NUCLEAR PHYSICS

LatticeQCD: Exascale Lattice Gauge Theory Opportunities and Requirements for Nuclear and High-Energy Physics

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Strong interactions between quarks and gluons represent 99% of the mass in the visible universe. Understanding these interactions and the phenomena that result from them is the central goal of nuclear physics. Over the past three decades, Quantum Chromodynamics (QCD) computations have been a driver of, and benefited from, the spectacular advances in HPC. Computing at the exascale is essential to reach two decadal challenges of central importance to nuclear and high-energy physics. The LatticeQCD project is implementing scalable QCD algorithms to realistically simulate the atomic nucleus to reveal a deeper understanding of the fundamental organization of matter at the subatomic level. These calculations will help us understand the fundamental interactions and nature of matter beyond "elementary" particles.

Atomic nuclei and most particles produced by high-energy accelerators are tightly bound composites of quarks and gluons. The fundamental interaction of these quarks and gluons is known as the strong (nuclear) force—one of the four fundamental forces of nature (i.e., strong, weak, electromagnetic, gravity). These nuclear interactions are explained with mathematical precision by QCD, and HPC is required to predict the consequences of this underlying theory. The properties of the resulting bound states and the nature of their strong, highly nonlinear interactions are the central focus of nuclear physics and an important context in which high-energy physics research must be conducted.

The couplings between the quarks and the W, Z, and Higgs bosons lie at the heart of the Standard Model of particle physics and can be studied, often with exquisite precision, by measuring the properties of the bound states formed from these quarks and gluons. Recent simulations of QCD on the previous generation of massively parallel computers have enabled a comparably precise theoretical understanding of these fundamental interactions of quarks and gluons.

Advances in exascale capability expected over the next decade offer to extend these exciting opportunities to even more groundbreaking discoveries in high-energy and nuclear physics. Exascale computing has the potential to realistically both simulate the atomic nucleus and discover the first harbingers of new laws of nature, revealing a deeper theory that underlies the present "elementary" particles. These possibilities can be achieved only if new and impending advances in computer science can be harnessed to provide a software framework that allows lattice QCD code to efficiently exploit exascale architectures, enabling application scientists to create and refine that code as new challenges and ideas emerge.

The challenge problem consists of six computations representative of three of the common fermion actions in current use by the worldwide lattice-QCD community. Each of these actions has specific advantages for different physical problems in nuclear and high-energy physics.

HISQ: The benchmark problem measures two rates—first, the rate of generating a new gauge configuration using a molecular dynamics (MD) algorithm for a Markov chain Monte Carlo, and second, the rate of making a representative set of "measurements" on the gauge–field configuration. Both steps are required for any campaign to calculate quantities of scientific importance.

DWF: As with the HISQ action, two figures of merit have been adopted for the DWF component of the application. The first measures the rate at which a current state-of-the-art gauge–field ensemble can be generated, and the second calculates a suite of observables using this ensemble.

Wilson-clover: The Clover benchmark has two components. The first is the rate at which dynamical Clover fermion lattices can be generated using a molecular dynamics (MD) algorithm. Several solutions of the Dirac equation are computed and contracted to construct observables as part of the second component of the benchmark.

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Progress to date

- Incorporated new Wilson-clover adaptive multigrid solver and force gradient integrator and achieved 100× reduction in GPU hours to generate gauge configurations on Summit over Titan.
- Implemented graph algorithms to perform Wick contractions in light nuclear matrix elements that yield greater than a 4× reduction in time and 10× reduction in memory.
- Implemented a new, fast eigensolver that combines Chebyschev preconditional with Block Lanczos and split grids that achieves a 3× speedup over previously used, implicitly restarted Lanczos iteration.

LatticeQCD's development of scalable algorithms for exascale systems will enable detailed physics investigations at the subatomic level that will lead to fundamental advances in our knowledge of the interactions of matter.