Chem 260 Project A

You must log on to biopathway to do this Project. For full credit complete this Project before 12:00AM (midnight) on Sunday, October 3, 2015. You can turn this in up to one week late (by midnight Sunday, October 10, 2015) for a 25% penalty**. If you choose to turn your Project in late, email me so I know to look for it the following week.**

Project overview:

In your **`~/projects/projectA`** directory you'll find a file **`MDSS.py`** which is a Python program that runs a classical molecular dynamics simulation of 108 Argon atoms held at constant volume and temperature. (This is known as the *canonical ensemble* in statistical mechanics in which N, V, and T are constants). This program takes 2 arguments, the temperature and the density (N/V) which are read in as integers and are immediately divided by 1000 inside the **`MDSS.py`** program. For example typing:

```
MDSS.py  850  1200
```

will run the simulation at a temperature of 0.850 and a density of 1.200. Note that these numbers are in so-called *reduced units*, but the program prints out the actual temperature and density in units of K and gm/ cm^3.

The range of sensible input values are:

Temperature: 500 to 2000 (corresponding to the range 60K to 240K)

Density: 100 to 1100 (corresponding to the range 0.17 to 1.85 gm/cm^3)

`MDSS.py` outputs many lines of output, indicating the progress of the simulation, but we are only interested in one output line, that looks like the following (and is the only output line containing the word "pressure"):

```
Average pressure=0.270784
```

Project assignment

Write a bash script called **`run_mdss.bash`** that will run as series of simulations over a range of temperatures and densities. Your script will take 4 arguments, the beginning and ending temperature and the beginning and ending density and will run simulations at every temperature and density combination in that range in steps of 100. For example, the command:

```
run_mdss.bash 1100 1300 150 450
```

will run MDSS.py runs at every combination of the following values:

Temperature = 1100, 1200, 1300

Density = 150, 250, 350, 450

That is, a total of 12 simulations (3 temperatures times 4 densities). The output of your program will be a set of lines echoed to the screen containing the temperature, the density and the pressure, for example:

```
1100  150   0.103380
1100  250   0.063609
   …
1300  450   0.107308
```

Your script should also do the following tests:

1. Test to be sure that MDSS.py is in the directory where you are running **`run_mdss.bash`**. If it is not, echo the message "**`Cannot find MDSS.py`**" and exit.

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2. Test to be sure that all four arguments to **`run_mdss.bash`** are numerical values. If any is not, echo the message: "**`All arguments must be integers`**" and exit.

3. Test to be sure that the entire range of temperatures and densities is within the range of "sensible" values listed above. If not, echo the message "**`Parameters out of range`**" and exit.

Note on the meaning of the pressures:

You'll notice that at higher densities and/or lower temperatures, your MDSS.py simulations will give negative pressure. This is not an error, but indicates that the system is at least partially in a *condensed phase* (liquid or solid).

Notes on the utility of the simulations:

Your script **`run_mdss.bash`** is mapping the Temperature-Density phase diagram (shown below), which is one of the important uses of molecular dynamics simulations. Note that the small size of the specific system simulated in **`MDSS.py`** (only 108 atoms), limits its accuracy for conditions that are a mix of two phases (e.g. liquid and gas) and therefore its accuracy for determining melting and boiling points.

Temperature-Density phase diagram for Argon: