The Role of Home-Built Software at User Facilities: The ORNL SANS experience

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Although most national and international synchrotron and neutrons scattering user facilities are making a push towards uniform and centrally-managed software for data reduction and analysis, home-grown software has historically and is continuing to play an important role in these facilities. An example of this is the instrument scientist developed data reduction and analysis routines for fixed-wavelength small-angle neutron scattering (SANS) developed for the instruments at the High Flux Isotope Reactor. Between first beam in May of 2007 and February 15, 2017, the CG2 General Purpose SANS and CG3 BioSANS have contributed over 350 articles to the scientific literature, more than 90% of which have relied on the in-house software described here for data reduction and often data analysis. The primary strength of home-grown software is its ability to take advantage of flexibility and access to expert knowledge about the instrumentation and technique to adapt to the special conditions of the equipment and develop to meet specialized needs of the users. The detectors on these instruments share a unique design that requires specialized corrections for normalization that were developed and coded in the home-grown software as the need for those corrections were identified in instrument commissioning. Flexible, modular design allows for freedom in correcting missing or incorrect metadata and exploring alternative data reduction pathways in instances where experimental problems compromise part of the data set. Furthermore, having access to the modular in-house code has allowed the instrument teams on the two instruments to independently introduce minor variations to the software and new capabilities that allow each instrument to better serve their separate scientific communities. Some of the instrument-specific corrections, special models, and examples of experimental troubleshooting are described here.