

## Remote running of XCE and model building on Diamond's filesystem

NX latency is a killer when trying to do anything graphical, like model building during *pandda.inspect* or during refinement. So instead use *Filesystem in Userspace* (FUSE), which mounts Diamond's disk from your computer using the ssh protocol. All you need is root privileges, or bribe your IT team.

### 1. Setup fuse (requires admin rights)

Install FUSE (<http://github.com/libfuse/libfuse>)

```
Centos: sudo yum install fuse-utils sshfs
```

```
Ubuntu: sudo apt-get install sshfs
```

See <https://gist.github.com/cstroee/e83681e3510b43e3f618> for details. FUSE is also available for Mac. Avoid building from source unless you really have to.

Create a /dls mount point and give your user ownership:

```
sudo mkdir /dls
```

```
sudo chown <yourUID>:<yourGID> /dls
```

### 2. Mount the Diamond filesystem

When you need it, run this from your own user account:

```
sshfs -o reconnect <your_fed_id>@nx.diamond.ac.uk:/dls /dls  
e.g. sshfs -o reconnect zqr16691@nx.diamond.ac.uk:/dls /dls
```

(Recommended): make your ssh client to keep the link alive by editing `~/.ssh/config` and adding these lines:

```
ServerAliveInterval 15  
ServerAliveCountMax 3
```

(The "reconnect" option is meant to do this too, but it slows down and eventually drops it anyway.)

### 3. Fire up XCE

```
cd <your-labxchem-visit-dir>  
e.g. cd /dls/labxchem/data/2017/lb18145-3/processing  
  
/dls/science/groups/i04-1/software/XChem/xce  
(See Note 1 below.)
```

### 4. When you're done, unmount the file system

```
fusermount -u /dls
```

## Notes:

1. Launching XCE this way avoids insane installation issues, because it runs the software directly off Diamond's drives, i.e. it's exactly what you use if physically at Diamond or through NX. This is therefore supported.

The trade-offs are currently (but we're trying to fix):

- a. It takes a very long time (up to 10 minutes in the UK and up to an hour in North America) to launch XCE and *pandda.inspect*. After that they are fully responsive.
  - b. The xce-coot plugin does not always work, due to a library mismatch.
2. IF YOU KNOW WHAT YOU'RE DOING and really hate (!) the lag on startup:
    - a. install XCE locally: <https://github.com/xchem/XChemExplorer>
    - b. update your PanDDA installation ([the ccp4 version is outdated](#)):

```
ccp4-python -m pip uninstall panddas
ccp4-python -m pip install pip --upgrade
ccp4-python -m pip install numpy --upgrade
ccp4-python -m pip install panddas
```

*(Note, this is not supported – you really are on your own! Recommended only for geeks.)*

3. If your IT team doesn't want to help you, try setting up a virtual machine – then you have root permissions and can do whatever you like. Performance ought to be okay.