

Worksheet

Tutorial: Electrostatic interactions in ESPResSo

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1 Good to know

- This time you will need the FFTW library¹ for P³M algorithm. Don't forget to recompile ESPResSo if you had to install it.
- The script used in this tutorial can be found on the workshop's homepage under "Course material".

2 Molten salt

The script `salt.tcl` is a simulation script for a simple molten salt, *e.g.* NaCl at 1400 K, one of the simplest possible systems with electrostatic interactions.

You can run this script with

```
mpirun -n 2 Espresso salt.tcl
```

3 Radial distribution functions

So far, the script only computes the radial distribution function (RDF) of opposite charges. Extend the script so that it also computes the RDF for both types of like charges. Compare the RDFs, and check that both like charges have the same RDF.

- Do the RDFs of like and opposite charges meet your expectations?
- Why is the RDF of like charges also highest at close contact?

¹<http://www.fftw.org>

Repeat the same experiments using MEMD instead of the default P³M, and verify that both algorithms give the same results. Try to play with the parameters and see, how they influence the speed of each method. Make sure that this does not introduce artifacts!

4 Salt crystal

Due to the small size of our system, we should have a relatively good chance to freeze it to obtain a NaCl crystal structure.

- Why is it *not* sufficient to lower the temperature?
Hint: check the definition of the Bjerrum length. What happens with electrostatic interactions at low temperatures at constant Bjerrum length?
- What do you obtain if you start with a low temperature immediately?
- To really obtain a crystalline structure, we need to be more careful. One approach is *simulated annealing*, *i.e.* slowly reducing the temperature to the desired value. Implement this in the script to finally investigate the NaCl crystal.
- Look at the crystal structure in VMD? How good is our sampling?
- Compare the RDF of the crystal with the melt. What are the differences? What do they come from?