# RESULTS LOG 9-26-2018 TO PRESENT

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## 1. 9/26/2018

(1) According to Professor de Pablo, the priority item for the path integral research project is to fix the path integral monte carlo barostat in DASH. So, we will start by investigating the code that Mike has already written for this barostat on the DASH github.
(2) First, let's compile the most recent version of DASH on Midway. Doing "git clone https://github.com/dreid1991/md_engine.git". Saving this compiled version on Midway 1 in DASH-9-26-2018.
(3) Information on BoostPython: https://wiki.python.org/moin/boost.python/GettingStarted.
The BoostPython library binds C++ and Python in a mostly-seamless fashion. It is just one member of the boost C++ library collection. Use the BoostPython library to quickly and easily export C++ to python such that the python interface is very similar to the C++ interface. Boost.Python bindings are written in pure C++, using no tools other than your editor and your C++ compiler.

## 2. 10/1/2018

(1) Created tip4pF_9-26-2018.py to run q-TIP4P/F water model in DASH 9/26/2018 version.
(2) Continuing to work on developing this basic test code, checking all possible options to make sure python script is correct.

## 3. 10/3/2018

(1) We will begin by running a series of tests on q-TIP4P/F water. We will use the following system: 1000 water molecules, 1 ns, initial density of 0.997, temperature of 298 K, pressure 1 atm, printing data every 1000 steps. We are using run_9-26-2018.sh and tip4pF_9-26-2018.py to run DASH version from 9/26/2018.
Tests using the Isotropic Monte Carlo Barostat:
Time Step: 0.5, rCut: 9, nBeads: 1, jobname MC-1, restart/traj every 50,000, RUNNING
Time Step: 0.5, rCut: 9, nBeads: 16, jobname MC-2, restart/traj every 50,000, RUNNING
Time Step: 0.5, rCut: 9, nBeads: 32, jobname MC-3, restart/traj every 50,000, RUNNING
Time Step: 0.5, rCut: 12, nBeads: 1, jobname MC-4
Time Step: 0.5, rCut: 12, nBeads: 16, jobname MC-5

*Date*: October 3, 2018.

Time Step: 0.5, rCut: 12, nBeads: 32, jobname MC-6
Time Step: 0.25, rCut: 9, nBeads: 1, jobname MC-7
Time Step: 0.25, rCut: 9, nBeads: 16, jobname MC-8
Time Step: 0.25, rCut: 9, nBeads: 32, jobname MC-9
Time Step: 1.0, rCut: 9, nBeads: 1, jobname MC-10
Time Step: 1.0, rCut: 9, nBeads: 16, jobname MC-11
Time Step: 1.0, rCut: 9, nBeads: 32, jobname MC-12

Tests using the Berendsen Barostat:

Time Step: 0.5, rCut: 9, nBeads: 1, jobname B-1
Time Step: 0.5, rCut: 9, nBeads: 16, jobname B-2
Time Step: 0.5, rCut: 9, nBeads: 32, jobname B-3
Time Step: 0.5, rCut: 12, nBeads: 1, jobname B-4
Time Step: 0.5, rCut: 12, nBeads: 16, jobname B-5
Time Step: 0.5, rCut: 12, nBeads: 32, jobname B-6
Time Step: 0.25, rCut: 9, nBeads: 1, jobname B-7
Time Step: 0.25, rCut: 9, nBeads: 16, jobname B-8
Time Step: 0.25, rCut: 9, nBeads: 32, jobname B-9
Time Step: 1.0, rCut: 9, nBeads: 1, jobname B-10
Time Step: 1.0, rCut: 9, nBeads: 16, jobname B-11
Time Step: 1.0, rCut: 9, nBeads: 32, jobname B-12

(2) On /home/swansonk1, Midway 1, go into openmm folder. On depablo-gpu, module load Anaconda3, source activate openmm-env. Downloaded pimd.py from Markland, called it pimd_original.py, and created new file pimd_modified.py. In the modified file, we change the nonbondedCutoff to 0.9*nanometers, comment out the platform and properties assignments (so that we use OpenCL by default), and change the Simulation() to get rid of platform and properties arguments.
(3) Searching for OpenMM code here: http://docs.openmm.org/development/api-python/
(4) Found RPMDMonteCarloBarostat. "This class is very similar to MonteCarloBarostat, but it is specifically designed for use with RPMDIntegrator. For each trial move, it scales all copies of the system by the same amount, then accepts or rejects the move based on the change to the total energy of the ring polymer."
(5) Having trouble understanding the kinetic energy units in DASH...not sure what is going on here. I just want to compute the total kinetic energy. For now we will leave it out then.

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