

18-660: Numerical Methods for Engineering Design and Optimization

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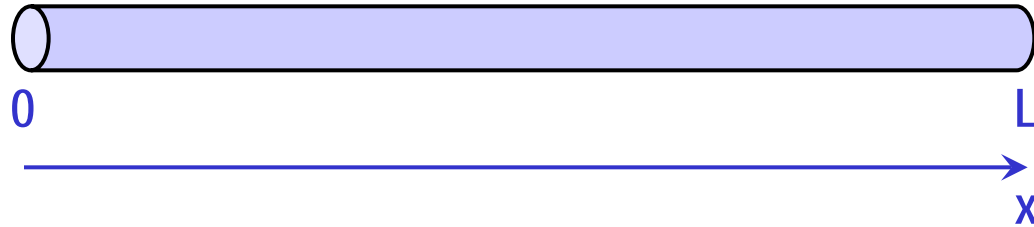
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Overview

- Thermal Analysis
 - ▼ 2-D / 3-D heat equation
 - ▼ Finite difference

1-D Heat Equation

- The complete PDE with boundary and initial conditions



PDE $\rho \cdot C_p \cdot T_t(x,t) = \kappa \cdot T_{xx}(x,t) + f(x,t) \quad (0 \leq x \leq L \quad 0 \leq t \leq \infty)$

BCs $\begin{cases} T(x=0,t) = T_1 \\ T(x=L,t) = T_2 \end{cases} \quad (0 < t \leq \infty)$

IC $T(x,t=0) = T_0 \quad (0 \leq x \leq L)$

2-D / 3-D Heat Equation

■ 2-D heat equation

$$\rho \cdot C_p \cdot \frac{\partial T(x, y, t)}{\partial t} = \kappa \cdot \nabla^2 T(x, y, t) + f(x, y, t)$$

■ 3-D heat equation

Density Laplace operator

$$\rho \cdot C_p \cdot \frac{\partial T(x, y, z, t)}{\partial t} = \kappa \cdot \nabla^2 T(x, y, z, t) + f(x, y, z, t)$$

Thermal capacity Thermal conductivity Heat source

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

2-D / 3-D Heat Equation

- Heat equation is a 2nd-order linear PDE

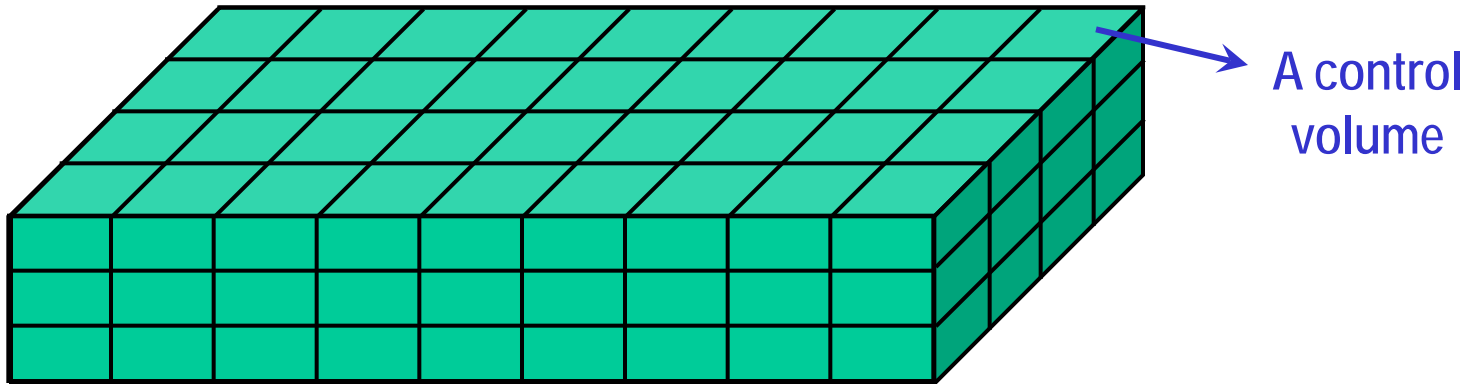
$$\rho \cdot C_p \cdot \frac{\partial T(x, y, z, t)}{\partial t} = \kappa \cdot \nabla^2 T(x, y, z, t) + f(x, y, z, t)$$

- Order of PDE – the order of the highest partial derivative
- Linearity – the dependent variable T and all its derivatives appear in a linear fashion
- Homogeneity
 - ▼ Homogenous if $f(x, y, z, t) = 0$
 - ▼ Non-homogenous if $f(x, y, z, t) \neq 0$

Finite Difference Method

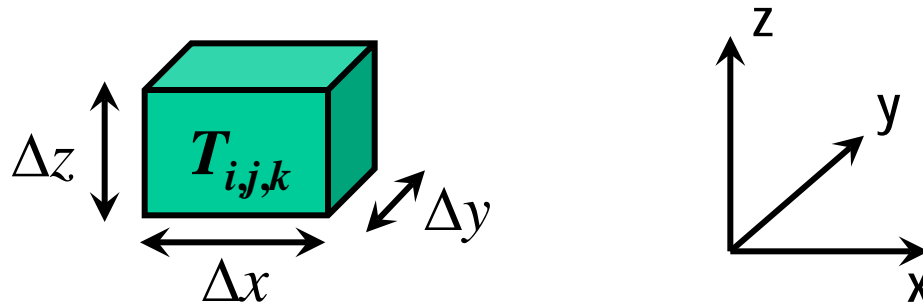
- PDE can be numerically solved using finite difference method
 - ▼ Discretize 3-D space into a number of small control volumes

$$\rho \cdot C_p \cdot \frac{\partial T(x, y, z, t)}{\partial t} = \kappa \cdot \nabla^2 T(x, y, z, t) + f(x, y, z, t)$$



Finite Difference Method

- A control volume



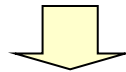
- Write PDE for each control volume

$$\rho \cdot C_p \cdot \frac{\partial T(i, j, k, t)}{\partial t} = \kappa \cdot \left[\frac{\partial^2 T(i, j, k, t)}{\partial x^2} + \frac{\partial^2 T(i, j, k, t)}{\partial y^2} + \frac{\partial^2 T(i, j, k, t)}{\partial z^2} \right] + f(i, j, k, t)$$

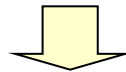
Finite Difference Method

- Discretize PDE over the control volume

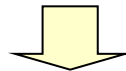
$$\frac{\partial^2 T(i, j, k, t)}{\partial x^2}$$



$$\frac{\frac{\partial T(i+1, j, k, t)}{\partial x} - \frac{\partial T(i, j, k, t)}{\partial x}}{\Delta x}$$



$$\frac{\frac{[T(i+1, j, k, t) - T(i, j, k, t)]}{\Delta x} - \frac{[T(i, j, k, t) - T(i-1, j, k, t)]}{\Delta x}}{\Delta x}$$

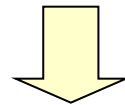


$$\frac{T_{i+1, j, k} - T_{i, j, k}}{(\Delta x)^2} - \frac{T_{i, j, k} - T_{i-1, j, k}}{(\Delta x)^2}$$

Finite Difference Method

■ Rewrite the finite difference discretization

$$\rho \cdot C_p \cdot \frac{\partial T(i, j, k, t)}{\partial t} = \kappa \cdot \left[\frac{\partial^2 T(i, j, k, t)}{\partial x^2} + \frac{\partial^2 T(i, j, k, t)}{\partial y^2} + \frac{\partial^2 T(i, j, k, t)}{\partial z^2} \right] + f(i, j, k, t)$$

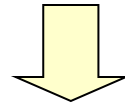


$$\rho \cdot C_p \cdot \frac{\partial T_{i,j,k}}{\partial t} = f_{i,j,k} + \frac{\kappa \cdot [T_{i+1,j,k} - T_{i,j,k}]}{(\Delta x)^2} - \frac{\kappa \cdot [T_{i,j,k} - T_{i-1,j,k}]}{(\Delta x)^2} +$$
$$\frac{\kappa \cdot [T_{i,j+1,k} - T_{i,j,k}]}{(\Delta y)^2} - \frac{\kappa \cdot [T_{i,j,k} - T_{i,j-1,k}]}{(\Delta y)^2} + \frac{\kappa \cdot [T_{i,j,k+1} - T_{i,j,k}]}{(\Delta z)^2} - \frac{\kappa \cdot [T_{i,j,k} - T_{i,j,k-1}]}{(\Delta z)^2}$$

Finite Difference Method

$$\rho \cdot C_p \cdot \frac{\partial T_{i,j,k}}{\partial t} = f_{i,j,k} + \frac{\kappa \cdot [T_{i+1,j,k} - T_{i,j,k}]}{(\Delta x)^2} - \frac{\kappa \cdot [T_{i,j,k} - T_{i-1,j,k}]}{(\Delta x)^2} +$$

$$\frac{\kappa \cdot [T_{i,j+1,k} - T_{i,j,k}]}{(\Delta y)^2} - \frac{\kappa \cdot [T_{i,j,k} - T_{i,j-1,k}]}{(\Delta y)^2} + \frac{\kappa \cdot [T_{i,j,k+1} - T_{i,j,k}]}{(\Delta z)^2} - \frac{\kappa \cdot [T_{i,j,k} - T_{i,j,k-1}]}{(\Delta z)^2}$$



$$I_{i,j,k} \leftarrow \boxed{f_{i,j,k} \cdot \Delta x \cdot \Delta y \cdot \Delta z} = \boxed{\rho \cdot C_p \cdot \Delta x \cdot \Delta y \cdot \Delta z} \cdot \frac{\partial T_{i,j,k}}{\partial t} +$$

$$G_x \leftarrow \boxed{\frac{\kappa \cdot \Delta y \cdot \Delta z}{\Delta x}} [T_{i,j,k} - T_{i+1,j,k}] + \frac{\kappa \cdot \Delta y \cdot \Delta z}{\Delta x} \cdot [T_{i,j,k} - T_{i-1,j,k}] +$$

$$G_y \leftarrow \boxed{\frac{\kappa \cdot \Delta x \cdot \Delta z}{\Delta y}} [T_{i,j,k} - T_{i,j+1,k}] + \frac{\kappa \cdot \Delta x \cdot \Delta z}{\Delta y} \cdot [T_{i,j,k} - T_{i,j-1,k}] +$$

$$G_z \leftarrow \boxed{\frac{\kappa \cdot \Delta x \cdot \Delta y}{\Delta z}} [T_{i,j,k} - T_{i,j,k+1}] + \frac{\kappa \cdot \Delta x \cdot \Delta y}{\Delta z} \cdot [T_{i,j,k} - T_{i,j,k-1}]$$

Finite Difference Method

- We have:

$$I_{i,j,k} = C \cdot \frac{\partial T_{i,j,k}}{\partial t} + G_x \cdot [T_{i,j,k} - T_{i+1,j,k}] + G_x \cdot [T_{i,j,k} - T_{i-1,j,k}] \\ G_y \cdot [T_{i,j,k} - T_{i,j+1,k}] + G_y \cdot [T_{i,j,k} - T_{i,j-1,k}] + G_z \cdot [T_{i,j,k} - T_{i,j,k+1}] + G_z \cdot [T_{i,j,k} - T_{i,j,k-1}]$$

▼ where

$$G_x = \frac{\kappa \cdot \Delta y \cdot \Delta z}{\Delta x} \quad G_y = \frac{\kappa \cdot \Delta x \cdot \Delta z}{\Delta y} \quad G_z = \frac{\kappa \cdot \Delta x \cdot \Delta y}{\Delta z} \\ C = \rho \cdot C_p \cdot \Delta x \cdot \Delta y \cdot \Delta z \quad I_{i,j,k} = f_{i,j,k} \cdot \Delta x \cdot \Delta y \cdot \Delta z$$

The discretized thermal equation has a form similar to a circuit equation

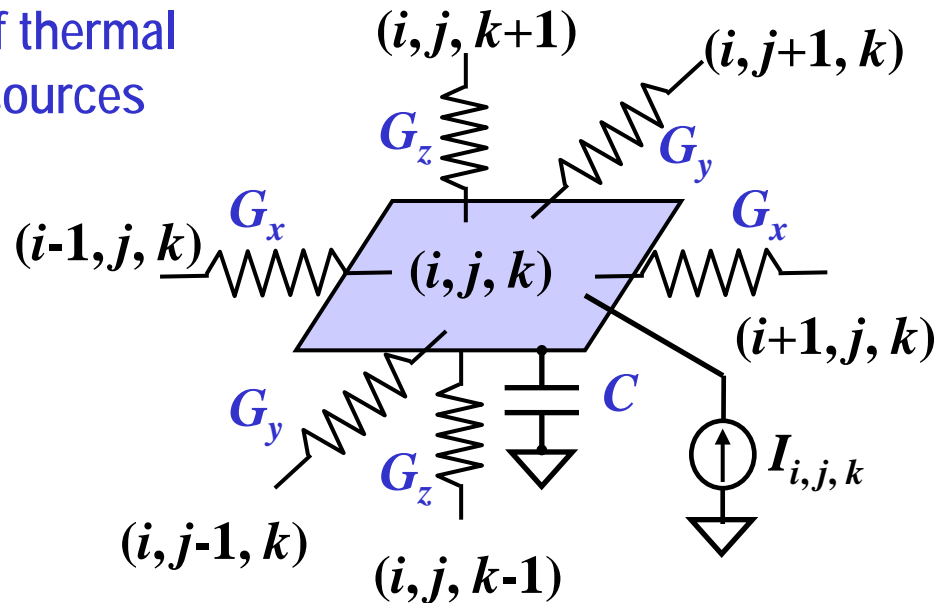
Finite Difference Method

$$I_{i,j,k} = C \cdot \frac{\partial T_{i,j,k}}{\partial t} + G_x \cdot [T_{i,j,k} - T_{i+1,j,k}] + G_x \cdot [T_{i,j,k} - T_{i-1,j,k}]$$
$$G_y \cdot [T_{i,j,k} - T_{i,j+1,k}] + G_y \cdot [T_{i,j,k} - T_{i,j-1,k}] + G_z \cdot [T_{i,j,k} - T_{i,j,k+1}] + G_z \cdot [T_{i,j,k} - T_{i,j,k-1}]$$

Equivalent circuit consisting of thermal resistors/capacitors and heat sources

T == nodal voltage

I == branch current



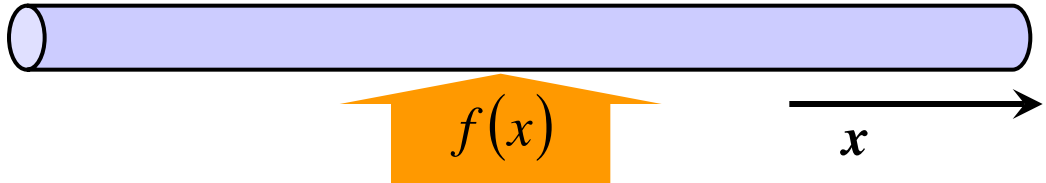
Finite Difference Method

$$I_{i,j,k} = C \cdot \frac{\partial T_{i,j,k}}{\partial t} + G_x \cdot [T_{i,j,k} - T_{i+1,j,k}] + G_x \cdot [T_{i,j,k} - T_{i-1,j,k}] \\ G_y \cdot [T_{i,j,k} - T_{i,j+1,k}] + G_y \cdot [T_{i,j,k} - T_{i,j-1,k}] + G_z \cdot [T_{i,j,k} - T_{i,j,k+1}] + G_z \cdot [T_{i,j,k} - T_{i,j,k-1}]$$

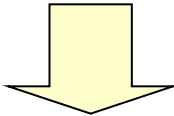
- The operator $\partial/\partial t$ can be handled by numerical integration
 - ▼ We need to solve a large-scale linear equation to find $T_{i,j,k}(t_n)$ at each time point t_n
- Generally interested only in steady state – thermal capacitance is not considered

1-D Thermal Analysis Example

- 1-D PDE to describe the steady-state temperature distribution along a uniform rod at $[0, 1]$

$$T(x,0) = T_{Init}$$
$$T(x=0,t) = T(x=1,t) = 0$$


$$\rho \cdot C_p \cdot \frac{\partial T(x,t)}{\partial t} = \kappa \cdot \frac{\partial^2 T(x,t)}{\partial x^2} + f(x,t)$$

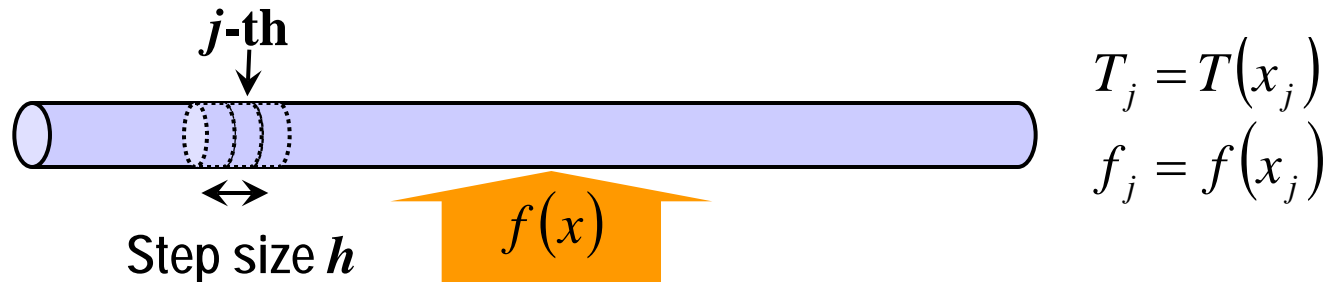
Steady state 

$$\frac{\partial T(x,t)}{\partial t} = 0$$

$$-\kappa \cdot T_{xx}(x) = f(x) \quad (0 < x < 1)$$

1-D Thermal Analysis Example

- Approximate 2nd order derivative using finite difference



$$T(x=0, t) = T(x=1, t) = 0 \quad -\kappa \cdot T_{xx}(x) = f(x) \quad T_{xx}(x_j) = \frac{T_{j+1} + T_{j-1} - 2T_j}{h^2}$$

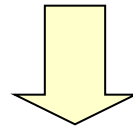
$$\kappa \cdot (-T_{j-1} + 2T_j - T_{j+1}) = h^2 \cdot f_j \quad (1 \leq j \leq N-1)$$
$$T_0 = T_N = 0$$

1-D Thermal Analysis Example

- The linear system is:

$$\kappa \cdot (-T_{j-1} + 2T_j - T_{j+1}) = h^2 \cdot f_j \quad (1 \leq j \leq N-1)$$

$$T_0 = T_N = 0$$



$$\kappa \cdot (-0 + 2T_1 - T_2) = h^2 \cdot f_1$$

$$\kappa \cdot (-T_1 + 2T_2 - T_3) = h^2 \cdot f_2$$

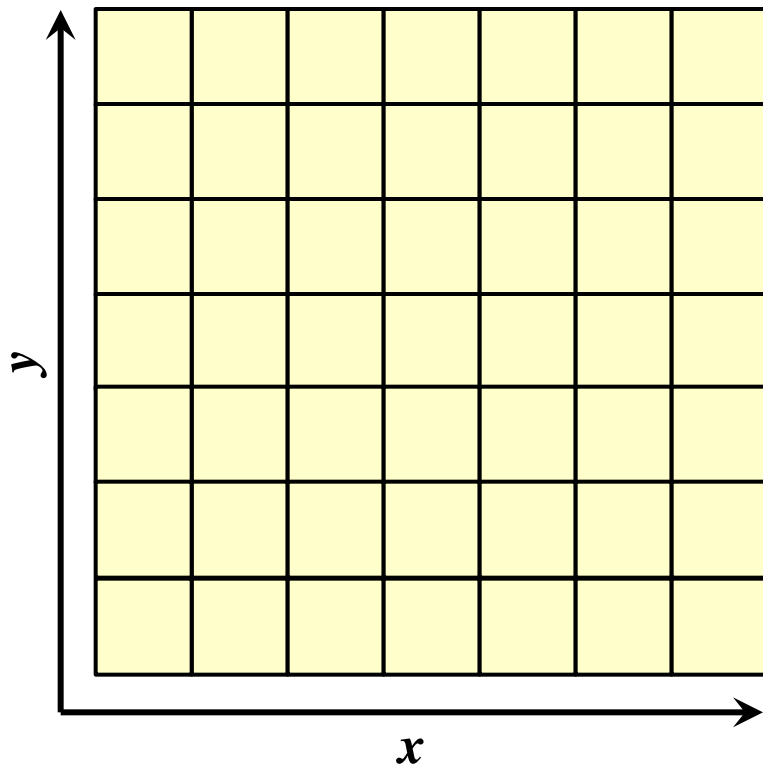
⋮

$$\kappa \cdot (-T_{N-2} + 2T_{N-1} - 0) = h^2 \cdot f_{N-1}$$

Solve linear equation to determine T_1, T_2, \dots, T_{N-1}

2-D Thermal Analysis Example

- 2-D PDE to describe the steady-state temperature distribution over a uniform plane $x, y \in [0, 1]$



$$T(x, y, 0) = T_{Init}$$

$$T(x = 0, t) = T(x = 1, t) = 0$$

$$T(y = 0, t) = T(y = 1, t) = 0$$

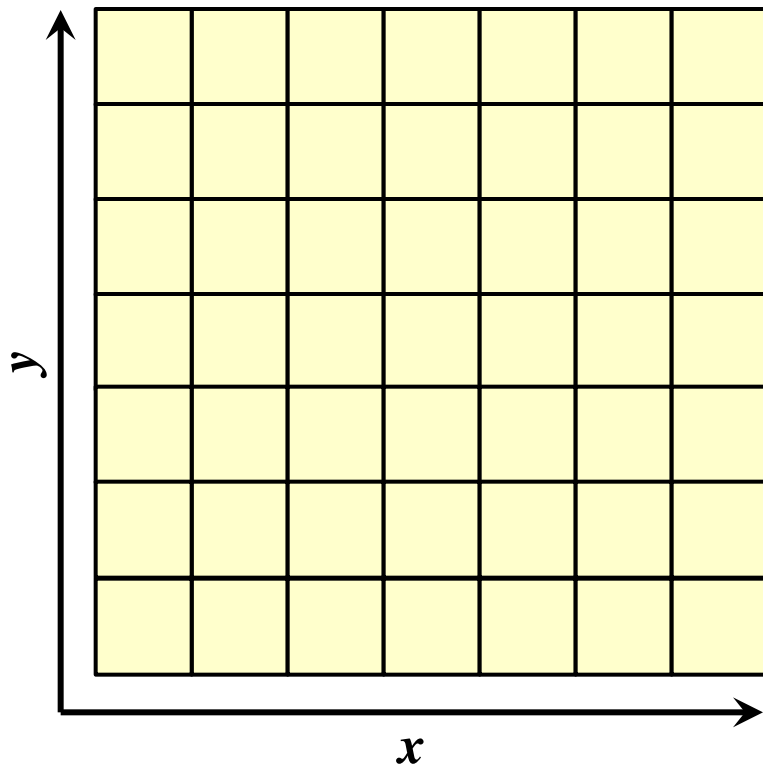
$$\rho \cdot C_p \cdot \frac{\partial T}{\partial t} = \kappa \cdot \left(\frac{\partial T^2}{\partial x^2} + \frac{\partial T^2}{\partial y^2} \right) + f(x, y, t)$$

Steady state \Downarrow $\frac{\partial T}{\partial t} = 0$

$$-\kappa \cdot (T_{xx} + T_{yy}) = f(x, y) \quad (0 < x, y < 1)$$

2-D Thermal Analysis Example

- Approximate 2nd order derivative using finite difference



$$T(x = 0, t) = T(x = 1, t) = 0$$

$$T(y = 0, t) = T(y = 1, t) = 0$$

$$-\kappa \cdot (T_{xx} + T_{yy}) = f(x, y)$$

$$T_{i,j} = T(x_i, y_j)$$

$$f_{i,j} = f(x_i, y_j)$$

$$T_{xx}(x_i, y_j) = \frac{T_{i+1,j} + T_{i-1,j} - 2T_{i,j}}{h^2}$$

$$T_{yy}(x_i, y_j) = \frac{T_{i,j+1} + T_{i,j-1} - 2T_{i,j}}{h^2}$$

2-D Thermal Analysis Example

- The linear system is:

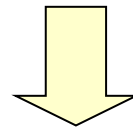
$$T(x=0, t) = T(x=1, t) = 0$$

$$T(y=0, t) = T(y=1, t) = 0$$

$$-\kappa \cdot (T_{xx} + T_{yy}) = f(x, y)$$

$$T_{xx}(x_i, y_j) = \frac{T_{i+1,j} + T_{i-1,j} - 2T_{i,j}}{h^2}$$

$$T_{yy}(x_i, y_j) = \frac{T_{i,j+1} + T_{i,j-1} - 2T_{i,j}}{h^2}$$



$$\kappa \cdot (-T_{i-1,j} + 2T_{i,j} - T_{i+1,j} - T_{i,j-1} + 2T_{i,j} - T_{i,j+1}) = h^2 \cdot f_{i,j} \quad T_{i,j} \text{ NOT at boundary}$$

$$T_{i,j} = 0 \quad T_{i,j} \text{ at boundary}$$

Solve linear equation to determine all temperature values

Thermal Analysis

- Thermal analysis generally requires to solve a large-scale linear equation

$$A \cdot X = B$$

- The matrix A is **symmetric** and **diagonally dominant**

$$A_{ij} = A_{ji} \quad \text{For all matrix elements}$$

$$|A_{ii}| \geq \sum_{j=1, j \neq i}^N |A_{ij}| \quad \text{For all diagonal elements}$$

Thermal Analysis

- A matrix "A" is **positive definite**, if
 - ▼ A is symmetric *and*
 - ▼ A is diagonally dominant *and*
 - ▼ All diagonal elements of A are non-negative *and*
 - ▼ A is not singular
 - ▼ *Sufficient* but *NOT necessary* condition

- Definition of positive definite matrix

$$P^T \cdot A \cdot P > 0 \quad \text{for any real-valued vector } P \neq 0$$

All eigenvalues of A are positive

Thermal Analysis

- Positive definite linear equation $AX = B$ can be solved by efficient numerical algorithms
 - ▼ Cholesky decomposition
 - ▼ Conjugate gradient method
 - ▼ Etc.

- We will try to cover some of these efficient algorithms in future lectures

Summary

- Thermal analysis
 - ▼ 2-D / 3-D heat equation
 - ▼ Finite difference