**Optimization involving MD**

1. Preparations prior to the optimization workflow:
   1. Generate an initial system
      1. configuration file (atomic coordinates)
      2. force field files (including topology)
   2. Template the force field files
      1. File defining force field keywords, bounds of actual values, and minimal step
   3. Create a template submission script file for MD
      1. Assess required wall time and number of processors
         1. Submit a job to debug queue on the cluster
         2. Retrieve job timing
      2. If necessary, enable partition of the simulation into consecutive submissions
      3. Define a scratch directory structure where files are produced
      4. Define a permanent directory structure where files are kept
      5. Define which files are parameter dependent, which are run dependent
   4. Create a template submission script file for Sassena
      1. Assess required wall time and number of processors
         1. Use previous debug MD job to run a job in debug
         2. Retrieve job timing
      2. Define a scratch directory structure where files are produced
      3. Define a permanent directory structure where files are kept
      4. Send the database to the cluster, or have the database stored in a place accessible to users
      5. Select the type of structure factor to be calculated
      6. Include the trajectory files to be used.
   5. Create script to Fourier transform and detailed balance Sassena output
   6. Define or select model to compare simulated and experimental S(Q,E)
   7. Write the first Dakota input file
      1. input parameters, bounds, and minimal variation step
      2. Select optimization protocol
2. Start Kepler workflow
3. Kepler calls the Dakota optimization loop
   1. Dakota output file filter
      1. Chek if simulation parameters were varied
      2. Intantiate force field files
      3. Instantiate MD submission script
   2. Remotely submit MD job
      1. Prepare scratch directory structure for new job
      2. Send new configuration and force field files
      3. Send the job request
   3. Monitor MD job
   4. Check MD files were created after job is finished
      1. Move files to permanent directory structure
   5. Remotely submit Sassena job
      1. Prepare scratch directory structure for new job
      2. Send new configuration file
      3. Send the job request
   6. Monitor Sassena job
   7. Check Sassena files were created after job is finished
      1. Move files to permanent directory structure
   8. Remotely submit Cost function job
      1. Run script to Fourier Transform and detailed balance
      2. Calculate cost function
         1. Load experimental S(Q,E)
         2. Load comparison model between experimental and simulated structure factor
         3. Write to file the calculated cost function in the simulated parameters
   9. Monitor Cost function job
   10. Dakota input filter
       1. Check Cost function output file was create
       2. Import the cost function output file
4. Write Results
   1. Output optimal set of parameters
   2. Output root directory of the permanent directory structure
   3. ICAT files?
   4. Plot a comparison between simulated and experimental structure factors?
   5. Plot Cost function versus sampled force-field parameters?