Carnegie Mellon

18-660: Numerical Methods for Engineering Design and Optimization

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Electrical & Computer ENGINEERING

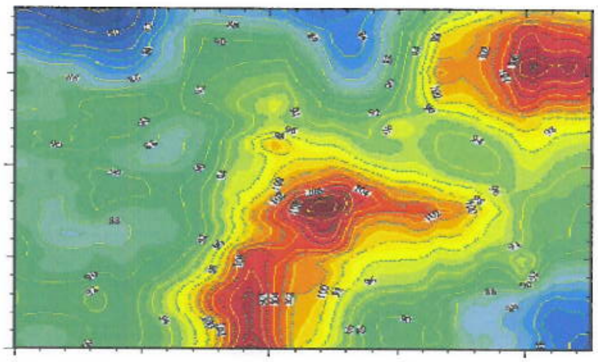
Overview

- Partial Differential Equation (PDE)
  - Heat equation
  - Boundary condition

Partial Differential Equation (PDE)

- **Partial differential equation is often used to describe a physical system or process**

- **Example: heat equation is an PDE for thermal analysis**
  - We will derive heat equation step by step in this lecture



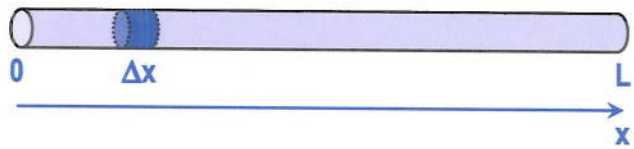
Heat Equation

- **Heat equation can be derived from several fundamental physics laws**
  - Fourier's law
  - Conservation of heat
  - Etc.

- **We will use a 1-D example to illustrate heat equation**
  - Help to get many insights about heat transfer process

1-D Heat Model

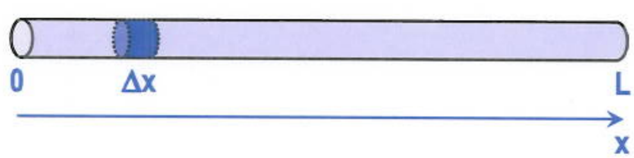
- We consider a 1-D rod of length L



- Three major assumptions
  - Rod is made of a single homogenous conducting material
  - Rod is laterally insulated (heat flows only in the x-direction)
  - Rod is thin (constant temperature at all points of a cross section)

Conservation of Heat

- Apply conservation of heat to the segment $[x, x+\Delta x]$

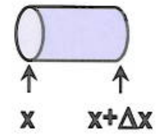


Net change of heat inside $[x, x+\Delta x]$ = Net flux of heat across boundaries + Total heat generated inside $[x, x+\Delta x]$

We will look at each of these three components in detail

Conservation of Heat

Net change of heat inside [x, x+Δx] = Net flux of heat across boundaries + Total heat generated inside [x, x+Δx]



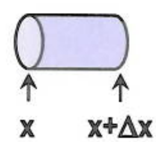
- Total heat inside [x, x+Δx] is equal to:

$$\int_{x}^{x+\Delta x} \rho \cdot C_p \cdot A \cdot T(s,t)\,ds$$

ρ: density
C_p: thermal Capacity
A: cross-section Area
T: temperature
s: x-Coordinate
t: time

Conservation of Heat

Net change of heat inside [x, x+Δx] = Net flux of heat across boundaries + Total heat generated inside [x, x+Δx]



- Net change of heat is equal to:

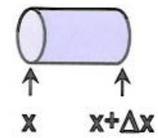
$$\frac{d}{dt}\left[\int_{x}^{x+\Delta x} \rho \cdot C_p \cdot A \cdot T(s,t)\,ds\right] \qquad \Delta x \to 0$$

$$= \frac{d}{dt}\left[\rho \cdot C_p \cdot A \cdot T(x,t) \cdot \Delta x\right]$$

$$= \rho \cdot C_p \cdot A \cdot \Delta x \cdot \frac{dT(x,t)}{dt}$$

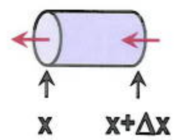
Conservation of Heat

Net change of heat inside [x, x+Δx] = **Net flux of heat across boundaries** + **Total heat generated inside [x, x+Δx]**



- **Fourier's law: heat flux across a boundary is proportional to the temperature gradient across the boundary:**

$$K \cdot A \cdot \frac{dT(x,t)}{dx}$$

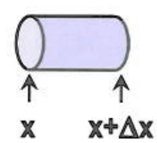


$$K \cdot A \cdot \frac{dT(x+\Delta x, t)}{dx}$$

K: thermal conductivity

Conservation of Heat

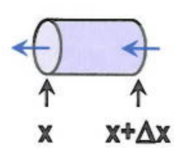
Net change of heat inside [x, x+Δx] = **Net flux of heat across boundaries** + **Total heat generated inside [x, x+Δx]**



- **Net flux of heat across boundaries is equal to:**

$$\kappa \cdot A \cdot \frac{\partial T(x,t)}{\partial x}$$

Heat flux at x



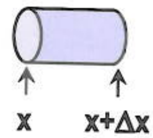
$$\kappa \cdot A \cdot \frac{\partial T(x+\Delta x,t)}{\partial x}$$

Heat flux at x+Δx

$$K \cdot A \cdot \frac{dT(x+\Delta x, t)}{dx} - K \cdot A \cdot \frac{dT(x,t)}{dx}$$

Conservation of Heat

Net change of heat inside [x, x+Δx] = Net flux of heat across boundaries + Total heat generated inside [x, x+Δx]



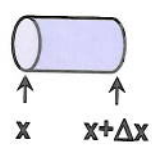
- Total heat generated inside [x, x+Δx] is equal to:

$$\int_{x}^{x+\Delta x} A \cdot f(s,t)\,ds$$

f: heat source

1-D Heat Equation

Net change of heat inside [x, x+Δx] = Net flux of heat across boundaries + Total heat generated inside [x, x+Δx]



- Overall, we have:

$$\rho \cdot C_p \cdot \cancel{A} \cdot \Delta x \cdot \frac{\partial T(x,t)}{\partial t} = \kappa \cdot \cancel{A} \cdot \left[\frac{\partial T(x+\Delta x,t)}{\partial x} - \frac{\partial T(x,t)}{\partial x} \right] + \int_{x}^{x+\Delta x} \cancel{A} \cdot f(s,t) \cdot ds$$

1-D Heat Equation

$$\rho \cdot C_p \cdot \frac{\partial T(x,t)}{\partial t} = \kappa \cdot \frac{1}{\Delta x}\left[\frac{\partial T(x+\Delta x,t)}{\partial x} - \frac{\partial T(x,t)}{\partial x}\right] + \frac{1}{\Delta x} \cdot \int_x^{x+\Delta x} f(s,t) \cdot ds$$

$\Delta x \to 0$

$$\rho \cdot C_p \cdot \frac{dT(x,t)}{dt} = k \cdot \frac{d^2 T(x,t)}{dx^2} + f(x,t)$$

$$\rho \cdot C_p \cdot T_t(x,t) = k \cdot T_{xx}(x,t) + f(x,t)$$

Partial Differential Equation (PDE)

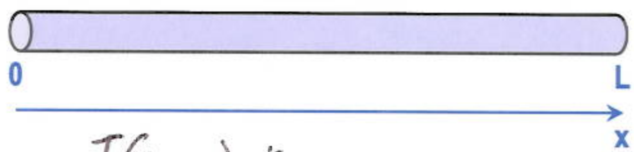
$$\rho \cdot C_p \cdot T_t(x,t) = \kappa \cdot T_{xx}(x,t) + f(x,t)$$

- T (which we differentiate) is called the **dependent variable**
- t and x (which we differentiate with respect to) are called **independent variables**
- In addition to this PDE, we further need to know the boundary and initial conditions to uniquely determine T(x,t)

Boundary Conditions

- Boundary conditions describe the physical nature of our problem on the boundaries

- A simple example
  - Rod temperature is fixed at the two ends



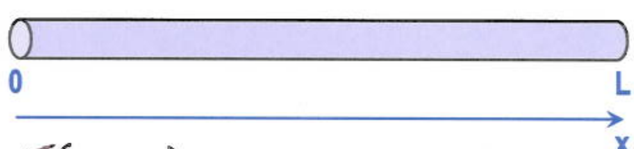
$T(x=0,t)=T_1$

$T(x=L,t)=T_2$

Initial Conditions

- Initial conditions describe the physical phenomenon at the beginning of the thermal transfer process

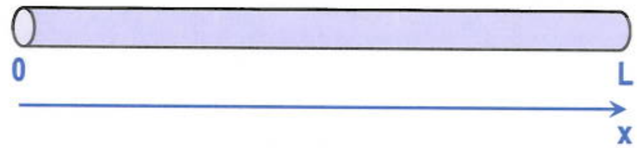
- A simple example
  - Rod is initially at an equilibrium point – constant temperature



$T(x,t=0)=T_0$

1-D Heat Equation

- The complete PDE with boundary and initial conditions



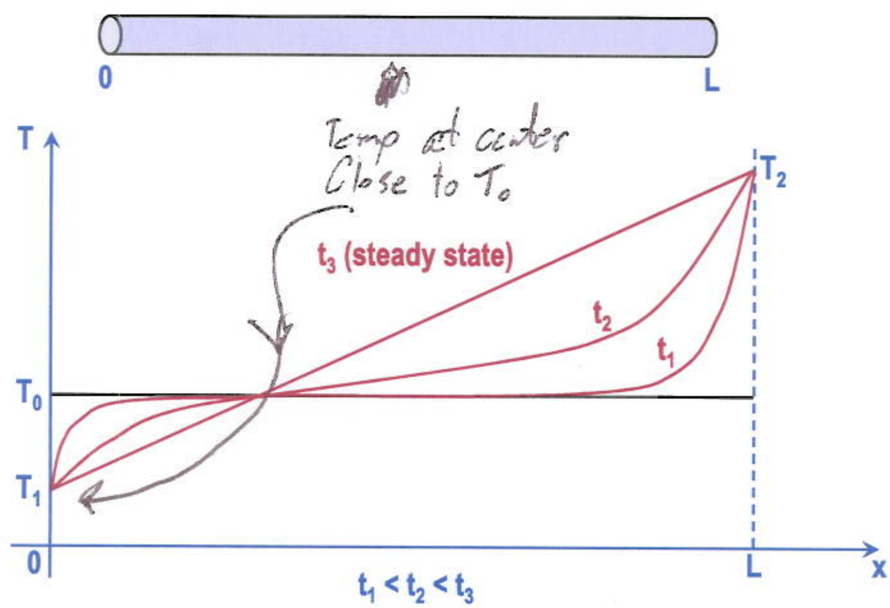
PDE $\rho \cdot C_p \cdot T_t(x,t) = \kappa \cdot T_{xx}(x,t) + f(x,t) \quad (0 \le x \le L \quad 0 \le t \le \infty)$

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

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

1-D Heat Equation

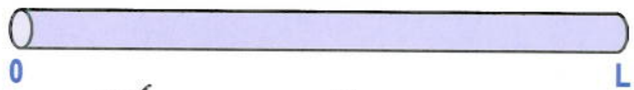
- The solution of this PDE can be analytically calculated



Boundary Conditions

- There are many ways to specify boundary conditions

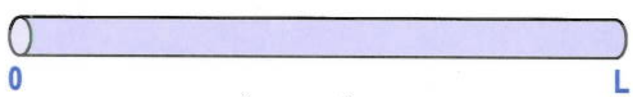
- Option 1: temperature is specified on boundaries



$$T(x=0,t)=g_1(t)$$
$$T(x=L,t)=g_2(t)$$

Boundary Conditions

- The BCs used for our 1-D rod belongs to this category

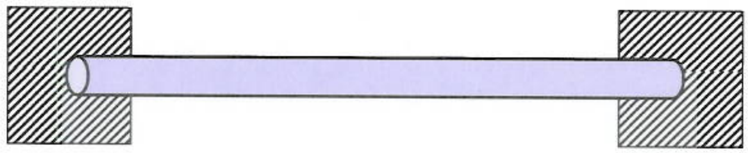


$$T(x=0,t)=T_1$$
$$T(x=L,t)=T_2$$

- Practically useful to force the temperature to behave in a suitable manner
  - E.g., boundary control in steel industry

Boundary Conditions

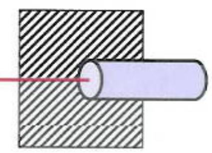
- **Option 2: temperature of the surrounding medium is specified**



  - Newton's law: heat flux across the boundary is proportional to the temperature difference

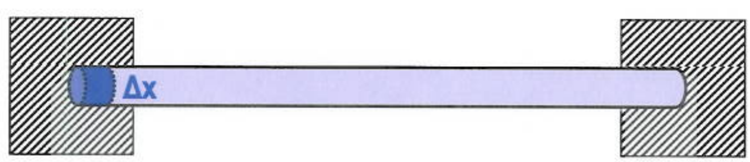
$h \cdot A \cdot [T(x=0,t) - g_1(t)]$

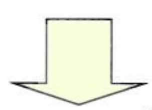
h: heat exchange coefficient



Boundary Conditions

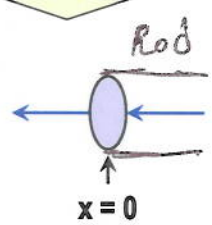
- **Consider Newton's and Fourier's laws at x = 0**





$h \cdot A \cdot [T(x=0,t) - g_1(t)]$

Newton's Law



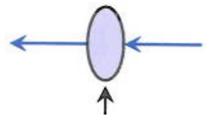
$k \cdot A \cdot \frac{\partial T(x,t)}{dx} \Big|_{x=0}$

Fourier's Law

Boundary Conditions

$h \cdot A \cdot [T(x=0,t) - g_1(t)]$

Heat flux at x = 0
(Newton's law)



$\kappa \cdot A \cdot \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0}$

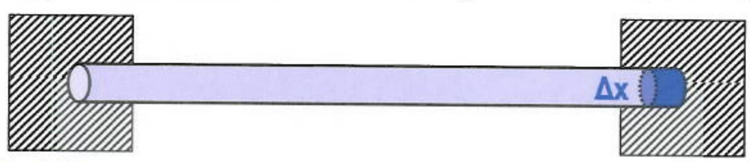
Heat flux at x = 0
(Fourier's law)

- **Apply conservation of heat flux to the boundary x = 0**

$$\kappa \cdot \cancel{A} \cdot \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = h \cdot \cancel{A} \cdot [T(x=0,t) - g_1(t)]$$

Boundary Conditions

- **Similarly, we can derive the boundary condition at x = L**



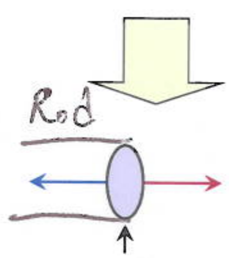
Liquid kept at temperature $g_1(t)$

Liquid kept at temperature $g_2(t)$

$k \cdot A \cdot \left.\frac{dT(x,t)}{dx}\right| X=L$

Fourier's Law

Rod



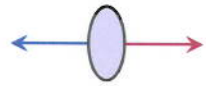
$h \cdot A \cdot [T(x=L,t) - g_2(t)]$

Newton's Law

Boundary Conditions

$$\kappa \cdot A \cdot \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=L}$$

Heat flux at x = L
(Fourier's law)



x = L

$$h \cdot A \cdot [T(x=L,t) - g_2(t)]$$

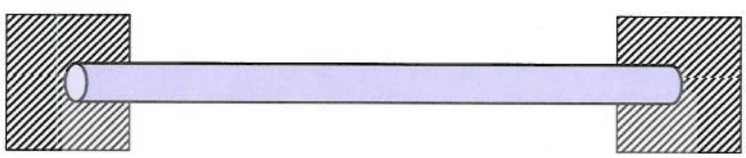
Heat flux at x = L
(Newton's law)

- **Apply conservation of heat flux to the boundary x = L**

$$\kappa \cdot \cancel{A} \cdot \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=L} = -h \cdot \cancel{A} \cdot [T(x=L,t) - g_2(t)]$$

Boundary Conditions

- **Option 2: temperature of the surrounding medium is specified**



Liquid kept at temperature $g_1(t)$

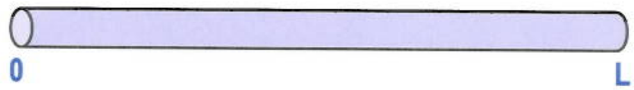
Liquid kept at temperature $g_2(t)$

$$\kappa \cdot \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = h \cdot [T(x=0,t) - g_1(t)]$$

$$\kappa \cdot \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=L} = -h \cdot [T(x=L,t) - g_2(t)]$$

Boundary Conditions

- **Option 3: heat flow across the boundaries is specified**

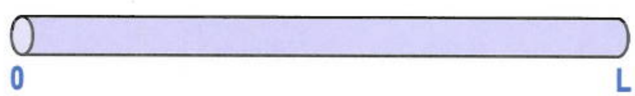


$$\frac{dT(x,t)}{dx}\bigg|_{x=0} = g_1(t)$$

$$\frac{dT(x,t)}{dx}\bigg|_{x=L} = g_2(t)$$

Boundary Conditions

- **Insulated boundaries (also referred to as reflective boundaries)**
  - No heat passes through boundaries



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

$$\frac{\partial T(x,t)}{\partial x}\bigg|_{x=L} = 0$$

Summary

- **Partial differential equation (PDE)**
  - Heat equation
  - Boundary condition

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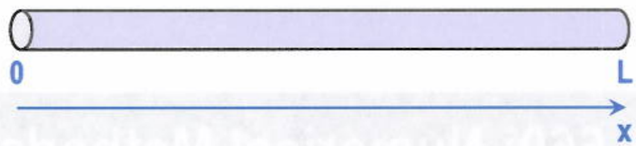
Electrical & Computer ENGINEERING

Overview

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

1-D Heat Equation

- The complete PDE with boundary and initial conditions



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

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

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

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**

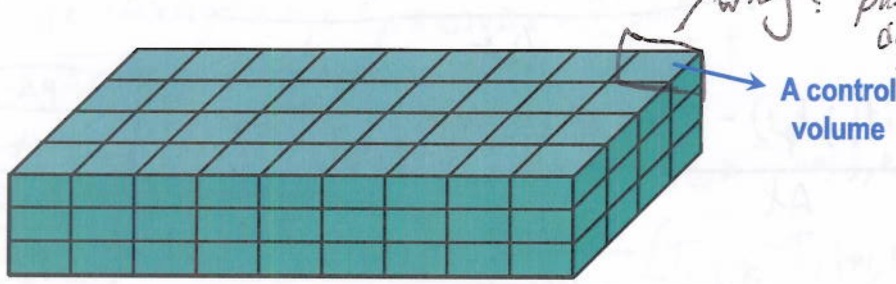
- **Homogeneity**
  - Homogenous if f(x,y,z,t) = 0
  - Non-homogenous if f(x,y,z,t) ≠ 0

Finite Difference Method

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

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

why? partial derivative of algebraic equations



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

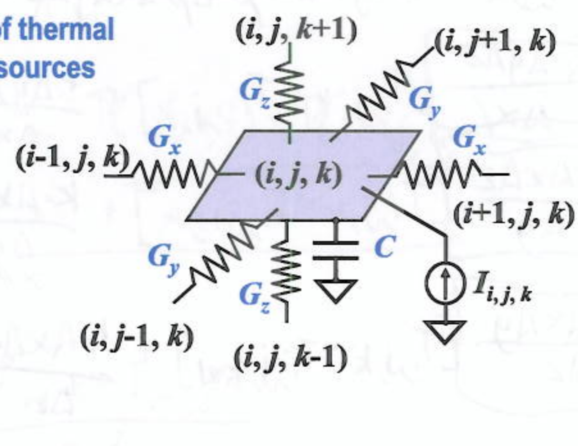
Finite Difference Method

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

Equivalent circuit consisting of thermal resistors/capacitors and heat sources

T == nodal voltage

I == branch current



Finite Difference Method

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

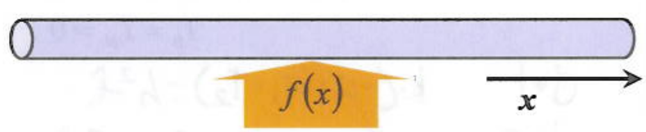
- **The operator ∂/∂t can be handled by numerical integration**
  - We need to solve a large-scale linear equation to find $T_{i,j,k}(t_n)$ at each time point t_n

- **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]**

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



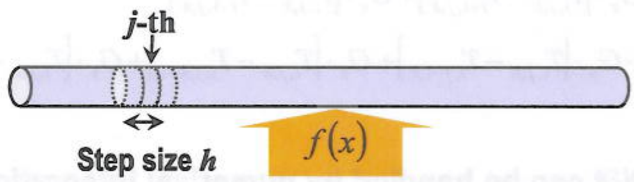
$$\rho \cdot C_p \cdot \frac{\partial T(x,t)}{\partial t} = \kappa \cdot \frac{\partial T^2(x,t)}{\partial x^2} + f(x,t)$$

steady state $\frac{dT(x,t)}{dt} = 0$

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

1-D Thermal Analysis Example

- **Approximate 2nd order derivative using finite difference**



$$T_j = T(x_j)$$
$$f_j = f(x_j)$$

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

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

$$-k \cdot [T_{j+1} + T_{j-1} - 2T_j] = h^2 \cdot f_j$$

$$T_0 = T_N = 0$$

1-D Thermal Analysis Example

- **The linear system is:**

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

$j=1 \quad k \cdot (-0 + 2T_1 - T_2) = h^2 f_1$

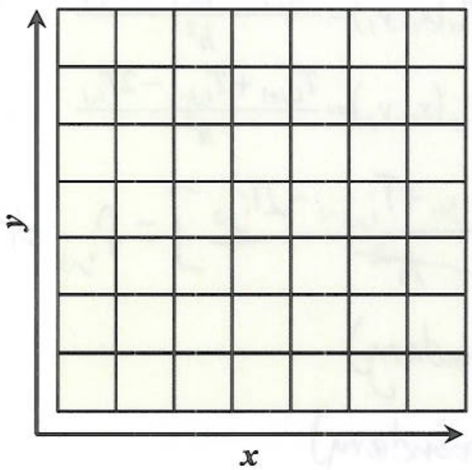
$j=2 \quad k \cdot (-T_1 + 2T_2 - T_3) = h^2 f_2$

$j=N-1 \quad k \cdot (-T_{N-2} + 2T_{N-1}) = h^2 \cdot f_{N-1}$

$T_1, T_2, T_3 \ldots T_{N-1}$

2-D Thermal Analysis Example

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



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

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

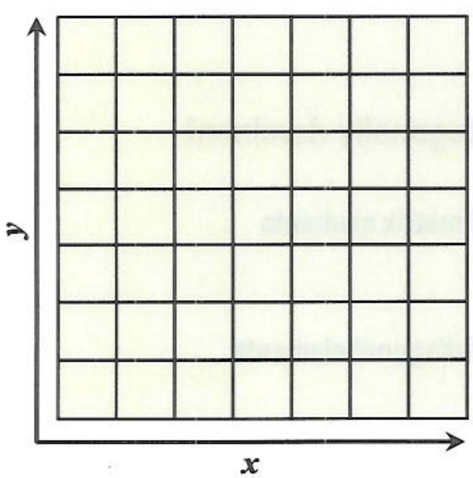
Steady state $\frac{dT}{dt}=0$

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

$(0<x,y<1)$

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:**

$$T(x=0,t)=T(x=1,t)=0 \qquad T_{xx}(x_i,y_j)=\frac{T_{i+1,j}+T_{i-1,j}-2T_{i,j}}{h^2}$$

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

$$-\kappa\cdot(T_{xx}+T_{yy})=f(x,y) \qquad T_{yy}(x_i,y_j)=\frac{T_{i,j+1}+T_{i,j-1}-2T_{i,j}}{h^2}$$

$$-k\left[\frac{T_{i+1,j}+T_{i-1,j}-2T_{i,j}}{\cancel{h^2}}+\frac{T_{i,j+1}+T_{i,j-1}-2T_{i,j}}{\cancel{h^2}}\right]=f_{i,j}\cdot h^2$$

(Not at boundary)

$T_{i,j}=0$ (at boundary)

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**

$A_{ij}=A_{ji}$ **For all matrix elements**

$|A_{ii}|\ge \sum_{j=1,j\ne i}^{N}|A_{ij}|$ **For all diagonal elements**

Thermal Analysis

- **1-D thermal analysis example**

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

$$T_0 = T_N = 0$$

$$\begin{array}{l} j=1 \\ j=2 \\ \\ \\ \\ \end{array} \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{N-1} \end{bmatrix} = \frac{h^2}{\kappa} \begin{bmatrix} f_1 \\ \vdots \\ \vdots \\ \vdots \\ f_{N-1} \end{bmatrix}$$

symmetric
diagonally dominant

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**

$P^T \cdot A \cdot P > 0$ **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