SimpleMD Tutorial: Charges in Liquid Argon

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The purpose of this exercise is to study the potential of mean force between two ions in liquid argon. You will build on what you learnt last week with the simpleMD on LJ particles. The exercise is divided into several steps:

1 Add Charges to LJ Potential

- Create a box of 500 argon atoms in a periodic box. Two of the atoms will be given some charge while all the rest will remain as neutral particles.
- On github there is a charge-partial.zip that builds on what you did for the LJ simulations. The code now reads the charges of all the atoms from a file called *chargefile*. For our exercise, only the first two atoms should be given a charge. The rest can be set to zero. In there you will find the regions of the code that need to be edited labeled *TO DO*. You need to modify the interaction energy between the particles to include the interaction of the two charges as well as the forces between the charge particles.
- The file *chargefile* has a file with the charges of all the atoms:
  1
  -1
  0
  0 ..
- In order to choose appropriate charges, we need to multiply the Coulomb interaction (-1/r) by an appropriate factor to convert into LJ units. As we learnt in class, the energy of a unitary positive and negative ion in contact distance is about $200k_BT$ which is about 120 kcal/mol which in LJ units corresponds to multiplying -1/r by about 15^2. Thus you should start your calculations by using a charge of ± 15.
- Run a simulation and make sure things are working properly: check the conserved quantity.
- Compute the distance between the two ions and make a histogram of the distance.

- Repeat the simulations using smaller charges: change the charge to $\pm$ 5 and then $\pm$ 1. Recompute the histogram. What do you observe?
- Visualize the two charges in VMD

2 Compute PMF Between Ions using Iterative Umbrella Sampling

- The next part of the exercise is for you to get an estimate of the potential of mean force between the ions. You will use a procedure similar to what you learnt in class for determining the free energy. You will perform a short simulation of the two ions and use that to build a bias that can be iteratively adapted to get an estimator of the underlying free energy.

- To build your intuition on the free energies, construct the PMF, for the simulations from the first step using charges of ± 15 and ± 1. What do you observe?

- If you had trouble finishing the previous exercise, please take the grid-partial.zip file from github which implements the charge-interactions for you. You then have to add the grid potential to the code (add the energies and forces coming from the potential on the grid). This has been labeled in the code *TO DO*. Both the energy and forces need to be updated using the grid. As you learnt in the lectures, your goal is to iteratively change the bias potential to get an estimate of the free energy.

- In grid-partial, the code needs a file called *gridfile* where the potential from the simulation is iteratively changed. The file with the grid should be something like:
  5 2 5
  1
  2
  3
  4
  5
  which corresponds to 5 bins with a range (2,5) and with 5 values: 1, 2, 3, 4, and 5.