Advanced Module for the GSS Summer-School 2015

Theory & Modelling – TIP5P-FQ: A polarizable force field for water

Well established and widely used non-polarizable water models like SPC[1] or TIP3P[2] struggle to accurately describe water under different conditions due to their fixed atomic charges. Since their parameters are static, they can not react to changes in the surrounding electric field and thus only approximately describe e.g. ion solvation or the behavior of water close to a charged surface.

More advanced models like AMOEBA[3] or TIP4P-FQ[4] include polarizability through different means, like introducing point dipoles[5] or using the EEM method[6]. While these models are capable of reacting to changes in their electrostatic environment, they still have their own drawbacks. In the case of TIP4P-FQ one of its shortcomings stems from the planar geometry which prevents polarization perpendicular to the molecular plane. We have derived a polarizable version of the five point water force field TIP5P, combining the additional lone pair sites with the EEM method. The figure shows ion solvation within this TIP5P-FQ water model.

During the advanced module the participants will use our Pydlpoly force field code to perform Molecular Dynamics simulations for established water force fields as well as TIP5P-FQ. Afterwards they will utilize analysis tools to calculate various properties from the collected data and draw a comparison between the different models.

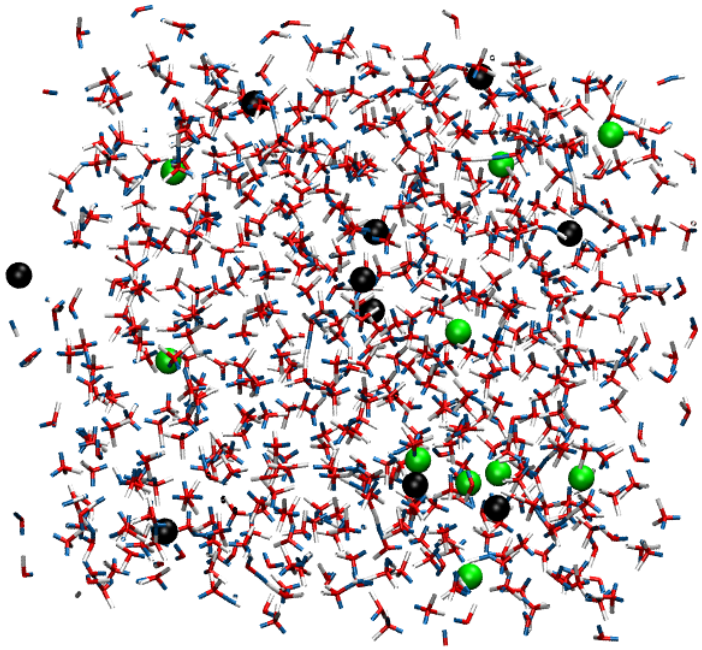

Fig 1: Water box containing 600 TIP5P-FQ water molecules and 10 sodium (green) and chloride (black) ions each. Hydrogen is shown in white, oxygen in red and the lone pairs in blue.

Literature:

[1] HJC Berendsen, *et al*. *Intermolecular Forces*, 331, 1981.

[2]: William L Jorgensen, *et al*. Comparison of simple potential functions for simulating liquid water. *The Journal of chemical physics* , 79(2):926-935, 1983.

[3] Jay W Ponder, *et al*. Current status of the amoeba polarizable force field. *The Journal of physical chemistry B* , 114(8):2549-2564, 2010.

[4] Jon Applequist, *et al*. Atom dipole interaction model for molecular polarizability. application to polyatomic molecules and determination of atom polarizabilities. *Journal of the American Chemical Society* , 94(9):2952-2960, 1972.

[5] Wilfried J Mortier, *et al*. Electronegativity equalization: application and parametrization. *Journal of American Chemical Society* , 107(4):829-835, 1985.