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, this proceeding summarizes contributions to a dedicated parallel session during the 41[st] 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 for participation in the session.

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[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 the CLS [8] For the JLQCD collaboration [9] For the TWEXT collaboration [10] For the ETM collaboration (ETMC) [11] For the RBC-UKQCD collaboration [12] For the RC* collaboration [13] For the OPEN LAT initiative [14] For the HotQCD collaboration [15] For the PACS collaboration [16] For the CLQCD collaboration [#] Conveners [*] Speaker

Contents

1 Introduction **2**

2 Contributions **3**
- 2.1 CLQCD 4
- 2.2 Jlab/W&M/LANL/MIT/Marseille 4
- 2.3 HotQCD 5
- 2.4 FASTSUM 5
- 2.5 TELOS 6
- 2.6 HAL QCD 6
- 2.7 TWEXT 7
- 2.8 QCDSF 7
- 2.9 RBC-UKQCD 8
- 2.10 OPEN LAT 8
- 2.11 RC* 9
- 2.12 ETMC 9
- 2.13 JLQCD 10
- 2.14 MILC 10
- 2.15 CLS 11
- 2.16 PACS 11

3 Summary **12**

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 this proceeding 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 during Lattice 2022 and a report of the contributions presented during that session can be found in Ref. [1].

These sessions are organized by the International Lattice Data Grid (ILDG) with the intention of obtaining, gathering, and summarizing the evolving needs of the lattice community in terms of data storage and management. The ILDG was setup in the early 2000s [2–5] 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 proceeding [9].

In the remainder of this proceeding, we present the status of ensemble generation of each of the 16 collaborations that contributed to the parallel session. We restrict ourselves to simulations of QCD, and at present these are carried out 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 [12–14] 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

2.3 HotQCD

2.4 FASTSUM

The FASTSUM collaboration use $N_{\rm f}$=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 [16, 17]. "Generation 2" ensembles were generated using the Chroma [11] software suite while the newer "Generation 2L" used a modfication [18] of the openQCD [19, 20] 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. Full details of these ensembles may be found in Refs. [21, 22]. 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 [18]. 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 [23] 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 [23, 24].

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) [25] (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) [26], (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 [27], (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($2N$) [28–30], 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 [31]. 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 [32, 33] and Grid [34, 35]. 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_f=1, 2 with Möbius domain wall fermions, and for SU(2) N_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

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 [36], topological properties of QCD and QCD axion [37], 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 [38–40] is used and the parameters of the ensembles were taken from the zero temperature simulations of the ETM collaboration [41]. 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 [42]. 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 [43]. Our approach to the physical point follows the $\bar{m}^R = (2m_\ell^R + m_s^R)/3 = const$ line [44], 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 [45] 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 RBC-UKQCD

2.10 OPEN LAT

2.11 RC*

2.12 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 [46]. Simulations are performed using the Hybrid Monte Carlo (HMC) algorithm implemented in the tmLQCD software package [38–40]. See Ref. [41] for details on the simulation program, including the parameter tuning. The DD-αAMG [47, 48] 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 [49] for a number of small shifts for the heavy sector. tmLQCD has interfaces to QPhiX [50] 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 [51–53] 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.

2.13 JLQCD

2.14 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. [54]. Our third generation calculations use the highly improved staggered quark (HISQ) action [55]. 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. [56–58].

The sharing policy for the MILC ensembles is available on GitHub [59]. 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.

2.15 CLS

The CLS (Coordinated Lattice Simulations) effort uses the openQCD code [20] to generate ensembles [60, 61] 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 [19, 62], 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 [63], 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.

2.16 PACS

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); #end: 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					
HotQCD					
FASTSUM	2,1	I	37	37,000	65
TELOS	1	P	250	800,000	120
HAL QCD					
TWEXT	1	P	80	70,000	80
QCDSF	1	P,U	24	20,000	55
RBC-UKQCD					
OPEN LAT					
RC*					
ETMC	1	P,U	24	12,000	3,000
JLQCD					
MILC	1	I	50	70,000	600
CLS	1	P,U	25	150,000	1,400
PACS					

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