Gauge generation and dissemination in OpenLat

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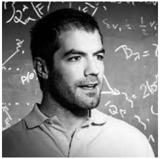
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https://openlat1.gitlab.io

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OPEN LATtice initiative

Bringing together researchers from different institutes. Our aim is to generate state-of-the-art QCD gauge ensembles for physics applications and to share them with the community to strengthen open science.

To us this means:

define and uphold quality
Standards for control observables, continue to research and improve best practices, consensus based decision making, frequent internal communication

share and maintain repository
Manage downloads, maintain data integrity, make control measurements available

community boosting
Use resource injections from members and interested/early access parties to expand set of gauges.

grant and enable access
Configurations will be made open access with accompanying first publication;
Early access through user agreement - get in touch with us!
No embargo time, no access vetting after publication

Action and algorithms

Stabilised Wilson fermions (SWF)

AF, Fritzsch, Lüscher, Rago ('19)

SMD = stochastic molecular dynamics $\rightsquigarrow$ (algorithm between HMC and Langevin)

- Algorithmic improvements:
  - SMD decreases fluctuations and makes for a generally more stable run
  - SMD algorithm shows net gain in reduced autocorrelations at same cost
  - increase precision of internal numbers to quad
  - use supremum-norm to ensure minimum solve quality
- Fermion discretisation:
  - exponentiated Clover action
  - bound from below and guaranteed invertibility for Clover term
  - indication of scaling benefits (see talks listed at the end)

SWF toolkit implemented from `openQCD-2.0` onwards

These go on top of the measures already deployed:

- twisted mass reweighting for light quarks
- mass preconditioning through Hasenbusch chains
- using improved solvers (for us: deflated SAP solver)
- high accuracy approximations for the strange quark RHMC

$\rightsquigarrow$ Combine all for the best, i.e. most stable in our experience, results.

Remark: Note that SWF preserve the pt-expansion, particularly important for renormalisation, and the change to the action is local only.

Actions and algorithms - algorithmic ingredients of SWF

$\rightsquigarrow$ `details given for reference, slides may be skipped 1/3`

Three ingredients to improve stability of MD evolution:

1. Use the SMD

In usual HMC:

- possible jumps in phase space trajectory, e.g. from accumulated integration errors.
- re-thermalisation necessary, can lead to extended autocorrelation times.

Alternative approach: **stochastic molecular dynamics (SMD)**

*Horowitz et al. ('85, '86, '91), Jansen et al. ('95)

1.	Refresh $\pi(x,\mu)$ and $\phi(x)$ by a random field rotation:		$\pi \rightarrow c_1\pi + c_2 v$ $\phi \rightarrow c_1\phi + c_2 D^\dagger\eta$ (v and η normal distributed)
	$c_1^2 + c_2^2 = 1$, $c_1 = e^{-\epsilon\gamma}$,	$\epsilon =$ MD integration time,	$\gamma =$ friction parameter
2.	short MD evolution		
3.	Accept/Reject-step		(algorithm exact)
4.	Repeat ↻		

- exact algorithm, coincides with HMC (for $\epsilon =$ fixed, $\gamma =$ large)
- shown to be ergodic for small ϵ
- effective reduction of unbounded energy violations $|\delta H| \gg 1$
- shorter autocorrelation times compensate longer time per MDU

Three ingredients to improve stability of MD evolution:

2. Use a volume-independent norm for solver stopping criterion

$\|\eta - D\tilde{\psi}\|_2 \leq w\|\eta\|_2,$	$\|\eta\|_2 = \left(\sum_x (\eta(x), \eta(x))\right)^{1/2} \propto \sqrt{V}$
uniform norm:	$\|\eta\|_\infty = \mathrm{sup}_x \|\eta\|_2$, V-independent

- norm guarantees the quality of a given solve
- gives insurance against precision losses from local effects in large but also traditional volumes

3. Use quadruple precision in global sums

For the global accept/reject step $\delta H \propto \epsilon^P \sqrt{V}$. This can lead to accumulation errors for global sums. Quadruple precision remedies this

Actions and algorithms - action ingredient of SWF

$\rightsquigarrow$ details given for reference, slides may be skipped 3/3

Improve aspects of the fermion discretisation:
$\rightarrow$ This marks a departure from the standard WCF setup and defines a new action.

The Wilson-Clover action reads:

$$D = \frac{1}{2}\Big[\gamma_\mu\Big(\nabla^*_\mu + \nabla_\mu - a\nabla^*_\mu\nabla_\mu\Big)\Big] + m_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}$$

Wilson term: $\rightsquigarrow$ unbounded below; Clover term: $\rightsquigarrow$ unbounded below

Typically one next classifies the lattice points as even/odd and writes the preconditioned form, $\hat{D} = D_{ee} - D_{eo}(D_{oo})^{-1}D_{oe}$ with diagonal part ($M_0 = 4 + m_0$):

$$D_{ee} + D_{oo} = M_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \quad .$$

Clover term can saturate $\|\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\|_2 \leq 3$ while $c_{sw} \geq 1$ and rising with g_0^2.
$\rightarrow$ Dirac operator is not protected from arbitrarily small eigenvalues

Solution: Define a bounded-from-below Clover term

$$D_{ee} + D_{oo} = M_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \;\rightarrow\; M_0 \exp\left[\frac{c_{SW}}{M_0}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\right] \quad .$$

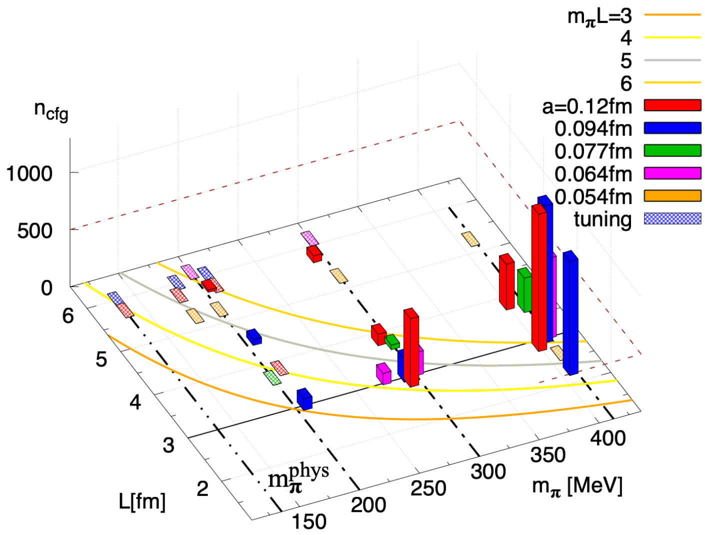
- local change of action
- valid in terms of Symanzik improvement
- guarantees invertibility of the Clover

Gauge generation status

Criteria that have to be fulfilled by a chain of configurations:

- $\phi_4 = 8t_0(m_K^2 + m_\pi^2/2) = 1.115$ within 0.5%, with an error of max. 1σ.
- The total reweighting factor fluctuations are mild, and ideally below 5%.
- The SMD step distance $\delta\tau$ maximises the backtracking period.
- The distribution of δH matches the one set by the acceptance rate.
- The distribution of the lowest $\sqrt{D^\dagger D}$ eigenvalue is well-behaved & gapped.
- The distribution of the lower and upper bounds of the spectral gap for the strange quark are within the input ranges, and the degree of the Zolotarev is sufficiently high, $12(V/2)\delta^2 < 10^{-4}$.
- There is no significant loss of precision caused by unbalanced contributions to the total action that might drive instabilities in the evolution.
- The distribution of the flowed topological charge is symmetric around zero with no signs of metastability.

Gauge generation status



⇝ 500 configurations at all $SU(3)$ flavor points is threshold for publication 1 and also making the ensembles openly accessible.

Data management

1. **Total amount of storage:**
   - Currently 71TB* data saved with $\sim$ 17k saved configurations, projected to 500+TB with completion of stage 2. *estimates include auxiliary measurement data, logs, etc.

2. **Management plan:**
   - Redundancy through mirrors (TPCC, NERSC)
   - Long term storage planned, currently tape option used
   - All metadata preserved on disk and in online repository
   - Main contacts: Andre Walker-Loud, Savvas Zafeiropoulos, Anthony Francis

3. **Metadata:**
   - Detailed provenance policy (runner, machine, code-version, time-stamps)
   - Auxilliary measurements include:
     - Run observables: plaquettes, δH, iteration counts, acceptance
     - Wilson flow observables: energy density (two operators), topological charge
     - Hadronic observables: pp, ap correlators
     - Other observables: reweighting factors, lowest eigenvalues, spectral range
   - Data integrity:
     - all configurations contain the plaquette in header
     - list of checksums for all configurations provided (using md5sum)

4. **Data accessibility:**
   - Main access point: `https://openlat1.gitlab.io`
   - All configurations and metadata are made openly available at time of publication.
   - Online repository connected to main site hosts metadata (currently only internal)

Production, publication and access

- **We follow a 3 stage production plan:**

1. Task: Perform high precision tuning and generate ensembles with 3 dynamical flavors at the SU(3) flavor symmetric point and $m_\pi = m_K = 412$MeV.
Minimum goal:

- 500+ independent configurations based on the larger of τ_Q or τ_E
- 4+ lattice spacings with $\phi_4 = 1.115$ within 0.5% and $\Delta\phi_4 \leq 1\sigma$.

2. Task: Reduce the light quark masses with $\mathrm{Tr}[M] = const$. Points in m_π[MeV] should match across all lattice spacings within a few MeV.
Minimum goal:

- $M_\pi = 300, 200$MeV for $a = 0.12, 0.094, 0.077, 0.064$fm.
- Additional lattice spacing $a = 0.055$fm (open boundary conditions)

3. Task: Go towards the physical values of the pion mass $m_\pi = 135$MeV.
Minimum goal:

- Supply at least 1+ ensemble at the physical point with 500+ configurations

1.-3. Remark: Multiple lattice volumes are generated at all stages. These are extended towards full ensembles with 500+ configurations, where reasonable (i.e. $L \gtrsim 3$fm, $m_\pi L \gtrsim 4$)

Production, publication and access

• Production plan overview:

Stage 1.: $SU(3)$ flavor symmetric point, $M_\pi = M_K = 412$MeV

Stage 2.: $M_\pi = 300$MeV and 200MeV

Stage 3.: $M_\pi = 135$MeV

• Publication plan:

1. Each completed stage is accompanied by a reference publication.
2. All configurations and metadata of that stage are made openly available.
3. No further embargo time.

- Users may obtain access to the configurations of ongoing stages.
- User-access is granted on a case-by-case basis.
- **OpenLat and ILDG**, main contact person: Antonio Rago

• Current status and results, towards publication of stage 1.:

- OpenLat — *Giovanni Pederiva, Tue. 9.08., 16:50

• Current user's projects include:

- nEDM — *Jangho Kim, presented at ECT* last week
- hadronic decays — *Fabian Joswig, Thu. 11.08., 12:30
- multi-nucleons — *Jeremy Green (BASC), Thu. 11.08., 12:10

Stage 1 production overview

Stage	m_π[MeV]	β	a[fm]	L	T	BC	N_{cfg}	MDU$^{(1)}$
1	412	3.685	0.12	24	96	P	1200	24800
				32	96	P	400	8300
		3.8	0.094	24	96	P	1200	35000
				32	96	P	1300	38800
		3.9	0.077	48	96	P	300	11000
		4.0	0.064	48	96	P	600	24500
2	300$^{(2)}$	3.685	0.12	24	96	P	600	13000
		3.8	0.094	32	96	P	300	8000
		4.0	0.064	48	96	P	200	6000

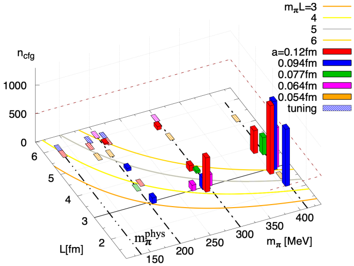
$^{(0)}$ all ensembles are currently still gathering more statistics
$^{(1)}$ converted from trajectory length in SMD
$^{(2)}$ openly available in stage 1 or 2 depending on progress but avoiding delays

Summary

- SWF toolkit of measures for more stable generation
- OPEN LATtice initiative founded to further research SWF and provide ensembles for physics applications under open science policy

OPEN LATtice initiative

openlat1.gitlab.io



Status overview

- 3 stage plan
- stage 1 nearing completion ($SU(3)_f$, $4 \times a$, $N = 500+$)
- tuning for stages 2, 3 continues
- access to ensembles at publication
- early access on case-by-case basis
- data management plan formulated
- ILDG contact person in place

SWF at Lattice'22 - come visit the talks and posters using SWF :o)

*Anthony Francis, Mon. 8.08., 14:40

*John Bulava, Tue. 9.08., 9:20

*Giovanni Pederiva, Tue. 9.08., 16:50

*Rocco Francesco Basta, Tue. 9.08., 20:00

*Justus Kuhlmann, Tue. 9.08., 20:00

*Marco Cè, Thu. 11.08., 11:50;

*Jeremy Green, Thu. 11.08., 12:10

*Fabian Joswig, Thu. 11.08., 12:30

*Patrick Fritzsch, Sat. 13.08., 9:20

Thank you for your attention.