Todd Martin

Dr. Johnson

Capstone Thesis

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[mart2612@pacificu.edu](mailto:mart2612@pacificu.edu)

**9-steps to Execute an MMAnalysis**

* Step 1: download MMAnalysis folder and MMTest folder to the same directory
  + Can be found on the google drive:
    - MD Research>workspace>MMAnalysis
    - MD Research>workspace>MMTest
  + Can be found on github:
    - Githublink1
    - Githublink2
* Step 2: install Anaconda
  + Download link for windows PCs: <https://conda.io/docs/user-guide/install/windows.html>
  + Download link for mac: <https://conda.io/docs/user-guide/install/macos.html>
* Step 3: create a new environment in conda with python version 2.7 and name it
  + Command-line code: conda create -n (insert environment name here) python=2.7
* Step 4: activate your python2.7 environment
  + For mac: source activate (environment name)
  + For windows: activate (environment name)
* Step 5: install numpy into the environment that you just activated
  + Command-line code: conda install numpy
* Step 6: download necessary OpenMM simulation files to MMTest folder (combo.log, frame\_Data.log, and sim\_variables.txt)
  + All three files must be in a folder titled with the same name as the .log and .txt files.
    - Ex: MMTest>8MgCl2>
      * 8MgCl2.frame\_Data.log
      * 8MgCl2.combo.log
      * 8MgCl2.sim\_variables.txt
* Step 7: open an anaconda prompt, with the newly activated environment and change the directory to the MMTest directory.
  + Command-line code: cd …...MMTest
* Step 8: enter the directory of the simulation you wish to analyze.
  + Ex: cd MMTest\8MgCl2
* Step 9: start the MMAnalysis program by running MMAnalysis.py and giving the .sim\_variable file name.
  + Command-line code if MMAnalysis and MMTest are in the same directory:
    - Ex: python ..\..\MMAnalysis\MMAnalysis.py 8MgCl2.sim\_variables.txt

Analysis files will be output to the directory with the name of the simulation. MMAnalysis will output these files: sim\_variables.txt.interfaces.txt, sim\_variables.txt.Density\_Analysis.txt, sim\_variables.txt.HOH.surface\_Height.txt, sim\_variables.txt.HOH.surface\_Type.txt, and sim\_variables.txt.ORG.surface\_Height.txt, sim\_variables.txt.ORG.surface\_Type.txt.

Reference time and memory considerations.

A simulation file with 9000 atoms, 5ns in duration, and 0.5femtosecond timesteps will take the typical central processing unit about 2 hours to complete. This large of a simulation will consume about 25Gb of RAM throughout the two hours of runtime. A simulation file with 36000 atoms, 5ns in duration, and 0.5femtosecond timesteps will take the average central processing unit 6 hours to complete. This large of a simulation will consume about 90Gb of RAM.

The simulations I ran with 9000 atoms were typically for 25ns long with 0.5femtosecond timesteps; as a result I had to run 5 simulations of 5ns each with each consecutive 5ns of simulation time loading the previous 5ns checkpoint file in order to be able to run MMAnalysis on computers with less than 64Gb of RAM. Splitting simulations in OpenMM also helped preserve simulation data in the result of a power outage or system crash because a checkpoint file was created between each 5ns of data collection that could be loaded into the simulation to continue where the simulation stopped.