Project MSI 2 – Water chemical potential
Deadline 20th May at 23.59

Objective. Create a python module which given a set of molecular dynamics trajectories computes the volumetric map of the chemical potential for water.

Assuming the simulations are in equilibrium, which is a reasonable assumption for water molecules, measure the average water occupancy p(x,y,z) from the Oxigen atom of water molecules on a 3-dimensional regular grid of 1A for each dimension. The chemical potential is obtained from the occupancy as $G(x,y,z) = -k_B T \log(p(x,y,z))$.

Use the function writeVoxel of VMD to save a volumetric file (.cube) which can then visualized on top of the PDB of the molecule as an isosurface.

OPTIONAL SECOND PART

1) Use a Gaussian with sigma=1.5 to distribute the occupancy of a water oxygen over neighboring grib points having the effect of interpolating between points. The results should be a much smoother isosurface.