Problem Sheet 2 - Answers

1. The centred difference approximation is

$$f''(x) \approx \frac{1}{h^2}\left\{f(x+h)+f(x-h)-2f(x)\right\}$$

in general, so for $f(x) = x\exp(-x)$ and $x = 2$ it is

$$f''(2) \approx \frac{1}{h^2}\left\{(2+h)\exp(-2-h)+(2-h)\exp(-2+h)-4\exp(-2)\right\}.$$

Since $f''(x) = \exp(-x)(x-2)$, the exact value is $f''(2) = 0$, so ε is just the absolute value of our approximation, in this particular case. Substituting $h = 1$, $h = 0.5$ and $h = 0.25$ in the approximation yields $\varepsilon = 0.0241$, 5.734×10^{-3} and 1.416×10^{-3} respectively. You could now take ratios of these to see whether ε is $O(h^2)$ as expected. If you are very keen, and that way inclined, you could write a program to compute ε for many different values of h, including much smaller values, and plot them on logarithmic axes.

2. The Taylor series are

$$f(x+\alpha h) = f(x) + \alpha h f'(x) + \frac{\alpha^2 h^2}{2} f''(x) + \cdots + \frac{\alpha^n h^n}{n!} f^{(n)}(x) + \cdots \quad (1)$$

$$\alpha f(x+h) = \alpha f(x) + \alpha h f'(x) + \alpha\frac{h^2}{2} f''(x) + \cdots + \alpha\frac{h^n}{n!} f^{(n)}(x) + \cdots \quad (2)$$

We want an approximation to $f''(x)$ in terms of values of f but not in terms of derivatives; terms with higher order derivatives are ignored (they form our discretisation error); terms with lower order derivatives (here $f'(x)$) must be made to disappear. This will happen if we take (1)-(2) to give

$$f(x+\alpha h) - \alpha f(x+h) = (1-\alpha)f(x) + \frac{\alpha h^2}{2}(\alpha - 1)f''(x) + \cdots,$$

so

$$f''(x) = \frac{2}{\alpha h^2(\alpha-1)}\left\{f(x+\alpha h) - \alpha f(x+h) - (1-\alpha)f(x)\right\} + \varepsilon,$$

where the error term ε is

$$\varepsilon = \frac{2}{\alpha h^2(\alpha-1)}\left\{-\frac{\alpha h^3}{6}(\alpha^2-1)f'''(x) - \frac{\alpha h^4}{24}(\alpha^3-1)f^{(iv)}(x) + O(h^5)\right\}.$$

So, to make an $O(h^2)$ approximation, the $f'''(x)$ term must disappear. In other words, $-h(\alpha+1)/3$=0. This is only true if $\alpha = -1$, for which we recover the familiar centred-difference approximation $f''(x) \approx [f(x+h)+f(x-h)-2f(x)]/h^2$.

Some choices of α are daft. For example, $\alpha = 0$ means neither (1) nor (2) is useful. $\alpha = +1$ means we are using $f(x+h)$ twice, so it isn't surprising that things look strange there.

3. We have a simple cubic grid, so we should just expand the derivatives in Cartesian coordinates and discretise each partial derivative in turn, using centred differences to achieve $O(a^2)$ discretisation errors. So with $\phi_{i,j,k}$ representing the discrete value of $\Phi(x,y,z)$ we have

$$\nabla\Phi = \mathbf{i}\frac{\partial\Phi}{\partial x} + \mathbf{j}\frac{\partial\Phi}{\partial y} + \mathbf{k}\frac{\partial\Phi}{\partial z}$$

$$\approx \frac{\mathbf{i}}{2a}(\phi_{i+1,j,k} - \phi_{i-1,j,k}) + \frac{\mathbf{j}}{2a}(\phi_{i,j+1,k} - \phi_{i,j-1,k}) + \frac{\mathbf{k}}{2a}(\phi_{i,j,k+1} - \phi_{i,j,k-1}).$$

Similarly,

$$\nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z},$$

and we approximate (for example)

$$\frac{\partial F_x}{\partial x} \approx \frac{1}{2a}\left\{F_x(x+a,y,z) - F_x(x-a,y,z)\right\}.$$

The curl generates a vector field, which we break down into components. So eg the x-component

$$(\nabla \times \mathbf{F})_x = \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}\right).$$

Our $O(a^2)$ discretisation approximates this as

$$\frac{1}{2a}\left\{F_z(x,y+a,z) - F_z(x,y-a,z) - F_y(x,y,z+a) + F_y(x,y,z-a)\right\}.$$

4. Because of the specific boundary conditions, we need to include $\xi = 0$, but we do not need $\xi = L$. Hence, our first point ($j = 1$) corresponds to $\xi_1 = 0$, and our last point ($j = N$) corresponds to $L - a$. With this, it is easy to see that $a = L/N$, and the discretised coordinate is $\xi_j = (j-1)a$.

   Using the "centred difference" approximation for the second-order derivative, the discretised equation for a generic point which is away from any boundary is:

$$-\frac{1}{a^2}(\psi_{j+1} + \psi_{j-1} - 2\psi_j) - U_0 \exp(-(j-1)^2 a^2/w^2)\psi_j = E\psi_j\ .$$

   At $\xi = 0$ we would have ($j = 1$):

$$-\frac{1}{a^2}(\psi_2 + \psi_0 - 2\psi_1) - U_0\psi_1 = E\psi_1\ .$$

   But ψ_0 is outside our grid! Need to apply boundary condition $d\psi/d\xi(0) = 0$. The discretised version of it is:

$$\frac{1}{2a}(\psi_2 - \psi_0) = 0\ ,$$

   which tells us that $\psi_0 = \psi_2$. Hence the equation for $j = 1$ grid point is:

$$-\frac{1}{a^2}(2\psi_2 - 2\psi_1) - U_0\psi_1 = E\psi_1\ .$$

   At the opposite boundary, $j = N$, applying the boundary condition $\psi(L) = 0$, we obtain:

$$-\frac{1}{a^2}(0+\psi_{N-1}-2\psi_N)-U_0\exp(-(N-1)^2a^2/w^2)\psi_N=E\psi_N\ .$$

Combining everything together, we can write this problem as the following matrix eigen-value problem:

$$\hat{M}\vec{\psi}=E\vec{\psi}\ ,$$

where $\vec{\psi}=[\psi_1,\psi_2,\psi_3,\ldots,\psi_N]^T$ is an N-element column vector, and the matrix $\hat{M}$ is defined as:

$$\hat{M}=\frac{1}{a^2}\begin{pmatrix} 2-a^2U_0 & -2 & 0 & 0 & \ldots & 0 \\ -1 & 2-a^2U_0e^{-a^2/w^2} & -1 & 0 & \ldots & 0 \\ 0 & -1 & 2-a^2U_0e^{-(2a)^2/w^2} & -1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & \ldots & 0 & 0 & -1 & 2-a^2U_0e^{-(N-1)^2a^2/w^2} \end{pmatrix}$$

5. Substitute the basis set expansion into the differential equation. This gives

$$\sum_n\left\{k_n^2+3\exp(-\pi x^2)\right\}\phi_n\exp(ik_nx)=0.$$

Now perform the "closure" procedure: multiply the equation by $\exp(-ik_mx)$ and integrate over the full window x:

$$\sum_n\left\{k_n^2\int_{-L/2}^{L/2}\mathrm{e}^{i(k_n-k_m)x}dx+3\int_{-L/2}^{L/2}\mathrm{e}^{-\pi x^2}\mathrm{e}^{i(k_n-k_m)x}dx\right\}\phi_n=0.$$

Use the orthogonality of the Fourier basis set:

$$\frac{1}{L}\int_{-L/2}^{+L/2}\exp\left[i(k_n-k_m)x\right]dx=\delta_{nm}\ .$$

Hence obtain:

$$\sum_n\left\{k_n^2\delta_{mn}+V_{n-m}\right\}\phi_n=0\ ,$$

where

$$V_{n-m}=\frac{3}{L}\int_{-L/2}^{L/2}\mathrm{e}^{-\pi x^2}\mathrm{e}^{i(k_n-k_m)x}dx=\frac{3}{L}\int_{-L/2}^{L/2}\mathrm{e}^{-\pi x^2}\mathrm{e}^{i2\pi(n-m)x/L}dx\ .$$

(Note that the coefficients V_{n-m} depend on the difference $(n-m)$, hence only single index).

And finally, using $k_n=2\pi n/L$, we obtain:

$$m^2\frac{4\pi^2}{L^2}\phi_m+\sum_n V_{n-m}\phi_n=0$$

You can now write down these equations in the matrix form, assuming $m,n=0,\pm1,\pm2$:

$$\begin{pmatrix} 16\pi^2/L^2+V_0 & V_1 & V_2 & V_3 & V_4 \\ V_{-1} & 4\pi^2/L^2+V_0 & V_1 & V_2 & V_3 \\ V_{-2} & V_{-1} & V_0 & V_1 & V_2 \\ V_{-3} & V_{-2} & V_{-1} & 4\pi^2/L^2+V_0 & V_1 \\ V_{-4} & V_{-3} & V_{-2} & V_{-1} & 16\pi^2/L^2+V_0 \end{pmatrix}\begin{pmatrix}\phi_{-2}\\ \phi_{-1}\\ \phi_0\\ \phi_1\\ \phi_2\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\end{pmatrix}.$$

For $|x| \gg 1/\sqrt{\pi}$ the integrand function in the definition of V_{n-m} decays to zero due to the factor $\exp(-\pi x^2)$. Hence, if $L \gg 1/\sqrt{\pi}$ the integral can be approximated as:

$$V_{n-m} \approx \frac{3}{L} \int_{-\infty}^{+\infty} \mathrm{e}^{-\pi x^2} \mathrm{e}^{i2\pi(n-m)x/L} dx$$

From the known Fourier transform pairs:

$$\mathcal{F}\left\{\mathrm{e}^{-\pi x^2}\right\} = \int_{-\infty}^{+\infty} \mathrm{e}^{-\pi x^2} \mathrm{e}^{-ikx} dx = \mathrm{e}^{-k^2/(4\pi)}$$

Hence we obtain:

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

6. First, need to re-write this as a system of two coupled first-order ODEs:

$$\begin{cases} \frac{dx}{dt} &= v \ , \\ \frac{dv}{dt} &= -2\gamma v - \omega_0^2 x \end{cases}$$

Assume time step a:

$$\begin{cases} x_{n+1} &= x_n + a v_n \ , \\ v_{n+1} &= v_n - a2\gamma v_n - a\omega_0^2 x_n \end{cases}$$

Splitting the solution into "exact" and perturbation, $x_n = x_n^{(e)} + \epsilon_n$, $v_n = v_n^{(e)} + \nu_n$, and Following the same steps as discussed on the lecture, it is easy to obtain the amplification matrix for this system:

$$\begin{bmatrix} \epsilon_{n+1} \\ \nu_{n+1} \end{bmatrix} = \begin{bmatrix} 1 & a \\ -a\omega_0^2 & 1-2a\gamma \end{bmatrix} \begin{bmatrix} \epsilon_n \\ \nu_n \end{bmatrix} = \hat{M} \begin{bmatrix} \epsilon_n \\ \nu_n \end{bmatrix}$$

To obtain eigen-values of $\hat{M}$ need to solve

$$\det\left[\hat{M} - \hat{I}\lambda\right] = 0$$

After some trivial algebra, obtain:

$$\lambda_{1,2} = 1 - a\gamma \pm a\sqrt{\gamma^2 - \omega_0^2} \ .$$

Next, we need to consider two cases.

(a) If $\gamma > \omega_0$ (the so-called over-damped oscillator), both eigen-values are real. For stability we require $|\lambda_{1,2}| \leq 1$. Let's look carefully at each of the eigen-values:

$$|\lambda_1| = |1 - a\gamma + a\sqrt{\gamma^2 - \omega_0^2}| \leq 1$$

If $1 - a\gamma + a\sqrt{\gamma^2 - \omega_0^2} > 0$ (which means $a < 1/(\gamma - \sqrt{\gamma^2 - \omega_0^2})$) this leads to the condition

$$a\gamma > a\sqrt{\gamma^2 - \omega_0^2}$$

which is always true.

If $1 - a\gamma + a\sqrt{\gamma^2 - \omega_0^2} < 0$ (which means $a > 1/(\gamma - \sqrt{\gamma^2 - \omega_0^2})$) this leads to the condition

$$-1 + a\gamma - a\sqrt{\gamma^2 - \omega_0^2} \leq 1 \ ,$$

and therefore:

$$a \leq \frac{2}{\gamma - \sqrt{\gamma^2 - \omega_0^2}} \ .$$

For the second eigen-value we have:

$$|\lambda_2| = |1 - a\gamma - a\sqrt{\gamma^2 - \omega_0^2}| \leq 1 \ .$$

It is easy to see that this eigenvalue can only exceed 1 by modulus if it is negative. Hence the condition is

$$-1 + a\gamma + a\sqrt{\gamma^2 - \omega_0^2} \leq 1 \ ,$$

which leads to:

$$a \leq \frac{2}{\gamma + \sqrt{\gamma^2 - \omega_0^2}} \ .$$

This second condition sets the lower threshold for the step size a. If a satisfies this condition, both eigen-values will not exceed 1 by modulus, and the scheme is stable.

(b) For $\gamma < \omega_0$ (under-damped oscillator), the eigenvalues become complex:

$$\lambda_{1,2} = 1 - a\gamma \pm ia\sqrt{\omega_0^2 - \gamma^2} \ .$$

Now we have:

$$|\lambda_{1,2}|^2 = (1 - a\gamma)^2 + a^2(\omega_0^2 - \gamma^2) = 1 - 2a\gamma + a^2\omega_0^2$$

Stability criterion: $|\lambda_{1,2}| \leq 1$, which gives us:

$$2a\gamma - a^2\omega_0^2 \geq 0 \qquad => \qquad a \leq 2\gamma/\omega_0^2$$