

- 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. <==
  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
```

```
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 |

Transferring Data

- After logging into the XSEDE Single Sign-On Hub, you can transfer data
 - using various commands in the terminal, including rsync, scp, and sftp
 - using specialized programs, as specified in the user manuals, but this requires installing programs, which you might not want to do
- On the terminal, I recommend rsync because you don't need to copy (and wait for) the whole directory
- A good template is: `rsync -Cuavz --port 2222 source_path destination_path`
 - Cuavz are options, which can be seen by ``man rsync``
 - port 2222 means that you go through the XSEDE SSO
 - the paths have the format `user_name@directory/file_name`
 - if `user_name@` is omitted, it assumes the same user name as on the current system
 - if `directory` is omitted, the home directory is assumed
 - if `file_name` is omitted, the whole directory is assumed