Performance, Portability, and Preservability for Strong Dynamics at the Exascale
Lattice Strong Dynamics (LSD) Collaboration
California Lattice (CalLat) Collaboration

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Introduction: Strongly interacting quantum field theories present a unique challenge to physicists due to our inability to use perturbation theory to explore regions of interest. The standard, alternative approach used to investigate these theories is to discretise, then simulate them on a computer using importance sampling and Markov Chain dynamics. The prototypical example of such a theory is Quantum Chromo-Dynamics (QCD) and its discrete analogue Lattice Quantum Chromo-Dynamics (LQCD). In addition, Composite Higgs [1, 2] and Composite Dark Matter[3, 4] models are strongly interacting fields theories. All of them require large computational effort to extract data, which has led to a proliferation of both open source and privately maintained code libraries, spanning a wide spectrum of available architectures and programming languages.

Strong dynamics in particle physics: CalLat and LSD rely heavily on code libraries to implement their respective research programs. CalLat uses LQCD as tool for computing nucleon scattering amplitudes[5], and has plans to measure more fundamental quantities of interest to Beyond Standard Model (BSM) physics (such as the proton radius) in the near future. This is the typical motivation for LQCD: to provide input for nuclear physics and to constrain searches for BSM physics by providing accurate data for QCD background. LSD uses code to investigate theories with a many degenerate fermion flavors for Composite Higgs models, and also to simulate SU(4) gauge theories which provide the basis for Stealth Dark Matter models. It is critical to note that none of these pursuits would be possible without the use of large scale computing resources, and good software to run on them. The majority of both CalLat's and LSD's code so far has been based largely on the CHROMA[6] library. However, as of mid 2020,

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CHROMA will no longer be maintained as an Exascale library for LQCD. This poses a severe problem for both collaborations as they both need a stable, performant code base for use in the Exascale era.

The task of continually upgrading LQCD software to take advantage of architectural developments can present a significant time sink for physics researchers. Furthermore, porting code written specifically for one architecture to work on another can be full time task, with no guarantee of performance. With three different types of architecture to cater for, and a variety of physics models to simulate, the problem of maintaining a competitive research program centered on strongly interacting theories would seem to dominated not by physics, but software development. This obstacle would be overcome if we could express all of these strongly interacting theories using a single code library that worked on all architectures. Such a library in the making.

The QUDA LQCD library: QUDA is written specifically for NVIDIA GPU architecture and is maintained by a team of software developers and engineers at NVIDIA. This is in addition to the many contributions coming from computational physicists in academia and national labs. As such it is at the cutting edge of High Performance Computing (HPC)[8–11] in terms of raw computational performance and algorithmic development. The advent of new Exascale architectures has motivated the QUDA community to coordinate with NVIDIA, AMD, and Intel developers, as well as national laboratory scientists from LLNL, ORNL, and ANL, to ensure that QUDA will be available and performant on all three of the proposed Exascale architectures.

Concurrent to this, key members of both CalLat and LSD will be able to conglomerate large portions of their respective physics code to utilize QUDA as their new base library with minimal overhead given to software development. For example, CalLat's nucleon scattering code (currently spread across three libraries and several years in the making) can be rewritten using QUDA syntax in a matter of months. With all the relevant code in one place, LSD can use it (along with some straightforward augmentations to QUDA) to create a code base that will simulate their Stealth Dark Matter program in its entirety. Furthermore, by porting the code to QUDA, both calculations would enjoy some 40-50x speed-up factors over the CHROMA based code via the use of accelerators, regardless of the manufacturer.

Summary: Strongly interacting quantum field theories provide a valuable insight into both Standard Model, and Beyond Standard model particle physics. By their non-perturbative nature, the only way we can extract information from them is via computationally intensive simulations. It is therefore vital to the particle physics community that research programs in this area maintain a presence in the HPC field with adequate computing allocations and efficient code libraries. QUDA, with its active community in industry, academia, and national laboratories is in an excellent position to cater for those needs.

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