

NXcanSAS: standard to store reduced SAS data of any dimension

Pete R Jemian¹, Andrew Jackson², Tobias Richter², Paul Butler³, Steve King⁴, Adrian Rennie⁵, Brian Pauw⁶

¹Advanced Photon Source, Argonne National Laboratory, Argonne, United States, ²European Spallation Source ESS AB, PO Box 176, Lund 221 00, Sweden, ³National Institute of Standards and Technology, 100 Bureau Drive, Bldg. 235, Stop 8562, Gaithersburg, MD 20899, United States, ⁴ISIS Pulsed Neutron Source, Science and Technology Facilities Council, Rutherford Appleton Laboratory, Harwell Campus, Didcot, OX11 0QX, United Kingdom, ⁵Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden, ⁶Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin, Germany
E-mail: jemian@anl.gov

The communication of experimental results is common to scientific investigation. The method of presentation varies widely across investigation technique, and may stymie fundamental scientific goals such as sharing of results and replication of experiments. Even within a limited community, such as small-angle scattering, the choice of how to organize stored information is fragmented, with the result that often, the data are deposited in ad hoc form.

To increase access to data produced from publicly-funded research, funding agencies are now requiring that proposals describe how data will be made available. With the increases in data volume due to higher-efficiency collection, increased experimental complexity, and larger and faster detectors, the plethora of ad hoc formats is a burden to the scientific community. Reliance on a few, well-considered standards facilitates automated processes for analysis and correlation of scientific data. Furthermore, it leads to development of common tools for data visualization and analysis, and data catalogues for access, reference, and data mining.

The Worldwide Protein Data Bank [1] is such an example where, by the provision of a standardized data format, scientific data and metadata from a vast range of methods has become available for research on the structures of proteins. Guidelines for structural modelling of small-angle scattering data from biomolecules in solution were adopted by the IUCr Commission on Small-Angle Scattering in 2012. [2]

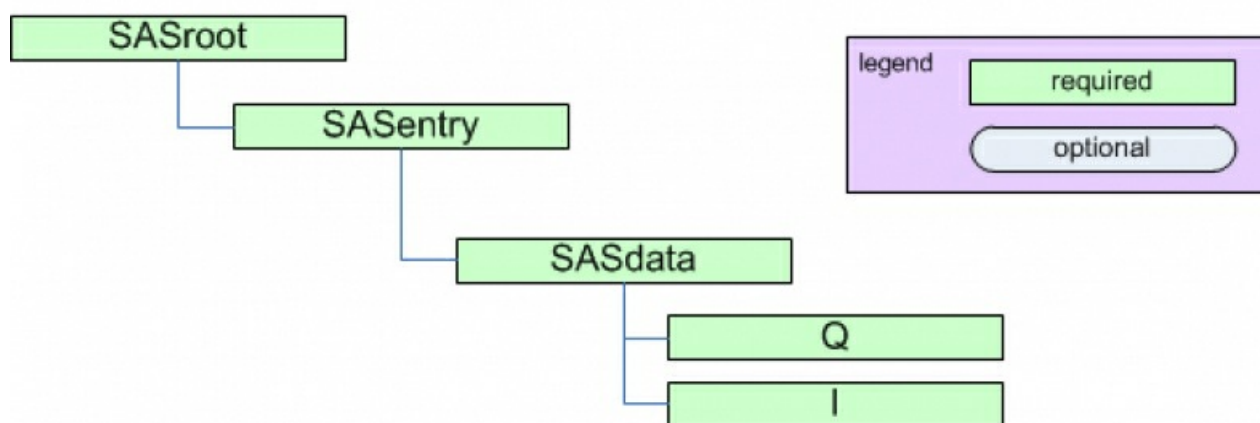
NXcanSAS [3] is a standard to store reduced small-angle scattering data of any dimension. It is sufficiently general that it may be used for any form of reduced SAS data in different scientific applications. The hierarchical structure of the canSAS (<http://www.cansas.org>) standard has been designed within the NeXus (<http://www.nexusformat.org>) data format. This presentation will describe the NXcanSAS standard, underlying concepts, and will give some examples.

This work was supported in part by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC-02-06CH11357.

[1] Worldwide Protein Data Bank, <http://www.wwpdb.org>

[2] Jacques, D. et al. (2012). Acta Cryst D Biol Crystallogr 68(6):620–626.

[3] NXcanSAS: <http://tinyurl.com/z4thyrn>



Keywords: [small-angle scattering](#), [data standard](#), [NeXus](#)