Phenix *Python-based Hierarchical ENvironment for Integrated Xtallography*

Install Cryo_fit

Contents

1. Install Phenix

See the installation notes for Phenix

2. Link cryo_fit to phenix

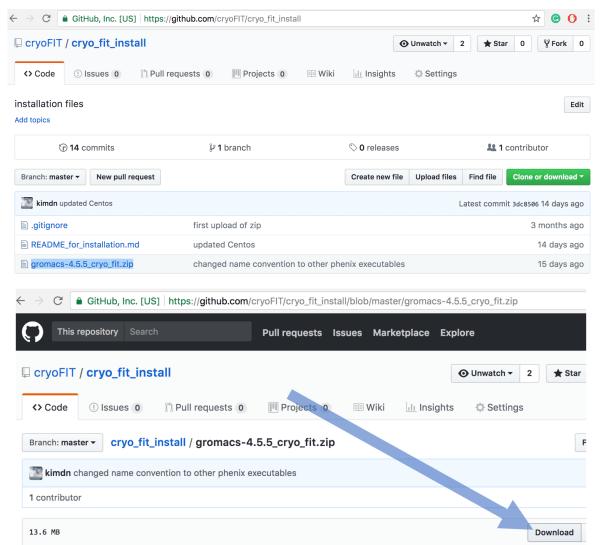At <user phenix>/modules

```
git clone git@github.com:cryoFIT/cryo_fit.git
```

At any folder,

```
libtbx.configure cryo_fit
```

3. Install gromacs_cryo_fit

Download gromacs-4.5.5_cryo_fit.zip from here

Install using a provided script.

```
python <user phenix>/modules/cryo_fit/steps/0_install_cryo_fit/install_cryo_fit.py <cryo_fit.zip>
```

For example,

```
python /Users/doonam/bin/phenix-dev-2906/modules/cryo_fit/steps/0_install_cryo_fit/install_cryo_fit.py ~/Downloads/gromacs-4.5
```

4. Troubleshooting

If user's OS doesn't have git

-> install git

If a user sees the error during git clone, "Permission denied (publickey).fatal: Could not read from remote repository. Please make sure you have the correct access rights and the repository exists.",

-> user's computer needs to be registered to his/her github account. Therefore, make github account (free), Generate a new SSH key and Add a new SSH key to your GitHub account

If user's macOS shows, "xcode-select: note: no developer tools were found at '/Applications/Xcode.app', requesting install. Choose an option in the dialog to download the command line developer tools."

```
download commandline as instructed (this may take ~7 minutes)
```

"-bash: libtbx.configure: command not found"

```
Run export PATH="/Users/.../phenix-xxxx/build/bin":$PATH
source /Users/.../phenix-xxxx/phenix_env.sh
in commandline, and try "libtbx.configure cryo_fit" again
```

"subprocess.CalledProcessError: Command '['which', 'phenix.cryo_fit']'"

```
It can't find phenix.cryo_fit, link (sync) cryo_fit by "libtbx.configure cryo_fit".
Open a new tab in your terminal (like iterm2), then your .bash_profile should run freshly.
```