Plan for week 35 FYS3150/4150

- Math from linear algebra
  (LU-decomp, matrix inv, Gaussian elimination ..)
- Programming Elements
  - write/read to/from file
  - Dynamical allocation of memory
    - vector, matrices, arrays
    - pointers
  - structure your program

Math of project 1

$$\frac{d^2u}{dx^2} = f(x) \qquad u(0) = u(1) = 0$$
$$x \in [0,1]$$

Discretize $\quad i = 0, 1, \ldots n$

$$x_i = x_0 + i \cdot h$$

$$h = \frac{x_n - x_0}{n}$$

$$x_0 = 0 \quad \wedge \quad x_n = 1$$

$$\frac{d^2u}{} \simeq \frac{u_{i+1} + u_{i-1} - 2u_i}{} = f_i$$

dx^2 $\qquad$ h^2

Truncation error $O(h^2)$

$i = \underline{1}$ $\qquad$ $h^2 f_i = g_i$

$$u_2 + \underset{\text{known}}{\boxed{u_0}} - 2u_{\underline{1}} = g_{\underline{1}}$$

$i = 2$

$$u_3 + u_1 - 2u_2 = g_2$$

$\vdots$

$$i = n-1 \quad \overset{\text{known}}{\boxed{u_n}} + u_{n-2} - 2u_{n-1} = g_{n-1}$$

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

Tridiagonal Töplitz matrix.

$$u^T = [u_1, u_2 \ldots u_{n-1}]$$

$$g^T = [g_1, g_2 \ldots g_{n-1}]$$

$$\boxed{Au = g}$$

$$u = A^{-1} g$$

$A \in \mathbb{R}^{n-1 \times n-1}$ $u, g \in \mathbb{R}^{n-1}$

$n-1 = 4$

$$A = \begin{bmatrix} d_1 & e_1 & 0 & 0 \\ e_1 & d_2 & e_2 & 0 \\ 0 & e_2 & d_3 & e_3 \\ 0 & 0 & e_3 & d_4 \end{bmatrix}$$

symmetric square matrix

Need to store two vectors

$d^T = [d_1, d_2, d_3\ d_4]$

$e^T = [e_1\ e_2\ e_3\ e_4]$ not needed.

Spell out in detail

$$d_1 \cdot u_1 + e_1 u_2 + 0 + 0 = g_1$$

$$e_1 u_1 + d_2 u_2 + e_2 u_3 + 0 = g_2$$

$$0 \quad e_2 u_2 + d_3 u_3 + e_3 u_4 = g_3$$

$$0 \quad 0 \quad e_3 u_3 + d_4 u_4 = g_4$$

e_1/d_1

$$\left|\begin{array}{ccccc} d_1 & e_1 & \underline{0} & 0 & g_1 \end{array}\right|$$

$$
\begin{matrix}
e_1 & d_2 & e_2 & 0 & g_2 \\
0 & e_2 & d_3 & e_3 & g_3 \\
0 & 0 & e_3 & d_4 & g_4
\end{matrix}
$$

$$
\begin{matrix}
d_1 & e_1 & 0 & 0 & g_1 \\
0 & \underbrace{d_2 - e_1^2/d_1}_{\tilde{d}_2} & e_2 & 0 & \underbrace{g_2 - g_1 e_1/d_1}_{\tilde{g}_2} \\
0 & \boxed{e_2} & d_3 & e_3 & g_3 \\
0 & 0 & e_3 & d_4 & g_4
\end{matrix}
$$

$$\frac{e_2}{d_2 - e_1^2/d_1} = \frac{e_2}{\tilde{d}_2} \qquad \tilde{g}_2 = g_2 - g_1\, e_1/d_1$$

$$
\begin{matrix}
d_1 & e_1 & 0 & 0 & g_1 \\
0 & \tilde{d}_2 & e_2 & 0 & \tilde{g}_2 \\
0 & 0 & \tilde{d}_3 & e_3 & \tilde{g}_3 \\
0 & 0 & \underline{e_3} & d_4 & g_4
\end{matrix}
$$

$e_3/\tilde{d}_3$

$$
\begin{matrix}
d_1 & e_1 & 0 & 0 & g_1 \\
0 & \tilde{d}_2 & e_2 & 0 & \tilde{g}_2 \\
0 & 0 & \tilde{d}_3 & e_3 & \tilde{g}_3 \\
0 & 0 & 0 & \tilde{d}_4 & \tilde{g}_4
\end{matrix}
$$

$$\underline{\tilde{d}_i} = \underline{d_i} - \underline{e_{i-1}^2} / \underline{\tilde{d}_{i-1}}$$

$$\underline{\tilde{g}_i} = \underline{g_i} - \underline{e_{i-1}}\,\underline{\tilde{g}_{i-1}} / \underline{\tilde{d}_{i-1}}$$

$$\tilde{d}_1 = d_1 \qquad \tilde{g}_1 = g_1$$

$i = 2, \dots n-1$

Have to define $g, \tilde{g}, d, \tilde{d}$
e, u
6 vectors

Floating point operations
FLOPs

$\tilde{d}_i \sim 3(n-2) \simeq 3n$

$\tilde{g}_i \sim 3(n-2) \simeq 3n$

Forward subst : 6n FLOPS

$$\begin{bmatrix} d_1 & e_1 & 0 & 0 \\ 0 & \tilde{d}_2 & e_2 & 0 \\ 0 & 0 & \tilde{d}_3 & e_3 \\ 0 & 0 & 0 & \tilde{d}_4 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} g_1 \\ \tilde{g}_2 \\ \tilde{g}_3 \\ \tilde{g}_4 \end{bmatrix}$$

$$\tilde{d}_4 u_4 = \tilde{g}_4$$

$$u_4 = \tilde{g}_4 / \tilde{d}_4$$

$$\tilde{d}_3 u_3 + e_3 \underline{u_4} = \tilde{g}_3$$

$$u_3 = (\tilde{g}_3 - e_3 u_4) / \tilde{d}_3$$

$$u_i = (\tilde{g}_i - \underline{e_i} \cdot u_{i+1}) / \tilde{d}_i$$

Backward substitution

Flops : $3(n-2)$

In total : $\underline{9n \text{ FLOPS}}$

$O(n)$ FLOPS

LU-decomposition $O(n^3)$

$\frac{2}{3} n^3$

our specific case

$$l_1 = l_2 \dots l_{n-2} = 1$$
$$d_1 = d_2 \dots d_{n-1} = -2$$

$$u_i = (\tilde{g}_i - u_{i+1})/\tilde{d}_i$$ 2 FLOPs

$$\boxed{\tilde{g}_i = g_i' - \tilde{g}_{i-1}/\tilde{d}_{i-1}}$$ 2 FLOPs

$$\boxed{\tilde{d}_i = d_i' - 1/\tilde{d}_{i-1}}$$ 2 FLOPs

analytic expression, pre-calculated.

$$d_i' = -2 \qquad l_i' = +1$$

$$d_1 = -2$$
$$\tilde{d}_2 = -2 - 1/\tilde{d}_1 = -3/2$$
$$\tilde{d}_3 = -2 + 2/3 = -4/3$$
$$\tilde{d}_4 = -5/4$$

$$\boxed{\tilde{d}_i = -\frac{(i+1)}{i}}$$ => 4n FLOPs

(Thomas algo)

- write algo (flow of data) before writing code

- read from file or terminal the input variables
- write to file
- initializations
  - n (number of integration points/mesh points)
  - allocation of memory vectors u, g, $\tilde{g}$, $\tilde{d}$, d, e
- algorithm

Forward part

FOR ($i = 1$, $n-1$)

update $\tilde{g}_i$, $\cancel{\tilde{d}_i}$

END FOR

Backward Part

$u_{n-1} = \tilde{g}_{n-1} / \tilde{d}_{n-1}$

FOR ($i = n-2$, 1)

update u_i

END FOR

WRITE RESULTS TO FILE

Analytical solution, $v(x)$

relative error $\quad \varepsilon_i = \left| \frac{v_i - u_i}{v_i} \right|$

$V \in \mathbb{R}^{100000}$ ~ 8 bytes per variable

vector ~ 1MB