Data Intensive and High Performance Computing: The View from High Energy Physics

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Computational efforts in many science communities are driven by a combination of computing tasks and managing large-scale data volume and data flow. Because of the complexity of such use cases, both performance/throughput and usability are equally important. Examples of such communities include astronomy, light source users, biology, climate/earth science, high energy physics (HEP) and materials science. The associated computation may come in the form of simulations or large-scale analysis on data generated by simulations, experiments, or observations. HEP is an example community whose computing use cases depend upon not only on high performance and data-intensive computing, but also on high throughput computing. Therefore, this community needs to have an optimal balance of compute, I/O, storage and networking.

HEP science focuses on three frontiers: the energy frontier, the intensity frontier and the cosmic frontier. The energy frontier is concerned with large experiments at colliders generating roughly 30PB a year, expected to reach 400PB per year in a decade. The intensity and cosmic frontiers deal with small to medium scale experiments, generating less than 1PB per year, though intensity frontier experiments are expected to grow to 10PB/year within 5 years, while the cosmic frontier is expected to reach about 10PB/year. The experimental data frequently requires fine-grained "event'' style analysis where data pipelines can be complex and need to be run many times. Each such campaign can last for months. Experiments themselves need support from theory, which involves simulations with variable scale data. Demands on I/O vary due to the nature of the simulations and the fine-grained nature of the outputs (many small files). Currently, the amount of data generated by simulations is mostly limited by available storage and I/O resources. High throughput computing is a major user of Grid resources in batch mode for long-duration loosely coupled analysis, and is fast approaching a potential breaking point as the experimental data volume reaches a threshold where the HEP community's own resources may no longer be sufficient to handle it.

From the perspective of the HEP community, the following are "ideal world'" requirements:

- *Software stack* --- ability to run arbitrarily complex software stack on demand
- *Resilience* --- ability to handle failures of job streams
- *Resource flexibility* --- ability to run complex workflows with changing computational 'width'
- *Wide-area data awareness* --- ability to seamlessly move computing to the data (and vice versa where possible); access to remote databases and data consistency
- *Automated workloads* --- ability to run automated production workflows
- *End-to-end simulation-based analyses* --- ability to run analysis workflows on simulations using a combination of in situ and offline/co-scheduling approaches

The aim is to bring to bear a combination of HPC, data-intensive, and high-throughput computing resources to solve HEP's broad range of problems. An important consideration in this is the design of edge services and the associated networking that would link a number of these resources together. These in turn must consider a number of factors such as security, resource flexibility, interaction with schedulers, external databases and requirements of the user community.