Analyze\_Traj\_Test, Analyze\_Traj, Angle: Fine

Aromodel\_lib:

    Line     101-106 Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

    Line 113-118 Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

    Line 1004-1009 Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

    Line 2577-2579 Cluster\_Location='/global/cscratch1/sd/andrewk/Find\_Charges'

    Line 2613-2619 OpenMP\_Location = "/home/andrewk/openmpi-3.1.4"

    Line 2738? Set\_Up\_Folders():

Atom, Aux\_Ring, Bond, Bonded\_Atom: Fine

Cluster\_IO: no hardcoded file locations, however some condition name might cause issue.

    Line 181: if End\_Condition == "SPE\_Orca":

Configure: good idea

Conjugated\_Polymer:

    Line 21: def \_\_init\_\_(self,Ring\_List,Scheduler = "Torque",Cluster\_Location='/oasis/tscc/scratch/andrewk/Optimized\_Monomers',Flip=10000000):

    Line 858: torsion\_file.write("EXTERNAL ARG=DIH\_%d,OOP\_%d FILE=/scratch/andrewk/job\_SLURM\_JOBID/%s\_Nonbonded.dat LABEL=ext\_%d\_nb\n\n" % (i,i,Bias\_File\_Name,i))

DA\_Main, DA\_Polymer, DA\_Strain, Dihedral, Improper, Lammps: Fine

Make\_DA\_Polymer:

    Line 5:  DA\_polymer = Molecule.Molecule('/Users/andrewkleinschmidt/DPP-HD.xyz')

Molecule:

    Line 634: os.system('/Users/andrewkleinschmidt/Library/Orca/orca %s > %s' %(File\_Name, File\_Out)) # Run Orca Job

OPLS, Parallel, Plot, Polymer: Fine

PolymerBuilder:

    Line 144: f = open('/Users/andrewkleinschmidt/AROMODEL/AROMODEL/%s.xyz' % Name,'w')

Post\_Process: Fine

Ring:

Line 20: Cluster\_Location='/oasis/tscc/scratch/andrewk/Optimized\_Monomers'

    Line 73: Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

    Line 74: Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

    Line 160 Read\_From\_Data\_File("./LigParGen\_Files/%s\_%d.lmp"

This one is fine, leave it

~~Line 310? config\_dict['Job\_Type'] = "Orca"~~

    Line 323-328 OpenMP\_Location = "/home/andrewk/openmpi-3.1.4"

    Line 340? os.system("mkdir ./Optimized\_Monomers")

    Line 667-672 Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

    Line 764-769 Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

    Line 867-862 Shared\_File\_Location = "/Users/andrewkleinschmidt/Shared\_Files\_Dihedral\_Parameterization"

Run\_Polymer\_Builder: Fine

sub\_PEDOT\_Ethyl…, submit\_orca: not sure what these are for

System:

    Line 1123-1127: torsion\_file.write("EXTERNAL ARG=DIH\_%d,OOP\_%d FILE=/scratch/andrewk/job\_SLURM\_JOBID/%s\_Nonbonded.dat LABEL=ext\_%d\_nb\n\n" % (i,i,Bias\_File\_Name,i))

Write\_Inputs: Fine

This is bad, should find a way to manage this with config or other file… we’ll need to cover this on Monday as it depends on cluster-specific stuff. The multi-line text should probably be replaced with a template file that is user-defined and then read in by this script

Write\_Submit\_Script:

    Line 60-63?: f.write('#!/bin/bash\n#SBATCH --job-name="%s"\n#SBATCH --output=%s\n#SBATCH --qos=%s\n#SBATCH --nodes=%d\n#SBATCH --ntasks-per-node=%d\n#SBATCH -A %s\n#SBATCH --export=ALL\n#SBATCH -t %d:00:00\n#SBATCH --constraint=%s\ncd %s\n' % (Name,Name,queue,nodes,proc\_per\_node,account,walltime,constraint,Cluster\_Location))

Line 117-119?: f.write('#!/bin/bash\n#SBATCH --job-name="%s"\n#SBATCH --output=%s\n#SBATCH --qos=%s\n#SBATCH --nodes=%d\n#SBATCH --ntasks-per-node=%d\n#SBATCH -A %s\n#SBATCH --export=ALL\n#SBATCH -t %d:00:00\n#SBATCH --constraint=%s\n%scd %s\n' % (Job\_Name,Job\_Name,queue,nodes,proc\_per\_node,account,walltime,constraint,spec\_core,Cluster\_Location))