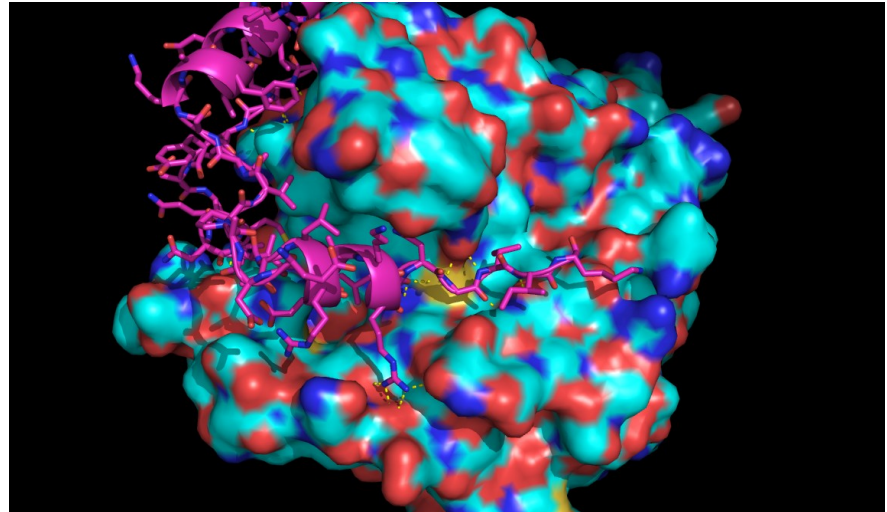


Introduction to CrystFEL

Data processing for serial crystallography



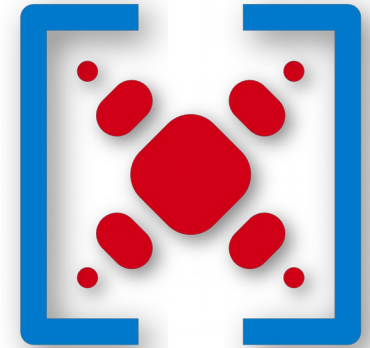
Thomas White
Serial Crystallography Data Analysis Workshop
ACA Annual Meeting
25 July 2015

Contributors to CrystFEL

- > Led by me, Thomas White (Center for Free-Electron Laser Science, DESY Hamburg).
- > Code contributions from:
 - Valerio Mariani, Alexandra Tolstikova, Lorenzo Galli, Kenneth Beyerlein, Cornelius Gati, Anton Barty, Fedor Chervinskii, Oleksandr Yefanov (CFEL).
 - Takanori Nakane (MRC-LMB, now Tokyo University).
 - Keitaro Yamashita (SPring-8)
 - Wolfgang Brehm (U Konstanz)
 - Rick Kirian, Nadia Zatsepin (ASU).
 - Karol Nass, Andrew Aquila, Andrew Martin, Chun Hong Yoon (previously CFEL).
- > Testing/feedback from the above people **and many more**.
- > Words of wisdom from many people, in particular:
 - Henry Chapman (CFEL), Petra Fromme (CFEL), James Holton (ALS/UC Berkeley), John Spence (ASU/LBL), Kay Diederichs (U Konstanz).

What is CrystFEL?

- CrystFEL: data processing for “snapshot serial” crystallography (usually using an FEL, but not necessarily).
- Development since late 2009. Version 0.6.1 to be released very soon.
- Licence: GPLv3 (*free and open source* software)
- User-oriented development.
- <http://www.desy.de/~twhite/crystfel>



CrystFEL

Welcome to the CrystFEL page!

CrystFEL is a suite of programs for processing diffraction data acquired “serially” in a “snapshot” manner, such as when using the technique of **Serial Femtosecond Crystallography (SFX)** with a free-electron laser source. CrystFEL comprises programs for indexing and integrating diffraction patterns, scaling and merging intensities, simulating patterns, calculating figures of merit for the data and visualising the results. Supporting scripts are provided to help at all stages, including importing data into [CCP4](#) for further processing.

The primary citation for CrystFEL is as follows:

T. A. White, R. A. Kirian, A. V. Martin, A. Aquila, K. Nass, A. Barty and H. N. Chapman. “CrystFEL: a software suite for snapshot serial crystallography”. *J. Appl. Cryst.* **45**, p335–341. doi:10.1107/S0021889812002312 — [Download PDF](#) — [Article on IUCr website](#)

Recent News

- **10th January 2013:** CrystFEL version 0.4.3 released. See the [download page](#) or the [changes page](#) for more information.
- **3rd October 2012:** CrystFEL version 0.4.2 released.
- **29th August 2012:** CrystFEL version 0.4.1 released.
- **31st July 2012:** CrystFEL version 0.4.0 released. See the [release notes](#) and the [download page](#) for more information.
- **20th June 2012:** Lysozyme test images available for download! Are you looking for some test data to work with? The images from a [recent Science article](#) have been made available via the Coherent Imaging Data Bank. [Download here!](#)
- **14th March 2012:** First public release of CrystFEL!

Acknowledgements

The development of CrystFEL is led by Thomas White at the [Center for Free-Electron Laser Science](#) at the [Deutsches Elektronen-Synchrotron DESY](#) in Hamburg, Germany. DESY is a research centre of the [Helmholtz-Gemeinschaft](#). See the [contact page](#) for more contact details.

Code has been contributed to CrystFEL by: Rick Kirian, Andrew Aquila, Andrew Martin, Lorenzo Galli, Kenneth Bayerlein, Chun Hong Yoon and Nadia Zatspein. It has been thoroughly tested by Karol Nass, Francesco Stellato, Linda Johansson, David Anlauf, Mark Hunter and many others. The design of CrystFEL and its algorithms has been influenced by Henry Chapman, Anton Barty, Petra Fromme, James Holton and John Spence.

You can read more information about some of the algorithms used in CrystFEL in the following article: Kirian et al., *Optics Express* **18** (2010) p5713. doi:10.1364/OE.18.005713

“Official” citation: White et al., *J. Appl. Cryst.* **45** (2012) p335

What do you get? Core programs

- > **indexamajig** Bulk indexing and integration of patterns
- > **ambigator** Resolve indexing ambiguities
- > **process_hkl** Merge using “Monte Carlo” technique
- > **hdfsee** View images in HDF5 format (with geometry)
- > **cell_explorer** Examine unit cell parameter distributions
- > **compare_hkl** Compare merged reflection data
- > **check_hkl** Evaluate merged reflection data
- > **pattern_sim** Simulate diffraction patterns
- > **partial_sim** Simulate partial reflection intensities
- > **get_hkl** Reflection data “Swiss army knife”
- > **render_hkl** Render plane sections of reciprocal space
- > **geoptimiser** Optimise multi-panel detector geometry
- > **list_events** Generate event lists
- > **whirligig** Detect rotation series
- > **partialator** Merge using partialities and post-refinement

What do you get? Documentation

> Manual pages: `$ man indexamajig`

> Help messages: `$ indexamajig --help`

> Website, particularly: tutorial, best practice, FAQ

> Mailing list for announcements

> User support

```
18:45:04 cfe4204w ~$ project % indexamajig --help
Syntax: indexamajig [options]

Process and index FEL diffraction images.

-h, --help          Display this help message.
-v, --version       Print CrystFEL version number and exit.
-i, --input=filename Specify file containing list of images to process.
-o, --output=filename Write output stream to this file. '-' for stdout.
                        Default: indexamajig.stream
--indexing=methods Use 'methods' for indexing. Provide one or more
                        methods separated by commas.
                        Set 'no_indexamajig' for details.
-g, --geometry=filename Get detector geometry from file.
-b, --beam=filename   Get beam parameters from file (provides nominal
                        wavelength value if no per-shot value is found in
                        the HDFS files.
-p, --pdb=filename   RDB file from which to get the unit cell to match.
                        Default: 'molecule.pdb'
--beamname          Remove the directory parts of the filenames.
-x, --prefix=prefix Prefix filenames from input file with 'prefix'.
--peaks=method      Use 'method' for finding peaks. Choose from:
                        'zarf' - use Zeffner (2000) gradient detection.
                        'hdfs' - get from a table in HDFS file.
                        'hdfs-peaks=mp' - Find peaks table in HDFS file here.
                        'integration=with' - Perform final pattern integration using 'method'.

For more control over the process, you might need:

--tolerance=tol    Set the tolerances for cell comparison.
                        Default: 5.5, 3.1, 5.
--filter-noise     Apply an aggressive noise filter which sets all
                        pixels in each 2d region to zero if any of them
                        have negative values. Intensity measurement will
                        be performed on the image as it was before this.
--median-filter=median Apply a median filter to the image data. Intensity
                        measurement will be performed on the image as it
                        was before this. The scan length of the median
                        filter box will be 20x10. (Default: 0 (no filter))
```

```
INDEXAMAJIG(1)                                INDEXAMAJIG(1)

NAME
  indexamajig - bulk indexing and data reduction program

SYNOPSIS
  indexamajig -i filename -o output_stream -g detector_geo -b beamline_beam --peaks=method --indexing=method (options) ...
  indexamajig --help

DESCRIPTION
  indexamajig takes a list of diffraction snapshots from crystals in random orientations and attempts to find peaks, index and
  integrate each one. The input is a list of diffraction image files in HDFS format and some auxiliary files and parameters.
  The output is a long text file ('stream') containing the results for each image in turn.

  For minimal basic use, you need to provide the list of diffraction patterns, the method which will be used to index, a file
  describing the geometry of the detector, and a PDB file which contains the unit cell which will be used for the indexing.
  Here is what the minimal use might look like on the command line.

  indexamajig patterns.lst -o g -g geometry_geo -indexing=mpsls.dirax --peaks=hdfs -b ayafel.beam -o test.stream -p
  mycell.pdb

  More typical use includes all the above, but might also include extra parameters to modify the behaviour. The HDFS files
  might be in some folder a long way from the current directory, so you might want to specify a full path name to be added in
  front of each filename. You'll probably want to run more than one indexing job at a time (i.e. MPI).

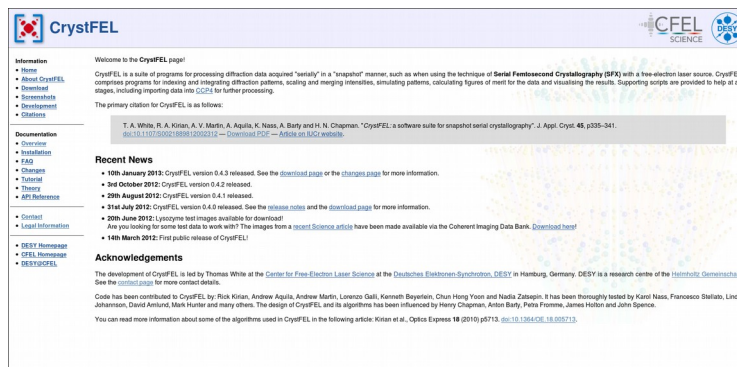
  See man crystfel\_geometry for information about how to create a geometry description file and a beam parameters file.

PEAK DETECTION
  You can control the peak detection on the command line. Firstly, you can choose the peak detection method using
  --peaks=method. Currently, two values for 'method' are available. --peaks=hdfs will take the peak locations from the HDFS
  file. It expects a low dimensional array, by default at processing/finder/peaks/ints. The first two columns contain the fast scan and
  slow scan coordinates, the third contains the intensity. However, the intensity will be ignored since the patterns will
  always be re-integrated using the unit cell provided by the answer on the basis of the peaks. You can tell indexamajig
  where to find this table inside each HDFS file using --hdfs-peaks=table.

  If you use --peaks=zarf, indexamajig will use a simple gradient search after Zeffner (2000). You can control the overall
  threshold and minimum squared gradient for finding a peak using --threshold and --minsq-gradient. The threshold has arbitrary
  units matching the pixel values in the data, and the minimum gradient has the equivalent squared units. Peaks will
  be rejected if the 'foot print' is further away from the 'waist' of the peak by more than the inner integration radius (see
  below). They will also be rejected if the peak is closer than twice the inner integration radius from another peak.

  You can suppress peak detection altogether for a panel in the geometry file by specifying the 'no_index' value for the panel
  as 'non-zero'.

INDEXING METHODS
  You can choose between a variety of indexing methods. You can choose more than one method, in which case each method will
  be used in turn until one of them appears that the pattern has been successfully indexed. Choose from:
  Manual page: indexamajig\(1\) line 4 \(press F for help\) \(press Q to quit\)
```



The screenshot shows the CrystFEL website. At the top, there is a navigation menu with links for Home, About CrystFEL, Download, Screenshots, Development, and Changelog. Below the menu, there is a 'Welcome to the CrystFEL page!' section followed by a paragraph describing CrystFEL as a suite of programs for processing diffraction data. A 'Recent News' section lists several updates, including the release of CrystFEL version 0.4.3 in January 2013 and version 0.4.2 in October 2012. An 'Acknowledgements' section at the bottom credits the developers and funding sources.



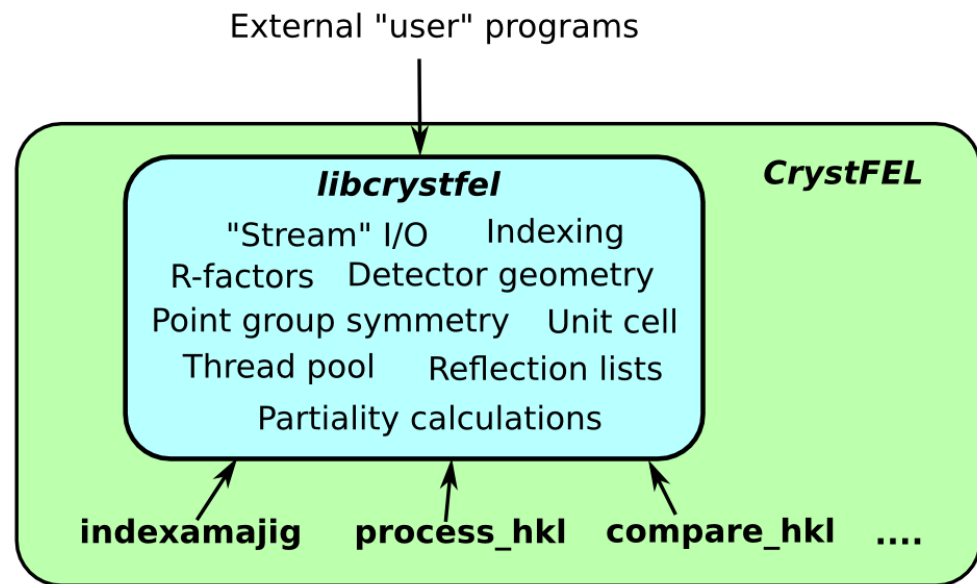
What do you get? Scripts

- > Auxiliary scripts for plotting graphs, collating results etc.
- > Difference from core programs: you're meant to copy them to your working directory and modify them

```
1#!/usr/bin/perl -w
2
3use strict;
4use File::Basename;
5
6my $args = join(" ", splice(@ARGV, 1, scalar(@ARGV)-1));
7if ( !($args eq "") ) {
8    printf("Extra arguments for hdfsee: %s\n", $args);
9} else {
10    # Default arguments - feel free to override!
11    $args = "--binning=2 --int-boost=10";
12    printf("Using default arguments for hdfsee: %s\n", $args);
13}
14
15open(FH, $ARGV[0]);
16open(TMP, "> list.tmp");
17
18my $in_image = 0;
```

What do you get? libcrystfel

- > libcrystfel: shared library exposing high-level functions, e.g. “index this pattern” or “calculate these partialities”.
- > Possible application: use CrystFEL for online data processing within a facility's monitoring software.
- > API docs on website



Where can you get it?

- > From the website: **<http://www.desy.de/~twhite/crystfel>**
(or just type “crystfel” into your favourite search engine)
- > “Release” versions: tested with a series of regression tests
- > Git repository: very latest code, maybe broken, maybe awesome, slightly harder to install (need autotools installed).
- > Packaged snapshots: like Git repository, but slightly easier to install.
- > Ubuntu, Red Hat, Debian packages, MacPort (back soon).

Where can you get it?

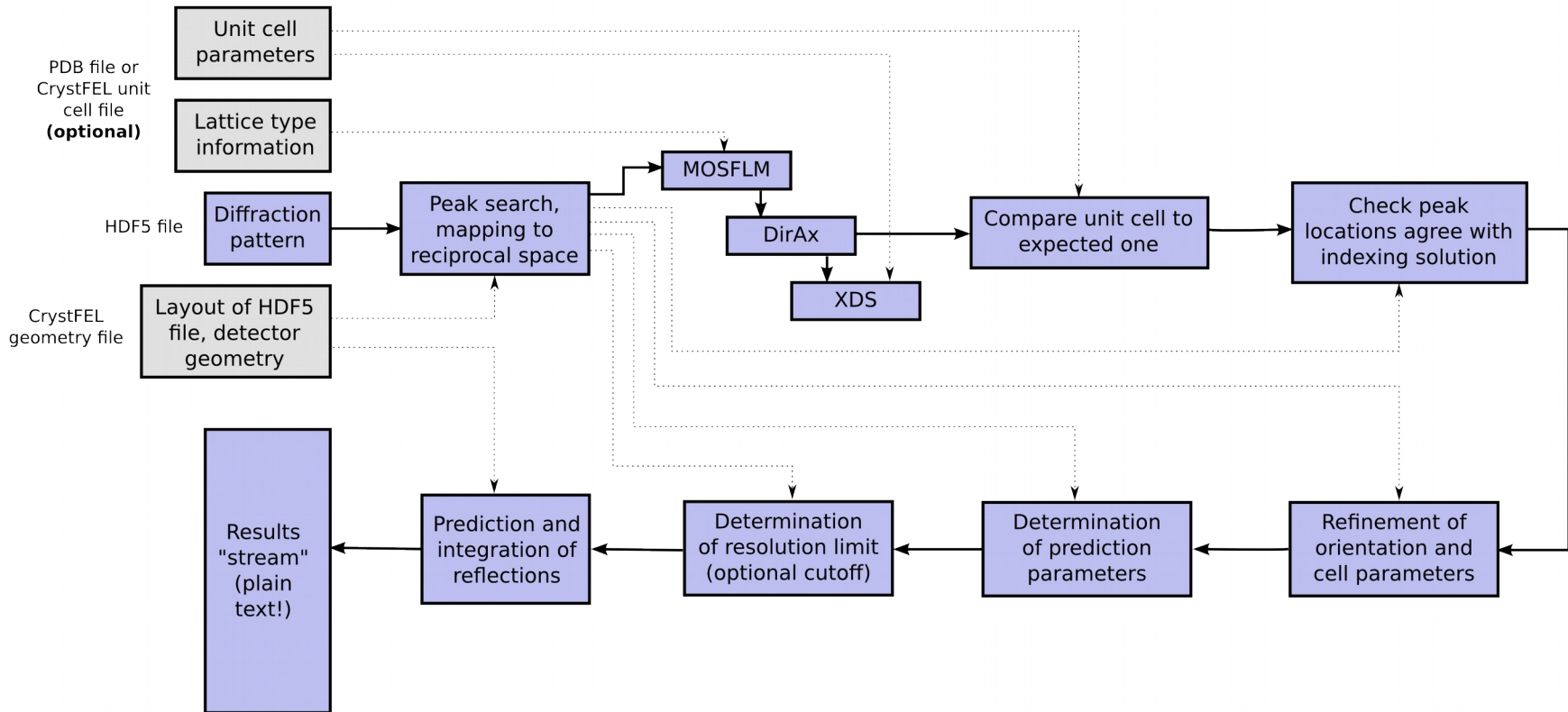
- > GNU General Public License (GPL):
“free” as in “freedom” (also as in “free beer”)
- > Freedom to use the software *for any purpose* (even commercially).
- > Freedom to study how the software works.
- > Freedom to change the software, e.g. to fix bugs or add features.
- > Freedom to share the software, even a modified version.
- > No license forms to sign, send etc.
- > The GPL ensures that these rights are never restricted.



Fundamental basis of CrystFEL

Every diffraction pattern is a new experiment and must be processed individually.

Pipeline in “indexamajig”



- > Input: HDF5 (very common scientific format, many language bindings)
- > Note: choice of methods for **peak search**, **indexing** and **integration**.
- > Output: plain text “stream” - don't be afraid to look inside!
(tip: use “less”, not “gedit” - file can be very large)

Peak search methods

- > `indexamajig [...] --peaks=hdf5 [...]`
... means “get peak list from HDF5 file”.
- > `indexamajig [...] --peaks=cxi [...]`
... means “get peak list from CXI file”.
- > `indexamajig [...] --peaks=zaef [...]`
... means “use internal peak search algorithm”.
- > More peak search algorithms will probably be added in the future.

Indexing methods

- > `indexamajig [...] --indexing=method1,method2,.. [.....]`
List of indexing methods will be tried in order.

- > **Example method:**

`mosflm - raw - latt`

Invoke mosflm to index the pattern using the peaks from the peak search

Skip the step where the unit cell parameters would be checked against the reference

Take the Bravais lattice information from the reference into account, e.g. “look for tetragonal P cells only”

Indexing methods

- > `indexamajig [...] --indexing=method1,method2,.. [.....]`
List of indexing methods will be tried in order.

- > **Example method:**

`mosflm-axes-latt`

Invoke mosflm to index the pattern using the peaks from the peak search

Check the unit cell parameters against the reference

Take the Bravais lattice information from the reference into account, e.g. “look for tetragonal P cells only”

Indexing methods

> `indexamajig [...] --indexing=method1,method2,.. [.....]`
List of indexing methods will be tried in order.

> Example method:

`mosflm-raw-nolatt`

Invoke mosflm to
index the pattern
using the peaks from
the peak search

Do not check the
unit cell parameters

Do not use
Bravais lattice
information

Indexing methods

> `indexamajig [...] --indexing=method1,method2,.. [.....]`
List of indexing methods will be tried in order.

> Example method:

`dirax-comb-nolatt`

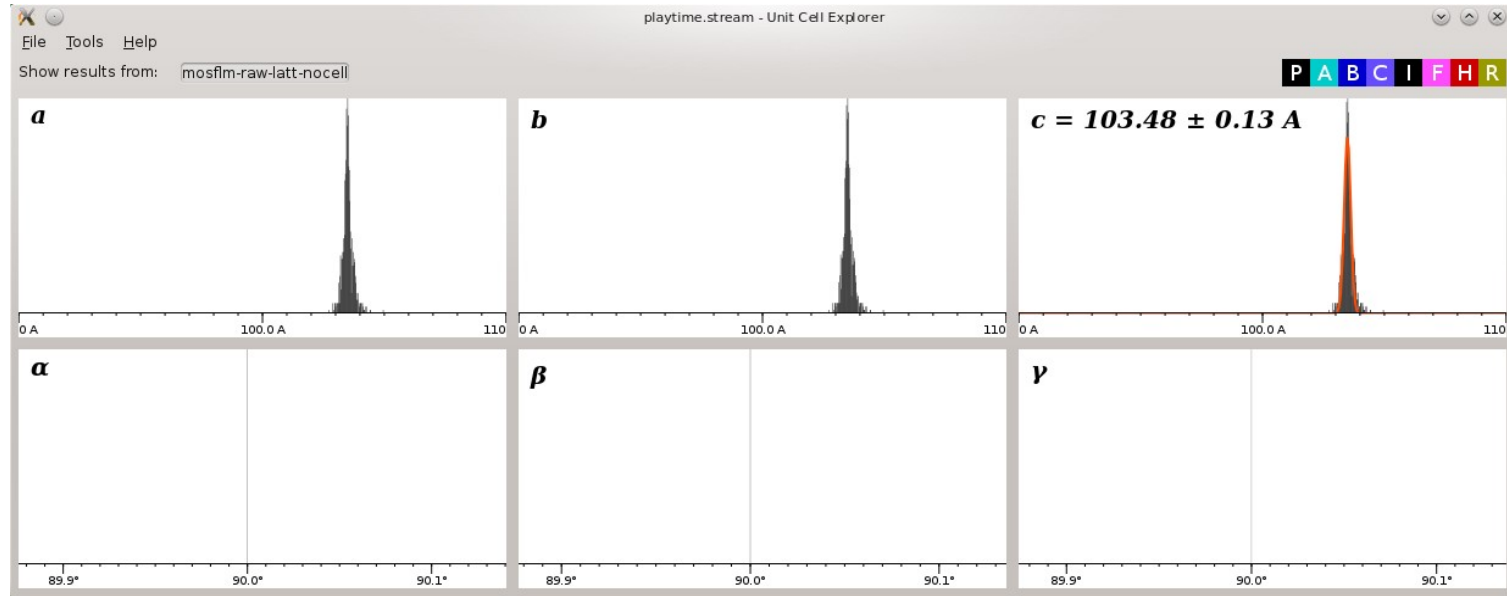
Invoke DirAx

Check the unit cell parameters against the reference, including doubling, halving, adding lattice vectors as necessary.

Do not use Bravais lattice information (DirAx cannot use this information)

The Unit Cell Explorer

> cell_explorer output.stream



$a = b = c = 103.5 \text{ \AA}$
 $\alpha = \beta = \gamma = 90.0^\circ$
Body centered (I).

Possible space groups: I23, I2₁3, I432, I4₁32, I422 I4₁22, I4₁, I4, I222

Indexing methods

> `indexamajig [...] --indexing=method1,method2,.. [.....]`
List of indexing methods will be tried in order.

> `--indexing=dirax,mosflm,xds,mosflm-raw-latt,dirax-raw`

Invoke DirAx (using defaults, i.e. match unit cell parameters)

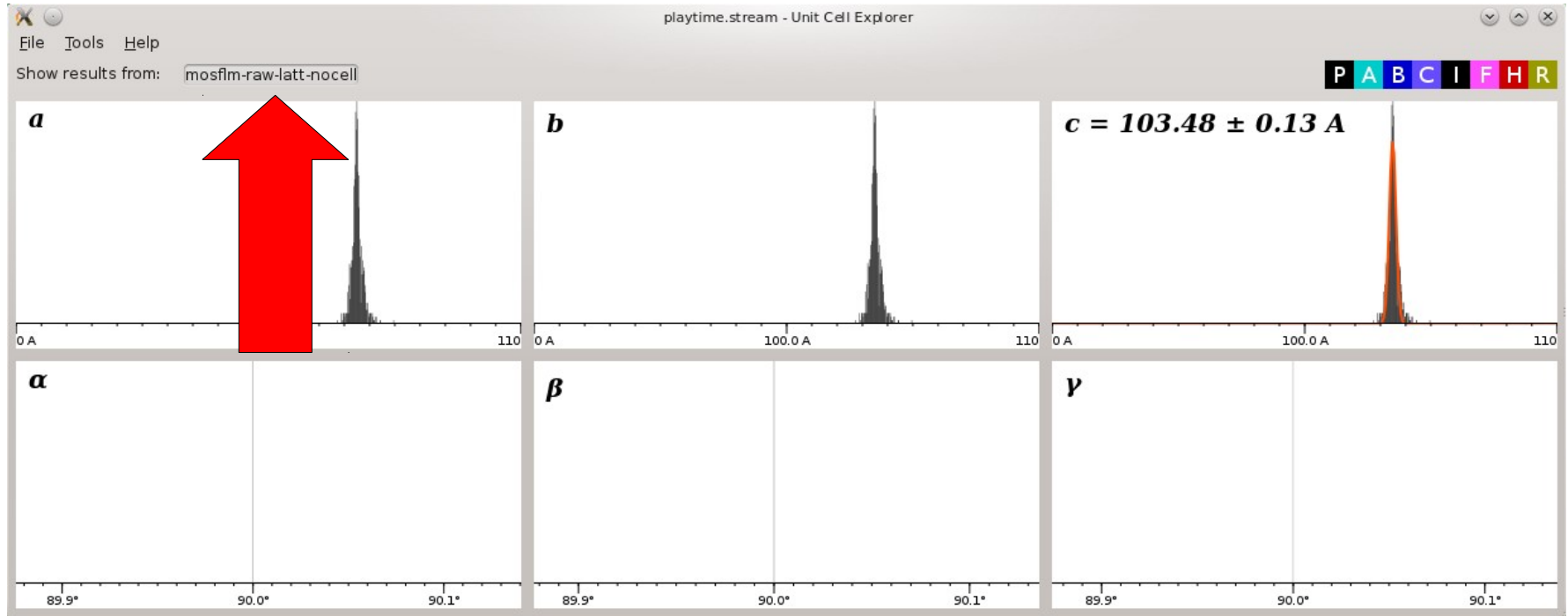
Invoke Mosflm (using defaults, i.e. match unit cell parameters, use lattice information)

Try XDS (defaults)

Still not indexed?
Try getting Mosflm to look for our lattice type, but any parameters

Last resort: see what DirAx finds on its own.

The Unit Cell Explorer



Geometry files

```
> indexamajig [...] --geometry=cspad.geom [.....]
```



Geometry file describes the layout of data in the file,
as well as the physical layout of the detector.

“man crystfel_geometry”, templates distributed with CrystFEL, or ask a
friendly PCS collaborator, beamline scientist or us.

Analysis in CrystFEL can be surprisingly robust to inaccurate geometry.

“Calibration mode” in hdfsee.

Geometry refinement tool (geoptimiser).

“Prediction refinement” stage updates central beam position.

(“Beam files” are no longer needed as of CrystFEL 0.6.0)

Integration methods

> `indexamajig [...] --integration=method [.....]`
(only one integration method allowed)

> Example method:

`rings-sat-cen`

Use “basic”
summation integration
(with background
subtraction)

Include saturated
reflections

Center the
integration position
on the peak first

Integration methods

> `indexamajig [...] --integration=method [.....]`
(only one integration method allowed)

> Example method:

`prof2d-nocen`

Use 2D profile fitting

Exclude saturated reflections (this is the default)

Do not center the integration box

Merging

```
> process_hkl -i input.stream -o output.hkl -y 6/m
```

Output: text file, can be imported into most structure solution programs. Alternatively: “create-mtz” and “create-xscale” scripts.

Actual symmetry (note: centre of symmetry added, i.e. merge Friedel pairs)

Confused about point group notation? “man crystfel” for a list of all possibilities.

Merging (advanced/experimental/dangerous/awesome)

```
> partialator -i input.stream -o output.hkl -y 6/m  
--model=unity -iterations=1
```

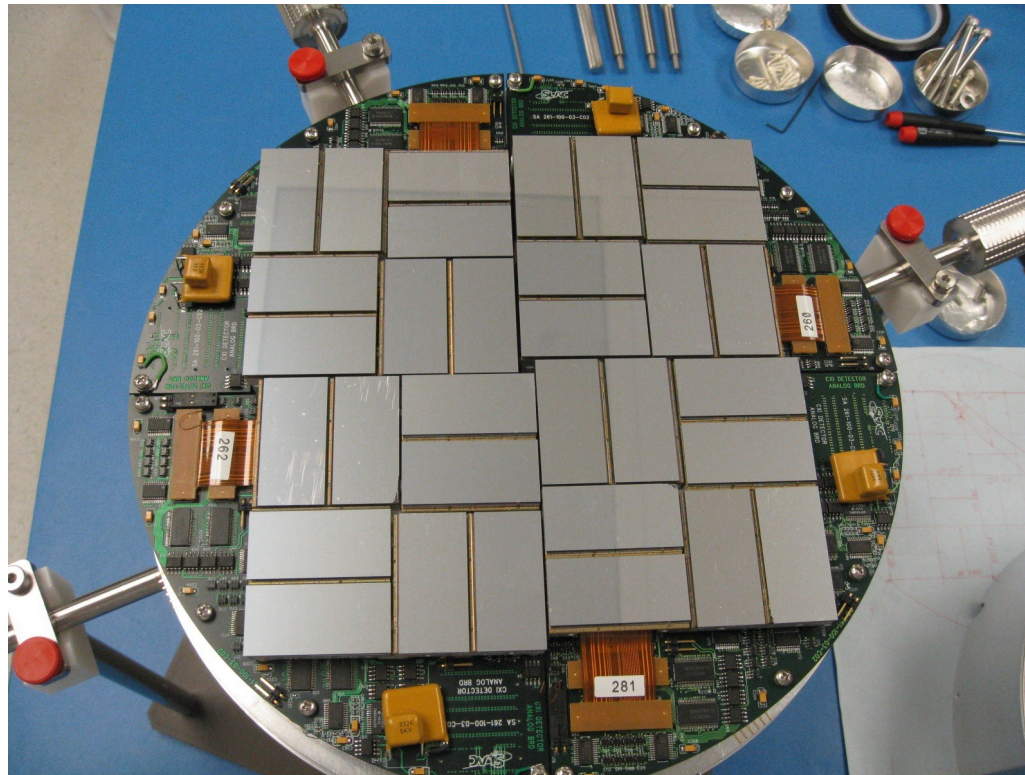
```
> partialator -i input.stream -o output.hkl -y 6/m  
--model=unity -iterations=3
```

```
> partialator -i input.stream -o output.hkl -y 6/m  
--model=scsphere -iterations=1
```

```
> partialator -i input.stream -o output.hkl -y 6/m  
--model=unity -iterations=0
```

CrystFEL 0.6.0 - detector geometry refinement

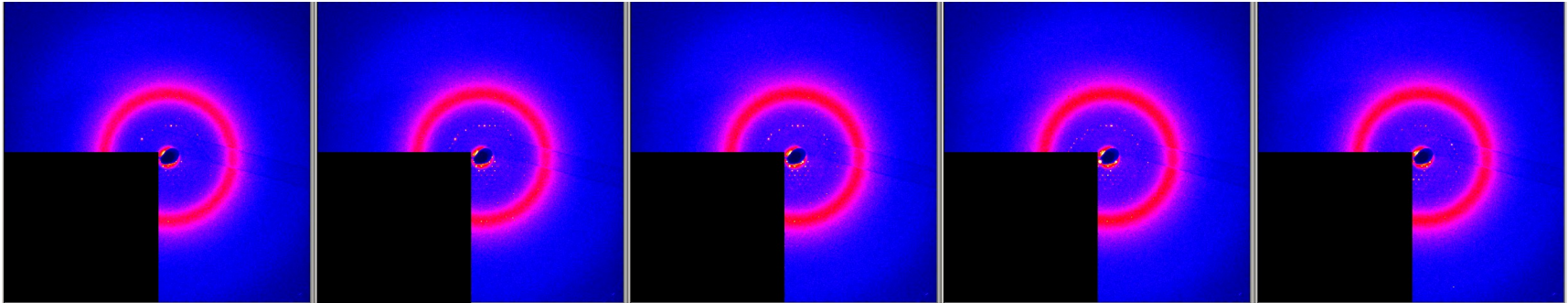
- > `geoptimiser -i input.stream -g input.geom -o output.geom`
 - Refines 3D position each part of the detector individually, or at a level of granularity you can specify (e.g. all tiles individually, quadrants as one, whole detector).



Finding “mini rotation series”

> whirligig input.stream

- Compares orientations of consecutive crystals, taking into account symmetry and indexing ambiguities. Outputs lists of events forming series.



P. Nogly, D. James, D. Wang, T. A. White et al., IUCrJ 2 (2015):

Occasionally, two or three consecutive hits were recorded on some of the larger (40–50 μm) crystals. Bragg spots appeared and disappeared within this sequence of consecutive images, indicating that the rotational diffusion of crystals in the LCP within the 80 ms between two exposures is larger than their mosaic spread. To investigate this further, a computer program was written to compare the orientations of crystals in adjacent frames using the data stream output from *CrystFEL*. For the fraction of data acquired with a 25 ms exposure time (81% of the total frames), 1088 frames (26% of the successfully indexed patterns) were found to be part of a rotation series. The mean series length was 2.2 frames and the maximum series length was 4 frames.

“Best practice” guidelines



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- [CFEL Homepage](#)
- [DESY@CFEL](#)

CrystFEL processing best practice

This page contains our most recent recommendations to processing SFX data using CrystFEL, as well as some hints and tips.

General

- Read all the messages written to the terminal by the various CrystFEL programs. They contain important information and useful advice.

Peak search

- Good peak detection is essential for indexing, so it's worth spending a long time optimising the peak search. Experiment with and use whichever combination you like from the peak detection options, which are: `--peaks=zaef`, `--peaks=hd15`, `--threshold`, `--gradient`, `--min-snr`, `--section-filter`, `--filter-noise`, `--no-use-saturated`, `--no-reval1data` and `--check-hd15-snr`. None of these options can do anything other than increase or decrease the indexing success rate.
- Note that `--use-saturated` has been the default since CrystFEL 0.5.1. This option states that saturated peaks are to be given to the indexing procedure. It does not mean that their intensities will be integrated and included in the final data.
- `--peaks=hd15` was the default behaviour prior to CrystFEL 0.5.3. Since then, the default behaviour has been not to check the SNR of peaks if you use `--peaks=hd15`. If your indexing rate dropped after upgrading to CrystFEL 0.5.3, add this option to restore the old behaviour.

Indexing

- When initially determining the unit cell parameters, try indexing with `mosflm-raw-no-latt-no-cell` first. Mosflm is the only indexing method which can guess the lattice type. Once you're convinced about the lattice type, use `mosflm-raw-latt` to constrain the search.
- Once you've determined the cell parameters, use as many indexing methods as you can, provided that they all use `--cell`, `--axes` or `--comp`. The more, the merrier! You can sometimes increase the indexing rate by combining multiple invocations of the same indexing program, for example: `--indexing mosflm-latt mosflm-no-latt`.
- At all stages, avoid using `--bad` anywhere in your list of indexing methods. Add this option only if it's really necessary.
- Do not use `--comb` if once of the cell parameters is a simple multiple of the others, e.g. if `a` is approximately equal to `2b`. **This happens with tetragonal lysozyme**, so don't assume it won't happen to you. `--comb` is the default for many indexing methods, so specify `--axes` explicitly. See the [tutorial](#) (step 10) for a discussion.
- Set the unit cell tolerances (`unit_cell_tol`) wide enough to capture the entire distributions of all the parameters, unless you have some reason to restrict it. The widths of the distributions vary between samples, so you have to

“Definitely use this option”

“Don't use this option except for testing”

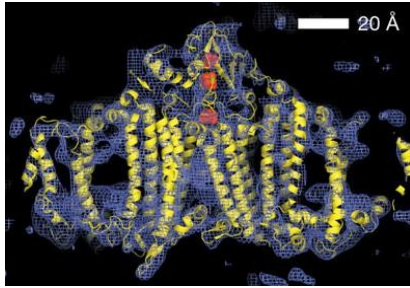
“Try this option and see what happens, might be good or bad”

“Watch out for this 'gotcha'”

... etc ...



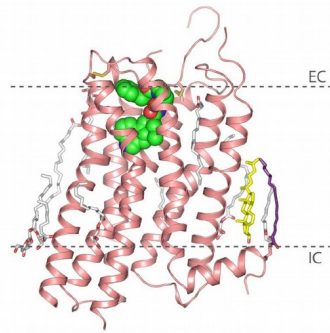
CrystFEL in the PDB (highlights)



3PCQ

Photosystem I (the first SFX experiment)

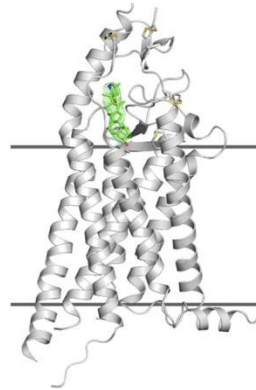
Chapman et al., Nature 2011



4NC3

Serotonin receptor bound to ergotamine

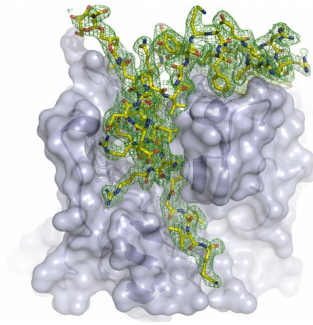
Lui et al., Science 2013



4O9R

Smoothed receptor using LCP injector

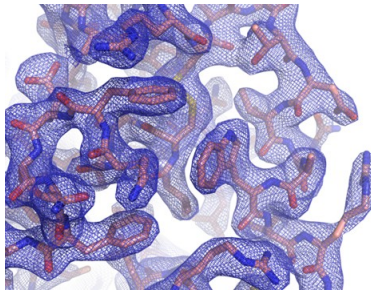
Weierstall et al., Nature Communications 2014



4HWY

Natively inhibited Cathepsin B

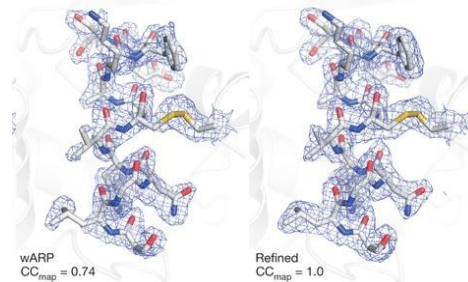
Redecke, Nass et al., Science 2013



4O34

Serial crystallography using a synchrotron beamline

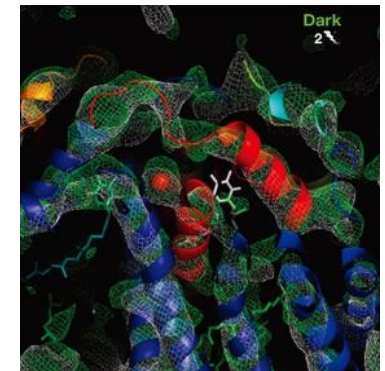
Stellato et al., IUCrJ 2014



4N5R

Lysozyme (Gd derivative) ab initio phasing using SAD

Barends et al., Nature 2013



4Q54

Photosystem II in putative S_3

excited state

Kupitz, Basu et al., Nature 2014

CrystFEL in the PDB / selected citations

2015

- Y. Kang, X. E. Zhou, X. Gao, Y. He et al. "Crystal structure of rhodopsin bound to arrestin by femtosecond X-ray laser". Nature (2015). **4ZWJ**.
- C. E. Conrad, S. Basu, D. Wang et al. "A novel inert crystal delivery medium for serial femtosecond crystallography". IUCrJ 2 (2015) p421. **4Z8K**.
- M. Bublitz, K. Nass, N. D. Drachmann, A. J. Markvardsen et al. "Structural studies of P-type ATPase-ligand complexes using an X-ray free-electron laser". IUCrJ 2 (2015) p409. **4XOU**.
- N. Coquelle, A. S. Brewser, U. Kapp, A. Shilova et al. "Raster-scanning serial protein crystallography using micro- and nano-focused synchrotron beams". Acta Cryst. D71 (2015) p1184. **4WG1, 4WG7, 4WL6 and 4WL7**.
- H. Zhang, H. Unal, C. Gati, G. W. Han et al. "Structure of the angiotensin receptor revealed by serial femtosecond crystallography". Cell (2015) p833. **4YAY**.
- S. Boutet, L. Foucar, T. R. M. Barends, S. Botha et al. "Characterization and use of the spent beam for serial operation of LCLS". Journal of Synchrotron Radiation 22 (2015) p634. **4RW1 and 4RW2**.
- K. Tono, E. Nango, M. Sugahara, C. Song et al. "DAPHNIS: application to serial protein crystallography using an X-ray free-electron laser". Journal of Synchrotron Radiation 22 (2015) p532. **3WUN**.
- G. Fenalti, N. A. Zatsépin, C. Betti, P. Giguere et al. "Structural basis for bifunctional peptide recognition at human δ -opioid receptor". Nature Structural & Molecular Biology (2015) p265. **4RWD**.
- P. Nogly, D. James, D. Wang, T. A. White et al. "Lipidic cubic phase serial millisecond crystallography using synchrotron radiation". IUCrJ 2 (2015). **4X31**.

2014

- J. Tenboer, S. Basu, N. Zatsépin, K. Pande et al. "Time-resolved serial crystallography captures high-resolution intermediates of photoactive yellow protein". Science 346 (2014) p1242. **4WL9 and 4WLA**.
- M. Sugahara, E. Mizohata, E. Nango, M. Suzuki et al. "Grease matrix as a versatile carrier of proteins for serial crystallography". Nature Methods (2014). **3WUL, 3WXT, 3WXU, 3WUM, 4W4Q, 3WXS and 3WXQ**.
- M. R. Sawaya, D. Cascio, M. Gingery, J. Rodriguez et al. "Protein crystal structure obtained at 2.9 Å resolution from injecting bacterial cells into an X-ray free-electron laser beam". PNAS 111 (2014) p12769.
- M. S. Hunter, B. Segelke, M. Messerschmidt, G. J. Williams et al. "Fixed-target protein serial microcrystallography with an x-ray free electron laser". Scientific Reports 4 (2014) 6026.
- C. Kupitz, S. Basu, I. Grotjohann, R. Fromme et al. "Serial time-resolved crystallography of photosystem II using a femtosecond X-ray laser". Nature (2014). **4PBU and 4Q54**.
- M. Caffrey, D. Li, N. Howe and S. T. A. Shah. "Hit and run" serial femtosecond crystallography of a membrane kinase in the lipid cubic phase". Phil Trans. Roy. Soc. B 369 (2014) 20130621.
- O. Yefanov, C. Gati, G. Bourenkov, R. A. Kirian et al. "Mapping the continuous reciprocal space intensity distribution of X-ray serial crystallography". Phil. Trans. Roy. Soc. B 369 (2014) 20130333.
- F. Stellato, D. Oberthür, M. Liang, R. Bean et al. "Room-temperature macromolecular serial crystallography using synchrotron radiation". IUCrJ 1 (2014). **4O34**.
- K. Qu, L. Zhou and Y.-H. Dong. "An improved integration method in serial femtosecond crystallography". Acta Cryst. D70 (2014) p1202.
- M. Frank, D. B. Carlson, M. S. Hunter, G. J. Williams et al. "Femtosecond X-ray diffraction from two-dimensional protein crystals". IUCrJ 1 (2014) p95.
- C. Gati, G. Bourenkov, M. Klinge, D. Rehders et al. "Serial crystallography on in vivo grown microcrystals using synchrotron radiation". IUCrJ 1 (2014) p87. **4N4Z**.
- U. Weierstall, D. James, C. Wang, T. A. White et al. "Lipidic cubic phase injector facilitates membrane protein serial femtosecond crystallography". Nature Communications 5:3309 (2014). **4O9R**.
- C. Song, K. Tono, J. Park, T. Ebisu et al. "Multiple application X-ray imaging chamber for single-shot diffraction experiments with femtosecond X-ray laser pulses". J. Appl. Cryst. 47 (2014) p18.

2013

- W. Liu, D. Wacker, C. Gati, G. W. Han et al. "Serial Femtosecond Crystallography of G Protein-Coupled Receptors". Science 342 (2013) p1522. **4NC3 and CXIDB ID 21**.
- L. C. Johansson, D. Arnlund, G. Katona, T. A. White et al. "Structure of a photosynthetic reaction centre determined by serial femtosecond crystallography". Nature Communications 4:2911 (2013). **4CAS**.
- T. R. M. Barends, L. Foucar, S. Botha, R. B. Doak et al. "De novo protein crystal structure determination from X-ray free-electron laser data". Nature (2013). **4N5R and CXIDB ID 20**.
- H. Dermirci, et al. "Serial femtosecond X-ray diffraction of 30S ribosomal subunit microcrystals in liquid suspension at ambient temperature using an X-ray free-electron laser". Acta Crystallographica F69 (2013) p1066.
- T. R. M. Barends, L. Foucar, R. L. Shoeman, S. Bari et al. "Anomalous signal from S atoms in protein crystallographic data from an X-ray free-electron laser". Acta Crystallographica D69 (2013) p838.
- L. Redecke, K. Nass et al. "Natively Inhibited Trypanosoma brucei Cathepsin B Structure Determined by Using an X-ray Laser". Science 339 (2013) p227. **4HWY**.

2012

- S. Boutet, L. Lomb, G. J. Williams, T. R. M. Barends et al. "High-Resolution Protein Structure Determination by Serial Femtosecond Crystallography". Science 337 (2012) p362. **4ET8 and 4ET9**.
- L. C. Johansson, D. Arnlund, T. A. White, G. Katona et al. "Lipidic phase membrane protein serial femtosecond crystallography". Nature Methods 9 (2012) p263. **4AC5**.

2011

- H. N. Chapman, P. Fromme et al. "Femtosecond X-ray protein nanocrystallography". Nature 470 (2011) p73. **3PCQ**.



(full list on the website)

