Chiral Lattice Fermions and the Computational Frontier

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1 Introduction

Lattice gauge theory is a systematically improvable theoretical tool for direct numerical evaluation of the Feynman path integral for Quantum Chromodynamics (QCD) in its nonlinear hadronic regime. Various discretisation approaches may be taken, which respect or break continuum flavour and chiral symmetries to various degrees. The authors of this letter of interest are members of the RBC-UKQCD collaboration. We have performed a series of calculations using pre-exascale computers with an approach that preserves continuum chiral and flavour symmetries. These have enabled calculations on grids up to $96^3 \times 192$ and inverse lattice spacing from $a^{-1} = 1.7$ to $a^{-1} = 2.7$ GeV with up, down and strange quark masses set to their physical values.

These calculations have represented significant theoretical input to experimental searches in flavor physics, and particularly in kaon physics[1–18]. Leptonic decay amplitudes and semileptonic form factors involve only the vector or axial current in isolation, however a much broader range of hadronic matrix elements are important to flavor physics and are best addressed using a formulation with chiral symmetry. This avoids unphysical lattice mixing between left and right handed currents. In neutral meson mixing, both within and beyond the standard model the chirally structured operator bases must be treated. Our calculations have contributed for example to the ϵ_K band in the unitarity triangle, and the two pion decay amplitudes of the kaon. This has explained QCD as the origin of the $\Delta I = 1/2$ rule, and combined with existing experimental results providing a wholly new constraint on the vertex of the unitarity triangle in the rho-eta plane. However, the error on these calculations must be improved by up to an order of magnitude to match current experimental precision.

2 2+1+1f chiral fermion simulations

Rare kaon decay amplitudes, the neutral kaon mass difference, and long distance contributions to ϵ_K are important theoretical inputs to intensity frontier experiments [19, 20]. These calculations receive contributions from internal charm loops which must be handled accurately and with the same fermion disretisation to ensure GIM cancellation occurs in our calculation as we take the continuum limit using multiple lattice spacings. Precison calculations incluing QED [21] enter tests of CKM unitarity and for the hadronic contributions to the anomalous magnetic moment of the muon [22].

The rich range of multi-hadron final state physics and complicated four-point functions discussed above in the kaon sector will be important to extend to the D and B meson systems [23]. Many daunting theoretical challenges that arise as we begin to treat many-particle states and physics farther into the Minkowski region. Examples may include $D \to \pi\pi$ or $D \to KK$ decays, or $D - \overline{D}$ mixing analogous to our recent kaon work[1, 5, 8, 11, 12]. For this ambitious programme to be viable, a significant computational challenge exists, in order to enable a series of calculations on ensembles from $a^{-1} = 3 - 5$GeV, and lattice volumes from $96^3 \times 192$ to $192^3 \times 384$. The challenges exist on multiple fronts: intellectual in developing algorithms that evade critical slowing down, software engineering to develop well performing and portable code on an evolving range of supercomputers and programming modes, and technical to remain engaged with the DOE HPC community as systems are planned and developed. USQCD has had senior-staff, post-doctoral researcher, post-graduate students funded under the Exascale Computing Project (ECP) and the SciDAC programme. The ECP project includes algorithmic programmes in “Critical Slowing Down”, and “multilevel solvers”[24–26]. It has also funded the development of high performance software portable to Exascale hardware[27, 28]. It is important that these gains continue to be realised, with continued funding throughout the Snowmass period, or an opportunity comparable to the available gains in computer performance will be lost. USQCD has written a computing whitepaper in 2019[26].

3 Algorithms

The development of numerical algorithms is an intellectual activity that spans physics, mathematics, and computer science, with many core algorithms such as Markov Chain Monte Carlo (MCMC) and Metropolis-Hastings algorithms emerging from theoretical physics. The Hybrid/Hamiltonian Monte Carlo algorithm was developed in Lattice Gauge theory and is one of several work horse algorithms used in training machine learning. Over the almost 40 year history of active lattice gauge theory calculations, the annual improvement from algorithm development has been broadly similar to the gain from Moore's law. The proposed simulations will require new algorithms with critical slowing down of MCMC auto-correlation times. Multi-level Dirac solvers are required to address the growing condition number of our PDE's.

4 Joint Lab-University Tenure Track Appointments

We seek to foster the continued development of intellectual leaders in computational quantum field theory. This is now done very well at the Labs with a large fraction of the leading personnel located there. The health of the field requires a similar cohort of individuals at the best universities, reflecting the intellectual vigor and potential of this area to contribute to DOE scientific goals. The creation of such positions can be stimulated by DOE-funded joint, five year, tenure-track appointments. Theoretical particle physics is one of the last area of physics to recognize the importance of computation in forefront research and continued effort is urgently required to overcome this historical bias, and create a vibrant pool of skilled young faculty, and around them their PhD students and research groups.

5 Lattice Gauge Theory Lab Software Positions

It is important that flexible high performance software is developed for a diverse range of architectures that tracks the DOE computing programme. The life cycle of scientific code is at least 10 years, and the health of a community depends on large code bases (up to 200,000 lines of code) which do not have a secure model for development and support which places investments at risk. Just as the large experiments require talented permanent staff at the Labs to engineer experiments and manage sophisticated long-term software systems, cost- and people-effective lattice QCD desperately requires that career paths be created to retain some of the most talented experts in software and algorithms.

These will address HPC architectures as they emerge under the Computational Frontier. We aim to develop performance portable high level data parallel code, with a write once and run anywhere approach that many domain scientists can modify effectively. Our aim is to abstract the parallelism through high level internal interfaces, while being able to target both CPU thread and vector parallelism and simultaneously multiple (GPU and FPGA) accelerators with API's such as OpenMP 5.0, OneAPI, CUDA, and HIP being compile time options. Architectural and programming model diversity has been growing rapidly and is expected to continue; this effort must track the evolution of computing.

The work is highly skilled. A key element of managing the science programme is the early engagement with DOE HPC laboratory sites during the development, and years prior to installation, of major new facilities. The lead time for porting to new architectures lies in the region of multiple years, and early engagement is required to ensure timely scientific exploitation. Our collaboration members have in the past developed bespoke academic Gordon Bell Prize winning supercomputers, worked with IBM on the design of the BlueGene/Q computer, participated fully in the Exascale Computing Project and Pathforward programme, and also worked with Intel on codesign, coauthoring patents with both IBM and Intel. A number of our gifted students and post-doctoral researchers have joined IBM, Intel and Nvidia.

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