Scalable HPC Workflow Infrastructure for Steering Scientific Instruments and Streaming Applications

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Linking scientific instruments to exascale machines and analyzing the large volumes of data produced by the instruments requires workflow infrastructure that scales along many dimensions. In this white paper we generalize this problem to include control systems, analysis of data produced by supercomputers, computational steering and data assimilation. The requirements of distributed computing problems which couple HPC and streaming data, are distinct from those familiar from large-scale parallel simulations, grid computing, data repositories and orchestration, which have generated sophisticated software platforms. Our analyses points to new research directions for a scalable infrastructure, to address this generalized streaming distributed workflows problem class.

Streaming HPC: A Workflow Infrastructure for Steering in Big Data Scientific Applications

Scientific experiments are increasingly producing large amounts of data that need to be processed on HPC platforms. These experiments often need support for real-time feedback to steer the instruments. Thus, there is a growing need to generalize computational steering to include coupling of distributed resources in real-time, and a fresh perspective on how streaming data might be incorporated in this infrastructure. In general, big data has spotlighted the importance of streaming as a computational paradigm, which is not a new idea but one of growing relevance. In Table 1, we list five problem areas that involve streaming data. These are all actively used today but without a software model focused on streaming aspects. All five problems areas have critical reliance upon high-performance computing (HPC), hence we propose generalization to a new paradigm of *Streaming HPC.*

	Streaming Application	Details
1	**Data Assimilation**	Integrate data into simulations to enhance quality. Distributed Data sources
2	**Analysis of Simulation Results**	Climate, Fusion, Molecular Dynamics, Materials. Typically local or in-situ data
3	**Steering Experiments**	Control of simulation or Experiment. Data could be local or distributed
4	**Astronomy, Light Sources**	Outlier event detection; classification; build model, accumulate data. Distributed Data sources
5	**Environmental Sensors, Smart Grid**	Environmental sensor data or Internet of Things; many small events. Distributed Data sources

Table 1: Five steering applications that involve data streaming

We suggest research on new infrastructure for Streaming HPC, which is contrasted with four other paradigms (outlined in Table 2.) In the first four paradigms of Table 2, the data is typically accessed systematically either at the start of or more generally at programmatically controlled stages of a computation. In today's workflow, multiple such data-driven computations are linked together. On the other hand, Streaming HPC absorbs data asynchronously throughout the computation.

Paradigm		Features and Examples
1	**Multiple Loosely-Coupled Tasks**	Grid computing, largely independent computing/event analysis, many task computing
2	**MapReduce**	Single Pass compute and collective computation
3	**BSP**	Iterative staged compute (map) and computation includes parallel machine learning, graph, simulations. Typically Batch
4	**Dataflow**	Dataflow linking functional stages of execution
5	**Streaming HPC**	Incremental data I/O feeding to long running analysis using other computing paradigms. Typically interactive

Table 2: Five Scientific Computing Paradigms

We argue that the applications of Table 1 are critical for next-generation scientific research and thus need research into a unifying conceptual architecture, programming models as well as scalable run time. For DOE applications, one needs to support a more general computation model including large parallel executions. In general, one should support linking of the buffered data to instances of any of the four other HPC paradigms in Table 2.

Streaming HPC: Defining and Distinctive Aspects

Streaming HPC is characterized by its distinctive data acquisition. However, Streaming HPC has multiple unique dimensions that requires rethinking the appropriate scalable infrastructure for steering scientific instruments and applications. We posit that Streaming HPC will affect many different dimensions of research including algorithms for data processing, storage and data management, resource management and scheduling.

For example, new algorithms are needed including online or streaming algorithms, which in addition to dealing directly with streaming data, aim at low computational complexity with data items looked at once and then discarded. In contrast most batch algorithms are iterative and have increased compute and data storage (memory use) needs.

Many of the applications that require steering of scientific instruments have real-time constraints. For example, scientists using the Advanced Light Source beamline often need real-time processing of the data, the results of which might be used for automated or manual steering of the experiment. Similarly, as extreme scale systems are used for analyses of data, there will be a need for interactive user sessions with the analyses that will require resource management infrastructure to support this. While in-situ analysis is proposed as a way to minimize I/O on next generation systems, there is a realization that it is insufficient when the type of analysis might not be known before hand and/or for domains where post-processing is critical.

Current HPC systems have been focused on fixed scaling where a user requests the resource for a fixed time and width. Streaming HPC necessitates a different resource management model that allows for dynamic scaling of resources to handle variable data rates in both buffering and computation stages. The problem of elastic computational scaling has been studied in the context of web or business applications. There is a need to study the impact of dynamic scaling to handle variable data rates in both the computation and data buffering stages in HPC environments.

Future Work

There is future work needed in this space to understand a number of different research topics related to distributed and HPC workflows.

- *Application Study:* Table 1 is a limited sampling of applications that critically depend upon Steering HPC. It is necessary to extend and refine Table 1 with broader set of application characteristics and requirements. This could benefit from collaboration with with other Federal Agency efforts, including but not limited to NIST Public Big Data working group and NSF and other commercial initiatives.
- *Scalable Architecture:* A critical challenge that follows is to come up with a scalable architecture that will support the different types of Streaming HPC for the range of applications types and infrastructure types. Existing approaches such as Apache Storm are elegant but for example, lack support for quality of service and HPC processing of events.
- *Novel programming and software paradigms:* There is a need to integrate features of traditional HPC such as scientific libraries and communication with the rich set of capabilities found in the commercial ecosystem. It is important in this context to understand the similarities and differences between the HPC workflows and distributed streaming workflows.