Numerical Analysis ~~in Mechanical Eng~~ for Eng. Appls.

$Ax = b$

Linear diff'l eqs.
Nonlinear " "
Steady diff'l eqs
Unsteady " "

Numerical $\Longrightarrow$ methods

System of algebraic eqs. (linear or nonlinear)

computer / numerical methods

Answers

$x = A^{-1}b$?

$\boxed{\text{Stability}} \leftrightarrow \boxed{\text{Precision, Cost}}$

Ch. 0 Linear Algebra

- Matrix-matrix multiplication

$$\underset{m\times n}{A} \quad \underset{n\times l}{B} \longrightarrow \underset{m\times l}{C} = AB$$

matrix elements $c_{ij} = a_{ik} b_{kj}$

$i = 1, 2, \cdots, m$
$j = 1, 2, \cdots, l$
$k = 1, 2, \cdots, n$

Let the columns of B be denoted $\underset{n\times 1}{\underline{b}^1}, \underline{b}^2, \underline{b}^3, \cdots, \underline{b}^l$

$$AB = [A\underline{b}^1, A\underline{b}^2, \cdots, A\underline{b}^l]$$

<u>Operation counts</u>

$A\underline{b}^1$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & & \cdots & a_{2n} \\ \vdots & & & & \vdots \\ a_{m1} & a_{m2} & & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

multiplications: $m \times n$

additions: $(n-1) \times m$

if $m = n$, $\Theta(n^2)$ operations are required.

$\underset{m \times n \quad n \times l}{A \quad B} \longrightarrow$ $m \times n \times l$ multiplications

$m \times (n-1) \times l$ additions

if $m = n = l$, $\Theta(n^3)$ operations.

ex) $n = 500 \rightarrow n^3 = 1.25 \times 10^8$

Intel Itanium 2 → 300 MFlops ↓ floating-point operation per second

≀

CRAY C90 3×10^8 operations/sec

For AB, $t = \frac{1.25 \times 10^8}{3 \times 10^8} \simeq 0.3$ sec

in mid 1980's, IBM PC → 8000 Flops ⇒ $t \doteq 4$ hrs.

NEC SX5 → 3G Flops → $t \simeq 0.03$ sec

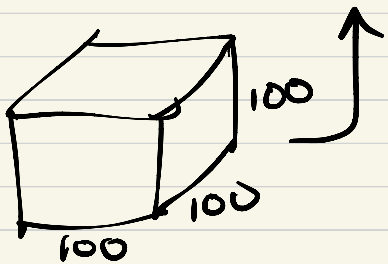
GAIA 1536 cores → 23.370 T Flops → $t = 0.5 \times 10^{-5}$ sec

GPU Nvidia A100 → 20 TFlops

CPU AMD Ryzen Threadripper 3990X

→ 3 TFlops → $t = 4 \times 10^5$ sec.

How about $n = 10^6$ → $n^3 = 10^{18}$



Intel Itanium 2 → $t = \dfrac{10^{18}}{3 \times 10^8} \simeq 10^6$ hrs

NEC SX5 → $t = 10^5$ hrs → 10^9 KW

(1M Korean Won for 100 CPU hrs)

GAIA $t = \dfrac{10^{18}}{23.37 \times 10^{12}} \simeq 42$ sec.

⇒ **Matrix-matrix multiplication is a very expensive job!**

$Ax = b$

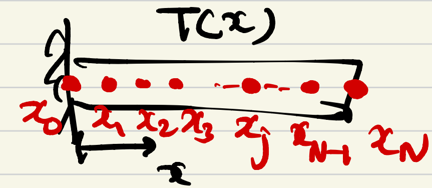
$x = A^{-1} b$

AB

- **Banded matrix**

diff'l eq $\xrightarrow[\text{method}]{\text{numerical}}$ system of algebraic eqs.

◎ ODE (ordinary diff'l eq)



$$\boxed{\frac{d^2T}{dx^2} - a^2T = Q(x)}$$

Introduce $\underbrace{\text{a discrete set of points}}_{\text{grid pts.}}$ x_j $\quad j = 0, 1, 2, \cdots, N$

Find $T(x_j)$ or T_j

finite difference method (FDM)

Taylor series expansion $\quad h_j = x_{j+1} - x_j$: grid spacing

$h_1 = h_2 = \cdots = h$: uniform grid spacing

$$T(x_{j+1}) = T(x_j) + h\frac{dT}{dx}\Big|_j + \frac{1}{2}h^2\frac{d^2T}{dx^2}\Big|_j + \frac{1}{6}h^3\frac{d^3T}{dx^3}\Big|_j + \frac{1}{24}h^4\frac{d^4T}{dx^4}\Big|_j + \cdots$$

$$-\ \ T(x_{j-1}) = \ '' \ - \ '' \ + \ '' \ - \ '' \ + \ '' \ + \cdots$$

$$T(x_{j+1}) - T(x_{j-1}) = 2h\frac{dT}{dx}\Big|_j + \frac{1}{3}h^3\frac{d^3T}{dx^3}\Big|_j + \cdots$$

$$\Rightarrow \boxed{\frac{dT}{dx}\Big|_j = \frac{T(x_{j+1}) - T(x_{j-1})}{2h}} \underbrace{- \frac{1}{6}h^2\frac{d^3T}{dx^3}\Big|_j}_{\text{leading error term}} + \cdots$$

FDM

$$\left(\frac{dT}{dx} = \lim_{\Delta x\to 0}\frac{T(x+\Delta x) - T(x)}{\Delta x}\right)$$

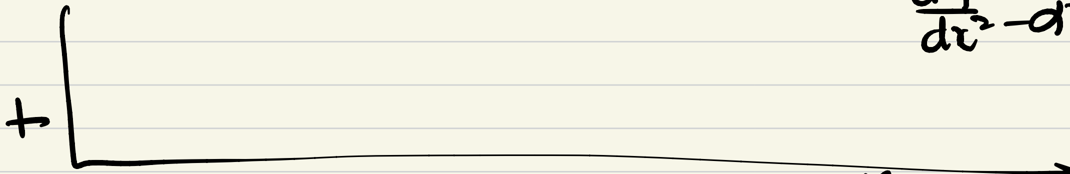
$O(h^2)$

Second-order FDM

$$\boxed{\frac{dT}{dx}\Big|_j = \frac{T(x_{j+1}) - T(x_j)}{h}} - \frac{1}{2}h\frac{d^2T}{dx^2}\Big|_j + \cdots$$

first-order FDM

$$\frac{d^2T}{dx^2} - \alpha T = Q$$



$$T(x_{j+1}) + T(x_{j-1}) = 2T(x_j) + h^2 \frac{d^2T}{dx^2}\Big|_j + \frac{1}{12} h^4 \frac{d^4T}{dx^4}\Big|_j + \cdots$$

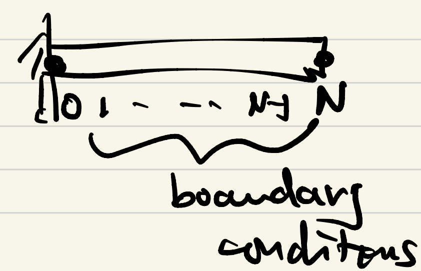
$$\Rightarrow \boxed{\frac{d^2T}{dx^2}\Big|_j = \frac{T(x_{j+1}) - 2T(x_j) + T(x_{j-1})}{h^2}} - \frac{1}{12} h^2 \frac{d^4T}{dx^4}\Big|_j + \cdots$$

second-order FDM

leading error term $O(h^2)$

→ substitute this to diff'l eq.

@ j, $\begin{cases} \dfrac{T_{j+1} - 2T_j + T_{j-1}}{h^2} - \alpha T_j = Q_j \\ T_0 = 0 \\ T_N = S \end{cases}$ $\quad j = 1, 2, \cdots, N-1$



$$\frac{d^2T}{dx^2} - \alpha^2 T = Q(x)$$

$$\begin{cases} \dfrac{T_{j+1} - 2T_j + T_{j-1}}{h^2} - \alpha^2 T_j = Q_j, \quad j = 1, 2, \cdots, N-1 \\ T_0 = 0 \\ T_N = S \end{cases}$$

System of algebraic eqs.

$$\rightarrow \begin{cases} T_{j+1} - (2 + h^2\alpha^2) T_j + T_{j-1} = h^2 Q_j \\ T_0 = 0 \\ T_N = S \end{cases}$$

$j=1$: $T_2 - (2+h^2\alpha^2) T_1 + T_0 = h^2 Q_1$, $T_0 = 0$

$j=2$: $T_3 -$ " $T_2 + T_1 = h^2 Q_2$

$\vdots$

$j=N-1$: $T_N -$ " $T_{N-1} + T_{N-2} = h^2 Q_{N-1}$, $T_N = S$

$$\begin{bmatrix} -(2+h^2\alpha^2) & 1 & 0 & \cdots & 0 \\ 1 & -(2+h^2\alpha^2) & 1 & 0 \cdots & 0 \\ & & \vdots & & \\ 0 \cdots 0 & 1 & -(2+h^2\alpha^2) & 1 & 0 \cdots 0 \\ & & & \ddots & \\ & & & 1 & -(2+h^2\alpha^2) \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_j \\ \vdots \\ T_{N-1} \end{bmatrix} = \begin{bmatrix} h^2 Q_1 \\ h^2 Q_2 \\ \vdots \\ h^2 Q_j \\ \vdots \\ h^2 Q_{N-1} - \varsigma \end{bmatrix}$$

tri-diagonal matrix $\quad \underline{A}x = b$

banded matrix : non-zero elements only around the main diagonal

↳ arises from FDM of diff'l eqs.

tri-diagonal matrix : $B[a_i, b_i, c_i]$

$$a_i = 1, \quad b_i = -(2+h^2\alpha^2), \quad c_i = 1$$

banded matrix $\longleftrightarrow$ sparse matrix

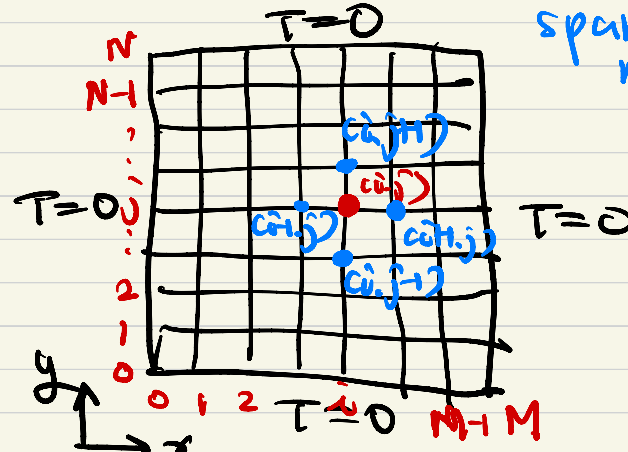
$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}$$

≠ sparse matrix

② PDE (partial diff'l eq.)

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = Q(x, y)$$

$$\left.\begin{aligned} \Delta x_i &= x_{i+1} - x_i = h \\ \Delta y_j &= y_{j+1} - y_j = h \end{aligned}\right\} \text{ uniform grid spacings}$$



2nd-order FDM

$$\boxed{\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{h^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{h^2} = Q_{i,j}}$$

$i = 1, 2, \cdots, M-1$

$j = 1, 2, \cdots, N-1$

$$\rightarrow T_{i+1,j} - 4T_{i,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} = h^2 Q_{i,j}$$

$$\begin{pmatrix} M=4 \\ N=4 \end{pmatrix}$$

$$i=1, j=1 : \; T_{2,1} - 4T_{1,1} + \underbrace{T_{0,1}}_{=0} + T_{1,2} + \underbrace{T_{1,0}}_{=0} = h^2 Q_{1,1}$$

$$i=2, j=1 : \; T_{3,1} - 4T_{2,1} + T_{1,1} + T_{2,2} + \underbrace{T_{2,0}}_{=0} = h^2 Q_{2,1}$$

$$\vdots$$

$$i=3, j=3 : \; \underbrace{T_{4,3}}_{=0} - 4T_{3,3} + T_{2,3} + \underbrace{T_{3,4}}_{=0} + T_{3,2} = h^2 Q_{3,3}$$

9 unknowns

$T_{1,1}$ --- $T_{3,3}$

$$\left[\begin{array}{ccc|ccc|ccc}
-4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\
\hline
1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\
\hline
0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4
\end{array}\right]
\begin{bmatrix} T_{1,1} \\ T_{2,1} \\ T_{3,1} \\ T_{1,2} \\ T_{2,2} \\ T_{3,2} \\ T_{3,1} \\ T_{3,2} \\ T_{3,3} \end{bmatrix}
=
\begin{bmatrix} h^2 Q_{1,1} \\ h^2 Q_{2,1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ h^2 Q_{3,3} \end{bmatrix}$$

Block-tridiagonal matrix

$$\begin{pmatrix} B_1 & C_1 & 0 & & 0 \\ A_2 & B_2 & C_2 & 0 & \\ 0 & A_3 & B_3 & C_3 & \\ 0 & & \ddots & \ddots & \ddots \end{pmatrix}$$

⊙ Solution technique

- diagonal matrix

$$\begin{pmatrix} 7 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

- upper triangular matrix

$$\begin{pmatrix} 1 & 2 & 3 \\ 0 & 4 & 5 \\ 0 & 0 & 6 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 8 \\ 9 \end{pmatrix}$$

- lower triangular matrix

$$\begin{pmatrix} 1 & 0 & 0 \\ 2 & 3 & 0 \\ 4 & 5 & 6 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 8 \\ 9 \end{pmatrix}$$

* Gauss elimination (GE) : to make upper triangular matrix

$$\begin{cases} 4x_2 - x_3 = 5 \\ x_1 + x_2 + x_3 = 6 \\ 2x_1 - 2x_2 + x_3 = 1 \end{cases} \rightarrow \begin{pmatrix} 0 & 4 & -1 \\ 1 & 1 & 1 \\ 2 & -2 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 5 \\ 6 \\ 1 \end{pmatrix}$$

Interchange the first two rows

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 4 & -1 \\ 2 & -2 & 1 \end{pmatrix} \begin{pmatrix} \\ \\ \\ \end{pmatrix} = \begin{pmatrix} 6 \\ 5 \\ 1 \end{pmatrix}$$

Subtract twice the first row from last row :

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 4 & -1 \\ 0 & -4 & -1 \end{pmatrix} \begin{pmatrix} \\ \\ \\ \end{pmatrix} = \begin{pmatrix} 6 \\ 5 \\ -11 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 & 1 \\ 0 & 4 & -1 \\ 0 & 0 & -2 \end{pmatrix} \begin{pmatrix} \\ \\ \\ \end{pmatrix} = \begin{pmatrix} 6 \\ 5 \\ -6 \end{pmatrix}$$

Stop GE.

upper triangular matrix

or, augmented matrix

$$\left(\begin{array}{ccc|c} 0 & 4 & -1 & 5 \\ 1 & 1 & 1 & 6 \\ 2 & -2 & 1 & 1 \end{array}\right) \xrightarrow{GE} \begin{pmatrix} 1 & 1 & 1 & 6 \\ 0 & 4 & -1 & 5 \\ 0 & 0 & -2 & -6 \end{pmatrix}$$

$$\to \begin{pmatrix} 1 & 1 & 1 & 6 \\ 0 & 4 & 0 & 8 \\ 0 & 0 & -2 & -6 \end{pmatrix} \to \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 3 \end{pmatrix}$$

$\to x_1 = 1,\ x_2 = 2,\ x_3 = 3$

Gauss - Jordan elimination

- General matrix system

$Ax = b$
$n \times n$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \times \frac{a_{21}}{a_{11}}$$

GE

0

To eliminate a_{21}, $l_2 = a_{21}/a_{11}$.
Multiply the first row by l_2, and subtract from 2nd row.
Continue until all elts below a_{11} are eliminated.

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22}' & \cdots & a_{2n}' \\ 0 & & & \\ \vdots & & & \\ 0 & a_{n2}' & \cdots & a_{nn}' \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2' \\ \vdots \\ b_n' \end{pmatrix}$$

By same way (we drop (′) for convenience)

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ & & \ddots & \vdots \\ & & & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Stop GE.

$\longrightarrow$ backward sweep

$$\begin{cases} x_n = b_n / a_{nn} \\ x_{n-1} = (b_{n-1} - a_{n-1\,n} x_n) / a_{n-1\,n-1} \\ x_j = \left(b_j - \sum_{k=j+1}^{n} a_{jk} x_k\right) / a_{jj} \end{cases}$$

$j = n-1, n-2, \ldots, 1$

* Operation counts for obtaining sol. of $Ax=b$

$Ax=b$ $\qquad$ A : full matrix

$$\ell = \frac{a_{21}}{a_{11}} \times \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & & a_{2n} \\ \vdots & & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

GE To eliminate a_{21} : 1 D, n M, n A

To " the first column : $(n-1)$ D, $n(n-1)$ M, $n(n-1)$ A

To " " 2nd " : $(n-2)$ D, $(n-2)(n+1)$ M, $(n-2)(n+1)$ A

$\vdots$

To " " $(n-1)^{th}$ " : 1 D, $1\cdot 2$ M, $1\cdot 2$ A

Total divisions : $\sum_{k=1}^{n-1} k = \frac{1}{2}n(n-1)$

" multiplications: additions $\sum_{k=1}^{n-1} k(k+1) = \frac{1}{3}(n^3-n)$

$\sum_{1}^{n} k^2 = \frac{1}{6}n(n+1)(2n+1)$

$\Rightarrow \frac{1}{2}n(n-1)\,D, \quad \frac{1}{3}(n^3-n)\,M, \quad \frac{1}{3}(n^3-n)\,A$ $\qquad \Theta(n^3)$

$\boxed{\text{Gauss elimination requires } \Theta(n^3/3)\,!}$

Backward sweep

$$x_n = b_n / a_{nn}$$

$$x_j = \Big(b_j - \sum_{k=j+1}^{n} a_{jk} x_k\Big) / a_{jj}, \quad j = n-1, n-2, \dots, 1$$

for each j, $\quad 1\,D, \ (n-j)M, \ (n-j)\,A$

total $\displaystyle\sum_{j=1}^{n-1} (n-j) = \frac{1}{2}n(n-1)\ A, \ M$ $\quad \Theta(n^2)$

$n\,D$

negligible as compared to GE requiring $\Theta(n^3)$ for $n \gg 1$.

* Gauss–Jordan elimination requires same operation counts.