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

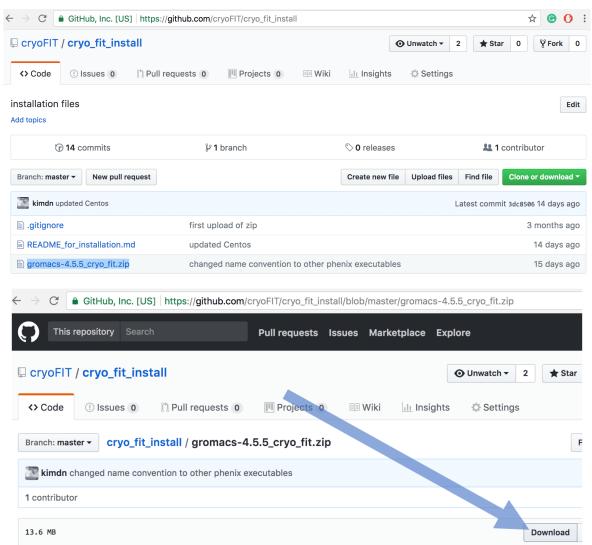At <user phenix>/modules

```
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 message 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"
  - (in commandline)
  - export PATH="/Users/.../phenix-xxxx/build/bin":$PATH
  - source /Users/.../phenix-xxxx/phenix_env.sh
  - libtbx.configure cryo_fit2