Stabilising complex Langevin simulations

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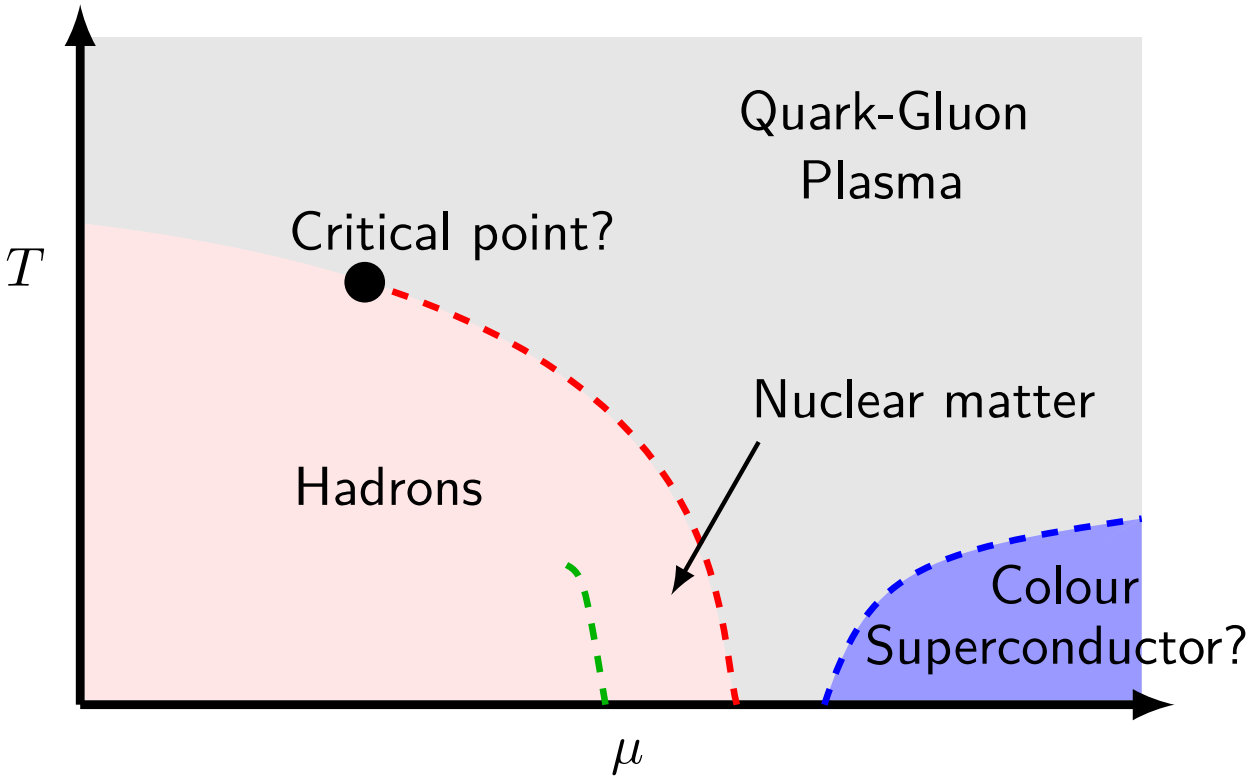
In collaboration with B. Jäger

CLE: Motivation

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 μ
- Traditional Monte-Carlo methods unreliable for severe sign problem

CLE: Stochastic quantization

On the lattice

[Damgaard and Hüffel, Physics Reports]

- Evolve gauge links according to the Langevin equation

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

with the Langevin drift

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

λ^a are the Gell-Mann matrices, ε 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

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

CLE: Complexification I

Complexification

[Aarts, Stamatescu, hep-lat/0807.1597]

- Allow gauge links to be non-unitary: $\mathrm{SU}(3) \ni U_{x\mu} \to U_{x\mu} \in \mathrm{SL}(3, \mathbb{C})$
- Use $U_{x\mu}^{-1}$ instead of $U_{x\mu}^{\dagger}$ as
  - keeps the action/observables holomorphic;
  - coincide on $\mathrm{SU}(3)$, but on $\mathrm{SL}(3, \mathbb{C})$ it is U^{-1} that represents the backwards-pointing link.
- Circumvents the sign problem by doubling the degrees of freedom

$$\text{similar to} \int_{-\infty}^{\infty} dx\, e^{-x^2} \to \sqrt{\int r\, dr d\theta\, e^{-r^2}}$$

CLE: Complexification II – Gauge cooling

Gauge cooling

[Seiler, Sexty, Stamatescu, hep-lat/1211.3709]

- SL$(3,\mathbb{C})$ is not compact $\Rightarrow$ gauge links can get arbitrarily far from SU(3)
- During simulations monitor the distance from the unitary manifold with

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

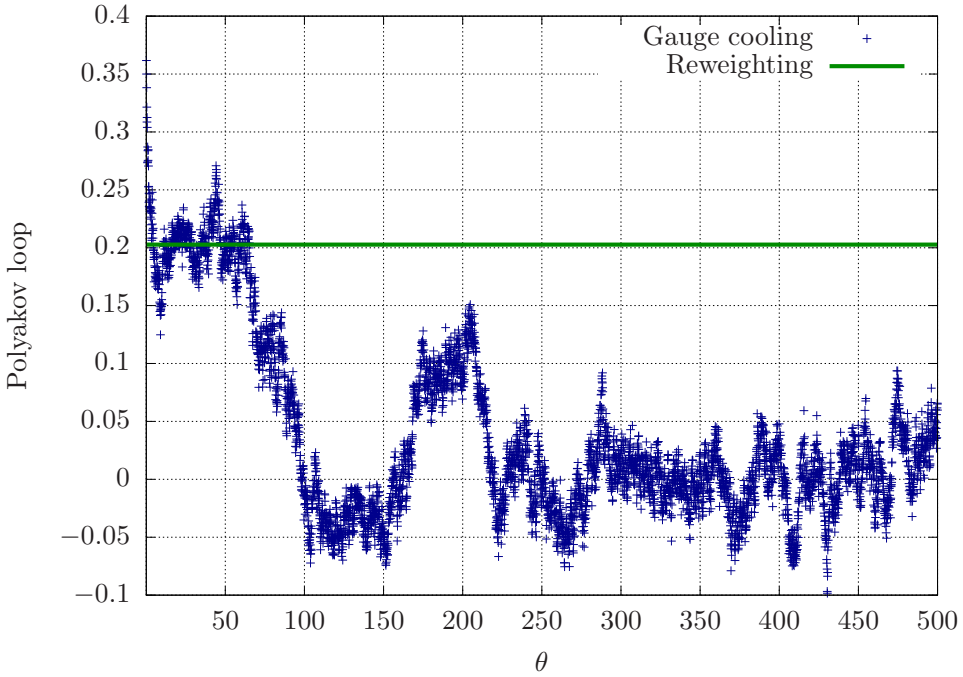
- Use gauge transformations to decrease d

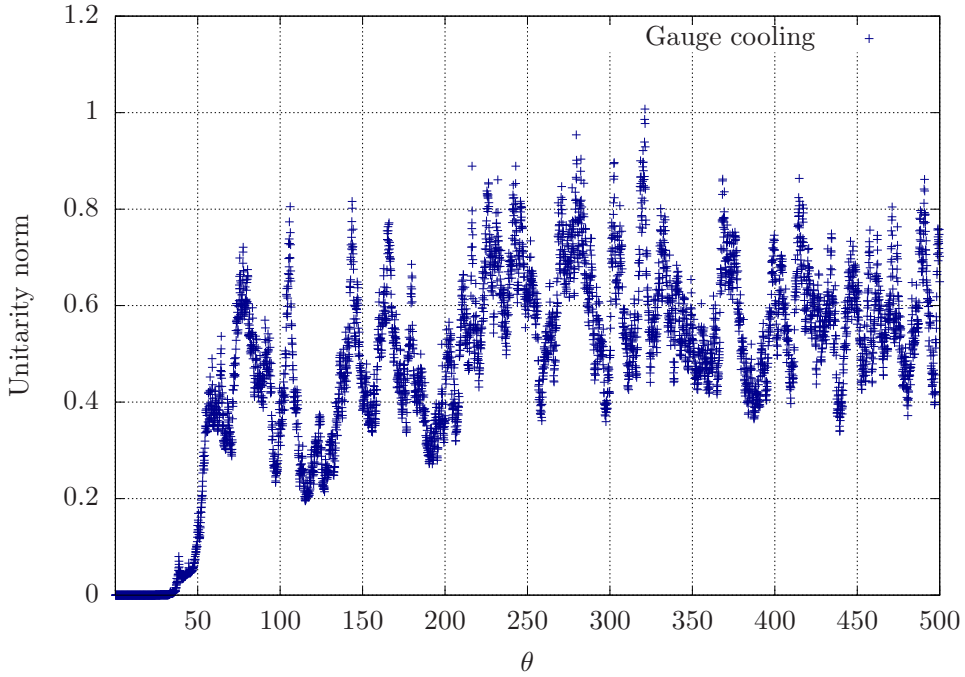
$$U_{x\mu} \to \Lambda_x U_{x\mu} \Lambda_{x+\mu}^{-1}$$

necessary, but not always sufficient

CLE: Complexification II – Gauge cooling

Gauge cooling (mild sign problem)





Left: Langevin time history of Polyakov loop
Right: Langevin time history of unitarity norm

CLE: Complexification III – Dynamic stabilisation

Dynamic stabilisation

[Attanasio, Jäger, hep-lat/1607.05642]

- New term in the drift to reduce the non-unitarity of $U_{x,\nu}$

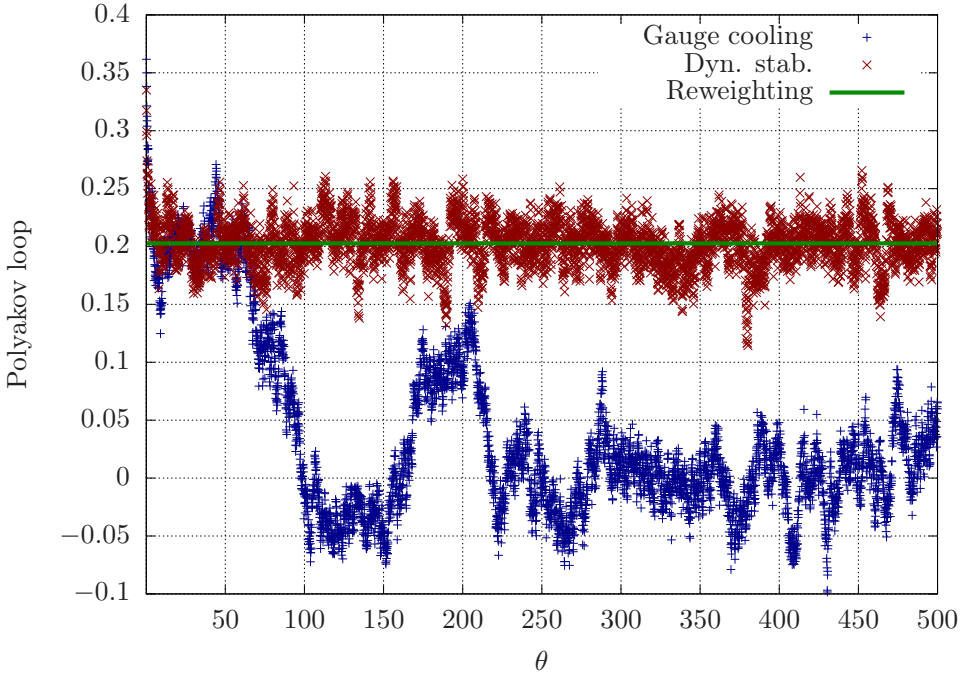
$$X_{x\nu} = i\lambda^a \left(-\epsilon D^a_{x,\nu} S - \epsilon \alpha_{\mathrm{DS}} M^a_x + \sqrt{\epsilon}\, \eta^a_{x,\nu}\right) .$$

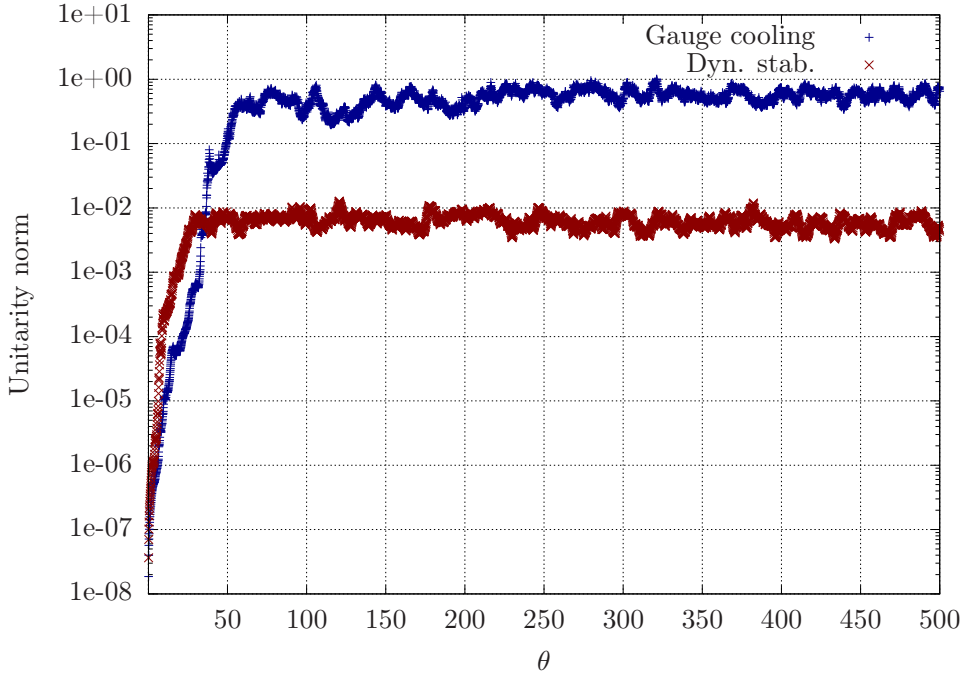
  with α_{DS} being a control coefficient

- 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)

CLE: Complexification III – Dynamic stabilisation

Dynamic stabilisation (mild sign problem)

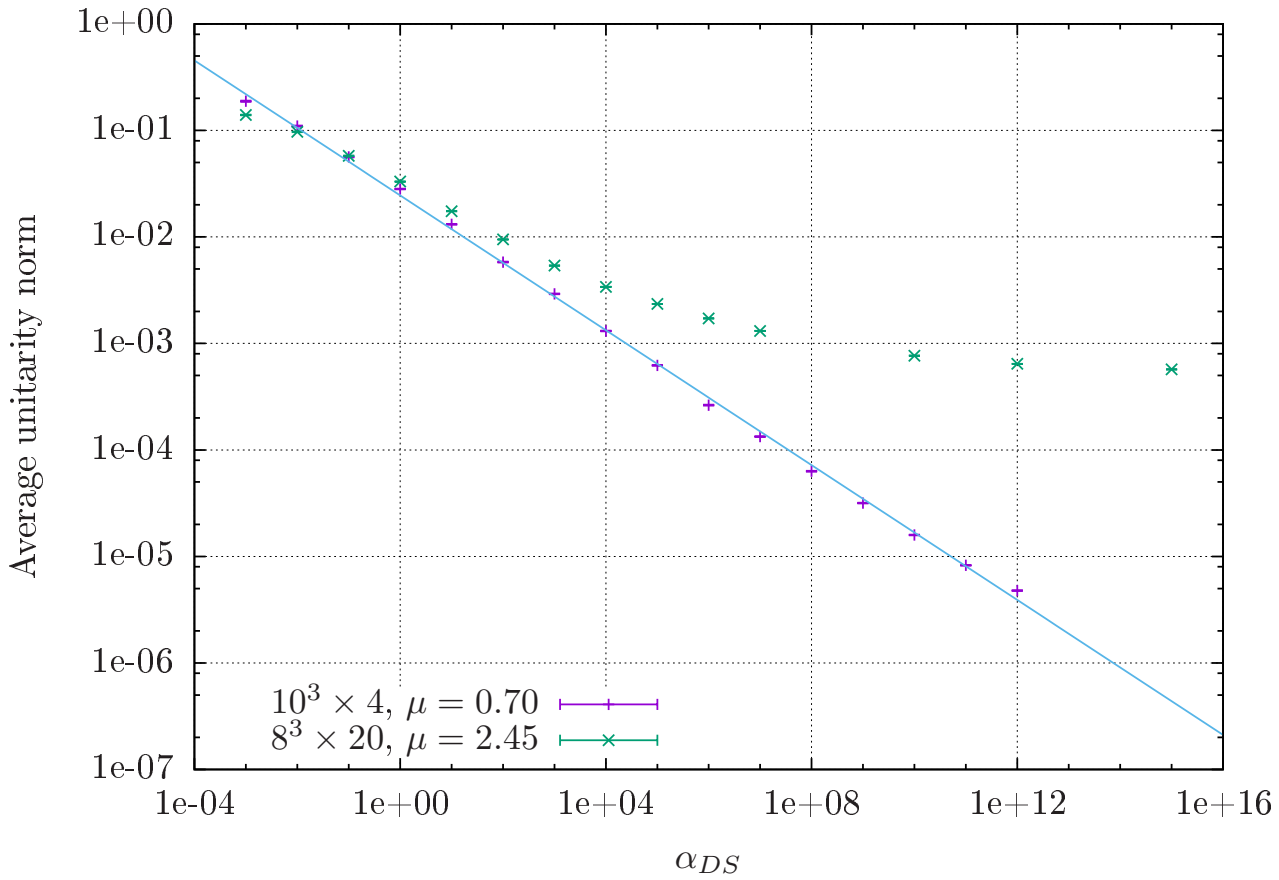




Left: Langevin time history of Polyakov loop
Right: Langevin time history of unitarity norm (notice log scale!)

CLE: Complexification III – Dynamic stabilisation

Dynamic stabilisation



Unitarity norm as a function of α_{DS} for HDQCD at $\beta = 5.8$ and $\kappa = 0.04$

Observables considered

- "Real part" of the Polyakov loop

$$P^s = \frac{1}{2}\left(\langle P\rangle + \langle P^{-1}\rangle\right) ,$$

- Chiral condensate (for dynamical quarks)

$$\langle\overline{\psi}\psi\rangle = \frac{T}{V}\frac{\partial \ln Z}{\partial m}$$

- Quark density

$$\langle n\rangle = \frac{T}{V}\frac{\partial \ln Z}{\partial \mu}$$

Heavy-dense QCD

Heavy-dense approximation

[Aarts, Stamatescu, hep-lat/0807.1597]

- Heavy quarks $\rightarrow$ quarks evolve only in Euclidean time direction:

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

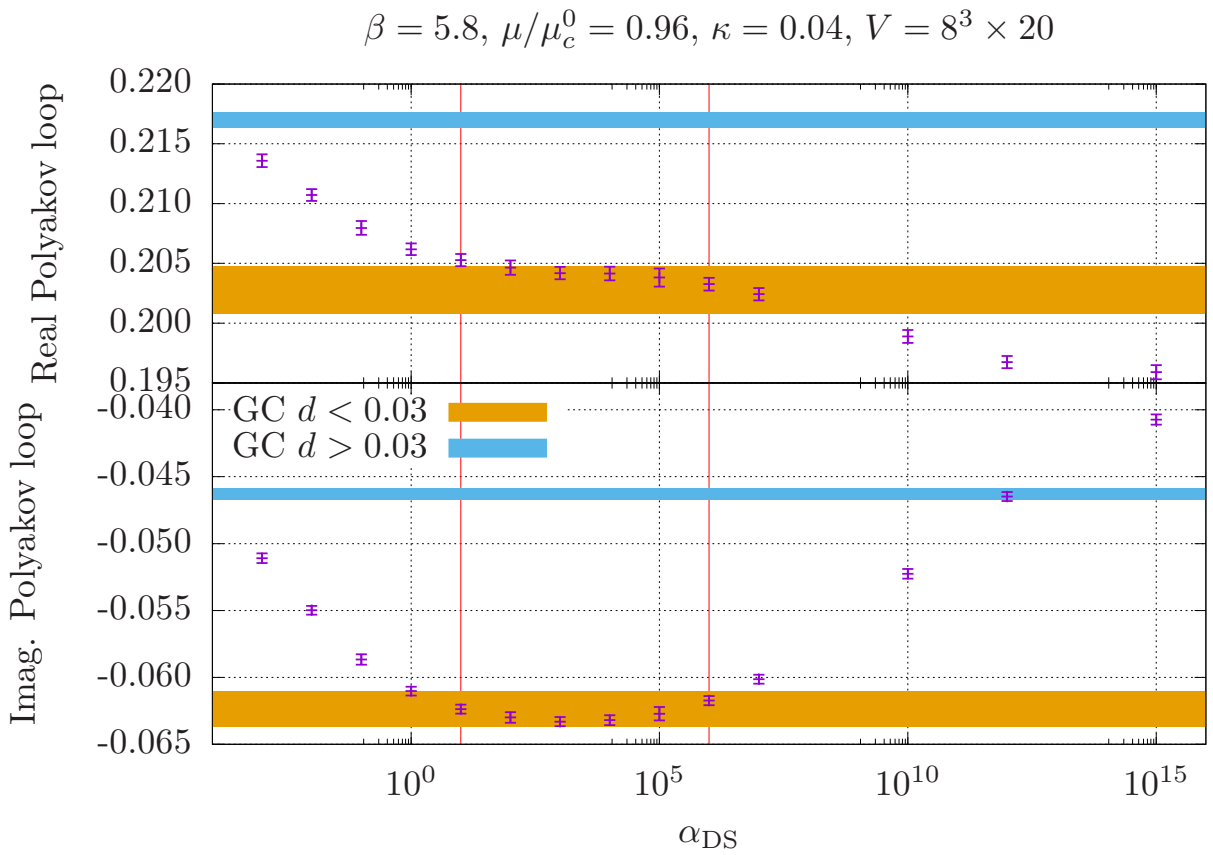
- Polyakov loop

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

- Exhibits the sign problem: $[\det M(U,\mu)]^* = \det M(U,-\mu^*)$
- Transition to higher densities (at $T=0$ it happens at $\mu = \mu_c^* \equiv -\ln(2\kappa)$)

Comparison of DS and GC

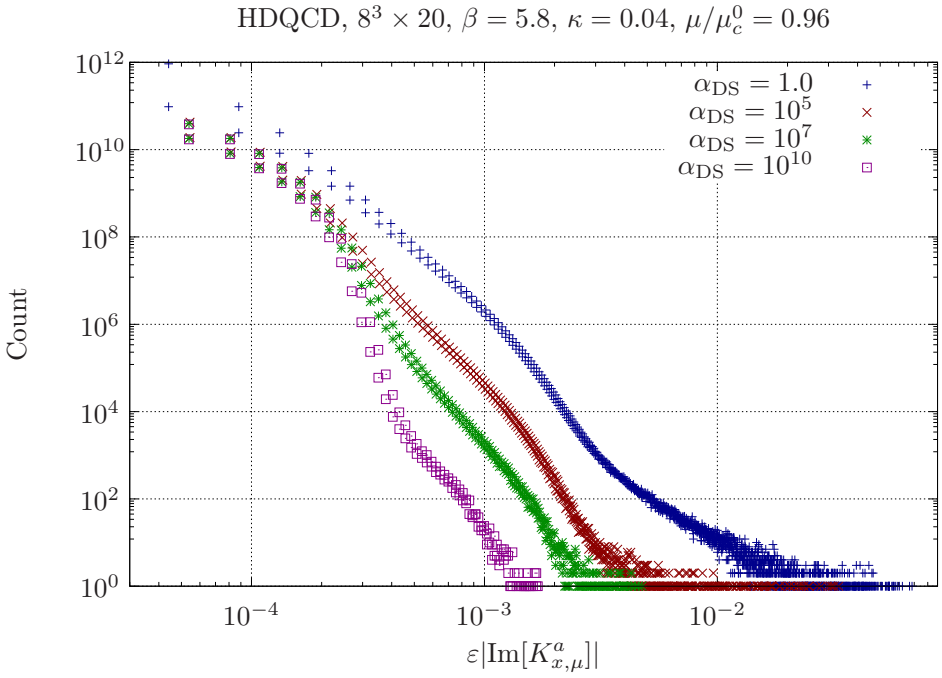
α_{DS} scan of the Polyakov loop, with results from gauge cooling

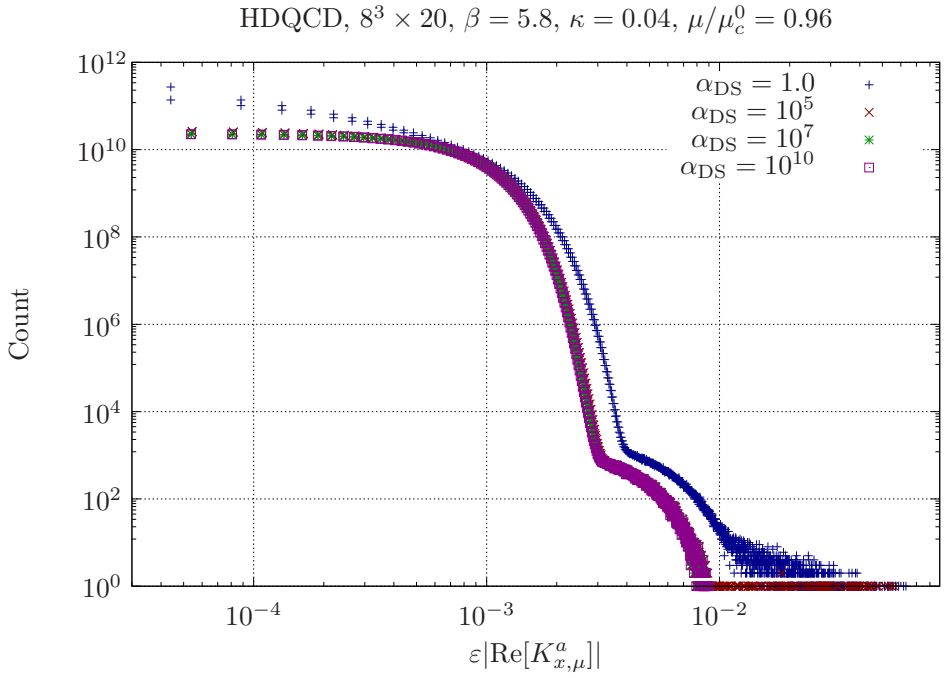


Wide region of α_{DS} where DS agrees with GC with low unitarity norm

Histograms I (HDQCD)

DS reduces only imaginary part of the Langevin drift

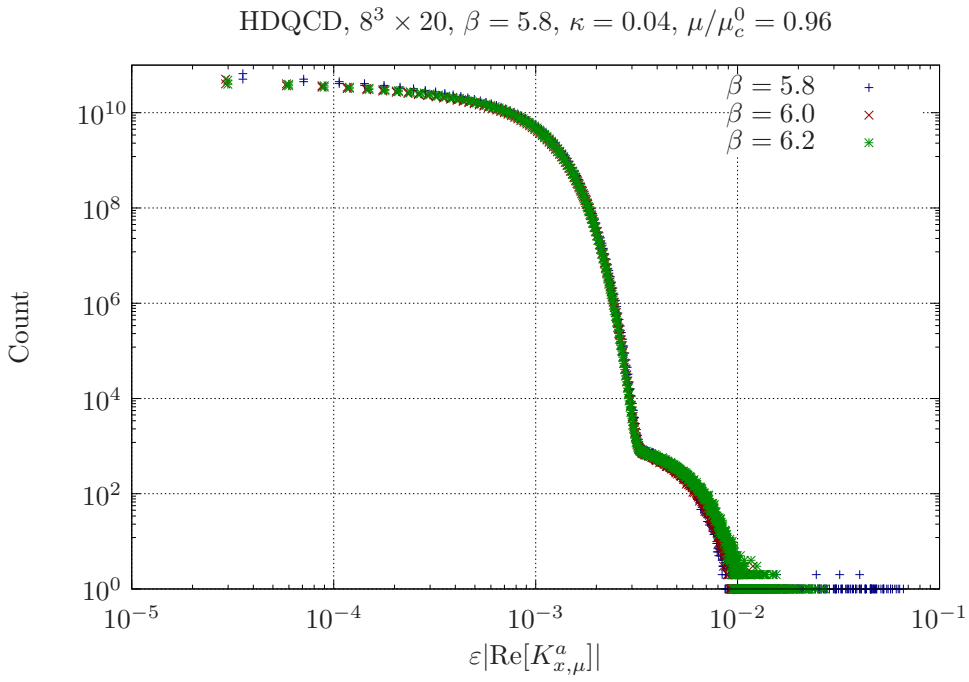


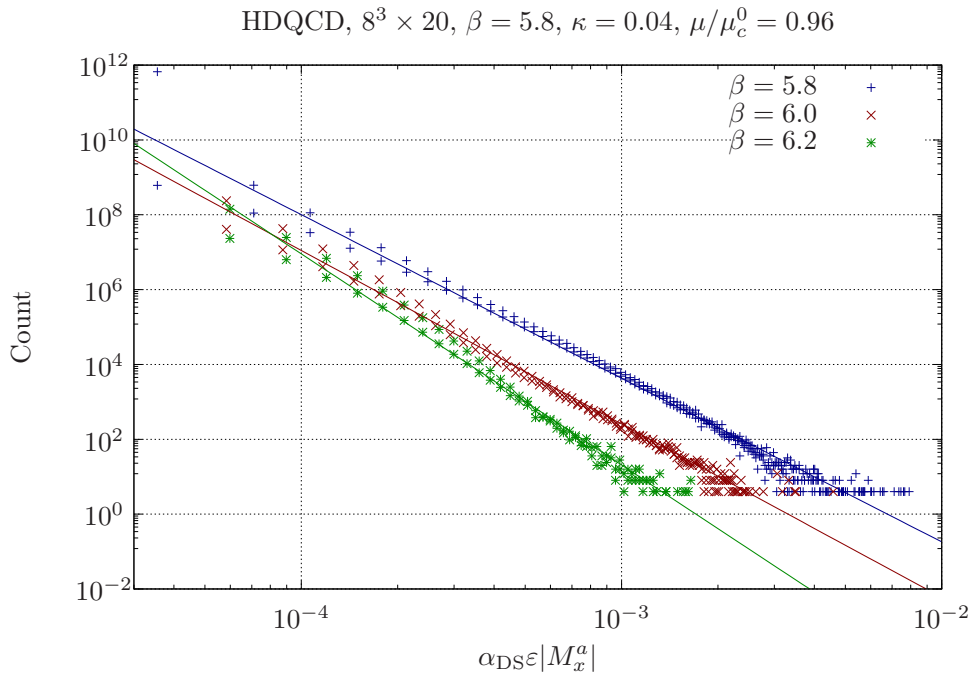


Histograms of the Langevin drift
Left: Imaginary part is clearly affected by larger $\alpha_{\rm DS}$
Right: For $\alpha_{\rm DS}$ large enough, the real part of the drift is essentially unchanged

Histograms II (HDQCD)

DS decreases with the lattice spacing

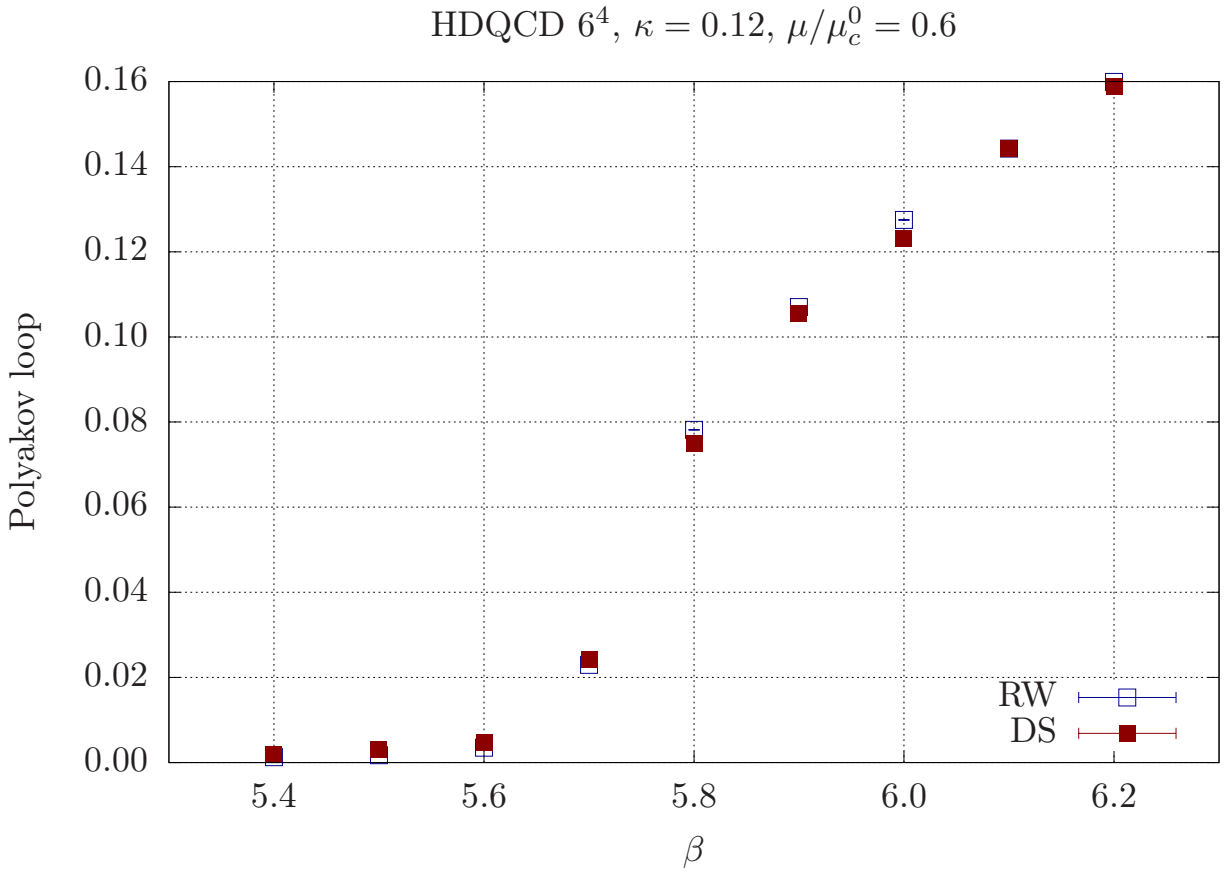




Histograms for different values of β
Left: Real part of the drift changes very little (a is changing)
Right: DS term decreases with a (higher β)

Deconfinement in HDQCD

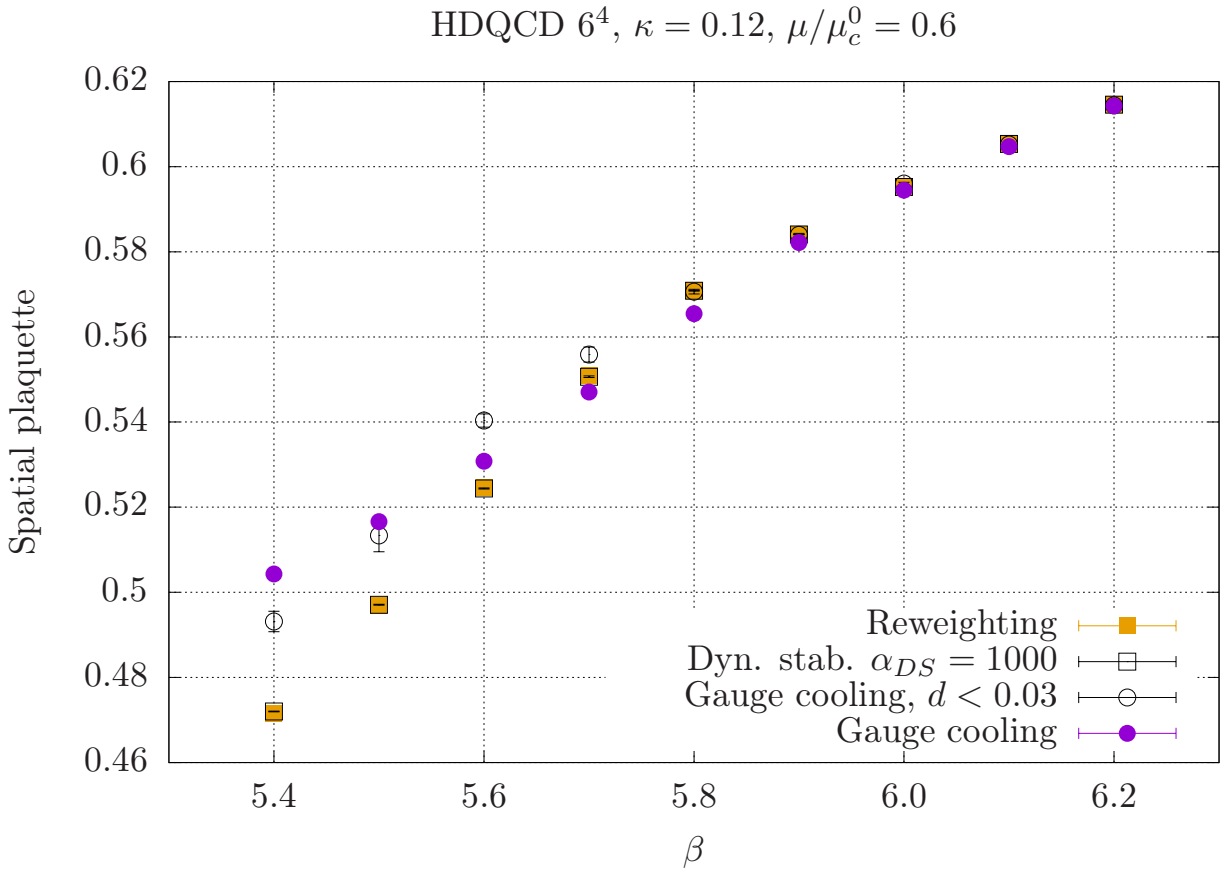
Good agreement with reweighting across the deconfinement region for fixed μ



Polyakov loop as a function of the inverse coupling β 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 β for HDQCD

Dynamical fermions

Staggered quarks

- The Langevin drift for N_f flavours of staggered quarks

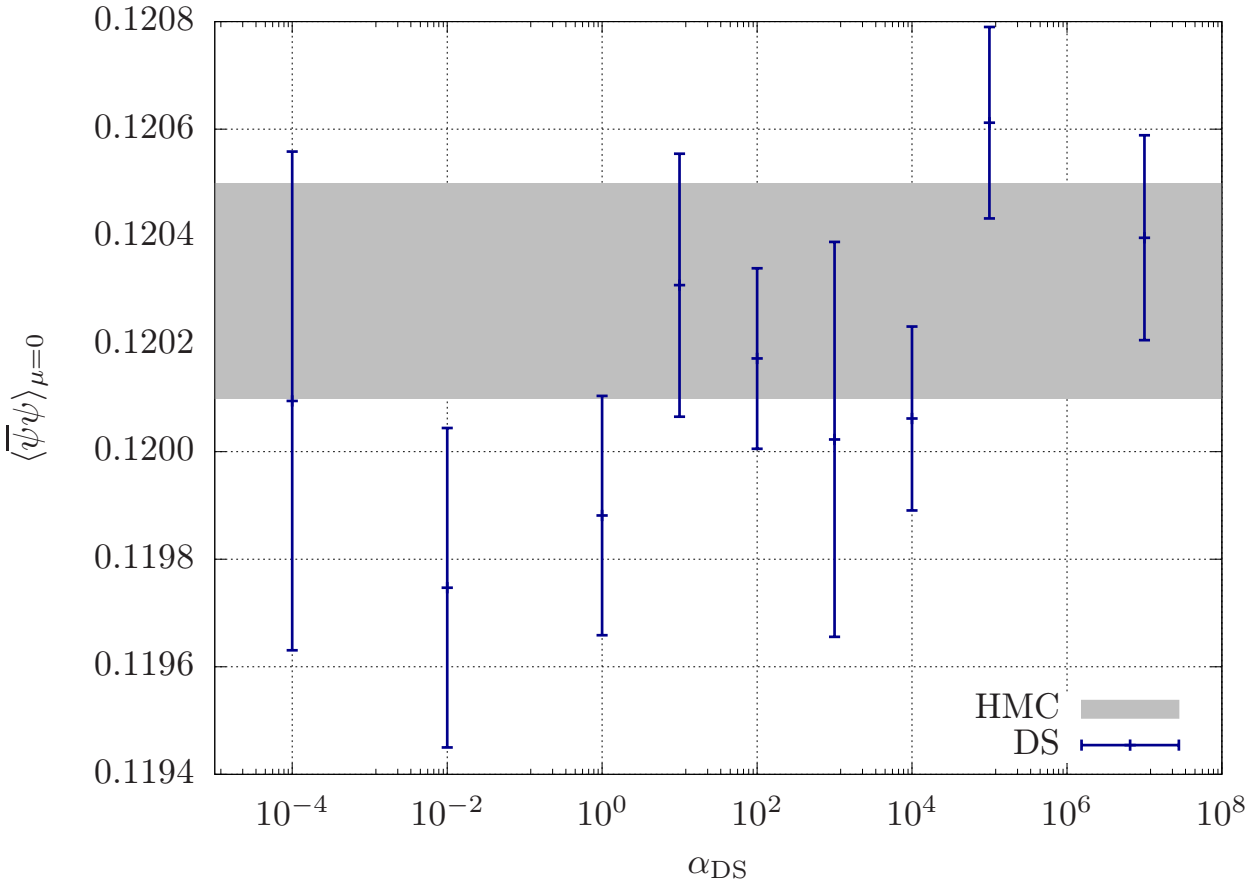
$$\begin{aligned} D^a_{x,\nu} S_F &\equiv D^a_{x,\nu} \ln \det M(U,\mu) \\ &= \frac{N_F}{4} \mathrm{Tr}\left[M^{-1}(U,\mu) D^a_{x,\nu} M(U,\mu)\right] \end{aligned}$$

- Inversion is done with conjugate gradient method

- Trace is evaluated by bilinear noise scheme – introduces imaginary component even for $\mu = 0$!

Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

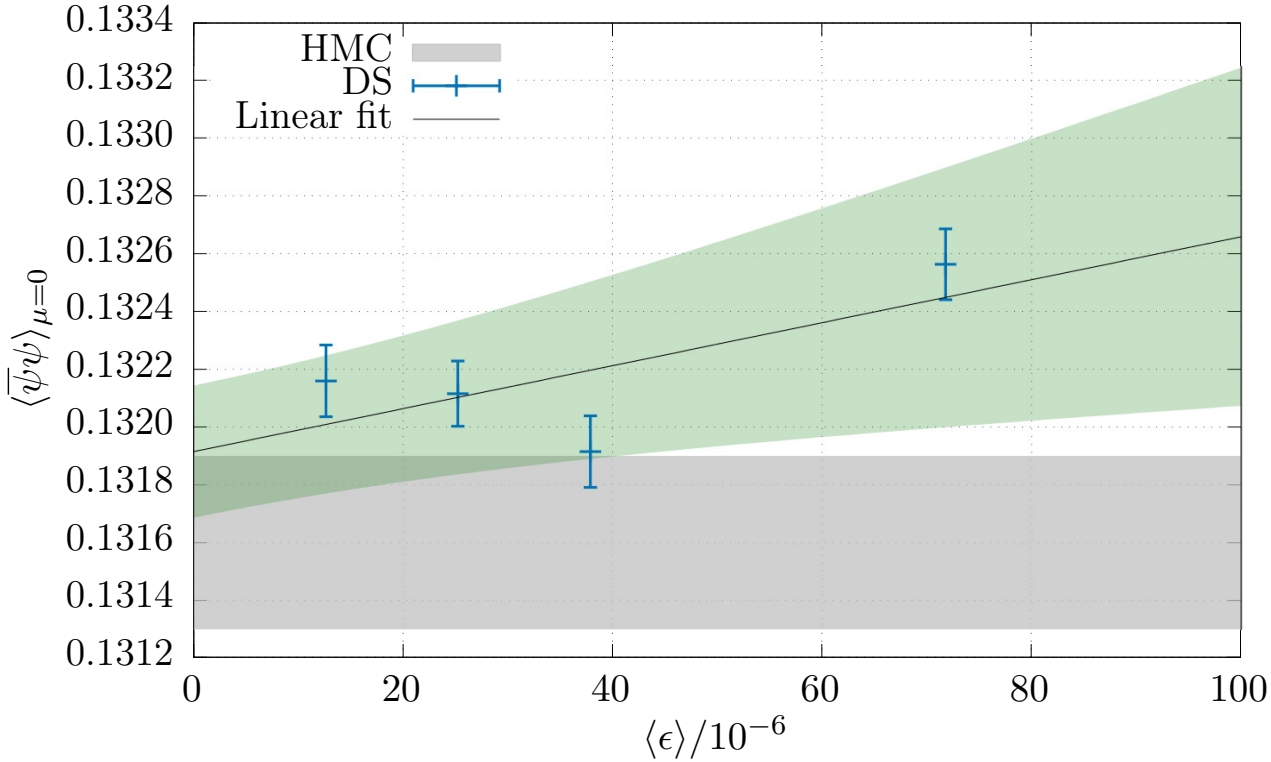
Comparison between CLE + DS runs and HMC (results by P. de Forcrand)



Grey band represents results from HMC simulations
α_{DS} scan of the chiral condensate for a volume of 6^4

Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

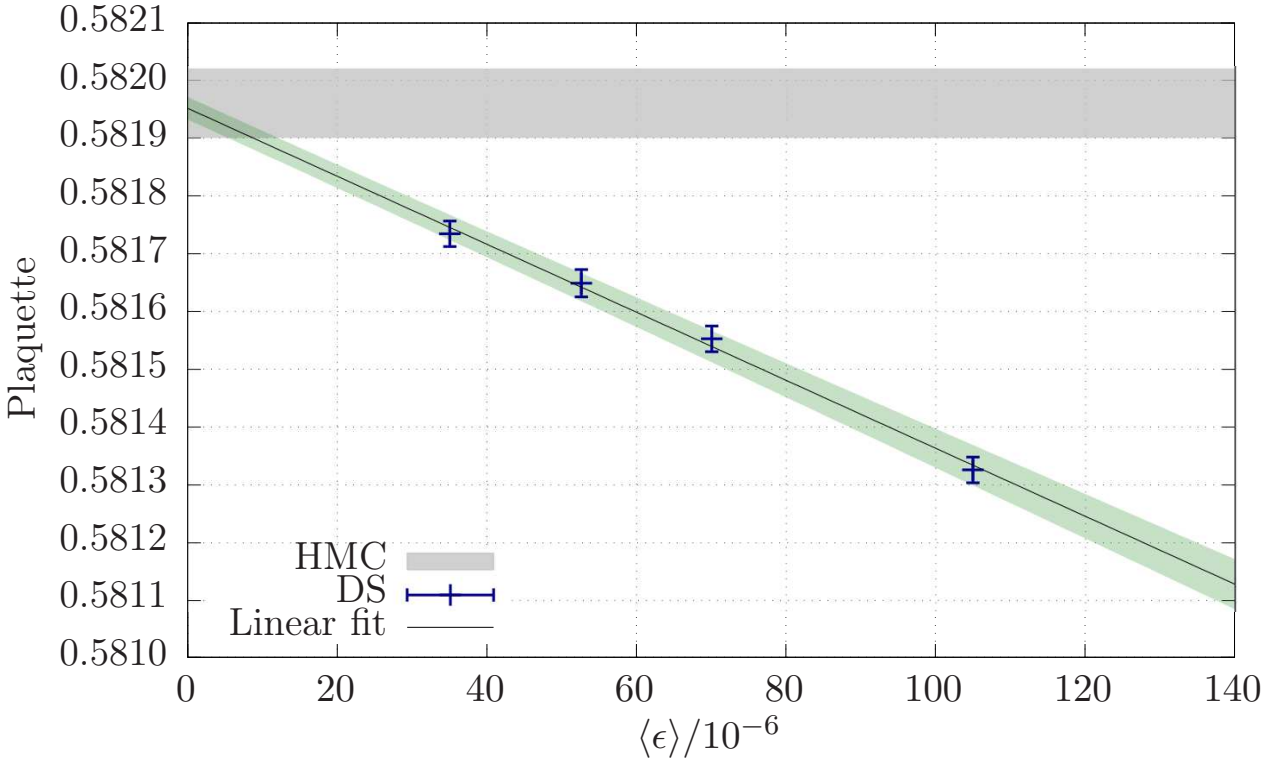
Comparison between CLE + DS runs and HMC (results by P. de Forcrand)



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 ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

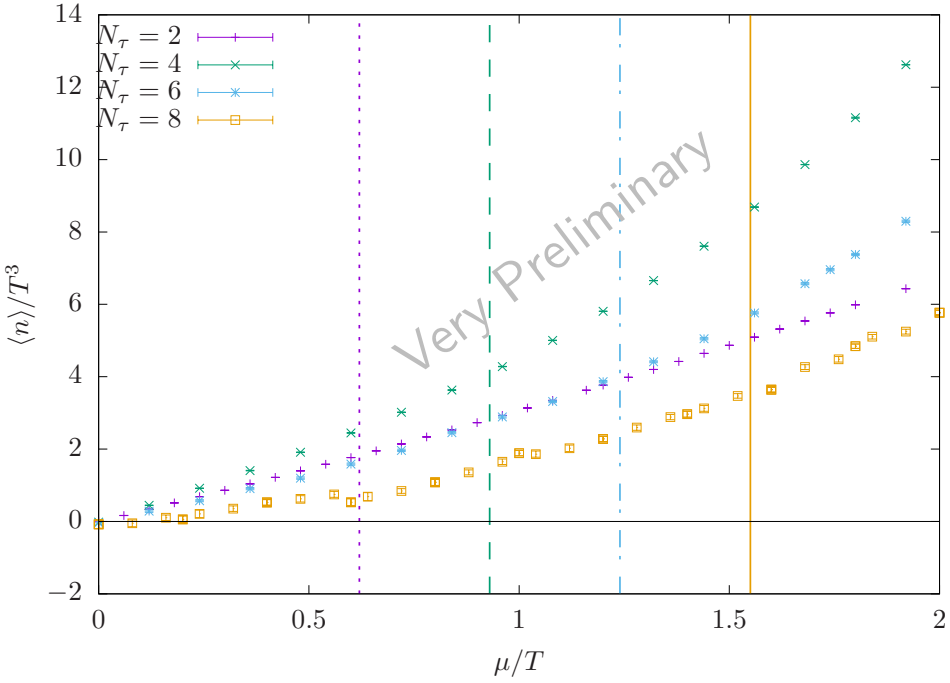
Comparison between CLE + DS runs and HMC (results by P. de Forcrand)

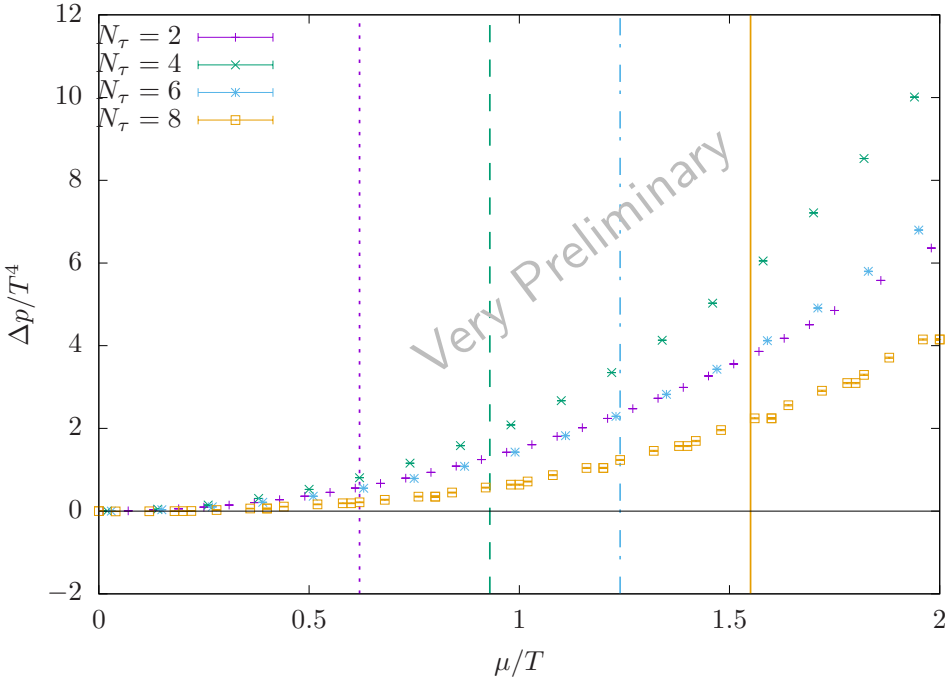
	Plaquette		$\overline{\psi}\psi$	
Volume	HMC	Langevin	HMC	Langevin
6^4	0.58246(8)	0.582452(4)	0.1203(3)	0.1204(2)
8^4	0.58219(4)	0.582196(1)	0.1316(3)	0.1319(2)
10^4	0.58200(5)	0.58201(4)	0.1372(3)	0.1370(6)
12^4	0.58196(6)	0.58195(2)	0.1414(4)	0.1409(3)

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 and Outlook

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