High Energy Physics Detector and Beamline Simulations in the 21st Century

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We describe the general High Energy Physics Detector and Beamline Simulations challenges and make proposals how to address them.

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Detector simulations, and modeling of beam interactions and particle production in fixed targets are indispensable in the design process of new detectors and facilities for High Energy Physics (HEP) experiments. Equally as important is the role these simulations play in the development of reconstruction algorithms, and validation and interpretation of experimental results.

As the sizes of datasets increase, physics measurements and theoretical predictions are made more precise, and experiments seek sensitivity to rarer processes, the demands for higher fidelity simulated events rapidly grow. While each of the HEP frontiers – Energy, Intensity, and Cosmic – have their own specific requirements for simulations, there are a number of overlapping needs. For some experiments, the growth of detector complexity – for instance, to accommodate higher beam energy, luminosity, beam intensity conditions and per-event multiplicities – will drive the development of fast parameterized or machine-learned models, or other novel techniques for detector simulation. For other experiments, the demand for more accurate simulations – such as needed for high-fidelity modeling of signal induction, LAr and other scintillation-based materials, as well as Cherenkov light propagation, condensed matter effects, low-energy response, and rare background processes – will push the development or more complete detector models. Apart from detector simulations, some experiments depend critically upon a detailed and precise understanding of the complex interactions of beams with fixed targets, such as needed for secondary beam production, stopping particles, etc.

The changing computing hardware landscape imposes new constraints on the way the simulations can and need to be performed. These new constraints make the old computing processing model – where many instances of a simulation code were run on separate computer cores – more difficult, if not impossible, to sustain. As the market-driven trends in hardware, which no longer are significantly influenced by HEP, evolve, the simulation software, algorithms and techniques must also evolve in order to satisfy the demands mentioned above. In parallel, it is also necessary to continuously adapt the software in response to the changes in operating systems and compilers. Research and development (R&D) into more accurate models, faster and more versatile codes, and efficient use of modern hardware – e.g. GPUs, FPGAs, etc. – is pivotal for the continued success of HEP experiments.

In order to satisfy the stringent and complex requirements of future programs, and to meet the computing challenges within the resource budgets, the HEP detector simulation community has established a multi-prong R&D and operations plan (see e.g. [1]). Detector simulation tools require effort for code modernization, improvement of physics models, maintenance and long-term support. Evolving computing architectures demand significant investment to adapt and optimize simulation software to run effectively and exploit the available hardware in modern supercomputing centers.

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This plan is not viable without a comprehensive and aggressive training plan of both application developers and end users.

The evolution of fast simulation tools and techniques is another element of the multi-prong approach. Machine learning (ML) is one of the most promising alternatives to traditional parameterization methods, provided the methods produce faithful physics output while achieving significant speed-ups. However, ML-based simulations still require computationally expensive training campaigns that typically rely heavily on some well-established simulation software – e.g. Geant4 [2–4]. Therefore, ML does not simply eliminate the need to establish long-term efforts to speedup existing software stacks, run on accelerators or efficiently on High-performance computing (HPC) hardware.

Some of the elements of a proposed R&D program which play to the strengths of the US simulation teams are listed below (described in their own, separate LOIs).

- "Celeritas - a nascent GPU detector simulation code" - is not a replacement for Geant4 but an application built based on Geant4 and SHIFT [5, 6] with the initial R&D phase including the implementation of elements of electromagnetic particle transport on GPUs to run on Exascale Computing (ECP) machines [7];
- “Simulating Optical Photons in HEP experiments on GPUs” – is an effort to Integrate Geant4 and Opticks [8, 9] in a hybrid CPU/GPU application using G4Tasking [10], a Task-Level Parallelization approach currently under development;
- “Pre-Learning Geant4 Geometry Using Machine Learning to Accelerate Detector Simulations” – is a project to speedup Geant4 tracking [11];
- “Simulation on HPCs” - proposes to investigate the interconnection of HPC systems for event simulation and task scheduling [12];
- “Simulations of Low-Energy Crystal Physics for Dark Matter Detectors” – describes the needs of a certain class of Dark Matter (DM) experiments and presents ideas on how to address them [13]; and
- “Generic Tasking Framework for Geant4” [10].

Due to the long lifetimes of current and future HEP experiments, it is crucial to continuously recruit, train and retain teams of experts, as well as to create attractive career paths for people developing and maintaining the software. Most importantly, the detector modeling requires multidisciplinary teams consisting of software developers and physicists with specializations in low-energy, electromagnetic, weak and condensed matter physics. Continuous funding is therefore required for High-Energy and Nuclear physicists, as well as software developers throughout the life cycles of software toolkits for HEP experiments.

To set the scale of the required detector simulation R&D and operations effort, we can use the Geant4 toolkit and the GeantV R&D projects [14] as examples. Geant4 is maintained by a 26 year-old collaboration, currently of 130 members (approximately 30 FTEs) distributed worldwide, serving a very diverse set of user domains; its developer and user bases extend from HEP to space and radiation studies, to medical applications. GeantV was an R&D project to redesign Geant4 to exploit the benefits of vectorization and increased code and data locality. It took about 5 years and 30 FTE-years to implement only a fraction of all Geant4 modules within GeantV, mainly in the transport and electromagnetic domains, leaving most of the code unvectorized. Based on this recent R&D experience and the size of the international Geant4 collaboration it is critical that the US contributes significantly to the global effort. A team of highly-skilled physicists and engineers is required to provide the necessary support and developments for Geant4 to meet the needs and challenges within the scope of the US HEP experimental program. The realization of Geant4 running on exascale computing hardware will require additional person-power — a team whose expertise lies in parallel and high-performance computing — to deliver production-quality framework on the timescale of the High-Luminosity Large Hadron Collider program [15] and future Intensity Frontier [16–18] and DM experiments [19].

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