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.

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