Boston University Project

Final Report for Award Number DOE DE-SC0008814
SciDAC-3: Searching for Physics Beyond the Standard Model:
Strongly-Coupled Field Theories at the Intensity and Energy Frontiers
Boston University Component
Report Date: Nov 8, 2016
Award Period: September 1, 2012- Aug 31, 2015

Lead Institution: Fermilab
Batavia IL 60510
This Institution: Boston University
Boston Principal Investigator: Prof. Richard C. Brower
Physics and ECE Departments, Boston University
Physics Research Building, Room 581
590 Commonwealth Ave. Boston, MA 02215
brower@bu.edu
617 353 6052
Office of Science Program Contact: Lali Chatterjee
High Energy Physics Program Manager: Glen Crawford

1 Project Report

This is a report on the Boston University component of the SciDAC project under the Project Director Paul Mackinzie at FNAL. Prof. Richard Brower is the co-Director for Computation, with overall responsibility for the software and algorithm work, providing direction and coherence to the work, and monitoring progress on all tasks. He coordinates work with other collaborators in USQCD, and our partners in the SciDAC FASTMath and SUPER Institutes and in the Emerging Applications Group at NVIDIA. He is the chair of Software Committee that has weekly teleconference to plan and track the projects and organizes the semi-annual face to face software workshops. Software for Multigrid algorithms [1, 2, 3] and GPU code optimization [4, 5], began at Boston University and continues as broad collaborative program under SciDAC-3. Two former BU SciDAC postdoctoral fellows, Mike Clark and Ron Babich continue to work on this as employees of NVIDIA.

The Boston University team under the direction of Prof. Claudio Rebbi and Prof. Richard Brower research focus in on the use of lattice gauge theory to investigate Higgs physics in the Energy Frontier [6, 7, 8, 11, 12] with the Lattice Strong Dynamics (LSD) collaborationhttp://www.yale.edu/LSD/. The goals are documented reports on the Lattice Gauge Theory at the Energy Frontier [13] and the Snowmas Report [14].

Prof Brower organized and chaired two SciDAC-3 workshops to monitor the progress toward these goals as well as the larger multi-Laboratory/University SciDAC software projects.

- Oct 18-19, 2013: USQCD SciDAC Software Workshop at FNAL
  On line status report: https://indico.fnal.gov
- April 17, 2014: USQCD SciDAC Software Workshop at Jlab
  On line status report: http://www.jlab.org/conferences/usqcd2014/program.html

All Software is distributed in github repositories. Access to these are provided at USQCD Software Release page http://usqcd-software.github.io/ The overall development of our software distribution and access to releases and documentation has been lead by Oliver Witzel the SciDAC supported postdoctoral fellow at Boston University.

Beyond the overall co-ordinating of these activity, several projects are the direct responsibility of the Boston University team. (see Sec. 2 below for the enumerated goals and milestones.) Briefly the status of these are as follows.

1. Developing multigrid software on GPUs : Mike Clark at NVIDIA and Michael Cheng at BU have extended the QUDA library (QCD in CUDA) for Nvidia GPUs to accommodate the Multigrid algorithm for Wilson-clover Dirac solver. A report on this milestone was presented by Mike Clark [10] on behalf of Brower and Cheng at the `31st International Symposium of Lattice Field Theory`, July 29 - Aug 3, 2013, Mainz, Germany. The software infrastructure is compliant with QCD SciDAC multi-GPU codes in QUDA targeted to the Titan. The multilevel framework is designed to accommodate other Dirac solvers in common use (staggered and Domain Wall) and to enable implementation of domain decomposition methods to mitigate data bottle necks antipated as architecture evolve to the Exascale. Performance of the first GPU implementation was presented at Jlab Workshop last month. The code is available at *https://github.com/lattice/quda*.

2. FASTmath HYPRE project: The HYPER/Qlua project is well underway. Rob Falgout, Christopher Schroeder and Andrew Pochinsky have completed an overall

design of a HYPRE/USQCD interface (HQL) and implementation. Rob has finished extending HYPRE to handle more than 3 dimensions and fully expects to finish implementing complex numbers on schedule. Chris and Rob are making progress on the implementation of the HQL interface. Rob and Andrew are proceeding with the HQL-Qlua interface. Andrew is finishing extending Qlua to handle data types and procedures required to support HQL. Brower visited the LLNL SUPER team with Andrew Polchinsky on March 8, 2013 to review the progress and plans.

3. Multigrid for Domain Wall and Staggered Fermions: Richard Brower, Andrew Pochinsky, Oliver Witzel have begun to develop the Domain Wall multigrid algorithm after a preliminary series of experiment by Saul Cohen [11], a former SciDAC postdoctoral fellow at Boston University who is since moved to the University of Washington. By using the Qlua system as a rapid prototyping and development environment, a first implementation of working Domain Wall multigrid algorithm can be tested at scale. In collaboration with a graduate student at Boston University, Evan Weinberg, the goal of this project is to begin to develop of the staggered multigrid solver QUDA frameworks.

3. FUEL framework for HMC multigrid: Brower worked closely with James Osborn and the new ANL SciDAC postdoctoral fellow, Meifeng Lin, to extend multigrid methods to HMC evolution of Wilson lattices on the leadership computers. This is very challenging project with great potential benefit to the generation of Wilson gauge configurations. The project uses the new framework FUEL (Framework for Unified Evolution of Lattices) created by James Osborn at Argonne Laboratory to accelerate the development of software for the Beyond the Standard Model at the Energy Frontier. At present the staggered code in FUEL currently supports Asqtad, HISQ and nHYP, using mass preconditioned HMC and RHMC, all for any N_f or N_c. $N_f = 8$, $N_c = 3$ HISQ and nHYP were/are being used for BSM. The extension to Wilson-colver for any N_f and N_c is well underway. Oliver Witzel and Evan Weinberg are starting to establish an interface between FUEL and the GPU QUAD library to apply GPU acceleration to the Energy Frontier beyond the standard model simulations.

2 Boston University Milestones

Boston University is part participant in the overall SciDAC-3 project on **Strongly-Coupled Field Theories at the Intensity and Energy Frontiers**. The specific miles for Boston University are

- *Year 1:*
  – work with NVIDIA to optimize this multigrid solver on multiple–GPU clusters
  – co-ordinate with FASTMath to optimize the Wilson-Clover multigrid in the HYPER framework
  – develop first version of level 3 multigrid solver for Domain Wall fermions.

- *Year 2:*
  – develop multigrid solver for Overlap fermions
  – work with NVIDIA on multi-precision multigrid solvers for Domain Wall fermions for GPUs
  – introduce communication mitigation of hybrid multigrid/domain decomposition solvers into HYPER with FASTMath collaborators.

- *Year 3:*
  – test & optimize multigrid/domain decomposition evolution in the FUEL framework in collaboration with ANL
  – work with NVIDIA to optimized multigrid/domain decomposition code for GPU systems (Titan, BlueWaters, USQCD Clusters).

Related Publications

[1] J. Brannick, R. C. Brower, M. A. Clark, J. C. Osborn and C. Rebbi, "Adaptive Multigrid Algorithm for Lattice QCD," Phys. Rev. Lett. **100**, 041601 (2008) [arXiv:0707.4018 [hep-lat]].

[2] R. Babich, J. Brannick, R. C. Brower, M. A. Clark, S. D. Cohen, J. C. Osborn and C. Rebbi, "The role of multigrid algorithms for LQCD," PoS **LAT2009**, 031 (2009)

[3] R. Babich, J. Brannick, R. C. Brower, M. A. Clark, T. A. Manteuffel, S. F. McCormick J. C. Osborn,and C. Rebbi, "Adaptive multigrid algorithm for the lattice Wilson-Dirac operator," Phys. Rev. Lett. **105**, 201602 (2010) [arXiv:1005.3043 [hep-lat]].

[4] K. Barros, R. Babich, R. Brower, M. A. Clark and C. Rebbi, "Blasting through lattice calculations using CUDA," PoS **LATTICE2008**, 045 (2008) [arXiv:0810.5365 [hep-lat]].

[5] M. A. Clark, R. Babich, K. Barros, R. C. Brower and C. Rebbi, "Solving Lattice QCD systems of equations using mixed precision solvers on GPUs," Comput. Phys. Commun. **181**, 1517 (2010) [arXiv:0911.3191 [hep-lat]].

[6] T. Appelquist, E. Berkowitz, R. C. Brower, M. I. Buchoff, G. T. Fleming, J. Kiskis, G. D. Kribs and M. Lin *et al.*, arXiv:1402.6656 [hep-lat].

[7] R. C. Brower *et al.* [LSD Collaboration], arXiv:1403.2761 [hep-lat].

[8] T. Appelquist, R. C. Brower, M. I. Buchoff, M. Cheng, G. T. Fleming, J. Kiskis, M. F. Lin and E. T. Neil *et al.*, Phys. Rev. Lett. **112**, 111601 (2014) [arXiv:1311.4889 [hep-ph]].

[9] T. Appelquist *et al.* [Lattice Strong Dynamics (LSD) Collaboration], Phys. Rev. D **88**, no. 1, 014502 (2013) [arXiv:1301.1693 [hep-ph]].

[10] M Clark, Michael Cheng, Richard Brower "Adaptive Multigrid Algorithms on GPUs" preentation by M. Clark at the 31st International Symposium of Lattice Field Theoyr, July 29- Aug 3, 2013, Mainz, Germany.

[11] S. D. Cohen, R. C. Brower, M. A. Clark and J. C. Osborn, "Multigrid Algorithms for Domain-Wall Fermions," PoS LATTICE **2011** (2011) 030 [arXiv:1205.2933 [hep-lat]].

[12] R. C. Brower, G. T. Fleming and H. Neuberger, PoS LATTICE **2012**, 061 (2012) [arXiv:1212.1757 [hep-lat]].

[13] T. Appelquist, R. Brower, S. Catterall, G. Fleming, J. Giedt, A. Hasenfratz, J. Kuti and E. Neil *et al.*, "Lattice Gauge Theories at the Energy Frontier," arXiv:1309.1206 [hep-lat].

[14] T. Blum, R. S. Van de Water, D. Holmgren, R. Brower, S. Catterall, N. Christ, A. Kronfeld and J. Kuti *et al.*, arXiv:1310.6087 [hep-lat].

[15] R. Babich, M. A. Clark, B. Joo, G. Shi, R. C. Brower and S. Gottlieb, "Scaling Lattice QCD beyond 100 GPUs," arXiv:1109.2935 [hep-lat].

[16] See 2013 whitepagers at USQCD website: http://www.usqcd.org/collaboration.html#2013Whitepapers

[17] See the programming language Lua website: *http://www.lua.org*