Advanced Methods on Computational Physics

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Exercise Set 14

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You can build and run the program by running 'main14.sh' script. gcc, 'armadillo' and 'openblas' are required.

A. Equation:

$$-\frac{d^2\phi(x)}{dx^2} + \phi(x) = f(x), 0 \leq x \leq 1, \phi(0) = \phi(1) = 0$$

In 1d space $\frac{d^2}{dx^2} = \nabla^2 \Rightarrow$

$$-\nabla^2\phi(x) + \phi(x) = f(x)$$

Let's multiply both sides by $\psi(x)$ and integrate them over the whole space ($0 \leq x \leq 1$)

$$-\int_0^1 \nabla^2\phi(x)\psi(x)\mathrm{d}x + \int_0^1 \phi(x)\psi(x)\mathrm{d}x = \int_0^1 f(x)\psi(x)\mathrm{d}x \quad (*)$$

Green's first identity:

$$\int \psi(x)\nabla^2\phi(x)\mathrm{d}\tau = -\int \boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}\psi \, \mathrm{d}\tau + \oint_S \phi \frac{\partial\psi}{\partial n}\mathrm{d}\boldsymbol{a}$$

$$\phi(x=0) = \phi(x=1) = 0 \xrightarrow{Dirichlet} \oint_S \phi \frac{\partial\psi}{\partial n}\mathrm{d}\boldsymbol{a} = 0$$

Since In 1d space $\nabla = \frac{d}{dx}$ & $d\tau = dx$ and from (*) and above relations we have

$$\boxed{(*) \Rightarrow \int \frac{d\phi}{dx}\frac{d\psi}{dx}\,\mathrm{d}x + \int_0^1 \phi(x)\psi(x)\mathrm{d}x = \int_0^1 f(x)\psi(x)\mathrm{d}x}$$

B.

- **Analytical solution**

$$-\frac{d^2\phi(x)}{dx^2} + \phi(x) = 1$$

Homogeneous equation

$$\frac{d^2\phi(x)}{dx^2} - \phi(x) = 0$$

Therefor this is an ODE with constant coefficients

$$\lambda^2 - 1 = 0 \rightarrow \lambda = \pm 1$$

$$\phi_h = Ae^{-x} + Be^{x}$$

Private solution $\phi_p = 1$

$$\Rightarrow \phi(x) = Ae^{-x} + Be^{x} + 1$$

From boundary conditions

$$\phi(0) = A + B + 1 = 0 \rightarrow B = -1 - A$$
$$\phi(1) = Ae^{-1} - (1 + A)e + 1 = 0$$
$$\rightarrow (e^2 - 1)A = e - e^2 \rightarrow A = \frac{e(1-e)}{(e-1)(e+1)} = -\frac{e}{e+1} \;\;, B = \frac{e}{e+1} - 1 = -\frac{1}{e+1}$$
$$\Rightarrow \boxed{\phi(x) = -\frac{1}{e+1}\left[e^{-x+1} + e^{x}\right] + 1}$$

- **FEM**

$$\phi(x) = \sum_i \alpha_i u_i(x)$$
$$\rightarrow \frac{d\phi(x)}{dx} = \sum_i \alpha_i \frac{du_i(x)}{dx}$$

In relation (*) from part A if we consider $\psi(x) = \sum_i u_i(x)$ we have

$$(*) \rightarrow \sum_{i,j} \left\{ \int \frac{du_i}{dx}\frac{du_j}{dx}\mathrm{d}x + \int_0^1 u_i(x)u_j(x)\mathrm{d}x \right\} \alpha_i = \sum_i \int_0^1 f(x)u_i(x)\mathrm{d}x$$

we need to solve this equation $A\alpha = F$

Where

$$A_{ij} = \int_0^1 \frac{du_i}{dx}\frac{du_j}{dx}\mathrm{d}x + \int_0^1 u_i(x)u_j(x)\mathrm{d}x$$

$$F_i = \int_0^1 u_i(x)\mathrm{d}x$$

We consider $u_i(x)$ as this function

$$u_i(x) = \begin{Bmatrix} \dfrac{x_{i+1} - x}{h} & , x_i \le x \le x_{i+1} \\ \dfrac{x - x_{i-1}}{h} & , x_{i-1} \le x \le x_i \end{Bmatrix}$$

$$\rightarrow u_i(x) = \frac{a(x)(x - b(x))}{h} \quad \& \quad \begin{Bmatrix} a(x) = -1, b(x) = x_{i+1} & , x_i \le x \le x_{i+1} \\ a(x) = 1, b(x) = x_{i-1} & , x_{i-1} \le x \le x_i \end{Bmatrix}$$

$$\rightarrow \frac{du_i}{dx} = \frac{a(x)}{h}$$

$$\Rightarrow (1) \int_0^1 \frac{du_i}{dx}\frac{du_j}{dx}\mathrm{dx} = \frac{1}{h^2}\int_0^1 a_i(x)a_j(x)\mathrm{dx} = \frac{1}{h^2}\sum_n \int_{x_n}^{x_n+h} a_i(x)a_j(x)\mathrm{dx}$$

$$\boxed{= \frac{1}{h}\sum_n a_i(x_n, x_n+h)a_j(x_n, x_n+h)}$$

$$\Rightarrow (2) \int_0^1 u_i(x)u_j(x)\mathrm{dx} = \int_0^1 \frac{a_i(x)a_j(x)}{h^2}\left[x^2 - (b_i(x)+b_j(x))x + b_i(x)b_j(x)\right]\mathrm{dx}$$

$$= \frac{1}{h^2}\sum_n \int_{x_n}^{x_n+h} a_i(x)a_j(x)\left[x^2 - (b_i(x)+b_j(x))x + b_i(x)b_j(x)\right]\mathrm{dx}$$

$$= \boxed{\frac{1}{h^2}\sum_n a_i(x_n\,, x_n+h)a_j(x_n\,, x_n+h)\left[\frac{x_n^3}{3} - \frac{x_n^2}{2}(b_i(x_n\,, x_n+h) + b_j(x_n\,, x_n+h)) + x_n b_i(x_n\,, x_n+h)b_j(x_n\,, x_n+h)\right]_{x_n}^{x_n+h}}$$

$$\boxed{\rightarrow A_{ij} = (1) + (2)}$$

$$F_i = \int_0^1 u_i(x)\mathrm{dx} = \frac{1}{h}\int_0^1 a_i(x)\big(x - b_i(x)\big)\mathrm{dx} = \frac{1}{h}\sum_n \int_{x_n}^{x_n+h} a_i(x)\big(x - b_i(x)\big)\mathrm{dx}$$

$$= \boxed{\frac{1}{h}\sum_n a_i(x_n, x_n+h)\left(\frac{x_n^2}{2} - b_i(x_n, x_n+h)x_n\right)_{x_n}^{x_n+h}}$$

where by $a_i(x_n, x_n+h)$ and $b_i(x_n, x_n+h)$ I mean

$$a_i(x_n, x_n+h) = \begin{cases} -1 & x_n \geq x_i \text{ and } x_n + h \leq x_{i+1} \\ 1 & x_n \geq x_i \text{ and } x_n + h \leq x_{i+1} \end{cases}$$

$$b(x_n, x_n+h) = \begin{cases} x_{i+1} & x_n \geq x_i \text{ and } x_n + h \leq x_{i+1} \\ x_{i-1} & x_n \geq x_i \text{ and } x_n + h \leq x_{i+1} \end{cases}$$

C.

- **Analytical solution**

$$-\frac{d^2\phi(x)}{dx^2} + \phi(x) = \sin x$$

Homogeneous equation

$$\frac{d^2\phi(x)}{dx^2} - \phi(x) = 0$$
$$\lambda^2 - 1 = 0 \rightarrow \lambda = \pm 1$$
$$\phi_h = Ae^{-x} + Be^{x}$$

Private solution $\phi_p = \frac{1}{2}\sin x$

$$\Rightarrow \phi(x) = Ae^{-x} + Be^{x} + \frac{1}{2}\sin x$$

From boundary conditions

$$\phi(0) = A + B = 0 \rightarrow B = -A$$

$$\phi(1) = Ae^{-1} - Ae + \frac{1}{2}\sin 1 = 0$$

$$\rightarrow A(e^{-1} - e^{1}) = -\frac{1}{2}\sin 1 \xrightarrow{e^{-1}-e^{1}=-2\sinh 1} A = \frac{1}{4}\frac{\sin 1}{\sinh 1}$$

$$\Rightarrow \boxed{\phi(x) = \frac{1}{4}\frac{\sin 1}{\sinh 1}(e^{-x} - e^{x}) + \frac{1}{2}\sin x = -\frac{1}{2}\frac{\sin 1}{\sinh 1}\sinh x + \frac{1}{2}\sin x}$$

- **FEM**

  The only difference between this part and part B is $f(x)$ so matrix A is the same as part B and we just need to calculate vector F

$$F_i = \int_0^1 \sin(x)\, u_i(x)\mathrm{d}x = \frac{1}{h}\int_0^1 \sin(x)\, a_i(x)\big(x - b_i(x)\big)\mathrm{d}x \rightarrow$$

$$F_i = \frac{1}{h}\sum_n \int_{x_n}^{x_n+h} \sin(x) a_i(x)\big(x - b_i(x)\big)\mathrm{d}x$$

$$= \frac{1}{h}\sum_n a_i(x_n, x_n + h)\left\{\int_{x_n}^{x_n+h} x\sin(x)\mathrm{d}x + b_i(x_n, x_n + h)\cos x \,\Big|_{x_n}^{x_n+h}\right\}$$

$$\boxed{= \frac{1}{h}\sum_n a_i(x_n, x_n + h)\,[-x\cos(x) + \sin x + b_i(x_n, x_n + h)\cos x]_{x_n}^{x_n+h}}$$