CVL867: Atomistic and multiscale modelling

Assignment 1

1) Select any 20 elements from the periodic table. Obtain the atomic number, mass, density, melting point, and boiling point using https://pypi.org/project/pyriodic-table/. Based on the data, perform the following:
    a. Write two algorithms to find the elements having maximum value of each of the properties.
    b. Sort the atoms in the increasing order of melting point, and boiling point using at least three different sorting algorithms.

2) Compute the correlation between: (i) mass and density, (ii) melting point and boiling point, (iii) density and melting point based on Pearson and Spearman correlation.

3) Repeat Problem 1 with 40 and 80 elements respectively. Analyse the scaling of the algorithms for (a), and (b) by computing the time taken. Draw a plot for the scaling with increasing dataset size.