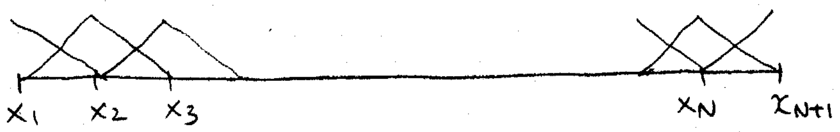
2. Problem Formulation



BVP

$$R(x) = \frac{d}{dx}\left((1+a\theta)\frac{dT}{dx}\right) = 0 \qquad \theta(0) = 0, \quad \theta(1) = 1$$

$$\theta(x) = \sum_{i=1}^{N+1} \alpha_i \Phi^i(x) \quad \text{— Linear Basis}$$

Galerkin eqn

$$\int_0^1 \Phi^i(x)\, R(x)\, dx = 0 \qquad i = 1, \cdots N+1$$

$$I = \int_0^1 \underset{u}{\Phi^i(x)} \frac{d}{dx}\underset{v'}{\left((1+a\theta)\frac{d\theta}{dx}\right)} dx$$

$$= \underbrace{\Phi^i(x)\,(1+a\theta)\frac{d\theta}{dx}\Big]_0^1}_{\text{Flux}} - \int_0^1 \frac{d\Phi^i}{dx}(1+a\theta)\frac{d\theta}{dx}\,dx$$

B.C's Look at $\theta(0) = 0$

$$\theta(0) = \sum_{i=1}^{N+1} \alpha_i \Phi^i(0)$$

$$= \alpha_1$$

Set Boundary data

$$\theta(0) = 0 \rightarrow \alpha_1 = 0$$

$$\theta(1) = 1 \rightarrow \alpha_{N+1} = 1$$

Satisfy essential BC's exactly

$$\theta(x) = 0 \cdot \Phi^1(x) + \sum_{i=2}^{N} \alpha_i \Phi^i(x) + 1 \cdot \Phi^{N+1}(x)$$

Look at Galerkin Eqn

$i = 2 \cdots N$

$$I = \underbrace{\left[\Phi^i(x)\,(1+a\theta)\,\frac{d\theta}{dx} \right]_0^1}_{=\,0} - \int_0^1 \frac{d\Phi^i}{dx}\,(1+a\theta)\,\frac{d\theta}{dx}\,dx = 0$$

since $\left. \begin{array}{l} \Phi^i(1) = 0 \\ \Phi^i(0) = 0 \end{array} \right\}$ for $i \neq 1, N+1$

Special case $a = 0$.

$$\int_0^1 \frac{d\Phi^i}{dx}\frac{d\theta}{dx}\,dx = \int_0^1 \frac{d\Phi^i}{dx}\left[\frac{d\Phi^{N+1}}{dx} + \sum_{j=2}^{N} \alpha_j \frac{d\Phi^j}{dx} \right] dx = 0$$

$$\int_0^1 \sum_{j=2}^{N} \frac{d\Phi^i}{dx}\frac{d\Phi^j}{dx}\,\alpha_j\,dx = -\int_0^1 \frac{d\Phi^i}{dx}\frac{d\Phi^{N+1}}{dx}\,dx$$

$$\sum_{j=1}^{N} \alpha_j \int_0^1 \frac{d\Phi^i}{dx}\frac{d\Phi^j}{dx}\,dx = -\int_0^1 \frac{d\Phi^i}{dx}\frac{d\Phi^{N+1}}{dx}\,dx$$

$i = 2 \cdots N.$

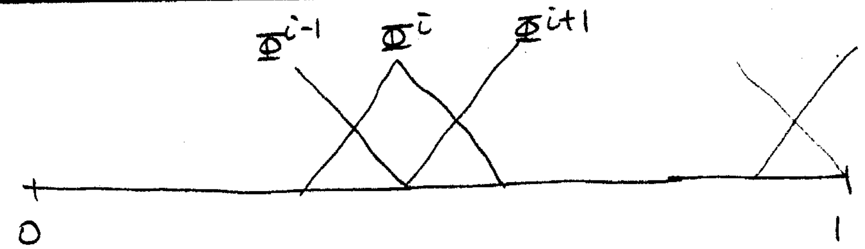
$$\sum A_{ij}\,\alpha_j = b_i$$

$$\underline{\underline{A}}\,\underline{\alpha} = \underline{b} \qquad \underline{\alpha}^T = (\alpha_2, \alpha_3 \cdots \alpha_N)$$

does not include α_1, α_{N+1}

$$A_{ij} = \int_0^1 \frac{d\Phi^i}{dx}\frac{d\Phi^j}{dx}\,dx$$

$$b_i = -\int_0^1 \frac{d\Phi^i}{dx}\frac{d\Phi^{N+1}}{dx}\,dx$$



compact support

Sparse matrix

$A_{ij} \neq 0 \quad \text{if } j = i, i-1, i+1$ > Tridiagonal matrix

$A_{ij} = 0 \quad \text{otherwise}$

$b_i \neq 0 \quad i = N,$

$ = 0 \quad \text{otherwise}$

Evaluate A_{ij} $\quad j = i, i-1, i+1$

$$\int_0^1 \frac{d\Phi^i}{dx}\frac{d\Phi^j}{dx}\,dx = \sum_{k=1}^{N} \int_{x_k}^{x_{k+1}} \frac{d\Phi^i}{dx}\frac{d\Phi^j}{dx}\,dx$$

i, j are combinations of $k, k+1$

<u>Map it</u>

$$\int_{x_k}^{x_{k+1}} \frac{d\Phi^i}{dx}\frac{d\Phi^j}{dx}\,dx = \int_{-1}^{1} \left(\frac{d\Phi^i}{d\xi}\right)\left(\frac{d\xi}{dx}\right)\left(\frac{d\Phi^j}{d\xi}\right)\cancel{\left(\frac{d\xi}{dx}\right)}\cancel{\left(\frac{dx}{d\xi}\right)}d\xi$$

$\Rightarrow$ Quadrature

$$A_{32} = \int_0^1 \frac{d\Phi^3}{dx}\frac{d\Phi^2}{dx}\,dx = \int_{x_2}^{x_3} \frac{d\Phi^3}{dx}\frac{d\Phi^2}{dx}\,dx$$

$$A_{33} = \int_0^1 \frac{d\Phi^3}{dx}\frac{d\Phi^3}{dx}\,dx = \int_{x_2}^{x_3} \frac{d\Phi^3}{dx}\frac{d\Phi^3}{dx}\,dx + \int_{x_3}^{x_4} \frac{d\Phi^3}{dx}\frac{d\Phi^3}{dx}\,dx$$

* Numerical Quadrature

$$\int_a^b f(x)\,dx \cong \sum_{i=1}^{n} c_i f(x_i)$$

Newton-Cotes formula (equal space)

$n=2$ Trapezoidal rule

$$\int_{x_0}^{x_0+h} f(x)\,dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right]$$

$n=3$ Simpson's rule

$$\int_{x_0}^{x_0+2h} f(x)\,dx = \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right]$$

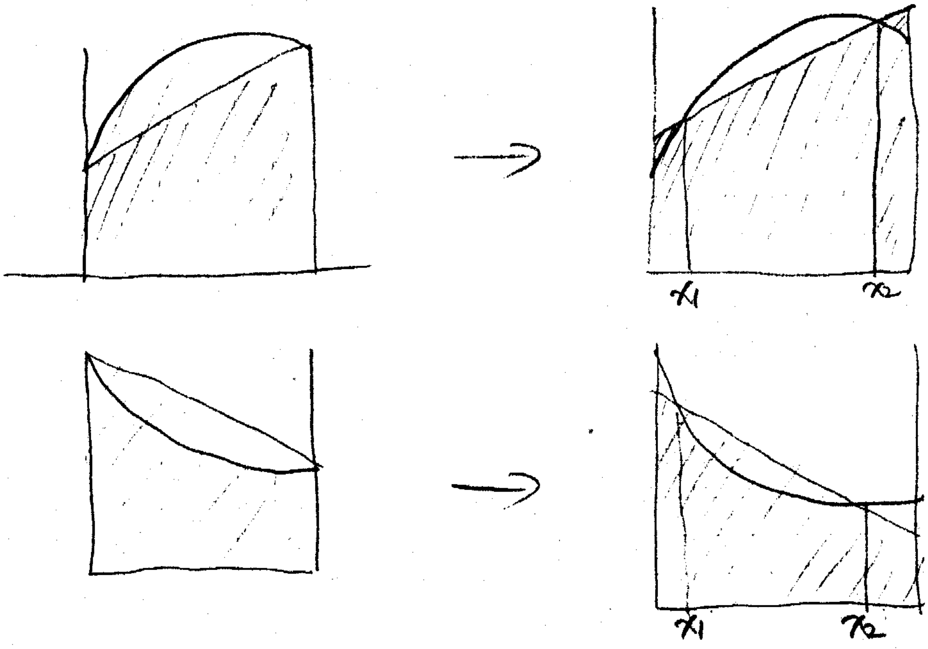
$n=4$ Simpson's three-eighths rule

$$\int_{x_0}^{x_0+3h} f(x)\,dx = \frac{3}{8}h\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right]$$

$n=5$

$$\int_{x_0}^{x_0+4h} f(x)\,dx = \frac{2h}{45}\left[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\right]$$

Gaussian Quddrature



Trapezoidal rule   Gaussian Quddrature

exact $p=1$ $p=?$

$$\int_{-1}^{1} f(x)\,dx = \sum_{i=1}^{n} c_i f(x_i)$$

$\sum_{i=1}^{n} c_i f(x_i)$: unknown $2n$

$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots a_m x^m$ unknown $m+1$

$2n = m+1 \qquad m = 2n-1$

$n=2 \longrightarrow p=3.$

$$\int_{-1}^{1} a_0 + a_1 x + a_2 x^2 + a_3 x^3 \, dx = c_1 f(x_1) + c_2 f(x_2)$$

$$a_0 \int_{-1}^{1} 1 \cdot dx + a_1 \int_{-1}^{1} x\,dx + a_2 \int_{-1}^{1} x^2 dx + a_3 \int_{-1}^{1} x^3 dx$$
$$= c_1 f(x_1) + c_2 f(x_2)$$

Exact when $f(x) = 1,\ x,\ x^2,\ x^3$.

$$c_1 + c_2 = \int_{-1}^{1} 1 \cdot dx = 2$$
$$c_1 \cdot x_1 + c_2 x_2 = \int_{-1}^{1} x\,dx = 0$$
$$c_1 x_1^2 + c_2 x_2^2 = \int_{-1}^{1} x^2 dx = \frac{2}{3}$$
$$c_1 x_1^3 + c_2 x_2^3 = \int_{-1}^{1} x^3 dx = 0.$$

$$\rightarrow\ c_1 = 1,\ c_2 = 1,\ x_1 = -\frac{1}{\sqrt{3}},\ x_2 = \frac{1}{\sqrt{3}}$$

$$\int_{-1}^{1} f(x)\,dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

exact up to $p = 3$.

$n = 3$. (exact upto $p = 5$)

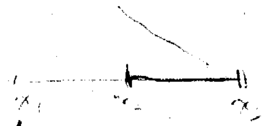
$$\int_{-1}^{1} f(x)\,dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

Roots of $P_n(x)$

Algorithm

1. Subdivide domain into elements $\rightarrow \{x_k\}$

2. Construct $\underline{\underline{A}}$ & $\underline{b}$



- Iterate over each element

  Construct pieces of $\underline{\underline{A}}$ & $\underline{b}$

- Integration loop.

  - $i = 1, 2$ $\quad [\Phi^i]$
  - $j = 1, 2$ $\quad [\Phi^j]$

$$\bar{A}_{ij} = \int_{x_k}^{x_{k+1}} \frac{d\Phi^i}{dx} \frac{d\Phi^j}{dx} \, dx$$

continue.

ex $\quad e = 2$

$$\begin{matrix} A_{23} & A_{22} \\ A_{32} & A_{33} \end{matrix}$$

$\bar{A} \in \mathbb{R}^{2\times 2}$

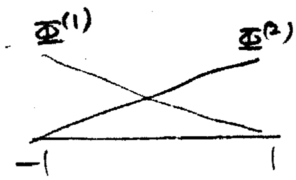
local matrix

Store $\bar{A}_{ij} \Rightarrow A_{ij}$

Global matrix.

3. Solve $\underline{\underline{A}}\,\underline{\alpha} = \underline{b}$

On the unit element



$$\bar{C}_{ij} = \int_{-1}^{1} \frac{d\Phi^{(i)}}{d\xi} \frac{d\Phi^{(j)}}{d\xi} \, d\xi$$

$$C_{11} = \int_{-1}^{1} \left(\frac{d\Phi^{(1)}}{d\xi}\right)^2 d\xi > 0$$

$C_{12} < 0, \quad C_{21} < 0, \quad C_{22} > 0.$

$a \neq 0$

$$\int_0^1 \frac{d\Phi^i}{dx} (1+a\theta) \frac{d\theta}{dx} \, dx = 0$$

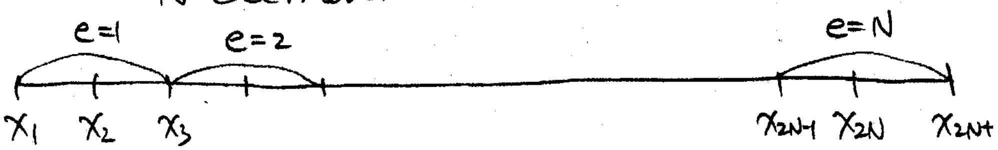
$$\int_0^1 \frac{d\Phi^i}{dx} \left(1 + a\left(\sum_{j=2}^{N} \alpha_j \Phi^j + \Phi^{N+1}\right)\right)\left(\frac{d\Phi^{N+1}}{dx} + \sum_{j=2}^{N} \alpha_j \frac{d\Phi^j}{dx}\right) dx$$
$= 0$

$\underline{R}(\underline{\alpha}) = 0$ non linear problem

Newton's method.

* Quadratic Basis Function

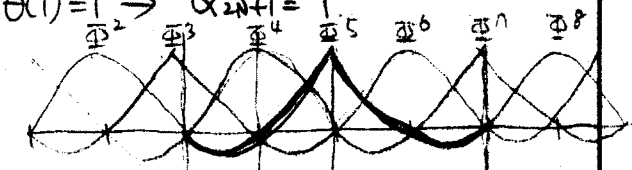
N element



Example Problem.

$$\theta(x) = \alpha_1 \Phi^1(x) + \sum_{i=2}^{2N} \alpha_i \Phi^i(x) + \alpha_{2N+1} \Phi^{2N+1}(x)$$

$\theta(0)=0 \rightarrow \alpha_1 = 0$ $\theta(1)=1 \rightarrow \alpha_{2N+1} = 1$



$\underline{\underline{A}}\, \underline{\alpha} = \underline{b}$

$$A_{ij} = \int_0^1 \frac{\partial \Phi^i}{\partial x} \frac{\partial \Phi^j}{\partial x} dx$$

A_{5j} A_{55} A_{54} A_{56} A_{53} A_{57} ~ non-zero

$A_{ij} \neq 0$ A_{ii}, $A_{i,i+1}$, $A_{i,i-1}$, $A_{i,i+2}$, $A_{i,i-2}$

$= 0$ otherwise.

3. FE with Flux BC

Ex 1

$$\frac{\partial}{\partial x}\left[(1+\theta)\frac{\partial \theta}{\partial x}\right] = f(x)$$

$$\theta(0) = 0 \qquad \text{(essential)}$$

$$(1+\theta)\frac{\partial \theta}{\partial x} + b\theta = q \quad \text{at } x=1 \qquad \text{(mixed)}$$

Lagrangian Quadratic Basis $\quad 0 \le x \le 1$

$$\theta(x) = \alpha_1 \Phi^1(x) + \sum_{i=2}^{2N+1} \alpha_i \Phi^i(x)$$

$$\alpha_1 = 0 \Leftarrow \theta(0) = 0.$$

Galerkin Eq.

$$\int_0^1 \Phi^i \left[\frac{\partial}{\partial x}\left((1+\theta)\frac{\partial \theta}{\partial x}\right) - f(x)\right] dx = 0 \qquad i = 2, \cdots 2N+1$$

$$\int_0^1 \frac{\partial}{\partial x}\left[\Phi^i (1+\theta)\frac{\partial \theta}{\partial x}\right] - \frac{\partial \Phi^i}{\partial x}\frac{\partial \theta}{\partial x}(1+\theta)\, dx$$

$$- \int_0^1 \Phi^i f(x)\, dx = 0$$

$$\left[\Phi^i(x)(1+\theta)\frac{\partial \theta}{\partial x}\right]_0^1 - \int_0^1 \frac{\partial \Phi^i}{\partial x}\frac{\partial \theta}{\partial x}(1+\theta)\, dx = \int_0 \Phi^i f(x) dx$$

forcing term

$i = 2, \cdots 2N+1$

$$\left[\Phi^i(1)(q - b\theta)\right]_{x=1} - \left.\Phi^i(0)(1+\theta)\frac{\partial \theta}{\partial x}\right]_{x=0}$$

$$- \int_0^1 \frac{\partial \Phi^i}{\partial x}\frac{\partial \theta}{\partial x}(1+\theta)\, dx = \int_0^1 \Phi^i f(x)\, dx$$

$\Phi^i(1) \neq 0$ only if $i = 2N+1$

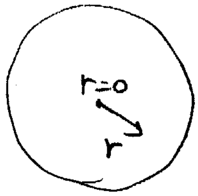
Substitute $\quad \theta = \sum_{j=2}^{2N+1} \alpha_j \Phi^j \implies \underline{R}(\underline{\alpha}) = \underline{0}$

Ex 2. Catalyst sphere

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dc}{dr}\right) = \phi^2 R(c)$$

$r=0 \quad \frac{dc}{dr} = 0$

$r=1 \quad -\frac{dc}{dr} = Bim(c-1)$



$c=1$

FE with Quadratic Basis Function (N elems)

$$c(r) = \sum_{i=1}^{2N+1} \alpha_i \Phi^i(r)$$

No essential BC.

$\rightarrow$ Apply Galerkin using entire expansion.

$$\int_0^1 \Phi^i(r)\left\{\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dc}{dr}\right) - \phi^2 R(c)\right\}\underbrace{r^2 dr}_{\text{correct volume element}} = 0$$

$$\int_0^1 \Phi^i(r)\cancel{\frac{1}{r^2}}\frac{d}{dr}\left(r^2\frac{dc}{dr}\right)\cancel{r^2}dr$$

$$= r^2\Phi^i\frac{dc}{dr}\Big]_0^1 - \int_0^1 r^2\frac{d\Phi^i}{dr}\frac{dc}{dr}dr$$

$$= r^2\Phi^i\frac{dc}{dr}\Big]_{r=1} - r^2\Phi^i\frac{dc}{dr}\Big]_{r=0} - \int_0^1 r^2\frac{d\Phi^i}{dr}\frac{dc}{dr}dr$$

$$= \Phi^i(1)\frac{dc}{dr}\Big|_{r=1} - \int_0^1\frac{d\Phi^i}{dr}\frac{dc}{dr}r^2dr$$

$$= \Phi^i(1)\,Bim(1-c(1)) - \int_0^1\frac{d\Phi^i}{dr}\frac{dc}{dr}r^2dr$$

$$-\int_0^1\left[\frac{d\Phi^i}{dr}\frac{dc}{dr} + \Phi^i(r)\phi^2R(c)\right]r^2dr + \Phi^i(1)\,Bim(1-c(1)) = 0$$

$$\Rightarrow \quad \underline{R}(\underline{\alpha}) = \underline{0} \qquad \underline{\alpha}^T = (\alpha_1 \cdots \alpha_{2N+1})$$

For linear kinetics

$$R(c) = c$$

$$\underline{R}(\underline{\alpha}) = -\int_0^1 \left(\frac{d\Phi^i}{dr} \frac{dc}{dr} + \phi^2 c\, \Phi^i \right) r^2 dr$$

$$+ \Phi^i(1)\, Bim\, (1 - c(1)) = 0$$

Substituting

$$c = \sum_{j=1}^{2N+1} \alpha_j \Phi^j$$

$$\underline{\underline{A}}\, \underline{\alpha} = \underline{b} \qquad b_i = -\Phi^i(1)\, Bim$$

$$A_{ij} = -\int_0^1 \left[\frac{d\Phi^i}{dr} \frac{d\Phi^j}{dr} + \phi^2 \Phi^i \Phi^j \right] r^2 dr$$

$$- \Phi^i(1)\, Bim\, \Phi^j(1)$$