Using the Complex Langevin equation to map out the phase diagram of QCD

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1. Introduction to the sign problem and CLE
2. Boundary terms
3. Review of results so far
4. Full QCD
   - Challenges of a full QCD simulation with CLE
   - Pressure
   - Improved actions
We are interested in a system described with the partition sum:

\[ Z = \text{Tr} \, e^{-\beta (H - \mu N)} = \sum_C W[C] \]

Typically exponentially many configurations, no direct summation possible.

If the weight is positive, build a Markov chain with the Metropolis alg.

... \rightarrow C_{i-1} \rightarrow C_i \rightarrow C_{i+1} \rightarrow ...

Probability of visiting \( C \):

\[ p(C) = \frac{1}{N_W} W[C] \]

\[ \langle X \rangle = \frac{1}{Z} \text{Tr} \, X \, e^{-\beta (H - \mu N)} = \frac{1}{N_W} \sum_C W[C] \, X[C] = \frac{1}{N} \sum_i X[C_i] \]

This works if we have \( W[C] \geq 0 \)

Otherwise we have a Sign problem.
Sign problems in high energy physics

Real-time evolution in QFT

“strongest” sign problem \( e^{i S_M} \)

Non-zero density (and fermionic systems)

\[
Z = \text{Tr} e^{-\beta (H - \mu N)} = \int DU e^{-S[U]} \det(M[U])
\]

Many systems: Bose gas
XY model
SU(3) spin model
Random matrix theory
QCD

Theta therm

\[
S = F_{\mu \nu} F^{\mu \nu} + i \Theta \epsilon^{\mu \nu \theta \rho} F_{\mu \nu} F_{\theta \rho}
\]

And everything else with complex action

\[
w[C] = e^{-S[C]} \quad w[C] \text{ is positive} \iff S[C] \text{ is real}
\]
How to solve the sign problem?

Probably no general solution – There are sign problems which are NP hard

Many solutions for particular models with sign problem exist

Transforming the problem to one with positive weights

\[ Z = \text{Tr} e^{-\beta (H - \mu N)} = \sum_{C} W[C] = \sum_{D} W'[D] \]  

Dual variables

Worldlines

\[ Z = \text{Tr} e^{-\beta (H - \mu N)} = \sum_{n} Z_n e^{\beta \mu n} \]  

Canonical ensemble

\[ Z = \text{Tr} e^{-\beta (H - \mu N)} = \int dE \rho_{\mu}(E) e^{-\beta E} \]  

Density of states

\[ Z = \text{Tr} e^{-\beta (H - \mu N)} = \sum_{C} W[C] = \sum_{S} \left( \sum_{C \in S} W[C] \right) \]  

Subsets
How to solve the sign problem?

Extrapolation from a positive ensemble

Reweighting

\[
\langle X \rangle_w = \frac{\sum_c W_c X_c}{\sum_c W_c} = \frac{\sum_c W'_c (W_c / W'_c) X_c}{\sum_c W'_c (W_c / W'_c)} = \frac{\langle (W / W') X \rangle_{w'}}{\langle W / W' \rangle_{w'}}.
\]

Taylor expansion

\[
Z(\mu) = Z(\mu = 0) + \frac{1}{2} \mu^2 \partial^2_\mu Z(\mu = 0) + ...\]

Analytic continuation from imaginary sources
(chemical potentials, theta angle, ..)

Using analyticity (for complexified variables)

Complex Langevin

Complexified variables - enlarged manifolds

Lefschetz thimble - Sign optimized manifolds
Integration path shifted onto complex plane
Complex Langevin Equation

Given an action $S(x)$

Stochastic process for $x$:
$$\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

Gaussian noise
$$\langle \eta(\tau) \rangle = 0$$
$$\langle \eta(\tau) \eta(\tau') \rangle = \delta(\tau - \tau')$$

Averages are calculated along the trajectories:
$$\langle O \rangle = \lim_{T \to \infty} \frac{1}{T} \int_0^T O(x(\tau)) d\tau = \frac{\int e^{-S(x)} O(x) dx}{\int e^{-S(x)} dx}$$

The field is complexified

real scalar $\rightarrow$ complex scalar

link variables: SU(N) $\rightarrow$ SL(N,C)
compact $\rightarrow$ non-compact

$\text{det}(U) = 1, \quad U^* \neq U^{-1}$

Analytically continued observables
$$\frac{1}{Z} \int P_{\text{comp}}(x) O(x) dx = \frac{1}{Z} \int P_{\text{real}}(x, y) O(x + iy) dx dy$$

$$\langle x^2 \rangle_{\text{real}} \rightarrow \langle x^2 - y^2 \rangle_{\text{complexified}}$$
\[
\frac{dx}{d\tau} = -\frac{\partial S}{\partial x} + \eta(\tau)
\]

Stochastic Quantisation [Parisi, Wu (1981)]

\[
S(x) \in \mathbb{C} \quad x \rightarrow x + iy
\]

[Klauder ‘83, Parisi ‘83]

“troubled past”: Lack of theoretical understanding
Convergence to wrong results
Runaway trajectories

Klauder '83, Parisi '83, Hueffel, Rumpf '83, Karsch. Wyld '84, Gausterer, Klauder '86.
Matsui, Nakamura '86, ...
Interest went down as difficulties appeared
Renewed interest in connection of otherwise unsolvable problems
applied to nonequilibrium: Berges, Stamatescu '05, ...
aimed at nonzero density QCD: Aarts, Stamatescu '08 ... many important results since revival
Status of Complex Langevin

Theoretically

Good understanding of the failure modes (boundary terms, poles)
Monitoring prescriptions allow for independent detection of failure
   unitarity norm, eigenspectrum, histograms, boundary terms
Is a cutoff allowed? (Dynamical stabilization)
How to cure problems? – No general answer, hit and miss

In practice

Many lattice models solved, crosschecked with alternative methods
   (Bose gas, SU(3) Spin model, HDQCD, kappa exp., cond. mat. systems...)
Some remain unsolved (xy model, Thirring,... )

Full QCD

High temperatures seem to be unproblematic
   checks with reweighting, Taylor expansion
Status of low T and near T_c is unclear – more work needed

See below for ongoing work
   concerning phase diag, EOS and improved actions
Gaussian Example

$S[x] = \sigma x^2 + i \lambda x$

$\frac{d}{d\tau} (x + iy) = -2\sigma (x + iy) - i\lambda + \eta$

$P(x, y) = e^{-a(x-x_0)^2-b(y-y_0)^2-c(x-x_0)(y-y_0)}$

Gaussian distribution around critical point $\frac{\partial S(z)}{\partial z} \bigg|_{z_0} = 0$

Measure on real axis

$\sigma = 1 + i \quad \lambda = 20$
Proof of convergence for CLE results

If there is fast decay \( P(x, y) \rightarrow 0 \) as \( x, y \rightarrow \infty \)

and a holomorphic action \( S(x) \)

then CLE converges to the correct result

[Aarts, Seiler, Stamatescu (2009)
Aarts, James, Seiler, Stamatescu (2011)]

Loophole 1: Non-holomorphic action for nonzero density

\[ S = S_w[U_\mu] + \ln \text{Det} M(\mu) \]

measure has zeros \( (\text{Det} M = 0) \)
complex logarithm has a branch cut

meromorphic drift

[Mollgaard, Splittorff (2013), Greensite(2014)]

Drift around a pole:

\[
\rho(x) = (x - z_p)^{n_f} e^{-S(x)}
\]

\[
K(z) = \frac{\partial z \rho(z)}{\rho(z)} = \frac{n_f}{x - z_p} + K_S(z)
\]
Langevin time evolved observables get singularities around pole
Zero of the distribution counteracts that
Proof goes through correct results
For HDQCD and full QCD at high temperatures this is satisfied

\[ \rho(x) = (1 + \kappa \cos(x - i\mu))^n e^{-\beta \cos(x)} \]

Poles can be inside the distribution

Pole pinches distribution
Acts as a bottleneck
might cause “separation phenomenon”
(potentially) wrong results

outside of the distribution

Langevin time evolved observables get singularities around pole
Zero of the distribution counteracts that
Proof goes through correct results
Loophole 2: decay not fast enough

What we want
\[ \int dx \rho(x) O(x) \]
What we get with CLE
\[ \int dx \, dy \, P(x, y) O(x + iy) \]

Using analyticity and partial integrations

boundary terms can be nonzero
explicit calculation of boundary terms

[Scherzer, Seiler, Sexty, Stamatescu (2018)]
Sketch of the proof

\[ P(x, y, t) \]: probability density on the complex plane at Langevin time \( t \)

\[ \rho(x, t) \]: complex measure evolving with the Fokker-Planck equation

\[ \partial_t \rho(x, t) = \partial_x (\partial_x + (\partial_x S)) \rho(x, t) \]

Stationary solution: \( \rho(x, \infty) = \exp(-S(x)) \)

CLE works, if

\[ \langle O(x) \rangle_{\rho(t)} = \langle O(x + iy) \rangle_{P(t)} \]

Interpolating function:

\[ F(t, \tau) = \int P(x, y, t - \tau) O(x + iy, \tau) \, dx \, dy \]

\[ F(t, 0) = \langle O(x + iy) \rangle_{P(t)} \]

\[ F(t, t) = \ldots = \langle O(x) \rangle_{\rho(t)} \]

\[ \partial_\tau F(t, \tau) = 0 \] can be seen with partial integrations

QED

\[ O(z, t) = e^{\tilde{L} t} O(z, 0) \]

with \( \tilde{L} = (\partial_z + K(z)) \partial_z \)

Use Cauchy-Riemann

\[ [\text{Aarts, Seiler, Stamatescu (2010)}] \]
Direct calculation of boundary terms

[Scherzer, Seiler, Sexty, Stamatescu (2018)]

Partial integration can give boundary terms:

\[ \int dy \partial_y G(y) = \lim_{Y \to \infty} \int_{-Y}^{Y} dy \partial_y G(y) = G(Y) - G(-Y) \]

In this case:

\[ B_O(Y; t, \tau) = \partial_\tau F(t, \tau)_Y \]

\[ B_O(Y; t, \tau) = \int dx \left[ K_y(x, Y) P(x, Y, t-\tau) O(x+iy, \tau) 
- K_y(x, -Y) P(x, -Y, t-\tau) O(x-iy, \tau) \right] \]

Only easy numerical evaluation at \( \tau = 0 \)

\[ O(x+iy, \tau) \quad \text{Calculable on the grid for toy models} \]

\[ O(z, t) = e^{\tilde{L}t} O(z, 0) \]

with \( \tilde{L} = (\partial_z + K(z)) \partial_z \)
Toy model study

\[ \rho(x) = \frac{1}{Z} \exp(-i \beta \cos(x)) \]

\[ O_k(x) = e^{ikx} \]

\[ \langle O_k \rangle = (-i)^k \frac{J_k(\beta)}{J_0(\beta)} \]

Analytical stationary solution for CLE [Salcedo (2017)]:

\[ P(x, y) = \frac{1}{4\pi \cosh^2(y)} \]

\[ \langle O_1 \rangle_P = 0 \neq \langle O_1 \rangle_{\rho} \]

This is reproduced by CLE and Fokker-Planck solutions.

For small times plateau at correct values, then converges to the wrong result.
Boundary term:

Using Fokker-Planck eq.

Using CLE
Calculating the boundary term for lattice systems

\[ B_O(Y; t, \tau = 0) = \int dx \left[ K_y(x, Y) P(x, Y, t) O(x + iY) \right. \]
\[ \left. - K_y(x, -Y) P(x, -Y, t) O(x - iY) \right] \]

Still too complicated for many variables:
need to define a surface in the 2N dimension complex manifold

\[ B(Y, t, \tau = 0) = \int_{-Y}^{Y} \partial_\tau F(t, \tau) = \]
\[ = -\int_{-Y}^{Y} (L^T P(x, y, t)) O(x + iy) \, dy \, dx + \int_{-Y}^{Y} P(x, y, t) L_c O(x + iy) \, dx \, dy \]
\[ \text{vanishes as } t \to \infty \]

\[ L_c = \sum_i \left( \partial_{z_i} + K_i \right) \partial_{z_i} \]
gives an eq. for various observables
with cutoff

“Schwinder-Dyson Eq.”
“consistency criteria”

Freedom to define cutoff

\[ \sum_i y_i^2 < Y \]
\[ \max_i |y_i| < Y \]
\[ \sum_i \text{Tr}(U U^{+1}) < Y \]
Regularized version of toy model:

\[ S(x) = i \beta \cos(x) + \frac{S}{2} x^2 \]

\[ L_c e^{ikz} = ik (ik + i \beta \sin z - s z) e^{ikz} \]

Currently being studied: Polyakov chain
HDQCD, Full QCD is next

\[ S = (\beta + \kappa e^{\mu}) \text{Tr } U + (\beta + \kappa e^{-\mu}) \text{Tr } U^{-1} \]
Some results of CLE so far

Bose Gas at zero temperature 

[Aarts '08]

Silver Blaze problem:

At zero temperature, nothing happens until first excited state (=1 particle) contributes

First spectacular success of complex Langevin

Gaugecooling and study of HDQCD

[Seiler, Sexty, Stamatescu '13]

Full QCD with light quarks

[Sexty '14]
Gauge cooling

[Seiler, Sexty, Stamatescu (2012)]

complexified distribution with slow decay \[\rightarrow\] convergence to wrong results

Keep the system from trying to explore the complexified gauge degrees of freedom

Minimize unitarity norm

Distance from SU(N)

\[
\sum_i \text{Tr}(U_i U_i^+ - 1)
\]

Dynamical steps are interspersed with several gauge cooling steps

Empirical observation:

Cooling is effective for \(\beta > \beta_{\text{min}}\)

but remember, \(\beta \rightarrow \infty\) in cont. limit

\(a < a_{\text{max}} \approx 0.1 - 0.2 \text{ fm}\)

Can we do more?

Dynamical Stabilization  soft cutoff in imaginary directions

[Attanasio, Jäger (2018)]
Chiral random matrix theory
[Mollgaard, Splittorff '13+'14]

Poles can be problematic

Study of the pole problem
[Nishimura, Shimasaki ‘15]
[Aarts, Seiler, Sexty, Stamatescu ‘17]

Distribution at poles (spectrum) should be monitored

Hopping parameter expansion
[Aarts, Seiler, Sexty, Stamatescu ‘15]

Very high orders easily calculated

Investigating Silver Blaze for QCD
[Kogut, Sinclair ‘16]
[Ito, Nishimura ‘16]
[Tsutsui, Ito, Matsufuru, Nishimura, Shimasaki, Tsuchiya ‘18]

Jury still out

0+1 dim Thirring model
[Fujii, Kamata, Kikukawa ‘17]

Reweighting or deformation makes CLE ok

Gauge cooling for eigenvalues
[Nagata, Nishimura, Shimasaki ‘16]

Shifts e.v.s away from origin in RMT

Gauge cooling for Random Matrix models
[Bloch, Glessaen, Verbaarschot, Zafeiropoulos ‘18]

1 hit 1 miss
Exact drift terms with selected inverse  
[Bloch, Schenk ‘17]

Fermionic drift term: \( \text{Tr} \left( M^{-1} D_{\alpha \mu x} M \right) \)
with sparse Dirac Matrix \( M \)

Use sparse LU decomposition to calculate inverse

No additional noise from stochastic estimator

Unitarity norm is better controlled

Reweighting complex Langevin trajectories  
[Bloch ‘17]

Reweighting from one non-positive ensemble to another
Equation of state for 1D non-relativistic fermions

\[ Z = \int d\sigma \det M_{\text{up}}(\sigma) \det M_{\text{down}}(\sigma) \]

\[ \sigma = \text{Hubbard-Stratonovich field} \]

Modify action to add an attractive force

\[ S(\sigma) = S_{\text{old}}(\sigma) + \xi \sigma^2 \]

Local interactions

2 parameters: coupling \( \lambda \), chemical pot. \( \mu \)

Attractive - pos. det

Repulsive - non pos. det
QCD sign problem

Euclidean SU(3) gauge theory with fermions:

$$Z = \int DU \exp(-S_E[U]) det(M(U))$$

for $det(M(U)) > 0$  Importance sampling is possible  $\rightarrow$ Hadron masses, EOS, ...

Non-zero chemical potential

For nonzero chemical potential, the fermion determinant is complex

$$det(M(U, -\mu^*)) = (det(M(U, \mu))^*)$$

Sign problem $\rightarrow$ Naive Monte-Carlo breaks down
In QCD direct simulation only possible at $\mu = 0$

Taylor extrapolation, Reweighting, continuation from imaginary $\mu$, canonical ens. all break down around

$$\frac{\mu_q}{T} \approx 1 - 1.5 \quad \frac{\mu_B}{T} \approx 3 - 4.5$$

Around the transition temperature
Breakdown at

$\mu_q \approx 150 - 200\text{ MeV} \quad \mu_B \approx 450 - 600\text{ MeV}$

Results on $N_T = 4, N_F = 4, ma = 0.05$

using Imaginary mu, Reweighting, Canonical ensemble

Agreement only at $\mu/T < 1$
Mapping the phase diagram of HDQCD

[Aarts, Attanasio, Jäger, Sexty (2016)]

Hopping parameter expansion of the fermion determinant
Spatial fermionic hoppings are dropped
Full gauge action

\[ \text{Det } M(\mu) = \prod_x \text{det}(1 + C_x P_x)^2 \text{det}(1 + C_x' P_x^{-1})^2 \]

Strategy to map \( T - \mu \) plane

fixed \( \beta = 5.8 \rightarrow a \approx 0.15 \text{ fm} \) \quad Unitarity norm is mostly under control

\( \kappa = 0.04 \)
onset transition at \( \mu = -\ln(2\kappa) \)

\( \mathcal{N}_t(6^3, 8^3, 10^3) \) lattice
\( \mathcal{N}_t = 2 \ldots 28 \)

Temperature scanning
\( T = 48 \ldots 671 \text{ MeV} \)
Mapping the phase diagram of HDQCD

Onset in fermionic density
Silver blaze phenomenon

Polyakov loop
Transition to deconfined state
Fits of the phase transition line

Deconfinement transition and onset transition meet in the middle
Errors from discretisation scheme
Volume dependence under control

much simpler phase diagram than full QCD
Reweighting

\[
\langle F \rangle_\mu = \frac{\int DU e^{-S_E} \det M(\mu) F}{\int DU e^{-S_E} \det M(\mu)} = \frac{\int DU e^{-S_E} R \frac{\det M(\mu) F}{R}}{\int DU e^{-S_E} R \frac{\det M(\mu)}{R}}
\]

\[
= \frac{\langle F \det M(\mu)/R \rangle_R}{\langle \det M(\mu)/R \rangle_R} \quad R = \det M(\mu=0), |\det M(\mu)|, \text{etc.}
\]

\[
\left\langle \frac{\det M(\mu)}{R} \right\rangle_R = \frac{Z(\mu)}{Z_R} = \exp \left( -\frac{V}{T} \Delta f(\mu, T) \right)
\]

\[
\Delta f(\mu, T) = \text{free energy difference}
\]

Exponentially small as the volume increases \( \langle F \rangle_\mu \to 0/0 \)

Reweighting works for large temperatures and small volumes

Sign problem gets hard at \( \mu/T \approx 1 \)
Comparison with reweighting for full QCD
[Fodor, Katz, Sexty, Török 2015]

Reweighting from ensemble at
\[ R = \text{Det} M(\mu = 0) \]
Comparisons as a function of beta

Similarly to HDQCD
Cooling breaks down at small beta

at $N_T=4$ breakdown at $\beta=5.1-5.2$

At larger $N_T$?
Comparisons as a function of beta

$N_T = 6$

$N_T = 8$

Breakdown prevents simulations in the confined phase for staggered fermions with $N_T = 4, 6, 8$

Two ensembles: $m_\pi \approx 4.8 \, T_c$

$m_\pi \approx 2.3 \, T_c$
Ongoing efforts concerning the QCD phase diag
with Manuel Scherzer and Nucu Stamatescu

1. Following phase transition line
   Do we meet a critical point?

2. Onset transition at small temperatures
   \[ \frac{m_\pi}{2} \text{ vs. } \frac{m_N}{3} \]

3. Calculating the pressure at high temperatures
   compare with know results

4. Implementing improved actions
   also for fermions
Mapping out the phase transition line

Follow the phase transition line starting from $\mu = 0$

Can follow the line to quite high $\mu/T$

Using Wilson fermions

$\beta = 5.9, \kappa = 0.15, N_f = 2, N_s = 8, 12, 20$

varying $N_t$ to change the temperature

$m_\pi \approx 1.3 \text{ GeV}$ on $N_s = 20$

Large finite size effects
Long runs with CLE

Unitarity norm has a tendency to grow slowly (even with gauge cooling)

Runs are cut if it reaches $\sim 0.1$

Thermalization usually fast
- might be problematic close to critical point or at low $T$
Getting closer to continuum limit

Test with Wilson fermions
Increase $\beta$ by 0.1 – reduces lattice spacing by 30%
change everything else to stay on LCP

behavior of Unitarity norm improves
How to detect the phase transition?

Chiral susceptibility

Renormalization procedure is hard for Wilson fermions
Costly

Polyakov loop susceptibility

$$P_{\text{ren}} = P_{\text{bare}} e^{-c(a) N_t}$$

Since we change $N_t$ peak position can have large shift

Binder cumulant of Polyakov loop

$$B(x) = \frac{\langle X^4 \rangle}{\langle X^2 \rangle^2}$$

Multiplicative renormalization drops out

Symmetrization for CLE  \( x = P + P^{-1} \),  \( x = \sqrt{P P^{-1}} \)

Finite size analysis gives order, critical exp.
Binder cumulant

$$T_{c}(\mu) = 1 - \kappa_{2} \left( \frac{\mu}{T_{c}(0)} \right)^{2}$$

Curvature of the transition line

$$\kappa_{2}^{\text{lit}} \approx 0.015$$  Near the physical point
Onset transition in QCD

Low temperature, chemical potential is increased

Nuclear matter onset at \( \mu_c = m_N/3 \)

"benchmark:" Phasequenched theory (equivalent to isospin chem. pot.)

\[ \text{det} \ M(\mu) \rightarrow |\text{det} \ M(\mu)| \]

Simulation with ordinary importance sampling

Pion condensation onset at \( \mu_{c,PQ} = m_\pi/2 \)

Can we see the difference?

Hard problem:
For large quark masses \( m_\pi/2 \approx m_N/3 \)
Low quark masses are expensive

Temperature effects might shift \( \mu_c \)
Low temperature is expensive

Huge finite size effects

Thermalization potentially slow
Pressure of the QCD Plasma at non-zero density

\[ \frac{p}{T^4} = \frac{\ln Z}{VT^3} \]

Derivatives of the pressure are directly measurable
Integrate from \( T=0 \)

Other strategies:

Measure the Stress-momentum tensor using gradient flow
[Suzuki, Makino (2013-)]

Shifted boundary conditions
[Giusti, Pepe, Meyer (2011-)]

Non-equilibrium quench
[Caselle, Nada, Panero (2018)]

First integrate along the temperature axis, then explore \( \mu > 0 \)

Taylor expansion [Allton et. al. (2002-), ... ]

Simulating at imaginary \( \mu \) to calculate susceptibilities
[Bud.-Wupp. Group (2018)]
Pressure of the QCD Plasma at non-zero density

\[ \Delta \left( \frac{p}{T^4} \right) = \frac{p}{T^4} (\mu = \mu_q) - \frac{p}{T^4} (\mu = 0) \]

If we want to stay at \( \mu = 0 \)

\[ \Delta \left( \frac{p}{T^4} \right) = \sum_{n>0, \text{even}} c_n (T) \left( \frac{\mu}{T} \right)^n \]

\[ c_2 = \frac{1}{2} \frac{N_T}{N_s^3} \frac{\partial^2 \ln Z}{\partial \mu^2} \]

\[ c_4 = \frac{1}{24} \frac{1}{N_s^3 N_T} \frac{\partial^4 \ln Z}{\partial \mu^4} \]

Measuring the coefficients of the Taylor expansion

\[ \frac{\partial^2 \ln Z}{\partial \mu^2} = N_F^2 \langle T_1^2 \rangle + N_F \langle T_2 \rangle \]

\[ \frac{\partial^4 \ln Z}{\partial \mu^4} = -3 \left( \langle T_2 \rangle + \langle T_1^2 \rangle \right) + 3 \langle T_2^2 \rangle + \langle T_4 \rangle + 4 \langle T_3 T_1 \rangle + 6 \langle T_1 T_2 \rangle + \ldots \]

\[ \frac{\partial^2 \ln Z}{\partial \mu^2} = N_F^2 \langle T_1^2 \rangle + N_F \langle T_2 \rangle \]

\[ \frac{\partial^4 \ln Z}{\partial \mu^4} = -3 \left( \langle T_2 \rangle + \langle T_1^2 \rangle \right) + 3 \langle T_2^2 \rangle + \langle T_4 \rangle + 4 \langle T_3 T_1 \rangle + 6 \langle T_1 T_2 \rangle + \ldots \]

\[ T_1 / N_F = \text{Tr} \left( M^{-1} \partial_\mu M \right) \]

\[ T_{i+1} = \partial_\mu T_i \]

\[ T_2 / N_F = \text{Tr} \left( M^{-1} \partial_\mu^2 M \right) - \text{Tr} \left( (M^{-1} \partial_\mu M)^2 \right) \]

\[ T_3 / N_F = \text{Tr} \left( M^{-1} \partial_\mu^3 M \right) - 3 \text{Tr} \left( M^{-1} \partial_\mu M M^{-1} \partial_\mu^2 M \right) + 2 \text{Tr} \left( (M^{-1} \partial_\mu M)^3 \right) \]

\[ T_4 / N_F = \text{Tr} \left( M^{-1} \partial_\mu^2 M \right) - 4 \text{Tr} \left( M^{-1} \partial_\mu M M^{-1} \partial_\mu^3 M \right) - 3 \text{Tr} \left( M^{-1} \partial_\mu^2 M M^{-1} \partial_\mu^2 M \right) - 6 \text{Tr} \left( (M^{-1} \partial_\mu M)^3 \right) + 12 \text{Tr} \left( (M^{-1} \partial_\mu M)^2 M^{-1} \partial_\mu^2 M \right) \]
Taylor expansion

Using naive staggered action with $N_F = 4$

Observables very noisy
state of the art calculations barely see a signal at 8th order

Disconnected terms
e.g. $\langle T_1^2 T_2 \rangle$
contribute most of the noise

16$^3 \times 8$, $N_F = 4$, $m = 0.02$
O(1000) configurations
64 noise vectors each
Pressure of the QCD Plasma using CLE

If we can simulate at $\mu > 0$

$$\Delta \left( \frac{p}{T^4} \right) = \frac{p}{T^4} (\mu = \mu_q) - \frac{p}{T^4} (\mu = 0) = \frac{1}{V T^3} \left( \ln Z(\mu) - \ln Z(0) \right)$$

$$\ln Z(\mu) - \ln Z(0) = \int_0^\mu d\mu \frac{\partial \ln Z(\mu)}{\partial \mu} = \int_0^\mu d\mu \Omega n(\mu)$$

$$n(\mu) = \langle \text{Tr} \left( M^{-1}(\mu) \partial_\mu M(\mu) \right) \rangle$$

Using CLE it’s enough to measure the density – much cheaper
Integration performed numerically
Jackknife error estimates

$T = 250 \text{ MeV}$, $T_c \approx 190 \text{ MeV}$

$T = 475 \text{ MeV}$

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$a$ (fm)</th>
<th>$c_2$ HMC</th>
<th>$c_4$ HMC</th>
<th>$c_2$ CLE</th>
<th>$c_4$ CLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.3</td>
<td>$0.099 \pm 0.001$</td>
<td>$1.986 \pm 0.042$</td>
<td>$0.27 \pm 0.23$</td>
<td>$2.117 \pm 0.1$</td>
<td>$0.152 \pm 0.05$</td>
</tr>
<tr>
<td>5.6</td>
<td>$0.052 \pm 0.0013$</td>
<td>$2.351 \pm 0.044$</td>
<td>$0.16 \pm 0.12$</td>
<td>$2.168 \pm 0.1$</td>
<td>$0.200 \pm 0.05$</td>
</tr>
</tbody>
</table>
Improved actions for lattice QCD

Carrying out continuum extrapolation \( a \to 0 \)

Simulate at multiple lattice spacings
Fitting some observable

\[ O(a) = O_0 + O_1 a + O_2 a^2 + \ldots \]

Change action such that \( O_1 \) is eliminated

Gauge improvement

Include larger loops in action

Symanzik action:

\[ S = -\beta \left( \frac{5}{3} \sum \text{ReTr} \square - \frac{1}{12} \sum \text{Re Tr} \begin{array}{c} \square \end{array} \right) \]

Straightforwardly implemented in CLE

Analyticity must be preserved:

\[ 2 \text{ReTr } U = \text{Tr } U + \text{Tr } U^+ \quad \Rightarrow \quad \text{Tr } U + \text{Tr } U^{-1} \]
Improved fermion actions

Changeing the Dirac operator

Wilson fermions: clover improvement       adds a clover term

Staggered fermions: naik or p4        take into account 3-link terms

Fat links

Smear the gauge fields inside the Dirac operator

APE, HYP

\[ V_\mu = (1 - \alpha) U_\mu + \alpha \sum \text{staples} \]

\[ U'_\mu = \text{Proj}_{SU(3)} V_\mu \]

Stout

\[ U'_\mu = e^{iQ_\mu} U_\mu \quad Q_\mu = \rho \sum \text{staples} \]

essentially one step of gradient flow with stepsize $\rho$
Stout smearing

\[ U'_\mu = e^{iQ_\mu} U_\mu \quad Q_\mu = \rho \sum \text{staples} \]

Usually multiple steps: \[ U \to U^{(1)} \to U^{(2)} \to \ldots \to U^{(n)} \]

Replace gauge fields in Dirac matrix \[ \det M(U) \to \det M(U^{(n)}) \]

For the Langevin eq. we need drift terms:
\[
\frac{\partial S_{\text{eff}}}{\partial U} = \frac{\partial S_{\text{eff}}}{\partial U^{(n)}} \frac{\partial U^{(n)}}{\partial U^{(n-1)}} \ldots \frac{\partial U^{(1)}}{\partial U}
\]

Calculated by “going backwards”

One iteration:
\[
\frac{\partial U'}{\partial U} = \frac{\partial e^{iQ}}{\partial U} U + e^{iQ} + \text{local terms} + \text{nonlocal terms from staples}
\]
Stout smearing and complex Langevin

\[ U'_\mu = e^{iQ_\mu} U_\mu \quad Q_\mu = \rho \sum \text{staples} \]

Adjugate is replaced with inverse for links

\[ Q^+ \text{ is not replaced with } Q^{-1} \quad (\text{because its a sum}) \]

\( Q \) is no longer hermitian

Calculation of \( \frac{\partial e^{iQ}}{\partial U} \) becomes trickier

Benchmarking with HMC at \( \mu = 0 \)

\[ a(\beta = 3.6) = 0.12 \text{ fm} \quad a(\beta = 3.9) = 0.064 \text{ fm} \]
What happens with the configurations?

Real part of gauge fields decay
Unitarity norm slightly rises

<table>
<thead>
<tr>
<th>smearing step</th>
<th>plaqavg</th>
<th>unitarity norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.562948</td>
<td>0.00913145</td>
</tr>
<tr>
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<td>0.0108531</td>
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<td>8</td>
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<tr>
<td>9</td>
<td>0.995831</td>
<td>0.0140539</td>
</tr>
<tr>
<td>10</td>
<td>0.996598</td>
<td>0.0141745</td>
</tr>
</tbody>
</table>
What happens with the drift terms?

\[
\frac{\partial S_{\text{eff}}}{\partial U} = \frac{\partial S_{\text{eff}}}{\partial U^{(n)}} \frac{\partial U^{(n)}}{\partial U^{(n-1)}} \cdots \frac{\partial U^{(1)}}{\partial U} \\
\frac{\partial S_{\text{eff}}}{\partial U^{(n)}} = F_0, \quad \frac{\partial S_{\text{eff}}}{\partial U^{(n)}} \frac{\partial U^{(n)}}{\partial U^{(n-1)}} = F_1, \quad \ldots \quad \frac{\partial S_{\text{eff}}}{\partial U} = F_n
\]

Average drift term is smaller

- Long tail
- More prone to runaways
- Smaller stepsize needed
Pressure with improved action

$C_4$ is measurable with this action at high $T$ (with O(500) configs.)
Pressure with improved action

Symanzik gauge action
stout smeared staggered fermions

\[
T = 260 \text{ MeV}
\]

\[
T = 385 \text{ MeV}
\]

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\beta & a(\text{fm}) & c_2 \text{ HMC} & c_4 \text{ HMC} & c_2 \text{ CLE} & c_4 \text{ CLE} & c_6 \text{ CLE} \\
\hline
3.7 & 0.094 \pm 0.001 & 2.127 \pm 0.026 & 0.122 \pm 0.046 & 2.143 \pm 0.07 & 0.151 \pm 0.02 & 0.0014 \pm 0.001 \\
3.9 & 0.064 \pm 0.001 & 2.302 \pm 0.026 & 0.138 \pm 0.021 & 2.314 \pm 0.04 & 0.143 \pm 0.007 & 0.0018 \pm 0.0003 \\
\hline
\end{array}
\]

Good agreement
CLE calculation is much cheaper
CLE is a versatile tool to solve sign problems

Potential problems with boundary terms and poles
  Monitoring of the process is required

Promising results for many systems:
  phase diagram of HDQCD mapped out

Ongoing effort for full QCD to get physical results
  Mapping out phase transition line
  Onset transition at small temperatures
  Calculating the pressure
  Using improved actions