

Advanced Software Tools and Workflows for Synchrotron X-Ray Scattering Analysis at ESRF: A User's Perspective

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The recent launch of the Extremely Brilliant Source (EBS)¹ at the ESRF has been accompanied by numerous advancements in software development, introducing sophisticated tools and workflows designed to provide the user community with the capability to generate high-quality scientific data. Understanding these tools is essential for efficient data analysis in synchrotron experiments.

Key collaborative software technologies employed at ESRF are introduced, including Extensible Workflow System (EWOKS)² for automated, reproducible, and traceable data processing integrated with Beam Line Instrumentation Support Software (BLISS)³ for beamline control, Scientific Library for eXperimentalists (SILX)⁴ as a Python package for data science and analysis, and specialized tools for reducing X-ray diffraction data from 2D detectors^{5,6,7}.

The digital ecosystem at ESRF is also introduced, highlighting the computing cluster for data analysis, the Virtual Infrastructure for Scientific Analysis (VISA) platform, and the web-based environment for interactive Jupyter notebooks. These tools and platforms are vital in accelerating scientific discoveries and enhancing synchrotron radiation research.

References

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