A(nother) file format? A standardized format for large azimuthally integrated area detector data

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Synchrotron-based powder diffraction and scattering techniques are powerful and ubiquitous tools for *in-situ* and *-operando* studies of materials, and all large-scale facilities have one or more beamlines designed for these types of experiments. For powder X-ray diffraction (PXRD), total scattering (TS), and small-angle X-ray scattering (SAXS), many beamlines use 2D area detectors to measure full or partial Debye-Scherrer rings with acquisition rates ranging from minutes to milliseconds, easily producing tens or hundreds of thousands of frames per measurement. The images from these detectors are reduced by azimuthal integration to yield intensity values as a function of scattering angle (1D) and, in some cases, also as a function of azimuthal angle (2D) (e.g. Kieffer et al., 2020, Jensen et al., 2022, Filik et al., 2017, Toby & Von Dreele, 2013 [1-4]). However, while the experimental geometry, data processing, and reduction are highly similar, today every facility – in many cases even each beamline – produces a distinct file format!
While various flavours of the human-readable multi-column ASCII files are the most widely used format for reduced scattering data and have historically worked well for earlier generation instruments, they quickly become impractical for the many thousands of scattering patterns produced with modern technology.

We present a standardized HDF5-based format within the NeXus framework (NXazint1D and NXazint2D [5-6]), designed to store 1D and 2D integrated data along with essential reduction metadata and sample data (time, temperature, pressure, position) for direct use in analysis software. This approach supports interoperability and reusability - in accordance with FAIR principles – significantly simplifies handling large datasets, and promotes compatibility across beamlines and facilities.
The file format has been accepted by the NeXus International Advisory Committee and is now part of the official NeXus release. The format is already implemented at the relevant beamlines across the MAX IV laboratory and can be used directly in the latest version of GSAS-II [4].
Here we will discuss the need for a standardized file format for azimuthally integrated data and its usefulness in the context of time-resolved scattering experiments. We will further show *plaid* [7], an application developed for fast visualization of the PXRD NXazint files.

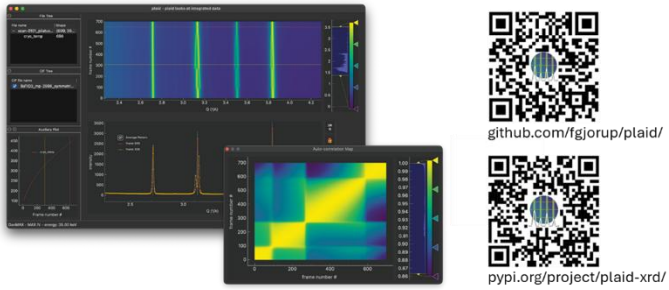


Figure 1. *plaid visualization software*

[1] Kieffer, J. et al. (2015). J Appl Crystallogr 48, 301-305.
[2] Jensen, A. B., et al. (2022). J Synchrotron Radiat 29, 1420–1428.
[3] Filik, J. et al. (2017). J Appl Crystallogr 50, 959-966.
[4] Toby, B. H. & Von Dreele, R. B. (2013). J Appl Crystallogr 46, 544-549.
[5] https://manual.nexusformat.org/classes/applications/NXazint1d.html
[6] https://manual.nexusformat.org/classes/applications/NXazint2d.html
[7] https://github.com/fgjorup/plaid/