

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
```

```
==> WARNING: A newer version of conda exists. <==
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Please update conda by running

```
$ conda update -n base -c defaults conda
```

```
## 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