

User Meeting 2020

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Data evaluation on the fly: Auto-Rickshaw at the MX beamlines of the Australian Synchrotron

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Auto-Rickshaw [1,2] is a system for automated crystal structure determination. It provides computer coded decision-makers for successive and automated execution of a number of existing macromolecular crystallographic computer programs thus forming a software pipeline for automated and efficient crystal structure determination.

Auto-Rickshaw (AR) is freely available to the crystallography community through the EMBL-Hamburg AR Server (<http://www.embl-hamburg.de/Auto-Rickshaw>).

Recently, it has been installed at the ASCI cluster at the Australian Synchrotron. The AS-AR server is accessible from the MX beamline computers during the X-ray data collection.

AR at the MX beamlines can be invoked through command line or a web-based graphical user interface (GUI) for data and parameter input and for monitoring the progress of structure determination. It can be also invoked via automatic data processing if the parameter inputs have been pre set at the GUI during X-ray diffraction experiment.

A large number of possible structure solution paths are encoded in the system and the optimal path is selected by the decision-makers as the structure solution evolves. The platform can carry out experimental (SAD, SIRAS, RIP or various MAD) and MR phasing or combination of experimental and MR phasing. The system can be used in evaluation of multiple datasets for any phasing protocols as well as for evaluation of ligand binding or fragment screening.

The new implementation and features will be discussed during the presentation.

References

- [1] Panjikar, S., Parthasarathy, V., Lamzin, V. S., Weiss, M. S. & Tucker, P. A. (2005). Auto-Rickshaw - An automated crystal structure determination platform as an efficient tool for the validation of an X-ray diffraction experiment. *Acta Cryst. D61*, 449-457.
- [2] Panjikar, S., Parthasarathy, V., Lamzin, V. S., Weiss, M. S. & Tucker, P. A. (2009). On the combination of molecular replacement and single-wavelength anomalous diffraction phasing for automated structure determination *Acta Cryst. D65*, 1089-1097.

Primary authors: Dr PANJIKAR, Santosh (Australian Synchrotron); MX TEAM

Presenter: Dr PANJIKAR, Santosh (Australian Synchrotron)

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