PROJECT TITLE

Celeritas: GPU-accelerated particle transport for detector simulation in high energy physics experiments

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Objective

High Energy Physics (HEP) is entering an incredibly exciting era for potential scientific discovery. The evidence that the Standard Model (SM) of particle physics is incomplete is overwhelming. A targeted program, as recommended by the Particle Physics Project Prioritization Panel (P5) [1], is being executed to reveal the nature and origin of the physics Beyond Standard Model (BSM). Two of the flagship projects are the planned high luminosity upgrades of the Large Hadron Collider (HL-LHC) and its detectors (ALICE, ATLAS, CMS and LHCb) and the Deep Underground Neutrino Experiment (DUNE) at the Sanford Underground Research Facility (SURF). The DUNE experiment will study neutrinos – via their interactions with liquid argon detectors – produced from both the Long-Baseline Neutrino facility and core-collapse supernovae to understand the role of these weakly interacting particles in the universe and search for signs of proton decay. The HL-LHC physics program includes further study of the Higgs boson as a means to look for new physics.

To further scrutinize the Standard Model and search for new physics, the volume and complexity of the data of the future particle physics experiments, notably the HL-LHC, will increase by orders of magnitude. To fully realize the physics potential of these new facilities, the computing capabilities have to be commensurate with the complexity and data-taking rate of the detectors. Unless significant advances in computing capabilities are made, the full potential of the HL-LHC physics program cannot be realized. Assuming an increase in computing power of 10% to 20% per year, the total computing needs to fully analyze the data from the HL-LHC experiments will still fall short by at least a factor of five [2–4]. Furthermore, the model of grid computing will not be sustainable anymore for these large data flows and would be completely cost-prohibitive.

Not only will the data volume increase substantially, also the events will be significantly more complex due to the much higher granularity and readout rate of the detectors. To extract the physics from these collider experiments, the recorded data is compared to detailed Monte Carlo (MC) simulations that describe the interactions in the detector of particles coming from the collision from known physics processes. There is an immediate and urgent need to be able to increase the modeling and simulation capacity that is out of reach of traditional software.

The current state-of-the-art and LHC baseline MC application for simulating the passage of particles through matter is Geant4 [5]. However, a major caveat is its runtime, as much as $\mathcal{O}(10)$ minutes, when simulating particles traversing complex detector geometries. One pathway to address this is to utilize advanced computational accelerator (e.g., GPUs) architectures; GPUs have become commodity hardware at DOE leadership computing facilities, and are becoming increasingly available on other institutional-scale computing clusters. GPUs offer far higher performance per watt than CPUs but are highly sensitive to memory access patterns, thread divergence and device occupancy, making them a difficult target platform for MC physics algorithms. Porting CPU physics codes to GPU-capable programming models is further complicated by common C++ language idioms – e.g., inheritance and dynamic memory allocation, both of which are used heavily within Geant4 – which are incompatible with vendor-independent device execution, potentially requiring fundamentally new algorithms to run on GPUs.

Recent work in the *ExaSMR: Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small Modular Reactors* project within the DOE Exascale Computing Project (ECP) has demonstrated speedups of 160× per CPU core on Summit for neutron MC transport on full-featured, three-dimensional reactor models [6]. However, there are several distinctions between that work and the necessary capabilities required for particle physics detector modeling. The reactor and nuclear technology applications targeted in *ExaSMR* are not characterized by large showers of secondary particles, and because the particles are neutral, there are no electromagnetic (EM) field interactions.

Our objective is to provide the needed HEP detector simulation modeling capacity using the new application *Celeritas* [7] that performs fast and accurate MC particle transport simulations on GPUs. This objective directly addresses Topic II of the SciDAC call; Celeritas will provide novel detector simulation and tracking models and data-driven analysis techniques for HEP physics experiments employing U.S. Department of Energy (DOE) leadership computing facilities. Celeritas is designed to complement, not replace, Geant4 and ultimately satisfy the detector response requirements as defined in Ref. [4] using the advanced architectures that will form the backbone of high performance computing (HPC) over the next decade.

Research Plan

The proposed work in this project is designed to increase the nascent capabilities in Celeritas for full HL-LHC detector modeling. During this five year effort we will extend Celeritas to address: (i) comprehensive SM physics including weak and strong interactions, (ii) integration with existing Geant4-defined workflows for offloading EM particle transport, (iii) a flexible scoring system for generating particle hit data in user-defined detector regions, and (iv) high-performance I/O that is compatible with the ROOT [8] framework.

In HEP detector simulation the desired outputs include particle history information and simulated detector response. Both outputs are tailored for each experiment and must be compatible with ROOT in order to be seamlessly integrated in HEP workflows. Efficient I/O between host and device is a challenge in HPC applications, and to fulfill HEP needs we will engage with the RAPIDS2 SciDAC institute. This collaboration will result in a set of workflow tools that provide compatibility layers between DOE federated computing facilities and current/future HEP computing centers.

The result of this proposed development plan for Celeritas will enable the use of DOE HPC resources to address HEP detector simulation needs for the HL-LHC. Through the collaboration with RAPIDS2, we will create the building blocks for better data integration and workflows between DOE leadership computing facilities and HEP experiments and their computing centers. Finally, physics components developed within Celeritas, e.g., EM physics transport, will be directly accessible within existing HEP workflows, thus providing an immediate benefit to experiments as a step towards full adoption of leadership class computing facilities.

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