Configuration

As explained in some parts of the documentation, the user can modify the built-in default configuration. In some installations, the default parameters might not be appropriate and this section will try to address some of the most common modifications any user might need to carry out.

Modification of pyMDMix defaults can be done in two ways:

1. Modify `settings.cfg` (or `md-settings.cfg`) file before installing the python package. This will affect all users in the system. Package config files can be found in `$INSTALL_DIR/pyMDMix/data/defaults/settings.cfg` and/ or `$INSTALL_DIR/pyMDMix/data/default/md-settings.cfg`. Where `$INSTALL_DIR` is the installation directory (before running `setup.py` or after).

2. Modify the user specific `settings.cfg` (`md-settings.cfg`) file. This will have impact only on current user configuration. The files are then located under the user home directory `$HOME/.mdmix/settings.cfg` or `$HOME/.mdmix/md-settings.cfg`. They contain same options as in the main package file and any un-commented parameter will over-write package defaults. This file will be written after the first attempt to run the program after installation. This first attempt will yield some warnings like the following:

```
### WARNING (SettingsManager) Could not find file with user-defined settings in /Users/dalvarez/.mdmix/se
### WARNING (SettingsManager) Creating new user configuration file /Users/dalvarez/.mdmix/settings.cfg.
### WARNING (SettingsManager) Could not find file with user-defined settings in /Users/dalvarez/.mdmix/md
### WARNING (SettingsManager) Creating new user configuration file /Users/dalvarez/.mdmix/md-settings.cfg
```

1. Modifying executable program names

By default, pyMDMix will call several programs from the AmberTools suite during operation. Default configuration calls `ptraj` for trajectory alignment, `tleap` for topology preparation and it will write in MD execution commands the following programs: `sander` for the minimization stage and `pmemd.cuda` for equilibration and production.

These default configuration can be modified in `settings.cfg` file under the following options (uncomment the lines if modifying the user settings):

```
AMBER_MIN_EXE = sander
AMBER_PROD_EXE = pmemd.cuda
AMBER_PTRAJ = ptraj
AMBER_TLEAP = tleap
NAMD_EXE = namd2
```

Just replace the executable name with your program. For instance, changing `ptraj` to `cpptraj` will be done uncommenting `AMBER_PTRAJ` line and changing `ptraj` to `cpptraj`. If you don't have a `pmemd.cuda` installation, in the same way, change `AMBER_PROD_EXE` to `pmemd.MPI`, for instance.