PHYS 511: Computational Modeling and Simulation - Fall 2018
Assignment #2, due Friday November 9, before class

Solving 2D Schrödinger equation on a grid

Consider a finite motion of a quantum particle in 2D. It is described by the stationary Schröedinger equation that has the following form for any given potential $V(x, y)$:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]\psi(x,y)+V(x,y)\psi(x,y)=E\psi(x,y). \tag{1}$$

Here $\hbar$ is the Plank constant divided by 2π and m is the mass of the particle. The (unknown) function $\psi(x, y)$ is the wave function of the particle, while E is its (unknown) energy. Thus, equation (1) is an eigenvalue problem. The existence of discrete energy levels, E, depends on the shape of the potential V. To insure this, we will consider a simple form of $V(x, y)$ – an infinite rectangular box of length $2a$ and width $2b$ centered at the origin:

$$V(x,y)=\begin{cases}0, & -a\le x\le a,\ -b\le y\le b\\ \infty, & \text{otherwise.}\end{cases}$$

1. Write a Fortran program (`main.f90`) that solves the Schrödinger equation with the above potential when $a = 1.5b$ (i.e. the box length is 50% larger than its width) and finds *four* lowest eigenvalues E as well as the corresponding eigenfunctions. Use the simplest (three-point) approximation for the second derivatives.

2. The first thing that you will need to do is introducing the natural scale for x (y), and E. That will eliminate constants $\hbar$ and m. After rescaling x should range from -1.5 to 1.5, while y should range from -1 to 1. Type the new equation in your report (`report.txt`) so that I understand what exactly you are solving. Feel free to use LaTeX syntax for math if you wish.

3. The grid in your calculations should be 76×51 points (which is equivalent of having $\Delta x = \Delta y = 0.04$). However, *do not hardcode* the number of grid points along each direction in any of your loops. Instead, define parameters (say $N = 76$ and $M = 51$) in the beginning of your code and use those. This way you can easily change the grid size if necessary.

4. Because the potential is infinite anywhere outside of the box, the boundary condition on ψ is such that is must vanish at the box exterior.

5. Use an appropriate subroutine from LAPACK (you will need to find out which one is suitable) to solve the resulting eigenvalue equation.

6. Include the four lowest eigenvalues in your report. These are your energies. The corresponding eigenvectors that you obtain when solving the eigenvalue equation are directly related to the wave functions. Your program should output the wave functions (as functions of x and y) into some data files so that you could later plot them.

7. Find a meaningful way to plot the wave functions (3D plot, density plot, countour plot, etc) so that you can look at them and check your solution visually . Save those plots as jpg or png files (`wf1.png`, `wf2.png`, `wf3.png`, `wf4.png`). Make sure the x:y aspect ratio is 1:1 and clearly label everything.

8. Upload your files to subdirectory `as2` in your google drive directory shared with the instructor. Files to be submitted: `main.f90` (program source), `report.txt`, `wf1.png`, `wf2.png`, `wf3.png`, `wf4.png`. Do not submit any intermediate data files that you may generate. You can submit your gnuplot script if you wish (assuming that you used gnuplot for plotting).