Complex Langevin for Lattice QCD at $T = 0$ and $\mu \geq 0$

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Introduction

Lattice QCD with a finite chemical potential μ has a complex fermion determinant. Hence standard simulation methods based on importance sampling fail.

The Langevin approach does not rely on importance sampling and can be extended to complex actions. For lattice QCD, this requires analytic continuation of the gauge fields from $SU(3)$ to $SL(3,C)$.

The long-time evolution of the fields under the Complex Langevin Equation (CLE) is not guaranteed to produce limiting values for observables. Even when it does, these values are not guaranteed to be correct.

For the CLE to produce the correct results, the fields should be confined to a compact domain, and the drift (force) term in the CLE should be holomorphic in the fields.

Early attempts at applying the CLE to QCD were frustrated by runaway trajectories, which were not controlled by adaptive adjustment of the time increment used for updating the fields.

Recent advances involving gauge transformations to keep the fields as close to the $SU(3)$ manifold as possible, avoid such runaway solutions provided the gauge coupling is not too large, by preventing large gauge excursions from well-behaved configurations. This is referred to as 'gauge cooling'.

When the gauge coupling is sufficiently small, the gauge fields do appear to be restricted to a compact domain. However, away from the SU(3) manifold, the Dirac operator has zero eigenvalues, which produce zeros in the fermion determinant, and the drift term is meromorphic, not holomorphic.

Much of the earlier work applying the CLE with adaptive updating and gauge cooling to lattice QCD at finite μ has been at large quark mass.

Simulations with light quark masses have been restricted to small lattices or to finite-temperature QCD, where they are used to study the finite-temperature transition at finite μ.

We are performing CLE simulations of lattice QCD at finite μ at zero temperature with quark masses light enough to clearly separate the expected phase transition from hadronic to nuclear matter at $\mu \approx m_N/3$ from any pseudo-transition at $\mu = m_\pi/2$.

Most of our simulations are performed with $N_f = 2$, $\beta = 5.6$ and $m = 0.025$ on a 12^4 lattice.

While many of the qualitative features of the zero-temperature phase diagram are observed, the observables show departures from known values in the low μ domain.

We are also performing simulations on a 16^4 lattice, which suggest that these departures are not a finite-size effect or a finite-dt effect. This larger lattice also enables us to run at $\beta = 5.7$, where we find significant improvement in the agreement between CLE measured observables and known values at $\mu = 0$. We will extend this to $\mu \neq 0$.

This suggests that the CLE produces correct results in the zero lattice-spacing (weak-coupling) limit.

This observation that the CLE approaches the wrong limit if the coupling is too large is observed by others in simulations of Lattice QCD at finite μ in other regimes as well as in models, and appears to be due to the poles in the drift term.

We are also performing some $N_f = 4$ simulations to determine how much of our departures are due to the known problems with rooting at finite μ.

Complex Langevin for finite density Lattice QCD

If $S(U)$ is the gauge action after integrating out the quark fields, the Langevin equation for the evolution of the gauge fields U in Langevin time t is:

$$-i\left(\frac{d}{dt}U_l\right)U_l^{-1} = -i\frac{\delta}{\delta U_l}S(U) + \eta_l$$

where l labels the links of the lattice, and $\eta_l = \eta_l^a \lambda^a$. Here λ_a are the Gell-Mann matrices for $SU(3)$. $\eta_l^a(t)$ are Gaussian-distributed random numbers normalized so that:

$$\langle \eta_l^a(t)\eta_{l'}^b(t')\rangle = \delta^{ab}\delta_{ll'}\delta(t-t')$$

The complex-Langevin equation has the same form except that the Us are now in $SL(3,C)$. S, now $S(U,\mu)$ is

$$S(U,\mu) = \beta\sum_{\Box}\left\{1-\frac{1}{6}Tr[UUUU+(UUUU)^{-1}]\right\} - \frac{N_f}{4}\mathrm{Tr}\{ln[M(U,\mu)]\}$$

where $M(U,\mu)$ is the staggered Dirac operator. Note: backward links are represented by U^{-1} not $U^{\dagger}$. Note also that we have chosen to keep the noise term η real.

To simulate the time evolution of the gauge fields we use a partial second-order formalism. For an update of the fields by a 'time' increment dt, this gives:

$$U^{(n+1/2)} = e^{X_0} U^{(n)}$$

$$X_0 = dt \frac{\delta}{\delta U} S(U^{(n)}, \mu) + i\sqrt{dt}\eta^{(n)}$$

$$U^{(n+1)} = e^{\gamma(X_0 + X_1)} U^{(n)}$$

$$X_1 = dt \frac{\delta}{\delta U} S(U^{(n+1/2)}, \mu) + i\sqrt{dt}\eta^{(n)}$$

where $\gamma = \frac{1}{2} + \frac{1}{4}dt$ and the Gaussian noise η is normalized such that:

$$\langle \eta_l^{a(m)} \eta_{l'}^{b(n)} \rangle = \left(1 - \frac{3}{2}dt\right) \delta^{ab} \delta_{ll'} \delta^{mn}$$

To proceed, we replace the spacetime trace with a stochastic estimator ξ

$$\mathrm{Tr}\{ln[M(U,\mu)]\} \rightarrow \xi^\dagger\{ln[M(U,\mu)]\}\xi\ ,$$

where ξ is a vector over space-time and colour of gaussian random numbers, normalized so that:

$$\langle \xi^{*i(m)}(x)\xi^{j(n)}(y)\rangle = \delta^{ij}\delta_{xy}\delta^{mn}$$

which means, in particular, that the ξs in X_0 and X_1 are independent, unlike the ηs. After performing $\frac{\delta}{\delta U}$ of $ln(M)$ it is useful to rearrange the terms proportional to U and U^{-1} so that this term is antihermitian when $\mu = 0$ and U is unitary. That way, in this special case, the complex-Langevin equation becomes the real-Langevin equation.

We apply adaptive updating, where if the force term becomes too large, dt is decreased to keep it under control.

After each update, we adaptively gauge fix to the gauge which minimizes the unitarity norm:

$$F(U) = \frac{1}{4V}\sum{}_{x,\mu} Tr\left[U^\dagger U + (U^\dagger U)^{-1} - 2\right] \geq 0$$

Zero Temperature Simulations on a 12^4 lattice

We simulate lattice QCD with $\beta = 5.6$ and $m = 0.025$ on a 12^4 lattice using the CLE.

On this size lattice finite-size effects could be expected to be large.

Here $m_\pi/2 \approx 0.21$ and $m_N/3 \approx 0.33$.

We simulate at a selection of μ values in the range $0 \leq \mu \leq 1.5$.

Our input $dt = 0.01$, and our runs at each β range in length from 0.9 to 3 million updates.

Adaptive rescaling of the update interval dt reduces it considerably. The length of the equilibrated part of the run at each β is then in the range 100 to 1000 time units.

Figure 1 shows the average plaquette values measured during these runs. The dashed blue line is the value of the plaquette for $\mu = 0$ from an RHMC simulation.

While the difference between the true(RHMC) value and the CLE value at $\mu = 0$ is small, it is significant.

For $\mu \leq 0.25$ the plaquette value does not appear to depend on μ, which is the expected result.

For $\mu \geq 0.35$ the plaquette increases with μ up until saturation.

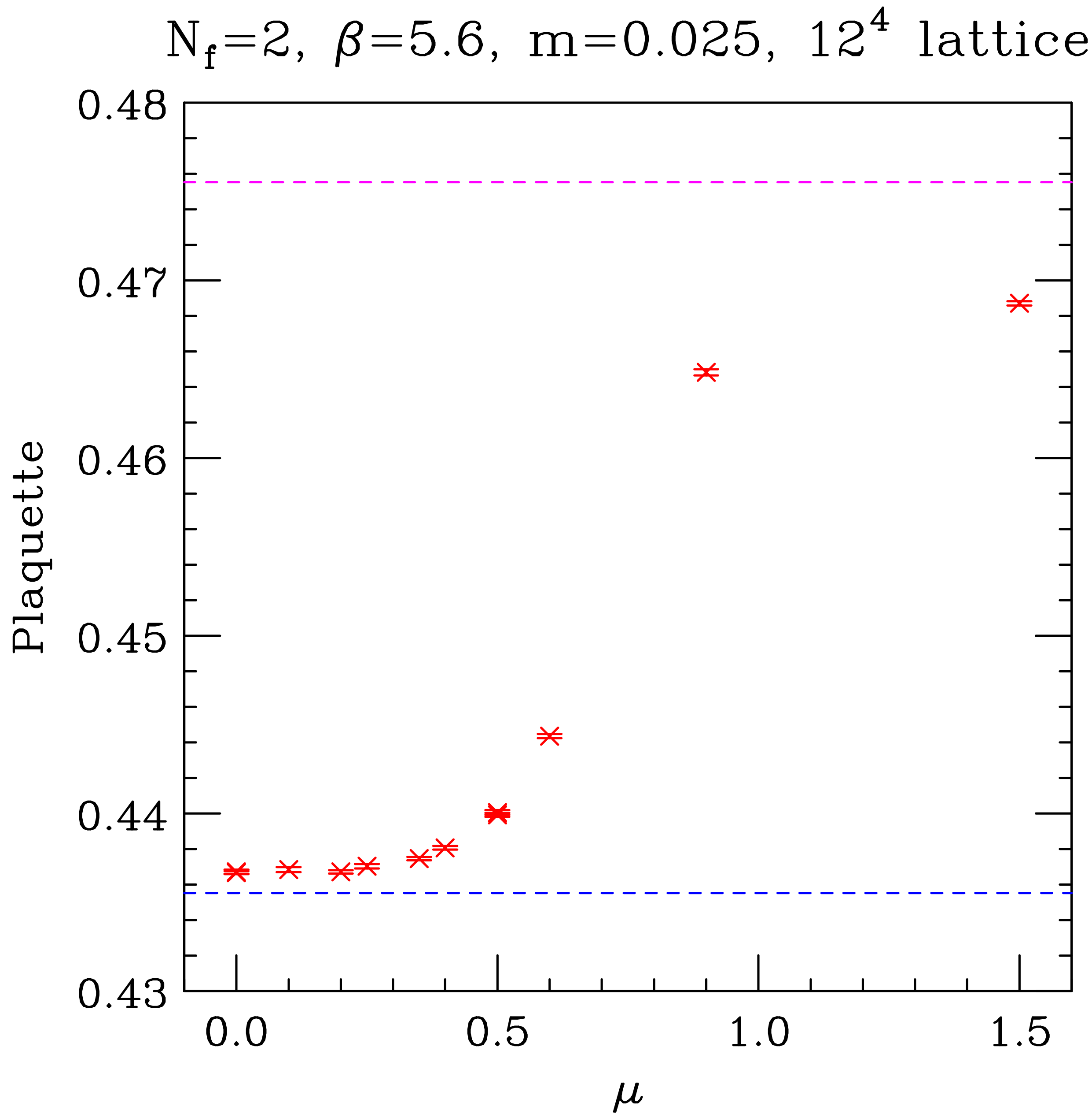

Figure 1: Plaquette as a function of μ. Dashed lines are the correct value at $\mu = 0$ and the quenched value.

Figure 2 shows the chiral condensates $\langle\bar{\psi}\psi\rangle$ measured during these runs. The dashed blue line is the true(RHMC) value at $\mu = 0$.

Note that the CLE value measured at $\mu = 0$ is appreciably below the correct value.

The chiral condensate decreases as μ is increased, rather than remaining constant up to the phase transition, which would be expected.

For large enough μ this condensate approaches zero, as expected for saturation.

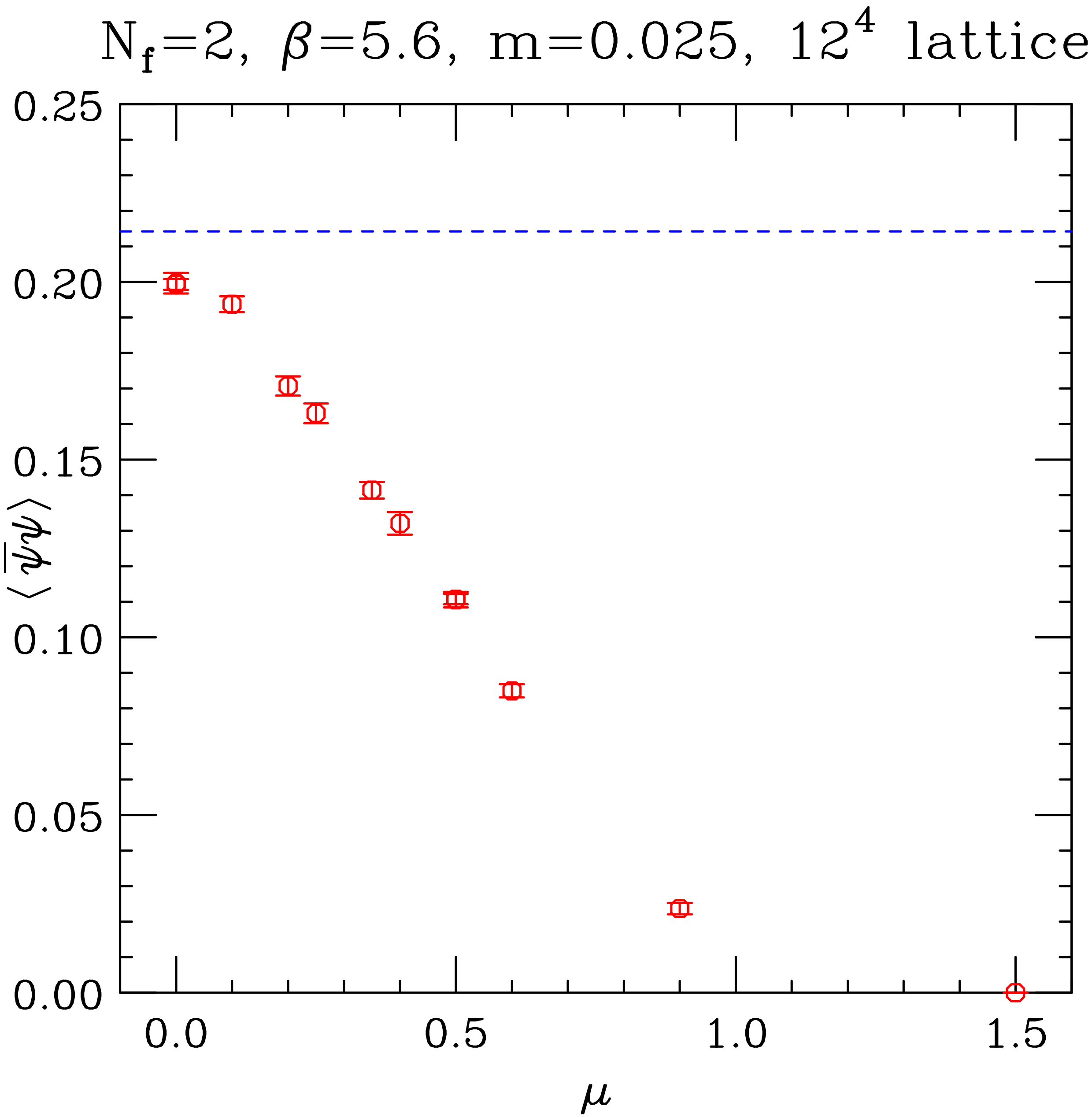

Figure 2: Chiral condensate as a function of μ. Dashed line is true value at $\mu = 0$.

Figure 3 shows the quark(fermion)-number density as a function of μ.

For $\mu \leq 0.25$ the number density is small (expected to be zero).

For $\mu \geq 0.35$ the number density increases, reaching the saturation value of 3 (3 quarks of different colours at each site), for large μ.

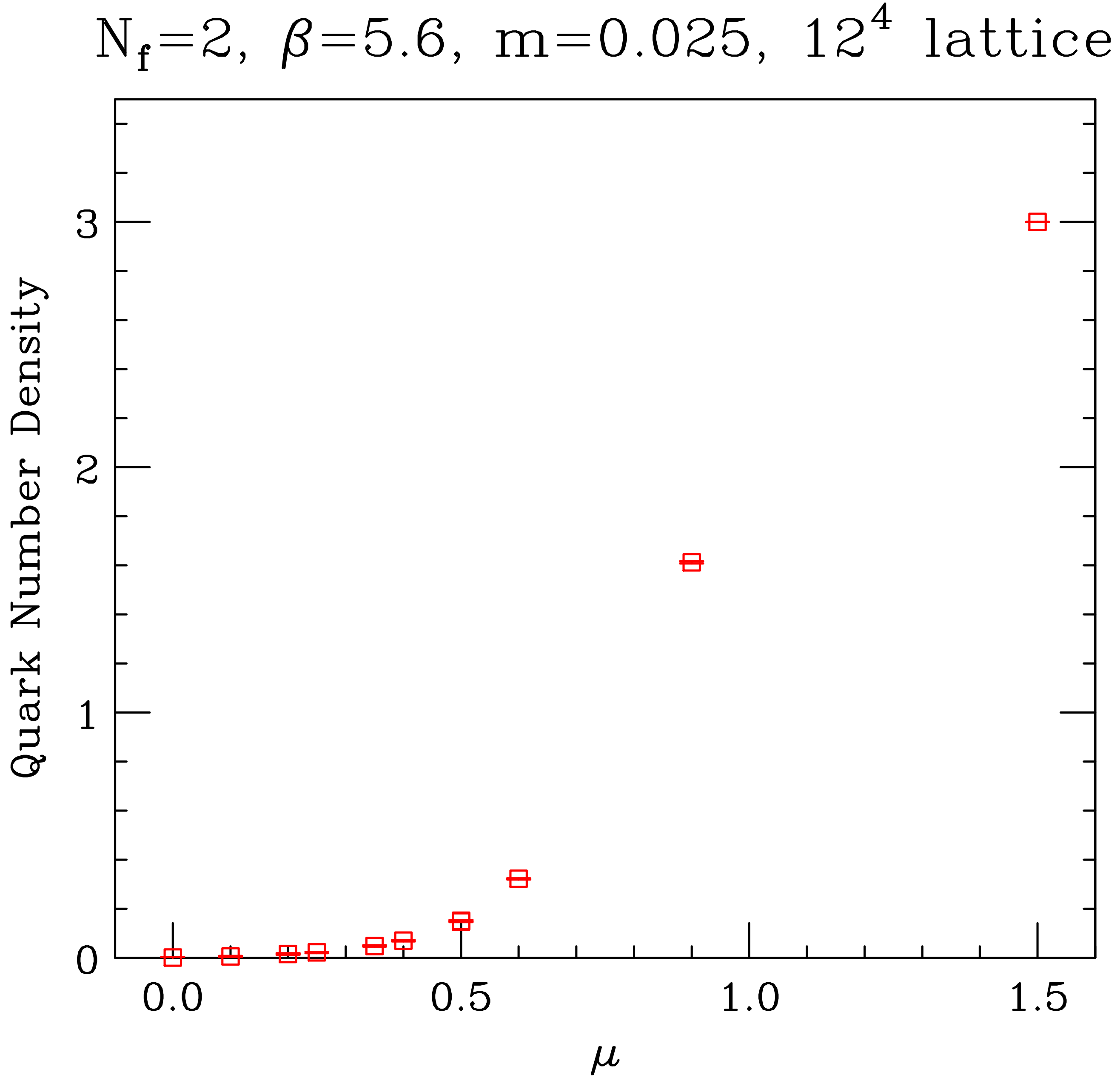

Figure 3: Quark number density as a function of μ.

These simulations reproduce some of the expected physics but fail in the details.

In particular they favour a phase transition near $\mu \approx m_N/3$ over one at $\mu \approx m_\pi/2$

The departures are most obvious (largest?) for the chiral condensate.

We now present evidence that the fields evolve over a compact domain, showing the time evolution of the unitarity norm defined above. If this norm evolves over a finite range, the fields do evolve over a compact domain.

Figures 4,5,6 show the time evolution of the unitarity norms at 3 different μ values. For the first 2 we present evolutions of this norm from ordered starts and from a configuration at saturation ($\mu = 1.5$).

It is clear from these that, after equilibration, the unitarity norm for each μ evolves over a finite range. The evolution from different starts suggests that this range is independent of the starting configuration.

The average unitarity norm has a minimum somewhere between $\mu = 0.35$ and $\mu = 0.9$. Does this mean that the CLE works if μ is sufficiently large?

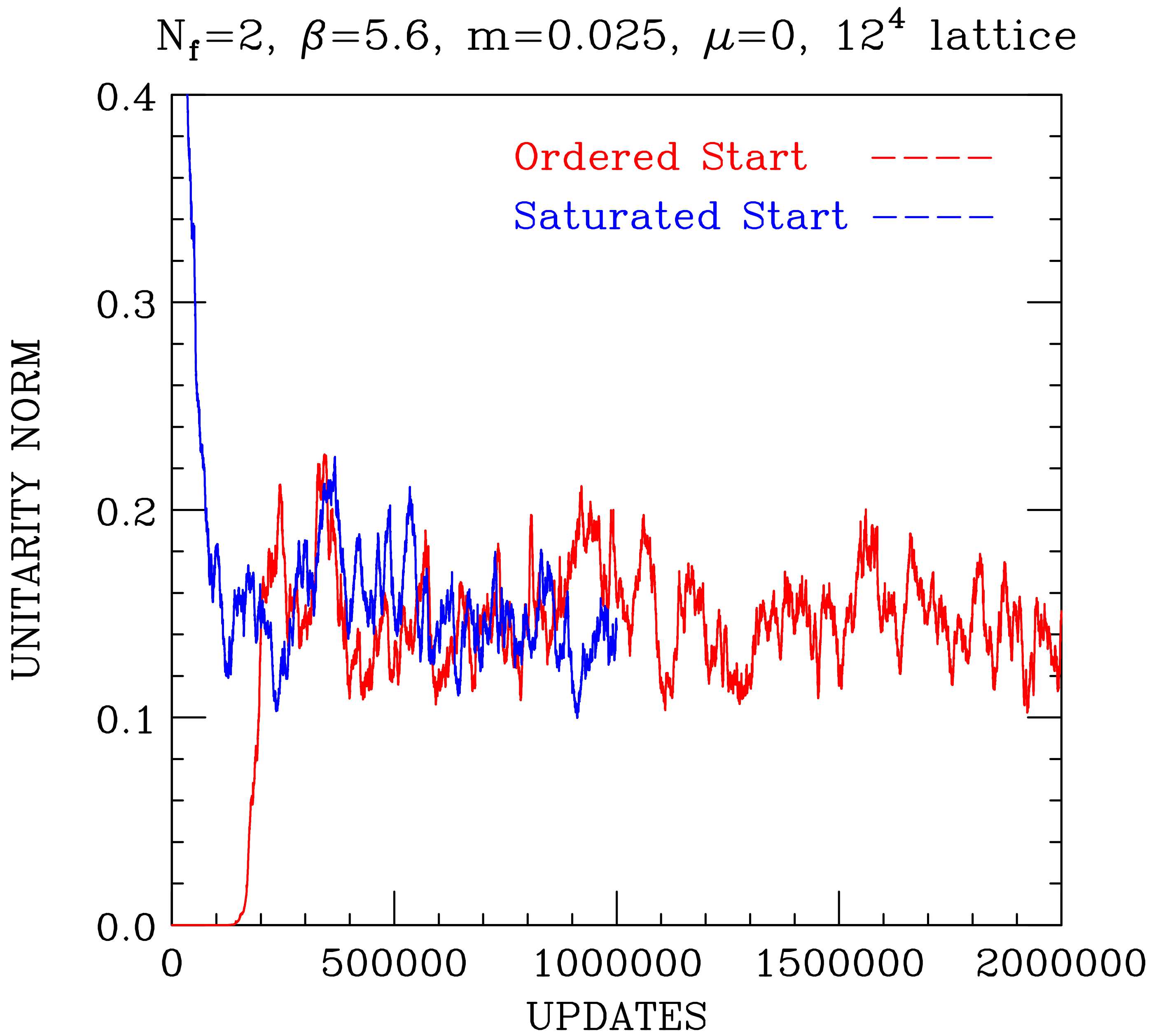

Figure 4: Evolution of unitarity norms for runs on a 12^4 lattice at $\mu = 0$. Red curve is for an ordered start. Blue curve starts from a $\mu = 1.5$ configuration.

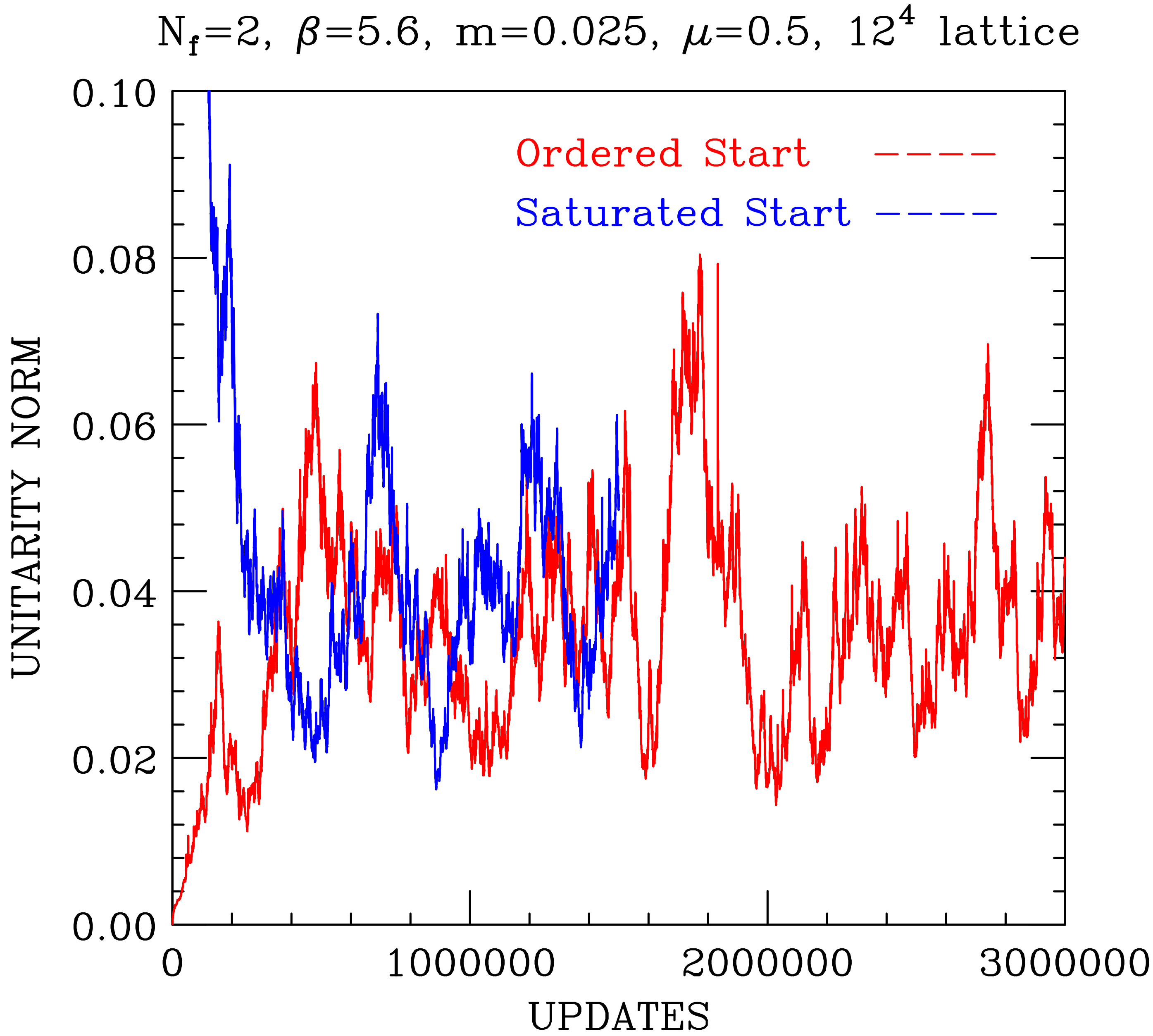

Figure 5: Evolution of unitarity norms for runs on a 12^4 lattice at $\mu = 0.5$. Red curve is for an ordered start. Blue curve starts from a $\mu = 1.5$ configuration.

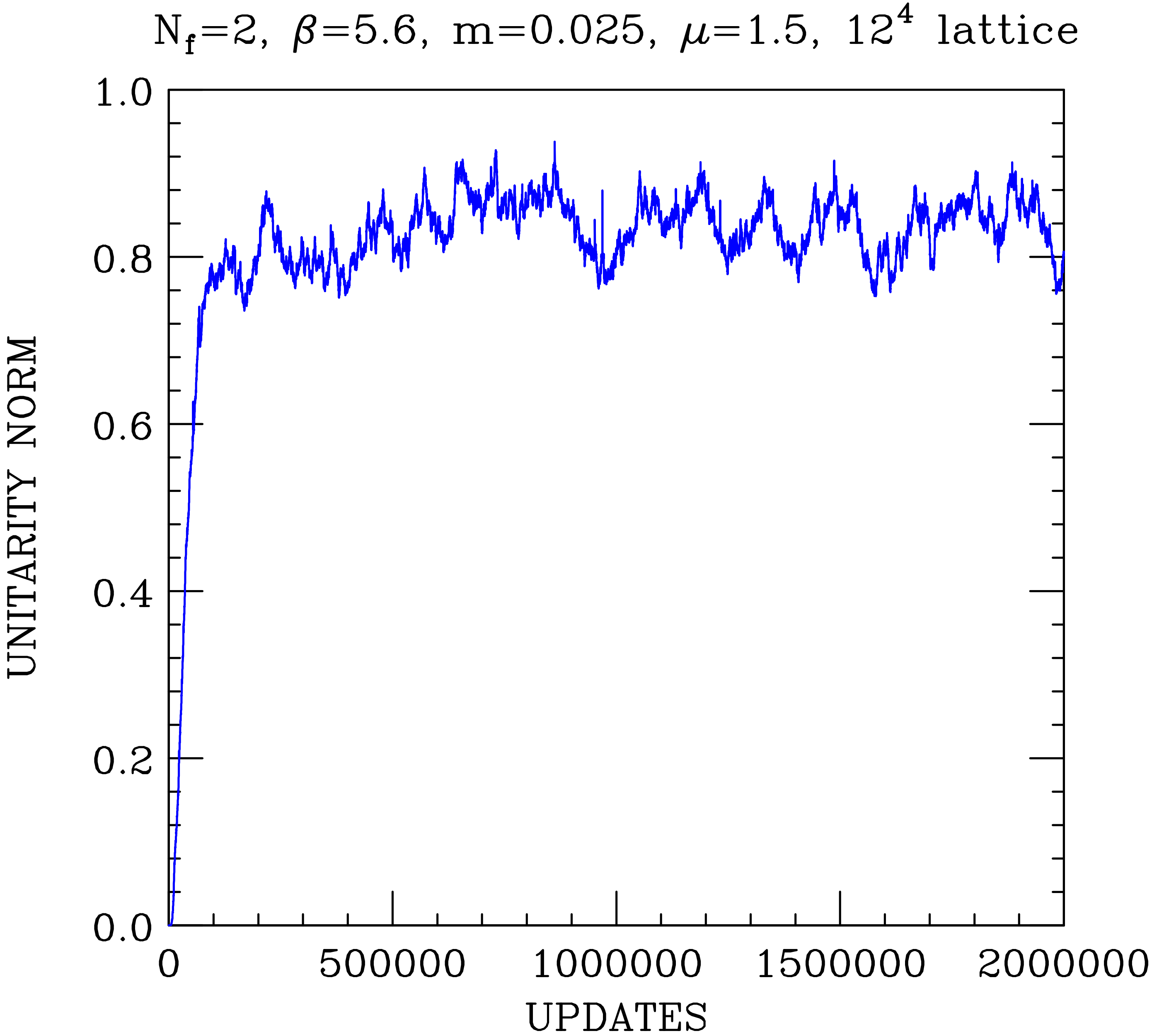

Figure 6: Evolution of unitarity norm for run on a 12^4 lattice at $\mu = 1.5$, from an ordered start.

Zero Temperature Simulations on a 16^4 lattice

We are also performing simulations on a 16^4 lattice.

Runs are being performed at $N_f = 2$,$\beta = 5.6$, $m = 0.025$ to measure finite size effects and finite dt effects.

So far runs have been performed at $\mu = 0$ and $\mu = 1.5$, and we are starting runs at $\mu = 0.2$. So far finite size (and finite dt) effects appear small.

At $\mu = 0$, the CLE measured plaquette value is $0.43690(6)$ compared with the RHMC value $0.43552(2)$, while the chiral condensate is $0.1974(7)$ compared with $0.2142(8)$ for the RHMC.

We are also running at $N_f = 2$, $\beta = 5.7$, $m = 0.025$. So far we have only run at $\mu = 0$.

Here the CLE measured plaquette value is $0.42374(4)$ compared with the RHMC value $0.42305(1)$, so the systematic error has been reduced by roughly a factor of 2.

For the chiral condensate the CLE value is $\mathbf{0.1738(11)}$ compared with the RHMC value of $\mathbf{0.1754(2)}$, almost an order of magnitude improvement.

We have also run $\boldsymbol{N_f = 4}$ simulations at $\boldsymbol{m = 0.02}$ and $\boldsymbol{\beta = 5.2}$ and $\boldsymbol{\beta = 5.4}$ at $\boldsymbol{\mu = 0}$. Again we find similar improvement for the smaller coupling.

Discussion and Conclusions

- We simulate Lattice QCD at finite μ on a 12^4 lattice at $\beta = 5.6$, $N_f = 2$, and light quark mass $m = 0.025$ using the CLE with gauge cooling.
- We see indications of the expected phase transition from hadronic to nuclear matter at $\mu \approx m_N/3$, and the passage to saturation at large μ.
- There are, however, systematic departures from known and expected results. At $\mu = 0$ the plaquette and chiral condensates disagree with known results. At small μ, the chiral condensate decreases with increasing μ rather than remaining constant. This does not appear to be a finite-size effect.
- We are extending our simulations to a 16^4 lattice. Preliminary results indicate that the failures of the CLE are not finite size or finite dt effects.
- At $\mu = 0$ we have also run at weaker coupling – $\beta = 5.7$. Here the systematic errors are significantly reduced suggesting that

the CLE will become valid in the continuum limit.

- We need to check if this improvement also occurs at $\mu \neq 0$, and on larger lattices.
- Methods suggested for reducing CLE failures need to be persued.
- Need simulations at lighter quark masses.
- We will also consider finite temperature.
- We will extend our $N_f = 4$ simulations, where the problems of rooting are absent.
- Once it is known that the CLE is generating correct results, we will study the high-μ phase for signs of colour superconductivity. This will also require simulations for $N_f = 3$ and $N_f = 2 + 1$.

These simulations are performed on Edison and Cori at NERSC, Comet at SDSC, Bridges at PSC, Blues at LCRC Argonne and Linux PCs in HEP Argonne.