1 PROJECT ACHIEVEMENTS

We have made significant progress on the research in quantum chromodynamics (QCD) set out in our 2017 proposal. There were five main programs of gauge configuration generation described in that proposal. These include the generation of gauge configurations for zero-temperature QCD with three different formulations of lattice quarks: highly improved staggered quarks (HISQ), Domain-Wall Fermions (DWF), and clover fermions, each stream being optimized for a different set of physics applications. We are also generating a stream of HISQ configurations to study high-temperature QCD and a stream of configurations for strongly coupled gauge theory beyond the standard model. The clover fermion calculations are being performed at the OLCF and the HISQ, DWF, BSM and high-temperature QCD streams at the ALCF. The ensembles of zero-temperature configurations are large data sets that are made available to all members of the USQCD Collaboration, which consists of nearly all the high energy and nuclear physicists in the United States involved in the numerical study of QCD. They are being used to perform a wide variety of calculations of importance to these fields.

1.1 Significance of Accomplishments to Date

Our Mira allocations were exhausted in April. Since then, we have continued to run in backfill time on Mira and have been able to extend the HISQ and DWF ensembles, as described below. We hope to make significant additional progress in the verburn period now beginning.

Tests and parameters of the standard model (HISQ): A major component of our work on the ALCF Blue Gene/Q, Mira, has been to generate and make measurements on gauge configurations ensembles produced with the **highly improved staggered quark (HISQ)** action [1, 2]. These configurations have proven to be especially useful for determining the basic parameters of the Standard Model of subatomic physics, and for making precise tests of it [3, 4, 5, 6]. In our program of HISQ configuration generation, we are including four flavors of quarks: up, down, strange and charm, and generating configurations with five lattice spacings $a \approx 0.15, 0.12, 0.09, 0.06$ and 0.042 fm. In most ensembles we tune the strange and charm quark masses, m_s and m_c, as close as possible to their physical values, and take the up and down quarks to be degenerate with a common mass m_l. At each lattice spacing, except $a \approx 0.042$ fm, we are generating ensembles with three values of m_l, corresponding to pion masses of approximately 315 MeV, 222 MeV, and 135 MeV, the last being the physical mass of the pion. (We refer to the ensembles with 135 MeV pions as physical quark mass ensembles). The availability of petascale computers, such as Mira, has made it possible for the first time to perform calculations at the physical value of the pion mass on very fine lattices. These calculations are having a major impact on our work, as described below.

We have completed all of the ensembles with lattice spacing $a \geq 0.06$ fm, except the one with $a \approx 0.06$ fm and physical quark masses. With this year's Mira time, we generated another 192 gauge configurations on this ensemble. This, together with the configurations generated last year on Mira, brings the total number of configurations to over 1000, which was our goal at the start of this project. This is already making major contributions to our measurement campaigns. We have also used this year's Mira time to analyze the 0.06 fm physical quark mass ensemble for a high-statistics calculation of the hadronic vacuum polarization corrections to the anomalous magnetic moment of the muon, which is of high priority to the DOE Office of High Energy Physics because of the currently running g-2 experiment at Fermilab. With the time requested in this year's proposal we expect to extend the physical-mass 0.06 fm ensemble further to address the precision needs of our analysis projects, the most urgent of which is the g-2 analysis.

The 0.042 fm ensembles will play an important role in future work because they will anchor extrapolations of physical quantities to the continuum (zero lattice spacing) limit. They will be particularly valuable because the lattice spacing is small enough to allow use of the HISQ action to describe b-quarks, which is expected to greatly increase the precision of all our work with these quarks. Indeed, we recently presented a first calculation of the B-meson decay constants [4] using this method which we obtained with unprecedented sub-percent precision. The 0.042 fm and 0.06 fm physical-mass HISQ ensembles were crucial for the success of this calculation. The generation and analysis of these ensembles are computationally very challenging, and so far, Mira has been the best suited resource for them of any computing system to which we have access. This past year, we also used Mira time to generate configurations for the most expensive 0.042 fm ensemble at physical pion mass.

Tests and parameters of the standard model (DWF): Significant progress was made toward three goals of our chiral fermion physics program which require the high degree of chiral symmetry realized by the domain-wall fermion formulation. First, we have more than doubled the number of equilibrated the $48^3 \times 64$ ensemble adding 351 molecular dynamics time units. This unusual ensemble exploits the surprisingly small finite lattice spacing errors of the combined Iwasaki and DSDR (dislocation suppressing determinant ratio) gauge action and the Möbius domain wall quark action to allow calculations with few-percent finite lattice spacing errors to be carried out using an inverse lattice spacing as small as $1/a = 1.0$ GeV. For such a large lattice spacing, this 48^3 lattice volume corresponds to a $(9.6\ \mathrm{fm})^3$ physical volume, an important resource for exploring the effects of finite volume at manageable computational cost. The most important use of this large-volume ensemble is to explore the finite volume errors present in our current calculation of the contribution of hadronic light-by-light scattering to the anomalous magnetic moment of the muon. Since we have now developed methods to treat the muon and photon lines in infinite volume [7], the only remaining source of systematic, finite-volume error is the finite size of the volume in which the hadronic Green's functions are computed — a question that can be studied with this new ensemble.

The second goal is the calculation of the $K_L - K_S$ mass difference, an extremely small ($\Delta M_K = 3.483(6) \times 10^{-12}$ MeV) but well-measured quantity that is highly sensitive to new phenomena that are not part of the standard model. This calculation was first proposed in 2010 and shown to be possible in 2014 [8]. A realistic calculation with controlled errors is now possible using Mira and we have developed the needed technique and obtained initial results in 2016 and 2017. During 62 M core hours have been devoted to this calculation during 2018 and 49 additional configurations have been analyzed. The added configurations have made the calculation much more reliable but not significantly decreased the systematic error. Our 2017 result of $5.7(1.5) \times 10^{-12}$ MeV has become $7.3(1.7) \times 10^{-12}$ MeV. The error has not decreased in spite of the inceased statistics, likely because a more accurate value for the η contribution lead to a more accurate estimate of its error. This calculation is now being run using overburn time which we expect will be sufficient to complete it.

Third, using 2018 Incite resources we were able to prepare for and begin calculation of the long-distance contribution to the rare kaon decay $K^+ \to \pi^+ \nu\bar{\nu}$, the rare decay process for which one hundred examples are being collected by the NA62 experiment at CERN. In addition to computing and performing a first analysis of the results from four gauge configurations, we have also developed code that allows an analysis of the statistical correlations between results obtained from different parts of the space-time volume. This is an important step in improving the analysis of many quantities where the large overheads needed by modern efficient methods require that many measurements be made on each configuration. This new approach [9] will allow a more accurate determination of the statistical errors for a result obtained as a volume average over relatively few configurations.

Cold Nuclear Physics: Aims of the Nuclear Physics program are to determine the origin and properties of mass directly from the QCD lagrangian. These calculations have been informing and guiding experimental searches at JLab, BNL, and a future FRIB program. Central to the goals of the project are the creation of gauge field ensembles upon which the analysis campaigns depend. With software development under SciDAC and Exascale, the gauge generation program has been substantially accelerated, and the original goals of our INCITE proposal have been exceeded.

The milestones for Years 1 and 2 involved generation 4000 Monte Carlo trajectories of dynamical

Clover lattices on a $64^3 \times 128$ lattice in the physical limit and a lattice spacing of 0.091 fm. The tremendous advance afforded by improved algorithms for the Clover gauge generation program has allowed us to exceed our goals early in the second year of the project. Originally a third year goal, we have also generated new ensembles on a $72^3 \times 192$ lattice at a smaller lattice spacing of 0.072 fm but at a non-physical pion mass. After this year's allocation time was consumed by May, we had also begun equilibrating a lattice in the physical limit.

Since the component of this Incite project targeting cold nuclear physics will be moved for the third year of this proposal into a new Summit Incite proposal, we do not include a more detailed account of the past accomplishments here. Additional details appear in that proposal and in the appropriate Titan year-end report.

QCD at High Temperature and Densities: The thermodynamic properties of matter interacting through the strong force is described by Quantum Chromodynamics (QCD). The only approach capable of providing quantitative results on the collective (thermal) behavior of matter at present is based on numerical calculations performed in lattice regularized QCD. Experimentally the phase structure of strongly interacting matter is studied in heavy ion collisions performed at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) and the Large Hadron Collider at CERN, Switzerland. While the latter allows to explore properties of matter at the highest energies and almost vanishing net baryon number, RHIC is capable of colliding heavy ions over a wide range of beam energies that allows to study matter with varying net baryon densities or, equivalently, net baryon chemical potential.

A central goal in theoretical and experimental studies of strongly interacting matter at nonzero temperature and baryon number density is to explore its phase diagram. A first beam energy scan (BES-I), varying the center-of-mass energy of the colliding beams in the range 7.7 GeV $\leq \sqrt{s_{NN}} \leq$ 200 GeV, has been performed at RHIC in 2010/11 and 2014. This allowed for a first exploration of the properties of matter in a range of baryon chemical potentials $\mu_B \leq 450$ MeV, or equivalently up to about $\mu_B = 3T_c$, with T_c denoting the transition temperature from hadronic matter to a quark-gluon plasma at $\mu_B = 0$. BES-I lead to a number of intriguing signals, in particular a pronounced non-monotonic behavior in the $\sqrt{s_{NN}}$-dependence of higher order cumulants of net-proton fluctuations, that has been expected to occur in the vicinity of a critical point. Strengthening evidence for the existence of such a critical point is a central goal of the next beam energy scan (BES-II) scheduled at RHIC for 2019/20 as well as theoretical lattice QCD calculations. This constitutes a central goal of the physics program at RHIC, as formulated in the 2015 NSAC Long Range Plan and is a central research objective of the Beam Energy Scan Theory (BEST) Topical Collaboration, which is funded by DOE since 2016.

Higher order cumulants of conserved charges, i.e. net-baryon number, net-electric charge and net-strangeness, have successfully been calculated in lattice QCD. Of particular interest for the comparison with experimental data are up to fourth order cumulants. However, in order to strengthen theoretical evidence for the existence of a critical point, one needs to go further and get control also over higher order cumulants. First results on 6^{th} order cumulants exist. Based on our calculations for 6^{th} order cumulants on lattices with temporal extent $N_\tau = 6$ and 8, that have been performed using also last year's INCITE allocation, we recently published results for the density dependence of the skewness and kurtosis of distributions of net-baryon number fluctuations [10, 11]. Related observables, the cumulants of net-proton number fluctuations, also get measured in the BES at RHIC. Our analysis of conserved charge fluctuations is based also on data that have been generated in earlier years with our INCITE allocation [12]. The calculations on large lattices, which became possible through the INCITE grant, also lead to a new, refined determination of the crossover temperature at vanishing baryon chemical potential as well as the dependence of the transition temperature on the baryon chemical potential. We reported on these results at the Quark Matter conference 2018 and are currently preparing a publication on these new results. Our new results [13] on the transition temperature and its dependence on the baryon chemical potential, μ_B, are shown in Fig. 1.

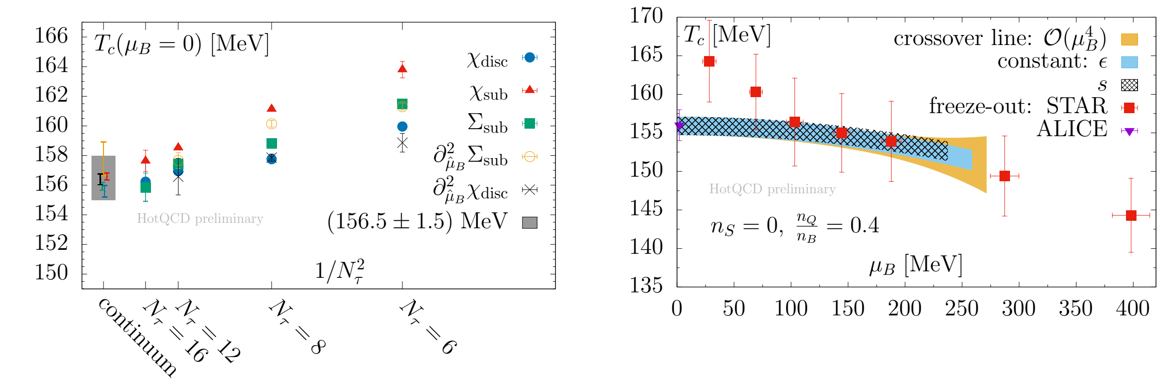

Figure 1. Continuum extrapolation of the crossover temperature at $\mu_B = 0$ (left). The crossover temperature has been extracted from several observables, which define pseudo-critical temperatures that extrapolated to a unique chiral phase transition temperature in the chiral limit. The right hand figure shows the dependence of the crossover temperature on μ_B. Lattice QCD results are compared to freeze-out temperatures measured in heavy ion collision experiments at RHIC (STAR) and the LHC (ALICE). Also shown are lines of constant energy and entropy density that also have been obtained in lattice QCD calculations.

Beyond the Standard Model (BSM): In CY 2018 of the USQCD INCITE award, the BSM effort within USQCD continued to lead world-wide efforts investigating the appearance of a new light scalar with 0^{++} quantum numbers (the same as the Higgs boson) in different strongly-coupled gauge theories. The emergence of this light state, which was discovered from lattice calculations, signals a dramatically different behavior from QCD, where the analogous σ meson is comparatively heavy. The co-existence of the light 0^{++} scalar with the pseudo-Goldstone-boson π mesons raises immediate questions about the nature of the corresponding low-energy effective field theory (EFT), which could provide a new template for the realization of the composite Higgs mechanism. Further investigation of the light 0^{++} scalar and the associated EFT requires significant and continued resources in CY 2019.

During the first six months of CY 2018, both the LSD and LatHC BSM groups have completed important project milestones. Both collaborations presented their results at the annual workshop on *Lattice for BSM Physics 2018* at the University of Colorado, April, 2018. [1] Members of the LSD and LatHC groups also have a number of scheduled talks reporting INCITE based CY 2018 results at The 36th Annual International Symposium on Lattice Field Theory, East Lansing, Michigan, July 2018. [2] Based on these presentations, several journal publications are in their final preparatory phase.

The LSD BSM group has finalized analysis of the SU(3) N_f=8 ensembles generated with nHYP-smeared staggered fermions during USQCD INCITE Year 1. The results are soon to be posted to the arXiv and submitted for publication in Physical Review D. The group also generated SU(3) N_f=4+6 $32^3 \times 64$ ensembles using Möbius domain wall fermions during the USQCD INCITE Year 2 Q1 using the `IroIro++` lattice gauge theory software on Mira BG/Q. Preliminary analysis shows a reasonable light hadron spectrum which varies with the ratio of the heavy and light quark masses m_ℓ/m_h. The group has started the generation of a new $48^3 \times 96$ ensemble with Möbius domain wall fermions during Q3 over-burn time. These larger volumes are essential for clearly demonstrating hyperscaling in an SU(3) N_f=4+6 system as a step towards validating composite Higgs models based on four flavors of light fermions. This

[1] A broad review of recent INCITE BSM lattice research from CY 2018 can be found on the website of the workshop http://www-hep.colorado.edu/ eneil/lbsm18/agenda/.

[2] INCITE BSM talks at the conference website https://indico.fnal.gov/event/15949/contributions.

represents a substantial increase in physics reach over what was initially proposed and was only made possible through the combined performance improvements made by the group plus additional resources available through overburn running.

Working toward the goals of important project milestones, in the first six months of CY2018 the LatHC BSM project continued gauge configuration generation and physics measurements in two ensembles of the near-conformal sextet model at fine lattice spacings with two fermion flavors in the two-index symmetric representation of the SU(3) color group on $64^3 \times 96$ lattices. The results emerging from the analysis of the gauge configurations include a more refined robust test of the dilaton interpretation of the emergent 0^{++} scalar from the analysis of the effective low energy theory incorporating chiral symmetry breaking and scale invariance [14, 15]. The results expose difficulties related to the dilaton interpretation. An important new method was tested for the precise determination of the renormalized mode number distribution of the Dirac operator with accurate analysis of the scale-dependent anomalous dimension of the chiral condensate in the sextet model.

In preparation for the FY 2019 SUSY project, the N=4 super-Yang-Mills code has been developed and tested on BlueGene/Q architecture, where it runs efficiently.

1.2 Allocation Use

We exhausted our Mira allocation by the beginning of April. As of the end of June we had used 304 M hours, or about 114% of our allocation. Our Titan allocation was consumed by May. Our Mira usage is divided approximately 50-50 between jobs running on partitions of 4K nodes or smaller and those using 8- or 12-rack partitions. This latter fraction will grow during the overburn period. On Titan, 80% of our running uses 20-30% of the machine and 15% uses 70-80% of the machine. Of our running on Titan 99% is classified by Oak Ridge as "at capability level".

We have two main users on Titan. On Mira we have two large users responsible for 50% of our running and 7 other users consuming between 10 and 40 M core hours.

1.3 Application Parallel Performance

We have an ongoing program to continue optimization of our codes for the Blue Gene and Cray architectures, which is funded by a DOE SciDAC grant. Members of USQCD have collaborated with Intel and Cray engineers under three different NESAP grants to prepare our codes for the Theta architecture.

Members of USQCD at Brookhaven National Laboratory and Columbia University, along with colleagues at the University of Edinburgh, participated in the design of the Blue Gene/Q, and at a very early stage developed high performance code for QCD with DWF quarks. The currently optimized version is called BFM. The DWF solver runs at 30.5% of peak, while code for the full evolution of gauge configurations and analysis runs at up to 25% of peak with exact performance depending on the specific problem. The scaling behavior of the solver is illustrated in Fig. 2. A new Lattice QCD software system called Grid is being developed by Peter Boyle (University of Edinburgh) and collaborators. Some components of this system are being incorporated into our codes. Although it is targeted specifically for Intel KNL/KNH processors, it also has support for the BG/Q.

Hand-written code for the HISQ solver achieves up to 23% of peak on Mira, and exhibits excellent weak scaling. We are working on a new code framework that will be better optimized for future architectures, such as KNL, and may also bring performance improvements for the BG/Q. The beyond-the-standard model work with the sextet action achieves a performance of approximately 30% of peak on $64^3 \times 128$ lattices on Mira, and demonstrates excellent strong scaling through 16 racks. The work on the composite Higgs model in the fundamental representation now uses Peter Boyle's new Grid code for

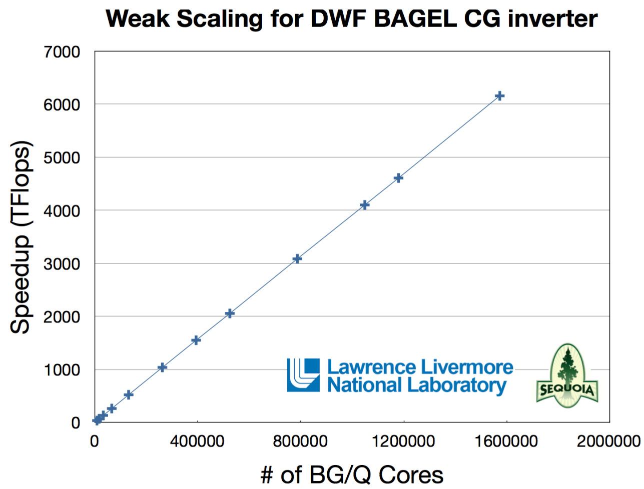

Figure 2. The performance in teraflop/s of the DWF solver on the Lawrence Livermore National Laboratory Blue Gene/Q, Sequoia, as a function of the number of compute cores on up to 98 Blue Gene/Q racks. This is a weak scaling plot with the number of lattice points per node fixed at 8^4.

lattice generation with ten flavors of domain-wall-fermion fermions, with the same excellent performance as that of the Brookhaven/Columbia code mentioned above.

Since we are requesting an allocation on Theta, an architecture that has not previously been used in this project, we will provide further information about our code performance for Theta. The proposed calculation of the HVP contribution to g-2 using DWF uses Grid-based code that has been highly optimized for KNL and run in production on Theta. The code runs efficiently on 1024 nodes. The deflated conjugate gradient inverter sustains 200 Gflops/node on 1024 nodes while the contraction part of the code runs significantly faster. The proposed BSM Theta calculation is also based on Grid code and is also a measurement, not an evolution job. Thus, a similar performance should be expected.

The KNL staggered measurement code that will be used in the QCD thermodynamics project is highly optimized by Patrick Steinbrecher and achieves as much as 800 Gflops per node. The code is parallelized using OpenMP, and vectorized using compiler intrinsics. Being able to change the vector register length at compile time we can take advantage of the KNL's AVX512 instruction set. We apply cache-blocking techniques in order to improve data re-use from L2. Compared to architectures with a large shared L3 cache, the speed-up achieved by cache-blocking on KNL is relatively small. If combined with optimal thread placement, i.e. let threads working on the same local volume share a tile, the Dslash runs about 10% faster.

On KNL, we achieve optimal performance using 2 threads per core. The Dslash kernel achieves a CPI of 0.8 per core. By using L2 software prefetching, we are able to improve the Dslash performance by 1.4x. Currently, the performance is limited by L2 to L1 forwarding. The memory-bandwidth bound linear algebra kernels achieve optimal performance of 400 GB/s. For this proposal, we can use KNL in quad cache or quad flat mode. In both modes, we plan to store the relatively large eigenvectors on the host. The overall performance impact by reading eigenvectors from the host instead from on-chip memory is less than 1%. We measure a performance difference of less than 1% between cache and flat mode. This is expected since all our kernels fit entirely into MCDRAM. For the RHMC, the whole program fits into MCDRAM requiring about 14 GB of memory. The single-node performance as a function of the number of right-hand sides for the set of equations being solved is shown in Fig. 3.

Finally for the KNL code that will be used in the staggered fermion flavor physics calculation being proposed for Theta is based on the QPhiX system originally developed for Wilson quarks at Jefferson Lab

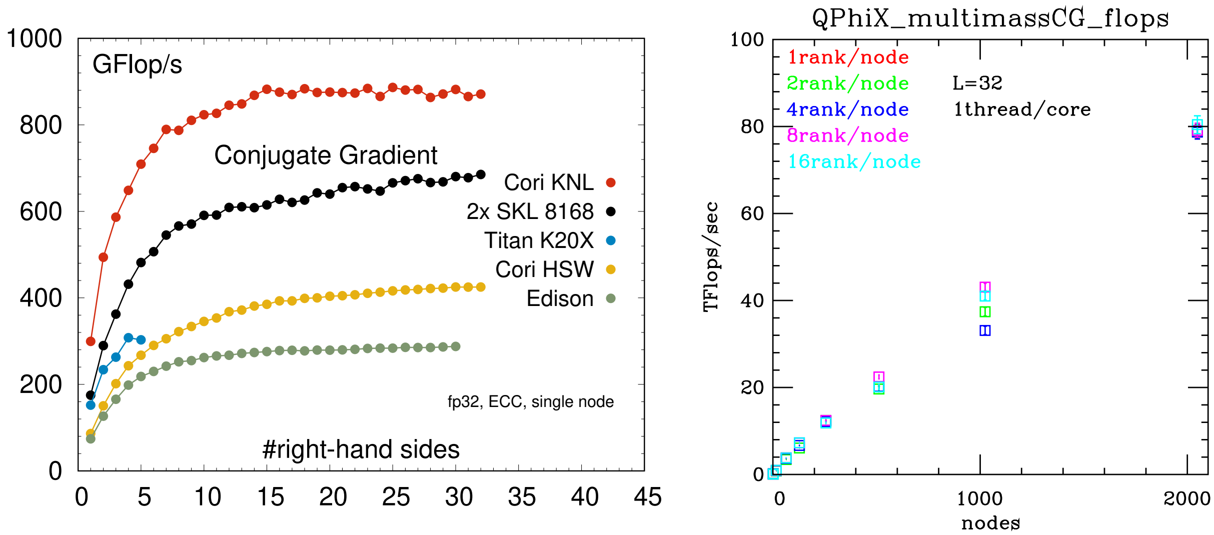

Figure 3. Left: Performance in Gflops/s for the single-node KNL code that will be used for the finite temperature calculations. Right: Weak scaling of double precision QPhiX conjugate gradient performance on Cori to be used for the HISQ flavor physics Theta calculation. This uses a volume of 32^4 per node for 1 to 16 MPI ranks per node. The number of OpenMP threads is adjusted so that all 64 cores of the Xeon Phi chip are used.

and Intel [16, 17]. We have made great progress on development of the QPhiX library for staggered quarks and have a fast conjugate-gradient solver for AVX512, and AVX2 that uses intrinsics to achieve good vectorization. We have run the code on Cori and Theta on up to 2,048 nodes. Our code uses both MPI and OpenMP for parallelization and we have experimented with different combinations of MPI ranks per node and threads per rank. Hyperthreading with two threads per core has been effective in some cases, but we have not seen gains from using four hyperthreads. Figure 3 contains results of a weak scaling study on Cori in which we use 32^4 grid sites on each node. We show the total performance for a multimass conjugate gradient solver running in double precision.

We also participated in the ALCF Theta Early Science Program for porting our code. We produced similar results on Theta during a workshop in August, 2016. In the coming year, we expect to be working on a block-conjugate gradient algorithm that should further improve our code. We have made presentations on our code optimization effort and performance at Lattice 2016 [18], and 2017, QCDNA 2016 and 2017, and most recently at the Intel Xeon Phi Users Group meeting held at TACC, Sept. 26–28, 2017.

1.4 Data Storage

At the ALCF we have about 500 TB of data stored on disk and 2,000 TB on tape. We have developed a highly effective eigenvector compression algorithm as part of our Exascale Computing Project Application Development project which reduces the required storage by a factor of eight and is already being used in the ΔM_K and rare kaon decay Incite projects on Mira. However, these eigenvector files must be decompressed before they can be used on Mira and their 40 TByte decompressed size requires approximately 200 Tbytes of working disk space to be used effectively in production.

The most important data we are creating at the LCFs are ensembles of gauge configurations. These are for the most part analyzed separately for various analysis projects. These ensembles are shared among all lattice groups in the US.

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