

Automated data processing pipelines for beamline P11

P11 at PETRA III (DESY, Hamburg) is a high-throughput instrument for macromolecular crystallography (1). P11 has tuneable photon energy between 5.5 - 28 keV having the Eiger2 X 16M as the stationary detector. The automatic sample changer at P11 has a total capacity of 23 sample pucks (total of 368 samples) having a mount-unmount cycle of approximately 36 s, which brings the beamtime spent per sample down to ca. 2min. All this enables enormous amounts of data being collected during every beamtime, which needs to be automatically processed preferably in real-time.

During the past two years mode of operation at P11 has changed from fully on-site to almost exclusively remote. Remote connection using FastX-access via a dedicated remote machine was established in 2020. Users have scientific accounts that can be used during and after the beamtime for manual data processing on Maxwell, where the autoproccessing is also migrated to dedicated P11 nodes. Currently there is only one, XDSAPP-based (2), autoproccessing pipeline running for each dataset through a simple script starting every time a data collection stops and a full dataset is detected. This workshop could help us establish parallel auto-processing pipelines, for which there are numerous options available, depending on the type of the experiment (standard, characterisation, large-scale screening, etc.). Furthermore, finding an alternative way of detecting the full dataset, which is currently done by a workaround having a batch script inside the processing batch script, and transferring all the data for users to have access to, would be ideal.

[1] Burkhardt A., et al., Status of the crystallography beamlines at PETRA III. Eur. Phys. J. Plus 131, 56 (2016).

[2] Sparta KM, et al., XDSAPP2.0. J. Appl. Cryst. 49, 1085-1092 (2016).

Accelerator or Beamline

PETRA III

Team Contacts

Team Name

Workflow Goals

Programming Languages

Publications

Data Volume

Team Speaker

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