# s and Software for Lattice Field Theory in the Coming US Program in High Energy Physics: Searchin
# National Computational Infrastructure for Lattice Gauge Theory

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## I. Background

We request a one year extension of the SciDAC-2 Project *The Secret Life of Quarks: National Computational Infrastructure for Lattice Gauge Theory*, from March 15, 2011 through March 14, 2012. The objective of this project is to construct the software needed to study quantum chromodynamics (QCD), the theory of the strong interactions of sub-atomic physics, and other strongly coupled gauge field theories anticipated to be of importance in the energy regime made accessible by the Large Hadron Collider (LHC). It builds upon the successful efforts of the SciDAC-1 project *National Computational Infrastructure for Lattice Gauge Theory*, in which a QCD Applications Programming Interface (QCD API) was developed that enables lattice gauge theorists to make effective use of a wide variety of massively parallel computers. This project serves the entire USQCD Collaboration, which consists of nearly all the high energy and nuclear physicists in the United States engaged in the numerical study of QCD and related strongly interacting quantum field theories. All software developed in it is publicly available, and can be downloaded from a link on the USQCD Collaboration web site, or directly from the URL usqcd.jlab.org/usqcd-software.

This extension covers a critical period for our research. During it we expect, for the first time, to have access to leadership class computers capable of sustaining one or more petaflop/s on our production codes (BlueGene/Q, Blue Waters, Cray XT6, ...). At the same time, the capabilities of the dedicated clusters we are building at the Fermi National Accelerator Laboratory (FNAL) and the Thomas Jefferson National Accelerator Facility (JLab) are undergoing rapid evolution with the inclusion of multi-core CPUs and multiple Graphics Processing Units (GPUs). The optimization of codes for both types of machines will be be a major component of our work under this proposal. It will require that our software integrate on node threads and inter node message passing. It will also require that new algorithms be developed to accelerate convergence in the presence of multiple scales in the underlying physics, and to map efficiently onto the heterogeneity of the architectures. As is discussed below, we have already made a substantial start. We are in the process of porting codes to Blue Waters and the BlueGene/Q; we are rapidly developing a new software library (QUDA) to efficiently map QCD onto multi-GPU clusters using Nvidia's CUDA language and development environment; and we are actively pursuing the development of new algorithms with applied mathematicians and computer scientists. The extension would be a major step in insuring that our codes are ready when the next generation of hardware becomes available.

# 1 Boston University Subproject

As software coordinator and Chair of the Software Coordinating Committee, Richard Brower guides the overall project. In addition Brower and Rebbi are leading an effort to exploit multi-scale algorithms and map then on to the heterogeneous environment of clusters with GPU accelerators. This is not only yielding immediate dividends in reducing the cost of the analysis of lattice gauge theory configurations, it is a natural environment for experimenting with algorithm and software design in anticipation of heterogeneous computing at the exascale.

The Boston University group, in collaboration applied mathematicians in the SciDAC TOPS project, is developing multigrid methods for lattice QCD. After nearly four years of effort, this team, which includes Mike Clark a postdoctoral fellow at BU who has recently moved to Harvard, Ron Babich, the current Boston University SciDAC postdoc, and applied mathematicians James Brannick (Penn State) Steve McCormick (Colorado University) and others, constructed the first successful multi-grid lattice Dirac inverter. James Osborn now at Argonne National Laboratory and Andrew Pochinsky at MIT have designed, and made a first implemented of, an extension to the QDP API to accommodate multiple lattices, providing a Level 3 multigrid inverter for the Wilson-clover operator, which is now being used in production code. At the lightest quark masses,the multigrid inverter out performs the best Krylov solver by a factor of 10-20. Saul Cohen, who joined the BU group in the summer of 2009, is doing research on a multigrid inverter for domain wall fermions.

## 2 Results of BU Subproject

The Boston University component has focussed on the algorithmic development of new Multigrid solver for the critical kernel for the Dirac propagators that dominated the both simulation require for lattice ensemble and the analysis of physical correlation functions.

Progress on this has meet the above objects, even exceeding them a bit. The result is the beginning if multi-scale lattice QCD applicable to future Exascale hardware and the development of the QUDA software for NVIDIA GPUs to give near optimal performance. As we approach exascale hardware and computation at that scale this provides the infrastructure for further advances.

Brower is also collaborates with lattice field theory for Beyond the Standard Model so that this advance can be incorporated into application code beyond the QCD theory.

### III. Recent Software Publications and Presentations.

- “Adaptive multigrid algorithm for the lattice Wilson-Dirac operator” R. Babich, J. Brannick, R. C. Brower, M. A. Clark, T. Manteuffel, S. McCormick, J. C. Osborn, and C. Rebbi, arXiv:1005.3043v2 [hep-lat] (2010).
- “Hardware developments for lattice QCD”, Ronald Babich, lectures given at the STRONGnet Conference on Hadron Physics in Lattice QCD, Paphos, Cyprus (2010)
- ”Parallelizing the QUDA Library for Multi-GPU Calculations In Lattice Quantum Chromodynamics” R. Babich, M. A. Clark, B. Joo, to be published in the proceedings of Supercomputing 2010, New Orleans (2010)
- ”Hadronic Physics using Lattice QCD and GPUs” B. Joo, R. Babich, R. C. Brower, M. A . Clark, J. Chen, J. Dudek, R. G. Edwards, M. J. Peardon, C. Rebbi, D. G. Richards, G. Shi, C. Thomas, W. Watson, USQCD Collaboration and Hadron Spectrum Collaboration, SciDAC 2010, Chattanooga, TN (2010).
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- “Multi-GPU Implementation of MILC”, Guochun Shi, Steven Gottlieb, Aaron Torok and Volodymyr Kindratenko, Supercomputing ’10, New Orleans, LA (2010)
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- “QUDA Programming for Staggered Quarks”, Steven Gottlieb, Guochun Shi, Aaron Torok and Volodymyr Kindratenko, Lattice 2010, Villasimius, Sardinia, Italy (2010).
- “Analysis and Visulizaiton tools for Lattice QCD”, M. Di Pierro and Y. Zhong, PoS **LAT2009**, 038 (2009).
- “Lattice QCD Software”, J. Osborn and M. Clark, tutorials given at the KITPC Lattice QCD Workshop, Beijing, China (2009).
- “Diagnosing performance bottlenecks in emerging petascale applications”, Nathan R. Tallent, John M. Mellor-Crummey, Laksono Adhianto, Michael W. Fagan and Mark Krentel, Proc. of Supercomputing ’09, 51 (2009).
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- “HISQ action in dynamical simulations”, S. Bazavov (MILC Collaboration), PoS **LATTICE2008**, 033 (2008)
- “Gauge Force Speedup”, S. Gottlieb, Pathways to Blue Waters Workshop, NCSA, Urbana, IL (2008).
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