HW Questions

Easy:

1. **Question:** What command do you use on the keyboard to run the cell?
    - **Answer:** Shift+Enter

2. **Question:** What is the button you press to clear out your progress and start again?
    - **Answer:** Click on "Kernel tab", and find "Restart and Clear Output"

3. **Question:** In the second block what must you do in order to make sure it runs correctly?
    - **Answer:** You must make sure the files you want to select from are listed within the embedded text, make sure everything is spelled correctly, and make sure your personal username is included in supposed to somebody else

(Example: '/home/nanohub/your.username/mdsandbox/simtool/mdsandbox1.ipynb')

Medium:

Definition Questions:

1. What is NVE?
2. What is NPT?
3. What is NVT?
4. What is NPH?
5. What is a Widget?

Answer:

1. Microcanonical: Constant Energy, Volume
2. Microcanonical: Constant Energy, Volume
3. Canonical: Constant Temperature, Volume
4. Isentropic-Isobaric: Constant Pressure, Enthalpy
5. A multi-purpose tool that makes the work easier (Slider, Dropdown, Textbox)

1. **Question:** If you forgot to switch a component or change the values of a number how would you proceed in running the cells again without restarting the kernel?
    - **Answer:** You would go to the cell you want to make changes to, simply change your desired function, and rerun every cell afterwards.

Hard:

1. **Question:** Describe the trajectory of the Time vs Volume graph of a simulation with the NVE or NVT ensemble.
    - **Answer:** The Time vs Volume graph do not have a trajectory, it is a straight line

2. **Question:** If the tinitial is set at 300 then you rerun it and it changes to 350. Will the difference in Temperature, Kinetic Energy, Pressure, Potential Energy, Total Energy, and Volume be drastic and if so would it have increased, decreased, or stayed the same. Explain?

- **Answer:** Temperature: Increased, Kinetic Energy: Decreased, Pressure: Stayed the Same, Potential Energy: Decreased, Total Energy: Increased, Volume: Stayed the Same