Cleo, Jonas SCC Interim report

Chemical equilibrium is often dynamic. In acid-base reactions, acidic species and base species are constantly reacting, simply due to energy and orientation. A system in equilibrium does not mean that the system no longer carries out reactions, hence dynamic equilibrium. Yet, equilibrium that is dynamic is oxymoronic. Chemical equilibria is defined by a constant found using the equation:

$$aA + bB \rightleftharpoons dD + eE$$

$$K_c = \frac{[D]^d[E]^e}{[A]^a[B]^b}$$

Where the square brackets, [ ], are the concentration of the species inside. This is at equilibrium when K_c is equal to 1 (unitless). The question we are trying to answer is, how far can K_c stray from 1 before the system is no longer in equilibrium. Essentially, how much precision is needed to have an accurate K_c.

Computationally, this is a very difficult problem to solve. Molecular dynamic models are often very large and take huge amounts of computational power. We started by writing the framework of a quantum based molecular dynamics model, and quickly realized we could not get any substantial information from our basic understand of dynamics. Therefore we started research into free, open source, molecular dynamics simulator. LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), written in C++, was an obvious choice, due to its speed and scope. Due to LAMMPS weak visualization tool (xmovie), we have also installed OVITO, a little higher level tool to visualize data.

So far, we have done a lot of research into LAMMPS, and OVITO. Both have been installed, and compiled. This was not trivial, as it required some knowledge into the workings of LAMMPS, which most of the documentation assumed we had. We are presently working on connecting LAMMPS and OVITO, again a task that is not easy as it assumes we have a computational knowledge we do not have. Our plan is to write an input file that allows for the dynamic reaction of weak acid and base in water solution.

As for expected results, our original goal of getting an answer to the variance of K_c is a little out of reach. LAMMPS is difficult to access for new users, and getting to the knowledge base necessary for full integration is huge. Therefore, our project is more about learning how to use LAMMPS then getting a numerical answer to the variance of K_c.

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