National Computational Infrastructure for Lattice Gauge Theory
SciDAC-2 Extension Closeout Report
Boston University

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Boston University SciDAC-2 Participation

At Boston University, Richard Brower serves as the Chair for the Software Coordinating Committee and as a member of the USQCD Executive Committee. For the 6 years of SciDAC-2 grant, a major activity for Brower has been monitoring the work of the ten universities and three national laboratories that are funded to carry out work under this grant. The Software Committee with all SciDAC developers has weekly teleconferences and annual face to face software workshops to plan and track the projects. In addition reports on the software status are given during our annual USQCD "All Hands Meetings" and at many lattice workshop such a the "Lattice Meets Experimentalist" series covering the 4 major topical areas: the Intensity Frontier, the Energy Frontier, Nuclear Structure and High Temperature QCD.

All Software is disctribute in githup repositories. Access to these are provided at USQCD Software Release page http://usqcd-software.github.io/

Under SciDAC-2, Boston University has focused on three software projects: (i) the development of the high performance GPU software library called QUDA [1] (or QCD in CUDA) for NVIDIA accelerated systems [2, 3, 4], (ii) the multi-scale algorithms for lattice Dirac solvers [5, 6] and (iii) the extension of lattice field theory method [7] to address Beyond the Standard Model (BSM) strong dynamics that may underly the Higgs phenomena under active experimental investigation at the Large Hadron Collider. While some initial steps were largely a result of efforts at Boston University, these activities have expanded greatly under SciDAC-2, so the role of Boston University increasingly includes substantial effort in co-ordinating these projects among participating SciDAC-2 institutions.

Under joint funding from SciDAC-2 and the National Science Foundation, Boston University has been fortunate to have a series of remarkably talented postdoctoral fellows: James Osborn (now the Computational Scientist at the ALCF and a Fellow of the Computation Institute at The University of Chicago), Michael A. Clark (visitor at Harvard-Smithsonian Center for Astrophysics and now full time software engineer at NVIDIA continuing with GPU lattice field theory software), Ron Babich (visitor at the Pittsburgh Super Computer Center and also full time at NVIDIA with continuing collaboration on lattice field theory software), Saul Cohen (now at University of Washington and INT in Seattle). The current Boston University postdoctoral fellows in lattice field theory are Michael Cheng and Oliver Witzel contributing to GPU, multigrid and BMS software development.

QUDA: GPU software development In the summer of 2008, Rebbi and Brower enlisted a graduate student in statistical physics, Kipton Barros, to explore the GPU architecture for lattice field theory. In collaboration with our postdoctoral fellow, Mike Clark, he obtained a performance in excess of 100 Gigaflops on a single 240 core Nvidia GTX280 GPU. Specifically, at Boston University methods developed by Mike Clark and Ron Babich using multiple precision solvers [3] and a variety of tricks to reduce bandwidth to the device memory on the GPU card have demonstrated an additional factor of two to three in performance for the Wilson inverter. The result has been the development of a software library, QUDA [9] for QCD Dirac solvers on GPUs, which has enabled substantial new analysis capability on the ARRA GPU cluster funding at Jefferson Laboratory and the LQCD funded GPU cluster at Fermi Laboratory. The CUDA coding effort has expanded to include work at Jefferson Laboratory by Balint Joo, Jie Chen and Robert Edwards focused on integration into production code and extensions to multi-GPU codes, work by Joel Giedt at Rensselaer focused on the Domain Wall operator, and work by Steve Gottlieb and Guochun Shi at NCSA and Carleton DeTar and Justin Foley at Utah on the MILC staggered code [8]. (See full QUDA team at *https://github.com/lattice/quda*.) The goal is to develop a new GPU implementation of the QCD API, which promises to reduce the cost/flop substantially both for analysis and lattice generation code [9].

Multigrid Research Brower, Rebbi and David Keyes have led an effort in collaboration with TOPS applied mathematicians to employ multigrid methods for lattice QCD. After nearly four years of effort this team, which includes Mike Clark, Ron Babich and applied mathematicians James Brannick (Penn State), Steve McCormick (Colorado University) and others, constructed the first successful multi-grid lattice Dirac inverter [5, 6, 10]. The inverter for Wilson Fermion propagators demonstrates uniform convergence in the chiral limit, and already shows a factor of ten to twenty improvement in execution time on large state of the art lattices. James Osborn and Andrew Pochinsky had designed and implemented an extension to the QDP API to accommodate multiple lattices, and, in collaboration with Clark and Saul Cohen, implemented a Level 3 multigrid inverter for the Wilson-clover operator in production code. Saul Cohen, who joined the BU group in the summer of 2009, has formulated the first multigrid inverter for domain wall fermions [11]. Recently simple version of Schwarz domain decomposition (or block Jacobi) preconditioner has been applied to communication mitigation for the multi-GPU solver for Wilson and Staggered lattice fermion allow for good strong scaling to 256 GPUs [4]. This is crucial step in the extension software for full gauge generation on capability platforms for the Titan and Blue Waters 2 hybrid systems.

Beyond the Standard Model (BSM) at the Energy Frontier In the last few years the research focus at Boston University has made a transition from lattice QCD to the study of new strongly interacting gauge theories for BSM studies at the TeV energy scale. Nearly five years ago Appelquist, Brower, Fleming, Osborn, Rebbi and Vranas have formed the Lattice Strong Dynamics collaboration (`http://www.yale.edu/LSD`) aimed at exploring non-perturbative scenarios beyond QCD, which may well be part of the new physics discovered at the LHC. A large range of options are described in an early white paper [12] in 2007 and an initial workshop on *Lattice Gauge Theory for LHC Physics* was held at Livermore May 2-3, 2008, followed by a second workshop at Boston University Nov. 6-7, 2009 and the most recent *Lattice Meets Experiment 2010: Beyond the Standard Model* at FNAL on October 14-15, 2011. To mitigate this risk and minimize software development time, initial projects were chosen in areas close to QCD itself [13]. Boston University's focus has been on the S-parameter [14], which places one of the most stringent constraints on technicolor models and problem of disconnected diagrams, specifically computing the $\bar{s}s$ condensate in the proton needed to estimate the cross section for the direct detection of SUSY neutralino as a possible candidate for dark matter. Both of these project are limited by the cost of the domain wall Dirac solvers. Collaboration with Andrew Pochinsky at MIT on a fast code [15] for the Möbius domain wall algorithm [16, 17, 18, 19] and the multi-GPU implementation on QUDA are two steps to address this problem. In addition in collaboration with James Osborn a new Framework for Unified Evolution of Lattices (FUEL), provides a tool that will enable the rapid development and testing of new algorithms for configuration generation based on top level control using the scripting language Lua [20] .

References

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