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# Simple CrystFEL demo

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# What is CrystFEL?

→ Suite of programs for processing serial crystallography data acquired at XFELs (and synchrotrons).

## What CrystFEL does?

... indexing, integrating intensities, merging, scaling, viewing, hit finding...

## How to get CrystFEL?

From Tom White, it's for free 😊

<http://www.desy.de/~twhite/crystfel/index.html>

*White, T. A., et al. (2012). "CrystFEL: a software suite for snapshot serial crystallography". J. Appl. Cryst. 45, p335-341.*

*White, T. A., et al. (2016). "Recent developments in CrystFEL". J. Appl. Cryst. 49, 680-689.*

# CrystFEL's core programs

**indexamajig** – peak finding, indexing, integration and data reduction program

**partialator** - merging and scaling partial intensities

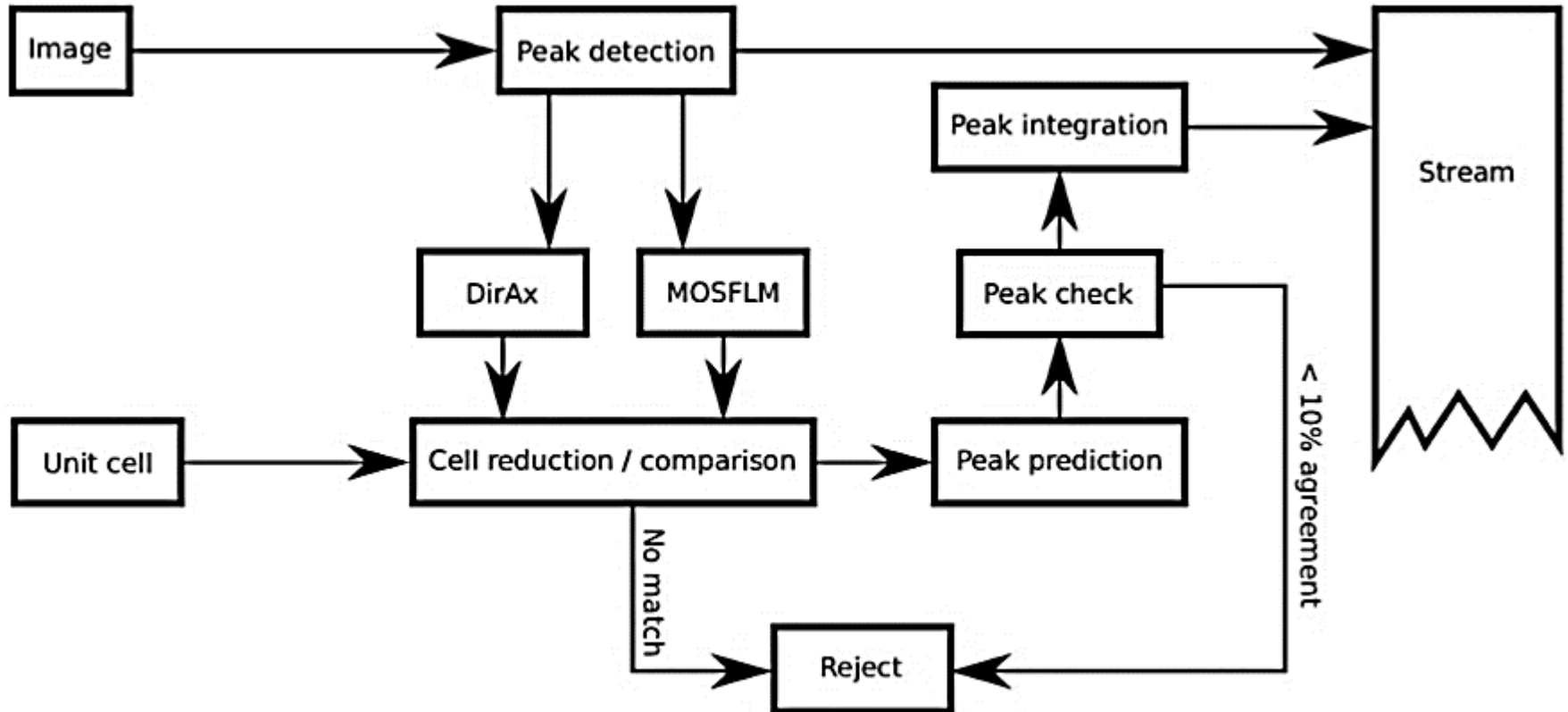
**compare\_hkl** and **check\_hkl** - programs for calculating figures of merit  
(R\_split, CC 1/2, Signal-to-Noise Ratio, etc.)

**cell\_explorer** – a tool for examining distributions of unit cell parameters

**hdfsee** - image viewer

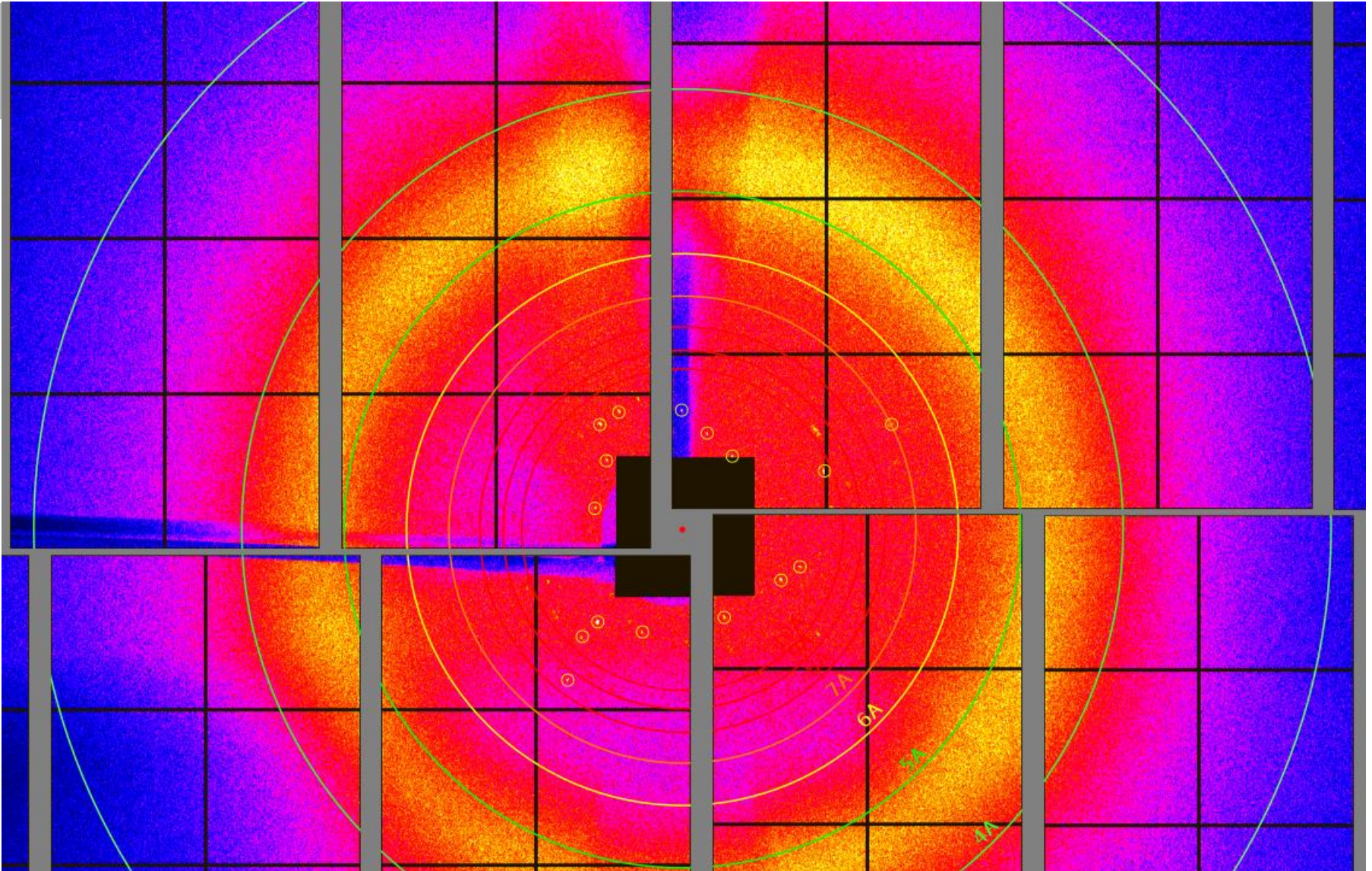
# Indexamajig – index and integrate diff. images

```
[nass_k@ra-1-002 merge4]$ indexamajig -j 12 -i list.lst -g g.geom -o list.stream --indexing=xgandalf
-latt-cell --peaks=peakfinder8 --threshold=50 -p c.cell --int-radius=4,6,9 --integration=rings-grad
--max-res=3000 --min-snr=5 --tolerance=9,9,9,2,2,2 --no-retry --no-multi --check-peaks --min-pix-co
unt=2 --local-bg-radius=4
```



# Hdfsee – useful image viewer

```
 hdfsee -i 5 -g div.geom run14.JF06T32V01.h5 |
```



## Merging using partialator

```
partialator -i mirr2.stream -o mirr2.hkl -y 422 --model=unity --iterations=1
```

## Calculating figures of merit (CC 1/2, Signal-to-Noise Ratio, etc.)

```
compare_hkl -y 422 -p c.cell --nshells=15 --highres=2.1 --fom=cc mirr2.hkl1 mirr2.hkl2
```

```
check_hkl -y 422 -p c.cell --nshells=15 --highres=2.1 mirr2.hkl
```



Thank you for your attention!

