Argonne NATIONAL LABORATORY

Intra-Laboratory Memo

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APS Renewal: Scientific Software in Five Years

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Each experiment performed at the APS requires three crucial ingredients: the powerful x-ray source, an optimized instrument to perform measurements, and computer software to acquire, visualize, and analyze the experimental observations. It is this combination that transforms a set of instruments into a research facility. Software underpins all aspects of the scientific output of the APS from data acquisition and reduction to real-time analysis, data visualization, modeling, and simulation software. As scientists attack problems of increasing sophistication and deal with larger and more complex data sets, the role of software expands. Demand for excellent and flexible scientific software can only be expected to increase as the upgrade of the APS facility and the implementation of advanced detectors and computational facilities create a host of new measurement capabilities. By taking a leading role in the development and maintenance of open-source software for the entire process of X-ray data analysis, and by partnering with APS users, scientists, and developers at universities, national laboratories, and other scientific facilities throughout the world, the APS has a unique opportunity to improve the state of the art of X-ray science.

High-performance computing capabilities, including computing clusters, high-speed/high-capacity file servers, and network access, are being delivered now to a few beam lines within XOR, providing dedicated access to real-time data processing and analysis. In the case of X-ray Photon Correlation Spectroscopy, access to HPC capabilities allows the instrument to exploit the 60 frame/second data acquisition on a continuous basis and provides real advancement in the XPCS facility. HPC advances the high throughput capability for X-ray tomography, providing APS users with both local and remote access to perform data reduction and analysis. New high frame-rate detectors for X-ray microdiffraction will rely on routine access to HPC resources as part of the routine data collection in addition to post-experiment support of users. Infrastructure is designed to support the expansion of HPC capabilities to other sectors as needs arise.

Data visualization tools are fundamental to the success of research investigations as they connect scientific data directly with scientific intuition. A finding from the 2006 XSD Scientific Software Workshop (ANL-APS-TB51) is emphasized as the APS assumes operating responsibility for a majority of the sectors that a facility-supported common tool set for viewing 1-D, 2-D, 3-D, and higher dimensional data is in strong demand.

APS users will rely on common software to support the flow of scientific data from experiment to HPC, data visualization, and through analysis. Upgrades in the small-angle facilities at sector 12, concentrating several SAXS instruments in one location, include the development of a common software tool set integrating data acquisition, reduction, analysis, visualization, modeling, and simulation. This tool set is expected to become the basis for a standard suite used at all APS small-angle instruments. Continued contributions to this tool suite are expected from the APS user community.