BE 276 Assignment

Gary Huber

February 3, 2017

This is a toy problem meant to show you how to set up a BrownDye simulation but avoids some of the complications and subtleties that come with a more realistic problem.

We have Molecule A and Molecule B. Each molecule is made of two spheres with a 5Å radius and a center-to-center distanc of 10Å. One sphere has a +1e charge at the center, and the other sphere has a -1e charge at the center. A reaction occurs when the surface of the positively-charged sphere of Molecule A comes within 2Å of the surface of the negatively-charged sphere of Molecule B. The solvent has a dielectric of 78 and the molecule has a dielectric of 4. The ionic strength is 0.1 M. Compute the 2nd-order rate constant within a precision of 10%.

Hints: You only need an APBS grid for one of the molecules. The b-radius can be computed automatically by bd_top. You want to make sure that your time steps can become small enough to resolve the reaction, so it's a good idea to set "minimum_dx" to be no larger than 0.01Å. Also, be sure to assign each sphere to a different "residue". By default, bd_top and the tools it calls lump the charges in a residue together, so if both spheres belong to the same "residue", you will have no charge. The two-charged-spheres example in the BrownDye distribution can be a good guide.

Due Monday, Feb. 13. When you turn in your answer, include your input file to APBS, your PQR files, and any other input files that you have typed in yourself. Also include the results file designated by "output" in your input file. You can email me or Sophie the files or use some other means to share them. If your answer is not close enough, we can figure out what is happening and help you get the correct answer, even if your final work is turned in after that date. But we do need something by the end of Feb. 13.

My email is gahuber95@gmail.com, and my phone number is 619-787-2164.