Complex Langevin Simulations of QCD at Finite Density – Progress Report

D. K. Sinclair and J. B. Kogut

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Introduction

Lattice QCD at a finite quark-number 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 $SL(3, C)$.

However, complex langevin (CLE) simulations cannot be guaranteed to work unless the trajectories are restricted to a finite domain and the drift (force) term is holomorphic in the fields.

In lattice QCD at weak coupling, potential runaway solutions are controlled by adaptively readjusting the updating 'time' increment and implementing gauge cooling.

For lattice QCD, the trajectories do appear to be confined to compact domains. However, zeros of the fermion determinant produce poles in the drift term, so that the drift term is meromorphic not holomorphic in the fields. Hence observables cannot be guaranteed to converge to the correct limits.

We have been testing the CLE for lattice QCD at finite μ at zero temperature, over a range of μ values from 0 to saturation.

For the state of knowledge on applications of the CLE to QCD at finite μ a good starting point is the papers of Aarts *et al.*.

Our earlier simulations at $\beta = 6/g^2 = 5.6$, $m = 0.025$ mainly on 12^4 lattices show some of the properties expected of finite density QCD, but fail in the details.

We are now extending these to weaker coupling, $\beta = 5.7$, on a 16^4 lattice, with $m = 0.025$. While this improves the agreement with known (RHMC) observables at $\mu = 0$, the behaviour for $\mu > 0$ through the transition region shows similar deficiencies to those at $\beta = 5.6$.

The one improvement over $\beta = 5.6$ is that the unitarity norm, which is a measure of the distance of the gauge fields from the $SU(3)$ manifold is significantly smaller for $\beta = 5.7$ than for $\beta = 5.6$. Since the experience of others has identified keeping this norm low as a a way of improving CLE results, this encourages one to try even weaker couplings.

Recent results from random matrix theory indicate that, when the complex Langevin fails, it produces results consistent with the phase-quenched theory. Preliminary indications from our simulations are that this is not true for lattice QCD at finite μ.

Complex Langevin for Lattice QCD at finite μ

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

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

where $M(U,\mu)$ is the staggered Dirac operator. Backward links are represented by U^{-1} not $U^\dagger$. We choose to keep the noise term η real. We simulate the time evolution of the gauge fields using a partial second-order formalism.

We apply adaptive updating: if the force term becomes too large, dt is decreased to keep it under control. After each update, we gauge cool, gauge fixing to the gauge which minimizes the unitarity norm:

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

We use unimproved staggered quarks.

Zero Temperature Simulations on a 16^4 lattice at $\beta = 5.7$

Since our earlier CLE simulations of lattice QCD at $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice correctly reproduced some aspects of the expected phase structure, but failed in the details, we are repeating such simulations at weaker coupling.

We are running simulations at $\beta = 5.7$, $m = 0.025$. In order to be sure that the $\mu = 0$ theory is confined, we have increased our lattice size to 16^4.

Important μ values are $m_\pi/2 \approx 0.194$ and $m_N/3 \approx 0.28$.

We are running 2 or 3 million updates at each μ, from $\mu = 0$ up to saturation. Our input $dt = 0.01$, and we perform 5 gauge-cooling steps after each update. After adaptive rescaling of dt this gives us between ≈ 80 and over 1000 equilibrated time-units per μ.

At $\mu = 0$ we find good agreement between the CLE observables and their exact values. (This was not true at $\beta = 5.6$.)

What follows are graphs of the average plaquette, the chiral condensate and quark-number density as functions of μ.

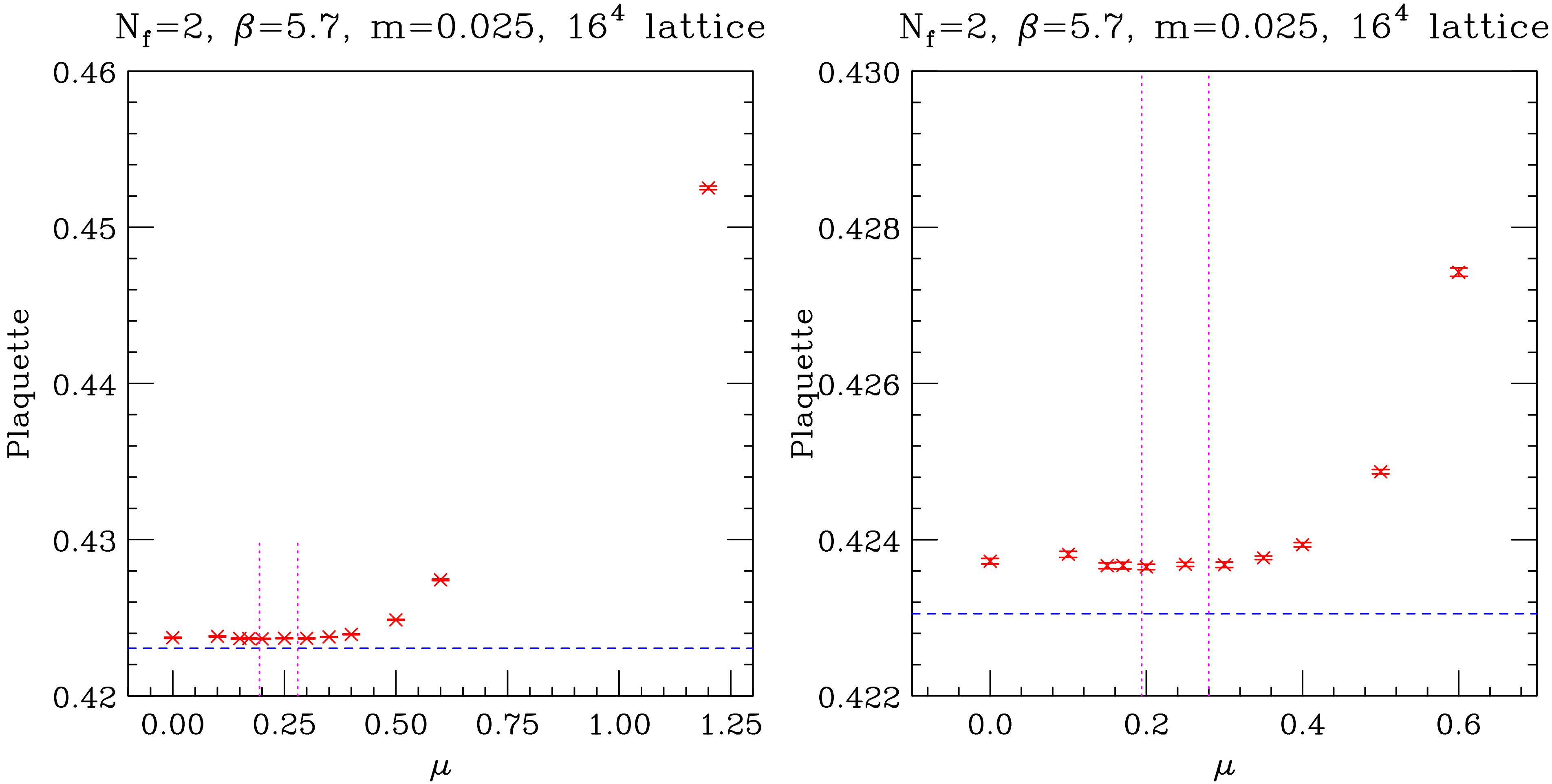

Figure 1: Average plaquette as a function of μ for $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice.

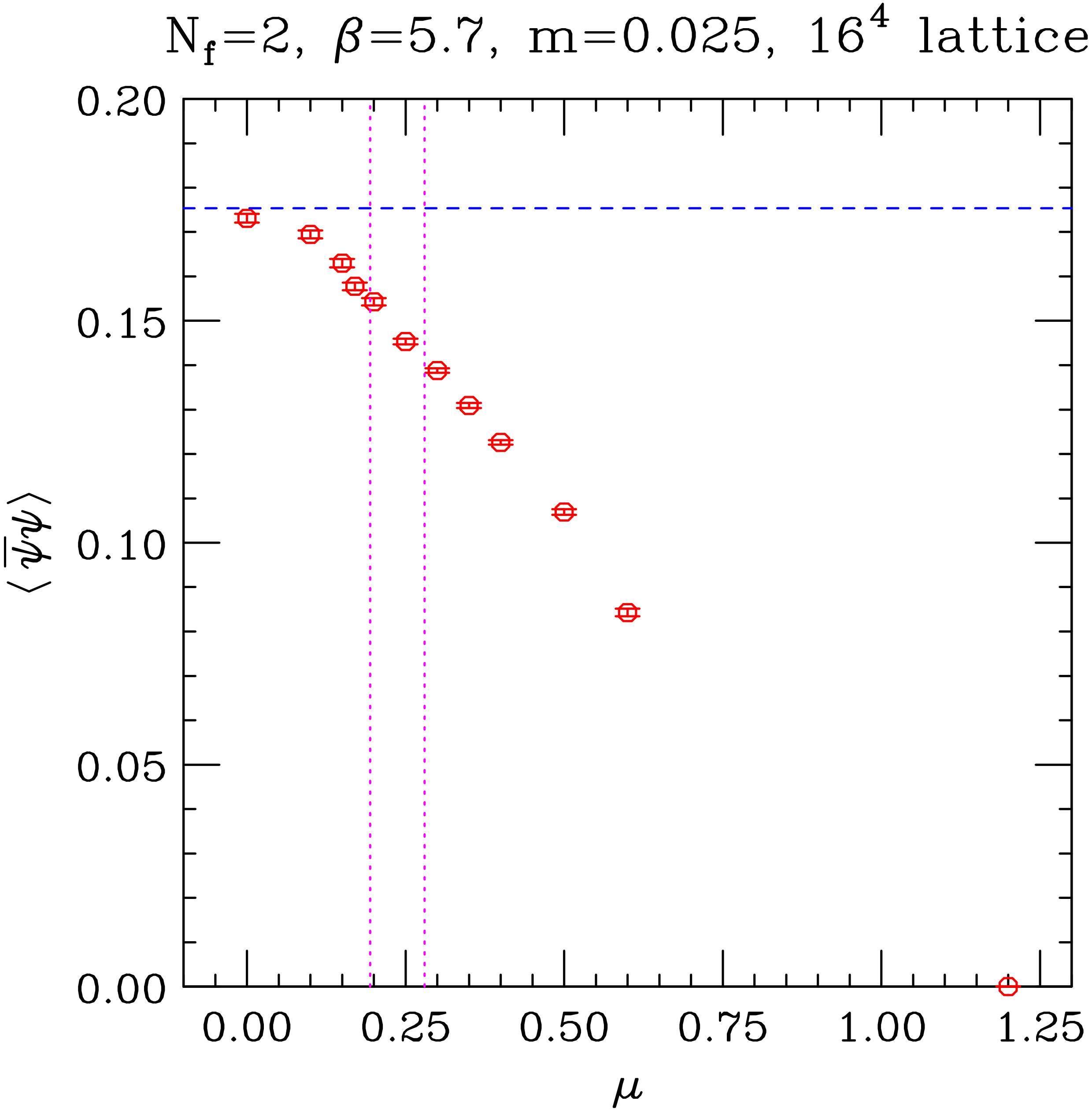

Figure 2: Chiral condensate as a function of μ for $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice.

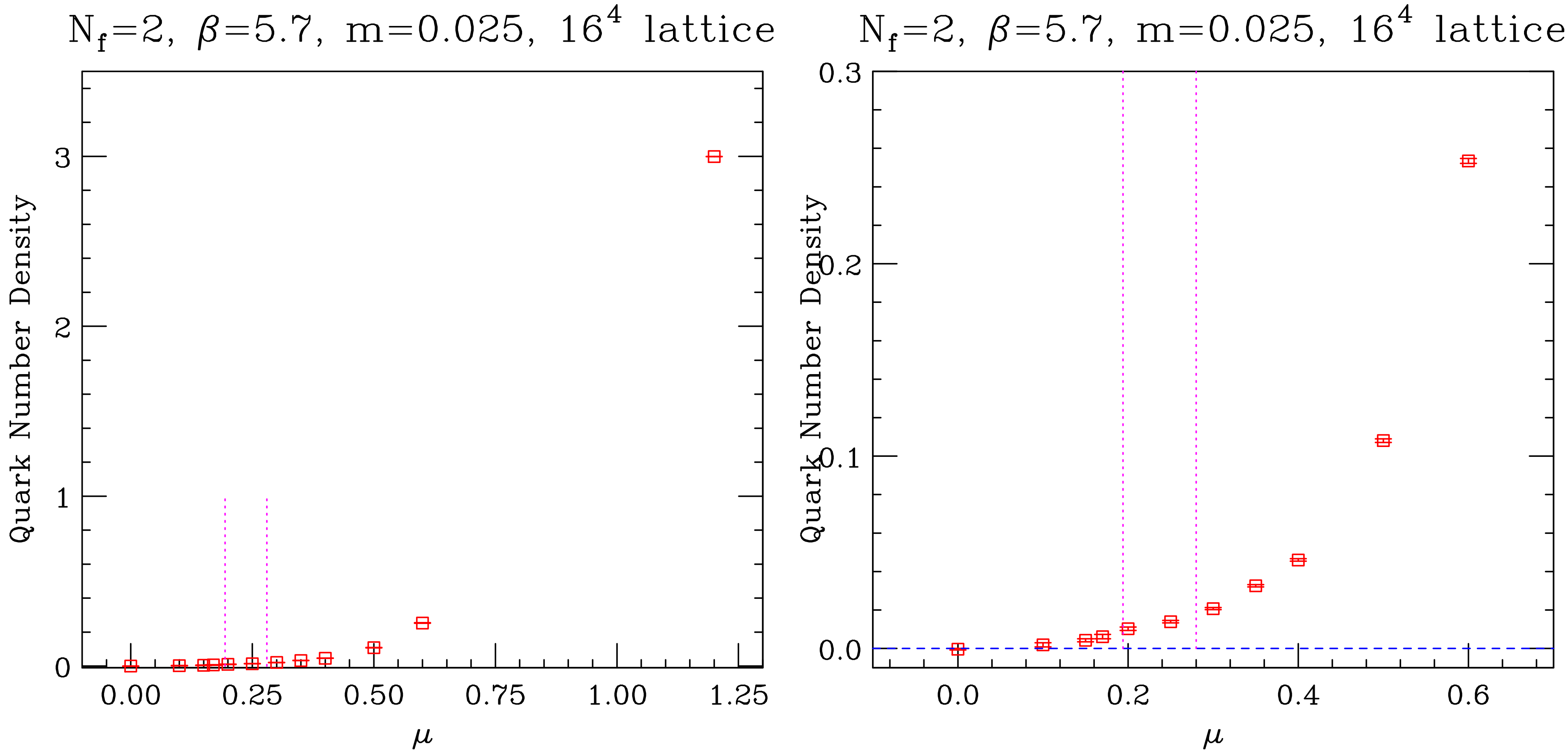

Figure 3: Quark-number density as a function of μ for $\beta = 5.7$, $m = 0.025$ on a 16^4 lattice.

The physics one expects is that all observables should remain at their zero μ values up to μ just below $m_N/3$.

Beyond this (1st order??) phase transition the chiral condensate $\langle\bar{\psi}\psi\rangle$ should fall rapidly approaching zero at saturation, if not before.

The quark number density should remain zero up to the transition. Above this it should rise, approaching 3 at saturation.

The plaquette should remain constant up to the transition. Above this it should increase towards its saturation value.

What we observe is that $\langle\bar{\psi}\psi\rangle$ starts to fall almost immediately μ is increased from zero, and by $\mu = m_N/3$ it is well below its $\mu = 0$ value. It does not show any clear transition. The main improvement over $\beta = 5.6$ is that its $\mu = 0$ value is close to the correct value.

The quark-number density does remain near zero for small μ. Its increase away from zero is so smooth and gradual that it is impossible to determine where this departure starts.

The plaquette is statistically constant for $\mu \leq 0.3$, above which it rises slowly.

Beyond the fact that the quark-number density and plaquette do not show as abrupt a transition as one might expect, they do not show as clear an indication that the CLE simulations are converging to the wrong limit in the low μ domain as does the chiral condensate.

In the following figure we show the average unitarity norm as a function of μ from our simulations on a 16^4 lattice at $\beta = 5.7$ and from our 12^4 runs at $\beta = 5.6$.

We note that the unitarity norms for $\beta = 5.7$ are significantly smaller than those for $\beta = 5.6$. Since it has been suggested that keeping unitarity norms small increases the chance that the CLE will converge to the correct results, it suggests one should try even weaker couplings.

Note also that both these graphs indicate that the unitarity norm has a deep minimum around $\mu = 0.5$ or 0.6. We suggest that the CLE simulations might converge to the correct distributions for μ above or even slightly below these minima.

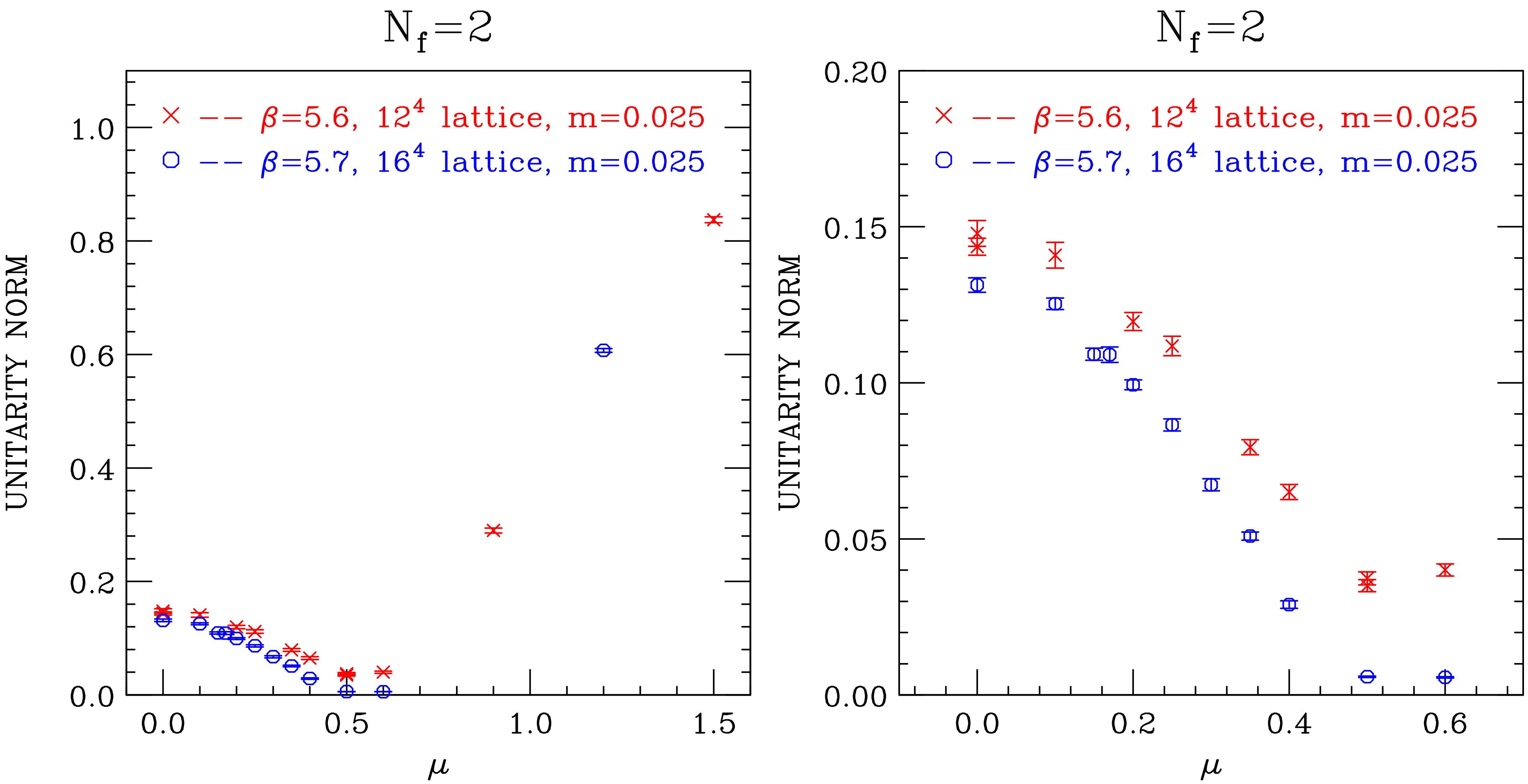

Figure 4: Average unitarity norm as a function of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice – red. Same, but for $\beta = 5.7$ on a 16^4 lattice – blue.

Comparison of the 12^4, $\beta = 5.6$ CLE simulations with the phase-quenched theory

A recent paper by Bloch $et\ al.$ has indicated that when CLE simulations of a random matrix theory at finite μ, which is a model for QCD at finite μ, converges to the wrong limit, it produces the results of the phase-quenched theory.

We are therefore testing to see if the same is true for lattice QCD at finite μ.

The following graphs show our preliminary results for 2-flavour lattice QCD at $\beta = 5.6$ on a 12^4 lattice.

Even making allowances for the fact that at $\beta = 5.6$, the CLE has relatively large systematic errors even at $\mu = 0$, the CLE and phase-quenched theories show significant differences.

The phase-quenched theory observables show little μ dependence below $\mu = m_\pi/2$. Beyond this value the chiral condensate decreases more rapidly and the quark-number density increases more rapidly than for the CLE results for the full theory.

We need to extend these comparisons to $\beta = 5.7$ on a 16^4 lattice.

Our results suggest that the pattern of failure of CLE simulations of random matrix theory is not a good guide to how CLE simulations fail for QCD at finite μ.

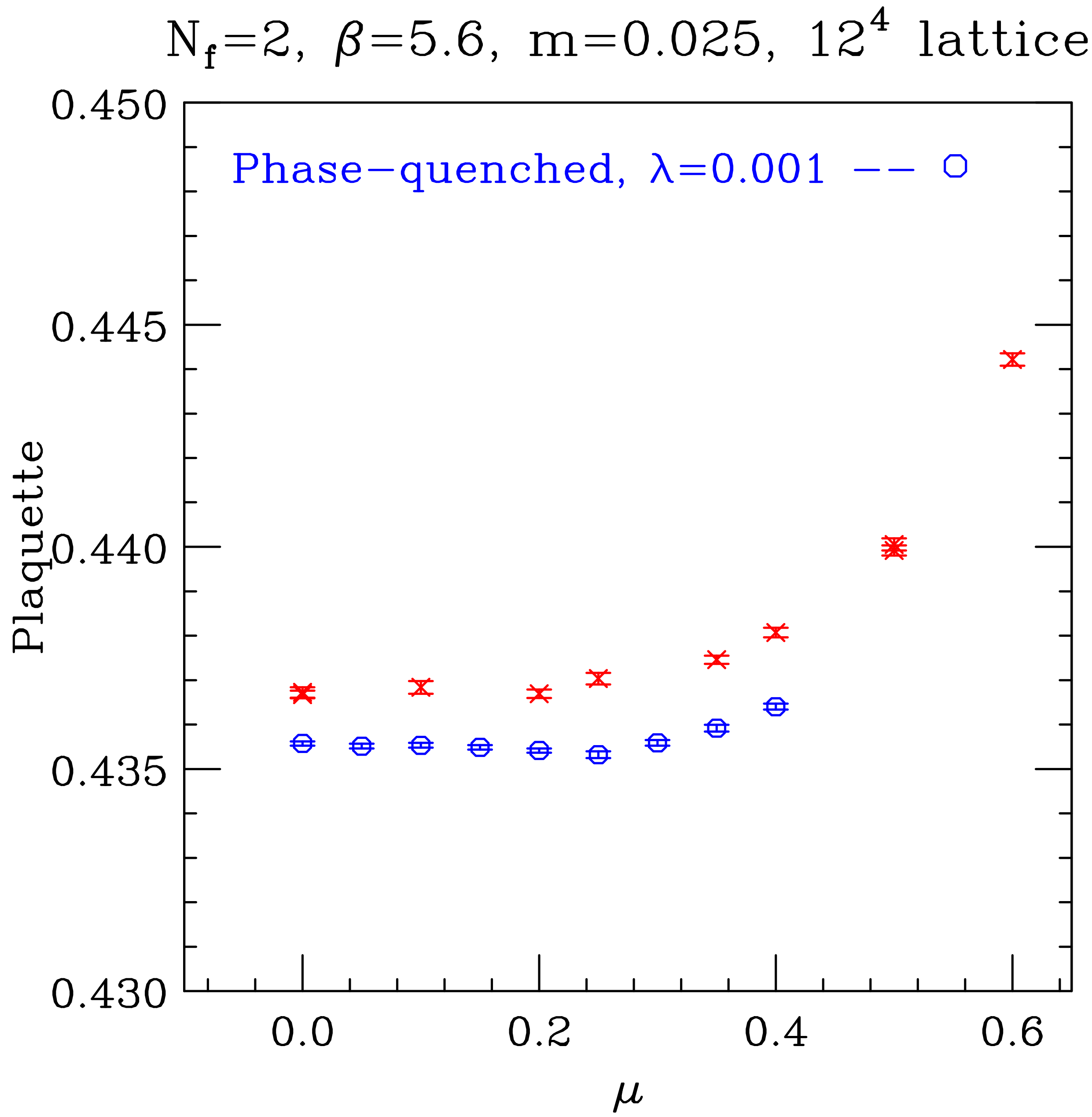

Figure 5: Average plaquette as a function of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice. Red – CLE prediction for full theory. Blue – phase-quenched results.

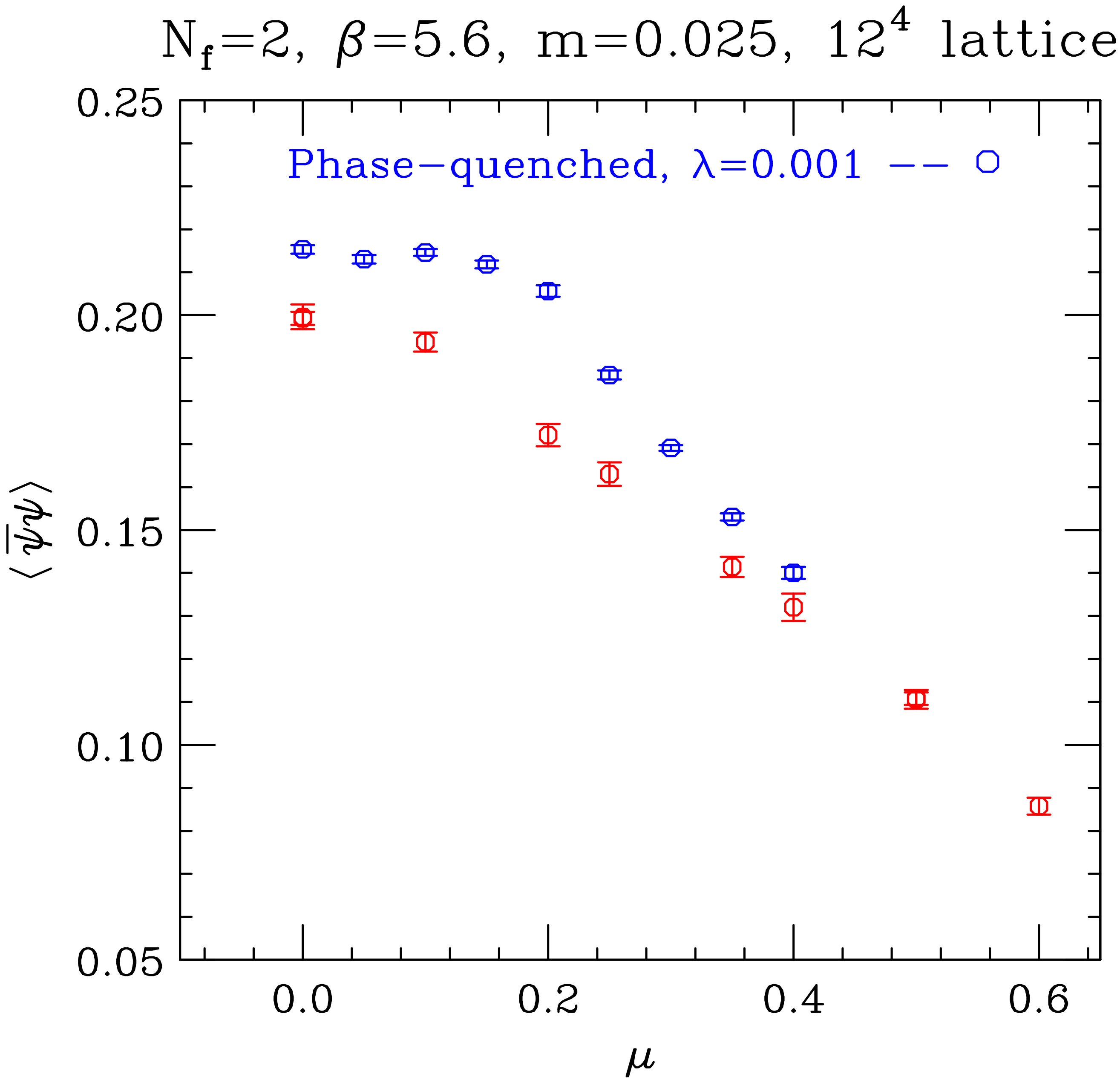

Figure 6: Chiral condensate as a function of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice. Red – CLE prediction for full theory. Blue – phase-quenched results.

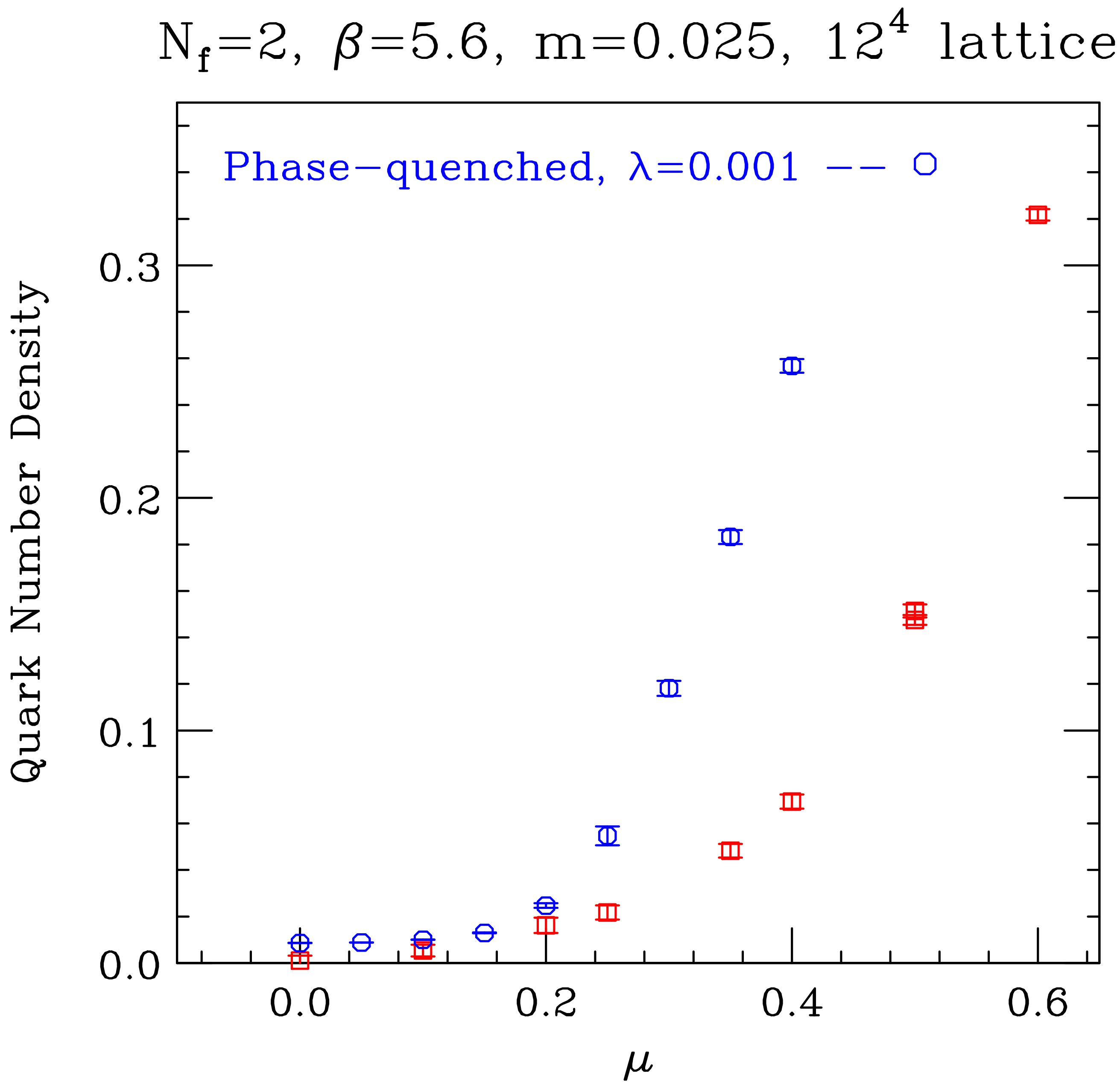

Figure 7: Quark-number density as a function of μ for $\beta = 5.6$, $m = 0.025$ on a 12^4 lattice. Red – CLE prediction for full theory. Blue – phase-quenched results.

Summary and Discussions

- We are extending our earlier CLE simulations of zero temperature lattice QCD at zero temperature and finite μ with $\beta = 5.6$ and $m = 0.025$ on a 12^4 lattice, to $\beta = 5.7$ and $m = 0.025$ on a 16^4 lattice.
- We find that the CLE simulations show a much smoother transition from hadronic to nuclear matter than is expected, as was observed at stronger coupling. This failure of the CLE at low μ is presumably due to the poles in its drift term.
- However, at least part of the problem is presumably that the chiral condensate and probably the quark-number density have poles at the zeros in the fermion determinant, and because of 'taste' breaking these zeros are not of high enough order to cancel the poles in these observables.

- The fact that the unitarity norm, which is a measure of the distance of the gauge fields from the $SU(3)$ manifold, decreases as one goes to weaker coupling suggests that we should investigate even weaker couplings.
- When the CLE converges to the wrong limits, these limits do not appear to be associated with the phase-quenched theory, contrary to what random matrix theory suggests. These comparisons need to be extended not only to weaker couplings, but also to smaller quark masses.

Where do we go from here?

- We need to finish out simulations at $\beta = 5.6$ and $\beta = 5.7$ adding more larger μ s, since this is the region where we suspect that the CLE gives the correct results. Simulations at smaller mass would be desirable. Exploration of even weaker couplings would be desirable.

- Extend our simulations to high temperatures, where the CLE is expected to give correct results, and search for the elusive critical endpoint.

- Because the so-called ‘taste-breaking’ is large for staggered fermions at these β s, the zeros of the fermion determinant are far apart. The order of these zeros is $N_f/4 = \frac{1}{2}$, and it is known from models that such low-order zeros do not repel CLE trajectories. We therefore suggest moving to Wilson fermions with their exact vector flavour symmetry which means that the zeros have order $N_f = 2$ which would tend to repel CLE trajectories. (Of course, such zeros can become bottlenecks, spoiling ergodicity.)

- Another approach is to add an irrelevant chiral 4-fermion interaction to the action. This moves the pion to the auxilliary field, where it cannot provide a spurious transition at $\mu = m_\pi/2$. The vacuum expectation value of the auxilliary field provides an alternative chiral order parameter, one which, unlike $\langle\bar{\psi}\psi\rangle$, does not have poles at those of the drift term.

These simulations are run on Cori and Edison at NERSC, Bridges at PSC, Comet at SDSC, Blues at LCRC, ANL and Linux PCs belonging to the HEP Division at ANL.