

SAXS Data Handling at the ESRF: Current Situation and Future Prospects

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Small angle X-ray scattering (SAXS) and related experimental methods, like anomalous SAXS (ASAXS), grazing incidence SAXS (GISAXS) and wide angle X-ray scattering (WAXS) are used on more and more beamlines at the European Synchrotron Radiation Facility (ESRF) in different scientific fields. However, a common strategy for processing data is currently not being undertaken, and is probably not even necessary in the present situation. In addition, there does not seem to be a strong users demand for it. The ESRF data format (EDF) is a commonly used internal exchange format, which is supported by the ESRF software groups and as such is easily portable between beamlines. However, its feature to save metadata and binary data in the same file is not always fully exploited. The common description is limited to the sizes of the images and of their pixels as well as the data type (integer, float, etc.). A general description of SAXS and WAXS metadata from pinhole cameras seems to be used only at the ESRF beamlines ID01 and ID02 (see ref. 1). The increasing demand for “fast” online data reduction can change this situation. During the last years the fast online correction program SPD, originally only used for SPatial Distortion corrections, has been extended to allow for basic SAXS data reduction. This program is now used by a host of ESRF beamlines, and not only SAXS beamlines. Depending on the beamline, the experimental data are distributed either in EDF format or in proprietary detector formats accompanied by log-files. Sometimes only 1D ASCII tables (q, I, standard deviation) of processed data are taken away by the users. The data are eventually backed up on movable hard disks or DVDs and carried along to the home labs. It should be mentioned that such a data backup is relatively cheap but not very safe.

The ESRF plans during the next years a major upgrade of the storage ring, the beamlines and the computing environment. The prospected higher photon flux will require faster detectors and faster analysis software. During time resolved experiments we are already now confronted with peak data rates in excess of 40 MBytes/s. We anticipate a significant increase in the future and a must of online data processing for most of the experiments. In order to cope effectively with the forthcoming challenges international collaborations (like the European FP7 project), the development of distributed computing (e.g. GRID), and the efforts to adopt internationally recognized data exchange formats (e.g. NEXUS) have been initiated.

References

1. P. Boesecke, Reduction of two-dimensional small- and wide angle X-ray scattering data, *J. Appl. Cryst.*, 40, s423-s427 (2007)