Lecture 12: Solving Transient Problems.

Going back to Lecture 3, a transient diffusion-reaction is:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + \lambda c + f \qquad (1)$$

Thus far have only looked at static or steady-state problems, where $\frac{\partial c}{\partial t} = 0$, i.e.

$$D\frac{\partial^2 c}{\partial x^2} + \lambda c + f = 0. \qquad (2)$$

Now would like to be able to solve the transient version given in Eqn (1).

First we will consider a general strategy for solving these transient problems, namely time integration or time stepping schemes, before applying them to finite element formulations.

Consider a general transient equation:

$$\frac{\partial c}{\partial t} = F(x, c, t) \qquad (3)$$

Integrating both sides of Eqn (3) w.r.t t between the times $t = t_n$ and $t = {}_{n+1}$

$$\int_{t_n}^{t_{n+1}} \frac{\partial c}{\partial t}\, dt = \int_{t_n}^{t_{n+1}} F(x, c, t)\, dt \qquad (4)$$

Eqn (4) becomes:

$$c(t_{n+1}) - c(t_n) = \int_{t_n}^{t_{n+1}} F(x,c,t)\,dt \qquad (5)$$

Using the trapezium rule on the RHS of Eqn (5).

$$\int_{t_n}^{t_{n+1}} F(x,c,t)\,dt = \frac{1}{2}\underbrace{\left(t_{n+1} - t_n\right)}_{\text{width}}\underbrace{\left(F(x,c,t_{n+1}) + F(x,c,t_n)\right)}_{\text{heights}}$$

Write $t_{n+1} - t_n$ as Δt, i.e. this is the time step.

$$\frac{c(t_{n+1}) - c(t_n)}{\Delta t} = \frac{1}{2}\left(F^{n+1} + F^{n}\right) \qquad \theta = 1/2$$

This is called the Crank-Nicolson scheme

Alternative schemes exist as follows:

$$\frac{c(t_{n+1}) - c(t_n)}{\Delta t} = F^{n}(x,c,t) \qquad \underline{\text{Forward Euler}} \quad \theta = 0$$

$$\frac{c(t_{n+1}) - c(t_n)}{\Delta t} = F^{n+1}(x,c,t) \qquad \underline{\text{Backward Euler}} \quad \theta = 1$$

General θ scheme:

$$\frac{c(t_{n+1}) - c(t_n)}{\Delta t} = \theta F^{n+1}(x,c,t) + (1-\theta) F^{n}(x,c,t)$$

Write the weighted residual form of Eqn. (1)

$$\int \left(\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} - \lambda c - f \right) v \, . \, dx = 0$$

Use the domain $x = [0,1]$ and integrate by parts:

$$\int_0^1 \left(v . \frac{\partial c}{\partial t} + D\frac{\partial c}{\partial x} . \frac{\partial v}{\partial x} - \lambda c v \right) dx = \int_0^1 f v \, dx + \left[v D \frac{\partial c}{\partial x} \right]_0^1$$

Only new term is the temporal derivative.

$v . \dfrac{\partial c}{\partial t}$ — which we can represent using the basis functions ψ_n

i.e. ~~[illegible]~~, $v = \psi_m$, $c = c_n \psi_n$

The local element matrix for this is therefore:

$$\int_{-1}^{1} \frac{d}{dt}(c_n \psi_n) . \psi_m \, J \, d\xi$$

Time derivative brought outside integral and $\dfrac{d}{dt}(\psi_n) = 0$

$$\frac{dc_n}{dt} \int_{-1}^{1} \psi_n \psi_m \, J \, d\xi$$

Now need to approximate the time derivative as:

$$\frac{dc_n}{dt} = \frac{c_n^{n+1} - c_n^{n}}{\Delta t}$$

where superscripts $n+1$ and n represent $c_n(t_{n+1})$ and $c_n(t_n)$

The other local element matrices were derived in previous lectures. We can gather them together and write the equation using the General θ scheme from page 12.2.

The element matrix that multiplies the time derivative we call the element mass matrix and assemble them into a global mass matrix, M

The local and global matrices that represent the diffusion and reaction terms we call the local and global stiffness matrices, K

$$M_{element} = \int_{-1}^{1} \psi_n \psi_m J \, d\xi$$

Note these are almost the same which reduces coding effort.

$$K_{element} = \int_{-1}^{1} D \frac{\partial \psi_n}{\partial \xi} \cdot \frac{\partial \xi}{\partial x} \cdot \frac{\partial \psi_m}{\partial \xi} \cdot \frac{\partial \xi}{\partial x} J \cdot d\xi$$

$$- \int_{-1}^{1} \lambda \psi_n \psi_m J \cdot d\xi$$

Writing our equation in terms of the global M, K

$$M \frac{\underline{c}^{n+1} - \underline{c}^{n}}{\Delta t} + K\left[\theta \underline{c}^{n+1} + (1-\theta)\underline{c}^{n}\right] = RHS$$

where $\underline{c}^n, \underline{c}^{n+1}$ are the global solution vectors at times t and $t+\Delta t$.

The RHS receives the same θ scheme:

$$RHS = \theta \underline{F}^{n+1} + (1-\theta)\underline{F}^{n} + \theta \underline{NBc}^{n+1} + (1-\theta)\underline{NBc}^{n}$$

$\underline{F}$: global vector for source term f

$\underline{NBc}$: global vector for Neumann Boundary Condition

Now need to rearrange our equation so that the unknowns $\underline{c}^{n+1}$ are on the LHS and the knowns $\underline{c}^{n}$ (calculated in the previous iteration) are on the RHS.

Also multiply by Δt, so we have:

$$[M + \theta \Delta t K]\underline{c}^{n+1} = [M - (1-\theta)\Delta t K]\underline{c}^{n} + \Delta t \theta [\underline{F}^{n+1} + \underline{NBc}^{n+1}] + \Delta t (1-\theta)[\underline{F}^{n} + \underline{NBc}^{n}]$$

Apply Dirichlet boundary conditions for $\underline{c}^{n+1}$ as before and solve this same matrix system using the same command in Matlab.

For the specific case of Crank-Nicolson i.e. $\theta = 1/2$, this is:

$$\left[M + \tfrac{1}{2}\Delta t K\right]\underline{c}^{n+1} = \left[M - \tfrac{1}{2}\Delta t K\right]\underline{c}^{n} + \tfrac{1}{2}\Delta t\left[\underline{F}^{n+1} + \underline{F}^{n} + \underline{NBc}^{n+1} + \underline{NBc}^{n}\right]$$

Solving this system at successive time steps will produce a series of $\underline{c}$ vectors as before, but one for each time step in the simulation.

Note that as $t \to \infty$ (in practice much before this) solving the transient problem for static boundary conditions will reach the solution found by solving the static version of this equation.

Note also that all the matrices and vectors calculated for solving the static problem using FEM can be reused here, they are just used in a slightly different form.