NUEN 618

Multiphysics computations in nuclear science and engineering

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Outline

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Diffusion equation

Diffusion

$$-\vec{\nabla}\cdot D\vec{\nabla}u + \sigma_a u = q \qquad \forall \vec{r} \in \mathcal{D} \tag{1}$$

Boundary conditions on $\partial\mathcal{D}$

$$u = f \qquad \forall \vec{r} \in \partial\mathcal{D}^d \tag{2}$$

$$-D\partial_n u = -D\vec{\nabla}u \cdot \vec{n} = g \qquad \forall \vec{r} \in \partial\mathcal{D}^n \tag{3}$$

$$au + b\partial_n u = h \qquad \forall \vec{r} \in \partial\mathcal{D}^r \tag{4}$$

(5)

Outline

1. Weak form approximation
   - Model problem
   - Finite element approximation of u
   - Weak formulation
   - Linear system
2. Implementation
   - Assembling the matrix
   - Numerical integration

Finite element approximation of u

1D mesh

N segments

$$x_L = x_1 < x_2 < \ldots < x_j < \ldots < x_{N+1} = x_R \tag{6}$$

Piecewise linear approximation

$$u \approx u_h = \sum_j \varphi_j u_j \tag{7}$$

φ_j

$\varphi_j(x) = 0$ for $x < x_{j-1}$ and $x > x_{j+1}$;
For $x \in [x_{j-1}, x_{j+1}]$, piecewise linear such that

$$\varphi_j(x_{j-1}) = 0 \tag{8}$$

$$\varphi_j(x_j) = 1 \tag{9}$$

$$\varphi_j(x_{j+1}) = 0 \tag{10}$$

Point-wise residual is not 0

Residual

$$-\vec{\nabla}\cdot D\vec{\nabla}u_h + \sigma_a u_h - q \neq 0 \tag{11}$$

Furthermore, we have **one** equation but $N+1$ unknowns (the u_j's).

Multiply residual by φ_i

$$-\varphi_i\vec{\nabla}\cdot D\vec{\nabla}u_h + \varphi_i\sigma_a u_h - \varphi_i q \neq 0 \tag{12}$$

for $j = 1, \ldots, N+1$

Require that the residual be zero in an integral sense

$$\int_{\mathcal{D}} \left(-\varphi_i\vec{\nabla}\cdot D\vec{\nabla}u_h + \varphi_i\sigma_a u_h - \varphi_i q\right) = 0 \tag{13}$$

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Weak formulation

double differentiation?

$\vec{\nabla} \cdot D \vec{\nabla} u_h$ may not exist for the piece-wise linear function u_h
Idea: integrate by parts
This will also make the Neumann and Robin boundary conditions come in play (they are called natural BC)

Integration by parts

$$\int_{\mathcal{D}} \vec{\nabla} \varphi_i D \vec{\nabla} u_h + \varphi_i \sigma_a u_h - \int_{\partial \mathcal{D}} \varphi_i D \partial_n u_h = \int_{\mathcal{D}} \varphi_i q \tag{14}$$

Boundary terms

On $\partial\mathcal{D}^n$,

$$-\int_{\partial\mathcal{D}^n} \varphi_i D\partial_n u_h = \int_{\partial\mathcal{D}^n} \varphi_i g \tag{15}$$

[fully goes to the rhs]

On $\partial\mathcal{D}^r$,

$$-\int_{\partial\mathcal{D}^n} \varphi_i D\partial_n u_h = \int_{\partial\mathcal{D}^n} \varphi_i D(au_h - h)/b \tag{16}$$

[some portion still depends on u_h, they stay on the lhs; some go to the rhs]

Outline

Linear system

It should be obvious that

$$\int_{\mathcal{D}} \vec{\nabla}\varphi_i D \vec{\nabla} u_h + \varphi_i \sigma_a u_h - \int_{\partial\mathcal{D}} \varphi_i D \partial_n u_h = \int_{\mathcal{D}} \varphi_i q \tag{17}$$

is equivalent to

$$AU = S \tag{18}$$

where the matrix entries are

$$a_{ij} = \int_{\mathcal{D}} \vec{\nabla}\varphi_i D \vec{\nabla}\varphi_j + \varphi_i \sigma_a \varphi_j + BC \tag{19}$$

and the rhs entries are

$$s_i = \int_{\mathcal{D}} \varphi_i q + BC \tag{20}$$

Outline

Assembling the matrix

Assembling the matrix

is **NOT** done row by row though it would seem easy on orthogonal grids.

In 1D, with a piece-wise linear approximation, non-zero entries are found on row i only for $j = i-1, i, i+1$, that is, only when φ_i and φ_j are both non-zero!!!

In general, A is a sparse matrix.

Assembling the matrix

Assembling the matrix

is **done** element by element.

$$a_{ij} = \int_{\mathcal{D}} \vec{\nabla}\varphi_i D \vec{\nabla}\varphi_j + \varphi_i \sigma_a \varphi_j = \sum_{K \in \mathcal{D}} \int_K \vec{\nabla}\varphi_i D \vec{\nabla}\varphi_j + \varphi_i \sigma_a \varphi_j \qquad (21)$$

Only look at a single element

$$\int_K \vec{\nabla}\varphi_i D \vec{\nabla}\varphi_j + \varphi_i \sigma_a \varphi_j \qquad (22)$$

In 1D, with a piece-wise linear approximation, this is a 2×2 elementary matrix: there are only two φ_i and two φ_j that are not zero for a given element K.

Connectivity array

For a given element K, the list of indices i, j such that $a_{ij} \neq 0$ is called the connectivity array.

Assembling the matrix

Add the element's contribution to A

Obvious, there is a summation over K so we add the contribution of each element K to the global matrix A ...

In 1D, for element $x \in [x_i, x_{i+1}]$, this 2×2 element matrix gets added to rows i and $i+1$ and columns i and $i+1$ of A. This is the connectivity array for 1D linear FEM.

It is easy to see how such a process can be effective for multi-D arbitrary possibly distorted grids with arbitrary polynomial trial spaces.

Outline

Numerical integration

Numerical integration

Each element K can be different, so how do we compute

$$\int_K \vec{\nabla}\varphi_i D \vec{\nabla}\varphi_j + \varphi_i \sigma_a \varphi_j \tag{23}$$

with integration bounds changing all of the time ????

Reference element

We do a change of variable to move the integration from K to $\hat{K}$, a reference element. In 1D, $\hat{K}$ is the $[-1, +1]$ interval.

$$\begin{aligned}\int_{x_i}^{x_{i+1}} \frac{d\varphi_i}{dx} D(x) \frac{d\varphi_j}{dx} + \varphi_i \sigma_a(x) \varphi_j \\ = \int_{-1}^{+1} \left(\frac{2^2}{(\Delta x_i)^2} \frac{d\hat{\varphi}_i}{d\hat{x}} D(\hat{x}) \frac{d\hat{\varphi}_j}{d\hat{x}} + \hat{\varphi}_i(\hat{x}) \sigma_a(\hat{x}) \hat{\varphi}_j(\hat{x}) \right) \frac{\Delta x_i}{2} d\hat{x}\end{aligned} \tag{24}$$

Numerical quadrature

Numerical quadrature

$$\int_{-1}^{+1} \left(\frac{4}{(\Delta x_i)^2} \frac{d\hat{\varphi}_i}{d\hat{x}} D(\hat{x}) \frac{d\hat{\varphi}_j}{d\hat{x}} + \hat{\varphi}_i(\hat{x}) \sigma_a(\hat{x}) \hat{\varphi}_j(\hat{x}) \right) \frac{\Delta x_i}{2} d\hat{x} \tag{25}$$

is computed using a quadrature (typically Gauss-Legendre in 1D)

$$\sum_q w_q \left(\frac{2}{\Delta x_i} \left. \frac{d\hat{\varphi}_i}{d\hat{x}} \right|_{\hat{x}_q} D(\hat{x}_q) \left. \frac{d\hat{\varphi}_j}{d\hat{x}} \right|_{\hat{x}_q} + \hat{\varphi}_i(\hat{x}_q) \sigma_a(\hat{x}_q) \hat{\varphi}_j(\hat{x}_q) \frac{\Delta x_i}{2} \right) \tag{26}$$