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
```

- To allow you to activate the environment, enter `conda init bash' and then `bash'
- Then to activate the environment, enter `conda activate openmm'
- Finally, to install OpenMM, enter
  - `conda install -c omnia -c conda-forge openmm'
  - `conda init bash'
- OpenMM may be tested using `python -m simtk.testInstallation'

```
(openmm) br006:[~]: conda install -c omnia -c conda-forge openmm
Collecting package metadata (current_repodata.json): done
Solving environment: done


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## Package Plan ##

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

  added / updated specs:
    - openmm


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    _libgcc_mutex-0.1          |      conda_forge           3 KB  conda-forge
    _openmp_mutex-4.5          |            0_gnu         435 KB  conda-forge
    ca-certificates-2019.11.28 |       hecc5488_0         145 KB  conda-forge
    certifi-2019.11.28         |           py37_0         148 KB  conda-forge
    cython-0.29.14             |   py37he1b5a44_0         2.2 MB  conda-forge
    ld_impl_linux-64-2.33.1    |       h53a641e_8         589 KB  conda-forge
    libblas-3.8.0              |      14_openblas          10 KB  conda-forge
```