Jan 21, 2022 | Homework 1 | Due: Feb 03, 2022, 5:00 PM
PHY 300/500 Lab | Total questions: 5 | Total points: 100

Please consider the following for full credit.

- Use informative variable names, for example, `atomic_radius` instead of `r`.
- Comment where necessary.
- Readability of code is as important as its functioning.
- Fewest possible lines of code taking advantage of the functionality and structure of Python.
- An authentic style guide for Python coding: https://www.python.org/dev/peps/pep-0008/
- Submit your solution in a single Jupyter notebook via LMS.

1. $\boxed{\text{5 points}}$ Write a program that prompts to read an email address and separately prints the username and the domain name.

2. $\boxed{\text{5 points}}$ Write a program that prompts to read a word and prints reversing the order of its characters.

3. $\boxed{\text{15 points}}$ Write a program that reads dates of birth of two people and returns the age difference in years, months, and days. A good program would perform sanity tests on the input, for example, it would not accept a date in the future.

4. $\boxed{\text{35 points}}$ You are given a time series data in the file `timeseries.txt`. It is temperature measured using a thermocouple at the sampling rate of 2 Hz.

   (a) Write a program that reads the file and plots the data (temperature vs time).

   (b) Write a program that computes and plots Fast Fourier Transform (FFT) of the data.

   (c) Write a program that calculates the average and subtracts it from the data before performing FFT.

   (d) Compare the FFT before and after subtracting the average and explain the difference.

   (e) What is on the x-axis of the FFT plot? It is frequency bins. Calculate the corresponding frequencies in Hz and replot the FFT results.

5. $\boxed{\text{40 points}}$ You are given a Molecular Dynamics (MD) trajectory of bulk silver (lattice constant = 4.03 Å) in the file `md_trajectory.txt`. That is 256 atoms of silver in a supercell (made of unit cells) of 16.12 × 16.12 × 16.12 Å. There are 500 frames, in each frame (after 1 ps) the positions (in units of the lattice constant) of atoms are updated depending on their initial velocities and forces acting on them. As you know from your elementary mechanics that the internal forces in such a system of particles, in the center of mass frame of reference, should add to zero. Due to the numerical nature of these simulations that is not always guaranteed. One way to quantify and fix this problem is to calculate the center of mass of such a system in each frame and plot it against time.

   Write a program that reads this file, calculates the center of mass in each frame and plots it against time. Instead of reading the whole file at once, read and process it frame by frame - because typical MD trajectories involve millions of atoms and millions of frames and are too large to be stored in the memory. MD trajectory file is in a given format, your reading program can be specific to this format however it should be able to read a different file in the same format - for example with different number of atoms and different number of frames.