

CrystFEL tutorial - “quick start”

> Start by setting up your environment:

- `source /reg/g/cfel/crystfel/crystfel-dev/setup-sh` (sh/bash/zsh users)
- `source /reg/g/cfel/crystfel/crystfel-dev/setup-csh` (tcsh users)

> Copy tutorial files to your working directory:

- `(cd /reg/data/ana13/cxi/cxi84914/scratch; mkdir myfolder; cd myfolder)`
- `cp -R /reg/data/ana13/cxi/cxi84914/scratch/crystfel-tutorial .`

> Examine files:

- `[nano | vim | emacs | less] run-indexing, tutorial.beam, tutorial.geom, tutorial.pdb` etc

> `./run-indexing`

CrystFEL tutorial - “quick start” - things to try 1

> Merge reflections and calculate completeness, SNR etc:

- `process_hkl -i tutorial.stream -o tutorial.hkl -y 4/mmm`
- `check_hkl tutorial.hkl -y 4/mmm -p tutorial.pdb`
- `cat shells.dat`

> Split stream into two, merge separately and calculate R_{split} , $CC_{1/2}$:

- `. /alternate-stream tutorial.stream t1.stream t2.stream`
- `process_hkl -i t1.stream -o t1.hkl -y 4/mmm`
- `process_hkl -i t2.stream -o t2.hkl -y 4/mmm`
- `compare_hkl t1.hkl t2.hkl -y 4/mmm -p tutorial.pdb --fom=rsplit`
- `cat shells.dat`
- `compare_hkl t1.hkl t2.hkl -y 4/mmm -p tutorial.pdb --fom=cc`
- `cat shells.dat`

CrystFEL tutorial - “quick start” - things to try 2

> Examine peaks from peak search:

- `./check-peak-detection tutorial.stream`
- To move to next image, simply close the viewer. To end, press Ctrl+C in the terminal.

> Examine integrated reflections (after spot “prediction”):

- `./check-near-bragg tutorial.stream`

> Examine unit cell distributions:

- `cell_explorer tutorial.stream`

> Visualise merged intensities:

- `render_hkl tutorial.hkl -y 4/mmm -p tutorial.pdb`
- Open `za.pdf` (may have to copy to own computer first). Note: unfortunately this doesn't work at SLAC, because of a bug in one of the system libraries on their system.

CrystFEL tutorial - long version

> `source /reg/g/cfel/crystfel/crystfel-dev/setup-sh (or setup-csh)`

> Copy `tutorial.geom` and `tutorial.beam` from the tutorial folder:

- `(cd /reg/data/ana13/cxi/cxi84914/scratch; mkdir myfolder; cd myfolder)`
- `cp /reg/data/ana13/cxi/cxi84914/scratch/crystfel-tutorial/tutorial.{beam,geom} .`

> Work through the tutorial on the CrystFEL website:

- <http://www.desy.de/~twhite/crystfel/tutorial.html>
- Do not download files from CXIDB, but use files already here:
`/reg/data/ana13/cxi/cxi84914/scratch/lysozyme-hdf5/`
- `files.lst` contains a list of 2000 files for tutorial purposes.
- `all-files.lst` has everything – nearly 300,000 frames – process this using `bsub` only!

> **Don't be shy about asking for help** - that's why we're all here!