Accelerating the Experimental Feedback Loop: Data Streams at the APS

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Increases in the volume and velocity of data from scientific experiments motivate significant changes in experimental protocols. Researchers often want quasi-instant feedback, so that one result can guide future observations and steer experimental processes. Such needs arise across DOE's Office of Science. Combining these high-speed data streams with high-performance computing has the capability to radically change experimental science.

Coupled experiment-computation systems provide a rich source of opportunities and challenges for stream processing tools, as a single experimental session can operate at multiple time scales; engage both distributed systems and tightly coupled parallel computers; and require interactions with data archives and human collaborators: see Figure 1. Timely and reliable execution of the resulting workflows can enable important new experimental modalities (e.g., real-time studies of battery charge-discharge cycles). They can also be essential to efficient use of expensive facilities: without online feedback, a vastly expensive experimental session, booked months in advance, can be entirely wasted.
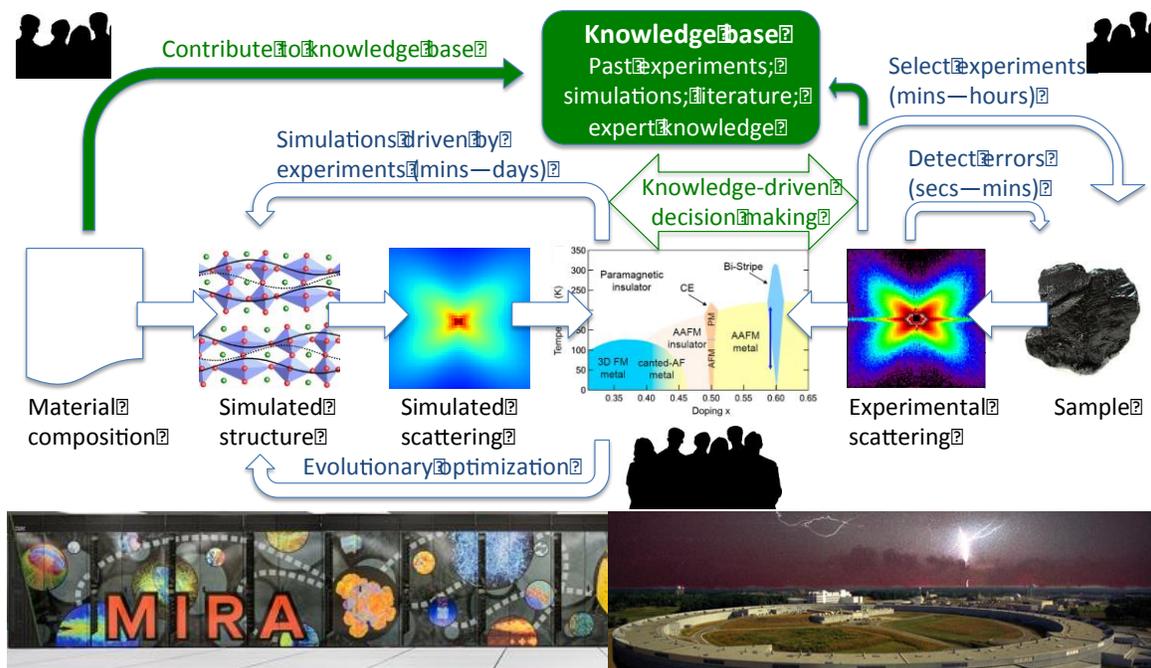
Figure 1: The analysis of defect structures in disordered materials can involve many different workflows with different time scales, computational needs, quality of service requirements, and resources. On the right, experiments are performed on Argonne's Advanced Photon Source (APS); on the left, computation is performed on the Argonne Leadership Computing Facility (ALCF)'s Mira supercomputer.

We use two application pilots from Argonne's Advanced Photon Source (APS) to illustrate some of the opportunities inherent in coupling experiment and computation. (The APS, a synchrotron light source, operates ~65 beamlines that support a wide range of experimental modalities, many scientific communities, and >5000 unique users every year.)

Single-crystal diffuse scattering (Osborn, Wozniak, Wilde, et al.) The goal of this work is to understand defect structure in disordered materials. We have developed a range of

workflows, illustrated in Figure 1, including rapid reconstruction during individual experiments (100s of cores), analysis of data from multiple experiments (1000s of cores), and evolutionary optimization for inverse modeling (100K+ BG/Q cores; Swift+OpenMP). Streaming data is ingested by our services, processed by automated pipelines, and made accessible via search and remote data access techniques.

Near-field high-energy X-ray diffraction microscopy (Almer, Sharma, et al.). This method is used to characterize microstructure in bulk materials. Reconstruction on 10K+ BG/Q cores returns results in ~10 min vs. >5 h on an O(100) core cluster or months if data is taken home. This workflow was recently used to detect errors in experiment configuration that would have otherwise resulted in a total waste of beamtime. Data here is streamed from the APS to a PC cluster to the BG/Q using a combination of high-performance techniques, including Globus and MPI-IO, in addition to compute-node caching.

These pilots also illustrate some key technical challenges that require substantial R&D if we are to make effective use of next-generation experimental facilities. For example:

Data-driven analysis: Experimental workflows are concerned, above all, with organizing, moving, analyzing, sharing, and tracking large quantities of data. In the examples above, we used Globus services to manage data flows and to track data products and provenance. But, much more work is required if we are automate and optimize ever-more-complex workflows, e.g., to track data products generated by large numbers of experiments, process data generated by many such experiments, integrate experiment streams with simulation streams or prior results, and introspect on behaviors of experiments, beamlines, and entire facilities to identify errors and plan future activities.

On-demand computation: Computation can link with experiments at multiple time scales: see Figure 2. The need to support a range of time scales, data volumes, and computational requirements has profound implications for computer systems architecture, scheduling methods, application configuration, and other factors. The computing systems best suited for modern experimental facilities are not yet clear. Given a selection of computing resources, the choice of resource(s) for individual workflow components may depend on resource availability, scheduling policies, performance, application characteristics, and other factors.

Real-time feedback implementation: Data- and compute-intensive near-real-time workflows pose simultaneous requirements for fast network transfers, high processing performance (often close-to-bare-metal performance); programmer productivity (because researchers often vary experimental protocols), and system scalability (because many workflows may execute simultaneously).
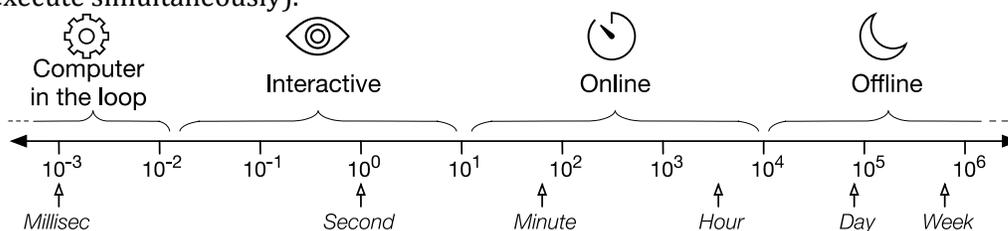
Figure 2: A rough categorization of the different time scales on which computation may be linked with experiments. (In practice, different categories and timescales may overlap.) *Computer-in-the-loop* activities may require timescales of a millisecond or less. For *interactive* activities, such as data subsetting to examine data features, delays of 0.1 to 10 seconds can be acceptable. *Online* computations, used for feedback during data acquisition, for example to detect errors in experiment setup, focus on an area of interest, or tune an experimental parameter, may range from minutes to an hour or more. *Offline* computations, performed periodically to say reprocess an entire data archive, may take hours or days.