Stabilising complex Langevin simulations

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In collaboration with B. Jäger
Description of QCD under different thermodynamical conditions

- Experimental investigations in progress (LHC, RHIC) and planned (FAIR)
- Perturbation theory only applicable at high temperature/density (asymptotic freedom)
- Full exploration requires non-perturbative (e.g. lattice) methods
CLE: Motivation

Description of QCD under different thermodynamical conditions

- **Sign problem**: chemical potential in Euclidean path integral $\Rightarrow$ complex action
- Expectation values $\Rightarrow$ precise cancellations of oscillating quantities
- In QCD: fermion determinant

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

is complex for real chemical potential $\mu$
- Traditional Monte-Carlo methods unreliable for severe sign problem
Evolve gauge links according to the Langevin equation

\[ U_{x\mu}(\theta + \varepsilon) = \exp [X_{x\mu}] U_{x\mu}(\theta) , \]

with the Langevin drift

\[ X_{x\mu} = i\lambda^a ( -\varepsilon D^a_{x\mu} S[U(\theta)] + \sqrt{\varepsilon} \eta^a_{x\mu}(\theta)) , \]

\( \lambda^a \) are the Gell-Mann matrices, \( \varepsilon \) is the stepsize, \( \eta^a_{x\mu} \) are white noise fields satisfying

\[ \langle \eta^a_{x\mu} \rangle = 0 , \quad \langle \eta^a_{x\mu} \eta^b_{y\nu} \rangle = 2\delta^{ab}\delta_{xy}\delta_{\mu\nu} , \]

\( S \) is the QCD action and \( D^a_{x\mu} \) is defined as

\[ D^a_{x\mu} f(U) = \frac{\partial}{\partial \alpha} f(e^{i\alpha\lambda^a} U_{x\mu}) \bigg|_{\alpha=0} \]
Complexification

- Allow gauge links to be non-unitary: $\text{SU}(3) \ni U_{x\mu} \rightarrow U_{x\mu} \in \text{SL}(3, \mathbb{C})$

- Use $U_{x\mu}^{-1}$ instead of $U_{x\mu}^\dagger$ as
  - keeps the action/observables holomorphic;
  - coincide on $\text{SU}(3)$, but on $\text{SL}(3, \mathbb{C})$ it is $U^{-1}$ that represents the backwards-pointing link.

- Circumvents the sign problem by doubling the degrees of freedom

  \[
  \int_{-\infty}^{\infty} dx \ e^{-x^2} \rightarrow \sqrt{\int} \ r \ dr \ d\theta \ e^{-r^2}
  \]
Gauge cooling

- \( \text{SL}(3, \mathbb{C}) \) is not compact \( \Rightarrow \) gauge links can get arbitrarily far from \( \text{SU}(3) \)

- During simulations monitor the distance from the unitary manifold with

\[
d = \frac{1}{N_s^3 N_\tau} \sum_{x, \mu} \text{Tr} \left[ U_{x\mu} U_{x\mu}^\dagger - 1 \right]^2 \geq 0
\]

- Use gauge transformations to decrease \( d \)

\[
U_{x\mu} \rightarrow \Lambda_x U_{x\mu} \Lambda_{x+\mu}^{-1}
\]

necessary, but not always sufficient
Gauge cooling (mild sign problem)

Left: Langevin time history of Polyakov loop
Right: Langevin time history of unitarity norm
New term in the drift to reduce the non-unitarity of $U_{x,\nu}$

$$X_{x,\nu} = i\lambda^a \left( -\epsilon D^a_{x,\nu} S - \epsilon \alpha_{DS} M^a_x + \sqrt{\epsilon} \eta^a_{x,\nu} \right).$$

with $\alpha_{DS}$ being a control coefficient

$M^a_x$: constructed to be irrelevant in the continuum limit

$M^a_x$ only depends on $U_{x,\nu} U^\dagger_{x,\nu}$ (non-unitary part)
Dynamic stabilisation (mild sign problem)

Left: Langevin time history of Polyakov loop
Right: Langevin time history of unitarity norm (notice log scale!)
Unitarity norm as a function of $\alpha_{DS}$ for HDQCD at $\beta = 5.8$ and $\kappa = 0.04$
Observables considered

- “Real part” of the Polyakov loop
  \[ P^s = \frac{1}{2} (\langle P \rangle + \langle P^{-1} \rangle) \],

- Chiral condensate (for dynamical quarks)
  \[ \langle \bar{\psi} \psi \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial m} \]

- Quark density
  \[ \langle n \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial \mu} \]
Heavy-dense approximation

- Heavy quarks → quarks evolve only in Euclidean time direction:

  \[ \det M(U, \mu) = \prod_{\vec{x}} \left\{ \det \left[ 1 + (2\kappa e^\mu)^N \mathcal{P}_{\vec{x}} \right]^2 \det \left[ 1 + (2\kappa e^{-\mu})^N \mathcal{P}_{\vec{x}}^{-1} \right]^2 \right\} \]

- Polyakov loop

  \[ \mathcal{P}_{\vec{x}} = \prod_\tau U_4(\vec{x}, \tau) \]

- Exhibits the sign problem: \[ [\det M(U, \mu)]^* = \det M(U, -\mu^*) \]

- Transition to higher densities (at \( T = 0 \) it happens at \( \mu = \mu_c^* = -\ln(2\kappa) \))
Comparison of DS and GC

\(\alpha_{DS}\) scan of the Polyakov loop, with results from gauge cooling

\(\beta = 5.8, \mu/\mu^0_c = 0.96, \kappa = 0.04, V = 8^3 \times 20\)

Wide region of \(\alpha_{DS}\) where DS agrees with GC with low unitarity norm
Histograms I (HDQCD)

DS reduces only imaginary part of the Langevin drift

Histograms of the Langevin drift
Left: Imaginary part is clearly affected by larger $\alpha_{DS}$
Right: For $\alpha_{DS}$ large enough, the real part of the drift is essentially unchanged
DS decreases with the lattice spacing

Histograms II (HDQCD)

HDQCD, $8^3 \times 20$, $\beta = 5.8$, $\kappa = 0.04$, $\mu/\mu_0 = 0.96$

Histograms for different values of $\beta$
Left: Real part of the drift changes very little ($a$ is changing)
Right: DS term decreases with $a$ (higher $\beta$)
Good agreement with reweighting across the deconfinement region for fixed $\mu$.

Polyakov loop as a function of the inverse coupling $\beta$ for HDQCD.
Deconfinement in HDQCD

Good agreement with reweighting – even when GC converges to the wrong limit

Spatial plaquette as a function of the inverse coupling $\beta$ for HDQCD
The Langevin drift for $N_f$ flavours of staggered quarks

$$D^a_{x,\nu} S_F \equiv D^a_{x,\nu} \ln \det M(U, \mu)$$

$$= \frac{N_F}{4} \text{Tr} \left[ M^{-1}(U, \mu) D^a_{x,\nu} M(U, \mu) \right]$$

- Inversion is done with conjugate gradient method

- Trace is evaluated by bilinear noise scheme – introduces imaginary component even for $\mu = 0$!
Staggered quarks \((\beta = 5.6, \ m = 0.025, \ N_F = 4)\)

Comparison between CLE + DS runs and HMC (results by P. de Forcrand)

Grey band represents results from HMC simulations

\(\alpha_{DS}\) scan of the chiral condensate for a volume of \(6^4\)
Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

Comparison between CLE + DS runs and HMC (results by P. de Forcrand)

Grey band represents results from HMC simulations
Langevin step size extrapolation of the chiral condensate for a volume of $8^4$
Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

Comparison between CLE + DS runs and HMC (results by P. de Forcrand)

Grey band represents results from HMC simulations
Langevin step size extrapolation of the plaquette for a volume of $12^4$
Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

Comparison between CLE + DS runs and HMC (results by P. de Forcrand)

<table>
<thead>
<tr>
<th>Volume $\times 4$</th>
<th>Plaquette $\bar{\psi}\psi$</th>
<th>HMC</th>
<th>Langevin</th>
<th>HMC</th>
<th>Langevin</th>
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<tr>
<td>$6^4$</td>
<td>0.58246(8)</td>
<td>0.582452(4)</td>
<td>0.1203(3)</td>
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<tr>
<td>$8^4$</td>
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<td>0.1372(3)</td>
<td>0.1370(6)</td>
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<tr>
<td>$12^4$</td>
<td>0.58196(6)</td>
<td>0.58195(2)</td>
<td>0.1414(4)</td>
<td>0.1409(3)</td>
<td></td>
</tr>
</tbody>
</table>

Expectation values for the plaquette and chiral condensate for full QCD Langevin results have been obtained after extrapolation to zero step size.
Staggered quarks ($\beta = 5.6, m = 0.025, N_F = 2$)

Preliminary results at $\mu > 0$ (not extrapolated to zero step size)

Vertical lines indicate position of critical chemical potential for each temperature
Left: Density as a function of chemical potential
Right: Pressure as a function of chemical potential
Summary

- Dynamic Stabilisation
  - improves convergence of complex Langevin simulations
  - allows for long runs

- HDQCD results with DS verified against reweighting across the deconfinement transition

- Very good agreement with HMC for full QCD at $\mu = 0$

Outlook

- Determine the QCD phase diagram, with particular attention phase boundaries and characteristics