partial x^2} \qquad \frac{d\phi_i}{dt} = -u_i \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} + \alpha_i \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$
  
$$\phi(0, t) = c_0; \ \phi(L, t) = c_L; \ \phi(x, 0) = f(x)$$

$$\begin{bmatrix} \frac{d\phi_1}{dt} \\ \frac{d\phi_2}{dt} \\ \frac{d\phi_3}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{2\alpha_1}{\Delta x^2} & -\frac{u_1}{2\Delta x} + \frac{\alpha_1}{\Delta x^2} & 0 \\ \frac{u_2}{2\Delta x} + \frac{\alpha_2}{\Delta x^2} & -\frac{2\alpha_2}{\Delta x^2} & -\frac{u_2}{2\Delta x} + \frac{\alpha_2}{\Delta x^2} \\ 0 & \frac{u_3}{2\Delta x} + \frac{\alpha_3}{\Delta x^2} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} + \begin{bmatrix} \frac{u_1 c_0}{2\Delta x} + \frac{c_0 \alpha_1}{\Delta x^2} \\ 0 \\ -\frac{u_3 c_L}{2\Delta x} + \frac{c_L \alpha_3}{\Delta x^2} \end{bmatrix}$$

Node Numbers:- 
$$0$$
  $1$   $2$   $i-1$   $i$   $i+1$   $m-1$   $m$   $x$ -values:-  $x_0$   $x_1$   $x_2$   $x_{i+1}$   $x_i$   $x_{i+1}$   $x_{m-1}$   $x_m$   $x_m$ 

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \qquad \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

$$\phi(0,t) = c_0; \ \phi(L,t) = c_L; \ \phi(x,0) = f(x)$$

$$\frac{\mathrm{d}\bar{\phi}}{\mathrm{dt}} = \mathbf{A}\bar{\phi} + \mathbf{b} \qquad \bar{\phi} = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} \qquad \bar{\phi}(0) = \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{bmatrix}$$

$$\frac{\mathrm{d}\bar{\phi}}{\mathrm{dt}} = \mathbf{A}\bar{\phi} + \mathbf{b} \qquad \bar{\phi} = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} \qquad \bar{\phi}(0) = \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{bmatrix}$$

$$\bar{\phi}^{n+1} = \bar{\phi}^n + \Delta t [\mu \{ \mathbf{A}^n \bar{\phi}^n + \mathbf{b}^n \} + (1 - \mu) \{ \mathbf{A}^{n+1} \bar{\phi}^{n+1} + \mathbf{b}^{n+1} \}]$$

 $\mu = 0$ : Euler Backward;  $\mu = 1$ : Euler Forward  $\mu = 1/2$ : Trapezoidal

$$[I - \Delta t(1 - \mu)\mathbf{A}^{n+1}]\bar{\phi}^{n+1}$$

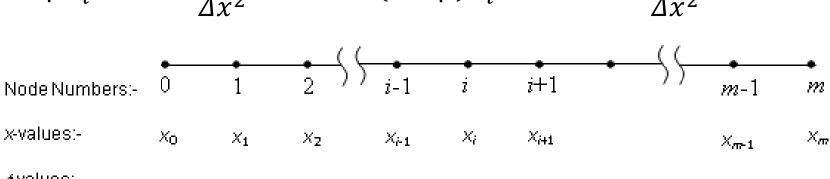
$$= [I + \mu \Delta t \mathbf{A}^n]\bar{\phi}^n + \Delta t[(1 - \mu)\mathbf{b}^{n+1} + \mu \mathbf{b}^n]$$

### Parabolic PDE: full-discretization

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

$$\phi(0,t) = c_0; \ \phi(L,t) = c_L; \ \phi(x,0) = f(x)$$

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \mu \alpha_i^n \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + (1 - \mu)\alpha_i^{n+1} \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}$$



$$\phi$$
 values:-  $\phi_0$   $\phi_1$   $\phi_2$   $\phi_{r_1}$   $\phi$   $\phi_{r+1}$   $\phi_{rr-1}$   $\phi_{rr}$ 

### Parabolic PDE: full-discretization

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

$$\phi(0, t) = c_0; \ \phi(L, t) = c_L; \ \phi(x, 0) = f(x)$$

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

Node Numbers:- 
$$0$$
  $1$   $2$   $i-1$   $i$   $i+1$   $m-1$   $m$  x-values:-  $x_0$   $x_1$   $x_2$   $x_{i+1}$   $x_i$   $x_{i+1}$   $x_{m-1}$   $x_m$   $x_{m-1}$   $x_m$   $x_$ 

## Types of Boundary Condition

- ✓ Dirichlet Condition (1<sup>st</sup> Type):
  - ✓ Variable value is specified

$$\phi(0,t) = c_0; \ \phi(L,t) = c_L$$

- ✓ Neumann Condition ( $2^{nd}$  Type):
  - ✓ Gradient is specified

$$\left. \frac{dj}{dx} \right|_{(0,t) \text{ and/or } (L,t)} = \epsilon$$

- ✓ Robin Condition (3<sup>rd</sup> Type):
  - ✓ A linear combination of the variable and gradient is specified at (0, t) and/or (L, t)

$$a\frac{dj}{dx} + bf = c$$

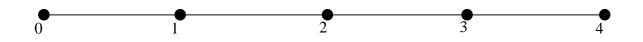
$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$$u = 0.1$$
;  $\alpha = 0.01$ ;  $T(0, t) = 0$ ;  $T(1, t) = 0$ ;  $T(x, 0) = 50 \sin \pi x$ 

#### Solve Using:

- (a) Euler Forward in time and Centeral Difference in space (EF-CD)
- (b) Euler Backward in time and Central Difference in space (EB-CD)
- (c) Crank Nicholson method
- (d) A 2<sup>nd</sup> order R-K method in time and Central Difference approximation in space.

Use 
$$\Delta x = 0.25$$
 and  $\Delta t = 0.5$ 



$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$$u = 0.1; \ \alpha = 0.01; T(0, t) = 0; \ T(1, t) = 0; \ T(x, 0) = 50 \sin \pi x$$

$$\frac{dT_{j}}{dt} + u \frac{T_{j+1} - T_{j-1}}{2Dx} = 2 \frac{T_{j+1} - 2T_{j} + T_{j-1}}{Dx^{2}}$$

$$\frac{dT_{j}}{dt} = \left(\frac{u}{2Dx} + \frac{\partial}{Dx^{2}}\right)T_{j-1} + \left(-\frac{2\partial}{Dx^{2}}\right)T_{j} + \left(-\frac{u}{2Dx} + \frac{\partial}{Dx^{2}}\right)T_{j+1}$$

$$\frac{dT_j}{dt} = 0.36T_{j-1} - 0.32T_j - 0.04T_{j+1}$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$$u = 0.1; \ \alpha = 0.01; T(0, t) = 0; \ T(1, t) = 0; \ T(x, 0) = 50 \sin \pi x$$

$$\frac{dT_{j}}{dt} = 0.36T_{j-1} - 0.32T_{j} - 0.04T_{j+1} \qquad \frac{d\mathbf{T}}{dt} = \mathbf{AT}$$

$$\mathbf{T} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} -0.32 & -0.04 & 0 \\ 0.36 & -0.32 & -0.04 \\ 0 & 0.36 & -0.32 \end{bmatrix} \qquad \mathbf{T}^0 = \begin{bmatrix} T_1^0 \\ T_2^0 \\ T_2^0 \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

$$\frac{d\mathbf{T}}{dt} = \mathbf{A}\mathbf{T} \quad \mathbf{T} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} -0.32 & -0.04 & 0 \\ 0.36 & -0.32 & -0.04 \\ 0 & 0.36 & -0.32 \end{bmatrix} \qquad \mathbf{T}^0 = \begin{bmatrix} T_1^0 \\ T_2^0 \\ T_2^0 \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

#### **Euler Forward:**

$$\mathbf{T}^{\mathbf{n}+\mathbf{1}} = \left[ I + \mathsf{D}t\mathbf{A} \right] \mathbf{T}^{\mathbf{n}}$$

$$\mathbf{T}^{0.5} = \begin{bmatrix} T_1^{0.5} \\ T_2^{0.5} \\ T_2^{0.5} \end{bmatrix} = \begin{bmatrix} 0.84 & -0.02 & 0 \\ 0.18 & 0.84 & -0.02 \\ 0 & 0.18 & 0.84 \end{bmatrix} \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix} = \begin{bmatrix} 28.6985 \\ 47.6568 \\ 38.6985 \end{bmatrix}$$

$$\frac{d\mathbf{T}}{dt} = \mathbf{A}\mathbf{T} \quad \mathbf{T} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} -0.32 & -0.04 & 0 \\ 0.36 & -0.32 & -0.04 \\ 0 & 0.36 & -0.32 \end{bmatrix} \qquad \mathbf{T}^0 = \begin{bmatrix} T_1^0 \\ T_2^0 \\ T_2^0 \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

$$\mathbf{A} = \begin{vmatrix} -0.32 & -0.04 & 0 \\ 0.36 & -0.32 & -0.04 \\ 0 & 0.36 & -0.32 \end{vmatrix}$$

$$\mathbf{T}^{0} = \begin{bmatrix} T_{1}^{0} \\ T_{2}^{0} \\ T_{2}^{0} \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

#### **Euler Backward:**

$$\begin{bmatrix} 1.16 & 0.02 & 0 \\ -0.18 & 1.16 & 0.02 \\ 0 & -0.18 & 1.16 \end{bmatrix} \begin{bmatrix} T_1^{0.5} \\ T_2^{0.5} \\ T_2^{0.5} \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

$$\mathbf{T}^{0.5} = \begin{bmatrix} T_1^{0.5} \\ T_2^{0.5} \\ T_2^{0.5} \end{bmatrix} = \begin{bmatrix} 29.6674 \\ 47.0556 \\ 37.7804 \end{bmatrix}$$

$$\frac{d\mathbf{T}}{dt} = \mathbf{AT} \quad \mathbf{T} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix}$$

$$\frac{d\mathbf{T}}{dt} = \mathbf{A}\mathbf{T} \quad \mathbf{T} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} -0.32 & -0.04 & 0 \\ 0.36 & -0.32 & -0.04 \\ 0 & 0.36 & -0.32 \end{bmatrix} \qquad \mathbf{T}^0 = \begin{bmatrix} T_1^0 \\ T_2^0 \\ T_2^0 \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

$$\mathbf{T}^{0} = \begin{bmatrix} T_{1}^{0} \\ T_{2}^{0} \\ T_{2}^{0} \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

#### **Crank-Nicholson:**

$$\left[I - 0.5Dt\mathbf{A}\right]\mathbf{T}^{n+1} = \left[I + 0.5Dt\mathbf{A}\right]\mathbf{T}^{n}$$

$$\begin{bmatrix} 1.08 & 0.01 & 0 \\ -0.09 & 1.08 & 0.02 \\ 0 & -0.09 & 1.08 \end{bmatrix} \begin{bmatrix} T_1^{0.5} \\ T_2^{0.5} \\ T_2^{0.5} \end{bmatrix} = \begin{bmatrix} 0.92 & -0.01 & 0 \\ 0.09 & 0.92 & -0.01 \\ 0 & 0.09 & 0.92 \end{bmatrix} \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix} = \begin{bmatrix} 32.0269 \\ 48.8284 \\ 37.0269 \end{bmatrix}$$

$$\mathbf{T}^{0.5} = \begin{bmatrix} T_1^{0.5} \\ T_2^{0.5} \\ T_2^{0.5} \end{bmatrix} = \begin{bmatrix} 29.2166 \\ 47.2923 \\ 38.2252 \end{bmatrix}$$

$$\frac{d\mathbf{T}}{dt} = \mathbf{A}\mathbf{T} \quad \mathbf{T} = \begin{bmatrix} T_1 \\ T_2 \\ T_3 \end{bmatrix} \qquad \mathbf{A} = \begin{bmatrix} -0.32 & -0.04 & 0 \\ 0.36 & -0.32 & -0.04 \\ 0 & 0.36 & -0.32 \end{bmatrix} \qquad \mathbf{T}^0 = \begin{bmatrix} T_1^0 \\ T_2^0 \\ T_2^0 \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix}$$

2<sup>nd</sup> Order Runge-Kutta (Heun's Predictor-Corrector Form):

$$\mathbf{T}_p^{n+1} = \left[ I + \mathsf{D}t\mathbf{A} \right] \mathbf{T}^n$$

This is same as Euler-Forward. EF solution is the Predictor.

$$\mathbf{T}_{c}^{n+1} = \mathbf{T}^{n} + \frac{\mathbf{D}t}{2} \left[ \mathbf{A} \mathbf{T}_{p}^{n+1} + \mathbf{A} \mathbf{T}^{n} \right] = \mathbf{T}^{n} + \frac{\mathbf{D}t}{2} \mathbf{A} \left[ \mathbf{T}_{p}^{n+1} + \mathbf{T}^{n} \right]$$

$$\mathbf{T}_{c}^{0.5} = \begin{bmatrix} T_{1c}^{0.5} \\ T_{2c}^{0.5} \\ T_{2c}^{0.5} \end{bmatrix} = \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix} + \begin{bmatrix} -0.08 & -0.01 & 0 \\ 0.09 & -0.08 & -0.01 \\ 0 & 0.09 & -0.08 \end{bmatrix} \begin{bmatrix} 28.6985 \\ 47.6568 \\ 38.6985 \end{bmatrix} + \begin{bmatrix} 35.3553 \\ 50.0 \\ 35.3553 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 29.2544 \\ 47.2118 \\ 38.2201 \end{bmatrix}$$

What about Consistency, Stability, Convergence?

How does one choose  $\Delta x$  and  $\Delta t$ ? Are they interdependent?

#### **Diffusion Equation:**

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \mu \alpha_i^n \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + (1 - \mu)\alpha_i^{n+1} \frac{\phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^2}$$

$$\left[ -\left(1 - m\right) a_{i}^{n+1} \frac{Dt}{Dx^{2}} \right] f_{i+1}^{n+1} + \left[ 1 + 2\left(1 - m\right) a_{i}^{n+1} \frac{Dt}{Dx^{2}} \right] f_{i}^{n+1} + \left[ -\left(1 - m\right) a_{i}^{n+1} \frac{Dt}{Dx^{2}} \right] f_{i-1}^{n+1} 
= \left[ m a_{i}^{n} \frac{Dt}{Dx^{2}} \right] f_{i+1}^{n} + \left[ 1 - 2m a_{i}^{n} \frac{Dt}{Dx^{2}} \right] f_{i}^{n} + \left[ m a_{i}^{n} \frac{Dt}{Dx^{2}} \right] f_{i-1}^{n}$$

### Advection-Diffusion Equation:

$$\begin{split} &\frac{\phi_{i}^{n+1} - \phi_{i}^{n}}{\Delta t} \\ &= \mu \left[ -u_{i}^{n} \frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\Delta x} + \alpha_{i}^{n} \frac{\phi_{i+1}^{n} - 2\phi_{i}^{n} + \phi_{i-1}^{n}}{\Delta x^{2}} \right] \\ &+ (1 - \mu) \left[ -u_{i}^{n+1} \frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} + \alpha_{i}^{n+1} \frac{\phi_{i+1}^{n+1} - 2\phi_{i}^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^{2}} \right] \\ &\left[ \left( 1 - m \right) \left( u_{i}^{n+1} \frac{\mathrm{D}t}{2\mathrm{D}x} - a_{i}^{n+1} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i+1}^{n+1} + \left[ 1 + 2\left( 1 - m \right) a_{i}^{n+1} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i}^{n+1} + \left[ \left( 1 - m \right) \left( -u_{i}^{n+1} \frac{\mathrm{D}t}{2\mathrm{D}x} - a_{i}^{n+1} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i-1}^{n} \\ &= \left[ m \left( -u_{i}^{n} \frac{\mathrm{D}t}{2\mathrm{D}x} + a_{i}^{n} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i+1}^{n} + \left[ 1 - 2ma_{i}^{n} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i}^{n} + \left[ m \left( u_{i}^{n} \frac{\mathrm{D}t}{2\mathrm{D}x} + a_{i}^{n} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i-1}^{n} \end{split}$$

Groups  $u \frac{\Delta t}{\Delta x}$  and  $\alpha \frac{\Delta t}{\Delta x^2}$  govern the equations.

✓ Peclet Number:

$$P_e = \frac{uL}{\alpha} = \frac{uL}{D}$$

✓ Grid Peclet Number:

$$P_g = \frac{u\Delta x}{\alpha} = \frac{u\Delta x}{D}$$

✓ CFL (Courant-Friedrich-Lewy) Number:

$$C = u \frac{\Delta t}{\Delta x}$$

Therefore,

$$\frac{C}{P_g} = \alpha \frac{\Delta t}{\Delta x^2}$$

### ✓ If u and $\alpha$ are constants (not function of x):

$$\left[ \left( 1 - m \right) \left( u \frac{\mathrm{D}t}{2\mathrm{D}x} - a \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i+1}^{n+1} + \left[ 1 + 2 \left( 1 - m \right) a \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i}^{n+1} + \left[ \left( 1 - m \right) \left( -u \frac{\mathrm{D}t}{2\mathrm{D}x} - a \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i-1}^{n+1}$$

$$= \left[ m \left( -u \frac{\mathrm{D}t}{2\mathrm{D}x} + a \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i+1}^{n} + \left[ 1 - 2ma \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i}^{n} + \left[ m \left( u \frac{\mathrm{D}t}{2\mathrm{D}x} + a \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right) \right] f_{i-1}^{n}$$

$$\left[ \left( 1 - m \right) \left( \frac{C}{2} - \frac{C}{P_{g}} \right) \right] f_{i+1}^{n+1} + \left[ 1 + 2 \left( 1 - m \right) \frac{C}{P_{g}} \right] f_{i}^{n+1} + \left[ \left( 1 - m \right) \left( -\frac{C}{2} - \frac{C}{P_{g}} \right) \right] f_{i-1}^{n+1}$$

$$= \left[ m \left( -\frac{C}{2} + \frac{C}{P_{g}} \right) \right] f_{i+1}^{n} + \left[ 1 - 2m \frac{C}{P_{g}} \right] f_{i}^{n} + \left[ m \left( \frac{C}{2} + \frac{C}{P_{g}} \right) \right] f_{i-1}^{n}$$

The the solutions depend on these two dimensionless groups or numbers. Therefore, stability and convergence will also depend on these two!

#### Diffusion Equation ( $\mu$ -CD scheme):

$$\begin{split} \frac{\phi_{i}^{n+1} - \phi_{i}^{n}}{\Delta t} &= \mu \alpha_{i}^{n} \frac{\phi_{i+1}^{n} - 2\phi_{i}^{n} + \phi_{i-1}^{n}}{\Delta x^{2}} + (1 - \mu)\alpha_{i}^{n+1} \frac{\phi_{i+1}^{n+1} - 2\phi_{i}^{n+1} + \phi_{i-1}^{n+1}}{\Delta x^{2}} \\ &\left[ -\left(1 - m\right)a_{i}^{n+1} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i+1}^{n+1} + \left[ 1 + 2\left(1 - m\right)a_{i}^{n+1} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i}^{n+1} + \left[ -\left(1 - m\right)a_{i}^{n+1} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i-1}^{n} \\ &= \left[ m a_{i}^{n} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i+1}^{n} + \left[ 1 - 2m a_{i}^{n} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i}^{n} + \left[ m a_{i}^{n} \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] f_{i-1}^{n} \end{split}$$

There are four kinds of terms that which to be expanded in Taylor's series:

$$\phi_{i\pm 1}^{n+1}$$
  $\phi_i^{n+1}$ 

$$\phi_i^{n+1}$$

$$\phi^n_{i\pm 1}$$

$$\phi_i^n$$

$$\left[ -\left(1 - m\right) a \frac{Dt}{Dx^{2}} \right] f_{i+1}^{n+1} + \left[ 1 + 2\left(1 - m\right) a \frac{Dt}{Dx^{2}} \right] f_{i}^{n+1} + \left[ -\left(1 - m\right) a \frac{Dt}{Dx^{2}} \right] f_{i-1}^{n+1} 
= \left[ ma \frac{Dt}{Dx^{2}} \right] f_{i+1}^{n} + \left[ 1 - 2ma \frac{Dt}{Dx^{2}} \right] f_{i}^{n} + \left[ ma \frac{Dt}{Dx^{2}} \right] f_{i-1}^{n}$$

$$\mathcal{T}_{i}^{n+1} = \mathcal{T}_{i}^{n} + Dt \frac{\mathcal{I}}{\mathcal{I}} \bigg|_{i}^{n} + \frac{Dt^{2}}{2!} \frac{\mathcal{I}^{2}f}{\mathcal{I}^{2}} \bigg|_{i}^{n} + \frac{Dt^{3}}{3!} \frac{\mathcal{I}^{3}f}{\mathcal{I}^{3}} \bigg|_{i}^{n} + HOT$$

$$\mathcal{F}_{i\pm 1}^{n} = \mathcal{F}_{i}^{n} \pm Dx \frac{\mathscr{N}f}{\mathscr{N}x} \bigg|_{i}^{n} + \frac{Dx^{2}}{2!} \frac{\mathscr{N}^{2}f}{\mathscr{N}x^{2}} \bigg|_{i}^{n} \pm \frac{Dx^{3}}{3!} \frac{\mathscr{N}^{3}f}{\mathscr{N}x^{3}} \bigg|_{i}^{n} + \frac{Dx^{4}}{4!} \frac{\mathscr{N}^{4}f}{\mathscr{N}x^{4}} \bigg|_{i}^{n} + HOT$$

$$f_{i\pm 1}^{n+1} = f_{i}^{n} + \left( Dt \frac{\mathscr{N}}{\mathscr{N}t} \pm Dx \frac{\mathscr{N}}{\mathscr{N}x} \right) f_{i}^{n} + \frac{1}{2!} \left( Dt \frac{\mathscr{N}}{\mathscr{N}t} \pm Dx \frac{\mathscr{N}}{\mathscr{N}x} \right)^{2} f_{i}^{n} + \frac{1}{3!} \left( Dt \frac{\mathscr{N}}{\mathscr{N}t} \pm Dx \frac{\mathscr{N}}{\mathscr{N}x} \right)^{3} f_{i}^{n} + HOT$$

$$\left[ -\left(1-m\right) a \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] \begin{cases} f_{i}^{n} + \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} + \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right) f_{i}^{n} + \frac{1}{2!} \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} + \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right)^{2} f_{i}^{n} + \frac{1}{3!} \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} + \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right)^{3} f_{i}^{n} \right) \\ + \frac{1}{4!} \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} + \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right)^{4} f_{i}^{n} + HOT \\ + \left[1+2\left(1-m\right) a \frac{\mathrm{D}t}{\mathrm{D}x^{2}}\right] \left\{ f_{i}^{n} + \mathrm{D}t \frac{\mathcal{H}f}{\mathcal{H}t} \right\}_{i}^{n} + \frac{\mathrm{D}t^{2}}{2!} \frac{\mathcal{H}^{2}f}{\mathcal{H}t^{2}} + \frac{\mathrm{D}t^{3}}{3!} \frac{\mathcal{H}^{3}f}{\mathcal{H}^{3}} + HOT \right\} + \\ \left[ -\left(1-m\right) a \frac{\mathrm{D}t}{\mathrm{D}x^{2}} \right] \left\{ f_{i}^{n} + \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} - \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right) f_{i}^{n} + \frac{1}{2!} \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} - \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right)^{2} f_{i}^{n} + \frac{1}{3!} \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} - \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right)^{3} f_{i}^{n} \right\} \\ + \frac{1}{4!} \left(\mathrm{D}t \frac{\mathcal{H}}{\mathcal{H}t} - \mathrm{D}x \frac{\mathcal{H}}{\mathcal{H}x}\right)^{4} f_{i}^{n} + HOT \\ = \left[ma \frac{\mathrm{D}t}{\mathrm{D}x^{2}}\right] \left\{ f_{i}^{n} + \mathrm{D}x \frac{\mathcal{H}f}{\mathcal{H}x} \right\}_{i}^{n} + \frac{\mathrm{D}x^{2}}{2!} \frac{\mathcal{H}^{2}f}{\mathcal{H}x^{2}} + \frac{\mathrm{D}x^{3}}{3!} \frac{\mathcal{H}^{3}f}{\mathcal{H}^{3}} + \frac{\mathrm{D}x^{4}}{4!} \frac{\mathcal{H}^{4}f}{\mathcal{H}x^{4}} + HOT \right\} + \left[1-2ma \frac{\mathrm{D}t}{\mathrm{D}x^{2}}\right] f_{i}^{n} \\ + \left[ma \frac{\mathrm{D}t}{\mathrm{D}x^{2}}\right] \left\{ f_{i}^{n} - \mathrm{D}x \frac{\mathcal{H}f}{\mathcal{H}x} \right\}_{i}^{n} + \frac{\mathrm{D}x^{2}}{2!} \frac{\mathcal{H}^{2}f}{\mathcal{H}x^{2}} - \frac{\mathrm{D}x^{3}}{3!} \frac{\mathcal{H}^{3}f}{\mathcal{H}x^{3}} + \frac{\mathrm{D}x^{4}}{4!} \frac{\mathcal{H}^{4}f}{\mathcal{H}x^{4}} + HOT \right\}$$

#### Diffusion Equation ( $\mu$ -CD scheme):

$$\frac{\P/f}{\P/t}\Big|_{i}^{n} - a\frac{\P/^{2}f}{\P/x^{2}}\Big|_{i}^{n} = -\frac{Dt}{2}\frac{\P/^{2}f}{\P/t^{2}}\Big|_{i}^{n} + (1-m)Dta\frac{\P/^{3}f}{\P/t}\|_{x^{2}}^{n} - \frac{Dt^{2}}{6}\frac{\P/^{3}f}{\P/t^{3}}\Big|_{i}^{n} + (1-m)\frac{Dt^{2}}{2}a\frac{\P/^{4}f}{\P/t^{2}}\Big|_{i}^{n} + a\frac{Dx^{2}}{12}\frac{\P/^{4}f}{\P/x^{4}}\Big|_{i}^{n} + HOT$$

#### **Truncation Error:**

$$TE = - + \frac{Dt}{2} \frac{\mathcal{I}^{2} f}{\mathcal{I}^{2}} \Big|_{i}^{n} - (1 - m) Dta \frac{\mathcal{I}^{3} f}{\mathcal{I}^{2} \mathcal{I}^{2}} \Big|_{i}^{n} + \frac{Dt^{2}}{6} \frac{\mathcal{I}^{3} f}{\mathcal{I}^{2}} \Big|_{i}^{n}$$
$$- (1 - m) \frac{Dt^{2}}{2} a \frac{\mathcal{I}^{4} f}{\mathcal{I}^{2} \mathcal{I}^{2} \mathcal{I}^{2}} \Big|_{i}^{n} - a \frac{Dx^{2}}{12} \frac{\mathcal{I}^{4} f}{\mathcal{I}^{2} \mathcal{I}^{4}} \Big|_{i}^{n} + HOT$$

$$TE = - + \frac{Dt}{2} \frac{\mathcal{I}^{2} f}{\mathcal{I}^{2}} \Big|_{i}^{n} - (1 - m) Dta \frac{\mathcal{I}^{3} f}{\mathcal{I}^{2} \mathcal{I}^{2}} \Big|_{i}^{n} + \frac{Dt^{2}}{6} \frac{\mathcal{I}^{3} f}{\mathcal{I}^{2}} \Big|_{i}^{n}$$
$$- (1 - m) \frac{Dt^{2}}{2} a \frac{\mathcal{I}^{4} f}{\mathcal{I}^{2} \mathcal{I}^{2}} \Big|_{i}^{n} - a \frac{Dx^{2}}{12} \frac{\mathcal{I}^{4} f}{\mathcal{I}^{2} \mathcal{I}^{2}} \Big|_{i}^{n} + HOT$$

### Identity from the original equation:

$$\partial \frac{\int_{0}^{3} f}{\int_{0}^{2} t} = \frac{\int_{0}^{4} \left(\partial \frac{\int_{0}^{2} f}{\int_{0}^{2} t}\right) = \frac{\int_{0}^{4} \left(\frac{\int_{0}^{4} f}{\int_{0}^{4} t}\right) = \frac{\int_{0}^{4} f}{\int_{0}^{4} t}$$

$$TE = \left(\mu - \frac{1}{2}\right)\Delta t \frac{\partial^2 \phi}{\partial t^2} \bigg|_i^n + \left(\mu - \frac{2}{3}\right) \frac{\Delta t^2}{2} \frac{\partial^3 \phi}{\partial t^3} \bigg|_i^n - \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} \bigg|_i^n + HOT$$

Method is  $O(\Delta t, \Delta x^2)$ . For  $\mu = \frac{1}{2}$ , the method is  $O(\Delta t^2, \Delta x^2)$ 

$$TE = \left(\mu - \frac{1}{2}\right) \Delta t \frac{\partial^2 \phi}{\partial t^2} \bigg|_i^n + \left(\mu - \frac{2}{3}\right) \frac{\Delta t^2}{2} \frac{\partial^3 \phi}{\partial t^3} \bigg|_i^n - \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} \bigg|_i^n + HOT$$

$$\frac{\sqrt{g^2 f}}{\sqrt{g^2 f}} = \frac{\sqrt{g}}{\sqrt{g} t} \left( \frac{\sqrt{g^2 f}}{\sqrt{g} t} \right) = \frac{\sqrt{g}}{\sqrt{g} t} \left( \frac{\sqrt{g^2 f}}{\sqrt{g} x^2} \right) = \frac{\sqrt{g^2 f}}{\sqrt{g} x^2} \left( \frac{\sqrt{g} f}{\sqrt{g} t} \right) = \frac{\sqrt{g}}{\sqrt{g} x^2} \left( \frac{\sqrt{g} f}{\sqrt{g} x^2} \right) = \frac{\sqrt{g}}{\sqrt{g} x^2} \left( \frac{\sqrt{g}}{\sqrt{g} x^2} \right) = \frac{\sqrt{g}}{\sqrt{g}$$

$$TE = \left\{ \left(\mu - \frac{1}{2}\right) \Delta t \alpha^2 - \alpha \frac{\Delta x^2}{12} \right\} \frac{\partial^4 \phi}{\partial x^4} \bigg|_i^n + \left(\mu - \frac{2}{3}\right) \frac{\Delta t^2}{2} \frac{\partial^3 \phi}{\partial t^3} \bigg|_i^n + HOT$$

In order to make the first term zero, one may choose:

$$\frac{\alpha \Delta t}{\Delta x^2} = \frac{1}{\left(\mu - \frac{1}{2}\right)12}$$

For  $\mu > \frac{1}{2}$ , it is also possible to make the method  $O(\Delta t^2, \Delta x^2)$  by carefully choosing  $\Delta t$  and  $\Delta x$ , e.g., for Euler Forward,  $\mu = 1$ :

$$\frac{\alpha \Delta t}{\Delta x^2} = \frac{1}{6}$$

Advection-Dispersion Equation:

$$\left[ \left( 1 - m \right) \left( u \frac{\mathsf{D}t}{2\mathsf{D}x} - \partial \frac{\mathsf{D}t}{\mathsf{D}x^2} \right) \right] f_{i+1}^{n+1} + \left[ 1 + 2\left( 1 - m \right) \partial \frac{\mathsf{D}t}{\mathsf{D}x^2} \right] f_i^{n+1} + \left[ \left( 1 - m \right) \left( -u \frac{\mathsf{D}t}{2\mathsf{D}x} - \partial \frac{\mathsf{D}t}{\mathsf{D}x^2} \right) \right] f_{i-1}^{n+1} \\
= \left[ m \left( -u \frac{\mathsf{D}t}{2\mathsf{D}x} + \partial \frac{\mathsf{D}t}{\mathsf{D}x^2} \right) \right] f_{i+1}^{n} + \left[ 1 - 2m\partial \frac{\mathsf{D}t}{\mathsf{D}x^2} \right] f_i^{n} + \left[ m \left( u \frac{\mathsf{D}t}{2\mathsf{D}x} + \partial \frac{\mathsf{D}t}{\mathsf{D}x^2} \right) \right] f_{i-1}^{n}$$

Putting the values of the Taylor's series expansion of the terms (like in diffusion equation) and simplifying

$$\frac{\sqrt{n}f}{\sqrt{n}t}\Big|_{i}^{n} + u\frac{\sqrt{n}f}{\sqrt{n}x}\Big|_{i}^{n} - a\frac{\sqrt{n}^{2}f}{\sqrt{n}x^{2}}\Big|_{i}^{n} = -u^{2}Dt\left(m - \frac{1}{2}\right)\frac{\sqrt{n}^{2}f}{\sqrt{n}x^{2}}\Big|_{i}^{n} + 2uaDt\left(m - \frac{1}{2}\right)\frac{\sqrt{n}^{3}f}{\sqrt{n}x^{3}}\Big|_{i}^{n} - a^{2}Dt\left(m - \frac{1}{2}\right)\frac{\sqrt{n}^{4}f}{\sqrt{n}x^{4}}\Big|_{i}^{n} + \frac{u^{3}Dt^{2}}{6}\left(\frac{m}{2} - \frac{1}{3}\right)\frac{\sqrt{n}^{3}f}{\sqrt{n}x^{3}}\Big|_{i}^{n} - \frac{uDx^{2}}{6}\frac{\sqrt{n}^{3}f}{\sqrt{n}x^{3}}\Big|_{i}^{n} + HOT$$

No surprises in the order of accuracy! The method is  $O(\Delta t, \Delta x^2)$ . For  $\mu = \frac{1}{2}$ , the method is  $O(\Delta t^2, \Delta x^2)$ 

#### New surprise is:

$$\frac{\sqrt{n}f}{\sqrt{n}t}\Big|_{i}^{n} + u\frac{\sqrt{n}f}{\sqrt{n}x}\Big|_{i}^{n} - \left[a - u^{2}Dt\left(m - \frac{1}{2}\right)\right]\frac{\sqrt{n}^{2}f}{\sqrt{n}x^{2}}\Big|_{i}^{n} = 2uaDt\left(m - \frac{1}{2}\right)\frac{\sqrt{n}^{3}f}{\sqrt{n}x^{3}}\Big|_{i}^{n} - a^{2}Dt\left(m - \frac{1}{2}\right)\frac{\sqrt{n}^{4}f}{\sqrt{n}x^{4}}\Big|_{i}^{n} + \frac{u^{3}Dt^{2}\left(\frac{m}{2} - \frac{1}{3}\right)\frac{\sqrt{n}^{3}f}{\sqrt{n}x^{3}}\Big|_{i}^{n} - \frac{uDx^{2}}{6}\frac{\sqrt{n}^{3}f}{\sqrt{n}x^{3}}\Big|_{i}^{n} + HOT$$

Numerical Diffusion!

### Strategies to compensate for Numerical Diffusion:

✓ Use modified Diffusion/Dispersion coefficient:

$$\mathcal{A}' = \mathcal{A} + u^2 \mathsf{D} t \left( m - \frac{1}{2} \right)$$

✓ Use Backward difference approximation for the advection term

If you thought that combining schemes that are consistent independently will always give you a consistent scheme for PDE, think again!

Let us look at one scheme that combines two consistent schemes!

### Consistency: inconsistent scheme

Consider the following approximation for the Diffusion equation:

$$\frac{\phi_i^{n+1} - \phi_i^{n-1}}{\Delta t} = \alpha \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} + O(\Delta t^2, \Delta x^2)$$

Replace:

$$\phi_i^n = \frac{\phi_i^{n+1} + \phi_i^{n-1}}{2} + O(\Delta t^2)$$

Resulting Scheme:

$$\left(1 + 2\alpha \frac{\Delta t}{\Delta x^2}\right)\phi_i^{n+1} = \left(1 - 2\alpha \frac{\Delta t}{\Delta x^2}\right)\phi_i^{n-1} + 2\alpha \frac{\Delta t}{\Delta x^2}\phi_{i+1}^n + 2\alpha \frac{\Delta t}{\Delta x^2}\phi_{i-1}^n$$

## Consistency: inconsistent scheme

$$\left(1+2\alpha\frac{\Delta t}{\Delta x^2}\right)\phi_i^{n+1} = \left(1-2\alpha\frac{\Delta t}{\Delta x^2}\right)\phi_i^{n-1} + 2\alpha\frac{\Delta t}{\Delta x^2}\phi_{i+1}^n + 2\alpha\frac{\Delta t}{\Delta x^2}\phi_{i-1}^n$$

It turns out that, this method is Unconditionally Stable!

Now, substitute the Taylor's series expansions of the terms!

$$\frac{\partial \phi}{\partial t} - \alpha \frac{\partial^2 \phi}{\partial x^2} = -\frac{\Delta t^2}{6} \frac{\partial^3 \phi}{\partial t^3} + \alpha \frac{\Delta x^2}{12} \frac{\partial^4 \phi}{\partial x^4} - \alpha \frac{\Delta t^2}{\Delta x^2} \frac{\partial^3 \phi}{\partial t^3} - \frac{\alpha}{12} \frac{\Delta t^4}{\Delta x^2} \frac{\partial^4 \phi}{\partial t^4} \cdots$$

#### It is an inconsistent scheme!

This is the Du Fort–Frankel scheme for the diffusion equation!

Let us now see brief stability analysis for the diffusion equation!

$$\frac{d\phi_i}{dt} = \alpha \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \implies \frac{d\overline{\phi}}{dt} = \mathbf{A}\overline{\phi} + \mathbf{b}$$

Assuming Dirichlet type zero boundary conditions!

$$\mathbf{A} = \frac{\partial}{Dx^2} \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & \cdots & 0 & 0 \\ 1 & -2 & 1 & 0 & \cdots & \cdots & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & \cdots & 0 & 0 \\ 0 & 0 & 1 & -2 & \cdots & \cdots & \cdots & 0 \\ \cdots & \cdots \\ 0 & 0 & \cdots & \cdots & \cdots & -2 & 1 & 0 \\ 0 & 0 & \cdots & \cdots & \cdots & 1 & -2 & 1 \\ 0 & 0 & \cdots & \cdots & \cdots & 0 & 1 & -2 \end{bmatrix}$$

#### Consider the grid:

Size of the matrix A is (m-1). It is a tri-diagonal matrix of the form A[l, d, u]. Eigenvalues of such a matrix is given by:

$$\lambda_k = \frac{\alpha}{\Delta x^2} \left( d + 2\sqrt{lu} \cos \frac{k\pi}{m} \right) = \frac{\alpha}{\Delta x^2} \left( -2 + 2 \cos \frac{k\pi}{m} \right)$$

Boundary conditions only affects the first and last row entries. For large *m*, that has little effect on the eigenvalues!

$$\lambda_k = \frac{\alpha}{\Delta x^2} \left( -2 + 2 \cos \frac{k\pi}{m} \right) \qquad k = 1, 2 \dots, m - 1$$

 $\checkmark$  For large m, the largest (absolute) eigenvalue is:

$$\lambda_{m-1} = -\frac{4\alpha}{\Delta x^2}$$

 $\checkmark$  For large m, the smallest (absolute) eigenvalue is:

$$\lambda_1 = \frac{2\alpha}{\Delta x^2} \left( \cos \frac{\pi}{m} - 1 \right)$$

✓ The ratio:

$$\left| \frac{\lambda_{m-1}}{\lambda_1} \right| = \left| \frac{2}{\left( \cos \frac{\pi}{m} - 1 \right)} \right| \approx \frac{4m^2}{\pi^2}$$

Larger the *m*, *stiffer* the system becomes!

#### Recall stability limits for such systems:

✓ Euler Forward:

$$h \le \frac{2}{|\lambda_{\text{max}}|} \implies \Delta t \le \frac{2}{|\lambda_{\text{m-1}}|} = \frac{\Delta x^2}{2\alpha}$$
$$\frac{C}{P_g} = \alpha \frac{\Delta t}{\Delta x^2} \le \frac{1}{2}$$

✓ For 4<sup>th</sup> order R-K:

$$h \le \frac{2.785}{|\lambda_{\text{max}}|} \implies \Delta t \le \frac{2.785}{|\lambda_{\text{m-1}}|} = 0.7 \frac{\Delta x^2}{\alpha}$$
$$\frac{C}{P_q} = \alpha \frac{\Delta t}{\Delta x^2} \le 0.7$$

Stability analysis of all numerical methods for linear PDE is done by *von-Neumann Analysis* (aka *Fourier Analysis*)!

# ESO 208A: Computational Methods in Engineering

Partial Differential Equation: Elliptic Equation

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## Laplace Equation: 1st Type BC

$$\frac{\sqrt{2}f}{\sqrt{x^2}} + \frac{\sqrt{2}f}{\sqrt{y^2}} = 0$$

$$x \hat{\mid} (0, L_x) \text{ and } y \hat{\mid} (0, L_y)$$

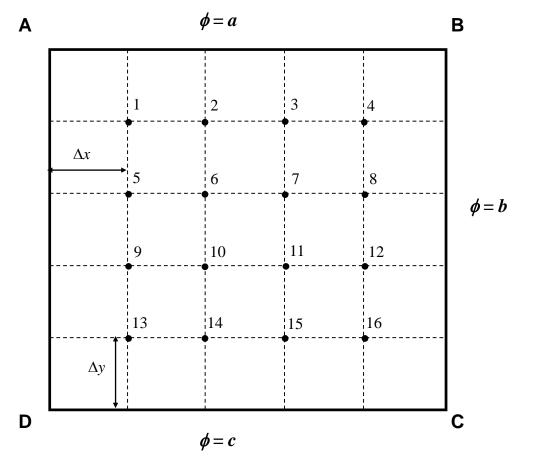
$$f(0,y) = d, \ f(L_x,y) = b$$

$$f(x,0) = c, \ f(x,L_y) = a$$

$$\phi = d$$

$$\Delta x = \frac{L_x}{5}$$

$$\Delta y = \frac{L_y}{5}$$



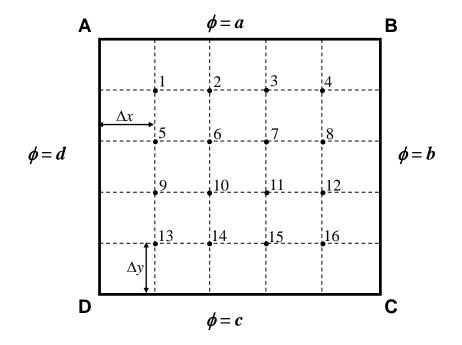
$$\frac{\sqrt{|f|^2 f}}{\sqrt{|x|^2}} + \frac{\sqrt{|f|^2 f}}{\sqrt{|y|^2}} = 0$$

$$\frac{\sqrt{|f|^2 f}}{\sqrt{|x|^2}} = \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{Dx^2}$$

$$\frac{\sqrt[q]{f}}{\sqrt[q]{y^2}}\bigg|_{i,j} = \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{Dy^2}$$

Transform the equation to the form:

$$A \phi = b$$

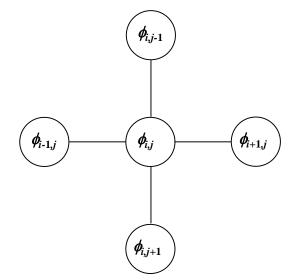


- Create a node number vs.
   co-ordinate look-up table
- ✓ Initialize a null matrix (A) of size N×N and a vector
  (b) of size N
- ✓ *N* is the total number of unknown nodes.

$$\frac{\sqrt[n]^2 f}{\sqrt[n] x^2} + \frac{\sqrt[n]^2 f}{\sqrt[n] y^2} = 0$$

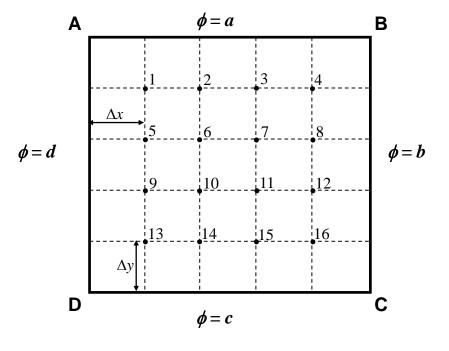
$$\frac{\mathscr{P}^{2}f}{\mathscr{T}x^{2}}\bigg|_{i,j} = \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{Dx^{2}}$$

$$\frac{\P^2 f}{\P y^2} \bigg|_{i,j} = \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{Dy^2}$$

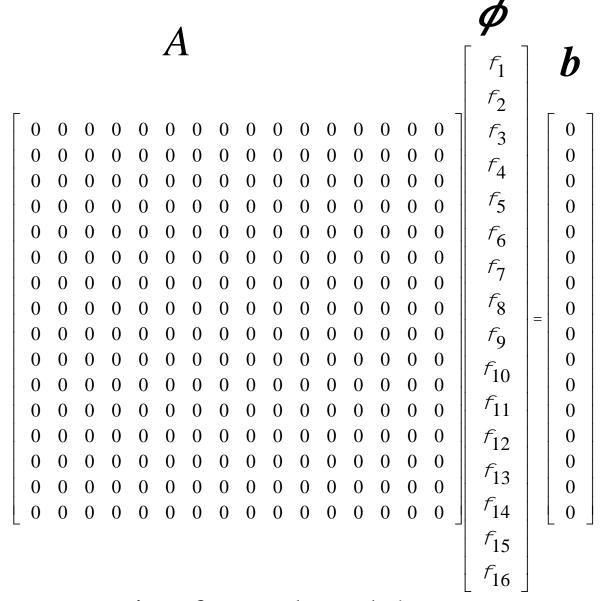


$$\left. \left( \frac{\P^2 f}{\P x^2} + \frac{\P^2 f}{\P y^2} \right) \right|_{i,j} = \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{\mathsf{D} x^2} + \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{\mathsf{D} y^2} = 0$$

$$\left(\frac{1}{Dy^{2}}\right)f_{i,j-1} + \left(\frac{1}{Dx^{2}}\right)f_{i-1,j} + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dy^{2}}\right)f_{i,j} + \left(\frac{1}{Dx^{2}}\right)f_{i+1,j} + \left(\frac{1}{Dy^{2}}\right)f_{i,j+1} = 0$$



Node No.	X	y	x-neighbour	y-neighbour
1	$\Delta x$	4∆y	$\phi = d, 2$	$5, \phi = a$
<b>:</b>	:	i i	<b>:</b>	:
3	3∆x	4∆y	2, 4	$7, \phi = a$
<b>:</b>	:	:	<b>:</b>	:
6	$2\Delta x$	3Ду	5, 7	10, 2
1	:	:	<b>:</b>	:
9	$\Delta x$	2Δy	$\phi = d, 10$	13, 5



$$\phi = a$$

$$\phi_{i,j-1}$$

$$\frac{1}{\Delta x}$$

$$\phi = b$$

$$\frac{\sqrt{2}f}{\sqrt{x^2}} + \frac{\sqrt{2}f}{\sqrt{y^2}} = 0$$

Denote:

$$\alpha = 1/\Delta x^2$$
;  $\beta = 1/\Delta y^2$ 

$$\phi_{i,j+1}$$

$$\dot{c} = c$$

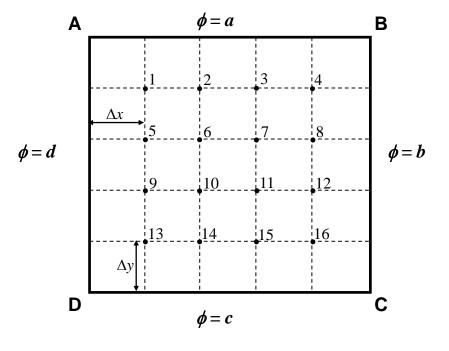
$$\left(\frac{1}{\mathsf{D} y^2}\right) f_{i,j-1}^- + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i-1,j}^- + \left(-\frac{2}{\mathsf{D} x^2} - \frac{2}{\mathsf{D} y^2}\right) f_{i,j}^- + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i+1,j}^- + \left(\frac{1}{\mathsf{D} y^2}\right) f_{i,j+1}^- = 0$$

 $\phi_{i-1,j}$ 

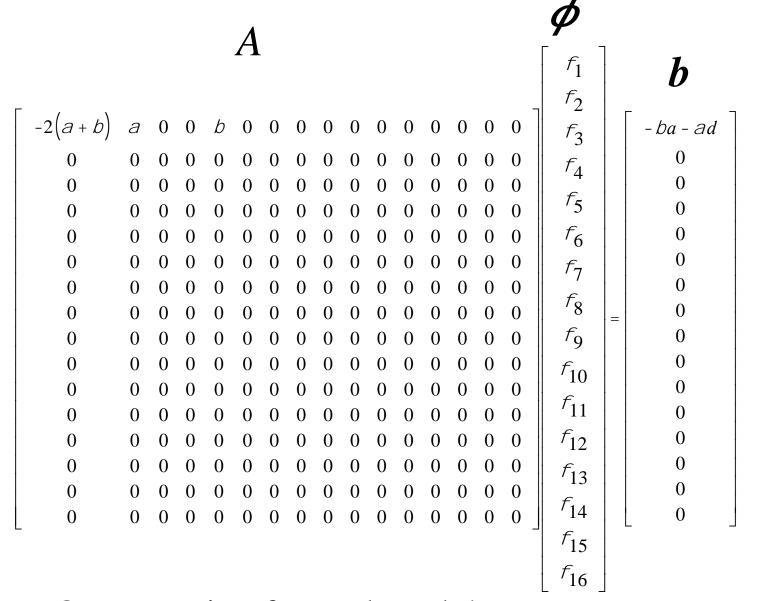
Node 1

$$\left(\frac{1}{\mathrm{D}y^2}\right)a + \left(\frac{1}{\mathrm{D}x^2}\right)d + \left(-\frac{2}{\mathrm{D}x^2} - \frac{2}{\mathrm{D}y^2}\right)f_1 + \left(\frac{1}{\mathrm{D}x^2}\right)f_2 + \left(\frac{1}{\mathrm{D}y^2}\right)f_5 = 0$$

$$\left(-\frac{2}{\mathsf{D}x^2} - \frac{2}{\mathsf{D}y^2}\right) f_1 + \left(\frac{1}{\mathsf{D}x^2}\right) f_2 + \left(\frac{1}{\mathsf{D}y^2}\right) f_5 = -\left(\frac{1}{\mathsf{D}y^2}\right) a - \left(\frac{1}{\mathsf{D}x^2}\right) d$$



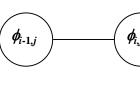
Node No.	X	y	x-neighbour	y-neighbour
1	$\Delta x$	4∆y	$\phi = d, 2$	$5, \phi = a$
<b>:</b>	:	i i	<b>:</b>	:
3	3∆x	4∆y	2, 4	$7, \phi = a$
<b>:</b>	:	:	<b>:</b>	:
6	$2\Delta x$	3Ду	5, 7	10, 2
1	:	:	<b>:</b>	:
9	$\Delta x$	2Δy	$\phi = d, 10$	13, 5



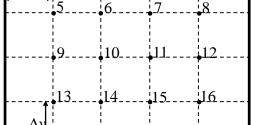
$$\phi_{i,j-1}$$

$$\phi = a$$

$$\frac{\sqrt{2}f}{\sqrt{x^2}} + \frac{\sqrt{2}f}{\sqrt{y^2}} = 0$$



$$\phi = a$$



#### Denote:

$$\alpha = 1/\Delta x^2$$
;  $\beta = 1/\Delta y^2$ 

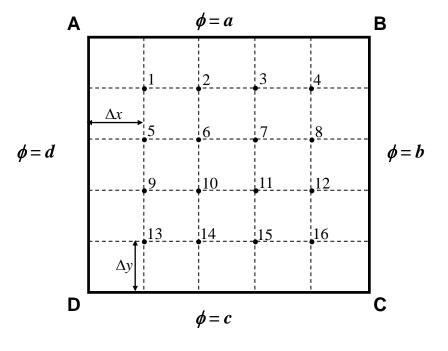
$$\left(\frac{1}{\mathsf{D} y^2}\right) f_{i,j-1}^- + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i-1,j}^- + \left(-\frac{2}{\mathsf{D} x^2} - \frac{2}{\mathsf{D} y^2}\right) f_{i,j}^- + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i+1,j}^- + \left(\frac{1}{\mathsf{D} y^2}\right) f_{i,j+1}^- = 0$$

a

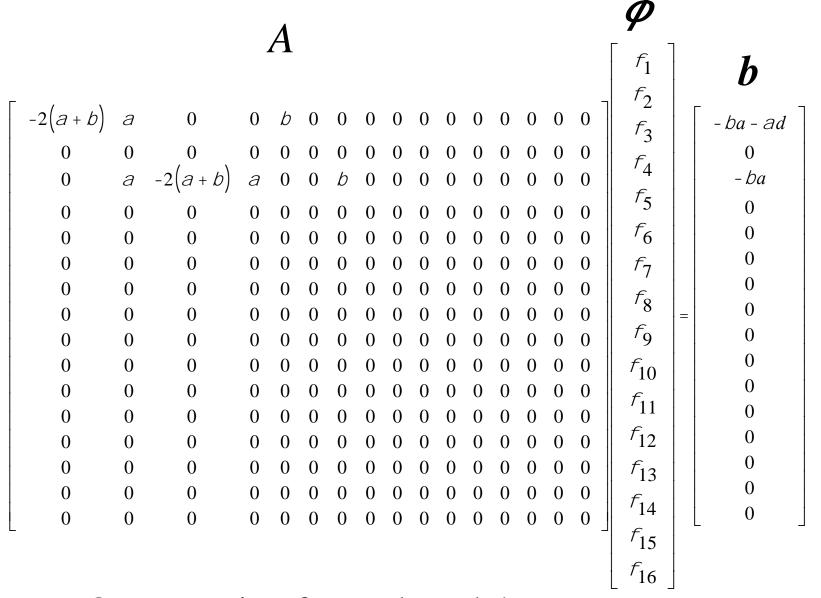
Node 3

$$\left(\frac{1}{Dy^{2}}\right)a + \left(\frac{1}{Dx^{2}}\right)f_{2} + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dy^{2}}\right)f_{3} + \left(\frac{1}{Dx^{2}}\right)f_{4} + \left(\frac{1}{Dy^{2}}\right)f_{7} = 0$$

$$\left(\frac{1}{Dx^{2}}\right)f_{2} + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dy^{2}}\right)f_{3} + \left(\frac{1}{Dx^{2}}\right)f_{4} + \left(\frac{1}{Dy^{2}}\right)f_{7} = -\left(\frac{1}{Dy^{2}}\right)a$$

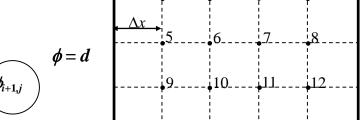


Node No.	X	y	x-neighbour	y-neighbour
1	$\Delta x$	4∆y	$\phi = d, 2$	$5, \phi = a$
:	:	<b>:</b>	<b>:</b>	:
3	$3\Delta x$	<b>4</b> Δy	2, 4	$7, \phi = a$
:	:	ŧ	:	:
6	$2\Delta x$	3Ду	5, 7	10, 2
:	÷	ŧ	ŧ	:
9	$\Delta x$	2Δy	$\phi = d, 10$	13, 5



$$\phi_{i,j-1}$$

$$\frac{\sqrt{2}f}{\sqrt{x^2}} + \frac{\sqrt{2}f}{\sqrt{y^2}} = 0$$



Denote:

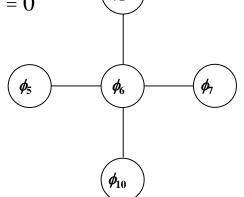
$$\alpha = 1/\Delta x^2$$
;  $\beta = 1/\Delta y^2$ 

$$\left(\phi_{i,j+1}\right)$$

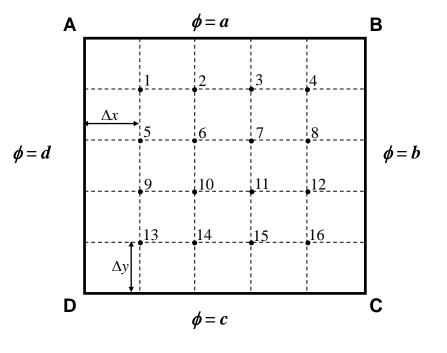
$$\left(\frac{1}{\mathsf{D} y^2}\right) f_{i,j-1}^* + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i-1,j}^* + \left(-\frac{2}{\mathsf{D} x^2} - \frac{2}{\mathsf{D} y^2}\right) f_{i,j}^* + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i+1,j}^* + \left(\frac{1}{\mathsf{D} y^2}\right) f_{i,j+1}^* = 0$$

 $\phi_{i-1,j}$ 

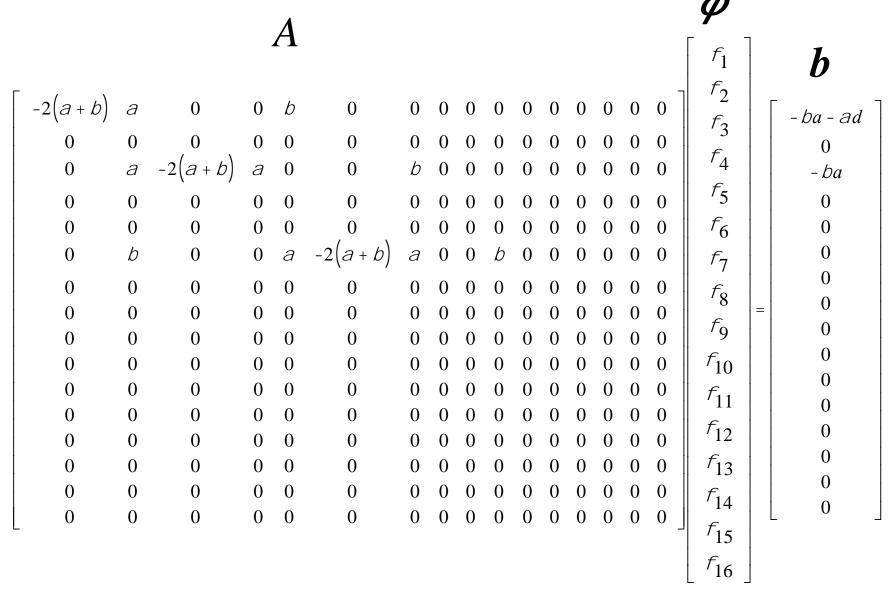
Node 6



$$\left(\frac{1}{Dy^{2}}\right)f_{2} + \left(\frac{1}{Dx^{2}}\right)f_{5} + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dy^{2}}\right)f_{6} + \left(\frac{1}{Dx^{2}}\right)f_{7} + \left(\frac{1}{Dy^{2}}\right)f_{10} = 0$$



Node No.	X	y	x-neighbour	y-neighbour
1	$\Delta x$	4∆y	$\phi = d, 2$	$5, \phi = a$
:	:	<b>:</b>	<b>:</b>	:
3	$3\Delta x$	<b>4</b> Δy	2, 4	$7, \phi = a$
:	:	ŧ	:	:
6	$2\Delta x$	<b>3</b> Δy	5, 7	10, 2
:	÷	ŧ	ŧ	:
9	$\Delta x$	2Δy	$\phi = d, 10$	13, 5



$$\phi_{i,j-1}$$

$$\phi = a$$

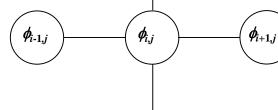
$$\phi_{i,j-1}$$

$$\phi_{i,j-1}$$



$$\phi = b$$

$$\frac{\sqrt{y^2 f}}{\sqrt{y^2}} + \frac{\sqrt{y^2 f}}{\sqrt{y^2}} = 0$$



#### Denote:

$$/\Delta y^2$$

$$\phi = a$$

$$\phi = c$$

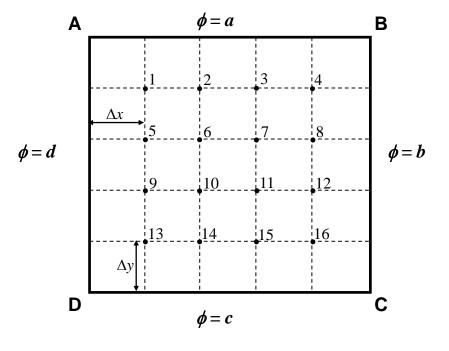
$$\alpha = 1/\Delta x^2$$
;  $\beta = 1/\Delta y^2$ 

$$\left(\frac{1}{\mathsf{D} v^2}\right) f_{i,j-1}^{-1} + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i-1,j}^{-1} + \left(-\frac{2}{\mathsf{D} x^2} - \frac{2}{\mathsf{D} v^2}\right) f_{i,j}^{-1} + \left(\frac{1}{\mathsf{D} x^2}\right) f_{i+1,j}^{-1} + \left(\frac{1}{\mathsf{D} v^2}\right) f_{i,j+1}^{-1} = 0$$

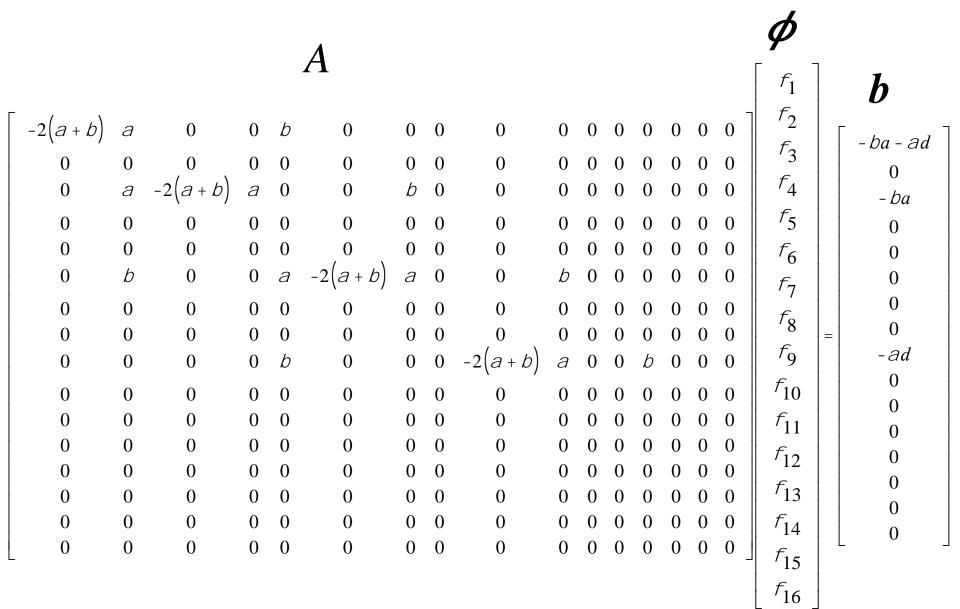
Node 9

$$\left(\frac{1}{Dy^{2}}\right)f_{13} + \left(\frac{1}{Dx^{2}}\right)d + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dy^{2}}\right)f_{9} + \left(\frac{1}{Dx^{2}}\right)f_{10} + \left(\frac{1}{Dy^{2}}\right)f_{5} = 0$$

$$\left(\frac{1}{Dy^{2}}\right)f_{5} + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dy^{2}}\right)f_{9} + \left(\frac{1}{Dx^{2}}\right)f_{10} + \left(\frac{1}{Dy^{2}}\right)f_{13} = -\left(\frac{1}{Dx^{2}}\right)d$$



Node No.	X	y	x-neighbour	y-neighbour
1	$\Delta x$	4∆y	$\phi = d, 2$	$5, \phi = a$
<b>:</b>	:	i i	<b>:</b>	:
3	3∆x	4∆y	2, 4	$7, \phi = a$
<b>:</b>	:	:	<b>:</b>	:
6	$2\Delta x$	3Ду	5, 7	10, 2
1	:	:	<b>:</b>	:
9	$\Delta x$	2Δy	$\phi = d, 10$	13, 5



## Laplace Equation: 1<sup>st</sup> and 2<sup>nd</sup> Type BC

$$\frac{\sqrt{2}f}{\sqrt{x^2}} + \frac{\sqrt{2}f}{\sqrt{y^2}} = 0$$

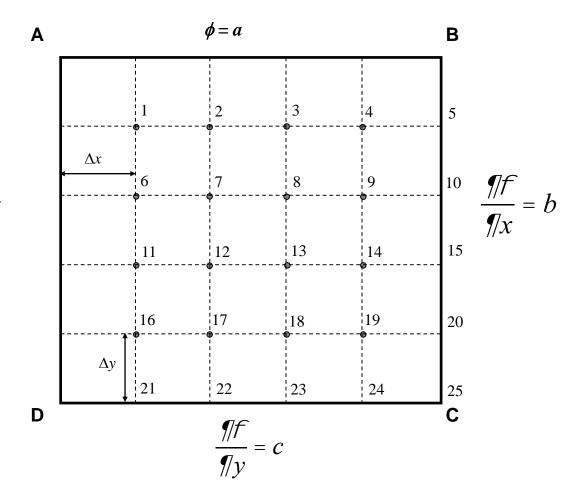
$$\frac{\mathscr{G}}{\mathscr{G}y}\bigg|_{(x,0)} = c, \ f(x,L_y) = a$$

$$f(0,y) = d$$
 and  $\frac{9/f}{9/x}\Big|_{(L,v)} = b$   $\phi = d$ 

$$\Delta x = \frac{L_x}{5} \qquad \Delta y = \frac{L_y}{5}$$

Number of unknowns increased from 16 to 25

$$x \hat{\mathsf{I}} \left(0, L_x\right) \text{ and } y \hat{\mathsf{I}} \left(0, L_y\right)$$



#### Neumann and Robin BC

#### Three Options for implementation:

- ✓ Backward Difference approximation with increased size of the matrix
  - ✓ asymmetric backward difference approximation
  - ✓ size of the matrix is increased
  - ✓ Solution at the boundary nodes are obtained together
- ✓ Ghost Node
  - ✓ Symmetric central difference approximation
  - ✓ Size of the matrix is increased
  - ✓ Solution at the boundary nodes are obtained together
- ✓ Backward Difference approximation without increasing the size of the matrix
  - ✓ asymmetric backward difference approximation
  - ✓ size of the matrix remains unaltered
  - ✓ Unknowns at the boundary nodes to be computed separately using the approximation of the BC after the solution have been computed for the interior nodes

#### Backward Difference

Number of equations is now 24 and the size of the matrix A is  $24 \times 24$  For Node 5, the 5<sup>th</sup> equation is:

$$\frac{f_{3} - 4f_{4} + 3f_{5}}{2Dx} = b \text{ or } \left(\frac{1}{2Dx}\right)f_{3} + \left(-\frac{2}{Dx}\right)f_{4} + \left(\frac{3}{2Dx}\right)f_{5} = b$$

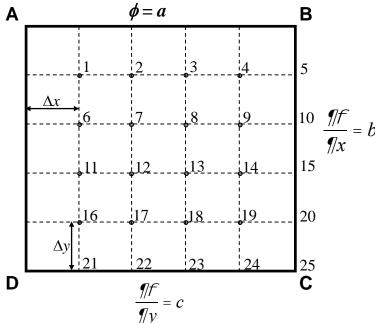
$$a_{53} = \left(\frac{1}{2Dx}\right), \ a_{54} = \left(-\frac{2}{Dx}\right), \ a_{55} = \left(\frac{3}{2Dx}\right), \ \text{and} \ b_{5} = b$$

For Node 21, the 21<sup>st</sup> equation is:

$$\frac{f_{11} - 4f_{16} + 3f_{21}}{2Dy} = c$$

$$\left(\frac{1}{2Dy}\right)f_{11} + \left(-\frac{2}{Dy}\right)f_{16} + \left(\frac{3}{2Dy}\right)f_{21} = c$$

$$a_{2111} = \left(\frac{1}{2Dy}\right), \ a_{2116} = \left(-\frac{2}{Dy}\right), \ a_{2121} = \left(\frac{3}{2Dx}\right), \ \text{and} \ b_{21} = c$$



#### **Backward Difference**

Number of equations will remain at 16 and the size of the matrix  $\mathbf{A}$  is  $16 \times 16$ 

For Node 16, the 16<sup>th</sup> equation is:

$$\phi = a$$

$$\phi = a$$

$$\frac{\Delta x}{5}$$

$$\frac{5}{9}$$

$$\frac{10}{13}$$

$$\frac{14}{14}$$

$$\frac{15}{16}$$

$$\frac{16}{7}$$

$$\frac{9}{7}$$

$$\frac{17}{7} = c$$

$$\left(\frac{1}{Dv^{2}}\right)f_{12} + \left(\frac{1}{Dx^{2}}\right)f_{15} + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dv^{2}}\right)f_{16} + \left(\frac{1}{Dx^{2}}\right)f_{16'} + \left(\frac{1}{Dv^{2}}\right)f_{16''} = 0$$

$$\frac{f_{15} - 4f_{16} + 3f_{16'}}{2Dx} = b \text{ or } \left(\frac{1}{2Dx}\right) f_{15} + \left(-\frac{2}{Dx}\right) f_{16} + \left(\frac{3}{2Dx}\right) f_{16'} = b$$

$$\frac{f_{12} - 4f_{16} + 3f_{16''}}{2Dy} = c \text{ or } \left(\frac{1}{2Dy}\right) f_{12} + \left(-\frac{2}{Dy}\right) f_{16} + \left(\frac{3}{2Dy}\right) f_{16''} = c$$

#### Backward Difference

Number of equations will remain at 16 and the size of the matrix  $\mathbf{A}$  is  $16 \times 16$ 

For Node 16, the 16<sup>th</sup> equation is:

$$\phi = d$$

$$\phi = d$$

$$\frac{\Delta x}{5}$$

$$\frac{6}{5}$$

$$\frac{7}{8}$$

$$\frac{8}{9}$$

$$\frac{9}{10}$$

$$\frac{11}{12}$$

$$\frac{12}{12}$$

$$\frac{13}{14}$$

$$\frac{14}{15}$$

$$\frac{16}{16}$$

$$\frac{9}{16}$$

$$\frac{17}{7} = c$$

$$\frac{9}{7}$$

$$\frac{18}{7} = c$$

$$\left(\frac{2}{3Dy^{2}}\right)f_{12} + \left(\frac{2}{3Dx^{2}}\right)f_{15} + \left(-\frac{2}{3Dx^{2}} - \frac{2}{3Dy^{2}}\right)f_{16} = -\frac{2b}{3Dx} - \frac{2c}{3Dy}$$

Recall, for Node 16, the 16<sup>th</sup> equation for the 1<sup>st</sup> type BC was:

$$\left(\frac{1}{Dy^{2}}\right)f_{12} + \left(\frac{1}{Dx^{2}}\right)f_{15} + \left(-\frac{2}{Dx^{2}} - \frac{2}{Dy^{2}}\right)f_{16} = -\frac{b}{Dx^{2}} - \frac{c}{Dy^{2}}$$