This program will run three main functions:

Given an input file containing position vectors for arbitrary atoms as a command line argument (default is input.txt) it will calculate the lennard jones potential of this cluster of atoms. It will also run a function to make a small adjustment to a random cartesian axis of a random atom in the cluster, and if this cluster has a lower energy than the original it will return this new geometry and its energy, else it will return the old geometry and energy.

The 3rd function takes the inputted cluster of atoms and runs the 2nd function many times to try and calculate a local minimum potential for the cluster of atoms. The output from this function is appended to a file called ‘minimums.txt’.

With the default settings, the program takes around half a minute to run fully.

This program takes command line arguments which can be seen by using -h in the command line,

Eg:

Write into command line:

* py testme.py -h

The command line will output useful information about the possible arguments that can be passed. All of these arguments are optional however, running the script in the same working directory as a workable input.txt file will work fine.

This program takes two arguments which could lead to the program taking a very long time to run, namely -i and -n. If either of these parameters are supplied a very large number it can lead to the program taking an impractically long time. In this case just use ctrl+c to cancel the script and try running again with smaller numbers.

If you want to supply multiple input files to the program here is an example:

py testme.py -f input.txt anotherinput.txt athirdinputfile.txt

This will run the program for each file that is supplied, with the usual outputs. If python can’t access any of the files those specific files will not be run but the rest of them will. If this occurs check that the correct path was supplied and that the file is in a place where python will be able to access it.