QCD simulations with stabilized Wilson fermions

Francesca Cuteri [1] Rocco Francesco Basta [1] Anthony Francis [2] Patrick Fritzsch [3] Jangho Kim [4]
Andrea Shindler [5 6] Antonio Rago [7] Giovanni Pederiva [4] Andre Walker-Loud [8] Savvas Zafeiropoulos [9]

[1]Goethe-Universität Frankfurt, Germany [2]National Yang Ming Chiao Tung University, Taiwan [3]Trinity College Dublin, Ireland [4]Forschungszentrum Jülich GmbH [5]FRIB& Michigan State University, USA [6]RWTH Aachen, Germany [7]University of Southern Denmark, Denmark [8]Lawrence Berkeley National Lab, USA [9]CNRS & Aix Marseille Université, France

OPEN LATtice initiative

HLRS High Performance Computing Center | Stuttgart

Introduction

Stabilized Wilson Fermions (SWF) are a new avenue for lattice quantum chromodynamics (QCD) calculations. The open lattice initiative (OpenLat) was founded to exploit & explore this new line of research.

- Gauge field ensembles in a setup very close to nature, with 2+1 fermion flavours across a wide range of lattice spacings $a = 0.055, 0.064, 0.077, 0.094, 0.12$ fm produced with resources in Germany, US, France and Finland.
- Most important contribution from HLRS at the finest resolution $a = 0.055$ fm.

SWF builds upon recent developments in the generation of gauge fields for use in lattice QCD. Initial studies [1–4] have shown a reduced c_{SW} compared to standard simulations, indications of positive scaling behaviours and other benefits. Good scaling in flow and hadronic observables going towards the continuum was also observed. SWF simulations give access to an extended parameter window. How far such window can be extended and with what scaling benefits is a key motivation for us to study this setup. A further motivation comes from the plan to exploit the produced gaugefields for renormalization purposes for thermodynamics studies that demand very fine lattices.

Together with HLRS we want to generate state-of-the-art QCD gauge ensembles for physics applications and share them with the community so that impactful particle physics research is accelerated under the FAIR principles and open science.

Stabilized Wilson Fermions

SWF [1] have been recently proposed as an improvement to the customary $O(a)$-improved Wilson Clover Fermions (WCF). First developed in order to allow simulations on very large volumes, they consist in:

- **SMD update algorithm** instead of HMC, which has been shown to be less affected from instabilities in MD evolution;
- **Exponentiated Clover action** to help protect the Dirac matrix from having arbitrarily small eigenvalues:

$$\mathcal{D} = \frac{1}{2}\gamma^\mu\left[\nabla^*_\mu + \nabla_\mu - a\nabla^*_\mu\nabla_\mu\right] + m_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \tag{1}$$

When using even-odd preconditioning, the term

$$D_{ee} + D_{oo} = 4 + m_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \tag{2}$$

can have arbitrarily small eigenvalues. To avoid this issue, we can change the improvement term without spoiling the continuum limit in the following way:

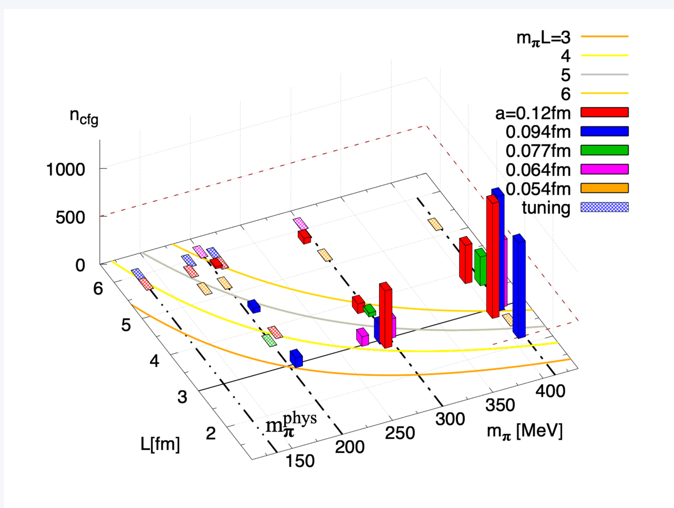
$$D_{ee} + D_{oo} = (4 + m_0)\exp\left[\frac{c_{SW}}{4+m_0}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\right] \tag{3}$$

- **Uniform norm solver stopping criterion**, which protects from precision loss from local effects;
- **Quadruple precision arithmetics**, in order to reduce precision loss effects.

Open science, FAIR principles and OpenLat

- Formation of OpenLat is the response to new challenges in data generation, access and usage in lattice gauge theory
- Our goals are to
  (1). transparently define and uphold quality for the data provided
  (2). share and maintain an easily accessible repository
  (3). gather resources towards a common community aim
  (4). grant access to any interested party freely and quickly
- Integration with ILDG (`hpc.desy.de/ildg/`) & zenodo (`zenodo.org`)
- Data adhere to the FAIR principles (`www.go-fair.org/`), i.e. they become: Findable, Accessible, Interoperable and Reusable.

Ensemble generation



The two separate stages in our gauge ensemble generation process are *Tuning* and *production*:

- In the tuning stage thermalization is performed and the algorithm's parameters are adjusted over a large number of SMD cycles.
- With all quality criteria fulfilled the run is considered ready for production.

The overview plot of the existing and planned ensembles shows the space of the pion mass, the physical volume and the number of available configurations, and with the lattice spacings distinguished by the colors. Colored lines depicting the regimes $m_\pi L = 3-4$, $4-5$ and $5-6$ are given for reference.

OpenLat on HAWK

- HLRS resources are a key component of the OpenLat strategy
  - 91% of the allocated resources steadily consumed over the past 23 months
- HAWK is uniquely capable of extending the OpenLat parameter window to finer lattice spacings, i.e. bringing them closer to nature
- HAWK presents near perfect scaling for our application

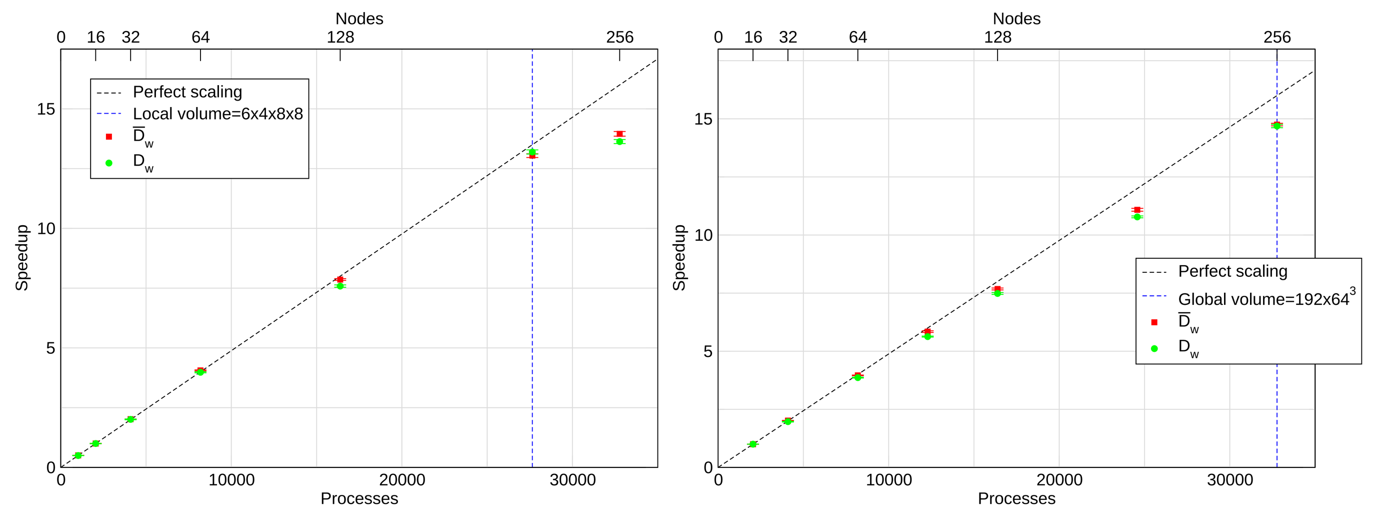


Figure 1. Strong (left) and weak (right) scaling of our software on HAWK @ HLRS.

OpenLat results

Through its unique open science philosophy OpenLat and the ensembles generated benefit the lattice QCD community. They enable further control over systematics, but importantly they also expand the accessible parameter window, pushing calculations to the next level in control and precision.

There are three levels of outcomes and results through OpenLat's research and ensembles:

(1.) Insights and physics results directly related to the generation process
- Algorithm research and tuning
- Pion related physics, e.g. the decay constant f_π
- Simple meson and baryon spectrum

(2.) The OpenLat extended physics research program
- Determination of the neutron electric dipole moment (nEDM) and the strong-CP problem
- Nuclear, flavor physics and exotic spectrum applications (in preparation)
- QCD phase diagram and thermodynamics at zero and non-zero isospin chemical potential [5]

(3.) User and early access projects
- Multi-hadron scattering, e.g. the H-dibaryon
- Hadronic decays, e.g. hadronic D-decays
- Masterfield simulations of QCD

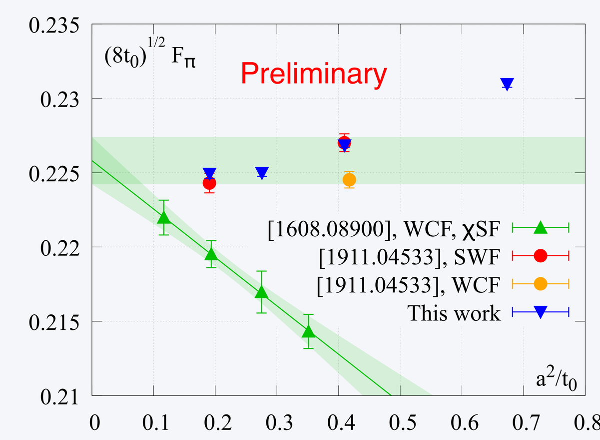


Figure 2. The pion decay constant f_π presented at Lattice'23

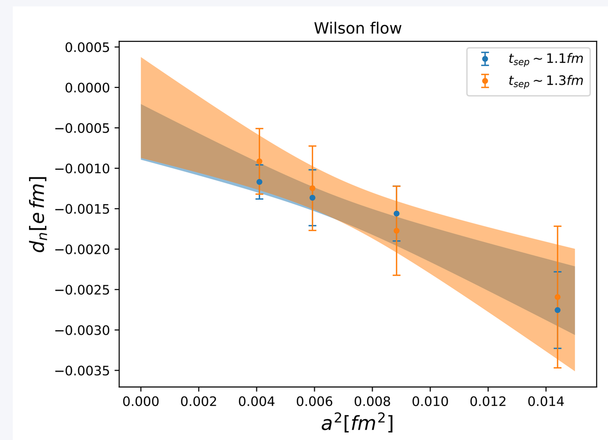


Figure 3. The nEDM is part of the OpenLat extended program.

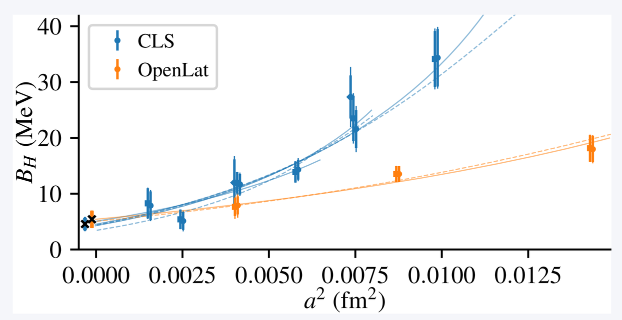


Figure 4. Multi-nucleons, here the the H-dibaryon by a user-group (Lattice'22).

Publications

[1] Anthony Francis, Patrick Fritzsch, Martin Lüscher, and Antonio Rago. Master-field simulations of O(a)-improved lattice QCD: Algorithms, stability and exactness. *Comput. Phys. Commun.*, 255:107355, 2020.

[2] Andrey Sebastian Francis, Francesca Cuteri, Patrick Fritzsch, Giovanni Pederiva, Antonio Rago, Andrea Schindler, Andre Walker-Loud, and Savvas Zafeiropoulos. Properties, ensembles and hadron spectra with Stabilised Wilson Fermions. *PoS*, LATTICE2021:118, 2022.

[3] Francesca Cuteri, Anthony Sebastian Francis, Patrick Fritzsch, Giovanni Pederiva, Antonio Rago, Andrea Shindler, Andre Walker-Loud, and Savvas Zafeiropoulos. Gauge generation and dissemination in OpenLat. *PoS*, LATTICE2022:426, 2023.

[4] Francesca Cuteri, Anthony Francis, Patrick Fritzsch, Giovanni Pederiva, Antonio Rago, Andrea Shindler, Andre Walker-Loud, and Savvas Zafeiropoulos. Benchmark Continuum Limit Results for Spectroscopy with Stabilized Wilson Fermions. *PoS*, LATTICE2022:074, 2023.

[5] Rocco Francesco Basta, Bastian B. Brandt, Francesca Cuteri, Gergely Endrődi, and Anthony Francis. QCD Thermodynamics with stabilized Wilson fermions. *PoS*, LATTICE2022:277, 2023.