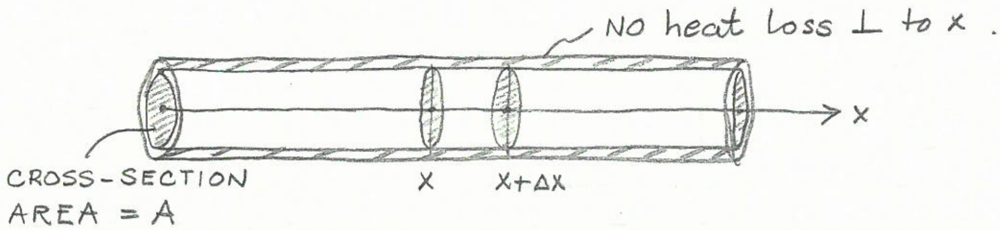
ILLUSTRATION USING THE ONE-DIMENSIONAL HEAT EQUATION :



"u" = temperature , "q_x" = heat flux (due to conduction) $\frac{J}{m^2 \cdot s}$

Rate of Heat Accumulation in CONTROL VOLUME between X AND X + ΔX	=	HEAT FLOW RATE IN	−	HEAT FLOW RATE OUT

$$\frac{\partial}{\partial t}\left(\rho C_p A \Delta x\, u\right) = q_x A - q_{x+\Delta x} A$$

$$\frac{1}{s}\cdot\frac{\cancel{kg}}{\cancel{m^3}}\cdot\frac{J}{\cancel{kg}\,°K}\cdot\cancel{m^3}\cdot °K \qquad\qquad \frac{J}{\cancel{m^2}\cdot s}\,\cancel{m^2}$$

DIFFERENTIAL CONTROL VOLUME ANALYSIS :

$$q_{x+\Delta x} = q_x + \frac{\partial q_x}{\partial x}\Delta x$$

$$\rho C_p \cancel{A \Delta x}\frac{\partial u}{\partial t} = -\frac{\partial q_x}{\partial x}\cancel{A\Delta x}$$

$q_x = -k\frac{\partial u}{\partial x}$: FOURIER'S LAW OF HEAT CONDUCTION. $\frac{\partial u}{\partial x}$ = THERMAL GRADIENT

k - THERMAL CONDUCTIVITY $\frac{J}{°K\,m\,s}$

$$\rho C_p\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}, \quad \text{OR WITH } b = \frac{k}{\rho C_p} \text{ THERMAL DIFFUSIVITY } \left(\frac{m^2}{s}\right)$$

$$\boxed{\frac{\partial u}{\partial t} - b\frac{\partial^2 u}{\partial x^2} = 0}$$

SECOND ORDER (PARABOLIC) PARTIAL DIFFERENTIAL EQUATION

x = SPACE , t = TIME

CONSIDER FINITE ROD , $0 \le x \le L$

Auxiliary conditions for Heat eqn. in one dimension $\frac{\partial u}{\partial t} - b\frac{\partial^2 u}{\partial x^2} = 0$

First-order in t : one auxiliary condition - INITIAL CONDITION (I.C.)

$$u(x, t=0) = u_0(x)$$

Second-order in x : two auxiliary conditions - BOUNDARY CONDITIONS (B.C.)

TYPES OF B.C. :

FIRST TYPE (DIRICHLET) : Value of u is specified at the boundary

e.g. $u(x=0, t) = T_1(t)$, $u(x=L, t) = T_2(t)$

SECOND TYPE (NEUMANN OR FLUX) : Heat flux is specified at the boundary

e.g. $-k\frac{\partial u}{\partial x}(x=0, t) = q_1(t)$ or $-k\frac{\partial u}{\partial x}(x=0, t) = q_2(t)$

e.g. insulated boundary, $-k\frac{\partial u}{\partial x} = 0 \Rightarrow \frac{\partial u}{\partial x} = 0$.

THIRD TYPE (ROBIN) : temperature-dependent flux at the boundary

e.g. heat is lost at $x=L$ to a well-mixed atmosphere at a rate proportional to the temperature difference between the rod and the atmosphere.

$$-k\frac{\partial u}{\partial x}(x=L, t) = \underbrace{h}_{\text{"Heat transfer coefficient"}}\big(u(L,t) - \overbrace{u_{atm}}^{\text{specified}}\big)$$

can be written in the general form: $c_1 u(L,t) + c_2 \frac{\partial u}{\partial x}(L,t) = f(t)$

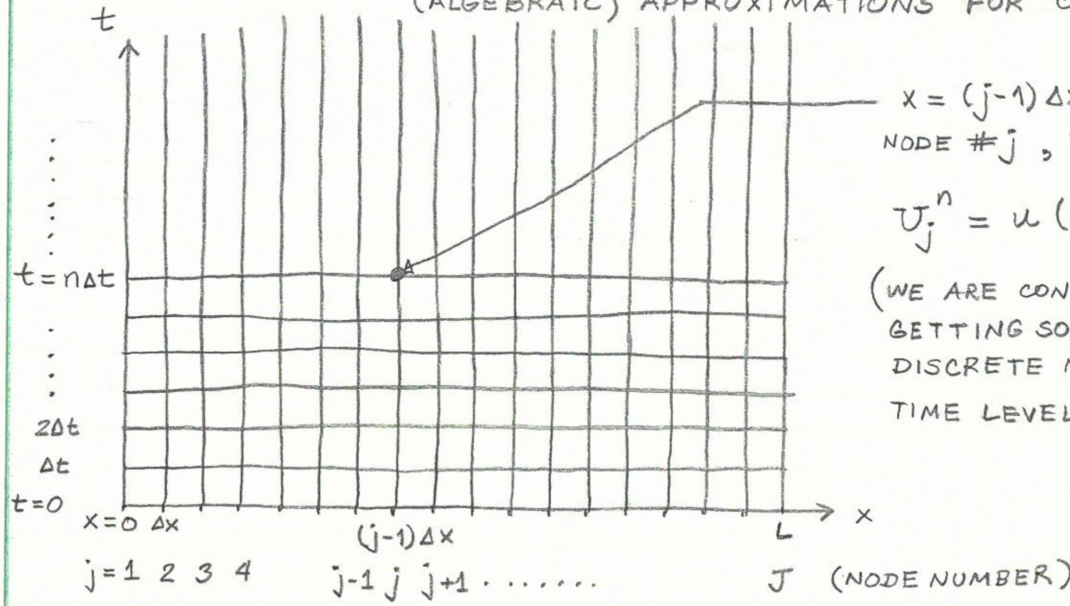
("MIXED" B.C.) not flux, some function

$\Rightarrow$ $\frac{\partial u}{\partial t} - b\frac{\partial^2 u}{\partial x^2} = 0$, $u(x,0) = u_0(x)$ has a unique solution if there are well-defined B.C. at each end $x=0$ & $x=L$. These can be of any of the 3 types listed above.

- Sometimes, we need to solve the heat eqn. in a semi-infinite domain, i.e. $L \to \infty$ or "large", we are interested in the behavior over some distance from $x=0$. For numerical solution in such cases, need to specify an artificial B.C. at some large distance (e.g. no flux)

NUMERICAL SOLUTION OF THE HEAT EQUATION : FINITE DIFFERENCE METHOD

ESSENCE OF FDM : REPLACE DERIVATIVES WITH FINITE-DIFFERENCE (ALGEBRAIC) APPROXIMATIONS FOR COMPUTATION.



$x = (j-1)\Delta x$, $t = n\Delta t$

NODE #j , TIME LEVEL n

$$U_j^n = u(x,t)$$

(WE ARE CONTENT WITH GETTING SOLUTION AT DISCRETE NODES AND TIME LEVELS)

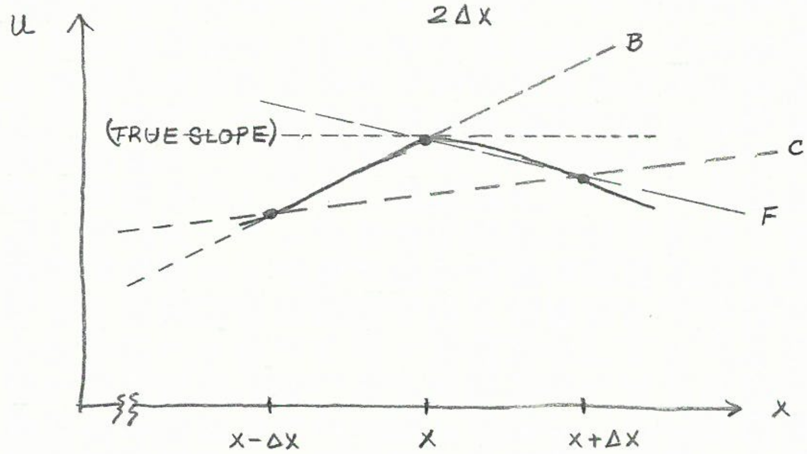
- ALGEBRAIC EQUATIONS TO SOLVE FOR U_j^n's ?
- APPROXIMATING SPATIAL DERIVATIVES USING DIFFERENCE APPROXIMATIONS.

FIRST DERIVATIVE : $\dfrac{\partial u}{\partial x}$ ... INTUITIVELY ... SLOPE

$$\frac{\partial u}{\partial x}(x) \cong \frac{u(x+\Delta x) - u(x)}{\Delta x} \quad \text{(FORWARD)}$$

$$\frac{u(x) - u(x-\Delta x)}{\Delta x} \quad \text{(BACKWARD)}$$

$$\frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} \quad \text{(CENTERED)}$$



ACCURACY OF APPROXIMATIONS : TAYLOR SERIES EXPANSIONS

$$u(x+\Delta x) = u(x) + \frac{\partial u}{\partial x}(x)\cdot\Delta x + \frac{\partial^2 u}{\partial x^2}(x)\cdot\frac{\Delta x^2}{2!} + \frac{\partial^3 u}{\partial x^3}(x)\cdot\frac{\Delta x^3}{3!} + \cdots$$

$$u(x-\Delta x) = \;'' \; + \;'' \;(-\Delta x) + \;'' \;\frac{(-\Delta x)^2}{2!} + \;'' \;\frac{(-\Delta x)^3}{3!} + \cdots$$

$$\frac{u(x+\Delta x) - u(x)}{\Delta x} = \frac{\partial u}{\partial x}(x) + \frac{\partial^2 u}{\partial x^2}(x)\cdot\frac{\Delta x}{2!} + \cdots$$

WHAT WE WANT — TRUNCATION ERROR — $O(\Delta x)$

$$\frac{u(x) - u(x-\Delta x)}{\Delta x} = \frac{\partial u}{\partial x}(x) - \frac{\partial^2 u}{\partial x^2}(x)\cdot\frac{\Delta x}{2!} + \cdots$$

$$\frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} = \frac{\partial u}{\partial x}(x) + 2\,\frac{\partial^3 u}{\partial x^3}(x)\cdot\frac{\Delta x^2}{3!}$$

$O(\Delta x^2)$! HIGHER-ORDER ACCURACY.

(... CAN ALSO USE MORE THAN TWO POINT VALUES)

HEAT EQN. HAS SECOND DERIVATIVE : $\frac{\partial^2 u}{\partial x^2}$ – FINITE-DIFFERENCE APPROX.?

$\longrightarrow$ "CURVATURE" : AT LEAST 3 POINT VALUES.

$$? \quad \frac{\partial^2 u}{\partial x^2}(x) \cong \alpha\, u(x-\Delta x) + \beta\, u(x) + \gamma\, u(x+\Delta x)$$

DETERMINE α, β, γ COEFFICIENTS FROM TAYLOR SERIES EXP.

$$\alpha\, u(x-\Delta x) = \alpha\left(u(x) - \frac{\partial u}{\partial x}\Delta x + \frac{\partial^2 u}{\partial x^2}\frac{\Delta x^2}{2!} - \frac{\partial^3 u}{\partial x^3}\frac{\Delta x^3}{3!} + \frac{\partial^4 u}{\partial x^4}\frac{\Delta x^4}{4!} + \cdots\right.$$

$$\beta\, u(x) = \beta \quad u(x)$$

$$\gamma\, u(x+\Delta x) = \gamma\left(\;'' + \;'' + \;'' + \;'' + \;'' + \cdots\right.$$

$$\text{SUM} = (\alpha+\beta+\gamma)\,u(x) + (\gamma-\alpha)\frac{\partial u}{\partial x}\Delta x + (\gamma+\alpha)\frac{\partial^2 u}{\partial x^2}\frac{\Delta x^2}{2!} + (\gamma-\alpha)\frac{\partial^3 u}{\partial x^3}\frac{\Delta x^3}{3!} + (\gamma+\alpha)\frac{\partial^4 u}{\partial x^4}\frac{\Delta x^4}{4!} + \cdots$$

FOR SUM TO $\approx \frac{\partial^2 u}{\partial x^2}$, NEED

$$\alpha+\beta+\gamma = 0$$
$$\gamma - \alpha = 0$$
$$(\gamma+\alpha)\frac{\Delta x^2}{2!} = 1$$

$$\gamma = \alpha$$
$$\alpha = \frac{1}{\Delta x^2}, \quad \gamma = \frac{1}{\Delta x^2}$$
$$\beta = \frac{-2}{\Delta x^2}$$

$$\frac{u(x-\Delta x) - 2u(x) + u(x+\Delta x)}{\Delta x^2} = \frac{\partial^2 u}{\partial x^2}(x) + \frac{2}{\cancel{\Delta x^2}}\cdot\frac{\partial^4 u}{\partial x^4}\cdot\frac{\cancel{\Delta x^4}\,\Delta x^2}{4!}$$

WHAT WE WANT — $O(\Delta x^2)$ TRUNCATION ERROR

WITH NODE NUMBER NOTATION, AT ANY NODE j,

$$\frac{\partial^2 u}{\partial x^2} = \frac{U_{j-1} - 2U_j + U_{j+1}}{\Delta x^2} \qquad \frac{\partial u}{\partial t} = \frac{dU_j}{dt}$$

SO, HEAT EQN. AFTER DISCRETE APPROX. IN SPACE BECOMES:

$$\text{(A)} \qquad \frac{dU_j}{dt} = b \, \frac{U_{j-1} - 2U_j + U_{j+1}}{\Delta x^2} \qquad \text{AT } j = 2 \ldots\ldots J-1$$

(INTERIOR NODES)

$+$

ALGEBRAIC APPROX. TO BOUNDARY CONDITIONS AT $j = 1$ AND J (BOUNDARY NODES)

(A) IS A SYSTEM OF <u>COUPLED</u> ORDINARY DIFFERENTIAL EQUATIONS (ODE) IN t.

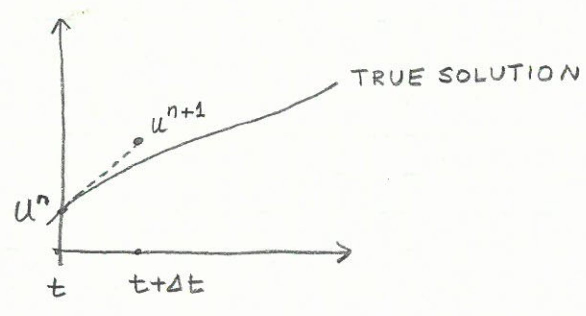
TO DEAL WITH TIME DERIVATIVES, SIMILAR DIFFERENCE APPROXIMATIONS IN TIME:

CONSIDER $\dfrac{du}{dt} = f(t,u)$ (ODE)

(SUPERSCRIPT, not power)

SIMPLEST ONE-STAGE ONE-STEP METHODS: LET $u^n = u(t = n\Delta t)$, $u^{n+1} = u(t+\Delta t)$

<u>EULER FORWARD</u>: $u^{n+1} = u^n + f^n \Delta t$ (EF)



EF approximates f based on current value of u at time t.

STRAIGHTFORWARD ALGEBRAIC CALCULATIONS: WHEN APPLIED TO HEAT EQN.,

$$U_j^{n+1} = U_j^n + \frac{b\Delta t}{\Delta x^2}\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n \right)$$

$\checkmark$ $\checkmark$ $\checkmark$ $\checkmark$ → ALL KNOWN AT CURRENT TIME

... <u>EXPLICIT</u> "FORMULA" FOR U_j^{n+1}'s

EULER FORWARD (EF) FOR HEAT EQN.

Consider the general form of the heat equation -

$$\frac{\partial u}{\partial t} - b\frac{\partial^2 u}{\partial x^2} = 0, \quad 0 \le x \le L.$$

$$u(x,0) = u_0(x); \quad c_1 u(0,t) + c_2 \frac{\partial u}{\partial x}(0,t) = f_1(t)$$

$$c_3 u(L,t) + c_4 \frac{\partial u}{\partial x}(L,t) = f_2(t)$$

($c_2 = 0$, $c_4 = 0$; $c_1 = 1$, $c_3 = 1$ for first-type B.C.)

THE DISCRETIZED FORM OF THE HEAT EQN. USING EF WOULD BE :

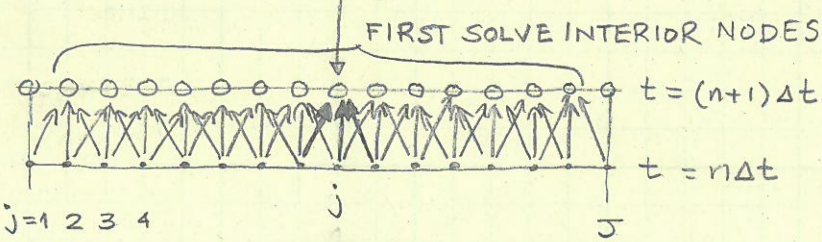
(A) $$U_j^{n+1} = U_j^n + \left(\frac{b\Delta t}{\Delta x^2}\right)\left(U_{j-1}^n - 2U_j^n + U_{j+1}^n\right), \quad j = 2, 3, 4 \dots J-1$$

(we are using EF for interior nodes; we will use B.C. for end nodes)

$$U_1^{n+1} = \frac{\Delta x f_1^{n+1} - c_2 U_2^{n+1}}{(c_1\Delta x - c_2)}, \quad U_J^{n+1} = \frac{\Delta x f_2^{n+1} + c_4 U_{J-1}^{n+1}}{(c_3\Delta x + c_4)}$$

So, in each time-step we start from U_j^n, known for $j = 1, 2, \dots J$, first advance interior node solutions

U_j^{n+1} is influenced by U_{j-1}^n, U_j^n, U_{j+1}^n



THEN SOLVE FOR U_1^{n+1}, U_J^{n+1} (B.C.)

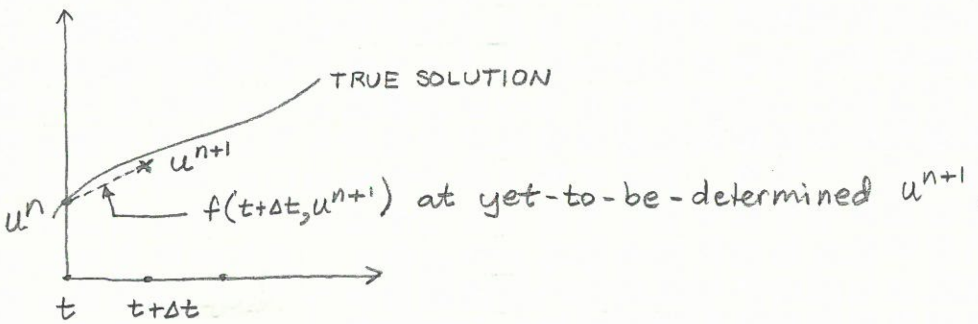
EF is very easy to implement! But could be unstable....

physics of instability: Note that U_j^n influences U_{j-1}^{n+1}, U_j^{n+1}, U_{j+1}^{n+1}, i.e. only 3 nodes, total region of influence of tempr. U_j^n extends over $(2\Delta x)$. But for large Δt, physically the influence may extend over a much larger region. By concentrating all the heat to a smaller region, EF may lead to instability and blow-up. You can also see that stability depends on Δt AND Δx. The true and EF regions of influence can be matched by increasing Δx?

OVERCOMING INSTABILITY:

EULER BACKWARD (EB) FOR $\frac{du}{dt} = f(t,u)$: $\underset{?}{u^{n+1}} = \underset{\text{KNOWN AT } t}{u^n} + f(t+\Delta t, \underset{?}{u^{n+1}})$

→ implicit formula for u^{n+1} → may need to solve a (nonlinear if f is nonlinear) equation for u^{n+1}.



when applied to heat equation,

$$\underset{?}{U_j^{n+1}} = \underset{\checkmark}{U_j^n} + \underbrace{\frac{b\Delta t}{\Delta x^2}}_{\text{CALL THIS "}\mu\text{"}} \left(\underset{?}{U_{j-1}^{n+1}} - 2\underset{?}{U_j^{n+1}} + \underset{?}{U_{j+1}^{n+1}} \right)$$

3 UNKNOWNS (MOVE TO LEFT)

$$-\mu U_{j-1}^{n+1} + (1+2\mu) U_j^{n+1} - \mu U_{j+1}^{n+1} = U_j^n$$

IMPLICIT EQN. (NOT EXPLICIT FORMULA) FOR U_j^{n+1}

CRANK-NICHOLSON SCHEME : $\frac{du}{dt} = f(t,u)$: $u^{n+1} = u^n + \frac{\Delta t}{2}(f^n + f^{n+1})$

TURNS OUT TO BE $O(\Delta t^2)$ ACCURATE, UNLIKE EF AND EB ($O(\Delta t)$)

$$\underset{?}{U_j^{n+1}} = \underset{\checkmark}{U_j^n} + \frac{\mu}{2}\left[\left(\underset{\checkmark}{U_{j-1}^n} - 2\underset{\checkmark}{U_j^n} + \underset{\checkmark}{U_{j+1}^n} \right) + \left(\underset{?}{U_{j-1}^{n+1}} - 2\underset{?}{U_j^{n+1}} + \underset{?}{U_{j+1}^{n+1}} \right) \right]$$

(IMPLICIT) → STILL 3 UNKNOWNS

$$-\frac{\mu}{2} U_{j-1}^{n+1} + (1+\mu) U_j^{n+1} - \frac{\mu}{2} U_{j+1}^{n+1} = \underbrace{\frac{\mu}{2} U_{j-1}^n + (1-\mu) U_j^n + \frac{\mu}{2} U_{j+1}^n}_{r_j^n \text{ (KNOWN)}}$$

just a different IMPLICIT EQN.

IMPLEMENTATION OF EB: note that U_j^{n+1} ARE ALL UNKNOWN at time level n. EB IS IMPLICIT

$$\frac{\partial u}{\partial t} - b\frac{\partial^2 u}{\partial x^2} = 0, \quad 0 \le x \le L;\ t>0 \qquad u(x,0) = u_0(x); \qquad c_1 u(0,t) + c_2 \frac{\partial u}{\partial x}(0,t) = f_1(t)$$

$$c_3 u(L,t) + c_4 \frac{\partial u}{\partial x}(L,t) = f_2(t)$$

Interior nodes: $(j = 2, 3, \ldots, J-1)$

$$U_j^{n+1} = U_j^n + \mu\left(U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}\right)$$

Rearrange unknowns on left side

$$\boxed{-\mu U_{j-1}^{n+1} + (1+2\mu)U_j^{n+1} - \mu U_{j+1}^{n+1} = U_j^n} \quad ☆$$

☆ is a linear eqn. in 3 unknowns. When ☆ is written for all interior nodes, get a system of J-2 equations in J unknowns.

We need 2 more equations – these come from B.C.

$$\left.\begin{aligned} c_1 U_1^{n+1} + c_2\frac{U_2^{n+1} - U_1^{n+1}}{\Delta x} &= f_1^{n+1} \\ c_3 U_J^{n+1} + c_4\frac{U_J^{n+1} - U_{J-1}^{n+1}}{\Delta x} &= f_2^{n+1} \end{aligned}\right\}$$

note that $\frac{\partial u}{\partial x}$ has been approximated only to $O(\Delta x)$ in these.

NOW WE HAVE A SYSTEM OF J EQS. IN J UNKNOWNS FROM EB (IMPLICIT) AS OPPOSED TO EF (EXPLICIT EXPRESSIONS FOR U_j^{n+1}'s). WE NEED TO SOLVE THIS SYSTEM OF EQS. IN EACH TIME-STEP WITH EB. IN MATRIX FORM, THE SYSTEM OF EQS. IS:

$$\begin{bmatrix} \left(c_1 - \frac{c_2}{\Delta x}\right) & \frac{c_2}{\Delta x} & 0 & \cdots & & & 0 \\ -\mu & (1+2\mu) & -\mu & \ddots & & & \vdots \\ 0 & \ddots & \ddots & \ddots & & & \\ \vdots & & & & & & \\ 0 & \cdots & 0 \ -\mu & (1+2\mu) & -\mu & 0 \cdots & 0 \\ \vdots & & & \ddots & \ddots & \ddots & 0 \\ & & & -\mu & (1+2\mu) & -\mu & \\ 0 & \cdots & & \cdots 0 & -\frac{c_4}{\Delta x} & \left(c_3 + \frac{c_4}{\Delta x}\right) \end{bmatrix} \begin{Bmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_{j-1}^{n+1} \\ U_j^{n+1} \\ U_{j+1}^{n+1} \\ \vdots \\ U_{J-1}^{n+1} \\ U_J^{n+1} \end{Bmatrix} = \begin{Bmatrix} f_1^{n+1} \\ U_2^n \\ \vdots \\ U_j^n \\ \vdots \\ U_{J-1}^n \\ f_2^{n+1} \end{Bmatrix}$$

NOTE MATRIX STRUCTURE – TRI-DIAGONAL

zeros everywhere except main diagonal, first upper and lower sub-diagonal

SOLVING A TRIDIAGONAL SYSTEM OF EQS. – THOMAS ALGORITHM

$$
\begin{bmatrix}
b_1 & c_1 & 0 & 0 & \cdots & & & & 0 \\
a_2 & b_2 & c_2 & 0 & \cdots & & & & 0 \\
0 & a_3 & b_3 & c_3 & & & & & \\
0 & 0 & a_4 & b_4 & c_4 & & & & \\
\vdots & & & & & & & & \\
0 & \cdots & 0 & a_j & b_j & c_j & 0 & \cdots & 0 \\
\vdots & & & & & & & & c_{J-1} \\
0 & & & & \cdots & & 0 & a_J & b_J
\end{bmatrix}
\begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_j \\ \vdots \\ x_J \end{Bmatrix}
=
\begin{Bmatrix} r_1 \\ r_2 \\ \vdots \\ r_j \\ \vdots \\ r_J \end{Bmatrix}
$$

$[A]$ $\qquad \underline{x} \qquad \underline{r}$

(Note, we only need to think of a tridiagonal matrix as 3 vectors)

THE FIRST STEP IS TO DETERMINE $[L]$, $[U]$ such that $[L][U] = [A]$.

LET US CHOOSE $[L]$ AND $[U]$ IN THE FORM:

$$
[L] =
\begin{bmatrix}
f_1 & 0 & 0 & \cdots & & & & 0 \\
e_2 & f_2 & 0 & \cdots & & & & 0 \\
0 & e_3 & f_3 & 0 & \cdots & & & 0 \\
0 & 0 & e_4 & f_4 & 0 & \cdots & & 0 \\
 & & & & & & & \\
0 & \cdots & 0 & e_j & f_j & 0 & \cdots & 0 \\
 & & & & & & & \\
 & & & & & & e_J & f_J
\end{bmatrix}
\qquad
[U] =
\begin{bmatrix}
1 & g_1 & & & & & \\
0 & 1 & g_2 & & & & \\
0 & 0 & 1 & g_3 & & & \\
\vdots & \vdots & 0 & 1 & g_4 & & \\
\vdots & \vdots & & & 1 & g_j & \\
\vdots & \vdots & & & & 1 & g_{J-1} \\
0 & 0 & & & & & 1
\end{bmatrix}
$$

IF WE FOLLOW THE STEPS OF MATRIX MULTIPLICATION, WE GET

$f_1 = b_1$

$f_1 g_1 = c_1 \Rightarrow g_1 = c_1/f_1$

$e_2 = a_2$

$e_2 g_1 + f_2 = b_2 \Rightarrow f_2 = b_2 - e_2 g_1$

$f_2 g_2 = c_2 \Rightarrow g_2 = c_2/f_2$

$e_3 = a_3$

$e_3 g_2 + f_3 = b_3 \Rightarrow f_3 = b_3 - e_3 g_2$

$f_3 g_3 = c_3 \Rightarrow g_3 = c_3/f_3$

---

etc.

suggests: $e_j = a_j$

$f_j = b_j - e_j g_{j-1}$

$g_j = c_j/f_j$

for $j = 2, \ldots, J$

NOW SOLVE $[L]\underline{y} = \underline{r}$: $y_1 = r_1/f_1$; $y_j = (r_j - e_j y_{j-1})/f_j$ for $j = 2, \ldots, J$

THEN SOLVE $[U]\underline{x} = \underline{y}$: $x_J = y_J$; $x_j = (y_j - g_j x_{j+1})$ for $j = J-1, \ldots, 1$