Problem Sheet 2 - Discretisation and ODE initial value problem

1. Consider the function $f(x) = x\exp(-x)$. Write down the "centred difference" approximation to $f''(x)$ for this function on a regularly-spaced grid with spacing h. Obtain numerical approximations to $f''(2)$ with $h = 1$, then $h = 0.5$ and $h = 0.25$. Calculate the exact value of $f''(2)$, and use it to work out the discretisation error ε for your 3 approximations. [Define ε as the modulus of the difference between the exact and approximate answers.] How do you think ε is scaling with h?

2. Use Taylor's theorem to express $f(x + \alpha h) - \alpha f(x + h)$ in terms of $f(x)$ and its derivatives, for any general function f. Hence determine a grid discretisation of $f''(x)$ using $f(x+\alpha h)$, $f(x+h)$ and $f(x)$. Show that this discretisation is $O(h^2)$ ONLY if α takes the value -1 , and that for all other values of α the discretisation error is $O(h)$. [What is happening at $\alpha = +1$?]

3. Use the derived on lectures "centred difference" approximations for derivatives to express the quantities $\nabla\Phi(\mathbf{r})$, $\nabla\cdot\mathbf{F}(\mathbf{r})$ and $\nabla\times\mathbf{F}(\mathbf{r})$ on a 3-dimensional cubic grid, with a grid spacing of a in x, y and z. $\Phi(\mathbf{r})$ is a scalar field, $\mathbf{F}(\mathbf{r})$ a vector field.

4. To find even-symmetry eigen-states of a Gaussian potential well, you need to solve the following dimensionless Schrödinger equation
$$\frac{-d^2\psi}{d\xi^2} - U_0\exp(-\xi^2/w^2)\psi = E\psi \ ,$$
where U_0 and w are positive constants which define the depth and width of the potential well, respectively. You need to solve this equation on the interval $(0 \le \xi \le L)$ with the following boundary conditions:
$$\frac{d\psi}{d\xi}(0) = 0 \ , \qquad \psi(L) = 0 \ .$$
Discretise this equation on a regular grid in ξ of spacing a; ensure the discretisation error is $O(a^2)$ at worst. What is the value of the step size a? What coordinates the first ($j = 1$) and the last ($j = N$) grid points correspond to? Apply the boundary conditions. Write down the corresponding matrix eigen-value problem, and specify the matrix. How the boundary conditions should be changed to find odd-symmetry eigen-states?

5. You need to solve the following equation:
$$\frac{d^2\Phi}{dx^2} - 3\exp(-\pi x^2)\Phi = 0 \tag{1}$$
on a symmetric interval $-L/2 \le x \le L/2$ with the periodic boundary condition $\Phi(x + L) = \Phi(x)$.
By expanding the solution in complex Fourier series,
$$\Phi = \sum_n \phi_n \exp(ik_n x) \ , \qquad k_n = \frac{2\pi n}{L}$$
show that the above differential equation may be re-written as
$$m^2\frac{4\pi^2}{L^2}\phi_m + \sum_n V_{m-n}\phi_n = 0. \qquad (2) \ ,$$

where V_{m-n} is an integral which you should define, but do not attempt to solve.

Write down equation (2) in the matrix form, assuming that m and n take the values 0, ± 1, and ± 2.

Show that for $L \gg 1/\sqrt{\pi}$ the coefficients V_{m-n} can be approximated as:

$$V_{m-n} \approx \frac{3}{L} \exp[-\pi(m-n)^2/L^2]$$

[Hint: use the known Fourier Transform pairs from the table in the formula book]

6. Write down Euler integration scheme for the following damped oscillator equation:

$$\frac{d^2x}{dt^2} + 2\gamma \frac{dx}{dt} + \omega_0^2 x = 0 \; .$$

Show that:

a) For $\gamma > \omega_0$ (over-damped oscillator), Euler scheme is stable if the time step is sufficiently small: $a \leq 2/(\gamma + \sqrt{\gamma^2 - \omega_0^2})$;

b) For $\gamma < \omega_0$ (under-damped oscillator), Euler scheme is stable if $a \leq 2\gamma/\omega_0^2$.

Note: In this example, I deliberately chose the model equation in standard physical units - many of you should be familiar with this oscillator equation from your year 1 courses. But you are more than welcome to try and de-dimensionalize it first, show that this model has only one parameter, $\Omega = \omega_0/\gamma$, and then implement the Euler scheme of your de-dimensionalized version of the oscillator equation. If you do everything correctly, the stability conditions of your model should be the same as those of the original oscillator equation.

Optional Extra-Curricular activities

Implement the integration scheme you derived in Q6 using a coding environment of your choice (Python, C, Matlab, etc).

Using the initial conditions

$$x(t=0) = 1; \qquad \frac{dx}{dt}(t=0) = 0,$$

integrate the oscillator equation in the time interval covering at least several oscillation periods: $0 \leq t \leq N \cdot 2\pi/\omega_0$, where $N = 3, 4, 5, ...$ is the number of periods. Try different combinations of the model parameters γ, ω_0 and different values of the time step to confirm your predictions about the stability of the Euler scheme.

Compare your numerical solutions with the known analytical solution:

$$x_o(t) = \exp(-\gamma t) \left[\cosh\left(\sqrt{\gamma^2 - \omega_0^2} t\right) + \frac{\gamma}{\sqrt{\gamma^2 - \omega_0^2}} \sinh\left(\sqrt{\gamma^2 - \omega_0^2} t\right) \right] , \quad \text{for} \quad \gamma > \omega_0 \, ,$$

$$x_u(t) = \exp(-\gamma t) \left[\cos\left(\sqrt{\omega_0^2 - \gamma^2} t\right) + \frac{\gamma}{\sqrt{\omega_0^2 - \gamma^2}} \sin\left(\sqrt{\omega_0^2 - \gamma^2} t\right) \right] , \quad \text{for} \quad \gamma < \omega_0$$