

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 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 for participation in the session.

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¹ For the TELOS collaboration ² For the FASTSUM collaboration ³ For the CSSM/QCDSF/UKQCD 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

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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 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 41st 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

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

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2.3 HotQCD

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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 $O(a^2)$ improved Symanzik gauge action and an $O(a)$ improved spatially stout-smearred Wilson-Clover action following the parameter tuning and zero-temperature ensembles of the Hadron Spectrum collaboration [11, 12]. “Generation 2” ensembles were generated using the Chroma [13] software suite while the newer “Generation 2L” used a modification [14] of the openQCD [15, 16] 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. [17, 18]. We are in the process of production for “Generation 3” - a parameter set similar to “Generation 2” but with twice the anisotropy $\xi \sim 7$ - using openQCD-FASTSUM [14]. 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 [19] 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 [19, 20].

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 $\text{Sp}(4)$ theory with two fundamental fermion flavours ($N_f=2$) [21] (five values of $\beta \in [6.9, 7.5]$, $V \leq 48 \times 42^3$, $m_{\text{PS}}/m_V \gtrsim 0.407(16)$), the $\text{Sp}(4)$ theory with three antisymmetric fermion flavours ($N_{\text{as}}=3$) [22], (six values of $\beta \in [6.6, 6.9]$, $V \leq 54 \times 36^3$, $m_{\text{PS}}/m_V \gtrsim 0.7954(44)$); and the $\text{Sp}(4)$ theory with $N_f=2$ and $N_{\text{as}}=3$ [23], (three values of $\beta \in [6.45, 6.5]$, $V \leq 56 \times 36^3$, $m_{\text{PS}}/m_V \gtrsim 0.8768(30)$, $m_{\text{PS}}/m_V \gtrsim 0.9022(27)$). 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 $\text{Sp}(2N)$ [24–26], 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 [27]. Specifically, these are $\text{SU}(2)$ with one adjoint flavour ($N_{\text{adj}}=1$) (seven values of $\beta \in [2.05, 2.4]$, $V \leq 96 \times 48^3$, $m_{2_s^+} \gtrsim 0.28$), and $N_{\text{adj}}=2$ ($V \leq 128 \times 64^3$, $m_{2_s^+} \gtrsim 0.47$). 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 [28, 29] and Grid [30, 31]. 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 $\text{Sp}(4)$ $N_f=2$ and for $\text{SU}(2)$ $N_f=1, 2$ with Möbius domain wall fermions, and for $\text{SU}(2)$ $N_f=1, 2$ with Wilson fermions and additional Pauli–Villars fields, which we aim to make available concurrently with the corresponding papers.

2.6 HAL QCD

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2.7 TWEXT

1 The TWEXT (Twisted Wilson @ Extreme conditions) collaboration studies the properties of
2 QCD at high temperature using Wilson Twisted Mass fermions. Problems under investigation in-
3 clude chiral properties of QCD, in particular the behavior of QCD around the chiral phase transition
4 and its scaling window [32], topological properties of QCD and QCD axion [33], hadron masses,
5 symmetries of QCD and others. For this purpose, TWEXT generated a set of configurations for
6 $N_f=2+1+1$ fermions at the physical pion mass and also uses older configurations with heavier pion
7 mass. Configurations with the physical pion mass have three lattice spacings $a \in (0.057, 0.080)$ fm
8 and cover a wide range of temperatures from ~ 120 MeV to ~ 900 MeV. It allows the TWEXT
9 collaboration to perform the continuum extrapolation for quantities of interest in this temperature
10 range. For the generation the tmLQCD software package [34–36] is used and the parameters of
11 the ensembles were taken from the zero temperature simulations of the ETM collaboration [37].
12 Currently, the TWEXT collaboration has 80 ensembles (one ensemble corresponds to one point in
13 the space temperature-pion mass-lattice spacing), which occupy ~ 80 TB of disk space. Configu-
14 rations are stored in the ILDG format. Possible collaborations are welcome and TWEXT plans to
15 make configurations public/use ILDG in the future, after performing the ongoing analysis.

2.8 CSSM/QCDSF/UKQCD

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2.9 RBC-UKQCD

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2.10 OPEN LAT

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2.11 RC*

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2.12 ETMC

1 The ETM collaboration focuses on hadron spectroscopy, hadron structure, and flavor physics
2 at zero temperature. Ensembles employ the twisted mass formulation, realizing $O(a)$ -improvement
3 by tuning to maximal twist, and include a clover term to further reduce the size of lattice artifacts.
4 The Iwasaki gauge action is used. The main simulation effort is for the generation of ensembles
5 with degenerate up- and down-, strange- and charm-quarks ($N_f=2+1+1$) with lattice spacing ranging
6 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
7 are available or in the process of being generated, with 8 of these at approximately physical values of
8 the quark masses. For a recent listing of the ensembles, see [38]. Simulations are performed using
9 the Hybrid Monte Carlo (HMC) algorithm implemented in the tmLQCD software package [34–36].
10 See Ref. [37] for details on the simulation program, including the parameter tuning. The DD-
11 α AMG [39, 40] multigrid iterative solver is employed for the most poorly conditioned monomials
12 in the light sector while mixed-precision CG is used elsewhere. Multi-shift CG is used together
13 with shift-by-shift refinement using DD- α AMG [41] for a number of small shifts for the heavy
14 sector. tmLQCD has interfaces to QPhiX [42] and QUDA [43, 44]. tmLQCD automatically writes
15 gauge configurations in the ILDG format, with meta-data including creation date, target simulation
16 parameters, and the plaquette. ETMC policy is to make ensembles publicly available after a grace
17 period. Older $N_f=2$ and $N_f=2+1+1$ ensembles [45–47] have made use of ILDG storage elements.
18 The current ensembles are available upon request and the collaboration intends to use ILDG in the
19 near future. For these ensembles, we expect storage requirements to reach 3 PB.

2.13 JLQCD

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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. [48]. Our third generation calculations use the highly improved staggered quark (HISQ) action [49]. 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 $0.2m_s$, 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. [50–52].

The sharing policy for the MILC ensembles is available on GitHub [53]. 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 [16] to generate ensembles [54, 55] 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 [15, 56], but also with (anti-)periodic boundary conditions in time (on some ensembles at $a \gtrsim 0.06$ 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 ($\text{Tr}[M] = \text{const.}$, $m_s \approx \text{const.}$, $m_s = m_l$) 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 [57], 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

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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) |
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| CLQCD | | | | | |
| 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 |
| CSSM/QCDSF/UKQCD | | | | | |
| 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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HAWK at Höchstleistungsrechenzentrum Stuttgart (HLRS), Germany,

SuperMUC and SuperMUC-NG at Leibniz Rechenzentrum (LRZ) in Garching, Germany,

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,
Tesseract at the DiRAC Extreme Scaling Service at the University of Edinburgh, United Kingdom,
DiRAC Data Intensive 2.5 & 3 at the University of Leicester, United Kingdom,
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the DiRAC Extreme Scaling and Data Intensive services, which are part of the UKRI Digital Research Infrastructure,

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