# Analysis pipeline for crystallographic data from FELs

Thomas A. White

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taw@physics.org

# Acknowledgements (first experiments)

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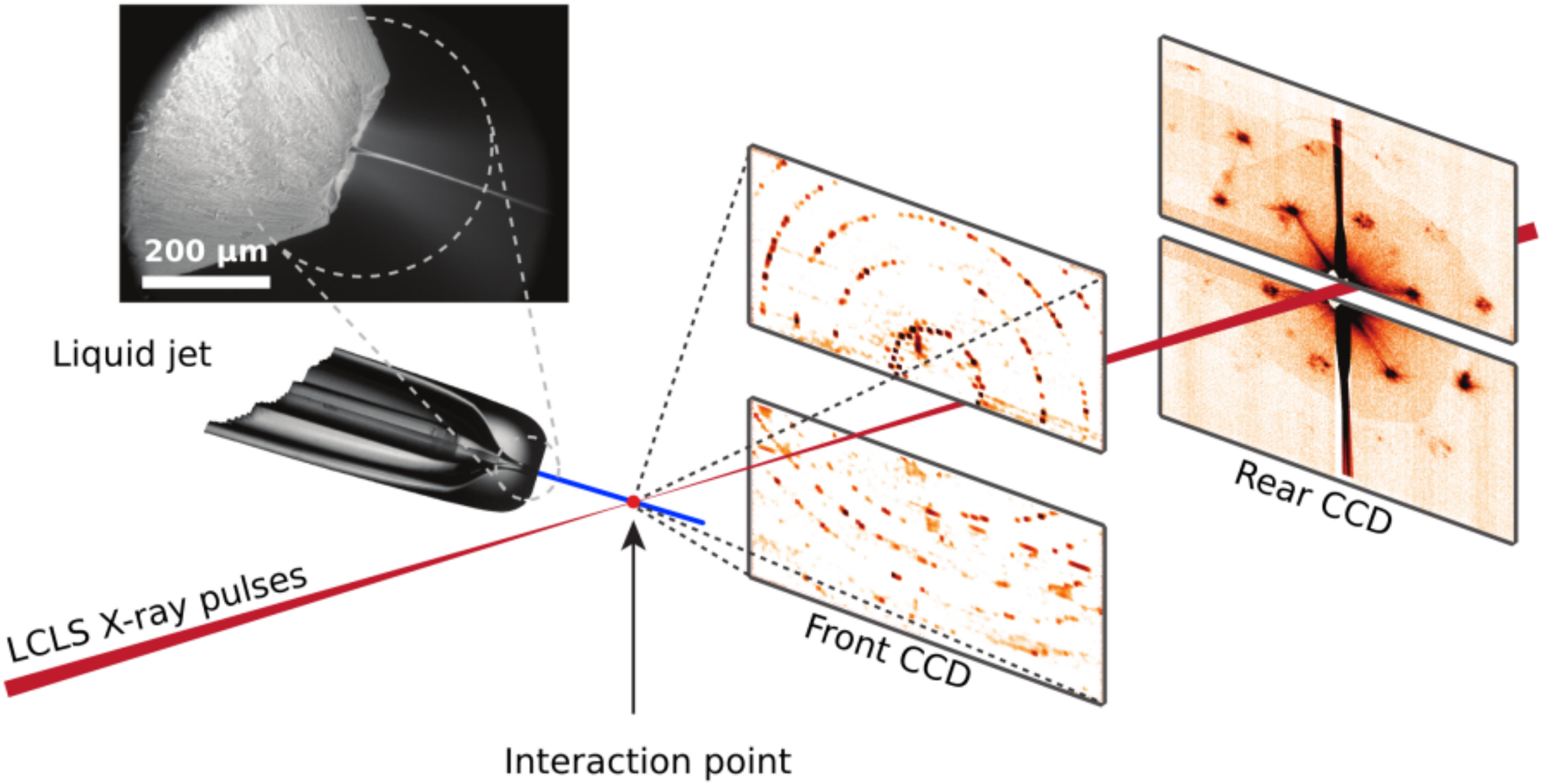
Biochemistry and Biophysics, UCSF, USA
Physical Biosciences, LBNL, USA

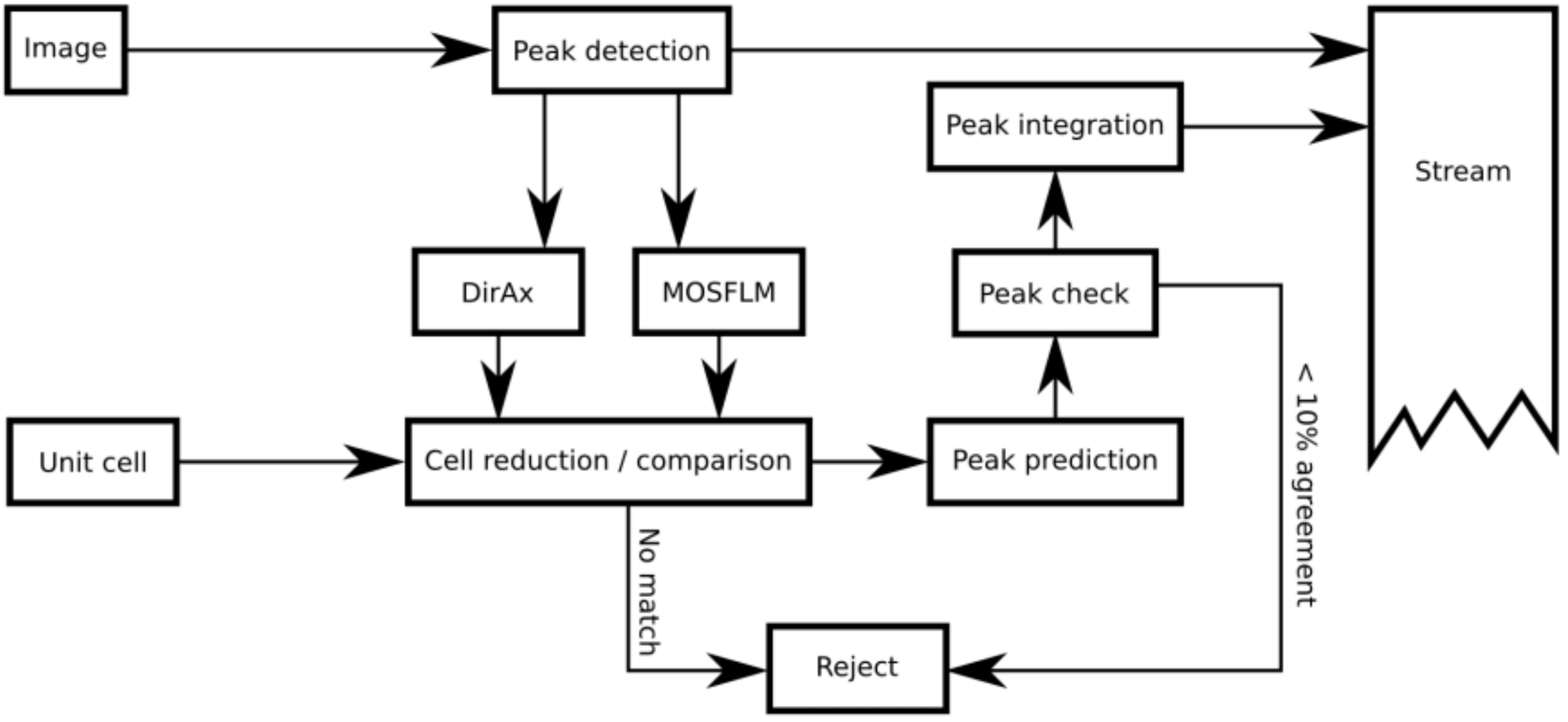
# Experimental setup for serial crystallography




One X-ray pulse, one detector readout, (hopefully) one crystal.

First published in Nature 470 (2011) p73-77

# CrystFEL indexing pipeline




Fully automated indexing and integration pipeline.

Parameters, e.g. for peak picking or unit cell tolerance, can be optimised to get the highest "yield".

# Data quantities in the "ideal" experiment

With current data processing methods, we need around 10,000 to 20,000 indexed diffraction patterns to solve the structure.

The indexing yield varies between 10% and 50%.

A good number of patterns to aim for is 100,000
- these will vary in quality and "indexability".

"Hit rate" varies between 1% and 10%, so we need about one million "shots".

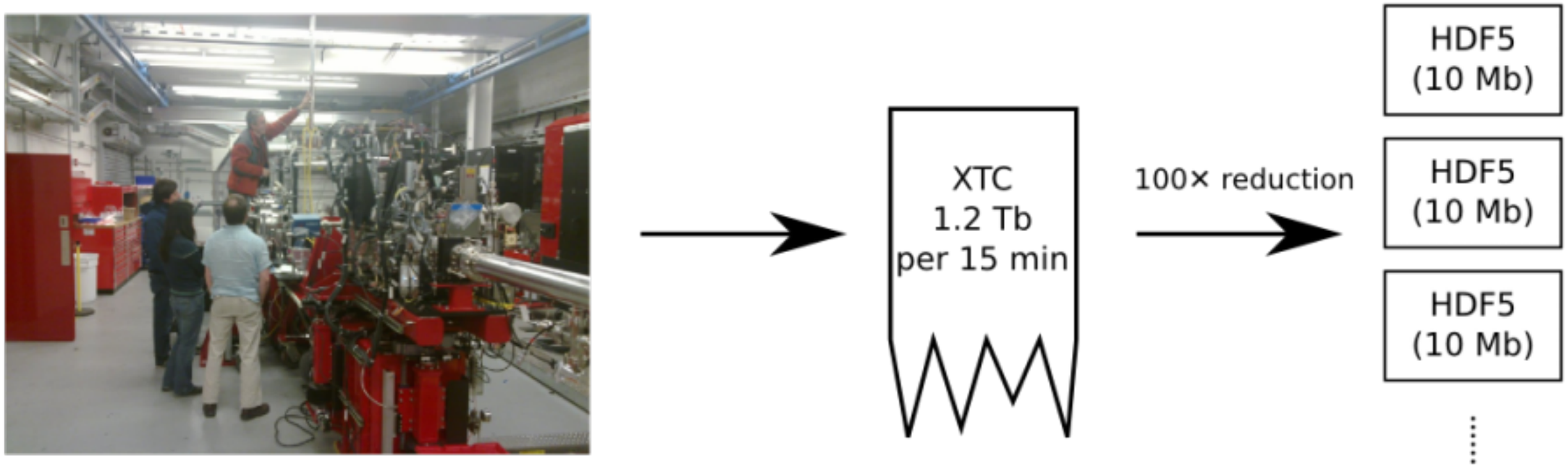
Two 2048 by 2048 pixel detectors, 16 bit readout = 16 Mb / shot.

At 120 Hz, this is about 2 Gb / second.

16 Tb for the whole dataset, acquired in just over two hours.

# Pre-processing software: Cheetah

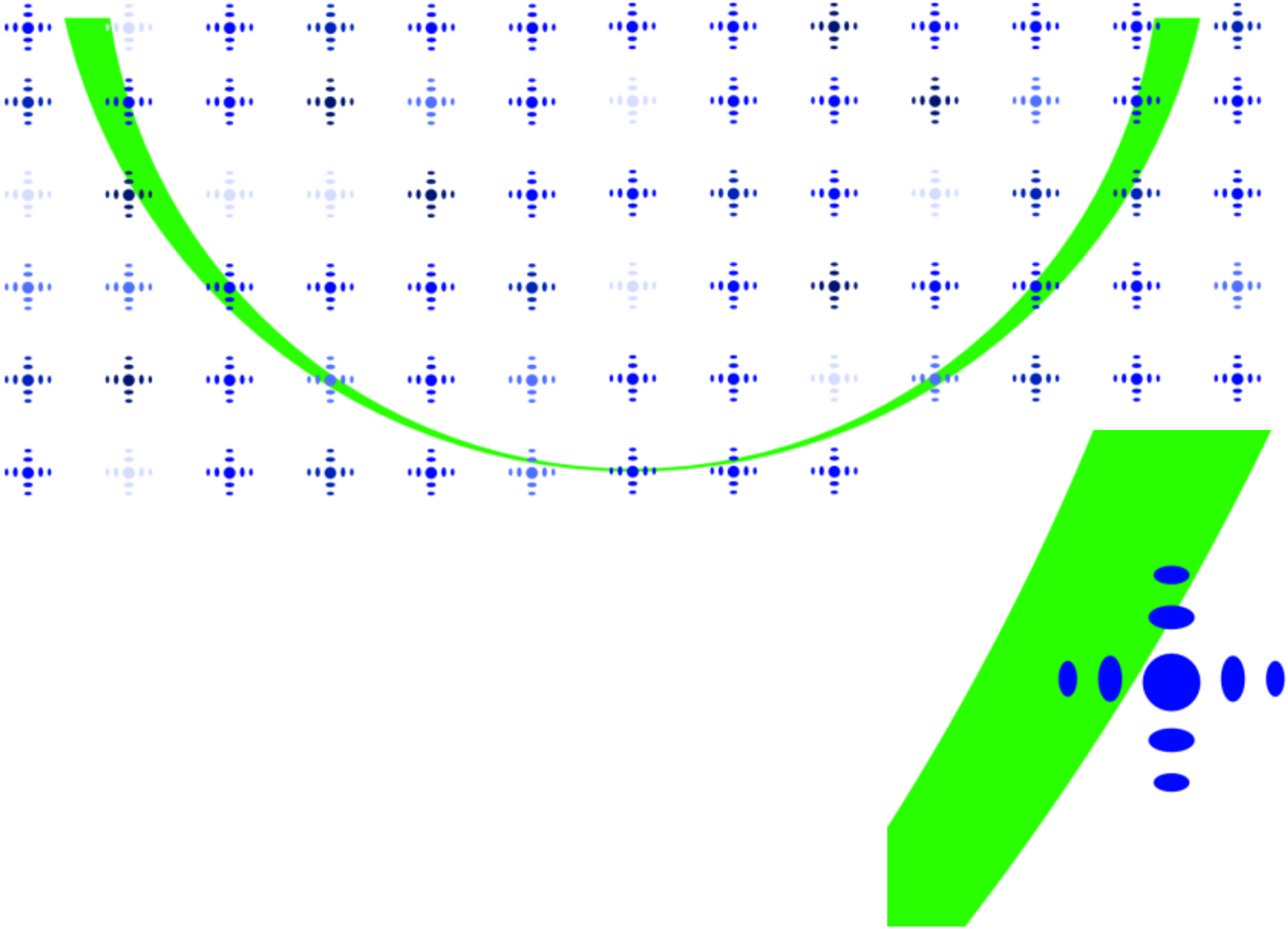
Cheetah performs detector corrections and finds the "hits".
Each "hit" is written to an individual HDF5 file for later processing.




Processing speed is almost the same as acquisition speed.

http://www.desy.de/~barty/cheetah/

# Snapshots are made up of partial reflections



# Every pattern is different...

Wavelength jitter

Crystal size

Quality of crystal

Bandwidth of X-ray pulse

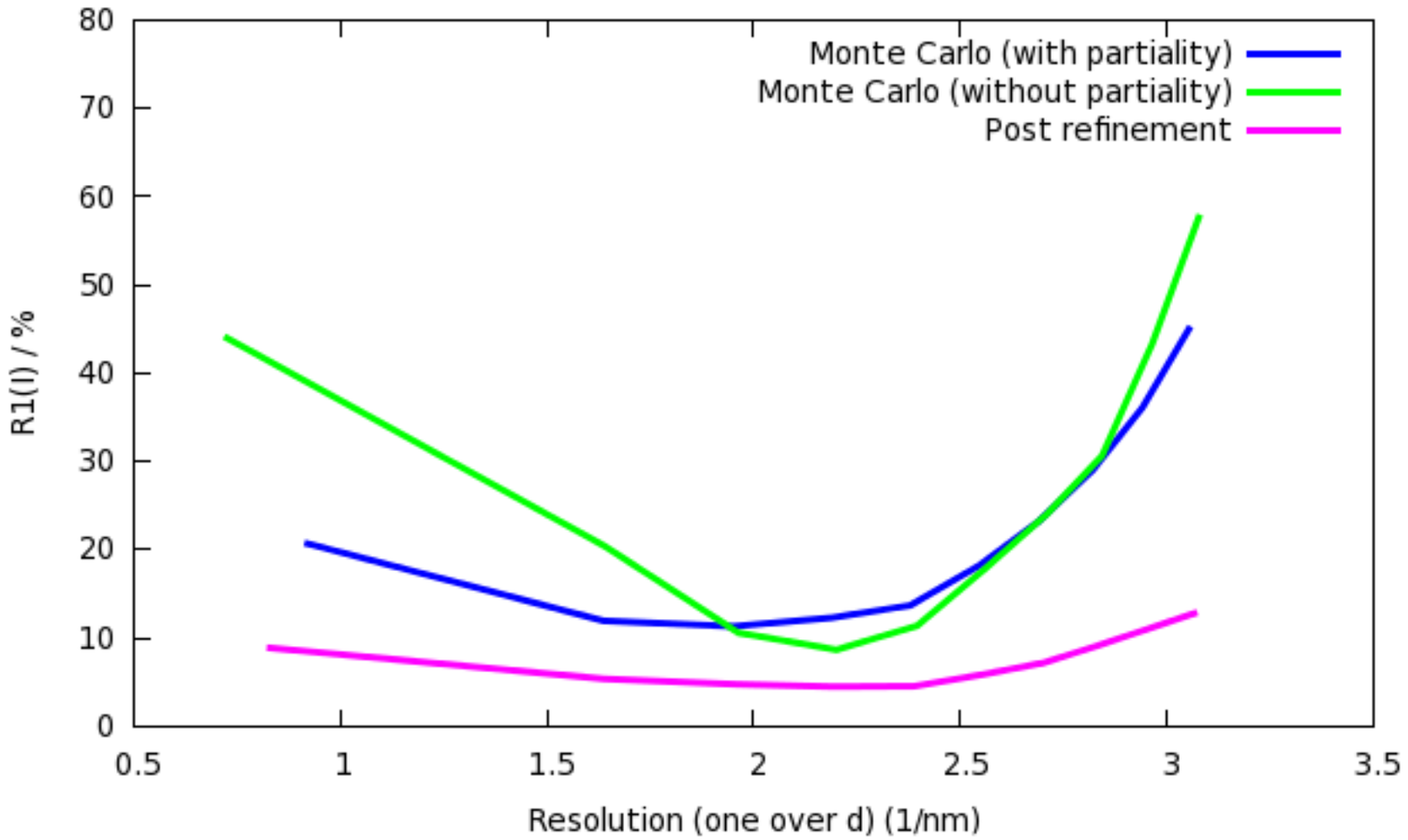
Spectrum of X-ray pulse

Incident intensity

Position of crystal in beam

....

# Improved analysis may reduce the amount of data



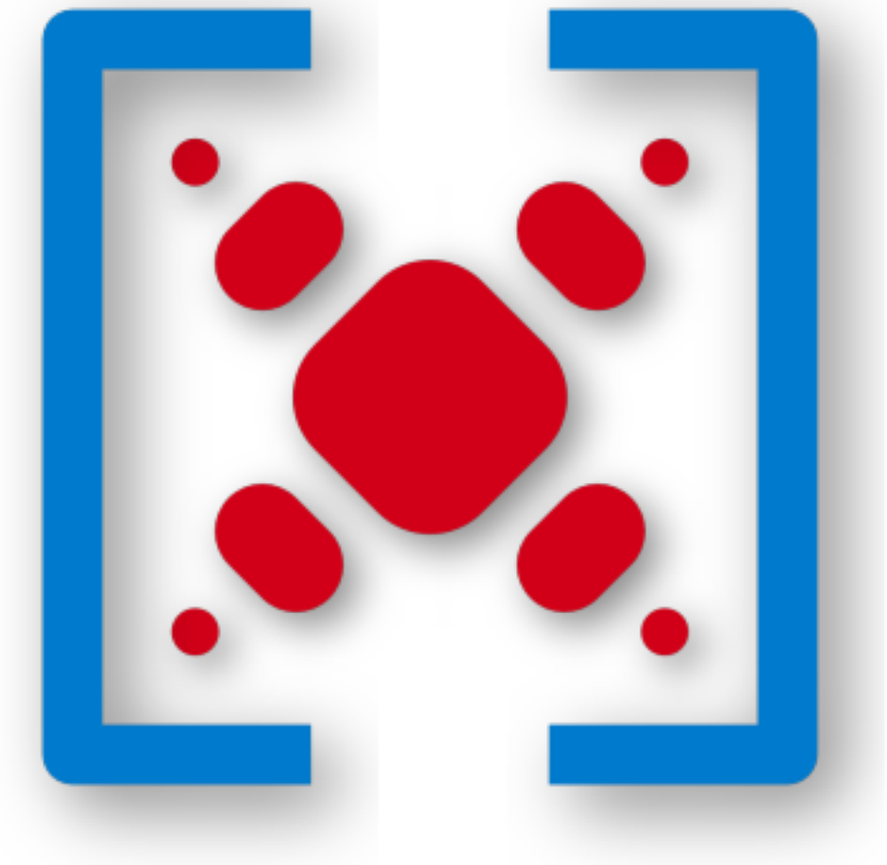

By modelling and reconstructing some of the things which vary between shots, we should be able to reduce the number of patterns required, perhaps significantly.

# CrystFEL software suite

Software suite for processing diffraction data from XFEL sources, and perhaps other experiments of a "serial crystallography" type.

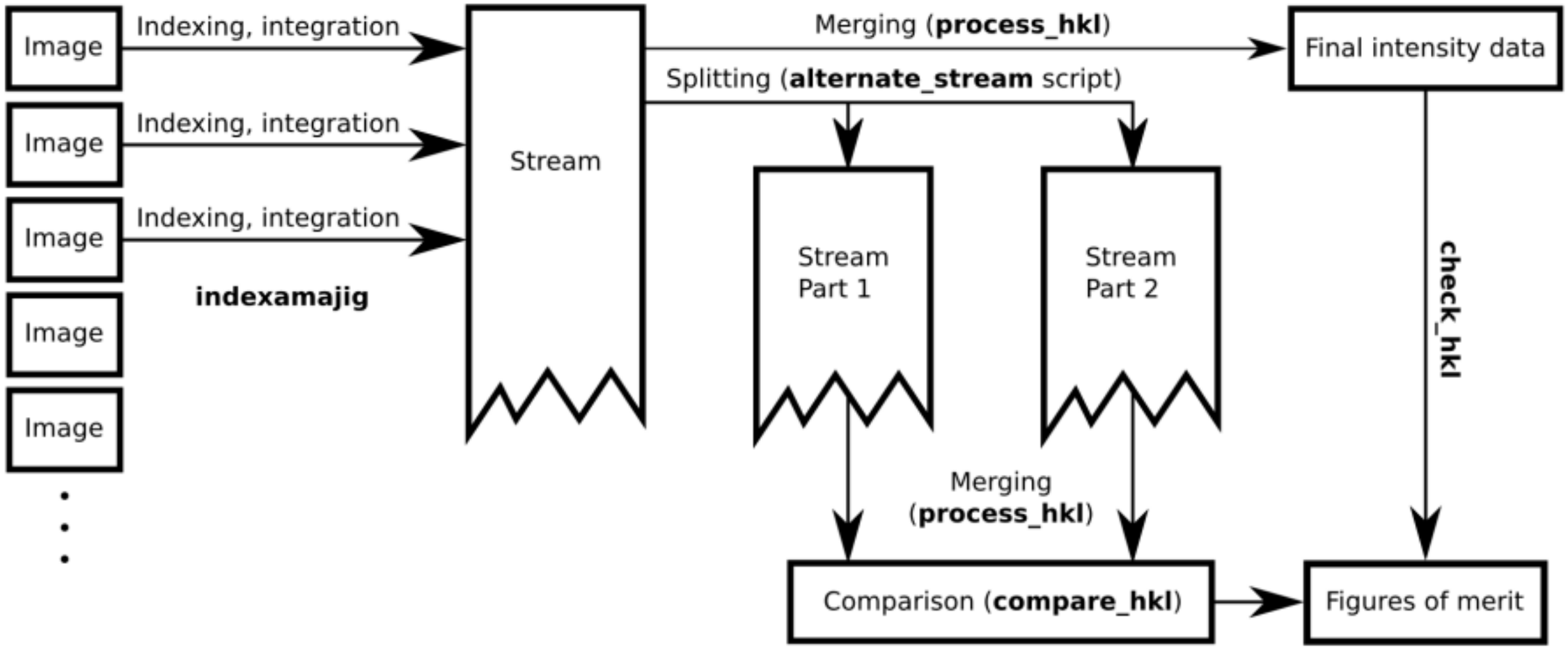
"Clean diffraction patterns to merged intensities."

Free and open-source software: GPLv3



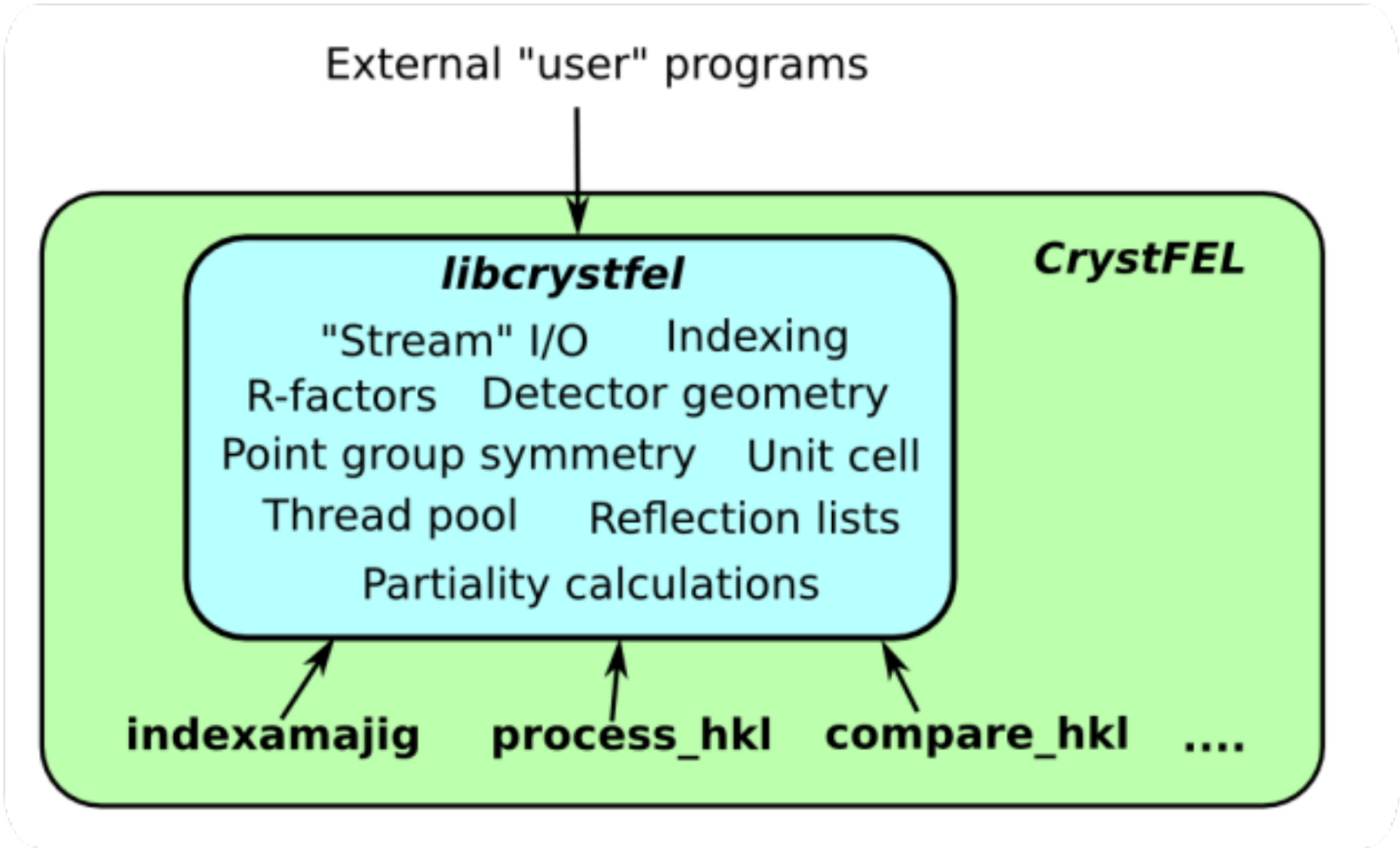
http://www.desy.de/~twhite/crystfel/

# CrystFEL software suite



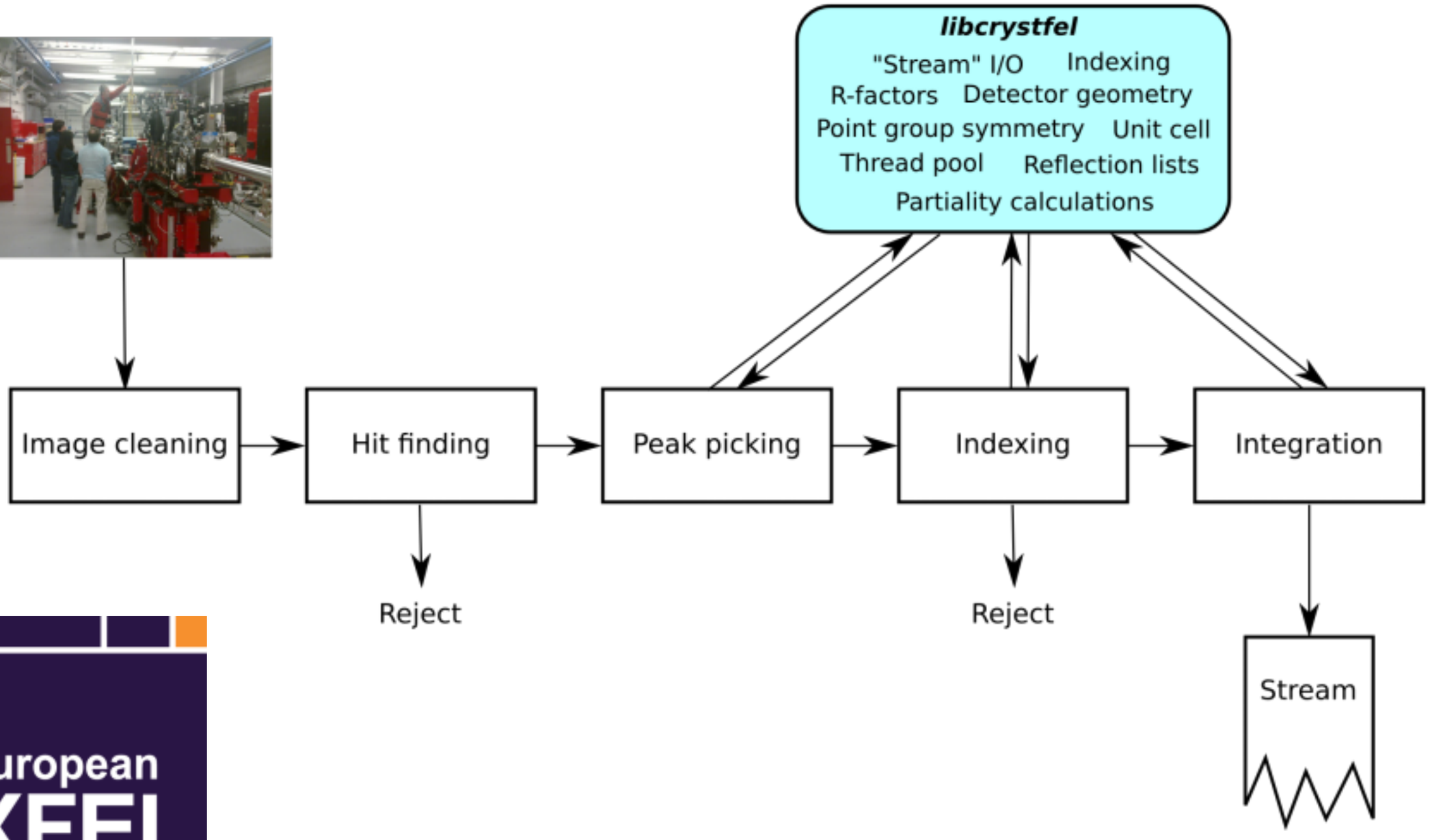

"Stream" contains all the relevant information in a series of "chunks". One chunk per pattern (whether indexed successfully or not).

# CrystFEL software suite



# The future ... ?






European XFEL

# References

T. A. White et al., "CrystFEL: A software suite for snapshot serial crystallography". J. Applied Crystallography 45 (2012) p334-341.

H. N. Chapman et al., "Femtosecond X-ray protein nanocrystallography", Nature 73 (2011) p73-77.

R. A. Kirian et al., "Structure-factor analysis of femtosecond micro-diffraction patterns from protein nanocrystals". Acta Crystallographica A68 (2011) p131-140.

http://www.desy.de/~twhite/crystfel

taw@physics.org