CHN-323

Computer Applications in Chemical Engineering

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Gauss-Jordon method

- Key idea: Converting the coefficient matrix to the identity matrix

Example:

$$
\begin{aligned}
x_1+2x_2-x_3-2x_4 &= -1\\
2x_1+x_2+x_3-x_4 &= 4\\
10x_1-5x_2+2x_3+x_4 &= 5\\
-x_1+5x_2-2x_3-3x_4 &= -3
\end{aligned}
$$

Example

$$\left[\begin{array}{cccc|c} 1 & 2 & -1 & -2 & -1 \\ 2 & 1 & 1 & -1 & 4 \\ 10 & -5 & 2 & 1 & 5 \\ -1 & 5 & -2 & -3 & -3 \end{array}\right] \to \left[\begin{array}{cccc|c} 1 & 2 & -1 & -2 & -1 \\ 0 & -3 & 3 & 3 & 6 \\ 0 & -25 & 12 & 21 & 15 \\ 0 & 7 & -3 & -5 & -4 \end{array}\right]$$

$$\left[\begin{array}{cccc|c} 1 & 2 & -1 & -2 & -1 \\ 0 & 1 & -1 & -1 & -2 \\ 0 & -25 & 12 & 21 & 15 \\ 0 & 7 & -3 & -5 & -4 \end{array}\right] \to \left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & -1 \\ 0 & 1 & -1 & -1 & -2 \\ 0 & 0 & -13 & -4 & -35 \\ 0 & 0 & 4 & 2 & 10 \end{array}\right]$$

Example

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & -1 \\ 0 & 1 & -1 & -1 & -2 \\ 0 & 0 & 1 & 4/13 & 35/13 \\ 0 & 0 & 4 & 2 & 10 \end{array}\right] \to \left[\begin{array}{cccc|c} 1 & 0 & 0 & -4/13 & 4/13 \\ 0 & 1 & 0 & -9/13 & 9/13 \\ 0 & 0 & 1 & 4/13 & 35/13 \\ 0 & 0 & 0 & 10/13 & -10/13 \end{array}\right]$$

$$\left[\begin{array}{cccc|c} 1 & 0 & 0 & -4/13 & 4/13 \\ 0 & 1 & 0 & -9/13 & 9/13 \\ 0 & 0 & 1 & 4/13 & 35/13 \\ 0 & 0 & 0 & 1 & -1 \end{array}\right] \to \left[\begin{array}{cccc|c} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 3 \\ 0 & 0 & 0 & 1 & -1 \end{array}\right] \Rightarrow x = \begin{bmatrix} 0 \\ 0 \\ 3 \\ -1 \end{bmatrix}$$

Tridiagonal systems

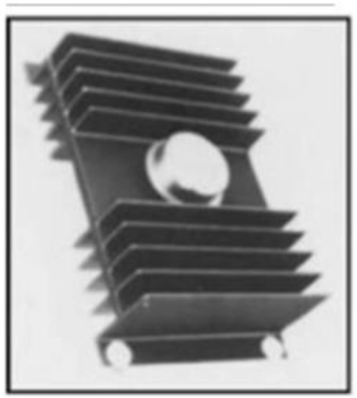
$$
\begin{aligned}
2x_1 - x_2 \qquad\qquad\qquad &= -1 \\
-x_1 + 2x_2 - x_3 \qquad\quad &= 0 \\
-x_2 + 2x_3 - x_4 &= 0 \\
-x_3 + 2x_4 &= 0
\end{aligned}
$$

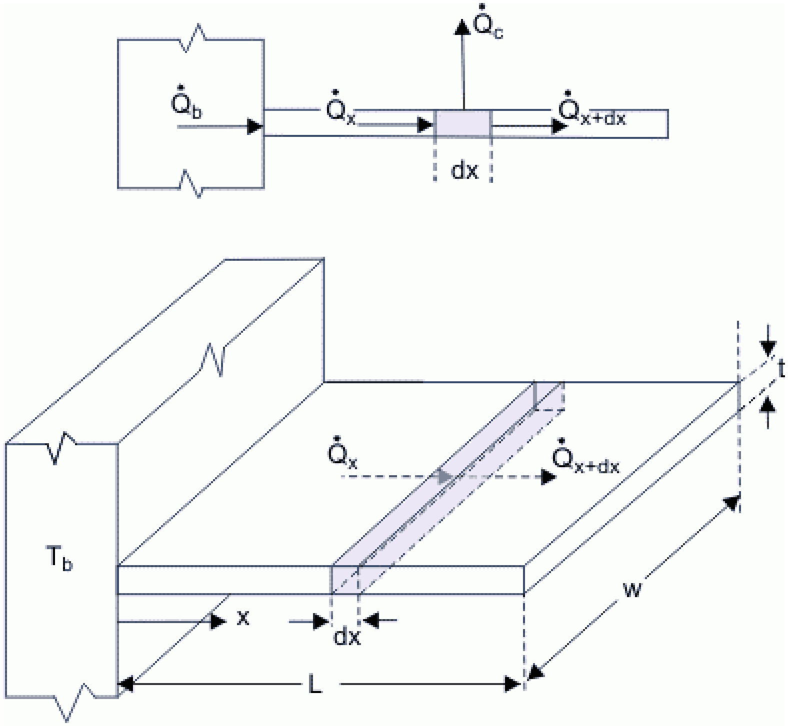
Coefficient matrix

$$A=\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$$

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:

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

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

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

Example: fin

- 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)

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

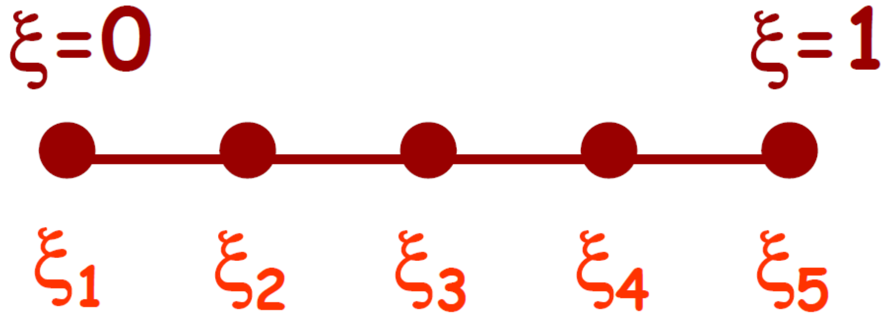
Centered Difference Formula for 2nd Derivative (2nd order accurate)

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

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 $\theta_1 = 1, \theta_5 = 0$

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

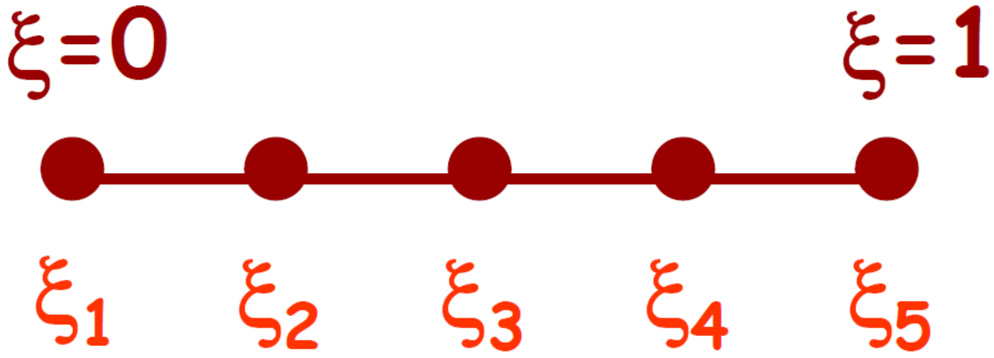
Example: fin

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

$\theta_1 - 2.0625\theta_2 + \theta_3 = 0$ (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

Solving tridiagonal systems

$$
\begin{aligned}
&b_1x_1+c_1x_2 &&= d_1\\
&a_2x_1+ b_2x_2 +c_2x_3 &&= d_2\\
&\qquad a_3x_2+ b_3x_3 +c_3x_4 &&= d_3\\
&\qquad\qquad \ddots\\
&a_{n-1}x_{n-2}+ b_{n-1}x_{n-1} +c_{n-1}x_n &&= d_{n-1}\\
&\qquad a_nx_{n-1}+b_nx_n &&= d_n
\end{aligned}
$$

Sparse systems

Solving tridiagonal systems

- Coefficient of x_1 is nonzero only in Eq. 2
- If x_1 is eliminated from eq. 2, eq. 2 will look like

$$b'_2 x_2 + c'_2 x_3 = d'_2$$

- Same structure as Eq. 1, only two unknowns

- Thus, at stage elimination, we will work with only two equations (of this form)

$$x_k + h_k x_{k+1} = p_k \quad \text{(Eq. A)}$$

$$a_{k+1} x_k + b_{k+1} x_{k+1} + c_{k+1} x_{k+2} = d_{k+1} \quad \text{(Eq. B)}$$

- After eliminating x_k from Eq. B, it will look like

$$x_{k+1} + h_{k+1} x_{k+2} = p_{k+1}$$

Solving tridiagonal systems

- Can we represent h_{k+1} and p_{k+1} in terms of b_{k+1}, d_{k+1}, c_{k+1}, a_{k+1}, h_k and p_k?

- Multiply Eq. A by a_{k+1} and subtract it from Eq. B

$$(b_{k+1}-a_{k+1}h_k)x_{k+1} + c_{k+1}x_{k+2} = d_{k+1} - a_{k+1}p_k$$

$$x_{k+1} + \frac{c_{k+1}}{b_{k+1} - a_{k+1} h_k} x_{k+2} = \frac{d_{k+1} - a_{k+1} p_k}{b_{k+1} - a_{k+1} h_k}$$

Thus, $h_{k+1} = \dfrac{c_{k+1}}{b_{k+1} - a_{k+1} h_k}$ **&** $p_{k+1} = \dfrac{d_{k+1} - a_{k+1} p_k}{b_{k+1} - a_{k+1} h_k}$

Solving tridiagonal systems

- The system will now look like

$$x_k + h_k x_{k+1} = p_k \quad (\text{for } k = 1,2,3,\ldots.,n-1)$$

$$x_n = p_n \quad (\text{for } k = n)$$

- We can now work backwards to get

$$x_k = p_k - h_k x_{k+1} \quad (\text{for } k = n-1,\ldots.,3,2,1)$$

Note that x_{k+1} is already known so that all RHS terms are all available during the computation of x_k from the above equation