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FY20 ASC IC L2 Milestone 7180: Performance Portability of SIERRA Mechanics Applications to ATS-1 and ATS-2

Executive Summary

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Introduction

The overall goal of this work was to accelerate simulations supporting the nuclear deterrence (ND) mission through improved performance of key algorithms in the ASC IC Sierra multi-physics application suite. This work focused on porting and optimizing algorithms for the graphics processing units (GPU) on the second ASC advanced technology system (ATS-2), while maintaining or improving performance on commodity technology systems (CTS) and ATS-1. Furthermore, these algorithmic developments used the ASC developed Kokkos performance portability abstraction library to maintain high performance across platforms using identical code, and enable sustainable reduced-cost migration and performance optimization to emerging hardware.

Milestone Description and Completion Criteria

As displayed in the ASC Implementation Plan (IP) and the Milestone Reporting Tool (MRT), the milestone description and completion criteria state:

Analyst provided W80-4 analysis use cases in the areas of Solid Mechanics, Structural Dynamics, and Thermal Transport will be benchmarked on the next generation platforms ATS-1 (Trinity), ATS-2 (Sierra), and Astra. Correctness of the physics applications will be demonstrated on these new platforms. Scalability and performance of the physics applications will be evaluated as compared to current production platforms such as CTS-1 (serrano). Performance improvement shall be demonstrated for the highest impact performance issues identified by the benchmarking.

Focus will be on providing optimization to the full analysis workflow including solves and pre and post processing. Kokkos, and Kokkos Kernels will be leveraged through the Sierra Toolkit ngp::Mesh to provide performance on these systems. A focused effort will be undertaken to optimize usability of these Kokkos tools for Sierra Mechanics applications.

Completion Criteria: Code Release, Test Suite, SAND Report

Impact Statement

The ASC IC Sierra multi-physics application suite was successfully ported to ATS-2 and demonstrated up to 4.9 times faster runtime compared to CTS-1 for W80-4 use cases in structural dynamics, solid mechanics, and thermal transport.

Summary of Work Done

The Sierra/SolidMechanics (SM), Sierra/StructuralDynamics (SD), and Sierra/ThermalFluids (TF) application teams gathered simulations representing W80-4 use cases from the analyst community to identify which algorithms should be implemented and/or optimized for GPU execution. The SM team used a mock W80-4 bare warhead drop simulation to drive performance improvement of the explicit transient dynamics solid mechanics simulation use case. The SD team used W80-4 component and assembly models to focus performance optimization of modal random vibration use cases common to normal environment structural mechanics and fatigue simulations. Finally, the TF team used a mock W80-4 bare warhead normal environment thermal analysis to improve performance of their thermal radiation and solver algorithms. Throughout the year, the application teams worked to implement or improve algorithms capable of performant GPU and CPU execution and demonstrated significant performance gains.

The TF team focused efforts on improving existing GPU-capable solver technology and implementing GPU thermal radiation view-factor computations. Compared with the beginning of FY20, the TF team realized 20 times faster runtime for their exemplar problem and up to 3.5 times faster runtime on ATS-2 than on CTS-1 compared node-to-node.

The SM team concentrated on development and integration of GPU capable element and material model formulations. By the end of the year, they realized up to 40% speedup compared to the equivalent CPU-only implementation on ATS-2 for the mock W80-4 drop simulation and faster execution on ATS-2 compared to CTS-1 using the same GPU-capable element and material formulation.

Finally, the SD team integrated a new GPU-capable domain decomposition linear equation solver into their eigenvalue extraction algorithms and leveraged Kokkos kernels to post-process modal random vibration response. Additionally, the GPU-capable solver was integrated into the SM application for implicit quasistatic solid mechanics simulations. Using these improved algorithms, the SD team was able to demonstrate up to 4.9 times faster computation of random vibration response on a part and over 2.5 times faster modal analysis of a W80-4 assembly, using ATS-2 compared to CTS-1.

This initial capability is included in the Sierra 4.57.7 and newer versions available on all supported SRN platforms, and will be included in the Sierra 4.58 release that will be installed on all production platforms. The Sierra 4.58 release is scheduled for October, 2020.

Path Forward

The successful completion of this effort has given Sandia the ability to support ND computations using the Sierra multi-physics applications on ATS-2 and future GPU accelerated computing platforms. Work remains to “harden” these newer capabilities for production ND computations and develop guidelines for analyst use of these fundamentally different computing architectures. With this new capability, analysts will have increased access to another, more powerful computing resource that will help them to complete their critical work. The ensuing reduced time-to-solution and broadened access to compute resources can improve throughput and/or allow for increased fidelity simulations.

In Support of Stewardship Capability Delivery Schedule (SCDS)?

Not Applicable.