Brian Keene
27 August 2015
Research Report - Slatt Fellowship

The main objective of my summer research was to facilitate simulations of porous solid materials in Cassandra, an open source Monte Carlo software package developed at Notre Dame. An additional objective was to implement the Drude polarizable force field within Cassandra. The final objective was to edit and improve the source code for the graphical user interface (GUI) previously designed by myself for use with Cassandra.

The porous solid materials I examined were zeolites – aluminosilicate structures with differing characteristics of pore size based on the underlying topology. The placement of aluminum atoms within the crystal structure affects the electric field of the zeolite, which in turn will cause different adsorption effects in simulation. The ratio of aluminum to silicon in the structure is known as the “Lowenstein Ratio”, and the placement of the aluminum is dictated by the “Lowenstein Rule”. The Lowenstein Rule says that there can be no (Al-O-Al) sequences within the zeolite structure.

My role in the analysis of zeolites was to create a generalized method which read in the zeolite structure from the common Protein Data Bank (PDB) format and converted to the ‘xyz’ file format used by Cassandra. Additionally, since these PDB files contain no aluminum within the structure, it was required that my script inject aluminum at allowed sites to achieve the specified Lowenstein ratio. In order to accomplish this, I learned Fortran and wrote a script that accepts a PDB created by the software program Vesta. The script is also capable of inserting aluminum atoms and swapping aluminum atoms with silicon atoms, all subject to the Lowenstein rule. During tests of the script, it was found to be able to reliably achieve a Lowenstein Ratio of 1.0 – the lowest allowed by the Lowenstein Rule, as this indicates a perfectly alternating (Si-Al) crystal lattice framework. The script is also useful for statistical analysis, as it is capable of generating an arbitrary number of configurations at the Lowenstein ratio specified by the user. The outputs of the script including ‘xyz’ data for all configurations, a new PDB file of the first configuration, and distribution data for the Al-Al distances for all configurations within a range specified by the user.

I also examined implementation of the Drude model for polarization, specifically applied to NPT ensemble water simulations. This consisted of several weeks consulting literature followed by modification of the main code in Cassandra to accommodate the idiosyncrasies of the Drude model. In the Drude model, polarization is simulated by creating a fictitious mobile charge and anchoring it to a specific atom within the molecule. The fictitious particle – or Drude particle – has no mass in the Monte Carlo interpretation, and does not have any van der Waals interactions. The Drude particle has charged scaling interactions identical to that of its anchor atom, and has a spring potential associated with its anchor rather than a charge-charge interaction. The overall charge within the molecule was conserved to match SPC/E Water, and rigid bonds were used for the H-O bonds. The H-O-H angle was also considered rigid. Initial testing of the model as implemented showed that similar energies were being obtained, which is promising. I will be continuing my work on the model this semester.

Finally, the source code for the GUI was heavily reworked. The functionality was preserved, although data management was changed for improved efficiency and more object oriented programming principles were used. A heavy emphasis was placed on ease-of-understanding when rewriting the code for the benefit of future programmers.