The Advanced Photon Source

The APS On-line Catalog of Data Analysis Software

The U.S. Department of Energy's (DOE's) Office of Science laboratories have long had a leadership role in the development of widely distributed scientific software. For instance, powder diffraction crystallography, as well as combined refinements from neutron and x-ray data, was pioneered in the 1980s by the GSAS software package from Los Alamos National Laboratory. To this day, GSAS (now hosted at Argonne National Laboratory) is utilized for more than 400 papers per year, with at least 15% of that usage from U.S. light sources.

The need for software for data collection and analysis is now even more acute; experiments are more ambitious, datasets are larger. The importance of software development is well appreciated at the APS, but detailed knowledge of each project often did not extend beyond specific beamline communities.

To help remedy that situation, an activity was initiated at the U.S. DOE's Advanced Photon Source (APS) to produce an on-line catalog of both nascent and mature active software development efforts. That on-line Catalog of Data Analysis Software can be accessed at https://www1.aps.anl.gov/Science/Scientific-Software/. More than 20 on-going software development projects have been documented through discussion of the scope of each code, how it is funded and distributed, and its impact and future development directions; additional projects are still being added. Another dozen or so smaller-scale projects, in the areas of data collection/visualization, were also documented, albeit with less extensive discussions.

From the catalog, we see that successful software creation is a long-term process of innovation, maintenance, and support, continued well after initial development is complete; many staff devote long hours at this, while also tending to their primary beamline activities. These efforts, however, can benefit greatly with more centralized support. The catalog has fostered much more discussion amongst the software development community and with management. We have also learned that at present there is a large diversity in programming environments, but most new work from scientists is done in Python, while software engineers tend to prefer C++. The catalog has also served to foster much more discussion among APS software developers, and between developers and beamline scientists.

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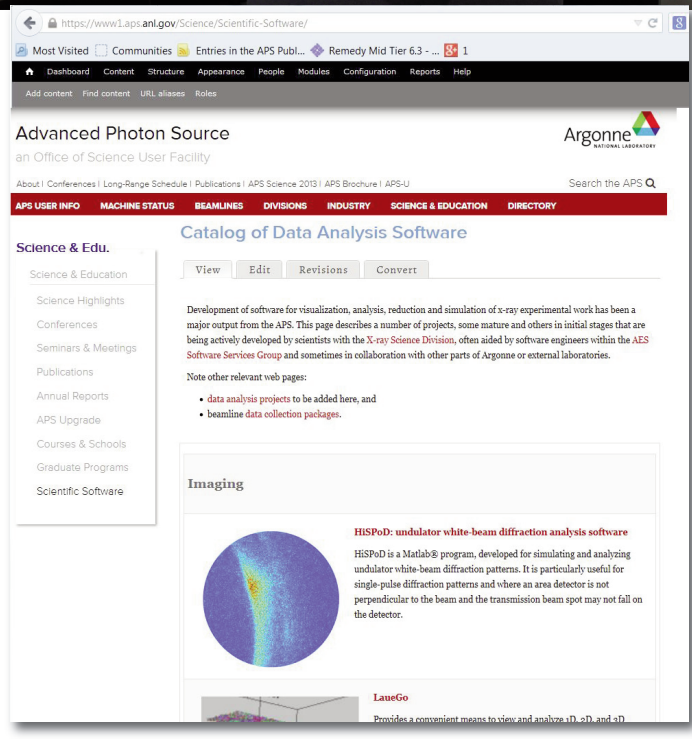

Top photo: Brian Toby, coordinator of the APS on-line Catalog of Data Analysis Software. The catalog web site is visible on the screen behind Toby; a small portion of the page is shown in the screen-grab (bottom).

Call for APS General-User Proposals

The Advanced Photon Source is open to experimenters who can benefit from the facility's high-brightness hard x-ray beams.

General-user proposals for beam time during Run 2015-3 are due by Friday, July 10, 2015.

Information on access to beam time at the APS is at https://www1.aps.anl.gov/Users-Information/About-Proposals/Apply-for-Time or contact Dr. Dennis Mills, DMM@aps.anl.gov, 630/252-5680.

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