Selected inversion as key to a stable Langevin evolution across the QCD phase boundary

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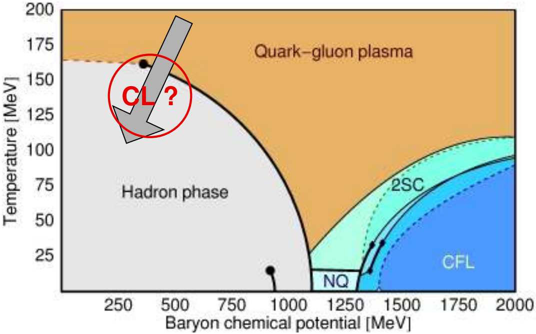
Complex Langevin results of PRD 92, 094516 (2015)

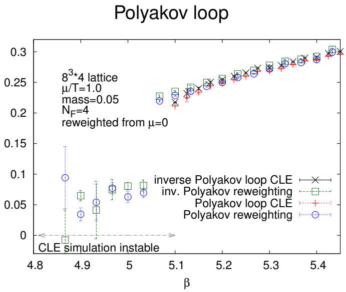
by Fodor, Katz, Sexty and Török

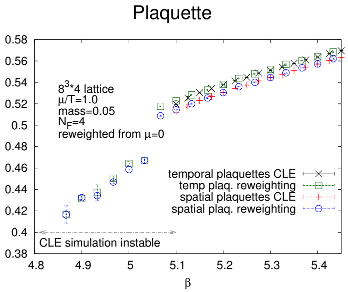
- Applied complex Langevin across QCD phase boundary
- Decreased temperature from deconfined to confined phase by decreasing β at constant μ/T
- Simulation parameters: $8^3 \times 4$ lattice, $m = 0.05$, $\mu/T = 1.0$, ($\beta_c \approx 5.04$ at $\mu = 0$).

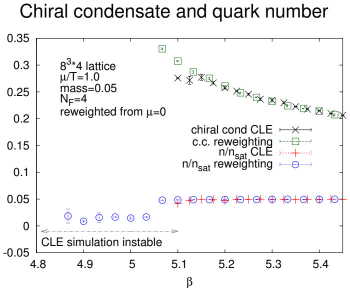


Breakdown of CL observed in PRD 92, 094516 (2015)

$8^3 \times 4$ lattice at $\mu/T = 1$ and $m = 0.05$







Lattice QCD partition function

Partition function of lattice QCD:

$$Z = \left[\prod_{x=1}^{V} \prod_{\nu=0}^{d-1} \int dU_{x\nu} \right] \exp[-S_g] \det D(m;\mu)$$

with Wilson gauge action S_g and staggered Dirac operator D and links

$$U_{x\nu} = \exp\left[i \sum_{a=1}^{8} z_{ax\nu} \lambda_a \right],$$

with Gell-Mann matrices λ_a and parameters $z_{ax\nu}$.

Complex Langevin for QCD

- Discrete Langevin evolution in SL$(3,\mathbb{C})$:

$$U_{x\nu}(t+1) = R_{x\nu}(t)\, U_{x\nu}(t)$$

where

$$R_{x\nu} = \exp\left[i \sum_a \lambda_a (\epsilon K_{ax\nu} + \sqrt{\epsilon}\, \eta_{ax\nu}) \right] \in \text{SL}(3,\mathbb{C}),$$

with Langevin step ϵ and Gaussian noise $\eta_{ax\nu}$.

- Total drift:

$$K_{ax\nu} = -\partial_{ax\nu} S = K^{\text{gauge}}_{ax\nu} + K^{\text{ferm}}_{ax\nu}$$

with complex action $S = S_g - \log\det D$.

- Fermionic drift:

$$K^{\text{ferm}}_{ax\nu} = \text{Tr}\left[D^{-1} \frac{\partial D}{\partial z_{ax\nu}} \right]$$

Discussion of breakdown

- **Question:** Is breakdown caused by violation of CL validity conditions or due to numerical approximations?
- **Argument:** Traces in drift term approximated by stochastic estimators $\longrightarrow$ can be unstable for indefinite matrices
- **Literature:** Bounds on estimator only for positive definite matrices.
- **Numerical tests:** Indefinite matrices *can* require huge number of estimators. Each Langevin step requires $8 \times 4 \times V$ traces.
- **Task:** Investigate if exact inversion stabilizes CL
- **Problem:** Full inversion too costly on four-dimensional lattices
- **Solution:** use Selected inversion

Drift term

- Complex Langevin evolution is delicate, irrespective of validity of CL

Problems

- Large drift → small ϵ to avoid runaways
- Large autocorrelation times → long trajectories to have enough independent configs

- Small ϵ and long trajectories → huge number of Langevin steps
  - Fermionic drift requires $D^{-1} \rightarrow \mathcal{O}(N^3)$: too expensive

Current solution

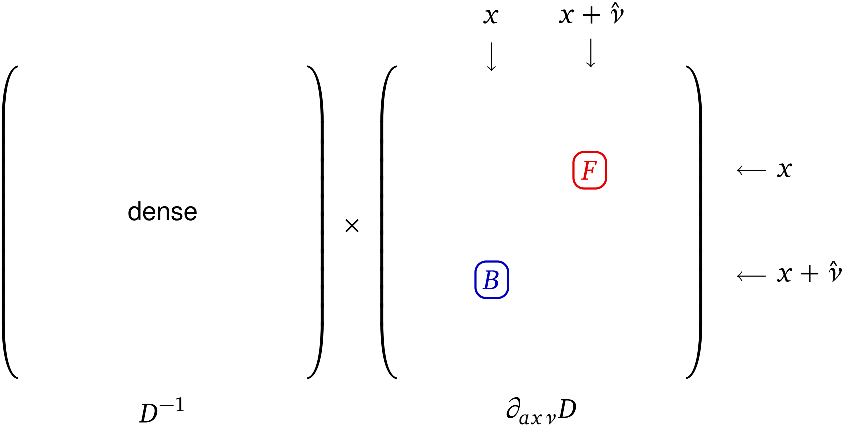
- Avoid computation of D^{-1} by using *stochastic estimator* of traces:

$$\mathrm{Tr}[D^{-1}\partial_{ax\nu}D] \approx \eta^\dagger D^{-1}\partial_{ax\nu}D\eta$$

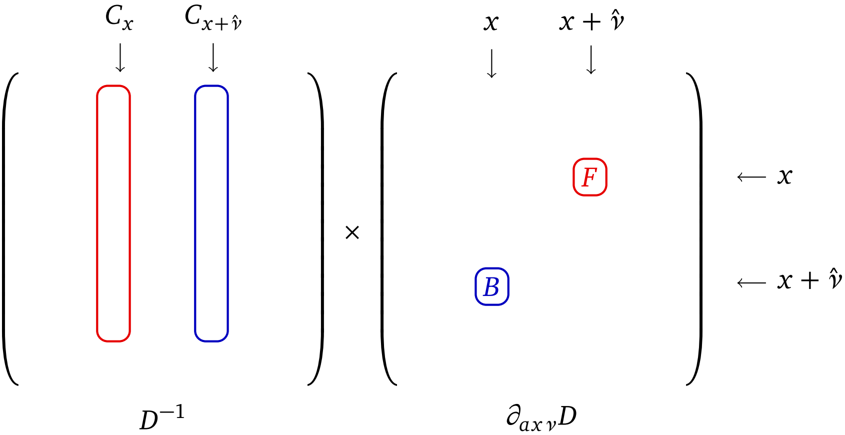
- Potential problem: stochastic technique unstable/costly for *indefinite* matrices → tiny ϵ → consecutive correlated CL steps provide many estimators of trace. Danger: wrong estimates may **destabilize** the discrete evolution.

Drift term

- Drift: $K_{ax\,\nu} = \mathrm{Tr}[D^{-1}\partial_{ax\,\nu}D]$
- $\partial_{ax\,\nu}D$: derivative of D wrt link $U_{x\,\nu}$ at site x and direction ν



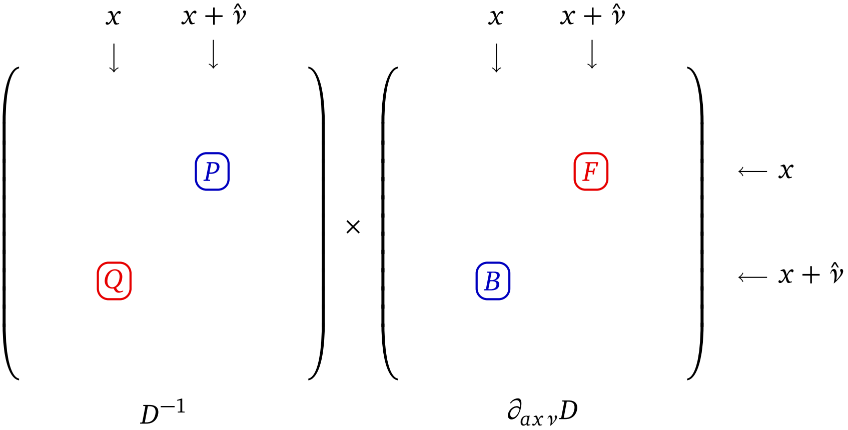
Drift term



- $C_{x+\hat{\nu}} \times B \to$ column x of $D^{-1}\partial_{ax\nu}D$
- $C_x \times F \to$ column $x+\hat{\nu}$ of $D^{-1}\partial_{ax\nu}D$

Drift term

AFTER TRACING



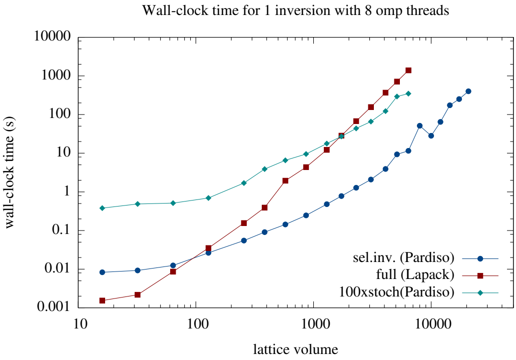
$K_{ax\nu} = \mathrm{Tr}[D^{-1}\partial_{ax\nu}D] = \mathrm{Tr}(P \cdot B) + \mathrm{Tr}(Q \cdot F)$

$\Rightarrow$ **ONLY USES ELEMENTS of D^{-1} where D itself is NONZERO.**

Selected inversion technique

- Presented in *Fast Methods for Computing Selected Elements of the Green's Function in Massively Parallel Nanoelectronic Device Simulations*, Euro-Par 2013, LNCS 8097, p. 533, 2013, Andrey Kuzmin, Mathieu Luisier and Olaf Schenk
- Sparse LU-factorization followed by selected inversion
- Selected inversion: exactly computes *selected* elements of the inverse A^{-1} of A. Subset of selected elements is defined by set of *nonzero entries* in A.
- Principle: this subset of A^{-1} can be evaluated without computing any inverse entry from outside of the subset → speedup
- Method implemented in latest verion of parallel sparse direct solver PARDISO
- Runs performed on Xeon cluster at ICS, Lugano

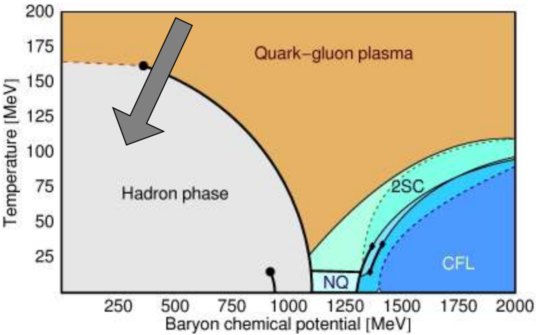
Performance gain using selected inversion



- Efficiency: Gain of factor 100 compared to Lapack dense inverse
- Storage: Dirac operator and selected inverse are stored in sparse format

Crossing the phase boundary

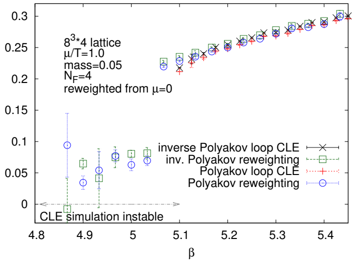
- Study QCD phase transition across roof of phase diagram, i.e. decrease temperature from deconfined to confined phase at constant μ/T
- Simulation parameters: $8^3 \times 4$ lattice, $m = 0.05$, $\mu/T = 1.0$, $\epsilon = 0.001$ (adaptive) ($\beta_c \approx 5.04$ at $\mu = 0$).
- Vary β from 5.45 down to 4.0.



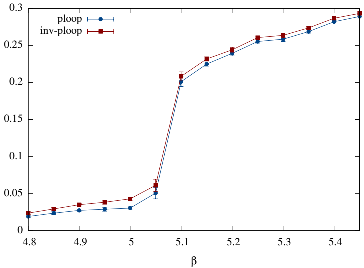
Polyakov loop versus β

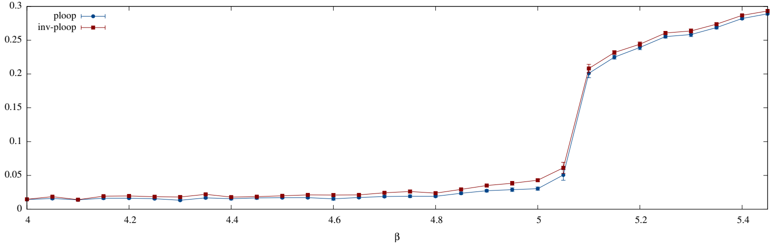
$8^3 \times 4$, $\mu/T = 1$, $m = 0.05$

PRD 92, 094516 (2015)



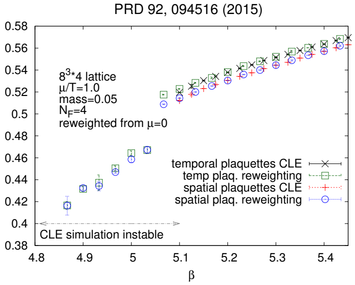
Polyakov loop and inverse Polyakov loop

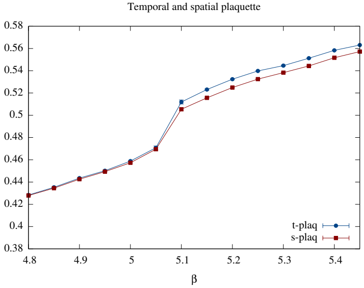


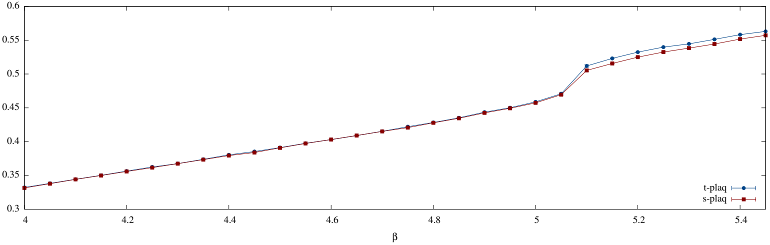


Plaquettes versus β

$8^3 \times 4$, $\mu/T = 1$, $m = 0.05$

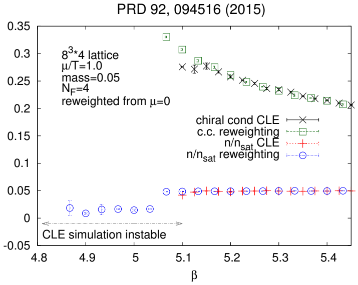


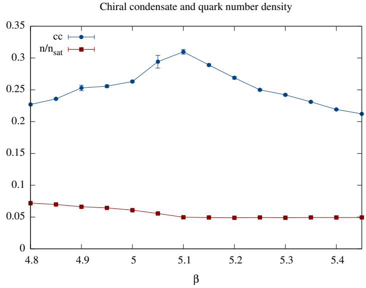


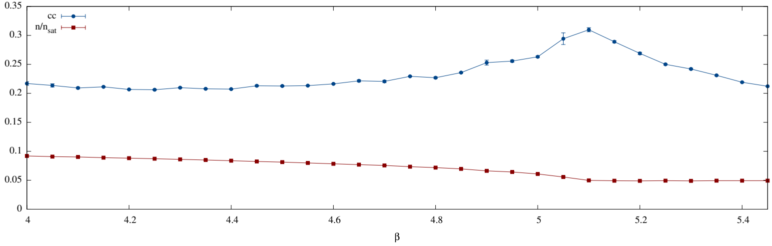


Chiral condensate and quark number density versus β

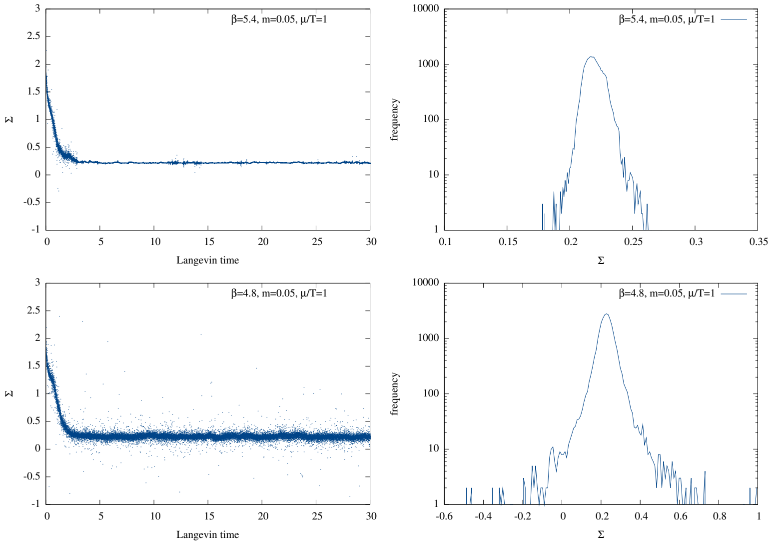
$8^3 \times 4$, $\mu/T = 1$, $m = 0.05$



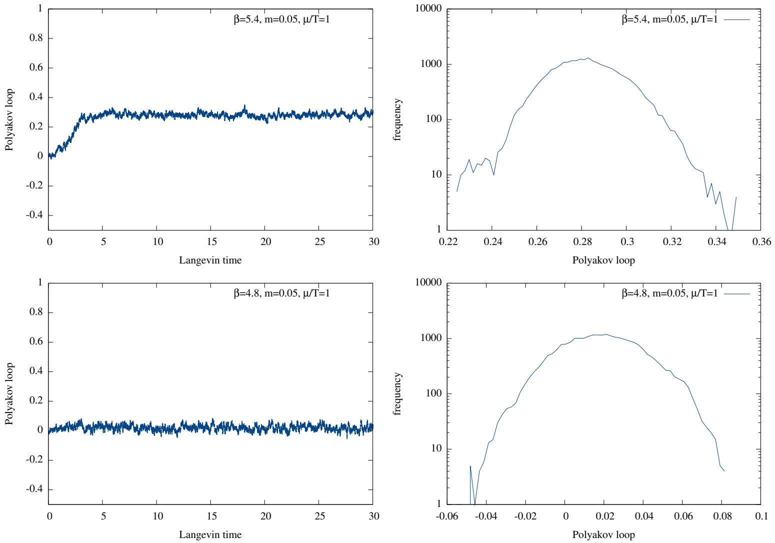




Langevin history and histogram of chiral condensate

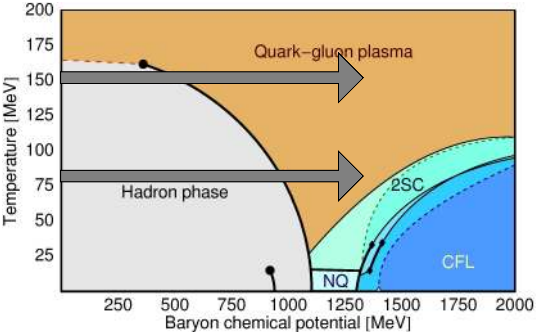


Langevin history and histogram of Polyakov loop



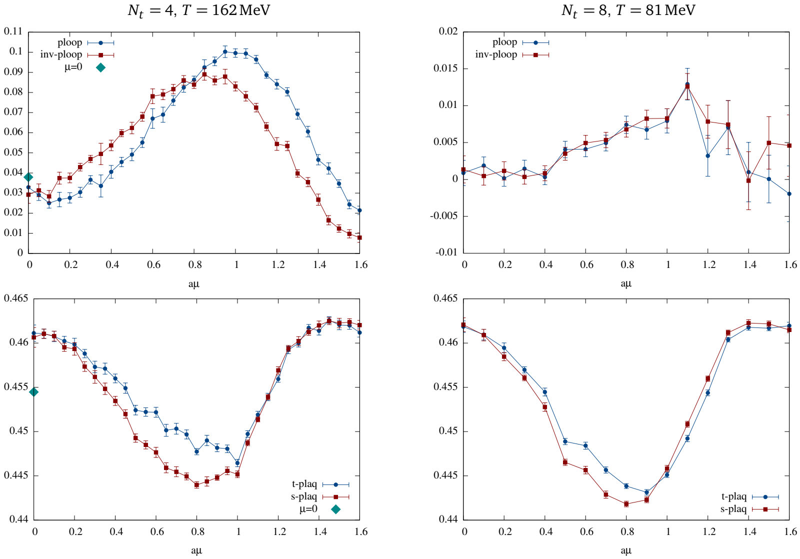
Evolution in μ

- Simulation parameters: $8^3 \times N_t$, $m = 0.05$, $\beta = 5.0$ ($\beta_c \approx 5.04$) $\rightarrow a = (0.3045 \pm 0.0001)\,\mathrm{fm}$, $1/a = 647\,\mathrm{MeV}$.
- Pion mass: $am_\pi = 0.5588 \pm 0.0002 \rightarrow m_\pi \approx 362\,\mathrm{MeV}$.
- Lattice size: $N_t = 4$ ($T = 161.74\,\mathrm{MeV}$) and $N_t = 8$ ($T = 80.87\,\mathrm{MeV}$)



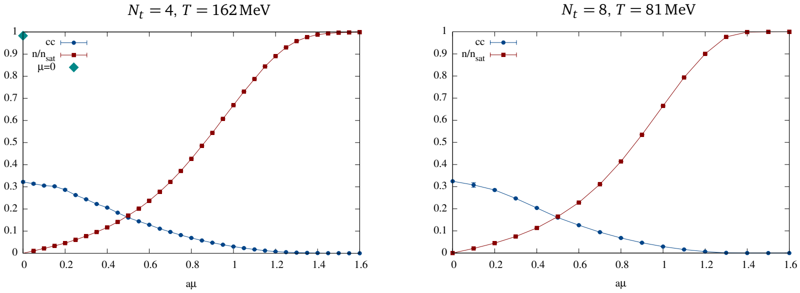
Polyakov loop and plaquette versus μ

$8^3 \times 4$, $\beta = 5$, $m = 0.05$



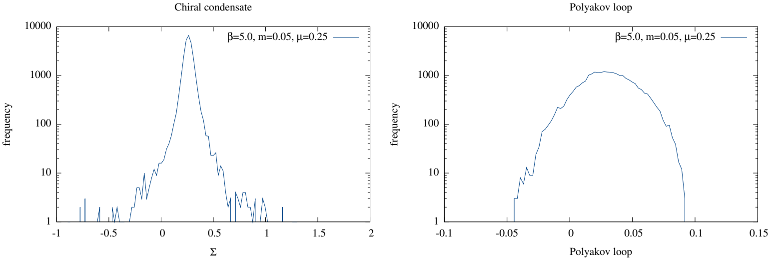
Chiral condensate and quark number density versus μ

$8^3 \times 4$, $\beta = 5$, $m = 0.05$



Histogram of chiral condensate and Polyakov loop

- Histograms for $N_t = 4$, $\beta = 5.0$, $m = 0.05$, $\mu = 0.25$



Summary and Outlook

- Breakdown of CL observed by Fodor et al. at QCD phase boundary → numerical artifact due to stochastic estimation of drift
- Full inversion too expensive, but selected inversion with PARDISO allows exact drift term calculation → Langevin evolution stable (with adaptive step size)
- Allows study of QCD phase transition across roof of phase diagram, i.e. decrease temperature from deconfined to confined phase at constant μ
- Study of QCD phase transition at fixed T as a function of μ

- Need detailed investigation into validity of CL results
- IF valid, move to larger lattice
- Apply reweighted complex Langevin where CL invalid