Final take-home exam (total 10 points), due date by Wednesday, 19 April 2023, 8 pm

By completing and submitting this exam, you commit to the university's section K. 'Integrity and Conduct' of the University Calendar.

This final take-home exam is open-book, i.e. you may consult and refer to your own notes, lecture notes, books, lecture video recordings, any material worked during the regular assignments, and consult websites. However, it is not allowed to solicit assistance from another person or from any online service (including any social media, forums, open AIs, and Q&A platforms) - or to offer such assistance to another person.

Instructions on how to prepare your final:

This final take-home exam contains 4 exercises in total. Create 1 notebook file per exercise and name them as demonstrated below:

- `final_exercise1.ipynb`
- `final_exercise2.ipynb`
- `final_exercise3.ipynb`
- `final_exercise4.ipynb`

Submit all 4 files onto the dropbox folder available in Gradescope.ca. Do not submit more than 4 files. Write your name and UCID on the first Markdown cell of each notebook file. UPLOAD ALL FILES AT ONCE. Your codes should output what each exercise requires (e.g., plots, numerical results, etc.). Plots should contain proper axis labels, units, and legends if necessary. Read carefully the requirements for each exercise. Additionally, your codes should be commented on a line-by-line basis where you should detail the implementation, variables, parameters, and methods used. The comments are supposed to clarify the programming instructions used in your codes. Points will be deducted from codes that do not provide sufficient comments and explanations. **No written report is required for this submission, only the 4 notebook codes. Only Notebook files are accepted.**

How to setup Markdown cells to add texts in your Notebook files

Discussions and supporting explanations should be provided using Markdown cells. In order to setup Markdown cells (fields where just texts can be added) in your Notebook file, select the cell you wish to cast as 'Markdown' then, on the top-bar menu, click on 'Cell' → 'Cell type' → 'Markdown' as exemplified on the figure below. Note that Jupyter Notebook menus and options may vary depending on your operating system, customized settings, Jupyter Notebook versions, etc. Consult the manuals of the Jupyter Notebook installed on your computer or, if you use `https://ucalgary.syzygy.ca/`, consult the Jupyter Notebook resources and links shared in week 1 of our course.

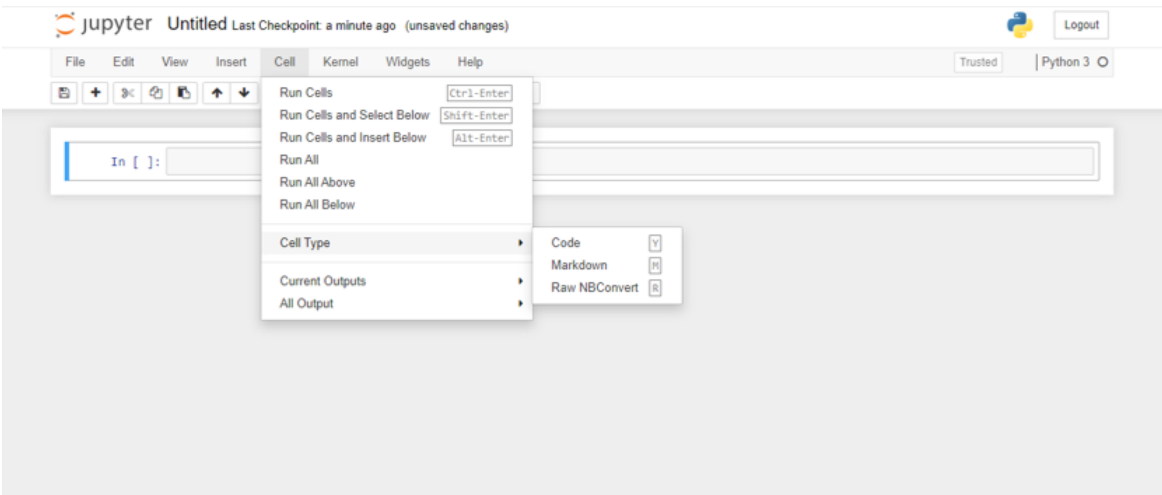

Figure 1: Screenshot that demonstrates how to set a notebook cell as Markdown to add texts and explanations in your Notebook file.

REMEMBER THAT ALL ANSWERS (BEING NUMERICAL OR GRAPHICAL) NEED TO BE GENERATED BY YOUR CODES. IF AN ANSWER IS SIMPLY MANUALLY TYPED AND NOT OUTPUTTED BY THE CODE IN ANY FORM, MARKS WILL BE DEDUCTED.

1 Fitting and finding minima of functions (total: 3 points)

The atomic interaction between two noble gas atoms can be described with the Lennard-Jones potential energy given below

$$U(r) = 4\epsilon \left\{ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right\} \tag{1}$$

where r is the interatomic separation, ϵ is the well-depth and a measure of how strongly the two particles attract each other, and σ is the distance at which the potential energy between the two particles is zero. σ gives a measurement of how close two nonbonding particles can get and it is also referred to as the van der Waals radius. The bonds between atoms held together by such van der Waals forces are weak with bond energies ranging just a few meV (milli-electron volts). For this reason, this interatomic potential energy can be used to describe bonds between noble gas atoms such as He, Ar, Ne, Kr.

The values of ϵ and σ can be obtained by fitting equation (1) onto data sets of potential energy versus atomic separation calculated by means of sophisticated quantum mechanics methods. In the D2L folder of this exam, you will find four text files named: `potential_He2_QM_d2.txt`, `potential_Ar2_QM_d2.txt`, `potential_Ne2_QM_d2.txt`, and `potential_Kr2_QM_d2.txt`. These are 2-column files containing atomic separation values (in Å) in the first column and values for the interatomic potential energy (in meV) in the second column for the noble gas molecules of He_2, Ar_2, Ne_2, and Kr_2, respectively.

(a) Choose a fitting method that you learned in *Assignment #5: Curve fitting, optimizations, and finite difference methods* to determine ϵ and σ parameters of the Lennard-Jones potential energy describing the bond of each of the gases introduced above. Apply the fitting method onto the given data points contained in the provided files and obtain the (ϵ, σ) fitting parameters for all gases. Write the name of the method you chose in a Markdown cell and print all (ϵ, σ) values determined by the method for each of the gases. *Hint: choose the simplest fitting method, i.e. the one that requires less amount of code lines!* **(1 point)**

(b) Use the values of (ϵ, σ) you found in the previous item and plot $U(r) \times r$ and $F(r) \times r$ where $F(r)$ is the interatomic force. Choose a method that you learned in *Assignment #1: Finding minima of functions* to determine the equilibrium properties of each noble gas molecule introduced above. In other words, determine the equilibrium separation between the atoms and the minimum of the potential energy for all gases. Mark with a scatter symbol (in all plots) the point characterizing the equilibrium properties of the molecules found by the method. Write the name of the method you chose in a Markdown cell and print all quantities characterizing the equilibrium properties determined by the method for all molecules. Write also how many iterations your method took to find the minimum of the potential energy for all molecules and write the tolerance information that the method requires. *Hint: remember to communicate physical quantities with their respective units!* **(1 point)**

(c) Write DETAILED explanations and document your Notebook file to explain how your codes work in the context of this physics problem. For example, explain what your codes use as input information, what your codes output, and the meaning of the variables and parameters defined throughout the codes; if you coded any function, method, conditions, and loops, explain what they do; if your codes conduct any recursive procedure, explain in detail how the procedure works, etc. *Hint: demonstrate that you fully understand what your codes do and their methods/algorithms!* **(1 point)**

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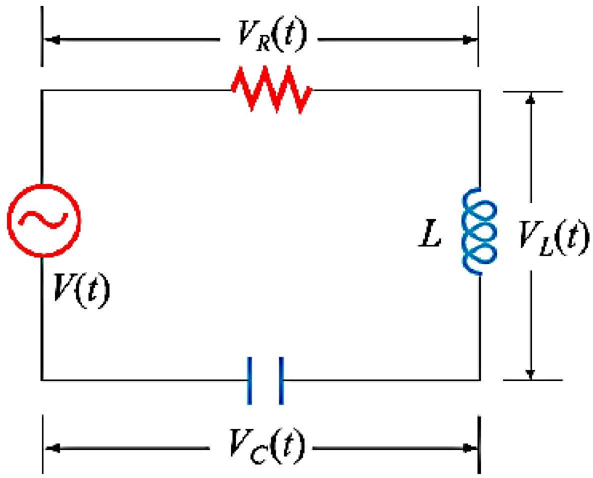
2 Numerical solution of ordinary differential equations (total: 2 points)

A RLC circuit (or LCR circuit) is an electrical circuit consisting of a resistor, an inductor, and a capacitor, connected in series or in parallel. Consider the driven RLC circuit in series shown in the Figure below.



Applying Kirchhoff's loop rule for the voltage drops depicted in the figure, we have:

$$V(t) - V_R(t) - V_L(t) - V_C(t) = V(t) - RI - L\frac{dI}{dt} - \frac{Q}{C} = 0 \tag{2}$$

where $V(t)$ is the voltage provided by the AC source as a function of time t. This is set as $V(t) = V_0 \cos(\omega t)$ with V_0 being the voltage amplitude and ω the angular frequency defined as $\omega = 2\pi f$ where f is the frequency. $V_R(t)$ is the voltage drop across the resistor and Ohm's law gives $V_R(t) = R\,I(t)$ where R is the resistance and I is the current flowing through the circuit. $V_L(t)$ is the voltage drop across the inductor and it is given by the derivative relation $V_L(t) = L\,dI/dt$ where L is the inductance. Finally, $V_C(t)$ is the voltage drop across the capacitor and it is given by $V_C(t) = Q(t)/C$ where C is the capacitance and Q is the charge on the capacitor. Using that $I = dQ/dt$, the equation above can be written as

$$L\frac{d^2Q}{dt^2} + R\frac{dQ}{dt} + \frac{Q}{C} = V(t) \tag{3}$$

Charge and current are variables that evolve in time and $\{L, R, C\}$ are constants fixed at values that you will obtain using the script provided `random_generator_circuit_values_ex2_final.ipynb`. The script will provide the values of the inductance (L in units of mH), resistance (R in units of

Ω), and capacitance (C in units of μF). Read carefully the instructions given in the script. Finally, the amplitude of the AC source is set at $V_0 = 10$ V and $f = 60$ Hz.

(a) Solve numerically equation (3) using the 4th order Runge-Kutta method. Recap from our Assignment #2 that we can write a set of first order differential equations as

$$\frac{dQ}{dt} = I \tag{4}$$

$$\frac{dI}{dt} = f(Q, I, t) \tag{5}$$

$$f(Q, I, t) = -\frac{R}{L}\frac{dQ}{dt} - \frac{1}{LC}Q + \frac{1}{L}V(t) \tag{6}$$

Set the initial conditions for the charge in such a way that the voltage drop at the capacitor is $V_C(t = 0) = Q(t = 0)/C = Q_0/C = 10$ V. The initial condition for the current is $I(t = 0) = I_0 = 0$ A. Plot the solutions of charge versus time and current versus time in different panels. Make sure that the steady-state solutions appear in your plots. **(0.5 points)**

(b) Create a phase portrait of $I(t) \times Q(t)$. Make sure that the steady-state solution appears in your plot. **(0.5 points)**

(c) Write DETAILED explanations and document your Notebook file to explain how your codes work in the context of this physics problem. For example, explain what your codes use as input information, what your codes output, and the meaning of the variables and parameters defined throughout the codes; if you coded any function, method, conditions, and loops, explain what they do. *Hint: demonstrate that you fully understand what your codes do and their methods/algorithms!* **(1 point)**

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3 Fourier transform analysis (total: 3 points)

The file `superposition_signal.txt` is a two-column data file containing time in its first column (in units of seconds) and sound amplitude in its second column (in arbitrary units). This signal is a function of time and it is a superposition of three sine waveforms of frequencies ν_1, ν_2, and ν_3, respectively.

(a) First, from the file, plot the signal as a function of time. You may need to restrict the time range when plotting the signal for better visualization of its fine oscillation patterns. Then, apply the Discrete Fourier Transform method learned in Assignment #4 to determine and plot the real and imaginary Fourier coefficients as a function of the component index. Overall, which Fourier contribution dominates: real or imaginary? Explain your answer. **(1 point)**

(b) Determine and plot the power spectrum of this signal and determine the values of ν_1, ν_2, and ν_3 in units of Hz. Reconstruct the signal using the Fourier coefficients obtained in the previous item and plot the reconstructed signal. **(1 point)**

(c) Write DETAILED explanations and document your Notebook file to explain how your codes work in the context of this physics problem. For example, explain what your codes use as input information, what your codes output, and the meaning of the variables and parameters defined throughout the codes; if you coded any function, method, conditions, and loops explain what they do. *Hint: demonstrate that you fully understand what your codes do and their methods/algorithms!* **(1 point)**

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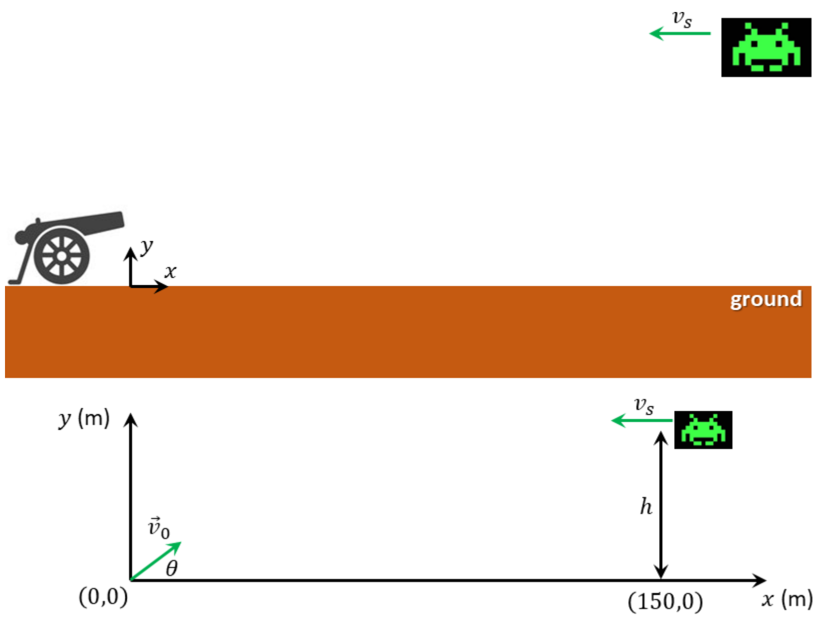
4 Space invaders game (total: 2 points)

You are a game developer and you are designing a target shooting game in which the player can control the initial settings of a static cannon sitting on the ground and the goal is to hit a space invader travelling horizontally at a fixed height from the ground as depicted in the schematics below:



The space invader is first spotted at a height $h = 30$ m and 150 m apart from the cannon. The space invader has a spherical shape with a radius of 1 meter and travels at constant velocity denoted by v_s. The value of v_s (given in m/s) is to be obtained using the script provided named `random_generator_space_invader_ex4_final.ipynb`. Read carefully the instructions given in the script.

The cannon makes an angle θ with the horizontal and a cannonball of a certain mass m and diameter D is shot from the cannon with an initial velocity of v_0. Similarly to what you worked in *Assignment #3: Projectile motion under air resistance*, write a code that will determine the trajectory of a cannonball of mass $m = 46$ g and diameter $D = 43$ mm shot from the cannon with $\theta = 50^o$ and an initial velocity v_0. The value of v_0 (given in m/s) is also to be obtained using the script provided named `random_generator_space_invader_ex4_final.ipynb`. Read carefully the instructions given in the script. Consider the quadratic contribution for the drag force (air resistance) on the cannonball with a drag coefficient of $c = CD^2$ where $C = 0.25$ Ns^2/m^4. Will the cannonball hit the space invader? Make trajectory and velocity plots to justify your answer. Do not forget to upload your code and document it to explain its procedures and methods in detail.

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