

The advection-diffusion-reaction equation

$$\frac{\partial c}{\partial t} + \underline{u} \cdot \nabla c = D \nabla^2 c + \lambda c + f \quad (1)$$

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 advection diffusion linear reaction source

Simplify

- static, not transient
- no fluid flow
- no reaction processes

$$\Rightarrow D \nabla^2 c + f = 0 \quad (2)$$

Move to a 1D situation:

$$D \frac{\partial^2 c}{\partial x^2} + f = 0 \quad (3)$$

This is the static/steady state diffusion equation.

For $f = 0$ known as Laplace's equation

For $f \neq 0$ known as Poisson's equation

We have written here what is known as the strong form of the equation.

Want to solve it on the following domain:



So, how do we solve :

5.2

$$D \frac{\partial^2 c}{\partial x^2} + f = 0 \quad ? \quad (4)$$

Suppose we had an approximate solution to eqn(4), given by c^A

Substituting c^A into (4) gives:

$$D \frac{\partial^2 c^A}{\partial x^2} + f = R \quad (5)$$

R = Residual i.e. the overall error in the equation.

If $c^A = c$, then $R = 0$.

\therefore Aim is to minimise R , to make c^A as close to c as possible. How?

Method of weighted residuals.

1. Multiply by a weighting function, v
2. Integrate over domain

$$\Rightarrow \left[\int_0^1 v \cdot \left(D \frac{\partial^2 c^A}{\partial x^2} + f \right) dx = 0 \right] \quad (7)$$

$$\int_0^1 R \cdot v \cdot dx = 0 \quad (6)$$

Weighted average of the error, to distribute it evenly over the domain

[Show slides on approximating data points]

Reminder: integration by parts.

5.3

Functions $u(x)$ and $w(x)$

Derivatives: $u'(x) = \frac{du}{dx}$, $w'(x) = \frac{dw}{dx}$.

$$\int u(x) w'(x) dx = u(x) w(x) - \int w(x) u'(x) dx. \quad (8)$$

In eqn (7) identify terms $u(x)$ and $w(x)$.

$$u(x) = v \quad \text{and} \quad w(x) = D \frac{\partial c}{\partial x}$$

$$\therefore \int_0^1 v \cdot D \frac{\partial^2 c}{\partial x^2} dx = \left[v \cdot D \frac{\partial c}{\partial x} \right]_0^1 - \int_0^1 D \frac{\partial c}{\partial x} \cdot \frac{\partial v}{\partial x} dx. \quad (9)$$

$$\Rightarrow - \int_0^1 D \frac{\partial c}{\partial x} \cdot \frac{\partial v}{\partial x} dx + \left[v \cdot D \frac{\partial c}{\partial x} \right]_0^1 + \int_0^1 v f dx = 0 \quad (10)$$

$$\Rightarrow \underbrace{\int_0^1 D \frac{\partial c}{\partial x} \cdot \frac{\partial v}{\partial x} dx}_{\text{unknown}} = \underbrace{\int_0^1 v \cdot f dx + \left[v \cdot D \frac{\partial c}{\partial x} \right]_0^1}_{\text{known}} \quad (11)$$

Note

$$\left[v \cdot D \frac{\partial c}{\partial x} \right]_0^1 = \text{Neumann or flux boundary condition.}$$

Fickian
diffusive
flux

i.e. diffusive flux at the
boundaries $x=0$ and $x=1$

What happened to the finite element method?

5.4

We have the domain:



Split into 3 equal elements.



Perform integral in each element i.e.

$$\int_0^1 dx = \int_0^{1/3} dx + \int_{1/3}^{2/3} dx + \int_{2/3}^1 dx.$$

How to integrate in 1 element?

Represent space, x , and solution, c , using the basis functions ψ_0 and ψ_1 introduced in Lecture 4

$$c = c_0 \psi_0(\xi) + c_1 \psi_1(\xi)$$

$$x = x_0 \psi_0(\xi) + x_1 \psi_1(\xi)$$

$$\text{where } \psi_0 = \frac{1-\xi}{2}, \quad \psi_1 = \frac{1+\xi}{2}$$

[Show slide]

Equally, the inverse holds:

5.5

$$\xi(x) = 2 \left(\frac{x - x_0}{x_1 - x_0} \right) - 1 \quad \text{For } x \text{ in that element between } x_0 \text{ and } x_1$$

Before integrating, need to define v .

The Galerkin Assumption

Choose v to be the basis functions ψ_0 and ψ_1 , i.e. same functions that represent the solution.

This can be thought of as being "optimal" for reducing error.

Finally, we perform integration in ξ coordinate rather than x .

$$\int_{x_0}^{x_1} dx = \int_{-1}^1 J d\xi$$

where $J = \left| \frac{dx}{d\xi} \right|$ is the Jacobian or

scaling between coordinates.

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