## MS41-O2

### Experiences developing and publishing a medium-sized software project: CrystFEL

Thomas White[1]

1. Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

**email: taw@physics.org**

CrystFEL [1,2] is a free and open-source suite of programs for processing data from "serial crystallography" experiments, starting from detector frames and ending with merged intensities ready to be imported into other packages such as CCP4 and PHENIX. As of June 2018, it has been in development for 8½ years and publicly available for just over 6 years. About 100 journal articles involved its use and 25 people from 8 different institutions have contributed code, with many more people contributing useful ideas and feedback.

This talk will describe our experiences developing CrystFEL and making it available to crystallographers around the world. How can the complexities of scientific data processing and high-performance computing environments be managed for the best overall results? What is the best way to get new users started, or to make changes to the software without tripping up the more experienced? And how can we encourage users who have programming skills to become contributors?

References:

[1] White, T. A. et al. (2016). J. Appl. Cryst. 49, 680-689.
[2] https://www.desy.de/~twhite/crystfel/

**Keywords: serial crystallography, CrystFEL, XFEL**

## MS41-O3

### Using Mathematica® as a platform for crystallographic computing

Stian Ramsnes[1], Helge Bøvik Larsen[1], Gunnar Thorkildsen[1]

1. Department of Mathematics and Physics, University of Stavanger, Stavanger, Norway

**email: stian.p.ramsnes@uis.no**

A comprehensive Mathematica® [1] package for crystallographic computations has been developed.

Complete representations of space groups (point groups) and cell transformations based on International Tables for Crystallography, volume A [2] together with scattering factors from International Tables for Crystallography, volume C [2] and cross sections from xraylib [3] are built into the package.

Featured functionalities include calculation of structure factors, linear absorption coefficients and various crystallographic transformations.

The crystal data used by the package is normally generated from external *.cif files.

The package comes with a dynamic documentation seamlessly integrated with the Mathematica system, including code, examples and options.

From the onset, minimal Mathematica experience is needed to make use of the package.

It may be a helpful supplement in research and teaching where crystallography and X-ray diffraction is essential.

Although Mathematica is a proprietary software, all the code of the package is open source.

It may easily be extended to cover user-specific applications.

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