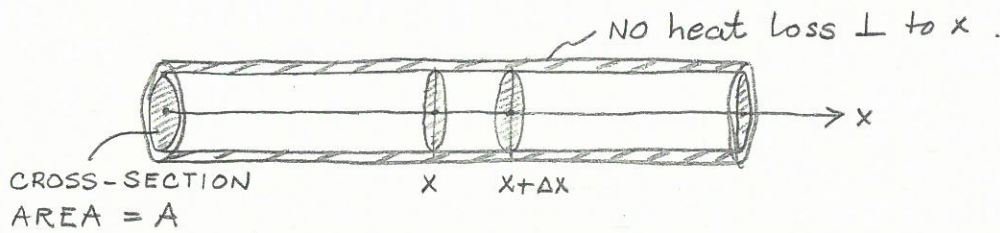


ILLUSTRATION USING THE ONE-DIMENSIONAL HEAT EQUATION :



"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

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

$\frac{1}{s} \cdot \frac{kg}{m^3} \cdot \frac{J}{kg \cdot K} \cdot K$ $\frac{J}{m^2 \cdot s} \cdot m^2$

DIFFERENTIAL CONTROL VOLUME ANALYSIS :

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

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

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

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

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

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

SECOND ORDER (PARABOLIC)

PARTIAL DIFFERENTIAL EQUATION

x = SPACE , t = TIME

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

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

$$\text{e.g. } u(x=0, t) = T_1(t), \quad u(x=L, t) = T_2(t)$$

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

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

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

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.

$$-k \frac{\partial u}{\partial x}(x=L, t) = h (u(L, t) - u_{atm})$$

↑ "Heat transfer coefficient"

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

$$\Rightarrow \frac{\partial u}{\partial t} - b \frac{\partial^2 u}{\partial x^2} = 0, \quad u(x, 0) = U_0(x) \text{ has a unique solution if}$$

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. $L \rightarrow \infty$ 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)

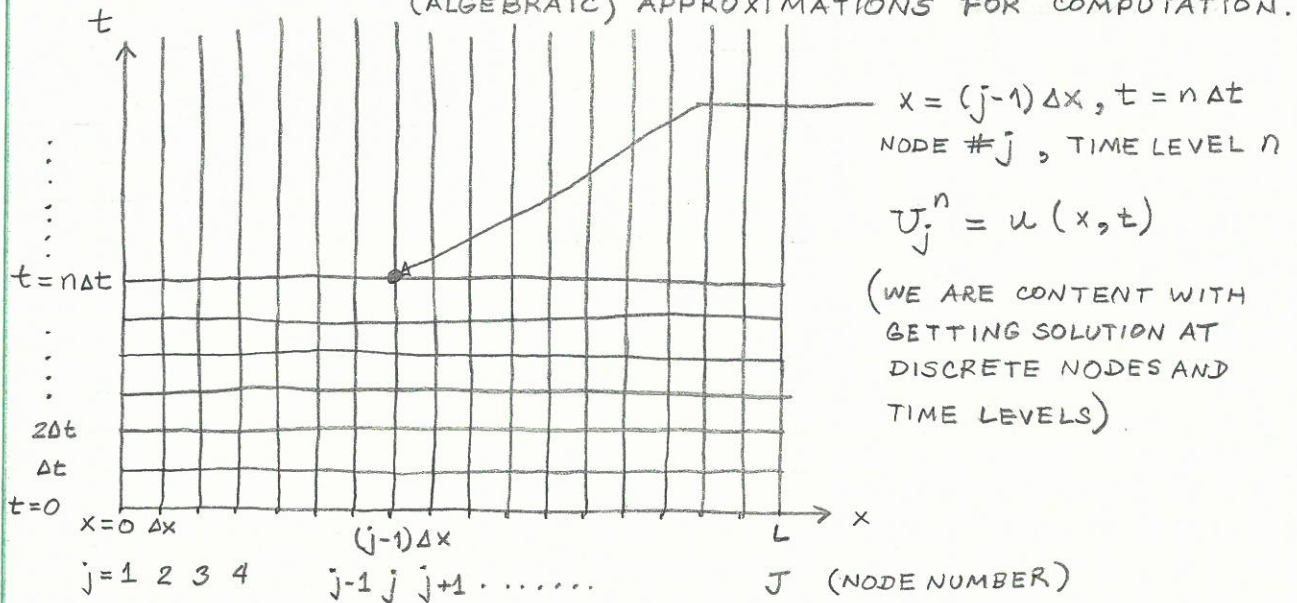
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NUMERICAL SOLUTION OF THE HEAT EQUATION: FINITE DIFFERENCE METHOD

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



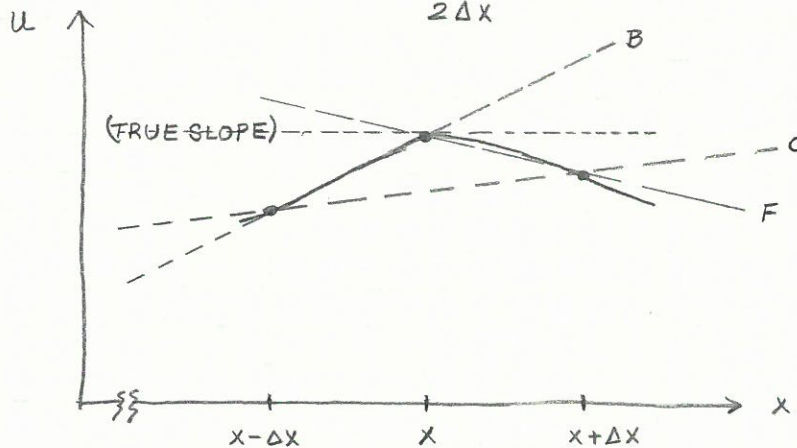
- ALGEBRAIC EQUATIONS TO SOLVE FOR U_j^n 's?
- APPROXIMATING SPATIAL DERIVATIVES USING DIFFERENCE APPROXIMATIONS.

FIRST DERIVATIVE: $\frac{\partial u}{\partial x}$... 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

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

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

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

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

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

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

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.?
 "CURVATURE" : AT LEAST 3 POINT VALUES.

$$\frac{\partial^2 u}{\partial x^2}(x) \approx \alpha u(x-\Delta x) + \beta u(x) + \gamma u(x+\Delta x)$$

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

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

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

$$\gamma u(x+\Delta x) = \gamma \left(\dots + \dots + \dots + \dots + \dots + \dots \right)$$

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

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

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

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

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

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

AMPAD

WITH NODE NUMBER NOTATION, AT ANY NODE j ,

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

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

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

+

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

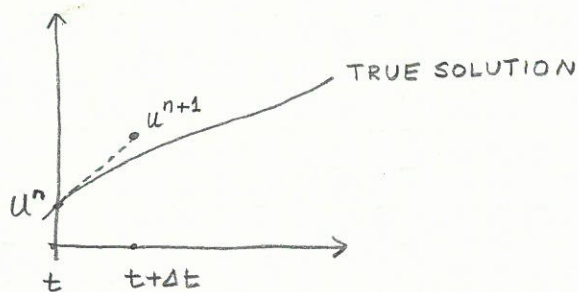
(A) IS A SYSTEM OF COUPLED ORDINARY DIFFERENTIAL EQUATIONS (ODE) IN t .

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

CONSIDER $\frac{du}{dt} = f(t, u)$ (ODE) (SUPERSCRIPT, not power)

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

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



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

STRAIGHTFORWARD ALGEBRAIC CALCULATIONS : WHEN APPLIED TO HEAT EQN.,

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

ALL KNOWN AT CURRENT TIME

... EXPLICIT "FORMULA"
FOR U_j^{n+1} 's

EULER FORWARD (EF) FOR HEAT EQN.

Consider the general form of the heat equation -

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

$$u(x,0) = u_0(x); \quad c_1 u(0,t) + c_2 \frac{\partial u}{\partial x}(0,t) = f_1(t) \quad (c_2=0, c_4=0; \\ c_1=1, c_3=1 \text{ for first-type B.C.}) \\ c_3 u(L,t) + c_4 \frac{\partial u}{\partial x}(L,t) = f_2(t)$$

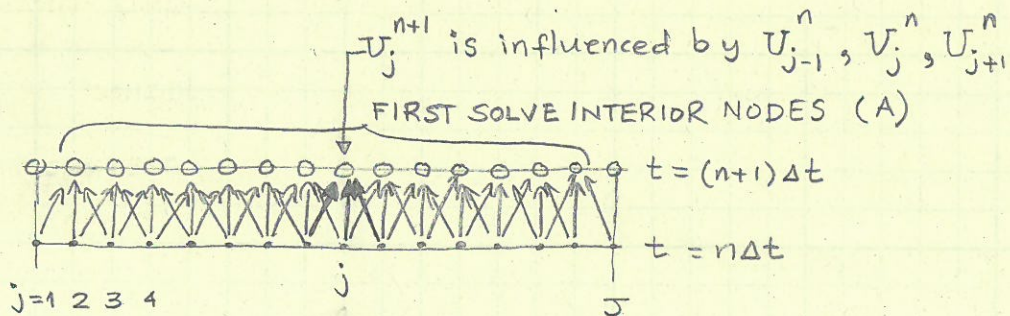
THE DISCRETIZED FORM OF THE HEAT EQN. USING EF WOULD BE :

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

(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



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 ?

IMPLEMENTATION OF EB: note that U_j^{n+1} ARE ALL UNKNOWN at

time level n . EB IS IMPLICIT

$$\frac{\partial u}{\partial t} - b \frac{\partial^2 u}{\partial x^2} = 0, \quad 0 \leq x \leq L; \quad u(x, 0) = U_0(x); \quad C_1 u(0, t) + C_2 \frac{\partial u}{\partial x}(0, t) = f_1(t)$$

$$C_3 u(L, t) + C_4 \frac{\partial u}{\partial x}(L, t) = f_2(t)$$

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

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

Rearrange unknowns on left side

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

\star is a linear eqn. in 3 unknowns. When \star 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.

$$\left. \begin{aligned} C_1 U_1^{n+1} + C_2 \frac{U_2^{n+1} - U_1^{n+1}}{\Delta x} &= f_1^{n+1} \\ C_3 U_J^{n+1} + C_4 \frac{U_J^{n+1} - U_{J-1}^{n+1}}{\Delta x} &= f_2^{n+1} \end{aligned} \right\} \begin{array}{l} \text{note that } \frac{\partial u}{\partial x} \text{ has been approximated} \\ \text{only to } O(\Delta x) \text{ in these.} \end{array}$$

NOW WE HAVE A SYSTEM OF J EQS. IN J UNKNOWNIS 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 :

$$\begin{bmatrix} (C_1 - \frac{C_2}{\Delta x}) & \frac{C_2}{\Delta x} & 0 & \dots & \dots & 0 \\ -\mu & (1+2\mu) & -\mu & & & \\ 0 & & & & & \\ \vdots & & & & & \\ 0 & & 0 & -\mu & (1+2\mu) & -\mu & 0 \\ \vdots & & & & & & \\ \vdots & & & & & & \\ \vdots & & & & & & \\ \vdots & & & & & & \\ \vdots & & & & & & \\ 0 & \dots & 0 & & -\mu & (1+2\mu) & -\mu \\ & & & & & & -\frac{C_4}{\Delta x} & (C_3 + \frac{C_4}{\Delta x}) \end{bmatrix} \begin{Bmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_{j-1}^{n+1} \\ U_j^{n+1} \\ U_{j+1}^{n+1} \\ \vdots \\ U_{J-1}^{n+1} \\ U_J^{n+1} \end{Bmatrix} = \begin{Bmatrix} f_1^{n+1} \\ U_2^n \\ \vdots \\ U_j^n \\ \vdots \\ U_{J-1}^n \\ f_2^{n+1} \end{Bmatrix}$$

NOTE MATRIX STRUCTURE - TRI-DIAGONAL
zeros everywhere except main diagonal, first upper and lower sub-diagonal

SOLVING A TRIDIAGONAL SYSTEM OF EQS. - THOMAS ALGORITHM

$$\begin{bmatrix}
 b_1 & c_1 & 0 & 0 & \dots & \dots & \dots & 0 \\
 a_2 & b_2 & c_2 & 0 & \dots & \dots & \dots & 0 \\
 0 & a_3 & b_3 & c_3 & \dots & \dots & \dots & 0 \\
 0 & 0 & a_4 & b_4 & c_4 & \dots & \dots & 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & \dots & \dots & 0 & a_j & b_j & c_j & 0 \dots 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & \dots & \dots & \dots & \dots & 0 & a_{j-1} & b_{j-1} & c_{j-1} \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & \dots & \dots & \dots & \dots & \dots & \dots & 0 & a_j & b_j & c_j & 0 \dots 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & 0 & a_j & b_j & c_j & 0 \dots 0
 \end{bmatrix}
 \begin{pmatrix}
 x_1 \\
 x_2 \\
 \vdots \\
 x_j \\
 \vdots \\
 x_j \\
 \vdots \\
 x_j
 \end{pmatrix}
 =
 \begin{pmatrix}
 r_1 \\
 r_2 \\
 \vdots \\
 r_j \\
 \vdots \\
 r_j \\
 \vdots \\
 r_j
 \end{pmatrix}$$

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

[A]

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

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

$$\begin{bmatrix}
 f_1 & 0 & 0 & \dots & \dots & \dots & 0 \\
 e_2 & f_2 & 0 & \dots & \dots & \dots & 0 \\
 0 & e_3 & f_3 & 0 & \dots & \dots & 0 \\
 0 & 0 & e_4 & f_4 & 0 & \dots & 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & \dots & \dots & 0 & e_j & f_j & 0 \dots 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 0 & \dots & \dots & \dots & \dots & e_j & f_j
 \end{bmatrix}
 \begin{bmatrix}
 1 & g_1 & & & & & \\
 0 & 1 & g_2 & & & & \\
 0 & 0 & 1 & g_3 & & & \\
 \vdots & \vdots & \vdots & 0 & 1 & g_4 & \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
 0 & 0 & & & & & 1 & g_{j-1} & \\
 & & & & & & & & 1
 \end{bmatrix}$$

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:

$$\begin{aligned}
 e_j &= a_j \\
 f_j &= b_j - e_j g_{j-1} \\
 g_j &= c_j / f_j \\
 &\text{for } j=2, \dots, J
 \end{aligned}$$

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

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

