Hands-On Tutorial: (H-)AdResS in ESPResSo++

Karsten Kreis and Torsten Stühn

ESPResSo summer school 2013, ICP, Stuttgart

10.10.2013

Good to know before you start...

This tutorial explains the implementation of the (Hamiltonian) Adaptive Resolution Scheme ((H-)AdResS) in ESPResSo++ by discussing and performing example calculations. All the files required for the tutorial can be found in the subfolder *hadress* in the examples folder of ESPResSo++.

For the theoretical background about (H-)AdResS we would like to refer you to the talk "ESPResSo++ and (H-)AdResS" given by Raffaello Potestio on 10.10.2013. Furthermore, there is a list of references at the end of this script.

We assume that, by now, you have a running version of ESPResSo++ installed on your machine. Otherwise, if you need help with the installation of ESPResSo++, let Torsten or me know.

Please ask Torsten or me whenever you have a question!

Exercises

1. H-AdRresS simulations explained

In the subfolder *hadressPlain*, you find a simulation script *hadress.py*, which runs a plain, typical H-AdResS simulation of a liquid composed of tetrahedral molecules. We have a slab geometry and the resolution of the molecules changes along the x-direction. The code is commented in detail.

Familiarize yourself with the way how H-AdResS simulations are performed in ESPResSo++ by understanding and running the script. You can follow the energy, which should stay constant, on your screen. Try to vary some parameters and see what happens. You can also uncomment the part which writes pdb trajectories and watch the trajectory with a program like vmd.

By changing *VerletListHadressLennardJones* to *VerletListAdressLennardJones* when defining the interaction in line 131, AdResS instead of H-AdResS simulations can be performed, in which the forces instead of the potential energies are interpolated. You should be able to see that now the energy is not conserved anymore.

However, continue performing H-AdResS simulations. It is also possible to perform thermostating. You can uncomment the corresponding parts in the script, which turn on a Langevin thermostat. It is implemented in ESPResSo++ as an integrator extension.

2. Density and pressure profiles

In (H-)AdResS simulations, typically, neither density nor pressure stay constant across the hybrid region. Have a look into the subfolder *hadressDensityPressure*. You find two scripts, which perform simulations calculating a density and a pressure profile respectively along the x direction. To be more precise, we calculate the molecular pressure and only the xx component of the pressure tensor. Unfortunately, we don't have enough time during the tutorial, to perform sufficiently long simulations for good statistics. Hence, you also find reference results in the folder which have been calculated previously. You can plot them.

3. Free Energy Corrections

To obtain a flat density *or* a flat pressure profile, we can perform Free Energy Corrections. We can either correct using the Helmholtz free energy difference, which leads to a flat pressure profile, or using the Gibbs free energy difference, which results in a flat density profile. You find the corresponding simulations in the subfolder *hadressFEC*. The free energy compensations are realized as an integrator extension in ESPResSo++. Also in this case, there is not sufficient time available for long simulations. However, you can find the reference profiles obtained from long simulations in the folder. You should see a flat density as well as a flat pressure profile.

4. Kirkwood Thermodynamic Integration

How can we actually calculate the free energy differences, which are needed as corrections? This can be realized by a Kirkwood Thermodynamic Integration (KTI). In the subfolder *hadressKTI* you find a script which performs such a KTI. Have a look and try to understand what is going on. Note that the output of the script still has to be flattened, normalized and integrated.

5. Do your own (H-)AdResS simulation!

Now, try to build your own H-AdResS simulation (in the subfolder *hadressOther* you find resources you can use for that).

You could use different potentials, e.g. simply other Lennard-Jones potentials. There is also another tabulated potential, which is a coarse-grained potential (via Iterative Boltzmann Inversion) reproducing the molecular structure of the tetrahedral liquid obtained from atomistic simulations (*table_potentialIBI_tetra.dat*).

Furthermore, you could use other input configurations. With the *Tetracryst.py* script for example, the tetrahedral liquid can be generated with the molecules being arranged on a lattice.

References

[1] **H-AdResS paper**: R. Potestio, S. Fritsch, P. Espanol, R. Delgado-Buscalioni, K. Kremer, R. Everaers, and D. Donadio, Phys. Rev. Let. **110**, 108301 (2013).

[2] **AdResS paper**: M. Praprotnik, L. Delle Site, and K. Kremer, J. Chem. Phys. **123**, 224106 (2005).

[3] **AdResS review paper**: M. Praprotnik, L. Delle Site, and K. Kremer, Annu. Rev. Phys. Chem. **59**, 454 (2008).

[4] **Simulation of liquid water with AdResS**: S. Fritsch, S. Poblete, C. Junghans, G. Ciccotti, L. Delle Site, and K. Kremer, Phys. Rev. Let. **108**, 170602 (2012).

[5] **ESPResSo++ paper**: J. Halverson, T. Brandes, O. Lenz, A. Arnold, S. Bevc, V. Starchenko, K. Kremer, T. Stühn, and D. Reith, Comp. Phys. Comm. **184**, 1129 (2012).

[6] **ESPResSo++ homepage**: https://www.espresso-pp.de/.