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Introduction

PDE	order	linearity
$\frac{\partial^2 u}{\partial x^2} + 2xy \frac{\partial^2 u}{\partial y^2} + u = 1$	2	<i>linear</i>
$\frac{\partial^3 u}{\partial x^2 \partial y} + x \frac{\partial^2 u}{\partial y^2} + 8u = 5y$	3	<i>linear</i>
$\left(\frac{\partial^2 u}{\partial x^2} \right)^3 + 6 \frac{\partial^3 u}{\partial x \partial y^2} = x$	3	<i>nonlinear</i>
$\frac{\partial^2 u}{\partial x^2} + xu \frac{\partial u}{\partial y} = y$	2	<i>nonlinear</i>

linear second-order PDEs

with two independent variable:

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + D = 0$$

$$\begin{cases} A, B, C : \text{functions of } x \text{ and } y \\ D : \text{functions of } x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \end{cases}$$

depending on the values of the coefficients of the second-derivative terms

$$\rightarrow B^2 - 4AC \begin{cases} < 0 : \text{elliptic} \\ = 0 : \text{parabolic} \\ > 0 : \text{hyperbolic} \end{cases}$$

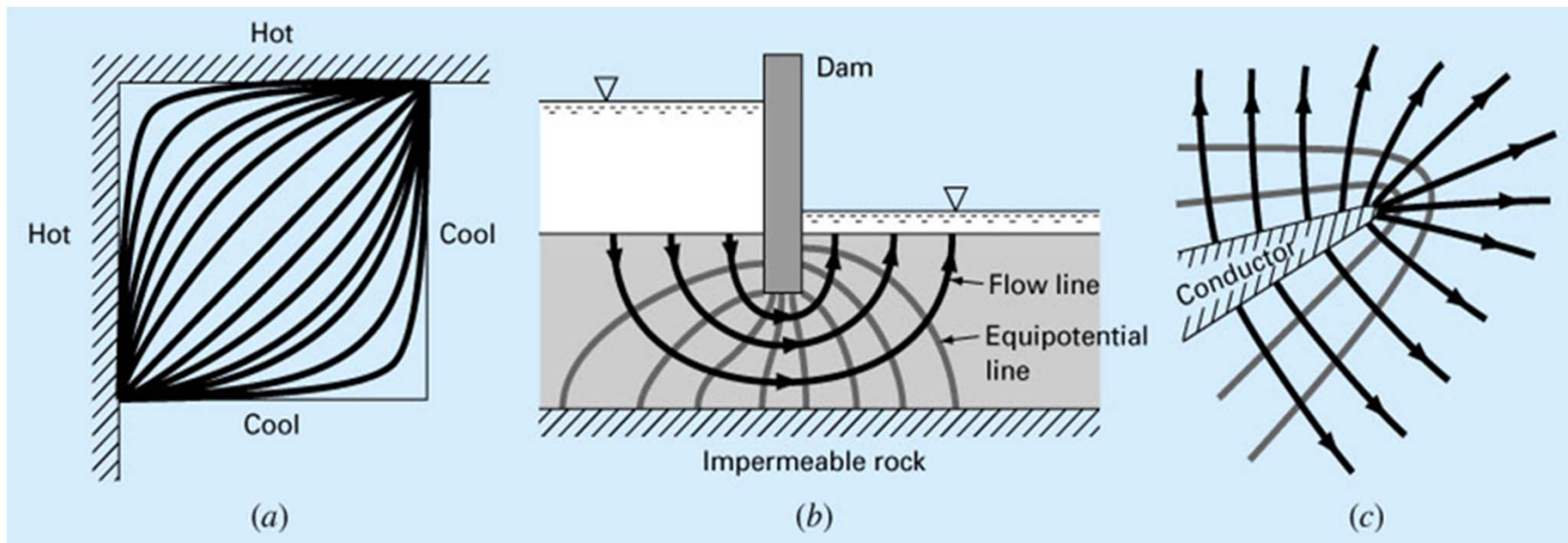
Classification of PDE

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} + D = 0$$

$B^2 - 4AC$	category	example
< 0	elliptic	$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \begin{cases} 0 & \text{(Laplace equation)} \\ f(x, y) & \text{(Poisson equation)} \end{cases}$
$= 0$	parabolic	$\frac{\partial T}{\partial t} = k' \frac{\partial^2 T}{\partial x^2}$ (heat conduction equation)
> 0	hyperbolic	$\frac{\partial^2 y}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 y}{\partial t^2}$ (wave equation)

Elliptic Equations

- Characterize steady-state systems
 - Steady-state distribution of an unknown in two spatial dimensions (no time derivative)
 - (a) temperature distribution on a heated plate
 - (b) seepage of water under a dam
 - (c) electric field near the point of a conductor

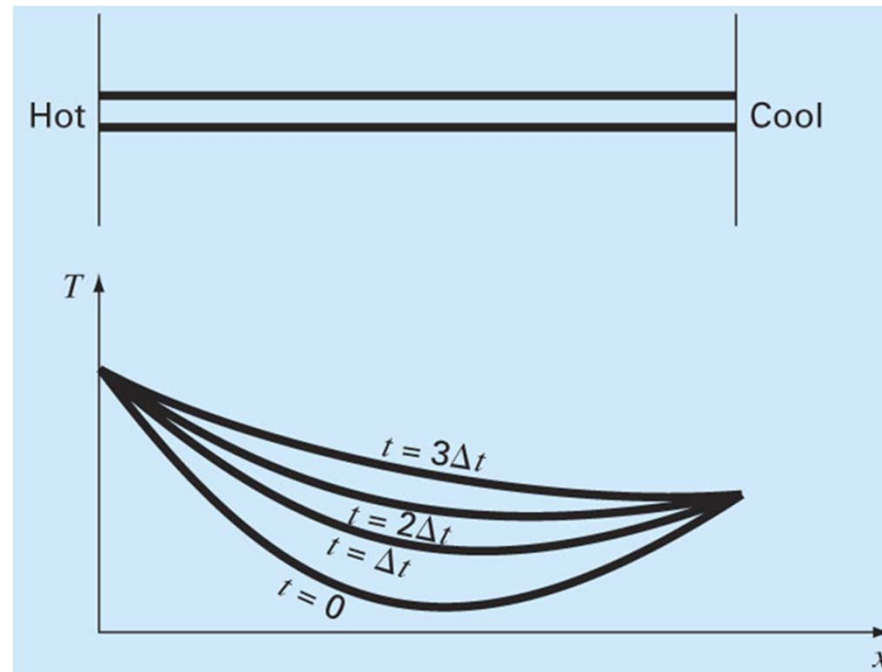


Comparison of Analogous Properties

Generic Term	Discipline		
	Elasticity	Heat Conduction	Magnetostatics
Potential function	$\{u\}$	u	$\{A\}$
“Strain”	$\{\varepsilon\}$	$-\{\nabla u\}$	$\{B\}$
“Stress”	$\{\sigma\}$	$\{q\}$	$\{H\}$
Load Density	$\{p\}$	$\{Q\}$	$\{J\}$
Boundary Load	$\{t\}$	$\{q^b\}$	$H \times n$
Definition of Strain	$\{\varepsilon\} = [L] \{u\}$	$-\{\nabla u\}$	$\{B\} = \nabla \times \{A\}$
Constitutive Relationship	$\{\sigma\} = [D] \{\varepsilon\}$	$\{q\} = -[K] \{\nabla u\}$	$\{H\} = [\mu]^{-1} \{B\}$
Potential Energy	$\frac{1}{2} \{\sigma\}^T \{\varepsilon\}$		$\frac{1}{2} \{H\}^T \{B\}$
Equilibrium	$\Sigma \sigma_{ij,j} = -P_i$	$\nabla \cdot \{q\} = Q$	$\nabla \times \{H\} = \{J\}$
Inertia Loading	$\{p^i\} = -\rho \{u_{,tt}\}$	$Q^s = -\rho c u_{,t}$	

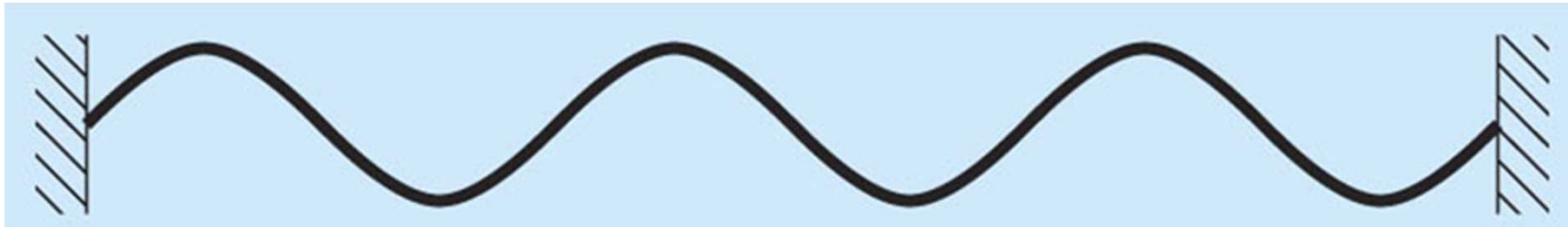
Parabolic Equations

- Determine how an unknown varies in both space and time
- Propagation problems: solution changes in time
 - Long, thin rod insulated everywhere but at its end



Hyperbolic Equations

- Propagation problems
 - Unknown is characterized by a second derivative w.r.t. time
 - Solution oscillates
 - Taut string vibrating at a low amplitude



COMSOL: Coefficient Form PDE

The diagram illustrates the physical interpretation of the terms in the wave equation:

$$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} - \nabla \cdot (c \nabla u + \alpha u - \gamma) + \beta \cdot \nabla u + a u = f$$

- Mass**: Points to the term $e_a \frac{\partial^2 u}{\partial t^2}$.
- Damping/Mass**: Points to the term $d_a \frac{\partial u}{\partial t}$.
- Diffusion**: Points to the term $c \nabla u$ within the divergence term.
- Convection**: Points to the term αu within the divergence term.
- Source**: Points to the term γ within the divergence term.
- Convection**: Points to the term $\beta \cdot \nabla u$.
- Source**: Points to the term $a u$.
- Conservative Flux**: A bracket under the entire divergence term $\nabla \cdot (c \nabla u + \alpha u - \gamma)$ points to this label.
- Absorption**: Points to the term $a u$.

$$\nabla = \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n} \right) \quad (\text{vector differential operator, gradient})$$

$$\nabla u = grad(u)$$

$$\nabla \cdot \mathbf{u} = \text{div}(\mathbf{u})$$

$$\nabla \times \mathbf{u} = \text{curl}(\mathbf{u})$$

$$\Delta = \frac{\partial^2}{\partial x_1^2} + \dots + \frac{\partial^2}{\partial x_n^2} \quad (\text{Laplace operator})$$

$$\nabla \cdot (c \nabla u) = \frac{\partial}{\partial x_1} \left(c \frac{\partial u}{\partial x_1} \right) + \dots + \frac{\partial}{\partial x_n} \left(c \frac{\partial u}{\partial x_n} \right)$$

$$\beta \cdot \nabla u = \beta_1 \frac{\partial u}{\partial x_1} + \dots + \beta_n \frac{\partial u}{\partial x_n}$$

COMSOL: Classical PDEs

EQUATION	COMPACT NOTATION	STANDARD NOTATION (2D)
Laplace's equation	$-\nabla \cdot (\nabla u) = 0$	$-\frac{\partial}{\partial x} \frac{\partial u}{\partial x} - \frac{\partial}{\partial y} \frac{\partial u}{\partial y} = 0$
Poisson's equation	$-\nabla \cdot (c \nabla u) = f$	$-\frac{\partial}{\partial x} \left(c \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(c \frac{\partial u}{\partial y} \right) = f$
Helmholtz equation	$-\nabla \cdot (c \nabla u) + au = f$	$-\frac{\partial}{\partial x} \left(c \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(c \frac{\partial u}{\partial y} \right) + au = f$
Heat equation	$d_a \frac{\partial u}{\partial t} - \nabla \cdot (c \nabla u) = f$	$d_a \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left(c \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(c \frac{\partial u}{\partial y} \right) = f$
Wave equation	$e_a \frac{\partial^2 u}{\partial t^2} - \nabla \cdot (c \nabla u) = f$	$e_a \frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x} \left(c \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(c \frac{\partial u}{\partial y} \right) = f$
Convection-diffusion equation	$d_a \frac{\partial u}{\partial t} - \nabla \cdot (c \nabla u) + \beta \cdot \nabla u = f$	$d_a \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left(c \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(c \frac{\partial u}{\partial y} \right) + \beta_x \frac{\partial u}{\partial x} + \beta_y \frac{\partial u}{\partial y} = f$

Elliptic: Laplace Equation

- Model a variety of problems involving the potential of an unknown variable

- Heated thin rectangular plate

- Insulated everywhere but at its edges
- Heat balance at steady state: (In) - (Out) = 0

$$\left\{ \begin{array}{l} k : \text{thermal diffusivity } [cm^2/s] \\ C : \text{heat capacity } [cal/(g \cdot ^\circ C)] \\ H = \rho CVT : \text{heat } [cal] \\ k' = k\rho C : \text{thermal conductivity} \\ [cal/(g \cdot cm \cdot ^\circ C)] \end{array} \right.$$

$$q(x)(\Delta y \Delta z) \Delta t + q(y)(\Delta x \Delta z) \Delta t = q(x + \Delta x)(\Delta y \Delta z) \Delta t + q(y + \Delta y)(\Delta x \Delta z) \Delta t$$

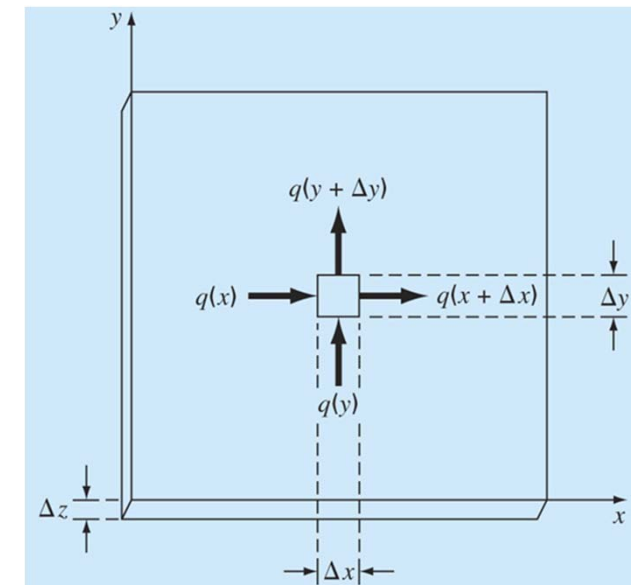
$$\xrightarrow{\div \Delta z \Delta t} [q(x) - q(x + \Delta x)] \Delta y + [q(y) - q(y + \Delta y)] \Delta x = 0$$

$$\rightarrow \frac{q(x) - q(x + \Delta x)}{\Delta x} \Delta x \Delta y + \frac{q(y) - q(y + \Delta y)}{\Delta y} \Delta x \Delta y = 0$$

$$\xrightarrow[\text{taking the limit}]{\div \Delta x \Delta y} -\frac{\partial q}{\partial x} - \frac{\partial q}{\partial y} = 0 \quad (\leftarrow \text{need heat fluxes at the plate's edges})$$

$$\left(\underbrace{\text{heat flux} \rightarrow \text{temperature}}_{\text{Fourier's law of heat conduction}} \right) q_i = -k' \frac{\partial T}{\partial i} \left\{ \begin{array}{l} \xrightarrow{k' = k\rho C} q_i = -k\rho C \frac{\partial T}{\partial i} \\ \xrightarrow{H = \rho CVT} q_i = -\frac{k'}{\rho CV} \frac{\partial H}{\partial i} \end{array} \right.$$

$$-\frac{\partial q}{\partial x} - \frac{\partial q}{\partial y} = 0 \rightarrow \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$



Analytic Solution

$$\begin{cases} \sinh x = \frac{e^x - e^{-x}}{2} \\ \sin x = \frac{e^{ix} - e^{-ix}}{2i} \\ \sin^2 x = \frac{1 - \cos 2x}{2} \end{cases}$$

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \text{ and BC } \begin{cases} \text{Dirichlet: } T(0, y) = T(a, y) = 0, T(x, 0) = 0, T(x, b) = f(x) \\ \text{Neumann: } \partial T / \partial n \\ \text{Mixed: } T \text{ and } \partial T / \partial n \end{cases}$$

$$T(x, y) = F(x)G(y) \rightarrow \frac{d^2 F}{dx^2} G + F \frac{d^2 G}{dy^2} = 0 \xrightarrow{\div FG} \frac{1}{F} \frac{d^2 F}{dx^2} = -\frac{1}{G} \frac{d^2 G}{dy^2} = -k$$

$$\begin{cases} T(0, y) = F(0)G(y) = 0 \\ T(a, y) = F(a)G(y) = 0 \end{cases} \rightarrow G(y) \neq 0, F(0) = 0 \text{ and } F(a) = 0$$

$$T(x, 0) = F(x)G(0) = 0 \rightarrow G(0) = 0$$

$$\begin{cases} \frac{d^2 F}{dx^2} + kF = 0 \rightarrow F = A \cos \sqrt{k}x + B \sin \sqrt{k}x \rightarrow \begin{cases} F(0) = 0 \rightarrow A = 0 \\ F(a) = 0 = B \sin \sqrt{k}a \rightarrow B \neq 0, \sqrt{k}a = n\pi \rightarrow k = \left(\frac{n\pi}{a}\right)^2 \end{cases} \\ \frac{d^2 G}{dy^2} - kG = 0 \rightarrow \frac{d^2 G}{dy^2} - \left(\frac{n\pi}{a}\right)^2 G = 0 \rightarrow G_n(y) = A_n e^{\frac{n\pi y}{a}} + B_n e^{-\frac{n\pi y}{a}} \rightarrow \{G(0) = 0 \rightarrow A_n + B_n = 0\} \end{cases}$$

$$T_n(x, y) = F_n(x)G_n(y) = \left(B \sin \frac{n\pi}{a}x\right) \left[A_n \left(e^{\frac{n\pi y}{a}} - e^{-\frac{n\pi y}{a}}\right)\right] = \tilde{A}_n \sin \frac{n\pi x}{a} \sinh \frac{n\pi y}{a} \rightarrow T(x, y) = \sum_{n=1}^{\infty} T_n(x, y)$$

$$T(x, b) = f(x) = \sum_{n=1}^{\infty} \tilde{A}_n \sin \frac{n\pi x}{a} \sinh \frac{n\pi b}{a} = \sum_{n=1}^{\infty} \left(\tilde{A}_n \sinh \frac{n\pi b}{a}\right) \sin \frac{n\pi x}{a}$$

$$\left(\tilde{A}_n \sinh \frac{n\pi b}{a}\right) = \frac{2}{a} \int_0^a f(x) \sin \frac{n\pi x}{a} dx \rightarrow \tilde{A}_n = 2 \int_0^a f(x) \sin \frac{n\pi x}{a} dx / a \sinh \frac{n\pi b}{a}$$

$$\begin{aligned} \int_0^a \sin^2 \frac{n\pi x}{a} dx &= \int_0^a \frac{1}{2} \left(1 - \cos \frac{2n\pi x}{a}\right) dx \\ &= \frac{1}{2} \left[x - \frac{a}{2n\pi} \sin \frac{2n\pi x}{a} \right]_0^a = \frac{a}{2} \end{aligned}$$

Solution Technique (1)

– PDE → algebraic difference equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \leftarrow \begin{cases} \frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} \\ \frac{\partial^2 T}{\partial y^2} = \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} \end{cases}$$

$$\rightarrow \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} = 0$$

$$\xrightarrow{\Delta x = \Delta y} T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$$

apply boundary conditions (fixed/Dirichlet)

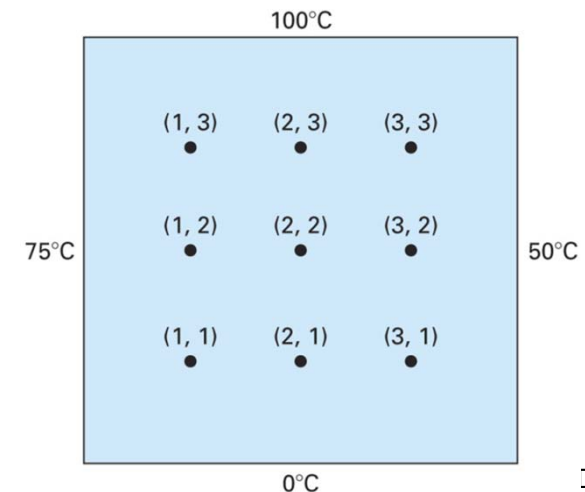
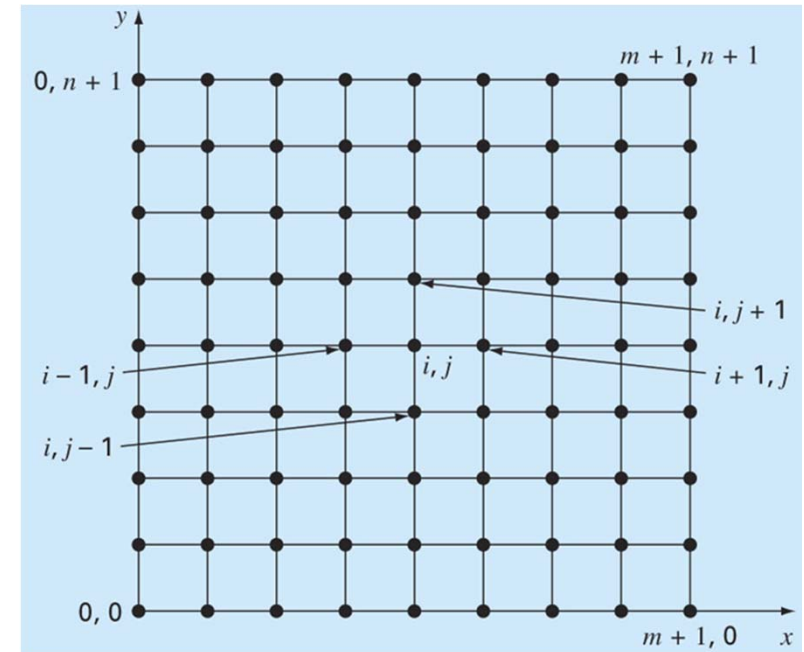
$$@ (1,1): T_{21} + \underbrace{T_{01}}_{75^\circ\text{C}} + T_{12} + \underbrace{T_{10}}_{0^\circ\text{C}} - 4T_{11} = 0 \rightarrow 4T_{11} - T_{21} - T_{12} = 75$$

$$@ (2,1): T_{31} + T_{11} + T_{22} + \underbrace{T_{20}}_{0^\circ\text{C}} - 4T_{21} = 0 \rightarrow -T_{11} + 4T_{21} - T_{31} - T_{22} = 0$$

$$@ (3,1): \underbrace{T_{41}}_{50^\circ\text{C}} + T_{21} + T_{32} + \underbrace{T_{30}}_{0^\circ\text{C}} - 4T_{31} = 0 \rightarrow -T_{21} + 4T_{31} - T_{32} = 50$$

⋮

9 equations



Solution Technique (2)

- How to solve linear algebraic equations (T_{ij})?
 - Gauss-Seidel (Liebmann in PDE) method

$$\begin{cases} x_1 - 0.25x_2 - 0.25x_3 = 50 \\ -0.25x_1 + x_2 - 0.25x_4 = 50 \\ -0.25x_1 + x_3 - 0.25x_4 = 25 \\ -0.25x_2 - 0.25x_3 + x_4 = 25 \end{cases}$$

$$\rightarrow \begin{cases} x_1^{(1)} = 0.25x_2^{(0)} + 0.25x_3^{(0)} + 50 \\ x_2^{(1)} = 0.25x_1^{(1)} + 0.25x_4^{(0)} + 50 \\ x_3^{(1)} = 0.25x_1^{(1)} + 0.25x_4^{(0)} + 25 \\ x_4^{(1)} = 0.25x_2^{(1)} + 0.25x_3^{(1)} + 25 \end{cases}$$

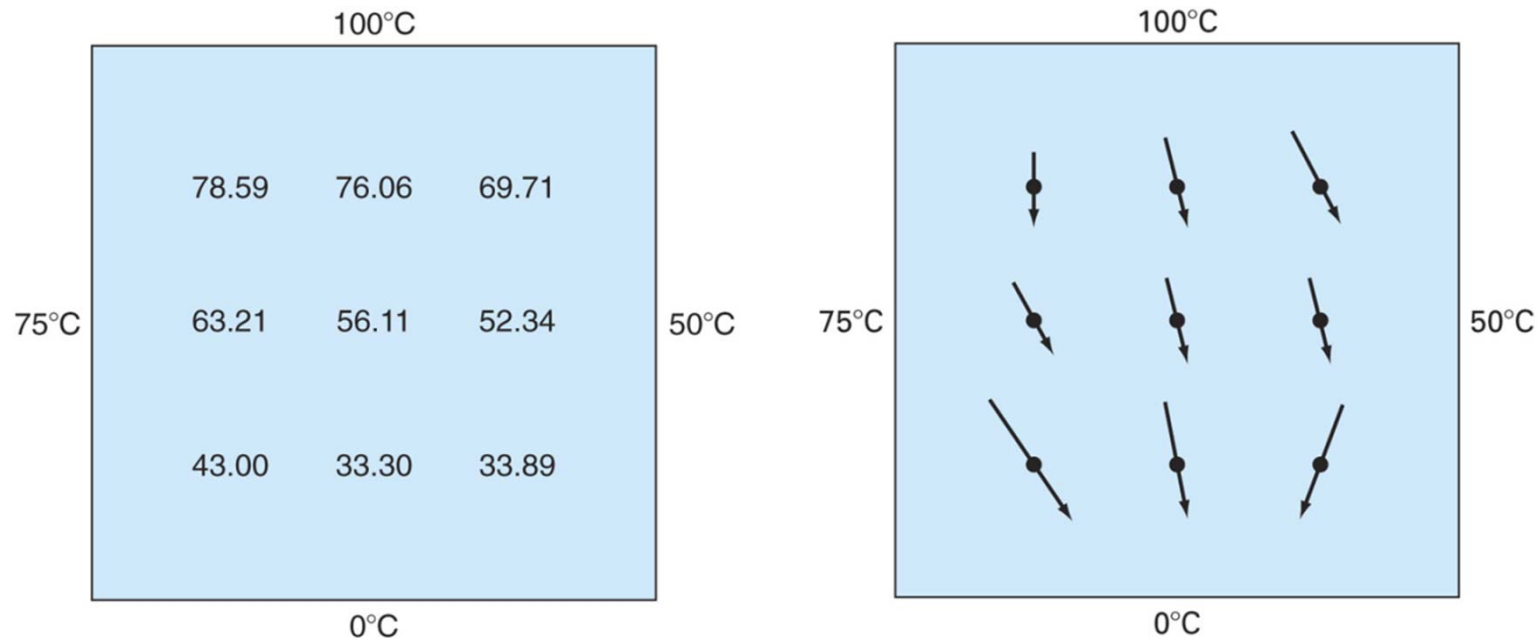
$$T_{i,j} = \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}}{4} \xrightarrow{\text{overrelaxation}} T_{i,j}^{new} = \lambda T_{i,j}^{new} + (1-\lambda)T_{i,j}^{old}$$

$$\xrightarrow{\text{stopping criterion}} \left| (\varepsilon_a)_{i,j} \right| = \left| \frac{T_{i,j}^{new} - T_{i,j}^{old}}{T_{i,j}^{new}} \right| 100\%$$

Example

- Primary variable (T_{ij}) $\rightarrow$ secondary variable ($q_{i,j}$)

$$q_l = -k' \frac{\partial T}{\partial l} \xrightarrow{\text{central difference}} \begin{cases} (q_{i,j})_x = -k' \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x} \\ (q_{i,j})_y = -k' \frac{T_{i,j+1} - T_{i,j-1}}{2\Delta y} \end{cases} \rightarrow \begin{cases} (q_{i,j})_n = \sqrt{(q_{i,j})_x^2 + (q_{i,j})_y^2} \\ \theta_{i,j} = \begin{cases} \tan^{-1}((q_{i,j})_y / (q_{i,j})_x) & \text{for } q_x > 0 \\ \tan^{-1}((q_{i,j})_y / (q_{i,j})_x) + \pi & \text{for } q_x < 0 \end{cases} \end{cases}$$



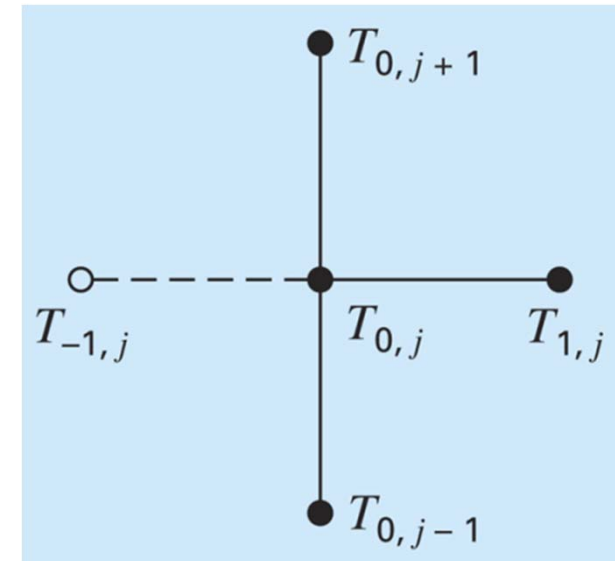
Derivative Boundary Conditions

- Neumann boundary condition
- For the heated plate problem
 - heat flux is specified at the boundary
 - If the edge is insulated, this derivative becomes zero

$$T_{1,j} + T_{-1,j} + T_{0,j+1} + T_{0,j-1} - 4T_{0,j} = 0$$

$$\frac{\partial T_{0,j}}{\partial x} \cong \frac{T_{1,j} - T_{-1,j}}{2\Delta x} \rightarrow T_{-1,j} = T_{1,j} - 2\Delta x \frac{\partial T_{0,j}}{\partial x}$$

$$2T_{1,j} - 2\Delta x \frac{\partial T_{0,j}}{\partial x} + T_{0,j+1} + T_{0,j-1} - 4T_{0,j} = 0$$



Example

$$@ (1,0): T_{2,0} + \underbrace{T_{0,0}}_{75^\circ\text{C}} + T_{1,1} + \underbrace{T_{1,-1}}_0 - 4T_{1,0} = 0 \leftarrow \left(\frac{\partial T_{1,0}}{\partial y} \cong \frac{T_{1,1} - T_{1,-1}}{2\Delta y} \rightarrow T_{1,-1} = T_{1,1} - 2\Delta y \underbrace{\frac{\partial T_{1,0}}{\partial y}}_0 \right)$$

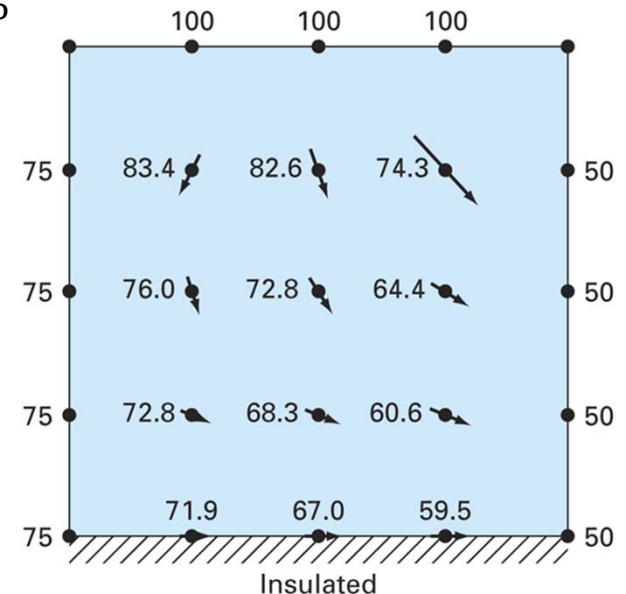
$$T_{2,0} + \underbrace{T_{0,0}}_{75^\circ\text{C}} + T_{1,1} + \left(T_{1,1} - 2\Delta y \underbrace{\frac{\partial T_{1,0}}{\partial y}}_0 \right) - 4T_{1,0} = 0 \rightarrow 4T_{1,0} - T_{2,0} - 2T_{1,1} = 75$$

⋮

$$@ (1,1): T_{2,1} + \underbrace{T_{0,1}}_{75^\circ\text{C}} + T_{1,2} + T_{1,0} - 4T_{1,1} = 0 \rightarrow -T_{1,0} + 4T_{1,1} - T_{2,1} - T_{1,2} = 75$$

⋮

12 equations



Irregular Boundaries

$$\left(\frac{\partial T}{\partial x}\right)_{i-1,i} \cong \frac{T_{i,j} - T_{i-1,j}}{\alpha_1 \Delta x}$$

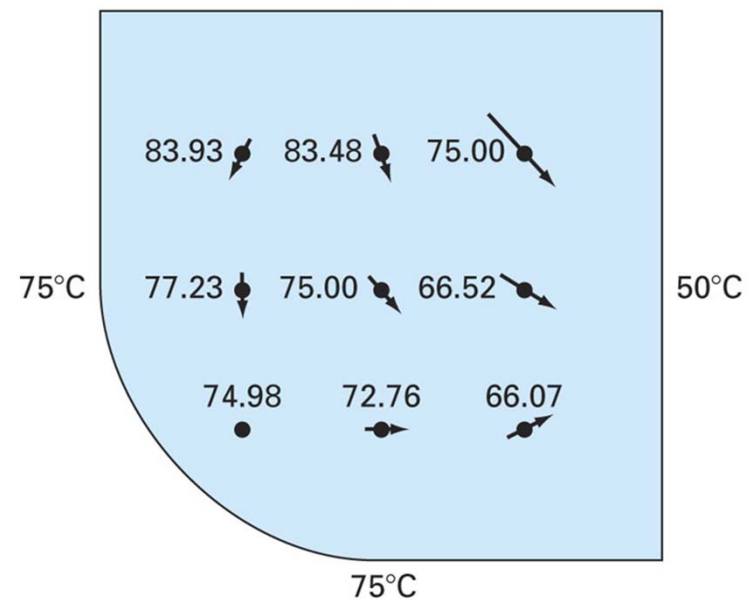
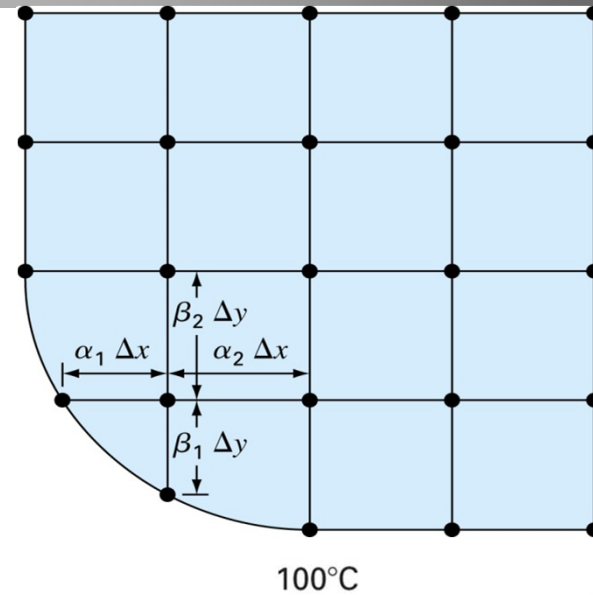
$$\left(\frac{\partial T}{\partial x}\right)_{i,i+1} \cong \frac{T_{i+1,j} - T_{i,j}}{\alpha_2 \Delta x}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial T}{\partial x} \right) = \frac{\left(\frac{\partial T}{\partial x}\right)_{i,i+1} - \left(\frac{\partial T}{\partial x}\right)_{i-1,i}}{\alpha_1 \Delta x + \alpha_2 \Delta x}$$

$$\frac{\partial^2 T}{\partial x^2} = 2 \frac{\frac{T_{i,j} - T_{i-1,j}}{\alpha_1 \Delta x} - \frac{T_{i+1,j} - T_{i,j}}{\alpha_2 \Delta x}}{\alpha_1 \Delta x + \alpha_2 \Delta x}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{2}{\Delta x^2} \left[\frac{T_{i-1,j} - T_{i,j}}{\alpha_1(\alpha_1 + \alpha_2)} + \frac{T_{i+1,j} - T_{i,j}}{\alpha_2(\alpha_1 + \alpha_2)} \right]$$

$$\frac{\partial^2 T}{\partial y^2} = \frac{2}{\Delta y^2} \left[\frac{T_{i,j-1} - T_{i,j}}{\beta_1(\beta_1 + \beta_2)} + \frac{T_{i,j+1} - T_{i,j}}{\beta_2(\beta_1 + \beta_2)} \right]$$



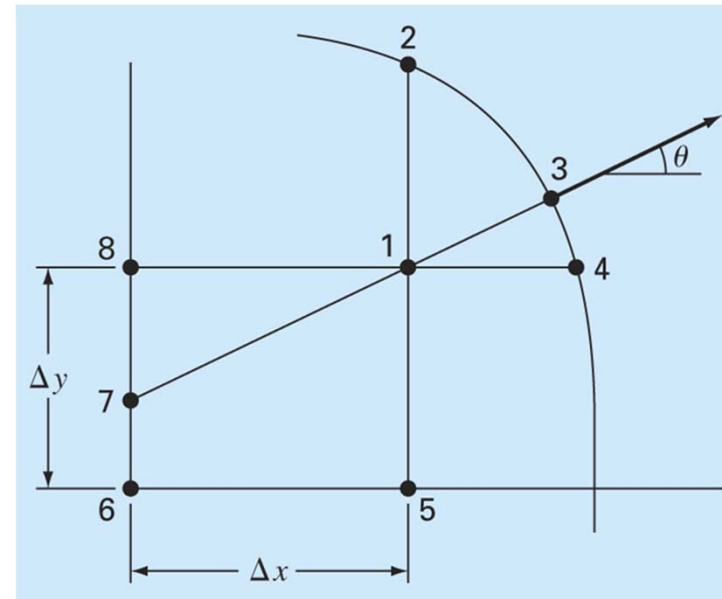
Derivative for Irregular Boundaries

$$\left(\frac{\partial T}{\partial \eta}\right)_3 = \frac{T_1 - T_7}{L_{17}} \rightarrow T_1 = \frac{\Delta x}{\cos \theta} \left(\frac{\partial T}{\partial \eta}\right)_3 + T_6 \frac{\Delta x \tan \theta}{\Delta y} + T_8 \left(1 - \frac{\Delta x \tan \theta}{\Delta y}\right)$$

$$L_{17} = \frac{\Delta x}{\cos \theta}$$

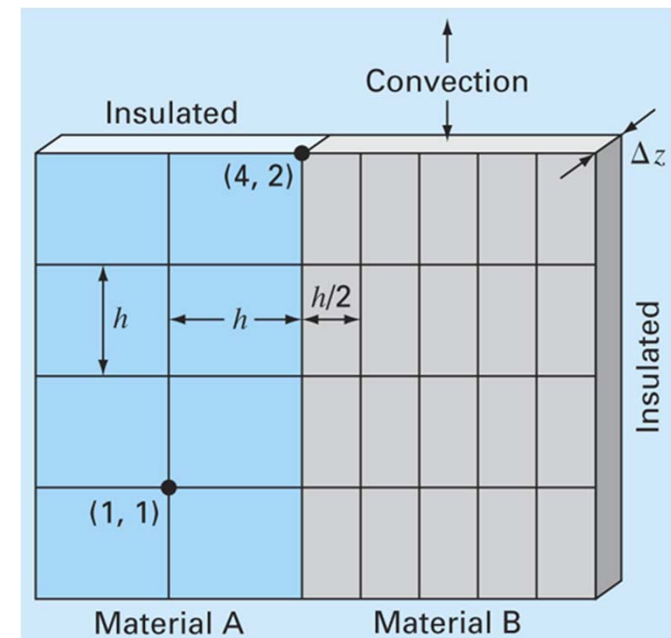
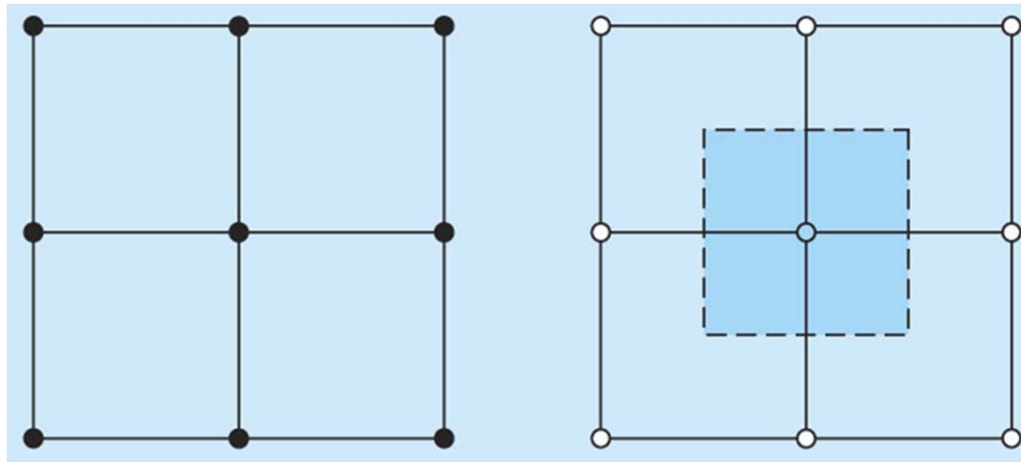
$$(T_7 - T_8) : (T_6 - T_8) = \Delta x \tan \theta : \Delta y$$

$$\rightarrow T_7 = T_8 + (T_6 - T_8) \frac{\Delta x \tan \theta}{\Delta y} \quad (\text{when } \theta < \pi/4)$$

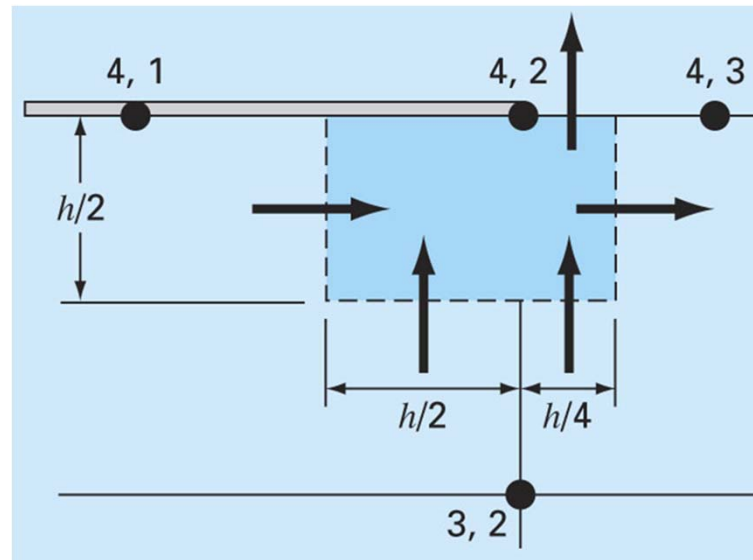


Control-Volume Approach

- Volume-integral approach
- points are determined across the domain
- approximation is applied to a volume surrounding the point rather than approximating the PDE at a point
 - Heated plate with unequal grid spacing, two materials, and mixed boundary conditions



Example



steady-state heat balance for the volume: $0 = (\text{In}) - (\text{Out})$

$$\left(\begin{array}{c} \text{left-side} \\ \text{conduction} \end{array} \right) + \left(\begin{array}{c} \text{lower} \\ \text{conduction} \\ \text{Material A} \end{array} \right) + \left(\begin{array}{c} \text{lower} \\ \text{conduction} \\ \text{Material B} \end{array} \right) = \left(\begin{array}{c} \text{right-side} \\ \text{conduction} \end{array} \right) + \left(\begin{array}{c} \text{upper} \\ \text{convection} \end{array} \right)$$

$$\left(-k'_A \frac{T_{42} - T_{41}}{h} \right) \left(\frac{h}{2} \Delta z \right) + \left(-k'_A \frac{T_{42} - T_{32}}{h} \right) \left(\frac{h}{2} \Delta z \right) + \left(-k'_B \frac{T_{42} - T_{32}}{h} \right) \left(\frac{h}{4} \Delta z \right) \\ = \left(-k'_B \frac{T_{43} - T_{42}}{h/2} \right) \left(\frac{h}{2} \Delta z \right) - h_c (T_a - T_{42}) \left(\frac{h}{4} \Delta z \right)$$

Parabolic: Heat Conduction Equation

- Conservation of energy can be used to develop an unsteady-state energy balance for the differential element in a long, thin insulated rod

$(In) - (Out) = (\text{heat stored in the element over a unit time period } \Delta t)$

$$q(x)(\Delta y \Delta z) \Delta t - q(x + \Delta x)(\Delta y \Delta z) \Delta t = \rho C (\Delta x \Delta y \Delta z) \Delta T$$

$$\frac{q(x) - q(x + \Delta x)}{\Delta x} = \rho C \frac{\Delta T}{\Delta t} \xrightarrow{\text{taking the limit}} -\frac{\partial q}{\partial x} = \rho C \frac{\partial T}{\partial t} \xrightarrow{q = -k \rho C \frac{\partial T}{\partial x}} k \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}$$



Analytic Solution (1)

$$k \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \quad \text{with} \quad \begin{cases} \text{BC: } T(0, t) = T_1 \text{ and } T(L, t) = T_2 \quad (t > 0) \\ \text{IC: } T(x, 0) = f(x) = 0 \end{cases}$$

$$T(x, t) = T_s(x) + T_T(x, t) \rightarrow \begin{cases} T_s(x) = T_1 + (T_2 - T_1) \frac{x}{L} \\ T_T(x, \infty) = 0 \\ T_T(0, t) = T_T(L, t) = 0 \quad (t > 0) \text{ since } T_s(x) \text{ satisfies BCs} \end{cases}$$

$$T_T(x, t) = F(x)G(t) \rightarrow kF''G = F\dot{G} \xrightarrow{\div kFG} \frac{F''}{F} = \frac{\dot{G}}{kG} = (\text{constant}) = -p^2 \quad (\text{why not 0 or positive?})$$

$$\left. \begin{aligned} F(0)G(t) &= 0 \\ F(L)G(t) &= 0 \end{aligned} \right\} \rightarrow G(t) \neq 0, F(0) = 0 \text{ and } F(L) = 0$$

$$\begin{cases} F'' + p^2 F = 0 \rightarrow F(x) = A \cos px + B \sin px \rightarrow \begin{cases} F(0) = 0 \rightarrow A = 0 \\ F(L) = 0 = B \sin pL \rightarrow B \neq 0, pL = n\pi \rightarrow p = \frac{n\pi}{L} \end{cases} \\ \dot{G} + kp^2 G = 0 \rightarrow G(t) = a \exp(-kp^2 t) = a_n \exp\left(-\frac{kn^2 \pi^2 t}{L^2}\right) \end{cases}$$

Analytic Solution (2)

$$T_{T,n}(x,t) = F_n(x)G_n(t) = \left(B \sin \frac{n\pi}{L} x \right) \left[a_n \exp \left(-\frac{kn^2\pi^2 t}{L^2} \right) \right]$$

$$T(x,t) = T_S(x) + \sum_{n=1}^{\infty} T_{T,n}(x,t) = T_1 + (T_2 - T_1) \frac{x}{L} + \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L} \exp \left(-\frac{kn^2\pi^2 t}{L^2} \right)$$

$$T(x,0) = f(x) = T_1 + (T_2 - T_1) \frac{x}{L} + \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}$$

$$\sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L} = f(x) - T_1 - (T_2 - T_1) \frac{x}{L}$$

$$a_n = \frac{2}{L} \int_0^L \left[f(x) - T_1 - (T_2 - T_1) \frac{x}{L} \right] \sin \frac{n\pi x}{L} dx = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi x}{L} dx + \frac{2}{n\pi} (T_2 \cos n\pi - T_1)$$

$$T_1 = 0, T_2 = \bar{T}, f(x) = 0$$

$$T(x,t) = \bar{T} \left[\frac{x}{L} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin \frac{n\pi x}{L} \exp \left(-\frac{kn^2\pi^2 t}{L^2} \right) \right]$$

$$\begin{aligned} & -\frac{2}{L} \int_0^L \left[T_1 + (T_2 - T_1) \frac{x}{L} \right] \sin \frac{n\pi x}{L} dx = -\frac{2T_1}{L} \int_0^L \sin \frac{n\pi x}{L} dx - \frac{2(T_2 - T_1)}{L^2} \int_0^L x \sin \frac{n\pi x}{L} dx \\ & = -\frac{2T_1}{L} \left[-\frac{L}{n\pi} \cos \frac{n\pi x}{L} \right]_0^L - \frac{2(T_2 - T_1)}{L^2} \left\{ \left[-\frac{Lx}{n\pi} \cos \frac{n\pi x}{L} \right]_0^L + \frac{L}{n\pi} \underbrace{\int_0^L \cos \frac{n\pi x}{L} dx}_{=0} \right\} \\ & = \frac{2T_1}{n\pi} (\cos n\pi - 1) + \frac{2(T_2 - T_1)}{n\pi} \cos n\pi = \frac{2}{n\pi} [T_1 (\cos n\pi - 1) + (T_2 - T_1) \cos n\pi] \\ & = \frac{2}{n\pi} (T_2 \cos n\pi - T_1) \end{aligned}$$

Explicit Methods

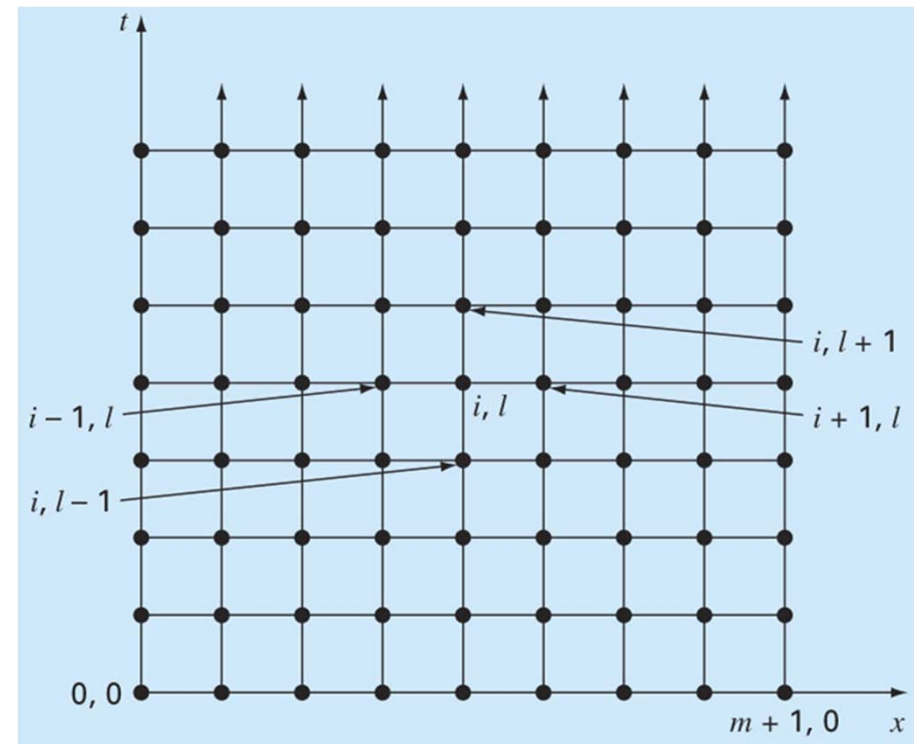
- approximations for the second derivative in space and the first derivative in time
- Time-variable: open-ended, stability problem

$$\left. \begin{aligned} \frac{\partial^2 T}{\partial x^2} &= \frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{\Delta x^2} \rightarrow O((\Delta x)^2) \\ \frac{\partial T}{\partial t} &= \frac{T_i^{l+1} - T_i^l}{\Delta t} \rightarrow O(\Delta t) \end{aligned} \right\}$$

$$\rightarrow k \frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{(\Delta x)^2} = \frac{T_i^{l+1} - T_i^l}{\Delta t}$$

$$T_i^{l+1} = T_i^l + \lambda (T_{i+1}^l - 2T_i^l + T_{i-1}^l) \text{ where } \lambda = \frac{k\Delta t}{(\Delta x)^2}$$

for all interior nodes



Convergence and Stability

$$\lambda = \frac{k\Delta t}{(\Delta x)^2} \leq \begin{cases} \frac{1}{2} \text{ (errors do not grow, but oscillate)} \rightarrow \Delta t \leq \frac{1}{2} \frac{(\Delta x)^2}{k} \\ \frac{1}{4} \text{ (ensure no oscillation)} \\ \frac{1}{6} \text{ (minimize truncation error)} \end{cases}$$
$$\left(\Delta x \rightarrow \frac{1}{2} \Delta x \right) \Rightarrow \left(\Delta t \rightarrow \frac{1}{4} \Delta t \right)$$

- Derivative boundary conditions

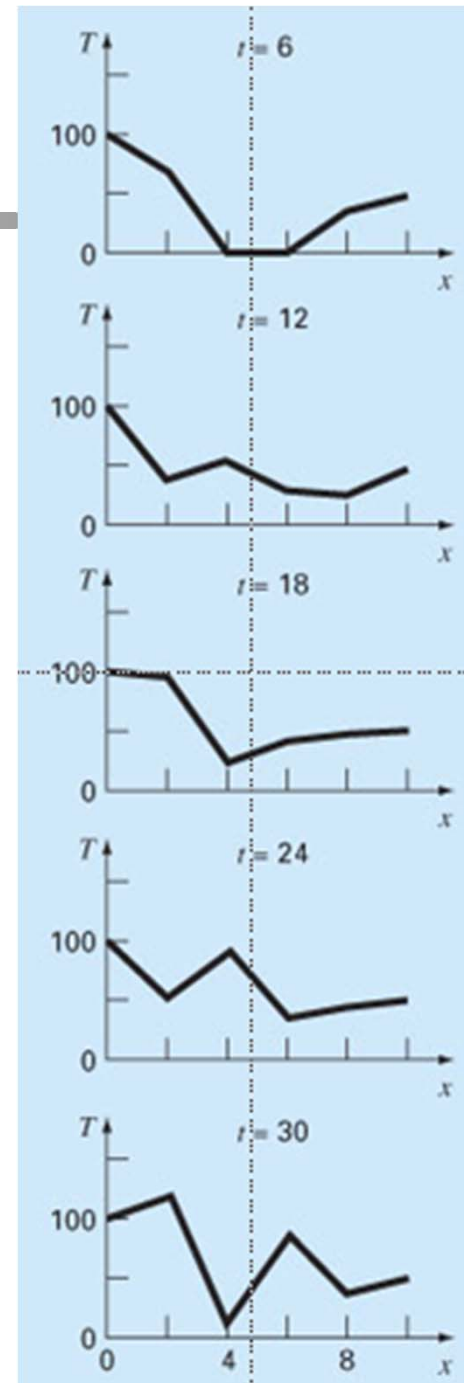
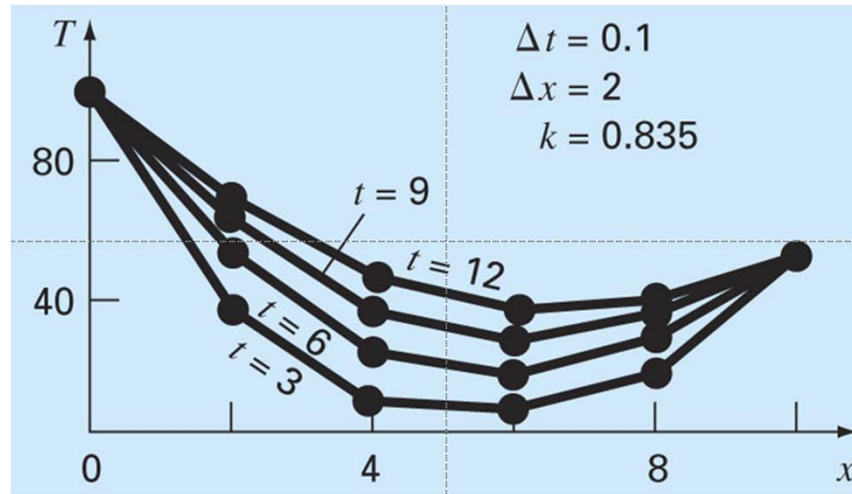
$$T_i^{l+1} = T_i^l + \lambda (T_{i+1}^l - 2T_i^l + T_{i-1}^l)$$

$$i = 0 : T_0^{l+1} = T_0^l + \lambda (T_1^l - 2T_0^l + \mathbf{T_{-1}^l})$$

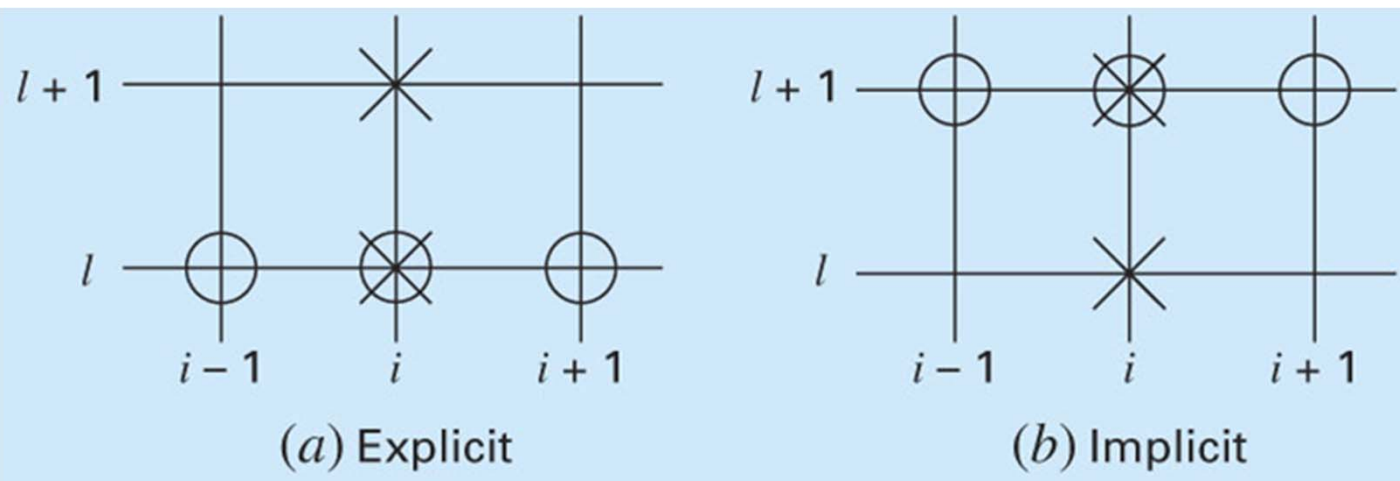
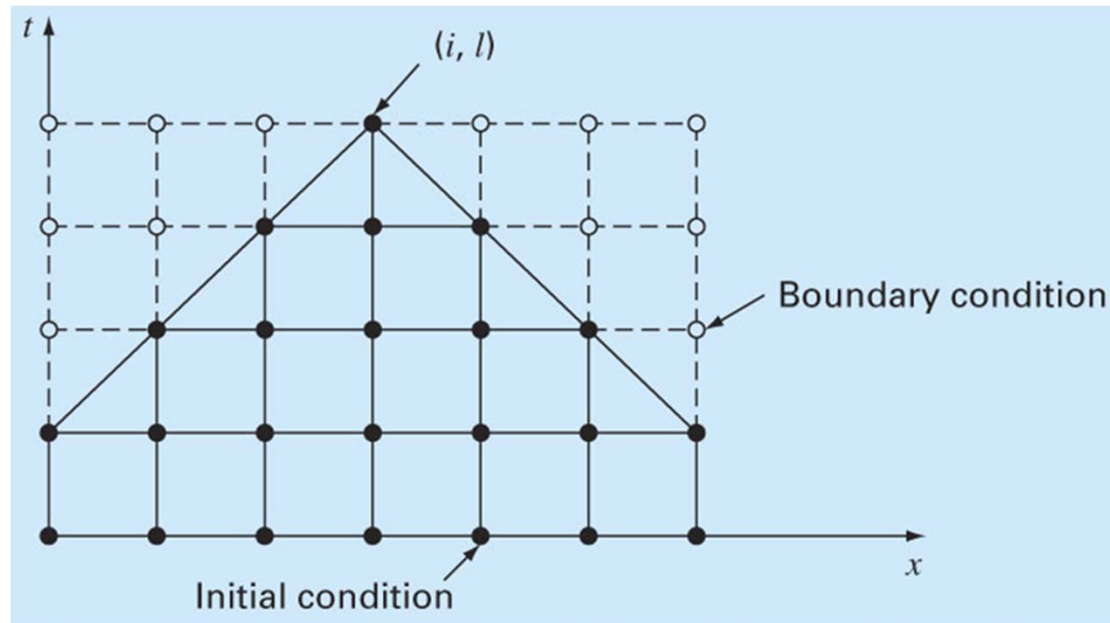
Example

$$\lambda = \frac{k\Delta t}{(\Delta x)^2} = 0.020875 (\ll 0.5)$$

$$\lambda = 0.735 (\gg 0.5)$$

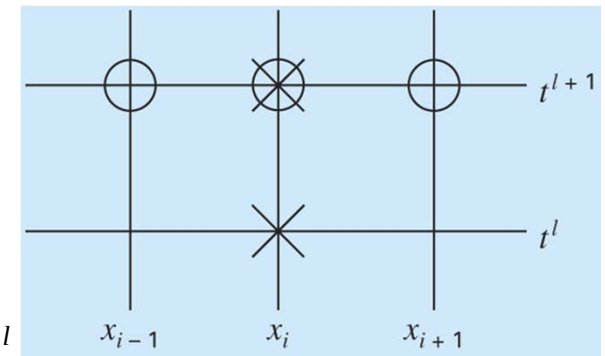


Explicit vs. Implicit



Simple Implicit Method

- overcome difficulties associated with explicit methods at the expense of somewhat more complicated algorithms
- spatial derivative is approximated at an advanced time interval $l+1$
- Unconditionally stable $\leftrightarrow$ accuracy limit
- Steady-state results in an efficient manner



$$k \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \frac{\frac{\partial^2 T}{\partial x^2} \cong \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2}}{\Delta t} \rightarrow k \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2} = \frac{T_i^{l+1} - T_i^l}{\Delta t}$$

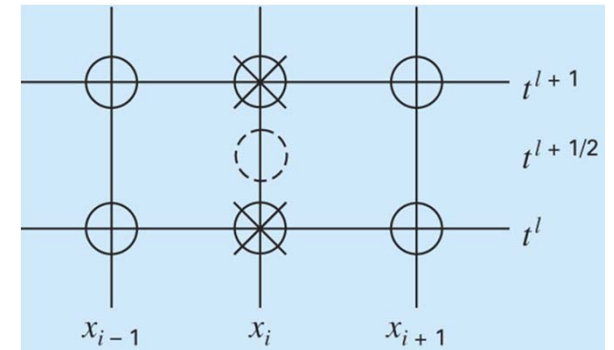
$$\begin{cases} i = 2, \dots, m-1: -\lambda T_{i-1}^{l+1} + (1+2\lambda)T_i^{l+1} - \lambda T_{i+1}^{l+1} = T_i^l \\ i = 1: -\lambda T_0^{l+1} + (1+2\lambda)T_1^{l+1} - \lambda T_2^{l+1} = T_1^l \rightarrow (1+2\lambda)T_1^{l+1} - \lambda T_2^{l+1} = T_1^l + \lambda f_0(t^{l+1}) \\ i = m: -\lambda T_{m-1}^{l+1} + (1+2\lambda)T_m^{l+1} - \lambda T_{m+1}^{l+1} = T_m^l \rightarrow -\lambda T_{m-1}^{l+1} + (1+2\lambda)T_m^{l+1} = T_m^l + \lambda f_{m+1}(t^{l+1}) \end{cases}$$

m equations / m unknowns

Crank-Nicolson Method

- alternative implicit scheme that is second order accurate both in space and time @ $t^{l+1/2}$
- difference approximations are developed at the midpoint of the time increment

$$k \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \leftarrow \begin{cases} \frac{\partial T}{\partial t} \cong \frac{T_i^{l+1} - T_i^l}{\Delta t} \\ \frac{\partial^2 T}{\partial x^2} \cong \frac{1}{2} \left[\frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{(\Delta x)^2} + \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2} \right] \end{cases}$$



$$k \frac{1}{2} \left[\frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{(\Delta x)^2} + \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2} \right] = \frac{T_i^{l+1} - T_i^l}{\Delta t}$$

$$\lambda (T_{i+1}^l - 2T_i^l + T_{i-1}^l + T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}) = 2(T_i^{l+1} - T_i^l)$$

$$\lambda T_{i-1}^{l+1} - 2(1+\lambda)T_i^{l+1} + \lambda T_{i+1}^{l+1} = -\lambda T_{i-1}^l - 2(1-\lambda)T_i^l - \lambda T_{i+1}^l$$

$$i=1: \lambda \mathbf{T}_0^{l+1} - 2(1+\lambda)T_1^{l+1} + \lambda T_2^{l+1} = -\lambda \mathbf{T}_0^l - 2(1-\lambda)T_1^l - \lambda T_2^l$$

$$i=m: \lambda T_{m-1}^{l+1} - 2(1+\lambda)T_m^{l+1} + \lambda \mathbf{T}_{m+1}^{l+1} = -\lambda T_{m-1}^l - 2(1-\lambda)T_m^l - \lambda \mathbf{T}_{m+1}^l$$

Parabolic Equations in 2-D

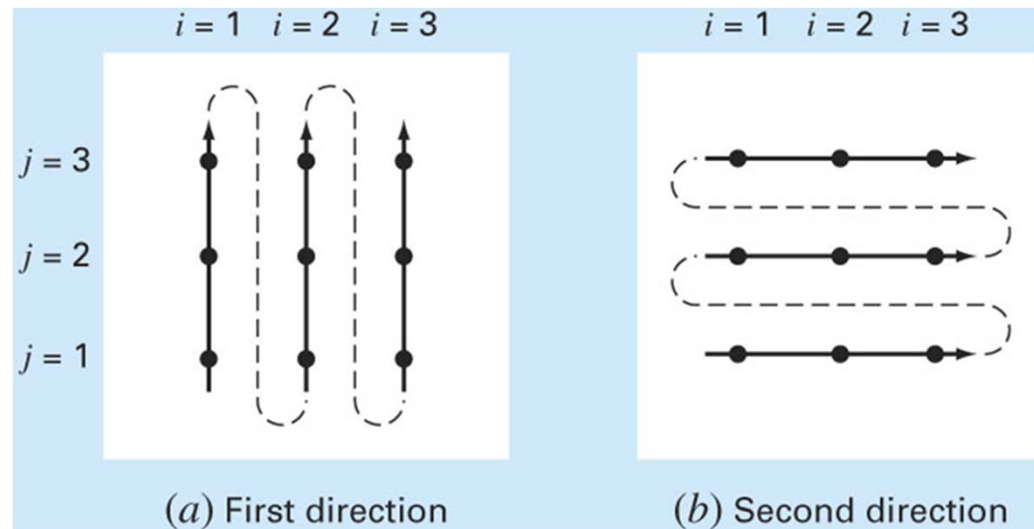
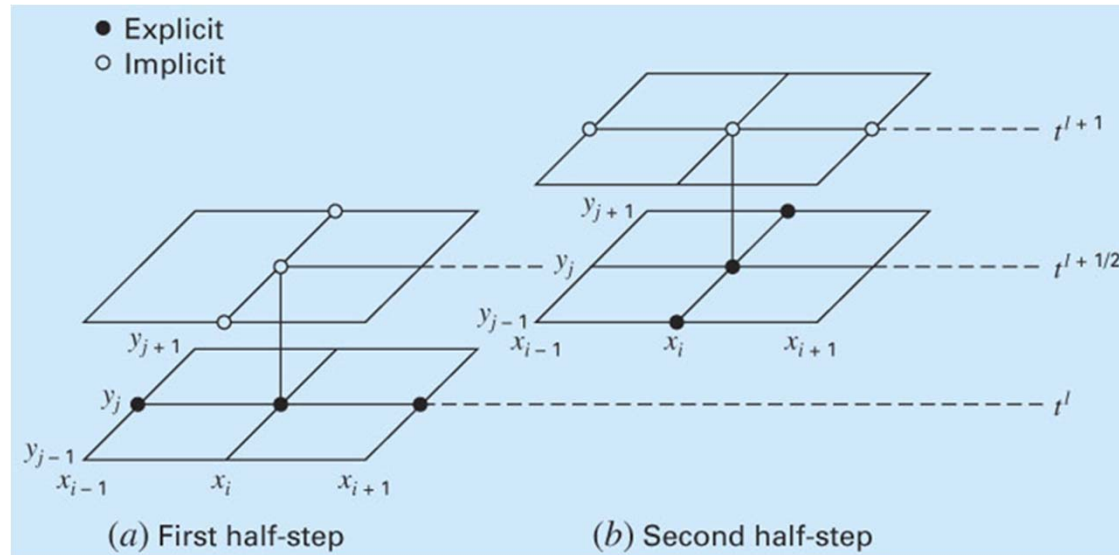
- alternating-direction implicit(ADI) scheme
 - solve parabolic equations in two spatial dimensions using tridiagonal matrices

$$\frac{\partial T}{\partial t} = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \rightarrow \text{stability: } \Delta t \leq \frac{1}{8} \frac{(\Delta x)^2 + (\Delta y)^2}{k}$$

$$\text{first step: } \frac{T_{i,j}^{l+1/2} - T_{i,j}^l}{\Delta t / 2} = k \left[\underbrace{\frac{T_{i+1,j}^l - 2T_{i,j}^l + T_{i-1,j}^l}{(\Delta x)^2}}_{\text{explicit}} + \underbrace{\frac{T_{i,j+1}^{l+1/2} - 2T_{i,j}^{l+1/2} + T_{i,j-1}^{l+1/2}}{(\Delta y)^2}}_{\text{implicit}} \right]$$

$$\text{second step: } \frac{T_{i,j}^{l+1} - T_{i,j}^{l+1/2}}{\Delta t / 2} = k \left[\underbrace{\frac{T_{i+1,j}^{l+1/2} - 2T_{i,j}^{l+1/2} + T_{i-1,j}^{l+1/2}}{(\Delta x)^2}}_{\text{implicit}} + \underbrace{\frac{T_{i,j+1}^{l+1} - 2T_{i,j}^{l+1} + T_{i,j-1}^{l+1}}{(\Delta y)^2}}_{\text{explicit}} \right]$$

ADI scheme



FDM vs. FEM

- FDM
 - Solution domain is divided into a grid of discrete points or nodes (pointwise approximation)
 - Shortcomings: irregular geometry, unusual boundary conditions, heterogeneous composition
- FEM
 - Solution domain is divided into simply shaped regions or elements

