

Building pyCHARMM and the python environment

To use pyCHARMM it is useful to build a python environment using anaconda (conda) that includes the following modules: python 3+, numpy, pandas, rdkit, jupyter, OpenMM (unless you have it installed as part of your Linux build environment), pymol, open babel, mpi4py, ...

In the folder python_environments I have created two separate environment configuration files, one from my MacBook pro laptop and the other from our linux environment. If you want to create a conda environment that's the same as either of these use:

```
conda install --name myenv --file spec-file.txt
```

To build pyCHARMM, as noted in the pyCHARMM Workshop pdf, one builds CHARMM using the following configure command, assuming you are building CHARMM in an empty folder (build_charmm) that sits below the main charmm folder.

In build_charmm:

```
../configure --without-mpi --with-blade --with-fftdock --as-library -p ../install-pycharmm-nompi
```

Note we build w/o MPI because we will utilize MPI calls directly in python using mpi4py, the --with-blade will incorporate the blade accelerated MSMD/MD kernels, the --with-fftdock will add the fft-based and OpenMM based CDOCKER functionality. If you have OpenMM installed on your system and available the output from the configure command will tell you it found OpenMM and will build linking with the OpenMM api libraries.

Once the configuring is done, you need to make the library:
make -j 8 install

This will compile all of the code and install it in the folder following the -p in the command above.

Lastly, with your conda environment active, you need to install the pyCHARMM functionality by:

- 1) setenv CHARMM_LIB_DIR <path_to_charmm_install_lib directory>
- 2) or export CHARMM_LIB_DIR=<path_to_charmm_install_lib directory>
- 3) pip install <path_to_charmm_tool_pycharmm directory>

So, if the top level CHARMM directory is /users/<user_name>/charmm, then CHARMM is configured and build from /users/<user_name>/charmm/build_charmm, the tool directory containing the pyCHARMM python functions is /users/<user_name>/charmm/tool/pycharmm and the CHARMM_LIB_DIR environment variable should point to /users/<user_name>/charmm/install-pycharmm-nompi/lib.