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Computational Physics Exam 1

# Instructions

You are to work all of the following problems by writing and running Python programs. Your solutions to the exam **must** be in the form of **one Jupyter notebook with your name** that includes the following:

* A header markup cell with **your name** and **Comp Phys Exam 1**
* Python code in code cells—one problem or section per cell
* **answers** to all questions in markup cells

**Place your completed documents in the Brightspace Dropbox by 5 p.m., Sunday September 25, 2022.**

The point value for each problem is shown. You will be graded on **the completeness** of your solutions, your **programming**, **refinements** to your output (such as formatting print statements, labeling axes, including legends, etc.), and your **answers** to questions. Notes, textbook, and other *non-human* resources are permitted. You probably will need to look up features of difference commands in SciPy or NumPy online. You *may not* discuss the exam or your solutions with anyone but your instructor.If you have questions, please contact me in my office or via e-mail over the weekend.

Best wishes and happy computing!

1. (10 pts) Python StufF:
   1. What is the difference between using  **np.arange**(1,10) and **np.linspace**(1,10,100)?
   2. What is the difference between NumPy **loadtxt()** and NumPy **genfromtxt**()? Which would you use for reading a CSV file? Why?
   3. What does vectorization of math refer to in Python? Give an example.

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* 1. What command lines are needed to plot four graphs in separates panels with two graphs next to each other as inside one figure.

1. (10 pts) Access the TESS file WASP24TESSexcerpt that can be found under Resource Files on Brightspace. **Produce a graph of the data.** Write code to read the file and rearrange values from least to greatest in the second column and write the rearranges data to a file called reordered.txt. **What are values in the first row of the rearranged data?**
2. (15 pts) In condensed matter physics the Madelung constant gives the total electric potential felt by an atom in a solid. It depends on the charges on the other atoms nearby and their locations. Consider for instance solid sodium chloride—table salt. The sodium chloride crystal has atoms arranged on a cubic lattice, but with alternating sodium and chlorine atoms, the sodium ones having a single positive charge +*e* and the chlorine ones a single negative charge −*e*, where *e* is the charge on the electron. If we label each position on the lattice by three integer coordinates (*i*, *j*, *k*), then the sodium atoms fall at positions where *i* + *j* + *k* is even, and the chlorine atoms at positions where *i* + *j* + *k* is odd.

Consider a sodium atom at the origin, *i* = *j* = *k* = 0, and let us calculate the Madelung constant. If the spacing of atoms on the lattice is *a*, then the distance from the origin to the atom at position (*i*, *j*, *k*) is  and the potential at the origin created by such an atom is



where the sign of the expression depend on whether *i* + *j* + *k* is even (+) or odd (-). The total potential felt by the sodium atom is therefore the sum of this quantity over all atoms. If we assume a cubic box around the sodium at the origin, with *L* atoms in all directions, we have

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where *M* is the Madelung constant (approximately for finite-sized lattice) and is given by



where the sign is + if the value of *i + j + k* is even and – if the value is odd.

This last expression is used by condensed matter researchers to characterize difference ionic molecules.

**Write a program to calculate and print the Madelung constant for sodium chloride for the value *L*  = 100. What value did you obtain?**

1. (15 pts) In 1910, Srinivasa Ramanujan, an Indian mathematician, found the rapidly converging infinite series for *π*

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**Using this series, determine π when the following number of terms, *n*, are used in the calculation: *n* = 1, 2**. You will need to use **np.float64**() for calculations. For each value of *n* print the NumPy value of π and then the value you calculated. Use Pythonic formatting with {:50.45} for a number. **What is amazing about this method of calculating π?**

1. (25 pts) Antarctic mass measurements from 04/2002 to 06/2020 taken from GRACE under the auspices of the NASA MEaSUREs program reveal trends in ice shelf mass. The file containing this data, Antarctica\_mass\_200204\_202006, can be found under Assignments and also Resource Files on Brightspace. To understand better the changes in ice shelf mass,

* 1. **Find the Pearson correlation coefficient for the data.**
  2. **Determine the linear regression for the data.**
  3. **Plot the data and the model curve (linear regression).**
  4. **Evaluate the goodness of the fit.**
  5. **What do you note about yearly and decadal changes in mass?**

1. (25 pts) One of the greatest discoveries of the 20th century is that of the expanding universe, which is attributed to Edwin Hubble (1929). What is not widely known is that the original treatise by Georges Lemaître (1927) contained a rich fusion of both theory and observation. The French paper was meticulously censored when printed in English: All discussion of radial velocities and distances (and the very first empirical determination of the “Hubble-Lemaître constant” *H*) were omitted. You will explore the quality of the data of both Hubble and Lemaître and decide which data and conclusions were better.
2. **Download the two files Lemaitre.txt and Hubble.txt from Brightspace.** You might want to open the files under Notepad to see what they look like. Each file contains data from the respective astronomer of the velocity of galaxies and their distances. Velocities are measured in km/s and distances in Mpc (Mega parsecs, but you don’t need to really know this unit).
3. **Run each set of data through your linear regression and print out the following values:**
   1. Number of data points, N,
   2. A and the uncertainty in A,
   3. B and the uncertainty in B,
   4. The slope of the straight line, B, is the Hubble- Lemaître constant.
   5. Chi-squared per degrees of freedom
   6. Correlation coefficient, *r*, and its uncertainty.
4. According to the raisin-bread cosmological model, the intercept of the graph of *velocity* vs. *distance* should be zero. Using arguments similar to those in class, you can show (but don’t have to prove this!) that in the case of fitting of fitting of fitting *y* = B*x*, the best estimate for B is

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**Modify your program in (b) to take A = 0 and compute B from above**. **Then determine for each data set the following**:

1. B and the uncertainty in B,
   * 1. The slope of the straight line, B, that is, the Hubble- Lemaître constant.
2. Chi-squared per degrees of freedom
3. Correlation coefficient, *r*, and its uncertainty.
4. **From your analysis, which data set has the stronger correlation? Which data set has the better chi-squared per degrees of freedom? For which data set does the value of the Hubble-Lemaître constant remain nearly the same for non-zero and zero intercept? Whose data would you say was better? Why?**