PROCEEDINGS OF SCIENCE

Lattice gauge ensembles and data management

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We summarize the status of lattice QCD ensemble generation efforts and their data management characteristics. Namely, these proceedings combine the contributions to a dedicated parallel session during the 41st International Symposium on Lattice Field Theory (Lattice 2024), during which representatives of 16 lattice QCD collaborations provided details on their simulation program, with focus on plans for publication, data management, and storage requirements. The parallel session was organized by the International Lattice Data Grid (ILDG), following an open call to the lattice QCD community for participation in the session.

The 41st International Symposium on Lattice Field Theory (LATTICE2024)
28 July - 3 August 2024
Liverpool, UK

[1] For the TELOS collaboration [2] For the FASTSUM collaboration [3] For the QCDSF collaboration [4] For the HAL QCD collaboration [5] For the MILC collaboration [6] For the Jlab/W&M/LANL/MIT/Marseille effort [7] For CLS [8] For the JLQCD collaboration [9] For the TWEXT collaboration [10] For the ETM collaboration (ETMC) [11] For the RC* collaboration [12] For the OpenLat initiative [13] For the HotQCD collaboration [14] For the PACS collaboration [15] For the CLQCD collaboration [#] Conveners [*] Speaker

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1. Introduction

The simulation of Quantum Chromodynamics (QCD) via its Euclidean-time, discrete formulation on a lattice, has been one of the most compute-intensive applications in scientific computing, consuming substantial fractions of computer time at leadership HPC facilities internationally. In particular, the generation of ensembles of gauge configurations, for multiple values of the QCD parameters such as the QCD coupling, the quark masses, and the extent of the finite volume, requires multi-year simulation campaigns, coordinated by multi-member research collaborations. It is thus common that collaborations store and reuse the same gauge ensembles for multiple observables of interest, and in many cases also share the ensembles with researchers external to the collaboration that generated them.

The purpose of these proceedings is to summarize the available gauge ensembles generated by various lattice QCD collaborations internationally, with a focus on the data management practices each collaboration employs. It follows a parallel session at the 41$^{\text{st}}$ International Symposium on Lattice Field Theory (Lattice 2024), during which 16 collaborations provided status reports of their simulation efforts, responding to an open call for participation addressed to the lattice QCD community prior to the conference. The first such session was held during Lattice 2022 and a report of the contributions presented during that session can be found in Ref. [1].

The sessions are organized by the International Lattice Data Grid (ILDG) as in-person continuations of a series of online workshops with the intention of collecting and gaining an overview of ongoing simulation efforts and the evolving needs of the lattice community in terms of data storage and management. The ILDG was setup in the early 2000s [2, 3, 4, 5] by the lattice community, which realized early on the value in standardizing data management practices across the field. ILDG is organized as a federation of autonomous *regional grids*, within a single Virtual Organization [6]. It standardizes interfaces for the services, which are to be operated by each regional grid, such as storage and a searchable metadata catalog, so that the regional services are interoperable. Within ILDG, working groups specify community-wide agreed metadata schemas (QCDml) [7] to concisely mark-up the gauge configurations and develop relevant middleware tools for facilitating the use of ILDG services. The middleware and metadata specifications developed by ILDG adhere to most of the FAIR (Findable, Accessible, Interoperable, Reusable) principles [8]. A summary of recent developments in ILDG, referred to as ILDG 2.0, was presented during the same session and can be found in a separate proceedings contribution [9].

In the remainder of these proceedings, we present the status of ensemble generation of the 15 collaborations that contributed to this proceedings contribution. The ensembles reported were generated using N_f=2+1, N_f=2+1+1, and N_f=1+1+1+1 sea-quark flavors with various fermion discretizations. The contributors were asked to specify whether their data are public or if they plan on making them public, their interest in using ILDG services and tools for that purpose, as well as some overall information regarding storage requirements. This information is collected in a table and summary section that follows the individual contributions.

2. Contributions

The contributions from each collaboration follow, in the order presented during the parallel session. The original presentations can be found on the conference website [10].

2.1 CLQCD

The CLQCD collaboration focuses on the first principles QCD study of the spectrum of exotic hadrons, parton structure of the nucleon, and other traditional hadron, N-point correlation functions related to high accuracy tests of the standard model, and also QCD in extreme conditions. For this purpose, CLQCD generated a set of configurations of N_f=2+1 fermions using the tadpole improved clover fermion action with stout smearing and the tadpole improved Symanzik gauge action, at 5 values of the lattice spacing $\in [0.05, 0.11]$ fm, several pion masses $\in [120, 350]$ MeV, several volumes with $m_\pi L \in [2.6, 5.8]$ fm, and several temperatures $\in (0, 464]$ MeV. In addition, there are several anisotropic ensembles using clover fermions with $\xi = 5$ at different lattice spacing, pion mass, volume and flavors which concentrate on the high precision studies related to glueball properties. For the gauge generation the Chroma package [11] with QUDA [12, 13, 14] is used at present, and we plan to switch to PyQUDA [15] with QUDA in the near future. Currently the CLQCD collaboration has ~20 ensembles (one ensemble corresponds to one point in the space lattice spacing-spatial volume-pion mass-temperature), which occupy $\sim$ 100 TB of disk space.

Configurations are stored in the SCIDAC format. Possible collaborations on the analysis of the correlation functions are welcome and CLQCD is preparing the hardware and software for the data sharing service.

2.2 Jlab/W&M/LANL/MIT/Marseille

The Jlab/W&M/LANL/MIT/Marseille collaborations are generating ensembles of (2+1)-flavor QCD including the Sheikholeslami-Wohlert (SW) term in the fermion action (the Wilson-clover action) and a tree-level tadpole improved Symanzik gauge action. To smooth the gauge fields, one iteration of four-dimensional stout smearing, with weight $\rho = 0.125$ for the staples, is used in the rational hybrid Monte Carlo (RHMC) algorithm. After stout smearing, the tadpole improved tree-level clover coefficient is found to be very close to the non-perturbative value as checked by using the Schrödinger functional method for determining the clover coefficient non-perturbatively. The two light flavors (u and d quarks) are taken to be degenerate and ensembles are generated with $M_\pi \approx 270,\ 220,\ 170$ and 130 MeV and with lattice spacings $a \approx 0.12,\ 0.091,\ 0.071$ and 0.056 fm. The strange quark mass is tuned close to its physical value by requiring the ratio $(2M^2_{K^+} - M^2_{\pi^+})/M_{\Omega^-}$ takes on its physical value 0.1678, which is independent of the light quark masses to lowest order in χPT. Current analyses of the 13 ensembles generated so far, however, show that the kaon mass varies between 490–570 MeV, necessitating all analyses be done with M_π and M_K as independent parameters. All eleven larger volume ensembles have $M_\pi L > 4$. The setting of the lattice scale a and quark masses m_l and m_s is being done using a global analysis of the octet and decuplet baryon spectrum, pion and kaon masses and decay constants and the flow parameters w_0 (or t_0). Details of the ensembles and their characterization, based on the results of this analysis of the spectral quantities, will be presented by April 2025. These ensembles constitute between 10K-20K thermalized trajectories, with every second one stored at the Oak Ridge Leadership Computing Facility, and constitute about 3.5 PB of data. They are available to USQCD mambers for non-competitive calculations.

2.3 HotQCD

The HotQCD collaboration generates finite temperature ensembles, using highly improved staggered quarks with a tree level improved Symanzik gauge action (HISQ/tree). The majority of the ensembles are with (2+1)-flavor of dynamical quark at the physical point, i.e. two degenerate light quarks (m_l) and one heavier strange quark, with a fixed ratio of $m_l/m_s = 1/27$. Here we have $O(10)$ different temperatures and lattices with aspect ratio $N_\sigma/N_\tau = 4$ and $N_\tau = 8, 12, 16$. These ensembles have been produced with high statistics for the Taylor expansion of the pressure at finite baryon chemical potential [16, 17]. In addition we have large lattices with $m_l/m_s = 1/5, 1/20$, $N_\sigma = 80, 96, 127$, $N_\tau = 20, 22, 24, 28, 32, 36$ and $T = 195, 220, 251, 293$ MeV, for the calculation of spectral functions and transport coefficients [18, 19]. Finally we have ensembles at lighter then physical quark masses: $m_l/m_s = 1/40, 1/60, 1/80, 1/160$, to study the chiral phase transition [20, 21]. Here we increase the aspect ratio with decreasing quark mass in order to keep the finite size effects under control. There is also a limited number of ensembles with three and 5 degenerate HISQ fermions, generated for a study of the Columbia plot [22, 23]. The lattices have been generated using the SIMULATeQCD code [24], using a Rational Hybrid Monte Carlo (RHMC) with a 3-level leap-frog or Omelyan integrator. The step sizes of light, strange and gauge force integrators are tuned to a meet an acceptance of 70%. The trajectory is usually between 0.5 and 1.0 time units. The configurations are stored in a compressed fp32 format and sum up to 1, 500 TB. We plan to upload these ensembles to ILDG 2.0, which is however subject to the available storage space.

2.4 FASTSUM

The FASTSUM collaboration use N_f=2+1 flavor anisotropic gauge ensembles in the fixed-scale approach to study the behavior of QCD as a function of temperature in hadronic and plasma phases. Specifically we have considered the behavior of hadronic states including light, strange, charm and bottom quarks, the electrical conductivity of QCD matter, the interquark potential and properties of the chiral transition. FASTSUM gauge fields utilise an $O\left(a^2\right)$ improved Symanzik gauge action and an $O\left(a\right)$ improved spatially stout-smeared Wilson-Clover action following the parameter tuning and zero-temperature ensembles of the Hadron Spectrum collaboration [25, 26]. "Generation 2" ensembles were generated using the Chroma [11] software suite while the newer "Generation 2L" used a modfication [27] of the openQCD [28, 29] package which introduces stout-link smearing and anisotropic actions. Generation 2 and 2L have an anisotropy $\xi = a_s/a_\tau \sim 3.5$ with $a_s \sim 0.12$ fm, $N_s = 24$ or 32 and a wide range of N_τ corresponding to $T \in [44, 760]$ MeV. mainly in their quark mass. Full details of these ensembles may be found in Refs. [30, 31]. We are in the process of production for "Generation 3" - a parameter set similar to "Generation 2" but with twice the anistropy $\xi \sim 7$ - using openQCD-FASTSUM [27]. We maintain a centralised metadata repository detailing (among other information) who was responsible for each run, on which machine that run was produced and where copies may be found. The gauge fields are redundantly stored on two (well-separated) storage servers managed by Swansea University in the openQCD format. The "Generation 2" ensembles are publically available [32] while other ensembles will be available after an embargo period. We anticipate making ensembles available through the next incarnation of the ILDG with supplementary information also available on Zenodo [33, 32].

2.5 TELOS

The TELOS collaboration performs **T**heoretical **E**xplorations on the **L**attice with **O**rthogonal and **S**ymplectic groups. Problems of interest focus on physics beyond the Standard Model, in particular composite Higgs models. Our work to date has made use of the Wilson gauge action and Wilson fermion action. Our ensembles include studies of the Sp(4) theory with two fundamental fermion flavours (N_f=2) [34] (five values of $\beta \in [6.9, 7.5]$, $V \leq 48{\times}42^3$, $m_\mathrm{PS}/m_\mathrm{V} \gtrsim 0.407(16)$), the Sp(4) theory with three antisymmetric fermion flavours (N_as=3) [35], (six values of $\beta \in [6.6, 6.9]$, $V \leq 54 \times 36^3$, $m_\mathrm{ps}/m_\mathrm{v} \gtrsim 0.7954(44)$); and the Sp(4) theory with N_f=2 and N_as=3 [36], (three values of $\beta \in [6.45, 6.5]$, $V \leq 56 \times 36^3$, $m_\mathrm{PS}/m_\mathrm{V} \gtrsim 0.8768(30)$, $m_\mathrm{ps}/m_\mathrm{v} \gtrsim 0.9022(27)$). In the latter two cases, the topological charge becomes slow running at small m_as, and at larger β. We do not retain our pure gauge ensembles, used for studies of the large-N limit of Sp($2N$) [37, 38, 39], since the costs of storage and data transfer are higher than those of regenerating the ensembles.

Additionally, we present ensembles generated by a subset of the collaboration, with applications to conformal and near-conformal dynamics, and to potential Walking Technicolor theories, again using the Wilson gauge and Wilson fermion actions [40]. Specifically, these are SU(2) with one adjoint flavour (N_adj=1) (seven values of $\beta \in [2.05, 2.4]$, $V \leq 96 \times 48^3$, $m_{2_s^+} \gtrsim 0.28$), and N_adj=2

($V \leq 128 \times 64^3$, $m_{2_s^+} \gtrsim 0.47$). In the former case, the majority of ensembles show ergodic topology, with $\beta = 2.4$ being marginal; in the latter, at large volumes we see significant topological freezing.

Ensembles are generated using HiRep [41, 42] and Grid [43, 44]. The above ensembles will be made available as soon as the infrastructure is in place to do so.

We are in the process of generating ensembles for Sp(4) N_f=2 and for SU(2) $N_\mathrm{f}=1, 2$ with Möbius domain wall fermions, and for SU(2) $N_\mathrm{f}=1, 2$ with Wilson fermions and additional Pauli–Villars fields, which we aim to make available concurrently with the corresponding papers.

2.6 HAL QCD

The Hadrons to Atomic nuclei from Lattice QCD (HAL QCD) collaboration studies multi-hadron systems on the lattice and determines the interactions among hadrons, which are crucial quantities to construct a bridge between QCD and nuclear physics as well as astrophysics. In order to perform the corresponding lattice calculations, it is necessary to prepare gauge configurations at the physical point with large physical volume(s) and a large number of ensembles, since the hadron interactions (whose ranges are typically $\sim 1/m_\pi$) are sensitive to quark masses, and statistical fluctuations of multi-hadron systems are known to be large.

For this purpose, we generate a new set of configurations with N_f=2+1 non-perturbatively improved Wilson-clover fermions with stout smearing and the Iwasaki gauge action on a 96^4 lattice [45]. Utilizing the simulation parameters taken from those used in the PACS10 configurations [46, 47], configurations were generated on the supercomputer Fugaku for 8,000 trajectories at a single lattice spacing, $a = 0.084$ fm, and at the physical point, $m_\pi = 137$ MeV, where we employ Hybrid Monte Carlo (HMC) with the domain-decomposed HMC algorithm and mass preconditioning for up and down quarks and with the rational HMC algorithm for the strange quark. The gauge configurations are stored for every fifth trajectory and thus amount to 1,600 configurations ($\sim$ 80 TB) in total. The set is named "HAL-conf-2023" [45]. We also performed Coulomb gauge fixing for the obtained configurations. Utilizing rotational symmetry, we have $1,600 \times 4$ (rotations) = 6,400 gauge-fixed configurations, which amount to $\sim$ 320 TB. We plan to to make these configurations public through JLDG/ILDG in the future, after performing the analyses which is currently on-going.

2.7 TWEXT

The TWEXT (Twisted Wilson @ Extreme conditions) collaboration studies the properties of QCD at high temperature using Wilson Twisted Mass fermions. Problems under investigation include chiral properties of QCD, in particular the behavior of QCD around the chiral phase transition and its scaling window [48], topological properties of QCD and QCD axion [49], hadron masses, symmetries of QCD and others. For this purpose, TWEXT generated a set of configurations for N_f=2+1+1 fermions at the physical pion mass and also uses older configurations with heavier pion mass. Configurations with the physical pion mass have three lattice spacings $a \in (0.057, 0.080)$ fm and cover a wide range of temperatures from $\sim$ 120 MeV to $\sim$ 900 MeV. It allows the TWEXT collaboration to perform the continuum extrapolation for quantities of interest in this temperature range. For the generation the tmLQCD software package [50, 51, 52] is used and the parameters of the ensembles were taken from the zero temperature simulations of the ETM collaboration [53]. Currently, the TWEXT collaboration has 80 ensembles (one ensemble corresponds to one point in the space temperature-pion mass-lattice spacing), which occupy $\sim$ 80 TB of disk space. Configurations are stored in the ILDG format. Possible collaborations are welcome and TWEXT plans to make configurations public/use ILDG in the future, after performing the ongoing analysis.

2.8 QCDSF

The main focus of the QCDSF collaboration is hadron spectrum and structure at zero temperature. Our ensembles are generated using the Symanzik improved gauge action and Stout Link Non-perturbative Clover (SLiNC) fermion action, for which the link variables appearing in the Dirac term are stout smeared, while the links in the clover term are not [54]. The clover coefficient is determined non-perturbatively. Our most recent set of ensembles are 2 + 1-flavour, which cover pion masses ranging $m_\pi^{phys} \lesssim m_\pi \lesssim 470$ MeV, and 5 lattice spacings in between $a = 0.052 - 0.082$ fm (inclusive). In total, there are 22 ensembles available and an additional 2 at almost-physical pion mass still being generated. A recent listing of available ensembles can be found in [55]. Our approach to the physical point follows the $\bar{m}^R = (2m_\ell^R + m_s^R)/3 = const$ line [56], i.e. we start from the SU(3) symmetric point where the renormalized masses of strange (m_s^R) and light quarks (m_ℓ^R) are equal to each other, $m_s^R = m_\ell^R = \bar{m}^R/3$ and we increase m_s^R as m_ℓ^R decreases. The BQCD software suite [57] is used to generate the ensembles, utilising the hybrid Monte Carlo (HMC) and rational HMC algorithms. All of our gauge configurations are stored in the ILDG format with metadata compliant with the ILDG scheme. We have made use of ILDG storage systems before, where the hub at the CSSM, Adelaide served as one of the regional grids, and some older configurations are still stored in the ILDG servers. The QCDSF collaboration kindly asks any prospective users to contact the collaboration before utilizing these configurations for their projects. We plan to make newly generated ensembles available upon request through ILDG, pending the collaboration's confirmation. QCDSF is open to new collaborative projects.

2.9 OpenLat

The Open Lattice Initiative is generating QCD ensembles using Stabilized Wilson Fermions (SWF) with N_f=2+1[58], based on the exponentially improved Dirac Wilson fermion formulation. The code used for the generation is OpenQCD[29]. These ensembles are intended to be general-purpose datasets, shared with the broader LQCD community in line with the principles of open science. Lines of constant physics are defined through the ϕ_4 parameter setting at a fixed trace M. The initial tuning was performed at the SU(3) flavor symmetric point. Additionally, a set of more chiral trajectories has been put into production, identified by four different pion masses, aiming to reach the physical point.

The generation has been divided into three stages, each to be released with a publication. The first stage, which is nearly complete, focuses on the flavor symmetric point; the second on $m_\pi = 300,\ 200$ MeV; and the third on the physical point. For each pion mass, there are four lattice spacings with periodic boundary conditions ($a = 0.12,\ 0.094,\ 0.077,\ 0.064$ fm) and one ensemble with open boundary conditions at a finer lattice spacing of $a = 0.054$ fm. The volumes have been chosen to always ensure that $m_\pi L > 4$. The collaboration is strongly in favor of uploading configurations to the ILDG, as it aligns with our core principles. The files are already stored in the ILDG format and a preliminary upload of a few configurations has been done before the

LATTICE24 conference. Our ensembles are publicly available for use after the publication of the corresponding stage has been completed. The total storage required is expected to be 0.5 PB.

2.10 RC*

The RC* Collaboration is generating QCD and QCD+QED ensembles with 3 or 4 flavours. We employ C-periodic (*aka* C*) boundary conditions in space, which allow to have a local and gauge-invariant formulation of QED in finite volume [59]. For the SU(3) gauge field we use the Lüscher-Weisz action, while for the compact U(1) field we use the Wilson action. The Wilson-clover discretization of the Dirac operator is used, which includes two Sheikholeslami-Wohlert (SW) terms for the coupling to the SU(3) and U(1) field-strength tensors. The coefficients are chosen in such a why that $O(a\alpha_{\mathrm{em}}^0)$ improvement is guaranteed non-perturbatively in α_{s}. All ensembles generated so far have a lattice spacing of about 0.05 fm, a heavier-than-physical charged pion with mass between 360 MeV and 500 MeV. We plan to move towards lighter pions in the near future. The spatial lattice extent L ranges between $2.9M_\pi^{-1}$ and $6.7M_\pi^{-1}$. Three values of the fine-structure constant α_{em} have been considered so far besides zero, i.e. its physical value, 2.7 and 5.5 times its physical value. In all cases, the β for the U(1) is smaller than 0.035, ensuring that the QED sector is deep in the perturbative regime and away from the bulk phase transition of the compact U(1) model. The configurations are generated with the publicly-available `openQ*D` code [60, 61], which is based on openQCD-1.6. Some of the ensembles as well as the used algorithms are described in [62]. At the moment we have 80Tb of data stored on the machines where they have been generated. This includes configurations, input and log files, histories of various reweigthing factors (to correct for the rational approximation and for occasional change of sign of the fermionic Pfaffian) and basic observables (gradient-flow observables and meson correlators). The RC* Collaboration has worked closely with the ILDG metadata working group to extend the XML schema in order to accommodate metadata for QCD+QED configurations with various finite-volume formulation of QED. We plan to generate the XML metadata and make our ensembles publicly available via ILDG as soon as possible.

2.11 ETMC

The ETM collaboration focuses on hadron spectroscopy, hadron structure, and flavor physics at zero temperature. Ensembles employ the twisted mass formulation, realizing $O(a)$-improvement by tuning to maximal twist, and include a clover term to further reduce the size of lattice artifacts. The Iwasaki gauge action is used. The main simulation effort is for the generation of ensembles with degenerate up- and down-, strange- and charm-quarks (N_{f}=2+1+1) with lattice spacing ranging between 0.049 and 0.091 fm. $M_\pi \cdot L$ varies from 2.5 up to ~5.5. At the time of writing, 24 ensembles are available or in the process of being generated, with 8 of these at approximately physical values of the quark masses. For a recent listing of the ensembles, see [63]. Simulations are performed using the Hybrid Monte Carlo (HMC) algorithm implemented in the tmLQCD software package [50, 51, 52]. See Ref. [53] for details on the simulation program, including the parameter tuning. The DD-αAMG [64, 65] multigrid iterative solver is employed for the most poorly conditioned monomials in the light sector while mixed-precision CG is used elsewhere. Multi-shift CG is used together with shift-by-shift refinement using DD-αAMG [66] for a number of small shifts for the heavy sector. tmLQCD has interfaces to QPhiX [67] and QUDA [12, 13]. tmLQCD automatically writes gauge configurations in the ILDG format, with meta-data including creation date, target simulation parameters, and the plaquette. ETMC policy is to make ensembles publicly available after a grace period. Older N_f=2 and N_f=2+1+1 ensembles [68, 69, 70] have made use of ILDG storage elements. The current ensembles are available upon request and the collaboration intends to use ILDG in the near future. For these ensembles, we expect storage requirements to reach 3 PB.

2.12 JLQCD

The JLQCD collaboration uses a tree-level Symanzik improved gauge action and Möbius domain wall fermions with the scale factor 2 and 3 levels of stout smearing, of which details are found in the supplemental material of [71]. We have two targets of physics to study: one is $T = 0$ 2+1 flavor focusing on B-physics, and the other is finite T focusing chiral symmetry (2 and 2+1 flavors) and investigation of the Columbia plot (3 and 2+1 flavors).

The $T = 0$ ensembles are $32^3 \times 64$ – $64^3 \times 128$ lattices with pion mass M_π between 230 – 500 MeV, and the lattice cutoff a^{-1} is 2.5, 3.6 and 4.5 GeV [71]. Together with 3 flavor ensembles with smaller volumes, we have more than 16 ensembles with 1.5k configurations.

Most of the finite-T 2+1 flavor sets are generated along the line of constant physics at $m_l = m_s^{\mathrm{phys}}/27.4$ and $m_l = m_s^{\mathrm{phys}}/10$ with $N_T = 12,\ 16$, and the remaining finite-T ensembles (2, 2+1 and 3 flavors) are generated with the fixed T approach. Some up-to-date details are found in [72] (2 flavor), [73] (3 flavor), and [74] (2+1 flavor). The recent configurations are generated mainly on the Fugaku supercomputer using Grid [75]. We employ the Hybrid Monte Carlo (HMC) and Rational Hybrid Monte Carlo algorithms. For the three flavor systems, we apply the same 2+1 flavor algorithm but with degenerate masses. The generated configurations are stored in a grid file system, the Japan Lattice Data Grid (JLDG). We are in close contact with ILDG members and plan to start uploading ensembles. The number of configurations and storage quoted in Table 1 assumes storing every 100 MD trajectories, which can be revised when uploading each ensemble.

2.13 MILC

The MILC Collaboration has been creating ensembles of gauge configurations for decades. Initial calculations used two dynamical flavors with naive staggered quarks. Second generation efforts used dynamical up, down, and strange quarks with the asqtad action, culminating with a review in Ref. [76]. Our third generation calculations use the highly improved staggered quark (HISQ) action [77]. They contain dynamical up, down, strange, and charm quarks. For most of the ensembles, up and down are degenerate. The charm quark is set near its physical value. For several ensembles, the light quarks are near their average physical value. There are also ensembles with $m_l = 0.1$, or $0.2 m_s$, where m_l (m_s) is the light (strange) quark mass. We have generated a number of ensembles with m_s less than its physical value to explore low energy constants and the chiral Lagrangian. Lattice spacings are in the range of $[0.15, 0.03]$ fm. In a few cases, multiple volumes are available. Details about the generation of configurations can be found in Refs. [78, 79, 80].

The sharing policy for the MILC ensembles is available on GitHub [81]. On that web page can be found links to 1) the sharing policy, 2) a Google Sheet detailing freely available ensembles, and 3) a document summarizing which papers to cite for the use of each ensemble. Anyone wishing to use an ensemble that is not listed in the Google Sheet, but has been used in a publication or noted in a talk, is welcome to contact a member of the Fermilab Lattice or MILC Collaborations to inquire as to whether the ensemble can be made available for a specific project. Many configurations are available on USQCD resources, making access relatively easy for USQCD members. The ILDG is not operational in the US, but should it become so, we would make an effort to use it. We have assisted transfer of configurations to other researchers both within and outside the US.

2.14 CLS

The CLS (Coordinated Lattice Simulations) effort uses the openQCD code [29] to generate ensembles [82, 83] with N_f=2+1 non-perturbatively O(a)-improved Wilson quarks and tree-level improved Symanzik glue, mostly with open boundary conditions in time to avoid topological freezing [84, 28], but also with (anti-)periodic boundary conditions in time (on some ensembles at $a \gtrsim 0.06\,\mathrm{fm}$), at six fine lattice spacings $a \in [0.039, 0.1]$ fm and quark masses from the symmetric to the physical point on three chiral trajectories ($\mathrm{Tr}[M]$ = const., $m_s \approx$ const., $m_s = m_l$) in large volumes satisfying $M_\pi L \geq 4$ throughout, with statistics typically $\gtrsim 2,000$ MDU.

Due to the algorithm used, two reweighting factors are needed to use CLS ensembles: one to correct for the twisted-mass stabilization of the light quarks, and one to correct for the rational approximation to $\sqrt{D^\dagger D}$ for the strange quark. In the latter case, $\det D < 0$ can occur [85], so that one also needs to correct for the wrong sign of the reweighting factor; fortunately, the fraction of configurations with a negative reweighting factor is very small (or zero) for most ensembles.

At the time of Lattice 2024, there were 149,766 configurations (1.384 PB) stored on tape in the openQCD (non-ILDG) data format. Metadata regarding data provenance, simulation setup, HMC stability, and data integrity are collected automatically via automated scripts, while reweighting factors and determinant minus signs are measured separately. A first batch of ensembles has been successfully uploaded to ILDG; several more ensembles will follow soon, and the remainder will follow after an embargo period. The XML metadata are generated automatically by extraction from the existing database; the (signed) reweighting factors are included in the Config XML.

2.15 PACS

In the past years, the PACS Collaboration has generated 2+1 flavor QCD configurations on very large lattices close to the physical point employing the stout-smeared $O(a)$-improved Wilson-clover quark action and Iwasaki gauge action. We use the stout smearing with six iterations. The improvement coefficient for the clover term is non-perturbatively determined using the Schrödinger functional scheme. These gauge configurations, which keep the space-time volumes larger than (10 fm)^4, are called "PACS10" configurations. We have finished generating three gauge ensembles of (lattice spacing, lattice size)=(0.085 fm, 128^4) [46], (0.064 fm, 160^4) [86], and (0.041 fm, 256^4), labeled as PACS10/L128, PACS10/L160, PACS10/L256, respectively. Using those PACS10 configurations, we have studied the hadron spectrum [46, 47], nucleon structure [87, 88, 89, 90], and physics beyond the standard model [86, 91, 92, 93]. For more precise determinations of physical quantities, we have started to generate the PACS10$_c$ configurations, which are 2+1+1 flavor QCD configurations satisfying the PACS10 conditions. In the configuration generation, the degenerate up- and down-quarks are simulated with the domain-decomposed HMC algorithm [94] and the strange quark with the rational HMC algorithm [95]. The up- and down-quark determinant is calculated by separating into UV and IR parts, with mass-preconditioning [96] for the IR part, even-odd preconditioning, and mixed precision nested BiCGStab [97] with the aid of the chronological inverter as a guess. Many gauge ensembles generated by the PACS Collaboration and its predecessors, the CP-PACS and PACS-CS Collaborations, are publicly available [98]. We plan to make the PACS10 and PACS10$_c$ ensembles (roughly 200 TB) public through the new generation of ILDG via JLDG after some embargo time. Details of the data policies are under discussion within the collaboration.

3. Summary

Table 1: Public: (2 = currently public, 1 = after an embargo period, 0 = no); ILDG: (N = no interest, I = interest, P = planned, U = already using); #ens: Number of ensembles; #cfg: Total number of configurations; storage: Total storage needed in TBytes.

Collaboration	Public	ILDG	#ens	#cfg	Storage (TB)
CLQCD	1	I	20	10,000	100
Jlab/W&M/LANL/MIT/Marseille	0	N	13	10,000	3,500
HotQCD	2,1	P	70	15,000,000	1,500
FASTSUM	2,1	I	37	37,000	65
TELOS	1	P	250	800,000	120
HAL QCD	1	P	1	8,000	400
TWEXT	1	P	80	70,000	80
QCDSF	1	P,U	24	20,000	55
OpenLat	2	U	12	40,000	500
RC*	1	P	14	28,000	60
ETMC	1	P,U	24	12,000	3,000
JLQCD	1	P	260	37,000	15
MILC	1	I	50	70,000	600
CLS	1	P,U	64	150,000	1,400
PACS	2,1	P,U	6	200	200

The contributions presented in this proceeding demonstrate the diverse approaches being taken in lattice QCD simulations. The fermionic actions used by the contributing groups include staggered quarks, particularly using the HISQ action (MILC, and CLQCD), improved Wilson quarks on isotropic lattices (CLQCD, Jlab/W&M/LANL/MIT/Marseille, PACS, CLS, and QCDSF), improved Wilson quarks on anisotropic lattices (FASTSUM and CLQCD), twisted mass fermions (ETMC and TWEXT), Domain Wall fermions (JLQCD), and Stabilized Wilson Fermions (OpenLat).

The simulations span both zero and finite temperature studies, with some collaborations focusing exclusively on $T > 0$, such as TWEXT, others on $T = 0$, and some pursuing both regimes, such as FASTSUM and MILC. Most simulations employ either N_f=2+1 or N_f=2+1+1 sea quark flavors, with all the more ensembles being tuned to their physical values.

A key development reflected in this year's contributions is the growing effort to generate ensembles at finer lattice spacings, with several collaborations now reaching $a \simeq 0.04$ fm or smaller. This push towards the continuum limit is particularly important for precision calculations involving heavy quarks and for controlling discretization effects in general.

The summary of ensemble generation efforts and data management characteristics is presented in Table 1. The collected data indicate that most collaborations plan to make their ensembles publicly available after an embargo period, with strong interest in utilizing ILDG infrastructure for data sharing. The total storage requirements reported by the collaborations are expected to exceed 10 PB, highlighting the substantial data management challenges faced by the community.

Several trends can be identified in the current ensemble generation efforts, namely: i) Increased focus on physical or near-physical quark masses; ii) Growing emphasis on large physical volumes, with some collaborations targeting $(10\text{ fm})^4$ or larger; iii) Development of new algorithmic approaches to address challenges in ensemble generation; iv) Enhanced attention to metadata collection and provenance tracking; and v) An interest in open science principles, with most groups planning public release of their data

The challenge of maintaining long-term storage infrastructure and providing reliable access to these valuable datasets remains a critical concern for the community. While ILDG 2.0 allows for standardizing data sharing, the responsibility for storage space and persistent accessibility remains with regional facilities and individual collaborations. This highlights the ongoing need for sustainable mechanisms to support storage resources required for lattice QCD calculations, similar to those currently available for computation.

The recorded level of interest in ILDG participation demonstrated by the contributing groups suggests there is an appreciation in the community for data sharing, and for frameworks with well-defined workflows that enable this. Thus, standardized data management and sharing practices may help to ultimately enhance the accessibility and reusability of lattice QCD ensembles.

Acknowledgments

We acknowledge the support of all members of the ILDG for making the data session possible. Y. A. and G. K. would also like to thank Hubert Simma for his assistance during the organization of the session and the authoring of these proceedings.

The work of E. B. is part-funded by the UKRI Science and Technology Facilities Council (STFC) Research Software Engineer Fellowship EP/V052489/1, the UKRI Engineering and Physical Science Research Council (EPSRC) ExCALIBUR programme ExaTEPP project EP/X017168/1, and the STFC Consolidated Grant ST/T000813/1. R. B. acknowledges support from a Science Foundation Ireland Frontiers for the Future Project award with grant number SFI-21/FFP-P/10186. K. U. C. is supported by the Australian Research Council grant DP190100297, DP220103098 and DP240102839. T. D. acknowledges support from HPCI System Research Project (Grants No. hp200130, hp210165, hp220174, hp230207, hp240213, hp220066, hp230075, hp240157, hp210212, and hp220240), the JSPS (Grants No. JP18H05407, JP18H05236, JP19K03879, JP21H05190, JP23H05439), JST PRESTO Grant No. JPMJPR2113, “Program for Promoting Researches on the Supercomputer Fugaku” (Grants No. JPMXP1020200105, JPMXP1020230411). S. G. acknowledges support from the Department of Energy, Office of High Energy Physics, DE-SC0010120. G. K. acknowledges support from EXCELLENCE/0421/0195, co-financed by the European Regional Development Fund and the Republic of Cyprus through the Research and Innovation Foundation and the AQTIVATE a Marie Skłodowska-Curie Doctoral Network GA No. 101072344. G. P. acknowledges funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - project number 460248186 (PUNCH4NFDI). The work of C. S. is supported by the European Union's Horizon 2020 research and innovation program under the Marie Sklodowska-Curie Grant Agreement No. H2020-MSCAITN-2018-813942 (EuroPLEx), by The Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project No. 315477589-TRR 211 and the PUNCH4NFDI consortium supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation). T. Y. acknowledges Grants-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (No. 19H01892, 23H01195, 23K25891), MEXT as "Program for Promoting Researches on the Supercomputer Fugaku" (JPMXP1020230409) and support from computational resources through the HPCI System Research Project (Project IDs: hp170022, hp180051, hp180072, hp180126, hp190025, hp190081, hp200062, hp200167, hp210112, hp220079, hp230199, hp240207). Y.-B. Y. is supported in part by NSFC grants No. 12293060, and 12435002.

The participating collaborations acknowledge the following HPC systems and HPC sites for the generation of the gauge ensembles reported here,

- National Computer Infrastructure (NCI) National Facility in Canberra, supported by the Australian Commonwealth Government and the Pawsey Supercomputing Centre, supported by the Australian Government and the Government of Western Australia, Australia;
- HPC Cluster of ITP-CAS, the Southern Nuclear Science Computing Center (SNSC) in Beijing and the Siyuan-1 cluster, supported by the Center for High Performance Computing at Shanghai Jiao Tong University, China;
- LUMI-C and LUMI-G at CSC, Finland;
- SuperMUC and SuperMUC-NG at the Leibniz Rechenzentrum (LRZ) in Garching, JUGENE, JUWELS, and JUWELS-Booster at the Jülich Supercomputing Centre (JSC) in Jülich, HAWK at Höchstleistungsrechenzentrum Stuttgart (HLRS), and the North-German Supercomputer Alliance (HLRN), Germany;
- Irène Joliot-Curie at Très Grand Centre de Calcul (TGCC) in Bruyères-le-Châtel, France;
- Kay and Stokes at the Irish Centre for High-End Computing (ICHEC) in Galway, Ireland;
- Leonardo, Marconi 100, and Marconi A2 at CINECA in Bologna, Italy;
- Polarie and Grand Chariot at Hokkaido University, the IBM Blue Gene system at KEK, SQUID at Osaka University, Supercomputer Fugaku at RIKEN, Oakforest-PACS at University of Tokyo, and Wisteria at University of Tsukuba, Japan;
- Cambridge Service for Data Driven Discovery (CSD3) in Cambridge, Tesseract at the DiRAC Extreme Scaling Service at the University of Edinburgh, DiRAC Data Intensive 2.5 & 3 at the University of Leicester, and Sunbird of Supercomputing Wales, supported by the European Regional Development Fund via the Welsh Government, United Kingdom;
- Cori, Edisson, and Perlmutter at the National Energy Research Scientific Computing Center (NERSC), California; Mira, Theta, Polaris at the Argonne Leadership Computing Center (ALCF), Illinois; Blue Waters and Delta at the National Center for Supercomputing Applications (NCSA), Illinois; Big Red 2, 2+, 3, 200 at Indiana University, Indiana; Computing at Los Alamos National Lab, New Mexico; Summit, Crusher, and Frontier at the Oak Ridge Leadership Computing Facility

(OLCF), Tennessee; Stampede, Stampede2, and Frontera at the Texas Advanced Computing Center (TACC), Texas; and the computing facilities at Jefferson Lab, Virginia, United States.

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