Snowmass2021 - Letter of Interest

Fast Simulations for Noble Liquid Experiments

Thematic Area: CompF2: Theoretical Calculations and Simulation
Additional Thematic Areas: CompF1: Experimental Algorithm Parallelization
CF1: Dark Matter, Particle-like; CF2: Dark Matter, Wave-like; NF1: Neutrino Oscillations
NF5: Neutrino properties; IF2: Photon Detectors; IF8: Noble Elements

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Abstract:

New computing paradigms featuring massively parallel hardware and dedicated accelerators can potentially reduce the time to discovery for HEP experiments. Several noble liquid experiments (DarkSide-20k [1], DUNE [2], LZ [3], nEXO [4], PandaX-4T [5], XENON-nT [6]) will come online in the next few years and run their simulation and reconstruction codes on novel supercomputing architectures. These experiments present a common computational challenge: identify a handful of possible "signal" events from several petabytes of background data. For this reason, the accuracy and speed of simulations is vital to the success of these experiments. In this letter we propose a trailblazing approach to the software needs of upcoming experiments, combining the use of standard HEP simulation frameworks, with novel Monte-Carlo solutions optimized for supercomputers at the exascale.

Introduction: Traditional computing in HEP is based on the many-cores approach and parallelizable algorithms, which are sequential and follow procedural templates. This is particularly suited for local, CPU-based computing clusters. The use of dedicated accelerators (GPUs, TPUs, FPGAs), requiring substantial redesign of simulation and reconstruction algorithms, is not largely adopted yet, but is expected to increase in the next decade.

The goal of this project is to develop a unique and innovative structure of detector simulation libraries specific to the most computationally challenging aspects across the majority of Noble Liquid experiments, such as the ray-tracing of optical photons. It is our goal to develop a system that can leverage the latest hardware capabilities. Graphical and Tensor Processing Units (GPUs and TPUs) will be used to reduce the required computation times to a fraction of what is needed today, without losing physics precision. Experiments will effectively increase their discovery potential thanks to increased statistics simulations. In addition, the validation of simulation software represents an interesting challenge that would allow experiments to reduce the risk of introducing bugs that would negatively impact the performances and the physics modeling. It is our goal to develop a system allowing us to test the code quality as long as the physics using continuous integration. Finally, the portability of the software is very important in large collaboration with many available data centers. We are aiming to develop a workflow that will be able to run simulations on any data center by using container technology and software distribution services.

Parallelization and Accelerators: In order to cope with the changes in hardware and computing expected in the next decade, we need to review some of the HEP computing paradigms we have used successfully in the field. This shift originates from the end of single-core scaling, which appeared in new generations of CPUs around 2005. Power consumption considerations have stalled the increase in clock frequency of general-purpose CPUs [7]. While the clock-speed does not increase anymore, the number of transistors continues to increase according to Moore's law. The increasing number of transistors has allowed for the introduction of more parallelism in the microarchitecture: larger number of cores and wider registers. The introduction of massively parallel accelerators (GPUs, TPUs, FPGAs) for general purpose computing, has further strengthened this hardware trend. These technologies require that the software used by specific experiments be substantially modified to take advantage of parallel capabilities.

Monte Carlo simulations are responsible for the largest fraction of the CPU hours spent by the typical HEP experiment; therefore, it is vital that this software be successfully modified to take advantage of larger parallelism. Previous experience [8, 9] has shown that significant speedup factors can be achieved by increasing parallelism. However, several experiments are still in a largely exploratory phase in which multiple technologies are being investigated. This exploratory phase can be facilitated by factorizing existing simulation frameworks into a set of independent kernels, which can function across a variety of hardware implementations. One would also want to develop a set of interface layers specific to the accelerator technology, with the goal to guarantee maximum flexibility.

One of the most time-consuming aspects of detector simulations (especially for noble liquid experiments) is the precise tracking of optical photons. This problem has some features that makes it the perfect candidate to explore their acceleration with the use of co-processors, specifically the tracking of many identical entities for a large number of steps, which makes them ideal candidates for the use of a ray-tracing algorithm. The combination of the Noble Element Simulation Technique (NEST) [10] software with existing GPU-based libraries for ray-tracing (such as NVIDIA OptiX) allows the straightforward exploitation of state-of-the-art technology in a mixed architecture, along with the most up-to-date physics model. The open-source Opticks package developed for the JUNO experiment, provides an integration to the NVIDIA OptiX library, and has produced a reduction in computation time of over a factor of 100 [11]. An extension of the Opticks model to a general set of parallelizable problems will serve as a starting point for our project. Experiments will effectively increase their discovery potential thanks to faster simulations.

Code and Physics Validation: An important challenge for Monte-Carlo software development in a collaboration is to guarantee the integrity of the simulation results during development. This can be done by adding validation procedures to the Continuous Integration (CI). We can distinguish two kinds of validation with different targets:

- **Code Validation:** code quality and reproducibility can be used by profiling CPU and memory usage, and by running unit tests. Code profiling allows for detecting inefficiencies and memory leaks before deployment. Unit tests are designed to inspect specific code components to track any differences in algorithm behavior. The combination of profiling and unit tests allows one to verify that code integrity is not altered by the addition of new features. Automated code validation can be performed within the CI, leveraging the facilities offered by commercial code repositories such as GitLab or GitHub.
- **Physics Validation:** the integrity and accuracy of physics modeling can be verified by automatically comparing the simulation output to a set of reference histograms. This validation stage can require chaining different software packages, and therefore relies on the ability to exchange input and output features between different repositories. Such validations can be very CPU-intensive and usually require linking the CI infrastructure with runners hosted at a data center.

Experiments will highly benefit from automatic tests of their simulation codes. A systematic battery of tests can reduce the risk of introducing bugs that can potentially impact performance and physics.

Simulation workflow portability: Data access across a large collaboration requires supporting a variety of hardware implementations, operating systems, and queue managers. Simulation workflow portability is crucial to exploit any and all available resources. This problem can be factorized into two main components:

- **Environment Portability:** environment portability is crucial to overcome the complexity of supporting different data centers. Environment unification can be accomplished by exploiting container technology, which allows running applications within containers that are isolated from their underlying implementation and carry their own OS, environment, and libraries. In addition, the deployment of containers across multiple data centers can be achieved by using a third-party repository such as Portus [12] or DockerHub [13]. Container technology raises a few issues concerning security and compatibility with HPC clusters, which are partially solved by Shifter [14] and Singularity [15].
- **Software Accessibility:** The accessibility of simulation frameworks and their dependencies can be addressed by using a software distribution service such as CVMFS [16]. Coupled with Continuous Deployment (CD), it allows for the automatic deployment of software binaries that will be accessible to any user.

This style of workflow, which combines containers and CVMFS, has been tested on HPC clusters across a variety of supercomputing centers in the USA, demonstrating its suitability for massive Monte-Carlo production. By adopting this workflow, experiments will effectively get access to more computing resources and drastically simplify user support. Given the increasing popularity of massively parallel accelerators, we will need to ensure compatibility with GPUs and TPUs for the next generation of container technology.

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