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Data Co-Processing for Extreme Scale Analysis Level II ASC Milestone (4745)

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Abstract

Exascale supercomputing will embody many revolutionary changes in the hardware and software of high-performance computing. A particularly pressing issue is gaining insight into the science behind the exascale computations. Power and I/O speed constraints will fundamentally change current visualization and analysis workflows. A traditional post-processing workflow involves storing simulation results to disk and later retrieving them for visualization and data analysis. However, at exascale, scientists and analysts will need a range of options for moving data to persistent storage, as the current offline or post-processing pipelines will not be able to capture the data necessary for data analysis of these extreme scale simulations. This Milestone explores two alternate workflows, characterized as *in situ* and *in transit*, and compares them. We find each to have its own merits and faults, and we provide information to help pick the best option for a particular use.

Executive Summary

Milestone 4745, Data Co-Processing for Extreme Scale Analysis, is successfully completed on time and demonstrated against the letter and spirit of the stated Milestone.

Visualization and data analysis on extreme scale platforms presents critical challenges in the management of data generated by simulations and the interface between simulation and data analysis. Computation speed will continue to outpace storage bandwidth, and power management will become much more of a workflow constraint on advanced architectures, so we anticipate that science on extreme scale machines will require a range of data analysis, filtering, and visualization workflows. With these tools, the analysts will determine the best computation profile for specific problems. In particular, in addition to current practices of post-processing and constrained writes, customers will need *in situ* and *in transit* workflows that allow them flexible options for getting results to persistent storage.

Milestone 4745 provides important study of the behavior of new workflows for visualization and data analysis. In particular, we examine the performance of two proposed workflows: an *in situ* workflow in which visualization and data analysis is coupled directly with a simulation as a library, and an *in transit* workflow in which visualization and data analysis is a separate service connected to the simulation via a network. Each workflow has its own characteristics, and our study details empirical evidence on their respective performances.

As we look ahead to the extreme architectures planned by ASC, it is critical to understand the strengths and weaknesses of these proposed analysis approaches, and to design experiments that will help us understand how to enhance scientific discovery on these new architectures. Milestones such as this one provide important foundations for evaluating our current technical approaches, and for strategic development of analysis capabilities for future architectures.

For this Milestone, we explored the performance characteristics of two proposed technologies developed with significant contributions from Sandia National Laboratories. These technologies leverage existing investments in data analysis, visualization and I/O research, and are part of a long term strategic plan for addressing ASC analysis needs across a spectrum of scales, codes, and science domains. We employ two critical software technologies developed with significant contributions from Sandia National Laboratories. First, we use the Catalyst library to provide *in situ* visualization and data analysis directly to a running simulation. Second, we use the Nessie framework to establish an *in transit* visualization and data analysis service connected to a running simulation.

Our primary motivation for this use case was to use a highly scalable code that provided an example of real physics, so that we could determine performance characteristics when applied against real data. There is significant community development in min-apps available in the community that scale well across large architectures, but whose output is not representative of a real science code. CTH is utilized as a test code for ASC platforms, and has been used in several exploratory in-situ tests in the past. Because of this, the team opted to use CTH as a driver for this large scale experiment.

Our empirical study comprises over 10 million core hours of running an instrumented simulation and data analysis use case. This use case, involving the fragmentation analysis of an explosion simulated in the CTH shock physics code, is designed in conjunction with a Sandia analysis customer as an exemplar of scientific work.

In addition to demonstrating the scalability of our frameworks, our study also provides insightful comparisons between the *in situ* and *in transit* workflows and the trade-off point between them. We also consider other important parameters such as memory overhead, initialization time, and scheduling.

This SAND report presents the full results of our milestone work and is available to anyone.

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