SciDAC-3 Project Title: Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics (LQCD)

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Principal Investigator: John W. Negele

Recipient: Massachusetts Institute of Technology

Final Technical Report

I. Introduction

Building on the success of two preceding generations of Scientific Discovery through Advanced Computing (SciDAC) projects, this grant supported the MIT component of a multi-institutional SciDAC-3 project that also included Brookhaven National Laboratory, the lead laboratory with P. I. Frithjof Karsch serving as Project Director, Thomas Jefferson National Accelerator Facility with P. I. David Richards serving as Co-director, University of Washington with P. I. Martin Savage, University of North Carolina with P. I. Rob Fowler, and College of William and Mary with P. I. Andreas Stathopoulos. Nationally, this multi-institutional project coordinated the software development effort that the nuclear physics lattice QCD community needs to ensure that lattice calculations can make optimal use of forthcoming leadership-class and dedicated hardware, including that at the national laboratories, and to exploit future computational resources in the Exascale era.

The two people in the MIT SciDAC3 research group were Professor John Negele, who was the Principal Investigator and received no support from the grant, and Principal Research Scientist Andrew Pochinsky, who was the Co-principal Investigator and was supported by the grant.

II. Research Topics

1. Qlua

A long-term goal in Pochinsky's SciDAC work has been creating tools for platform-independent software development that make efficient use of both human time and computer hardware. During SciDAC2, he developed Qlua, a framework for integration and optimization that was used extensively for developing optimized solvers and as a platform for rapid algorithm research, software prototyping and for hadron structure calculations. In SciDAC3, he refined it for use on emerging architectures and used it for software development and investigations of algorithms at scale.

2. Multigrid Propagator Solvers

The inverter algorithms for solving the Dirac equation based on low eigenmodes that were effective for heavy masses and small lattices do not scale well and it is essential to develop new algorithms that are efficient in the physical regime. The multigrid family of algorithms is a particularly promising alternative, which obtains speed-up by exploiting discretization at different scales. However, it is important to note that there is not a single, unique algorithm that one simply programs efficiently, but rather a large algorithmic space of options that must be explored and optimized for lattice QCD in the physical regime.

3. Monte Carlo Equilibration

Generation of QCD lattice configurations at the physical pion mass or at small lattice spacing requires extraordinary computer resources. Existing evolution algorithms tend to get stuck in a given topological sector, which makes exploration of the full configuration space very problematic. Exploration of new algorithms is needed to attain rapid equilibration of gauge configurations.

III. Research Accomplishments

1. Qlua

Pochinsky has refined Qlua so that the resulting implementation shares a common front end and scripting language interpreter, but has machine-specific back ends targeting each of the architectures used by USQCD. He converted Qlua to use OpenMP, improving machine utilization on BG/Q and other platforms.

Advanced sampling techniques, such as all mode averaging (AMA), are considerably sped up by approximate solution of the domain wall Dirac equation. Hence, Pochinsky has included in Qlua an extension of the Möbius DWF with complex hopping terms in the fifth direction, called zMöbius DWF, that is beneficial for AMA. He also added another DWF acceleration method that uses the twisted mass Wilson inverter to start the DWF solver.

Qlua support for HDF5 file storage has been improved to the point where storage intensive LQCD computations, such as AMA and disconnected diagrams production, are no longer dominated by I/O time, and can be divided into shorter jobs to better utilize time available at national HPC installations.

Pochinsky, in collaboration with Stefan Meinel of U. Arizona, Jeremy Green of U. Mainz, Sergey Syritsyn of SUNY Stony Brook, and other members of the Lattice Hadron Physics collaboration, used Qlua to explore the hierarchical probing algorithm for disconnected diagrams at scale. It proved to be significantly more efficient for calculating nucleon electromagnetic form factors than existing algorithms and yielded the first calculation of the strange nucleon electromagnetic form factors that are statistically distinct from zero.

2. Multigrid Propagator Solvers

Pochinsky initiated a collaboration with Evan Berkowitz, Philip Powell, Robert Falgout, Pavlos Vranas, and Chris Schroeder of the FASTMath Institute to utilize their multigrid expertise to explore multigrid algorithms for lattice QCD calculations at the physical pion mass. They defined an abstraction layer HQL between FASTMath's multigrid software suite HYPRE and USQCD software. Pochinsky extended Qlua to accommodate multigrid algorithms and to interface with HQL. Schroeder developed the interface between HQL and HYPRE and Falgout added the extensions needed in HYPRE for QCD, including complex numbers and arbitrary user-defined dimensions.

A major result was that they found that the common multigrid techniques, such as SMG, PFMG, or FAC, that work well in other domains do not work for the Wilson Dirac operator, the basic discretization of QCD for which any viable algorithm must work.

On the other hand, multigrid methods based on the algebraic properties of the operator are more promising, as they directly exploit the structure of the near-null space. One such method is Bootstrap Algebraic Multigrid (BAMG) which they explored extensively. Solver convergence speedups of a factor of 8 were observed which is comparable to EigCG. In addition, the interface has been extended to consistently support an arbitrary number of colors as well as arbitrary stencil structures.

3. Monte Carlo Equilibration

Pochinsky, in collaboration with Will Detmold and Michael Endres of MIT, Rich Brower of BU, and Kostas Orginos of ODU, developed a multiscale thermalization algorithm for lattice gauge theory, which enables efficient parallel generation of uncorrelated gauge field configurations. The algorithm combines standard Monte Carlo techniques with ideas drawn from real space renormalization group and multigrid methods. They demonstrated the viability of the algorithm for pure Yang-Mills gauge theory for both heat bath and hybrid Monte Carlo evolution, and showed that it ameliorates the problem of topological freezing up to controllable lattice spacing artifacts.

IV. Research Metrics

1. Refereed Publications (8/15/12 to 8/14/17)

[1] J. R. Green, J. W. Negele, A. V. Pochinsky, S. N. Syritsyn, M. Engelhardt and S. Krieg, "Nucleon Scalar and Tensor Charges from Lattice QCD with Light Wilson Quarks," Phys. Rev. D **86**, 114509 (2012) doi:10.1103/PhysRevD.86.114509 [arXiv:1206.4527 [hep-lat]].

[2] J. R. Green, M. Engelhardt, S. Krieg, J. W. Negele, A. V. Pochinsky and S. N. Syritsyn, "Nucleon Structure from Lattice QCD Using a Nearly Physical Pion Mass," Phys. Lett. B **734**, 290 (2014) doi:10.1016/j.physletb.2014.05.075 [arXiv:1209.1687 [hep-lat]].

[3] J. R. Green, J. W. Negele, A. V. Pochinsky, S. N. Syritsyn, M. Engelhardt and S. Krieg, "Nucleon electromagnetic form factors from lattice QCD using a nearly physical pion mass," Phys. Rev. D **90**, 074507 (2014) doi:10.1103/PhysRevD.90.074507 [arXiv:1404.4029 [hep-lat]].

[4] W. Detmold, M. McCullough and A. Pochinsky, "Dark Nuclei I: Cosmology and Indirect Detection," Phys. Rev. D **90**, no. 11, 115013 (2014) doi:10.1103/PhysRevD.90.115013 [arXiv:1406.2276 [hep-ph]].

[5] W. Detmold, M. McCullough and A. Pochinsky, "Dark nuclei. II. Nuclear spectroscopy in two-color QCD," Phys. Rev. D **90**, no. 11, 114506 (2014) doi:10.1103/PhysRevD.90.114506 [arXiv:1406.4116 [hep-lat]].

[6] J. Green *et al.*, "High-precision calculation of the strange nucleon electromagnetic form factors," Phys. Rev. D **92**, no. 3, 031501 (2015) doi:10.1103/PhysRevD.92.031501 [arXiv:1505.01803 [hep-lat]].

[7] C. Alexandrou, J. W. Negele, M. Petschlies, A. V. Pochinsky and S. N. Syritsyn, "Study of decuplet baryon resonances from lattice QCD," Phys. Rev. D **93**, no. 11, 114515 (2016) doi:10.1103/PhysRevD.93.114515 [arXiv:1507.02724 [hep-lat]].

[8] M. G. Endres, R. C. Brower, W. Detmold, K. Orginos and A. V. Pochinsky, "Multiscale MonteCarlo equilibration: Pure Yang-Mills theory," Phys. Rev. D **92**, no. 11, 114516 (2015) doi:10.1103/PhysRevD.92.114516 [arXiv:1510.04675 [hep-lat]].

[9] B. Yoon *et al.*, "Controlling Excited-State Contamination in Nucleon Matrix Elements," Phys. Rev. D **93**, no. 11, 114506 (2016) doi:10.1103/PhysRevD.93.114506 [arXiv:1602.07737 [hep-lat]].

[10] J. Green *et al.*, "Up, down, and strange nucleon axial form factors from lattice QCD," Phys. Rev. D **95**, no. 11, 114502 (2017) doi:10.1103/PhysRevD.95.114502 [arXiv:1703.06703 [hep-lat]].

2. Preprints submitted to refereed journals 8/15/12 to 8/14/17 and published after 8/14/17

[1] C. Alexandrou *et al.*, "P-wave $\pi\pi$ scattering and the ρ resonance from lattice QCD," Phys. Rev. D **96**, no. 3, 034525 (2017) doi:10.1103/PhysRevD.96.034525 [arXiv:1704.05439 [hep-lat]].

[2] B. Yoon *et al.*, "Nucleon Transverse Momentum-dependent Parton Distributions in Lattice QCD: Renormalization Patterns and Discretization Effects," Phys. Rev. D **96**, no. 9, 094508 (2017) doi:10.1103/PhysRevD.96.094508 [arXiv:1706.03406 [hep-lat]].

3. Conference proceedings 8/15/12 to 8/14/17

[1] J. Green, M. Engelhardt, S. Krieg, J. Negele, A. Pochinsky and S. Syritsyn, "Nucleon structure with pion mass down to 149 MeV," PoS LATTICE **2012**, 170 (2012) [arXiv:1211.0253 [hep-lat]].

[2] J. Green, M. Engelhardt, S. Krieg, S. Meinel, J. Negele, A. Pochinsky and S. Syritsyn, "Nucleon form factors with light Wilson quarks," PoS LATTICE **2013**, 276 (2014) [arXiv:1310.7043 [hep-lat]].

[3] S. Syritsyn *et al.*, "Initial nucleon structure results with chiral quarks at the physical point," PoS LATTICE **2014**, 134 (2015) [arXiv:1412.3175 [hep-lat]].

[4] T. Kurth, A. Pochinsky, A. Sarje, S. Syritsyn and A. Walker-Loud, "High-Performance I/O: HDF5 for Lattice QCD," PoS LATTICE **2014**, 045 (2015) [arXiv:1501.06992 [hep-lat]].

[5] M. Engelhardt *et al.*, "Nucleon transverse momentum-dependent parton distributions from domain wall fermion calculations at 297 MeV pion mass," PoS LATTICE **2014**, 167 (2014).

[6] C. Alexandrou, J. W. Negele, M. Petschlies, A. V. Pochinsky and S. Syritsyn, "Calculation of the decay width of decuplet baryons," PoS LATTICE **2015**, 084 (2016) [arXiv:1511.02752 [hep-lat]].

[7] B. Yoon *et al.*, "Lattice QCD calculations of nucleon transverse momentum-dependent parton distributions using clover and domain wall fermions," Proceedings of Science LATTICE 2015 (2016) 116 [arXiv:1601.05717 [hep-lat]].

[8] M. Engelhardt *et al.*, “Aspects of Lattice QCD Calculations of Transverse Momentum-Dependent Parton Distributions,” PoS QCDEV **2015**, 018 (2015).

[9] M. Engelhardt *et al.*, “Lattice QCD calculations of transverse momentum-dependent parton distributions (TMDs),” EPJ Web Conf. **112**, 01008 (2016). doi:10.1051/epjconf/201611201008

[10] M. Engelhardt *et al.*, “Lattice QCD calculations of nucleon transverse momentum-dependent parton distributions (TMDs) at 170 MeV pion mass,” PoS LATTICE **2015** (2016) 117.

[11] L. Leskovec *et al.*, “A study of the radiative transition $\pi\pi \to \pi\gamma^*$ with lattice QCD,” PoS LATTICE **2016** (2016) 159 [arXiv:1611.00282 [hep-lat]].

[12] N. Hasan, M. Engelhardt, J. Green, S. Krieg, S. Meinel, J. Negele, A. Pochinsky and S. Syritsyn, “Computing the nucleon Dirac radius directly at $Q^2 = 0$,” PoS LATTICE **2016**, 147 (2016) [arXiv:1611.01383 [hep-lat]].

4. Software developments posted on the web

Web sites are actively used by Qlua users, with more than 10,000 hits on the tutorial and reference pages so far.

- Qlua and Level III libraries distributions: https://usqcd.lns.mit.edu/gitweb/
- Qlua tutorials: https://usqcd.lns.mit.edu/w/index.php/QLUA_tutorials
- Qlua reference: https://usqcd.lns.mit.edu/w/index.php/Category:Qlua_reference
- https://usqcd.lns.mit.edu/redmine/projects/qlua_code
- https://usqcd.lns.mit.edu/redmine/projects/clover
- https://usqcd.lns.mit.edu/redmine/projects/mdwf
- https://usqcd.lns.mit.edu/redmine/projects/qa0
- https://usqcd.lns.mit.edu/redmine/projects/build
- https://usqcd.lns.mit.edu/redmine/projects/qlua
- https://usqcd.lns.mit.edu/redmine/projects/hql