Excercise 1

Assignment 1. (4/5) Radial distribution function (RDF) is a statistical measure of microsolvation structure. Among other definitions, it is defined as an ensemble average

$$g_{ab}(r) = \frac{V}{N^2} \left\langle \sum_i \sum_{j \neq i} \delta(\mathbf{r} - \mathbf{r}_{ij}) \right\rangle .$$

A numerical recipe for calculation of $g_{ab}(r)$ includes steps

- Choose r_{min}, r_{max} and Δr, and generate grid points $\{r_i\}$, $i = 1, ..., N_{grid}$.
- Generate a histogram $h_{ab}^{(c)}(i)$, $i = 1, ..., N_{grid}$,$c = 1, ..., N_{conf}$, counting the number of times the two atoms of type a and b lies between r_i and r_{i+1}. Use all atoms of proper type in the snapshot, one histogram for each snapshot (total N_{conf}) to obtain best possible statistics. As we are deling with bulk, one has to include pbc and minimum image convention.
- Once the histograms $h_{ab}^{(c)}$ have been generated, normalize them point-by-point (for each r_i, $i = 1, ..., N_{grid}$)

  $$g_{ab}^{(c)}(r_i) = \frac{h_{ab}^{(c)}(i)}{4\pi\rho_b r_i^2 \Delta r N_a},$$

  where ρ_b is the number density (N_b/V) of atoms of type b, and N_a is the number of atoms of type a, you used in generating histogram $h_{ab}^{(c)}(i)$.
- To account for a varying box size, calculate $g_{ab}(r)$ as the average over $g_{ab}^{(c)}(r)$ of snapshots $c = 1, ..., N_{conf}$.

Prepare a code that reads in *mystery.xyz* of the previous excercise and calculates $g_{OO}(r)$ from it using periodic boundary conditions in all three dimensions. Play a bit with the bin size Δr and select a reasonable one. Incude the source code as a separate file, and attach a plot of your result in the report. **Note you can use any programming language you know. With `MATLAB` this code took approximately 80 lines.**

Turn the page! →

Assignment 2. (1/5) Please answer.

- By definition, all RDFs should $g(r) \to 1$, when $r \to \infty$. Give this an verbal (written) interpretation based on the RDF you just calculated. How far (r-wise) is it reasonable to calculate the RDF in the given case?

- Based on the RDF you just calculated, what would be your first guess for the distance of the minimum in the potential energy curve for O-O? Neglect dependence on molecular orientations here, but in future remember that they naturally play a role.

- In this excercise we studied a system in a cubic unit cell. How should the minimum image vector be calculated in a case of orthorhombic (rectanglar) box of side lengths L_x, L_y and L_z?

Return your solutions to Ville *moleculardynamicssimulations@gmail.com*, **latest Wed 18.9.2013 10:15**. To maintain good relations with the assistant, you might want to consider sending a single PDF with all your solutions and then your code as a separate file.