Computational Physics: PHAS0030, 2018-2019
Problem Sheet 3

Hand in your answers by **Monday 4 March**, *on Moodle through the link provided. Marks per section are shown in square brackets. Your answers should ideally be a Jupyter Notebook, though Python code is acceptable. Ensure that you comment your code, and give every function a docstring.*

1. (a) Write a successive over-relaxation (SOR) function for a two-dimensional potential, taking the potential, its size and the value of `omega` as parameters. Write a clear docstring explaining the function. [4]

   (b) For a 2D box with side lengths of one unit (we will not specify units here), create an appropriate 2D array for the potential (use 50-100 points per side). We will impose the boundary conditions $\phi = 0$ at the edges, $\phi = 1$ for $(0.2, 0.2 \to 0.8)$ and $\phi = -1$ for $(0.8, 0.2 \to 0.8)$. Plot your initial potential. [2]

   (c) Using your SOR function, iterate until you have a converged potential; be sure to be clear about the tolerance and include a maximum number of iterations. Explore the effect of varying `omega` (do not exceed $0.1 < \omega < 0.9$). Plot your potential with `plt.imshow` (and optionally also using `mplot3d`). [4]

2. (a) Write a function to perform an update step on a wave in two dimensions, taking the wave at $n-1$ and n and $r = c\Delta t/\Delta x$ as parameters. [2]

   (b) For a wave with wavelength 1m and frequency 1Hz, create appropriate arrays in x and y to hold three wavelengths and create the initial waves defined by $\theta_0(x, y) = \sin(kx - \omega t), x < \lambda$ and zero otherwise, for $t = 0$ and $t = \Delta t$. Plot one of your waves. (Use 50-100 points in each dimension.) [2]

   (c) Now create an array to hold r; you will model the change of refractive index of a medium by changing r. Set $r = 0.1$ except when $y < 1.5(x - \lambda)$, where you should set $r = 0.05$. Plot the resulting array. [2]

   (d) Using Δt calculated in the *starting* medium, propagate the wave forward by 1,800 steps, and plot the resulting disturbances every 150 steps. Comment *briefly* on what you observe. (NB in this simulation, we are assuming *periodic* boundaries, so do not change the wave at the boundaries.) Use an array of subplots.. [4]

3. (a) Create two functions to build the Crank-Nicolson matrices used in propagating the time-dependent Schrödinger equation (you may base them on the functions from class). [2]

   (b) For a domain $-100 < x < 100$ with $\Delta x = 0.1$, create an initial wavefunction that is a Gaussian, centred on $x = 0$ with $\sigma = 10.0$: $\psi(x, 0) = e^{-(x-x_0)^2/\sigma^2}$. Also create a potential $V(x) = \alpha x^2$ and set $\alpha = 5 \times 10^{-4}$. Plot the initial wavefunction and potential. [3]

   (c) For $\Delta t = 0.1$, propagate the wave forward for 2,000 steps, plotting the real and imaginary parts every 200 steps, using an array of subplots. Comment on the behaviour (briefly!). [3]

   (d) Now make the initial wavefunction $\psi(x, 0) = e^{ikx}e^{-(x-x_0)^2/\sigma^2}$ with $k = 1$, and do the same propagation. Why does this wave behave differently? [2]