Problem Sheet 4 - The FDM and FEM

1. Several of the questions on this sheet are about solving the ODE

$$\frac{d^2F}{dx^2} + F = 0 \tag{1}$$

with boundary conditions $F(0) = 0$ and $F(1) = 1$, using the FDM and the FEM. For the purposes of comparison with later approximations, first find the analytic solution of the ODE at $x = 0.5$

2. Calculate the value the FDM gives for the solution to (1) with a single unknown grid value when the grid spacing is $h = 0.5$. Write down the difference equations needed to find the FDM solution $f(0.5)$ for regular grids with $h = 0.25$ and $h = 0.125$. If you are happy doing the computing, find $f(0.5)$ for these grids, and look at the convergence of the FDM answer towards the true answer as a function of h.

3. In cylindrical coordinates, Laplaces's equation is

$$\nabla^2\Psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\phi^2} + \frac{\partial^2\Psi}{\partial z^2} = 0.$$

Show that any problem with cylindrical symmetry in which Laplace's equation is obeyed may be modelled using the finite difference method on a 2-d rectangular grid. Derive the difference equation for a general point (i, j) in your grid.

4. Use variational methods to show that the functional

$$I[f] = \int_0^1 \left[\left(\frac{df}{dx}\right)^2 - f^2\right] dx$$

is minimized by the solution of equation (1) in Q1, with the same Dirichlet conditions at $x = 0$ and $x = 1$. Evaluate I for the exact solution to (1), and compare this with the value of I for a simple trial function $f(x) = x$ (which satisfies the Dirichlet conditions).

5. Let us try a slightly better FEM solution to the problem in Q4. Let us suppose that we have a single node at $x = 0.5$ with (unknown) value ϕ, and linear interpolants. Verify that the two "elemental" trial functions in this case are $2\phi x$ for $0 \le x \le 0.5$ and $2(1-\phi)x + (2\phi - 1)$ for $0.5 \le \phi \le 1$. Then show that the value of the functional in Q4 for this trial function is

$$I = \frac{11}{3}\phi^2 - \frac{25}{6}\phi + \frac{11}{6}.$$

Use this to find the approximate FEM solution to the ODE in Q1 for this segmentation.

Optional Extra-Curricular activities

Find the ground state of a 2D square quantum well. For this, you need to solve numerically the following eigen-value problem:

$$-\frac{d^2\psi}{dx^2} - \frac{d^2\psi}{dy^2} + V(x,y)\psi = E\psi\ ,$$

where x and y are dimensionless coordinates, the square well potential is defined as

$$V(x,y) = \begin{cases} -V_0, & \text{if } |x| \le 1 \text{ and } |y| \le 1 \\ 0 & \text{elsewhere} \end{cases}$$

and E is the energy of the eigenstate (to be determined). All localized eigenstates are expected to have $-V_0 < E < 0$, and the ground state should have the minimal energy (closest to the bottom of the quantum well $E_{min} = -V_0$.

You can play with the bottom level of the potential well V_0. For example, set it initially to $V_0 = 250$ (like in our example on Lecture 6 in a similar 1D problem), and then see what happens as you "push" V_0 up or down.

Formally, the problem is defined on an infinite 2D space. But the ground state $\psi(x, y)$ is expected to be localized in a vicinity of the quantum well, and it should decay exponentially as $|x|, |y| \to \infty$. For the numerical purposes, you should set a square domain: $|x| \leq L$ and $|y| \leq L$, with L being "sufficiently large". As you do not know in advance how strongly the ground state is localized, expect to make several iterations, adjusting the overall size L until you no longer see any boundary effects. A good starting point would be $L = 2$ (i.e. twice as large as the quantum well).

Since the wave function is expected to decay exponentially towards the boundaries, it is convenient to set Dirichlet boundary conditions at all boundaries: $\psi(\pm L, y) = \psi(x, \pm L) = 0$.

Use FDM method, make a sensible step size in each coordinate (at least ten discretization points across the well). To save computational time, consider using symmetries and working with a quarter of the full domain, $0 \leq x \leq L$, $0 \leq y \leq L$, with the appropriately modified boundary conditions at $x = 0$ and $y = 0$ (check how this was done in the RF waveguide example on Lecture 15).

You can solve the eigenvalue problem using some available eigenvalue routines in various numerical libraries (e.g. in matlab you can use "eig" or "eigs"). Alternatively, consider using the modified Power method (since you are interested in one eigenvalue only, which is the closest to the bottom of the potential well).