**National Computational Infrastructure for Lattice Gauge Theory**
**SciDAC-2 Closeout Report**
**Indiana University Component**

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# 1 Introduction

The overall structure and accomplishments of this project are described in the project-wide final report, while this report identifies the part done by the three MILC collaboration institutions, the University of Arizona, Indiana University, and the University of Utah.

The MILC collaboration consists of approximately ten senior and seven junior members at ten institutions, mostly in the USA. [1] Almost all of its scientific work is done with the MILC code, an integrated package of some 200,000 lines of scientific application codes and a library of generic supporting codes. It has been in use worldwide and freely available to the public since the early 1990's, and has grown and evolved over the years to meet our evolving physics goals and rapid changes in computer architecture and capability.

Under SciDAC-2 three MILC-collaboration institutions, the University of Arizona, Indiana University, and the University of Utah, were responsible for a large number of important revisions to the code that exploit the evolving SciDAC code suite. These institutions have also contributed important new SciDAC modules. These changes have made the MILC code much more flexible,

[1] A. Bazavov, R.S. Van de Water (Brookhaven), C. Bernard, M. Lightman (Washington U.), C. DeTar, J. Foley, L. Levkova, M. Oktay (U. Utah), J. Kim, D. Toussaint (U. Arizona), S. Gottlieb, R. Zhou (Indiana U.), U.M. Heller (APS), J.E. Hetrick (U. Pacific), J. Laiho (Glasgow U.), J. Osborn (Argonne), R.L. Sugar (UC, Santa Barbara)

they have allowed us to keep abreast of our changing scientific objectives, and, consequently, they have enabled rapid scientific progress.

Over the six years of the SciDAC-2 grant, the MILC institutions received support for approximately 1/2 postdoctoral research associate each. We list accomplishments and publications resulting from this support:

## 1.1 Arizona

Work at the University of Arizona was done by postdoctoral researchers Dru Renner (–Sep. 2007), Alexei Bazavov (Sep. 2007–Aug. 2010) and Jongjeong Kim (Nov. 2010–present), under the supervision of the PI, Doug Toussaint.

**Operation of the QCDOC** During the first part of the proposal period the University of Arizona was responsible for the implementation and operation of the MILC code on the QCDOC, the special purpose machine at Brookhaven National Laboratory (BNL). This included testing the codes and making the necessary modifications to get them to run on the QCDOC, and developing and maintaining the scripts needed at the top level to use the QCD codes in projects. This also required arranging for the movement of lattices and output files to and from BNL. The QCDOC was used successfully in generating many of the lattice ensembles made with the Asqtad fermion action, and these ensembles were later used by many lattice projects in both high energy and nuclear physics [1].

**Implementation of the highly improved staggered quark (HISQ) algorithm** Following the retirement of the QCDOC, the postdocs at the University of Arizona concentrated on the development of the "Highly Improved Staggered Quark" (HISQ) action introduced by the HPQCD collaboration. Specifically, they completed the programming of the code for the "fermion force", which is necessary to generate ensembles with dynamical HISQ quarks, and for the projection of intermediate matrices onto unitary matrices. These routines were integrated into the MILC code suite, making possible the generation of large lattice ensembles using this action.

This algorithm has become a mainstay of our current physics efforts. It is yielding greatly improved control of discretization errors, which, in turn, is producing higher precision results [2, 3, 4, 5, 6].

**Porting the HISQ algorithm into SciDAC Level 3** Optimized QOP (Level 3) versions of the HISQ routines were developed, and these have now been placed in the production environments for this project. This step is essential for taking advantage of architecture-specific optimizations in the SciDAC code suite [7].

**Production of gauge field configurations with HISQ** These gauge configurations are the basis for many physics analyses, including spectroscopy, decay constants, and a wide variety of weak matrix elements [1]. We publish worldwide the gauge field configurations we produce [8].

## 1.2 Indiana University

Work at Indiana University was done by postdoctoral researchers Subhasish Basak (Jan. 2007–Sep. 2008) and Aaron Torok (Sep. 2009–June 2011) under the supervision of the PI, Steven Gottlieb.

**Single-GPU code for asqtad lattice generation** This work, done in collaboration with Guochun Shi of NCSA developed all the major components for asqtad lattice generation. The code was incorporated into the SciDAC QUDA library. [9, 10]. This is a milestone on the path to multi-GPU capability.

**Multi-GPU gauge-force and fat-Naik solver** This work, again with G. Shi, developed and benchmarked an improved gauge-force routine and a fat-Naik solver for multi-GPU operation [11, 12].

**Integration of the MILC code with the SciDAC QUDA multi-GPU fat-Naik solver** This capability gives our code a factor of four or more speedup for some of our analysis projects. [11, 12, 13]. The code has been put into production measuring electromagnetic splittings of hadron masses [14].

**Development of code for heavy baryon spectroscopy** This new MILC code module made it possible to do the spectroscopy of baryons containing a charm or bottom quark [15, 16].

## 1.3 University of Utah

Work at the University of Utah was done by postdoctoral researchers Tommy Burch (Oct. 2007–Sep. 2008), Bugra Oktay (Sep. 2008–Feb. 2011), Ludmila Levkova (Aug. 2011) and Justin Foley (Oct. 2010–present) under the supervision of the PI, Carleton DeTar.

**Two major releases of the MILC code suite** These revisions provide support for the HISQ algorithm, greatly expanded support for hadron interpolating source operators, the FFTW (Fourier transform) package, the PRIMME (eigenvalue) package, random color-wall sources, momentum twists, open-meson code for B Bbar mixing calculation, HISQ equation of state, etc. [17]. The new features of the code are yielding new physics results [18, 19, 20, 21, 22, 23, 24, 25, 26].

**A user manual for the MILC code suite** This 70-page user manual, developed and provided with the code release, describes how to build and operate the code [17].

**Development of QUDA GPU HISQ link-fattening and fermion force modules** These are the first steps toward developing the ability to do full HISQ hybrid molecular dynamics calculations on multiple GPU's.

**Testing the improved heavy-quark Oktay-Kronfeld action** This action is designed to do for heavy quarks what the asqtad and HISQ actions do for light quarks, namely reducing considerably the lattice discretization errors. Work is still under way [27].

# 2 Publications and conference proceedings resulting from this work

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