The Bridges File System

- As described in the Bridges user guide under “File Spaces”, Bridges allows you to store data in
  - your home directory ($HOME) - shared across nodes, backed up, smaller quota (10 GB)
  - a “scratch” directory ($SCRATCH) - shared across nodes, not backed up, faster than $HOME, larger quota shared by class
  - the worker node for a job ($LOCAL) - only accessible by local node, not backed up and immediately deleted after job, faster than shared disk space, many terabytes of available space
  - the local memory for a job ($RAMDISK) - only accessible by local node, not backed up and immediately deleted after job, fastest storage
  - $(VARIABLE_NAME) is a variable that contains the actual location. The variable is available while logged onto Bridges
- Try `cd $SCRATCH’, ‘pwd’, `cd $HOME’, and ‘pwd’

Installing OpenMM

- The easiest way to install OpenMM is through the conda package manager
- Conda is available on bridges, but needs to be loaded by entering `module load anaconda'
- Then you need to create an conda environment that you can write to by entering `conda create --name openmm'

```
br005:[~]: conda create --name openmm
Collecting package metadata (current_repodata.json): done
Solving environment: done


==> WARNING: A newer version of conda exists. <==
  current version: 4.7.12
  latest version: 4.8.1

Please update conda by running

    $ conda update -n base -c defaults conda



## Package Plan ##

  environment location: /home/dminh/.conda/envs/openmm



Proceed ([y]/n)? y

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate openmm
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```