CHN-323
Computer Applications in Chemical Engineering

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Boundary value problem (BVP)

- Diffusion followed by 1st order Rxn in a Slab

$$\frac{d^2y}{dx^2} - y = 0$$

- Boundary conditions

1. $\frac{dy}{dx} = 0$ at $x = 0$
2. $y = 1$ at $x = 1$

Finite Difference Method

- <u>Key idea</u>:

  Convert the ODE's and boundary conditions into a set of algebraic equations (linear or nonlinear) using Numerical differentiation formulas.

  Solve the resulting algebraic equation system using the methods studied earlier.

Steps

- Step 1: Break the solution domain into equal sized sub-domains using equidistant grid points.

Steps

- Step 2: Replace the derivatives in the ODE's and B.C.'s by appropriate finite difference approximations.
  - In doing so, make sure that the truncation error of all approximations are of the same order
  - This converts the DAE system into an algebraic system.

- Step 3: Set up the algebraic equation system and solve it

Numerical differentiation formula

- Finite-difference approximations provide a means to transform derivatives into algebraic form

Forward Difference Formula (1st order accurate)

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

Backward Difference Formula (1st order accurate)

$$f'(x) = \frac{f(x) - f(x-h)}{h}$$

Centered Difference Formula (2nd order accurate)

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

Centered Difference Formula for 2nd Derivative (2nd order accurate)

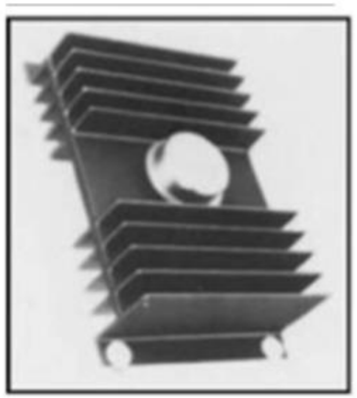
$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

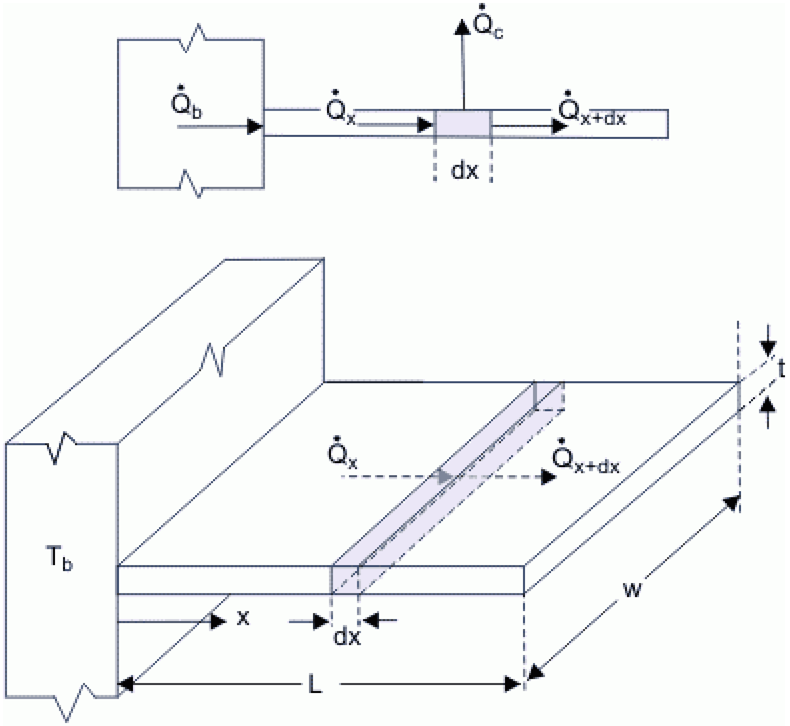
First Derivative		
Method	**Formula**	**Truncation Error**
Two-point forward difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Three-point forward difference	$f'(x_i) = \dfrac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$
Two-point backward difference	$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Three-point backward difference	$f'(x_i) = \dfrac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$	$O(h^2)$
Two-point central difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$

Second Derivative		
Method	**Formula**	**Truncation Error**
Three-point forward difference	$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2}$	$O(h)$
Four-point forward difference	$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{h^2}$	$O(h^2)$
Three-point backward difference	$f''(x_i) = \dfrac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2}$	$O(h)$
Four-point backward difference	$f''(x_i) = \dfrac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Three-point central difference	$f''(x_i) = \dfrac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2}$	$O(h^2)$

Example

- Heat transfer through a fin
- https://web.mit.edu/16.unified/www/FALL/thermodynamics/notes/node128.html





Example: fin

- Equation governing the heat transfer in the fin

$$\frac{d^2\theta}{d\xi^2} - \frac{hPL^2}{kA}\theta = 0$$

- Boundary conditions:

$$\theta(\xi = 0) = 1; \theta(\xi = 1) = 0$$

$$\theta = \frac{T - T_\infty}{T_0 - T_\infty}$$

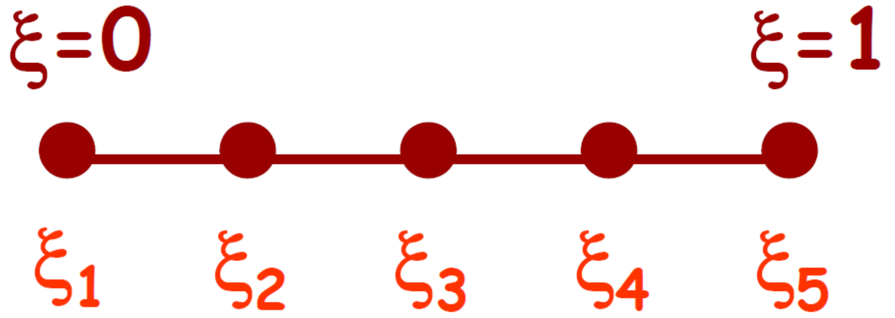
- Let $\frac{hPL^2}{kA} = 1$. This gives

$$\frac{d^2\theta}{d\xi^2} - \theta = 0$$

Example: fin

$$\frac{d^2\theta}{d\xi^2} - \theta = 0$$

- Divide the fin into 5 equispaced nodes
- 5 grid points; 3 internal grid points; 2 boundary grid points
- For internal grid points



$$\frac{\theta_{i+1} - 2\theta_i + \theta_{i-1}}{\Delta\xi^2} - \theta_i = 0$$

$$\Delta\xi = 1/4$$

$$\theta_{i+1} - 2\theta_i + \theta_{i-1} - 0.0625\theta_i = 0$$

We know that $\theta_1 = 1, \theta_5 = 0$

$$\theta_{i-1} - 2.0625\theta_i + \theta_{i+1} = 0$$

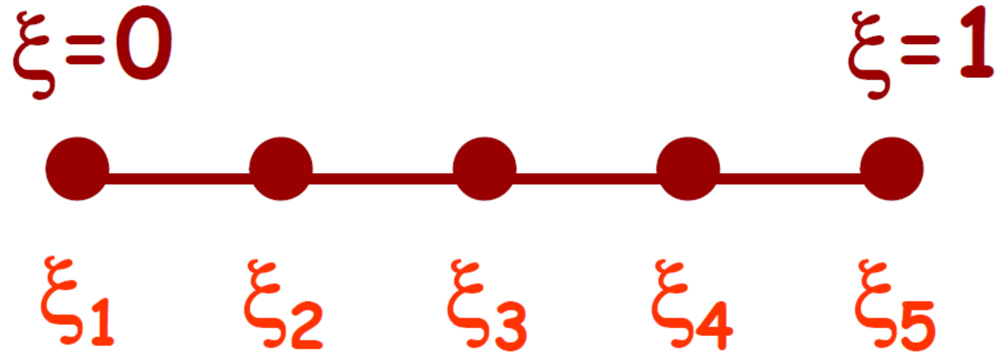
Example: fin

$$\theta_{i-1} - 2.0625\theta_i + \theta_{i+1} = 0$$

$\theta_1 - 2.0625\theta_2 + \theta_3 = 0$ (for node 2)

$\theta_2 - 2.0625\theta_3 + \theta_4 = 0$ (for node 3)

$\theta_3 - 2.0625\theta_4 + \theta_5 = 0$ (for node 4)



$\Delta\xi = 1/4$

We know that $\theta_1 = 1, \theta_5 = 0$

$$-2.0625\theta_2 + \theta_3 = -1$$

$$\theta_2 - 2.0625\theta_3 + \theta_4 = 0$$

$$\theta_3 - 2.0625\theta_4 = 0$$

Example: fin

$$\begin{bmatrix} -2.0625 & 1 & 0 \\ 1 & -2.0625 & 1 \\ 0 & 1 & -2.0625 \end{bmatrix} \begin{bmatrix} \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}$$

A tridiagonal structure

Example 2

- Heat Transfer through a variable Cross section area Fin

$$A(\xi)\frac{d^2\theta}{d\xi^2}+\frac{dA(\xi)}{d\xi}\frac{d\theta}{d\xi}-\frac{hPL^2}{k}\theta=0$$

$$\theta\left(\xi=0\right)=1;\quad \left.\frac{d\theta}{d\xi}\right|_{\xi=1}=0$$

$$Let\ \frac{hPL^2}{k}=2$$ **and $A(\xi) = 5 - 4\xi$**