Computational Physics
Problem Set 1, September 2, 2025

Due: Monday, September 8, 2025 by 11:59 PM

Link to join GitHub classroom to submit homework solution: **Click here**.

Submit to the TA a link to the repository checked into your GitHub account containing a Jupyter Notebook including solutions for homework problems. The directory tree of the repository should include a directory for "homework" with subdirectories for each individual homework assignment.

You *must* label all axes of all plots, including the units if applicable.

1 Coordinate Conversions (10%)

The formulas for converting from Cartesian coordinates (x, y, z) to spherical coordinates (r, θ, ϕ) and vice-versa are given by

$$
\begin{aligned}
x &= r \sin\theta \cos\phi \\
y &= r \sin\theta \sin\phi \\
z &= r \cos\theta
\end{aligned} \tag{1}
$$

and

$$
\begin{aligned}
r &= \sqrt{x^2 + y^2 + z^2} \\
\theta &= \arctan\left(\frac{\sqrt{x^2 + y^2}}{z}\right) \\
\phi &= \arctan\left(\frac{y}{x}\right)
\end{aligned} \tag{2}
$$

A) Write a program that asks the user to enter a set of Cartesian coordinates and outputs the spherical coordinates in radians.

B) Write a program that asks the user to enter a set spherical coordinates in radians and outputs the Cartesian coordinates.

C) Use your programs from parts A and B to take the set of Cartesian coordinates $(x, y, z) = (3.5, -7.2, 5.357)$, convert it to spherical coordinates, then convert it back to Cartesian coordinates. Do you get the coordinates you started with? If not, what is the difference in the starting and final Cartesian coordinates?

2 Quantum Tunneling (25%)

A) Exercise 2.5 in *Newman* (pg. 36).

B) Taking the parameters from part A, compute the probabilities for the step values $V = 0 - 10$ eV. Write the results into a file with columns (V, T, R). Include the file in your repository.

3   Madelung Constant for NaCl (25%)

Exercise 2.9 in *Newman* (pg. 74). Terminate the sum when the next term adds less than 0.1% to the current total.

4   Fibonacci Sequence (25%)

The Fibonacci sequence is given by

$$
\begin{aligned}
f_0 &= 1 \\
f_1 &= 1 \\
f_n &= f_{n-1} + f_{n-2}
\end{aligned}
\tag{3}
$$

A) Write a user-defined function that computes the nth element in the sequence in a recursive manner. For an example of a recursive function, see Exercise 2.13 on pg. 83 of *Newman*.

B) Use your function from part A to find the 58th element of the sequence.

5   Latex practice (15%)

Create a short LaTeX document. You may use code on your laptop or you may use an online LaTeX editor such as Overleaf. In this document describe your goals for this course, your background in programming and/or numerics, and (to the extent you know them) your plans after your degree is finished (grad school? industry? law school? etc.). A paragraph is sufficient. If you write more than a page, you have written way too much. You won't be graded on the content of this, just whether you do it.