MOFF IDP Guide

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1. Setup template and pdb
    a. Run write_MOFF.py. Should be up to 2 arguments. The first is the pdb file for the protein that you want to simulate. The second is the template file. Unless doing further development, this should be template_MOFF.top.
    b. The output should be a CA only pdb file and a template file. These will be input for gromacs
2. Generate a table potential
    a. Use write_table.py to make a tabulated potential for MOFF. There are up to 6 input possibilities:
    (python write_table.py ionic_strength outputfile cut cut2 table_length dr)
        i. ionic_strength is for the debye-huckel electrostatic interactions, in mM (default=150 mM)
        ii. outputfile is the name of the table (default=table.xvg)
        iii. cut is the distance at which electrostatic interactions are cut to 0 with a fifth degree polynomial switching function (default=1.5 nm)
        iv. cut2 is the distance at which electrostatic interactions are dampened with a fifth degree polynomial switching function (default=1.2 nm)
        v. table_length is the length of the generated table (default=15 nm)
        vi. dr is the minimal distance at which the table is calculated (default=0.002 nm)

3. Run simulation
    a. Minimize energy
    b. Place in an empty simulation box
    c. Run your simulation

Check out the Example folder for an example on how to do a simple simulation.

Starting in the example folder:
1. python ../Scripts/write_MOFF.py An16 ../Scripts/template_MOFF.top
2. python ../Scripts/write_table.py
3. Run the corresponding commands in Gromacs from job.pbs

Compatible with any version of GROMACS that uses tabulated potentials (used GROMACS 4.5 in published work)
Email aplatham@mit.edu with any questions