Contribution ID: **5** Type: **Oral**

The Scientific Computing Strategy for the Upgraded Advanced Photon Source

Thursday 22 September 2022 13:30 (20 minutes)

The Advanced Photon Source (APS) at Argonne National Laboratory (ANL) will replace the entire storage ring with a ring based on a multi-bend achromat lattice design. The new storage ring will increase the APS' s brilliance by factors of 100-1,000s, depending on x-ray energy, and make the APS the brightest hard x-ray synchrotron source in the world. Because of the greatly enhanced brightness, coherence, and signal at high x-ray energies along with new state-of-the-art high-bandwidth commercial detectors, beamlines require significant improvements in networking, controls and data acquisition, computing, workflow, data reduction, and analysis tools to operate effectively.

All aspects of APS operation depend on computation, but data analysis software and beamline control and computing infrastructure are of particular importance for facility productivity. Demands for increased computing at the APS are driven by new scientific opportunities, which are enabled by new measurement techniques, technological advances in detectors, multi-modal data utilization, and advances in data analysis algorithms. The priority for the APS is to further improve its world-class programs that benefit most from high-energy, high-brightness, and coherent x-rays. All of these require advanced computing. The revolutionized high-energy synchrotron facility that the APS will deliver will increase brightness and coherence, leading to further increases in data rates and experiment complexity, creating further demands for advanced scientific computation.

Over the next decade, the APS anticipates a multiple-order-of-magnitude increase in data rates and volumes generated by APS instruments. This necessitates 10s of petaflop/s of on-demand computing resources and increased data management and storage resources to process and retain this data and the analyzed results. Advanced data processing and analysis methods will be required to keep up with the anticipated data rates and volumes and to provide real-time experiment steering capabilities.

The key elements of the scientific computing strategy at the upgraded APS, include upgrading networking infrastructure within the APS and between the APS and the Argonne Leadership Computing Facility (ALCF), deploying state-of-the-art experiment control software at beamline instruments, expanding the capabilities and use of common data management and workflow tools and science portals, deploying sufficient local and edge computing resources, and utilizing new supercomputers at the ALCF for large on-demand data processing and analysis tasks, developing high-speed, highly parallel data processing and analysis software, and extensively applying novel mathematical and AI/ML methods to solve challenging data reduction and analysis problems, and collaborating with other light sources, experimental facilities, large-scale computing and networking facilities, and the APS user community.

*Work supported by U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

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Track Classification: NOBUGS 2022