



Contribution ID: 29

Type: Talk

Cross-Facility Workflow Development for Live Analysis and Visualization on the Web

Monday, 16 October 2023 17:40 (20 minutes)

For users to make informed decisions about adapting their experimental setup or inspect the decisions of an autonomous experiment, it is essential to extract and visualize relevant features from scattering patterns as they are collected. Making use of browser-based technologies further enables remote, device-independent and installation-free access, as well as providing standards-based authorization capabilities.

We present a browser interface and infrastructure setup to configure a reduction workflow for small- and wide-angle scattering in transmission and grazing-incidence geometry at beamline P03, the micro- and nano-focus small- and wide-angle X-ray scattering beamline (MiNaXS) at PETRA III (DESY, Hamburg), and beamline 7.3.3, the SAXS/WAXS/GISAXS/GIWAXS beamline at the Advanced Light Source (ALS, Berkeley).

Our setup relies on Tiled [<https://blueskyproject.io/tiled/>] for unified data access, pyFAI [<https://pyfai.readthedocs.io/en/v2023.1/>] and additional Python routines for 1d reduction and feature extraction, Prefect [<https://docs.prefect.io/2.11.3/>] for workflow management, SciCAT [<https://scicatproject.github.io/>] for data cataloging, and Dash Plotly [<https://dash.plotly.com/>] for visualization and interactivity. This project aims for limited customization to a particular instrument and facility-specific computing infrastructure. We plan to expand support for additional beamlines and close the autonomous loop with optimization frameworks such as gpCAM [<https://gpcam.readthedocs.io/en/latest/>] in the near future.

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Session Classification: Automation & software