Solving $\mathrm{SU}(3)$ Yang-Mills theory on the lattice: a calculation of selected gauge observables with gradient flow

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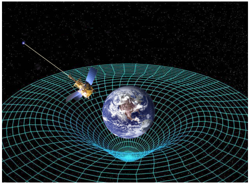
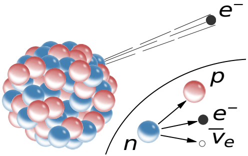
The four forces of nature

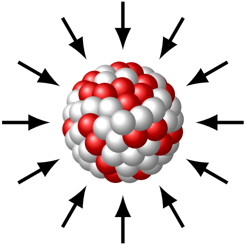


Gravity

Electromagnetism



Weak nuclear force



Strong nuclear force

What is the strong force?

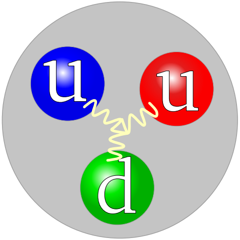
Consists of:

- 6 quark flavors: up, down, strange, charm, bottom and top
- 8 gluons

A **proton** consists of: up-, up- and down-quarks
Mass discrepancy:

$$m_p \neq m_u + m_u + m_d,$$

936 MeV $\neq 3$ MeV $+ 3$ MeV $+ 6$ MeV.



Comparing the strong force and QED

Electromagnetism or **Quantum Electrodynamics**(QED), a U(1) symmetry theory:

$$\mathcal{L}_{\mathrm{QED}} = \sum_{f=\text{fermions}} \bar{\psi}_f(i\gamma^\mu(\partial_\mu + ieQ_f A_\mu) - m_f)\psi_f - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$

Field strength tensor:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

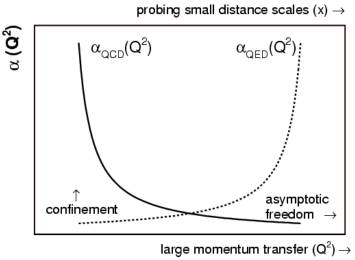
The **strong nuclear force** or **Quantum Chromo Dynamics**(QCD), a $\mathrm{SU}(3)$ symmetry theory:

$$\mathcal{L}_{\mathrm{QCD}} = \sum_{f=u,d,\ldots} \bar{\psi}_f(i\gamma^\mu(\partial_\mu + ig_S A_\mu^a T^a) - m_f)\psi_f - \frac{1}{4}G^a_{\mu\nu}G^{a\mu\nu}$$

Field strength tensor:

$$G^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g_S f^{abc} A^b_\mu A^c_\nu$$

Why is the strong force strong?

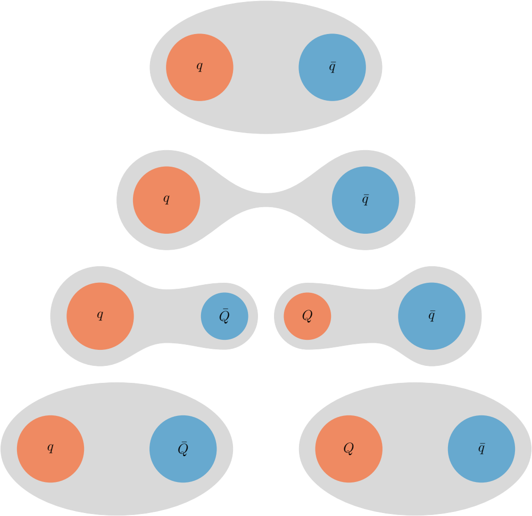


https://www-cdf.fnal.gov/~group/WORK/DISS_PAGE/diss_page.htm

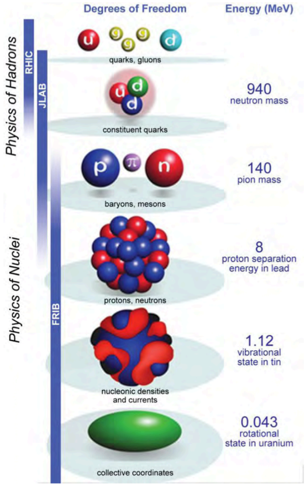
- Coupling constant α is the strength of the force in an interaction.
- QED becomes stronger - QCD becomes weaker at higher energies.
- Can't use perturbation theory on strong force in low-energy regime!
- Need to understand the low-energy regime to understand phenomenas such as **confinement**.

Confinement: a low-energy phenomena

No free quarks in nature!



QCD and nuclear physics



- Need to understand the low-energy regime in order to better understand nuclear physics!
- Want to bridge the gap between theories that operate at different scales.
- $\rightarrow$ numerical methods(e.g. lattice QCD)

FRIB Users Organization for the NSAC Long Range Plan Implementation Subcommittee

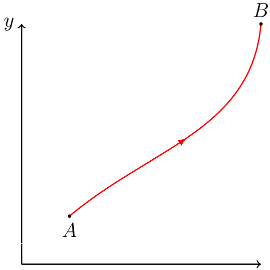
We currently have...

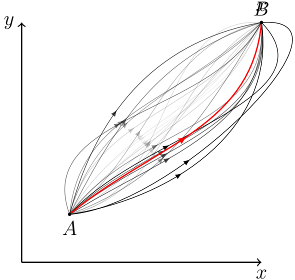
- A theory for QCD in the **continuum**.
- Which we solve QCD by a Feynman **path integral**.
- We want to solve this **numerically**.
- $\rightarrow$ need to **discretize** the path integral.

But first, we need to know *what* a path integral is.

How we measure: path integrals

Going from t_0 at A to a time t_1 at B can be given in terms of a path integral.





Path integrals

Given a field ϕ_M in Minkowski space, the *partition function* Z is given by

$$
\begin{aligned}
Z &= \int \mathcal{D}\phi_M \mathrm{e}^{\frac{i}{\hbar} S_M[\phi_M]} \\
&\downarrow \quad \hbar = 1, \quad \tau \to -it \qquad \text{imaginary time}(\to \text{Euclidean space})! \\
&= \int \mathcal{D}\phi \mathrm{e}^{-S[\phi]}
\end{aligned}
$$

where $\mathcal{D}$ is an integration of all possible paths in space.
An observable O becomes,

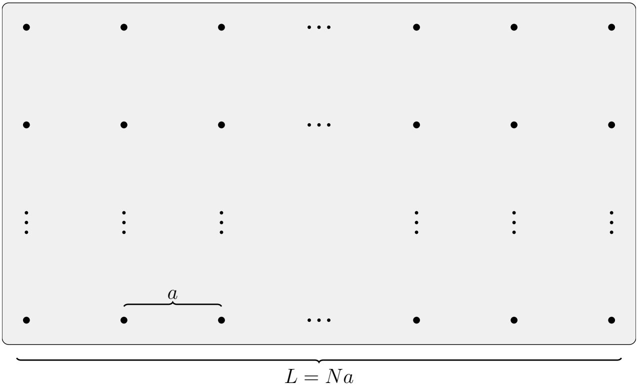
$$
\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi O[\phi] \mathrm{e}^{-S[\phi]}
$$

with action given in terms of spacetime integral of the Lagrangian $\mathcal{L}$

$$
S = \int \mathrm{d}^4 x \mathcal{L}
$$

Difficult to calculate the all possible paths $\to$ discretize spacetime

Discretizing the path integral



Discretizing the path integral

Path integral integration measure becomes

$$\int \mathcal{D}\phi = \prod_{x_\mu} \int \mathrm{d}\phi_{x_\mu}$$

We integrate over each spacetime point.
$32 \times 32 \times 32 \times 32 = 2^{20} \to n^{2^{20}}$ integration points.
A **statistical approach** using importance sampling is needed for generating gauge configurations.

Configurations: comparing QCD and the Ising model

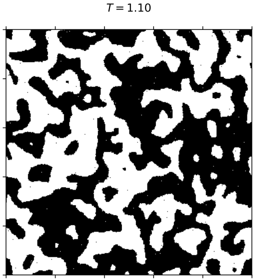
The 2D Ising model is given by:

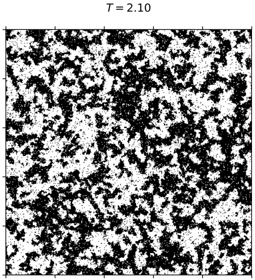
$$H = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

- Ising model only has two possible values at a spin site S_i: $\uparrow$, $\downarrow$
- QCD many more degrees of freedom: quarks, gluons, color, charge, …
- With $N = 10$, a lattice in the Ising model has the size $10 \times 10 = 100$.
- A lattice in LQCD is however $N^4 = 10000$.

Then what is a configuration?

Looking at a spin lattice of the Ising model,





- A **configuration** in the Ising model is a given *arrangement of the spins*.
- A **configuration** in LQCD is a given *arrangement of the gauge field*.

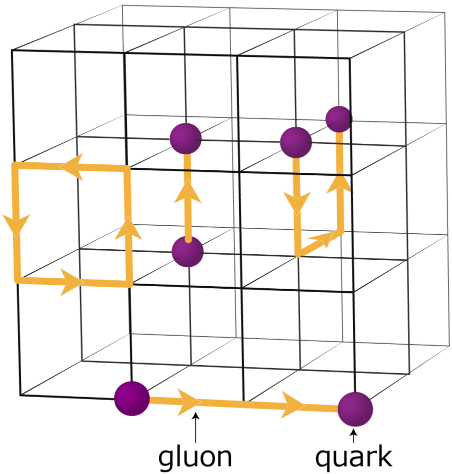
Sampling configurations

An expectation value becomes

$$\langle O \rangle = \frac{1}{N_{\mathrm{cfg}}} \sum_{i=1}^{N_{\mathrm{cfg}}} O[\phi_i] + \mathcal{O}\left(\frac{1}{\sqrt{N_{\mathrm{cfg}}}} \right)$$

where ϕ_i is a generated gauge configuration(or just a general configuration).

QCD on the lattice



http://www.jicfus.jp/en/wp-content/uploads/2012/12/LatticeQCD.png

From QCD to pure $\mathrm{SU}(3)$ Yang-Mills

We exclude fermions to only look at the gauge fields,

$$S_G = \frac{1}{2} \int \mathrm{d}^4 x \mathrm{tr} \left(G_{\mu\nu} \right)^2$$

Links

- *Links* $U_\mu(n)$ tell us how the gauge field at lattice location n changes in a given direction $\hat{\mu}$
- Four links at every lattice site(one for each Lorentz index). Opposite direction given by its inverse.
- Links are complex 3×3 matrices of the group $\mathrm{SU}(3)$ with properties of,

$$U_\mu^\dagger(x) = U_\mu^{-1}(x), \qquad \det\left(U_\mu(x)\right) = 1.$$

From this we can build a lattice action,

$$S_G[U] = \frac{\beta}{3} \sum_{n \in \Lambda} \sum_{\mu < \nu} \mathrm{Re}\,\mathrm{tr}\left[1 - U_\mu(n)\, U_\nu(n+\hat{\mu})\, U_\mu(n+\hat{\nu})^\dagger\, U_\nu(n)^\dagger\right],$$

with $\beta = 6/g_S^2$

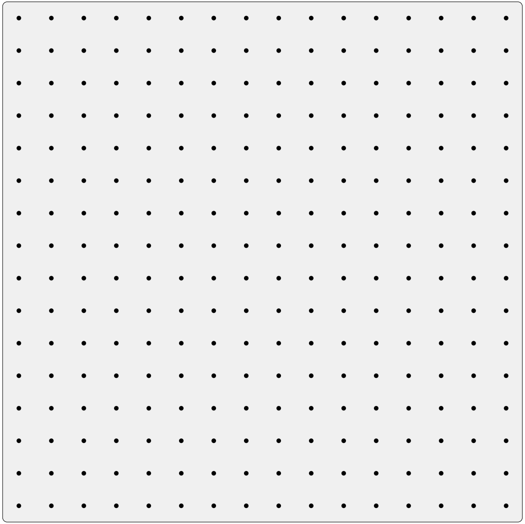
Parallelization: distributing the problem

Number of points in a lattice:

$$\underbrace{N^3}_{\text{Spatial}} \times \underbrace{N_T}_{\text{Temporal}} \times \underbrace{4}_{\text{Links}} \times \underbrace{9}_{\mathrm{SU}(3)\text{ matrix}} \times \underbrace{2}_{\mathbb{C}\text{-numbers}} = 72N^3N_T,$$

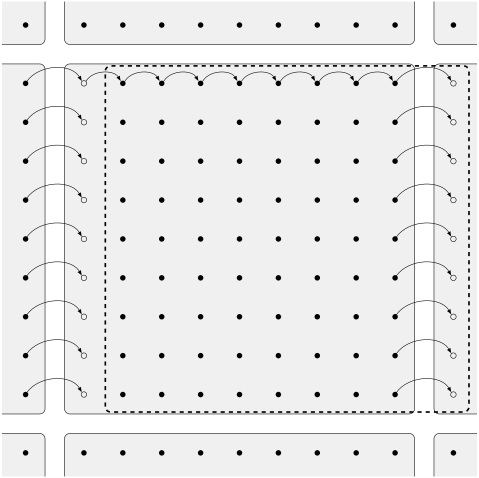
Too large to solve on any single computer.

Parallelization: splitting the hypercube



Parallelization: shifts

We need a message passing interface for communication(MPI).
Implemented *shifts* for sharing data.



So far, we have ...

- a procedure for calculating the action using links.
- a statistical Monte Carlo method for solving the path integral.
- We have a method for parallelization for handling the computations.

However, some observable are problematic...

Gradient flow

$$\partial_{t_f} B_\mu(x, t_f) = D_\nu G_{\nu\mu}(x, t_f)$$
$$B_\mu(x, t_f)\Big|_{t_f=0} = A_\mu(x)$$

- Solves this by integrating along t_f called *flow time* [1]
- $B_\mu(x, t_f)$ is the gauge field $A_\mu(x)$ at a flow time t_f.
- $D_\nu = \partial_\nu + [B_\mu(x, t_f), \cdot]$
- Field strength tensor:
  $G_{\mu\nu}(x, t_f) = \partial_\mu B_\nu(x, t_f) - \partial_\nu B_\mu(x, t_f) - i[B_\mu(x, t_f), B_\nu(x, t_f)]$

An analogy: the diffusion equation:

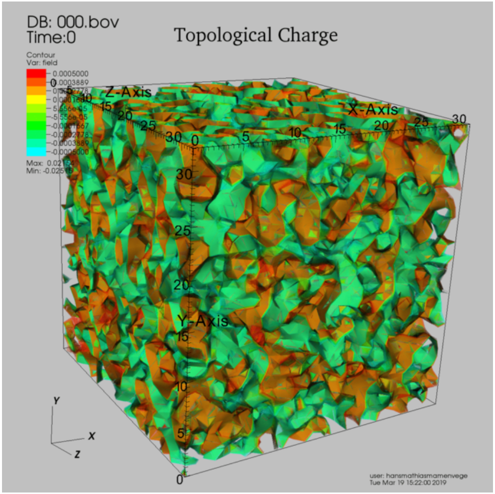
$$\frac{\partial}{\partial t_f} B_\mu(x, t_f) \approx \partial_x^2 B_\mu(x, t_f)$$

[1] Lüscher [2010]

Gradient flow II

- The gauge field at $t_f > 0$ is a **smooth, renormalized field**.
- Allows us to measure certain quantities such as the **topological charge**, Q

Gradient flow III: topological charge



Animation created using LatViz.

Results

Ensembles

Points in lattice given by $N^3 \times N_T$.

Ensemble	$\beta = 6/g_S^2$	N	N_T	N_{cfg}	a [fm]	Config. size[GB]
A	6.0	24	48	1000	$0.0931(4)$	0.356
B	6.1	28	56	1000	$0.0791(3)$	0.659
C	6.2	32	64	2000	$0.0679(3)$	1.125
D_1	6.45	32	32	1000	$0.0478(3)$	0.563
D_2	6.45	48	96	250	$0.0478(3)$	5.695

A scale t_0 was set using the energy and gradient flow.

Topological charge

- QCD vacua(i.e. gauge fields) can be classified by their topological properties.
- In this vacua, **instantons** are local minima of the Yang-Mills action in Euclidean space, as they are solutions to the e.o.m.
- **Topological charge** Q can be viewed as a "measure" of instantons.

$$Q = a^4 \sum_{n \in \Lambda} q(n),$$

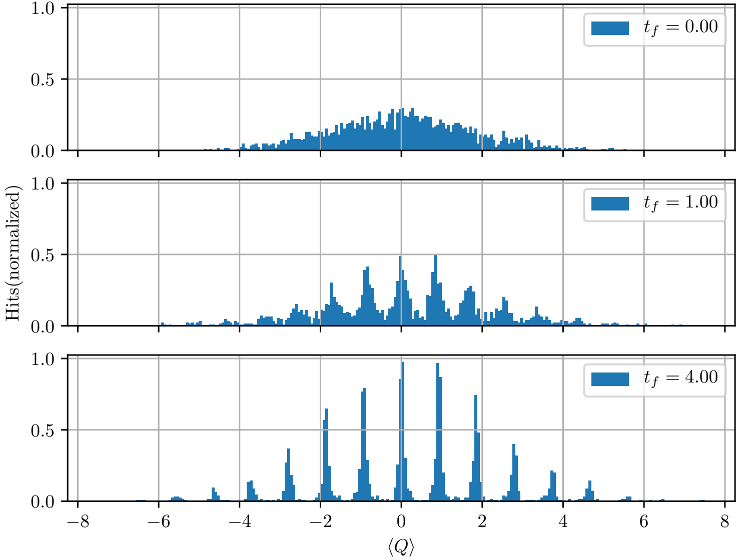
with the charge density given by

$$q(n) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathrm{tr} \left[G_{\mu\nu}(n) G_{\rho\sigma}(n) \right].$$

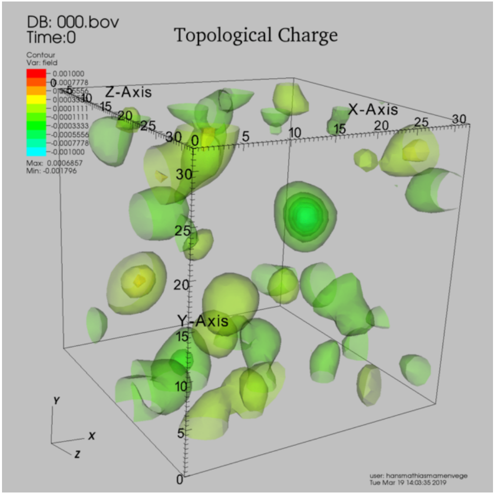
Integer valued and equally probably to have negative charge as positive,

$$\langle Q \rangle = 0$$

Topological charge distribution

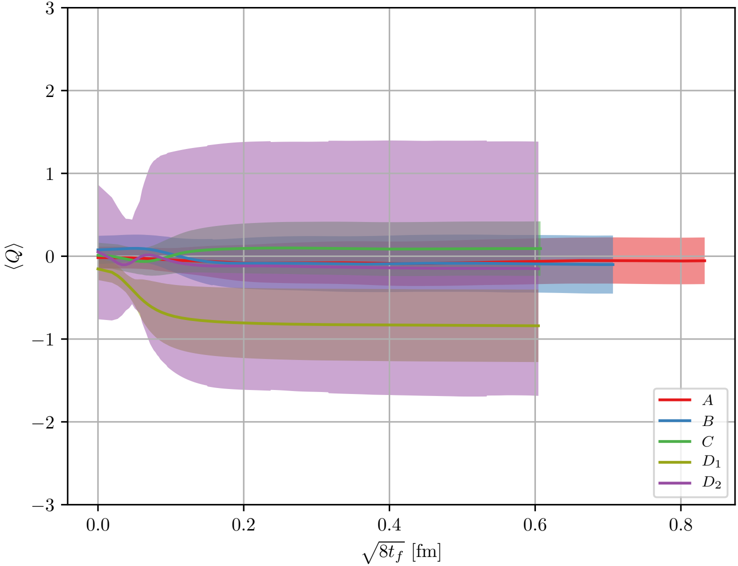


Topological charge



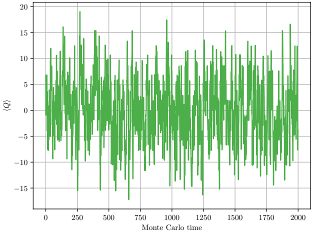
Animation created using LatViz.

Topological charge for our main ensembles

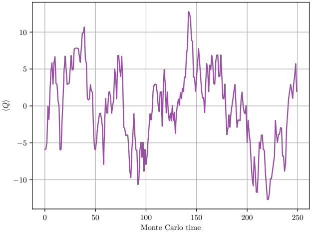


Autocorrelations

- Why is the charge not centered around zero for certain ensembles?
- Let us look at the **autocorrelation** - the measure for correlations between gauge configurations in Monte Carlo time.
- The autocorrelation is given as $\Gamma(t) = \langle (x_i - x)(x_{i+t} - x) \rangle$ and $\tau_{\text{int}} = \frac{1}{2} + \sum_{t=1}^{\infty} \frac{\Gamma(t)}{\Gamma(0)}$.
- **Zero autocorrelation** corresponds to $\tau_{\text{int}} = 0.5$

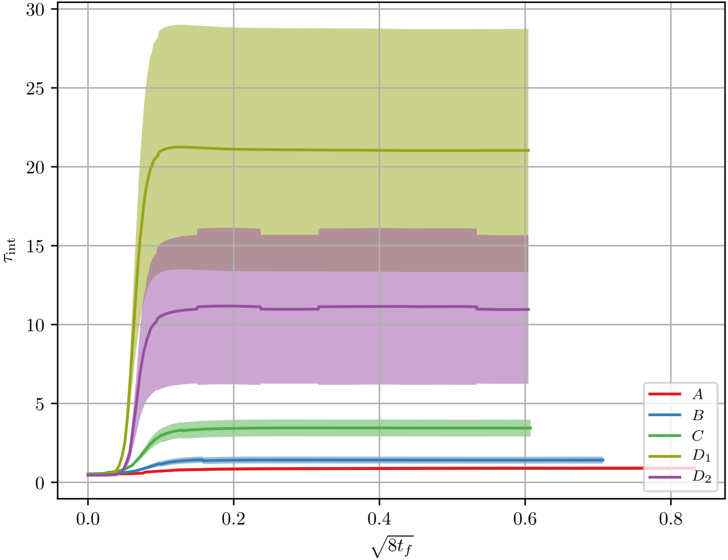


Ensemble C, $32^3 \times 64$, $\beta = 6.2$



Ensemble D_2, $48^3 \times 96$, $\beta = 6.45$

Topological charge autocorrelation



Critical slowing down

- Critical slowing down is the phenomena where we as the lattice spacing a *decreases* the required energy to tunnel from one topological sector to another *increase*.
- In the continuum, going from one topological sector, a region with similar topological charge, to another require infinite energy. As $a \to 0$, the amount of effort required to change the configuration increases.
- $\rightarrow$ many more lattice updates are required in order to have independent gauge configurations.

Topological susceptibility

The *topological susceptibility* is given by

$$\chi_{\text{top}}^{1/4} = \frac{1}{V^{1/4}} \left\langle Q^2 \right\rangle^{1/4}$$

with V being the lattice volume and $\left\langle Q^2 \right\rangle$ is the second momenta of the charge.

The *Witten-Veneziano relation* is given by

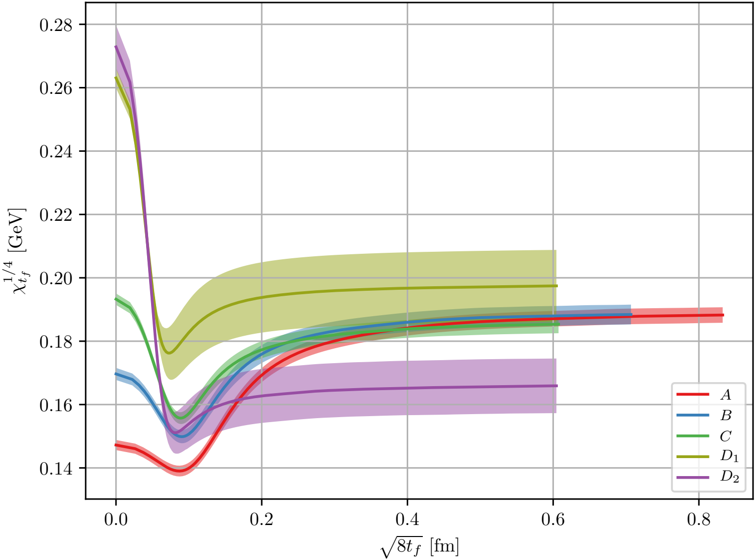
$$m_{\eta'}^2 = \frac{2N_f}{f_\pi^2} \chi_{\text{top}}$$

with

- pion decay constant $f_\pi = 0.130(5)/\sqrt{2}$ GeV.
- η' meson mass $m_{\eta'} = 0.95778(6)$ GeV.
- N_f is the number of flavors(i.e. quark species involved in η'.).

We expect $N_f = 3$.

Topological susceptibility



Topological susceptibility continuum extrapolation

Ensembles	$\chi_{t_f}^{1/4}\left(\langle Q^2\rangle\right)$ [GeV]	N_f	$\chi^2/\mathrm{d.o.f}$
A, B, C, D_2	$0.179(10)$	$3.75(29)$	2.38
A, B, C, D_1	$0.186(6)$	$3.21(25)$	0.83
A, B, C	$0.184(6)$	$3.37(26)$	0.33

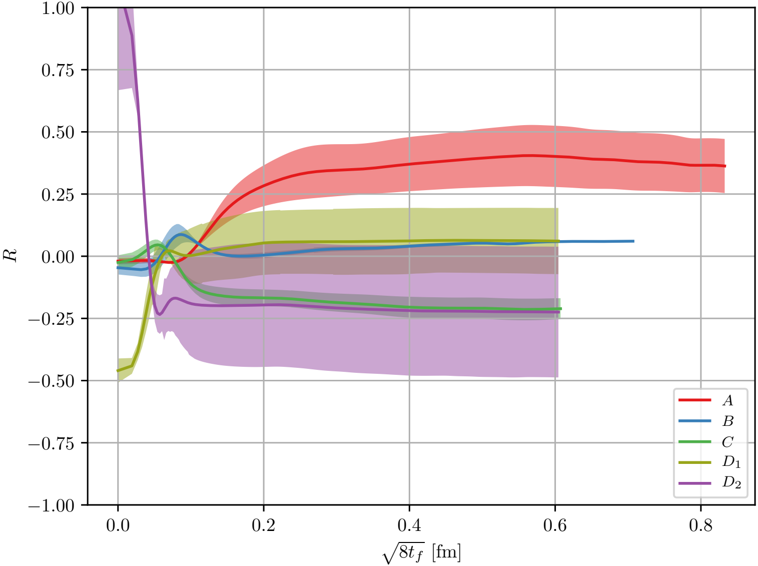
The fourth cumulant

$$\left\langle Q^4 \right\rangle_c = \frac{1}{V^2}\left(\left\langle Q^4 \right\rangle - 3\left\langle Q^2 \right\rangle^2\right).$$

From this, we can also measure the ratio R,

$$R = \frac{\left\langle Q^4 \right\rangle_c}{\frac{1}{V}\left\langle Q^2 \right\rangle} = \frac{1}{V}\frac{\left\langle Q^4 \right\rangle - 3\left\langle Q^2 \right\rangle^2}{\left\langle Q^2 \right\rangle},$$

The fourth cumulant



The fourth cumulant at reference flow times

Ensemble	L/a	t_0/a^2	$\langle Q^2 \rangle$	$\langle Q^4 \rangle$	$\langle Q^4 \rangle_C$	R
A	2.24	3.20(3)	0.78(4)	2.13(27)	0.282(67)	0.359(65)
B	2.21	4.43(4)	0.81(5)	1.98(23)	0.036(11)	0.044(11)
C	2.17	6.01(6)	0.77(4)	1.6(2)	−0.174(40)	−0.226(64)
D_1	1.53	12.2(1)	1.00(20)	3.01(1.07)	0.03(12)	0.03(12)
D_2	2.29	12.2(1)	0.497(100)	0.64(20)	−0.103(95)	−0.21(23)

Comparing fourth cumulant

We can compare with article by Cè et al. [2015]

Ensemble	β	L/a	L [fm]	a [fm]	t_0/a^2	t_0/r_0^2	N_{cfg}
F_1	5.96	16	1.632	0.102	2.7887(2)	0.1113(9)	1 440 000
B_2	6.05	14	1.218	0.087	3.7960(12)	0.1114(9)	144 000
$\tilde{D}_2$		17	1.479		3.7825(8)	0.1110(9)	
B_3	6.13	16	1.232	0.077	4.8855(15)	0.1113(10)	144 000
$\tilde{D}_3$		19	1.463		4.8722(11)	0.1110(10)	
B_4	6.21	18	1.224	0.068	6.2191(20)	0.1115(11)	144 000
$\tilde{D}_4$		21	1.428		6.1957(14)	0.1111(11)	

Article	Thesis	Ratio($\langle Q^2 \rangle$)	Ratio($\langle Q^4 \rangle$)	Ratio($\langle Q^4 \rangle_C$)	Ratio(R)
F_1	A	1.08(6)	1.34(18)	19.03(5.81)	17.64(4.48)
B_2	A	1.02(5)	1.15(15)	3.60(1.09)	3.54(90)
	B	1.04(6)	1.06(11)	0.480(74)	0.46(4)
$\tilde{D}_2$	A	1.02(5)	1.19(15)	8.31(1.99)	8.15(1.56)

The topological charge correlator and the effective glueball mass

The **topological charge correlator**

$$C(n_t) = \langle q(n_t) q(0) \rangle \,,$$

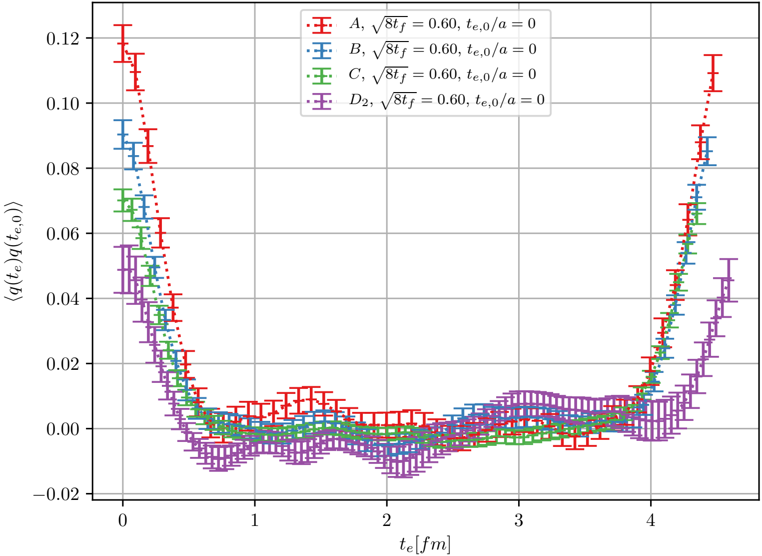
is the correlator between two topological charge densities in Euclidean time.
The ground state in the correlator is given as

$$C(n_t) = A_0 \mathrm{e}^{-n_t E_0} + A_1 \mathrm{e}^{-n_t E_1} + \dots$$

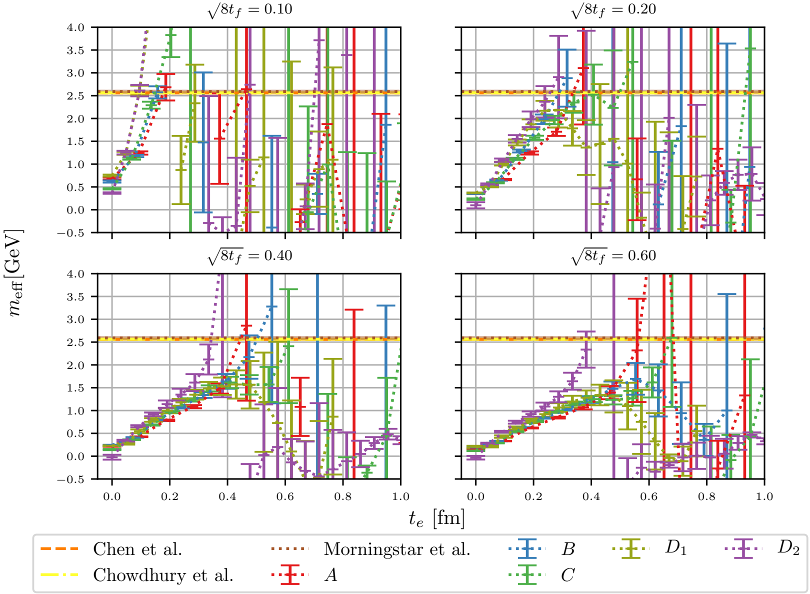
from which the **effective glueball mass** can be extracted as

$$a m_{\mathrm{eff}} = \log \left(\frac{C(n_t)}{C(n_t + 1)} \right),$$

The topological charge correlator



The effective glueball mass



Conclusion, future developments and final thoughts

Conclusion

- Created a code (GLAC) capable of generating and flowing gauge configurations.
  - Verified to match other code bases down to machine precision.
- Created a code (LatViz) for visualizing gauge fields.
- $\langle Q \rangle \neq 0$ for some ensembles $\rightarrow$ understood with autocorrelation.
- The topological susceptibility $\chi_f^{1/4}$ and N_f
- $\left\langle Q^4 \right\rangle_C$ and R. Sensitive quantities - need large statistics.
- Topological charge correlator $\langle q(n_t) q(0) \rangle$ and glueball mass.
- Statistics, autocorrelation and critical slowing down.
- The energy, the scale t_0 and w_0 were also calculated match what is found in the literature, i.e. Lüscher [2010] and Cè et al. [2015].

Future developments and final thoughts

- Better statistics - more gauge configurations.
- Implement better actions with operators that have smaller error contributions.
- Fermions and HMC(Hybrid Monte Carlo).

Thank you for listening.

Questions?

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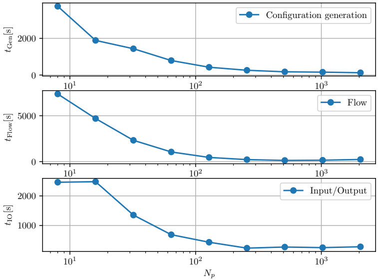
Extra slides

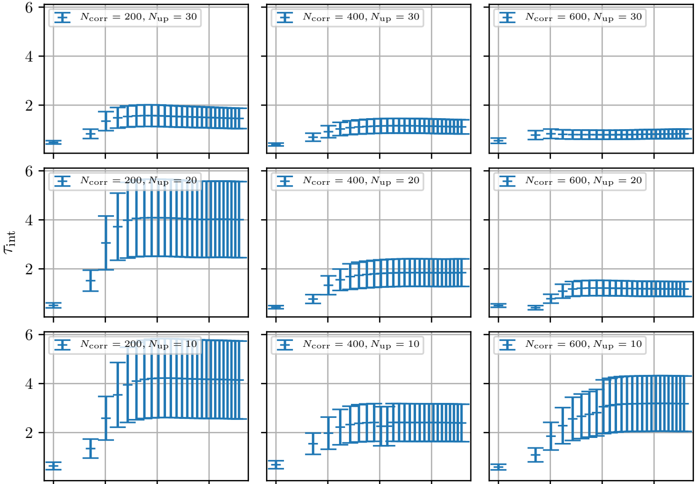
We checked three types of scaling,

- **Strong scaling:** *fixed problem* and a *variable N_p cores*
- **Weak scaling:** *fixed problem per processor* and a *variable N_p cores.*
- **Speedup:** defined as $S(p) = \frac{t_{N_p}}{t_{N_p,0}}$.



Optimizing the gauge configuration generation

Generated 200 configurations for a lattice of size $N^3 \times N_T = 16^3 \times 32$ and $\beta = 6.0$, for combinations of $N_{\mathrm{corr}} \in [200, 400, 600]$ and $N_{\mathrm{up}} \in [10, 20, 30]$.



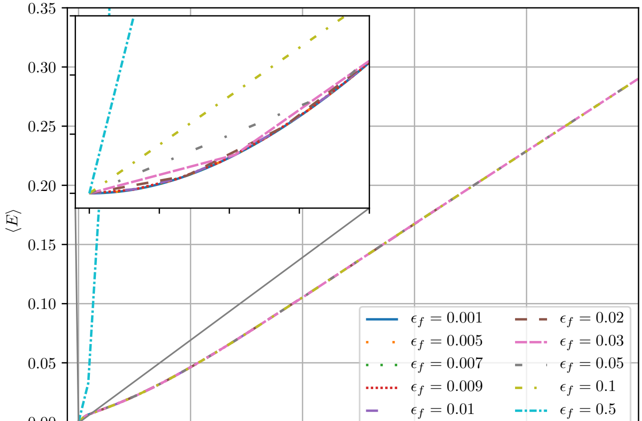
Verifying the code

- Unit testing. $\mathrm{SU}(3)$, $\mathrm{SU}(2)$ multiplications.
- Integration testing. Random matrix generation, lattice objects, parallelization, ect.
- Validation testing. Cross checking results with a configuration from Chroma.

Testing the integrator for different integration steps ϵ_f.

ϵ_f	0.001	0.005	0.007	0.009	0.01	0.02	0.03	0.05	0.1	0.5

Lattice size $N^3 \times N_T = 24^3 \times 48$ with $\beta = 6.0$.



The non-linearity of QCD

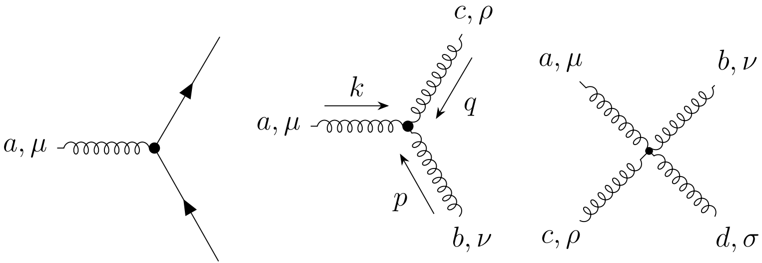
The QCD Lagrangian

$$\mathcal{L}_{\mathrm{QCD}} = \sum_{f=1}^{N_f} \bar{\psi}^{(f)} \left(i\not{D} - m^{(f)} \right) \psi^{(f)} - \frac{1}{4} G^a_{\mu\nu} G^{a\mu\nu},$$

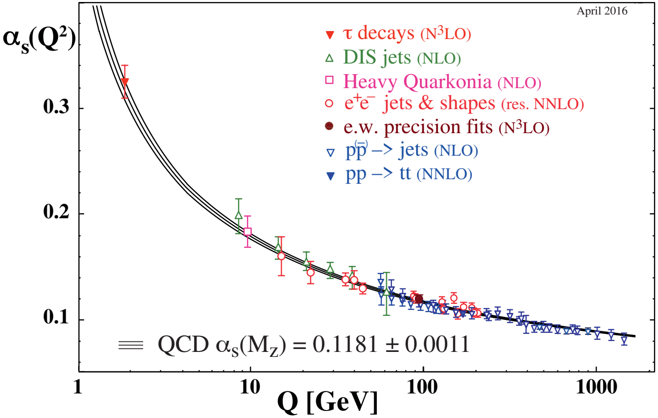
with action

$$S = \int \mathrm{d}^4 x \mathcal{L}_{\mathrm{QCD}}, \tag{1}$$

is invariant under a $\mathrm{SU}(3)$ symmetry.



Asymptotic freedom



Solving gradient flow with Runge-Kutta 3

With

$$\dot{V}_{t_f} = -g_S^2 \left\{\partial_{x,\mu} S_G[V_{t_f}]\right\} V_{t_f} = Z(V_{t_f}) V_{t_f},$$

and $Z_i = \epsilon_f Z(W_i)$ we get

$$\begin{aligned}
W_0 &= V_{t_f}, \\
W_1 &= \exp\left[\frac{1}{4} Z_0\right] W_0, \\
W_2 &= \exp\left[\frac{8}{9} Z_1 - \frac{17}{36} Z_0\right] W_1, \\
V_{t_f+\epsilon_f} &= \exp\left[\frac{3}{4} Z_2 - \frac{8}{9} Z_1 + \frac{17}{36} Z_0\right] W_2,
\end{aligned}$$

with coefficients from Lüscher [2010].

Additional ensembles

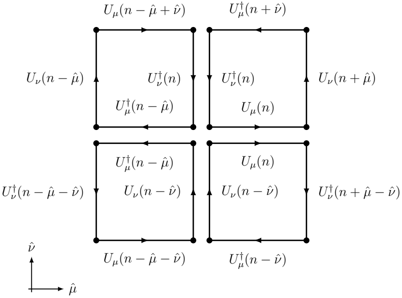
Ensemble	N	N_T	N_{cfg}	N_{corr}	N_{up}	a [fm]	L [fm]
E	8	16	8135	600	30	0.0931(4)	0.745(3)
F	12	24	1341	200	20	0.0931(4)	1.118(5)
G	16	32	2000	400	20	0.0790(3)	1.265(6)

Energy definition

We use t_0

$$E = \frac{a^4}{2|\Lambda|} \sum_{n \in \Lambda} \sum_{\mu,\nu} \left(F^{\text{clov}}_{\mu\nu}(n) \right)^2$$

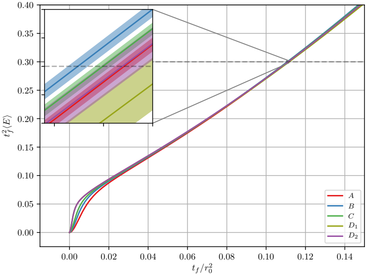
$F^{\text{clov}}_{\mu\nu}(n)$ is given by

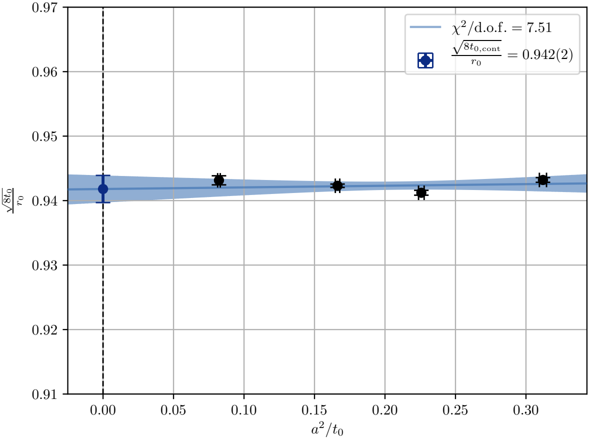


Energy

Using scale definition t_0 from Lüscher [2010],

$$\left\{ t_f^2 \langle E(t) \rangle \right\}_{t_f = t_0} = 0.3.$$





Continuum extrapolation using ensembles A, B, C, and D_2 gives $t_{0,\text{cont}}/r_0^2 = 0.11087(50)$. This matches the values retrieved by Lüscher [2010],

a = 0.05 fm 0.07 fm 0.1 fm

Scale setting t_0

Ensemble	L/a	L [fm]	a [fm]
A	24	2.235(9)	0.0931(4)
B	28	2.214(10)	0.0791(3)
C	32	2.17(1)	0.0679(3)
D_1	32	1.530(9)	0.0478(3)
D_2	48	2.29(1)	0.0478(3)

Ensemble	t_0[fm^2]	t_0/a^2	t_0/r_0^2
A	0.02780(2)	3.20(3)	0.11121(9)
B	0.02769(2)	4.43(4)	0.11075(10)
C	0.02775(2)	6.01(6)	0.11099(8)
D_1	0.02779(5)	12.2(1)	0.1112(2)
D_2	0.02794(9)	12.2(1)	0.1117(3)

Scale setting t_0

Extrapolations for different ensemble-combinations

Ensembles	$t_{0,\mathrm{cont}}/r_0^2$	$\chi^2/\mathrm{d.o.f}$
A, B, C, D_2	$0.11087(50)$	7.51
B, C, D_2	$0.1115(3)$	0.41
A, B, C, D_1	$0.1119(6)$	0.88

Scale setting w_0

Can also set a scale using the derivative which offers more granularity for small flow times,

$$W(t)|_{t=w_0^2} = 0.3,$$
$$W(t) \equiv t_f \frac{\mathrm{d}}{\mathrm{d}t_f} \left\{ t_f^2 \langle E \rangle \right\}.$$

First presented by Borsanyi et al. [2012].

Ensembles	$w_{0,\mathrm{cont}}$[fm]	$\chi^2/\mathrm{d.o.f}$
A, B, C, D_2	$0.1695(5)$	7.12
B, C, D_2	$0.1702(3)$	0.53
A, B, C, D_1	$0.1706(6)$	0.86

Comparable to Borsanyi et al. [2012] which included dynamical fermions, with $w_{0,\mathrm{cont}} = 0.1755(18)(04)$ fm.

Autocorrelation in the energy