for long-term maintenance and new developments. CCP4 libraries have been created and shaped over many years, and concentrate a vast experience of building crystallographic software. In the talk, I will give an overview of CCP4 libraries and describe their general concepts and functionality.

Keywords: crystallography, computations, CCP4

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Libraries and software development at rigaku

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Software development at Rigaku relies on strategic leveraging of 3rd party software, both commercial and open source. For example, the *Computational Crystallography Toolbox* [1] is integral to our current methods development efforts. The cctbx library was especially useful in expediting the development of our new space group determination program, XPlain, in which the determination of the Patterson symmetry (Laue group + lattice centering) from an unreduced unit cell relies heavily on cctbx functions. The cctbx library was also found useful for transforming space group symbols and for associating observed absences with compatible space groups.

On the user interface side, we use Nokia's Qt software for rapid development of user interfaces to Mac/Linux/Windows compatible programs, such as our new CollectionStrategy program (a complementary part of Rigaku's HKL3000R suite), and our new reciprocal space exploration program, RSV3D.

[1] W. Ralf Grosse-Kunstleve, K. Nicholas Sauter, W. Nigel, *Moriarty and Paul* D. Adams, *J. Appl. Cryst.* **2002,** *35*, 126-136.

Keywords: software, libraries, programming

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DiffPy - an open-source library for powder crystallography

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DiffPy is an open-source collection of applications and libraries for structure analysis from powder diffraction data. DiffPy is written in Python and C++ and has been developed as a part of DANSE, the Distributed Data Analysis for Neutron Scattering Experiments. The library is focused on nanoscale structure analysis using atomic Pair Distribution Functions (PDF), and on sequential Rietveld refinements of multiple datasets that are obtained with latest, high-throughput neutron instruments. For such studies the library provides user-friendly GUI applications PDFgui [1] and SrRietveld [2], which are intended for general, non-programmer users. The library can be also accessed at a lower level to calculate various structure quantities (e.g., PDF, bond valence sums, Rietveld refinement residuum) or to setup a specialized structure refinement that combines multiple experimental probes in a single fit (e.g., x-ray and neutron PDFs). DiffPy can be used as a library from both Python or C++ layer, where Python interface has been designed for ease of use and the C++ layer for speed. The object-oriented design makes the library easy to extend or customize, for example the PDF calculator can be easily switched to use user-defined peak profiles, that can be implemented either in Python or C++. The DiffPy library includes the Liga algorithm for structure determination from experimental PDFs. [3] The presentation will provide an overview of the DiffPy functionality, demo several examples for accessing the library from Python and C++, and describe its usage for structure analysis of metallofullerene molecules from experimental PDF.

[1] C.L. Farrow, P. Juhas, J.W. Liu, D. Bryndin, E.S. Bozin, J. Bloch, Th. Proffen, S.J.L. Billinge, *J. Phys. Condens. Matter* **2007,** *19*, 335219. [2] P. Tian, W. Zhou, J. Liu, Y. Shang, C.L. Farrow, P. Juhas, S.J.L. Billinge, *arXiv: 1006.0435,* **2010.** [3] P. Juhas, D.M. Cherba, P.M. Duxbury, W.F. Punch, S.J.L. *Nature* **2006,** *440*, 655-658.

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MyTARDIS: Managing the Lifecycle of Crystallography Data

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MyTARDIS is an automated solution for cataloging, managing and assisting the sharing of data in a private and secure way. TARDIS is its counterpart that that provides a central index for published data. MyTARDIS is currently deployed at the Australian Synchrotron to automatically catalogue and store a scientist's raw data. Together, MyTARDIS and TARDIS provide a complete end-to-end solution for data management, from the initial generation of the data through to its eventual publication.

As a scientist collects data at the Australian Synchrotron, it's routed to a MyTARDIS federated node hosted at the their home institution. This allows them to log in to the MyTARDIS web interface using their standard institutional log in credentials, browse their data locally and its associated metadata parameters and download all or parts of an experiment. Researchers can freely add derived data alongside their raw data via a simple dataset upload mechanism. MyTARDIS has been designed to provide researchers with the ability to regularly archive, share and preserve their data across time and has already resulted in raw and derived data being published and cited within publications in journals such as Nature.

This presentation will demonstrate the entire workflow of the MyTARDIS/TARDIS systems, from the initial collection of raw diffraction images, to its eventual publication. Additionally, new features planned and prototyped such as molecular replacement in the cloud via the MyTARDIS interface will be explained and demonstrated.

Keywords: data, publishing, synchrotron

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Structural and magnetic transitions of Cd_6R approximants

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