Linear second order ODE - boundary value problem
<method of finite differences>)

Equation given:

$$\frac{d^2}{dx^2}y + g(x)_3 \cdot \frac{d}{dx}y + g(x)_2 \cdot y = g(x)_1 \qquad x = x1 .. x2$$

Boundary conditions (Robin type):

$x = x1$ $\quad A_1 \cdot y + B_1 \cdot \frac{d}{dx}y = C_1$

$x = x2$ $\quad A_2 \cdot y + B_2 \cdot \frac{d}{dx}y = C_2$

Finite difference equation transformed:

$$\frac{y_{i+1} - 2 \cdot y_i + y_{i-1}}{h^2} + g(x_i)_3 \cdot \frac{y_{i+1} - y_{i-1}}{2 \cdot h} + g(x_i)_2 \cdot y_i = g(x)_1 \qquad i = 2 .. n$$

Integrating step,h with number of subintervals,n:

$$h := \frac{x2 - x1}{n}$$

Finite difference boundary conditions transformed:

$i = 1$ $\quad A_1 \cdot y_1 + B_1 \cdot \frac{y_2 - y_1}{h} = C_1$

$i = n + 1$ $\quad A_2 \cdot y + B_2 \cdot \frac{y_{n+1} - y_n}{h} = C_2$

EXAMPLE:

$$\frac{1}{Pe} \cdot \frac{d}{dx}y - \frac{d}{dx}y - Da \cdot y = 0$$

Concentartion profile allong the tubular reactor with axial dispersion:

Boundary conditions:

$x = 0$ $\quad y - \frac{1}{Pe} \cdot \frac{d}{dx}y = 1$

$x = 1$ $\quad \frac{d}{dx}y = 0$

$Pe := 1 \qquad Da := 2$

Given parameters

Vector function,g(x) and constants A,B,C
*change for some other equation

$$g(x) := \begin{pmatrix} 0 \\ -Da \cdot Pe \\ -Pe \end{pmatrix} \qquad A_1 := Pe \quad B_1 := -1 \quad C_1 := Pe$$

$$A_2 := 0 \quad B_2 := 1 \quad C_2 := 0$$

Number of subintervals:
*could be changed

$n := 50$

Integration step:
*change for some other integration range

$x1 := 0 \quad x2 := 1 \quad h := \frac{x2 - x1}{n}$

Independent variable points:

for $i \in 0..n$

$x_{i+1} := x1 + i \cdot h$

Applaying Thomas algorithm:

$a_{n+1} := -B_2$

$b_1 := h \cdot A_1 - B_1$

$b_{n+1} := h \cdot A_2 + B_2$

$c_1 := B_1$

$d_1 := C_1 \cdot h$

$d_{n+1} := C_2 \cdot h$

for $i \in 2..n$

$$a_i := 1 - g(x_i)_3 \cdot \frac{h}{2}$$

$$b_i := g(x_i)_2 \cdot h^2 - 2$$

$$c_i := 1 + g(x_i)_3 \cdot \frac{h}{2}$$

$$d_i := g(x_i)_1 \cdot h^2$$

$\beta_1 := b_1 \quad \gamma_1 := \frac{d_1}{\beta_1}$

for $i \in 2..n+1$

$$\beta_i := b_i - \frac{a_i \cdot c_{i-1}}{\beta_{i-1}}$$

$$\gamma_i := \frac{d_i - a_i \cdot \gamma_{i-1}}{\beta_i}$$

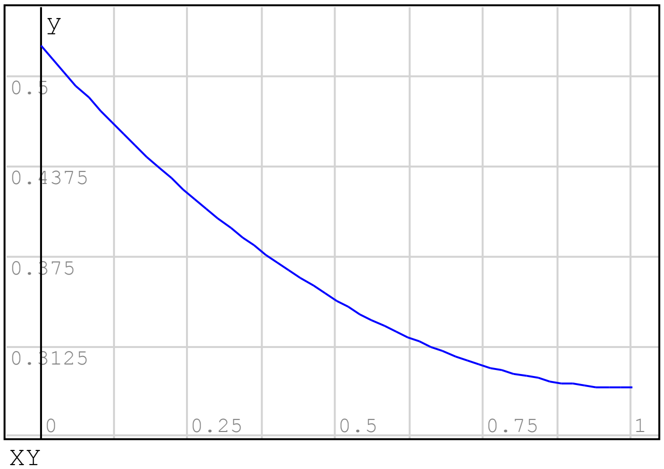
$y_{n+1} := \gamma_{n+1}$

for $i \in n, n-1..1$

$$y_i := \gamma_i - \frac{c_i \cdot y_{i+1}}{\beta_i}$$

Final concentration profile, y(x)
*the scaling should be changed acordingly

$XY := \text{augment}(x, y)$



Inlet concentartion: $y_1 = 0.5224$

Outlet concentration: $y_{length(y)} = 0.2839$