Supercomputing Project Proposal- Cleo and Jonas

Weak Acid-Base Chemical reactions exist in dynamic equilibrium states. The dynamic equilibrium is controlled by a constant, calculable by the concentrations of all the solutes. Chemical reactions occur when orientation and kinetic energy of two molecules are in the required position. Thus, despite two molecules coming in contact with each other, they may not react. Therefore, dynamic equilibrium depends on the general kinetic energy and orientation of molecules as they move through solution. So, dynamic equilibrium is truly dynamic. Our question is: “How far from the calculable equilibrium does dynamic equilibrium differentiate?”

This question will be explored by using a physics based molecular model in a programming language called Julia. This language is a very new, and high powered language, however lacks in the graphical side, making models difficult to analyze. We will use Octave, a free version of Matlab, to visualize the time step results. We will start with very few molecules, and incredibly simple acid base pairs in solution. If this model works, we will ramp up the complexity. We will ignore H_2O’s acid base properties simply for clarity.