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CLS 2+1 flavor simulations at physical light- and strange-quark masses

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Abstract. We report recent efforts by CLS to generate an ensemble with physical light- and strange-quark masses in a lattice volume of 192×96^3 at $\beta = 3.55$ corresponding to a lattice spacing of 0.064 fm. This ensemble is being generated as part of the CLS 2+1 flavor effort with improved Wilson fermions. Our simulations currently cover 5 lattice spacings ranging from 0.039 fm to 0.086 fm at various pion masses along chiral trajectories with either the sum of the quark masses kept fixed, or with the strange-quark mass at the physical value. The current status of simulations is briefly reviewed, including a short discussion of measured autocorrelation times and of the main features of the simulations. We then proceed to discuss the thermalization strategy employed for the generation of the physical quark-mass ensemble and present first results for some simple observables. Challenges encountered in the simulation are highlighted.

1 Introduction

The CLS (Coordinated Lattice Simulations) consortium with members in Denmark, Germany, Italy, Spain, and Switzerland has embarked on a program to generate 2+1 flavor gauge ensembles with $O(a)$ improved Wilson fermions and a Lüscher-Weisz gauge action with tree-level coefficients. A special feature is the use of open boundary conditions in the time direction (to avoid topological freezing at fine lattice spacings [1]) for the bulk of ensembles generated to date. Another feature is the introduction of a small twisted-mass term for the light (up and down) quarks in the simulation together with subsequent reweighting to zero twisted mass (twisted mass reweighting) [2], to avoid accidental near-zero modes of the lattice Dirac operator. Most of the ensembles generated initially [3] are along a trajectory keeping the trace of the bare quark-mass matrix fixed, $\mathrm{Tr}(M) = \mathrm{const.}$ More recently, these ensembles have been supplemented by ensembles along a trajectory with fixed strange quark mass $m_s \approx m_{s,phys}$ [4] and with $m_s = m_l$ at different values of $\mathrm{Tr}(M)$.

For the simulation, the highly flexible `openQCD` package [5] is used. Among its main features are the use of nested hierarchical integrators (for the implementation see [2]), Hasenbusch-style frequency splitting [6] with an arbitrary number of pseudofermion pairs, RHMC [7] (plus reweighting) for the strange quark, deflation acceleration along the HMC trajectory [8, 9] and a chronological inverter [10]. The package implements a number of solvers.

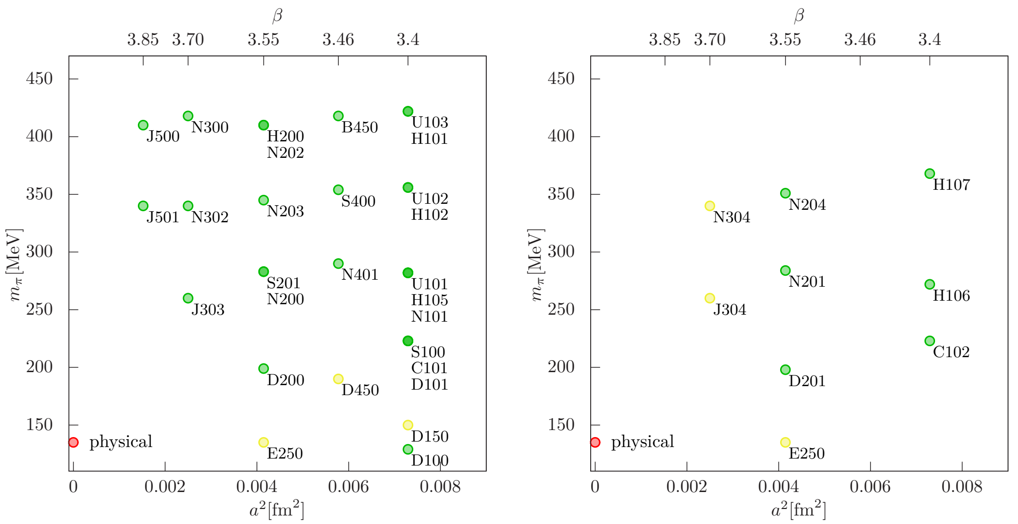

Figure 1: Landscape of CLS 2+1-flavor ensembles with $\mathrm{Tr}(M)$ = const (left pane) and m_s = const (right pane). In both cases the lattice spacing squared is displayed on the x-axis, while the y axis shows the pion mass. Ensembles still in production are shown in yellow, while ensembles considered complete are shown in green. The physical light-quark mass ensemble E250 discussed in these proceedings is shown in both plots. Multiple ensemble names next to a single dot indicate ensembles with different volumes at the (otherwise) same set of simulation parameters.

Figure 1 shows the current set of ensembles for both $\mathrm{Tr}(M)$ = const (left pane) and m_s = const (right pane). The ensembles are labeled by a letter (denoting the aspect ratio T/L) and three numerical digits (the first digit encodes β and therefore the lattice spacing). Our current library features ensembles at 5 lattice spacings (ranging from 0.039 fm to 0.086 fm) and with a range of pion masses $M_\pi \leq 420$ MeV. For some sets of parameters, multiple lattice volumes exist, enabling us to control finite volume effects. Figure 2 shows the same set of ensembles, now highlighting the current set of statistics. We typically generate chains of roughly 4000 molecular dynamics units (MDU), and save a gauge configuration every 4 MDU. The choice of target statistics is made considering the largest integrated autocorrelation time τ_{int} (often given by the Yang Mills action density at finite flow time).

Finally, Figure 3 shows the spatial extent L of the ensembles. Most production ensembles feature $m_\pi L \geq 4$, ensuring that exponentially suppressed volume effects are small. For some parameter sets, smaller volumes to check for and control finite size effects have also been generated.

2 Autocorrelation times towards the physical point

In this section we will provide a brief update on estimated autocorrelation times for the Yang-Mills action density at flow time t_0 determined by the condition $t^2\langle E\rangle = 0.3$ [11]. While the open boundary conditions in time [1] avoid topological freezing at fine lattice spacing a, it is expected that the autocorrelation time in this observable increases significantly as the lattice spacing is decreased. In a previous global fit [3] of data from the initial set of 2+1 flavor CLS ensembles, the autocorrelation time was determined to be well described by $\tau_{\exp} = 14(3)\frac{t_0}{a^2}$.

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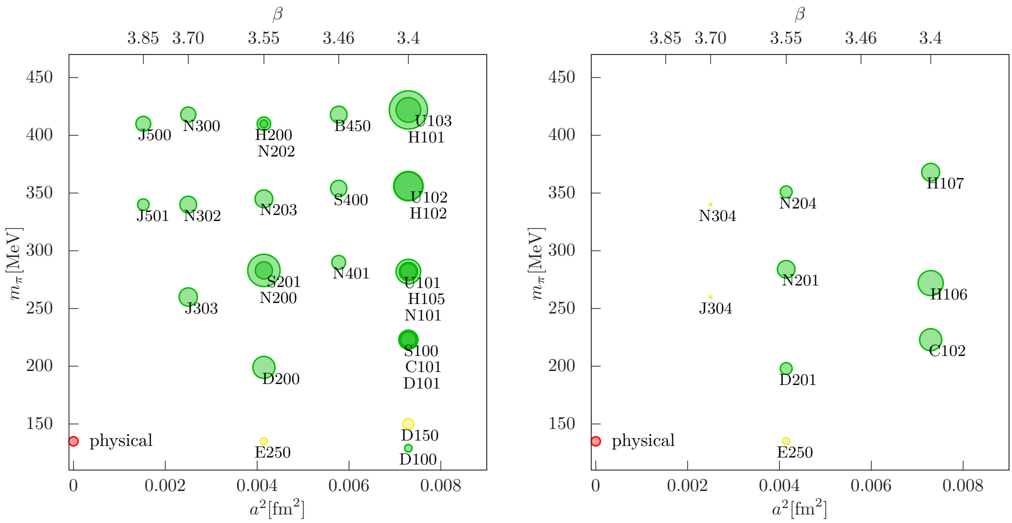

Figure 2: Landscape of CLS 2+1-flavor ensembles with Tr(M) = const (left pane) and m_s = const (right pane). The area of the circles in this plot is proportional to the number of MDU divided by the largest integrated autocorrelation time τ_{int}

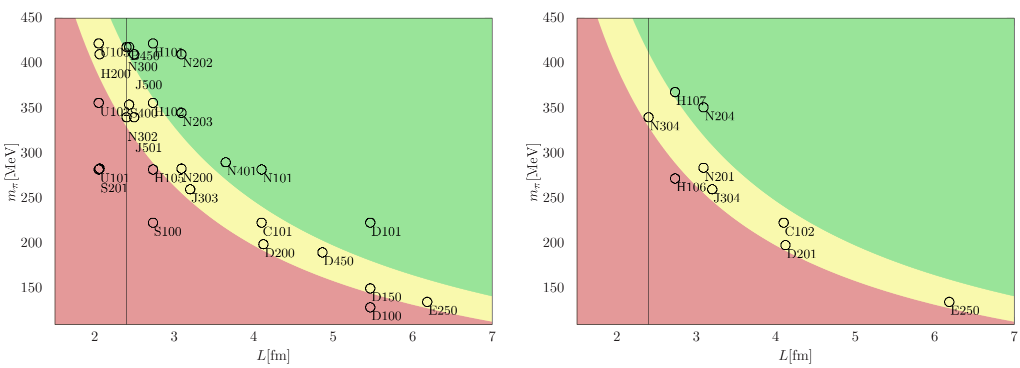

Figure 3: Landscape of CLS 2+1-flavor ensembles with Tr(M) = const (left pane) and m_s = const (right pane). The spatial extent L of the ensemble is used as the x-axis value. The region of the plot with $m_\pi L \leq 4$ is colored red, the region with $4 \leq m_\pi L \leq 5$ is colored yellow and the region with $5 \leq m_\pi L$ is colored green.

Figure 4 shows the MD history of the YM action density at flow time t_0 for fixed pion mass $m_\pi \approx 340$ MeV and for three lattice spacings. The corresponding integrated autocorrelation time τ_{int} is given above each subfigure. Even with chains longer than 3000 MDU the statistical uncertainty on τ_{int} is large. The current results are consistent with the expected increase of the autocorrelation time [3]. Figure 5 shows the MD history of the YM action density at flow time t_0 for three different pion masses along the trajectory with Tr(M) = const. Unlike in simulations by the MILC collaboration at fixed strange-quark mass [12], no clear pattern is seen with our current statistics.

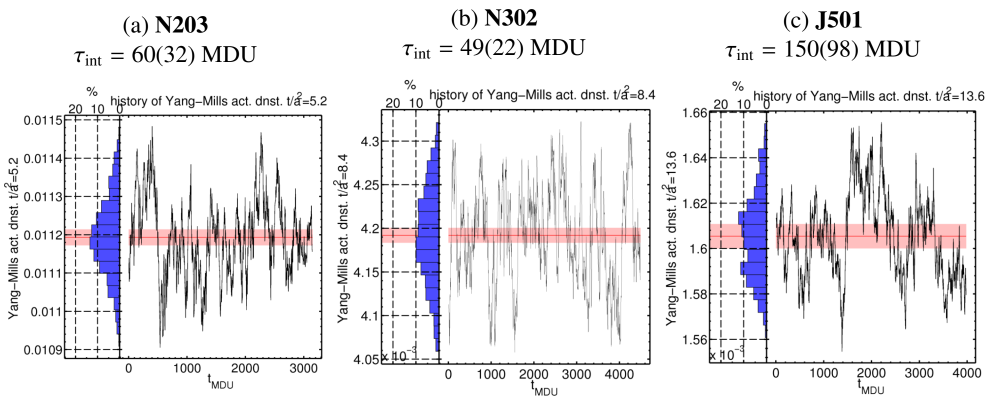

Figure 4: History of the YM action density at flow time t_0 along the MD trajectory.The three panes show results for $a \approx 0.064$fm (a), $a \approx 0.050$fm (b), and $a \approx 0.039$fm (c).

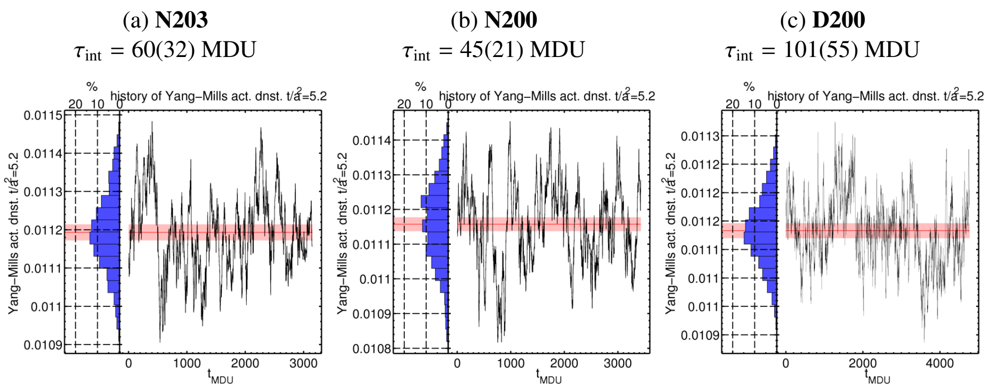

Figure 5: History of the YM action density at flow time t_0 along the MD trajectory.The three panes show results at fixed lattice spacing $a \approx 0.064$fm for $m_\pi \approx 340$ MeV (a), $m_\pi \approx 280$ MeV (b), and $m_\pi \approx 200$ MeV (c).

3 Thermalization of a physical light-quark mass ensemble

While the current CLS 2+1 flavor ensembles cover a wide range of parameters, the accurate determination of some quantities of phenomenological interest are currently limited by our control of systematic uncertainties associated with the chiral extrapolation. An important example is the calculations of the hadronic contributions to the anomalous magnetic moment of the muon (see [13] for a CLS based determination). Beyond specific observables, our determination of the lattice scale [14] would also greatly benefit from simulations with physical light- and strange-quark masses.

In these proceedings we report on our efforts to thermalize an ensemble (E250) at physical light- (mass degenerate up and down) and strange-quark mass and with $\beta = 3.55$ corresponding to a lattice spacing $a \approx 0.064$ fm. At this lattice spacing, the exponential autocorrelation time τ_{exp} is not yet

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completely dominated by topology, and therefore periodic boundary conditions are chosen. To keep $m_\pi L \geq 4$, we choose a lattice volume $T \times L^3 = 192 \times 96^3 a^4$. We work with the following thermalization strategy:

- Start from an SU(3) run with $T \times L^3 = 64 \times 48^3 a^4$, 3 mass-degenerate light quarks and periodic boundary conditions generated for non-perturbative renormalization. Perform a number of runs (updating the light- and strange-quark hopping parameters to their target values) and thermalize this small volume.
- Triple the time extent and partially thermalize this intermediary ensemble of size $192 \times 48^3 a^4$.
- Double the spatial extent and thermalize the resulting ensemble of size $192 \times 96^3 a^4$.

3.1 Status of gauge field generation for E250

The thermalization runs on the small and intermediate volume have been successfully completed and we are currently producing a first production chain. At the time of Lattice2017, there was a chain of 436 MDU, corresponding to 109 saved configurations, some of which might not be fully thermalized. The measured acceptance is 0.872(27). Figure 6 shows plots for the history of the hamiltonian deficit ΔH seen in the Monte-Carlo accept/reject step, for the average plaquette, and for the topological charge at the center of the lattice. While a proper analysis will need a much longer Monte-Carlo chain, the right panel of of Figure 6 suggests that at this lattice spacing, the slowing down of topological tunneling is not yet a serious issue.

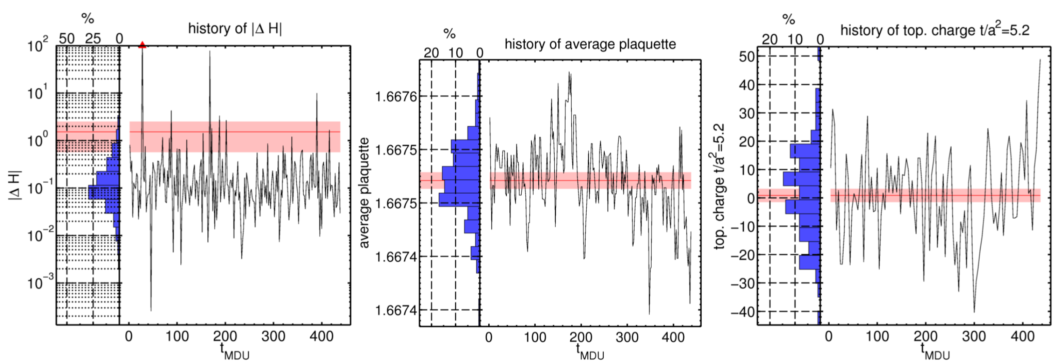

Figure 6: Left pane: MD history of ΔH for the physical mass run E250. Mid pane: MD history of the average plaquette. Right pane: History of the topological charge at the center of the lattice.

Figure 7 shows the reweighting factors associated with the rational approximation for the strange quark and for the reweighting to zero twisted mass. The reweighting factor for the twisted mass reweighting is estimated using 24 random sources and no intermediate value for the twisted mass parameter μ. For the full ensemble, this estimate might have to be improved, as occasional small reweighting factors are not estimated very accurately. [1]

Figure 8 shows results for the pion correlator and pion effective mass using random wall sources on the same time slice for 70 configurations. With this procedure, autocorrelations in the pion correlator are clearly visible. For future measurements we will make use of the large time extent of the lattice

[1] The fluctuations of the twisted mass reweighting factor are also somewhat larger than desirable and a slightly smaller twisted mass parameter (chosen as $\mu = 0.0001$ for the current run) might have been a better choice.

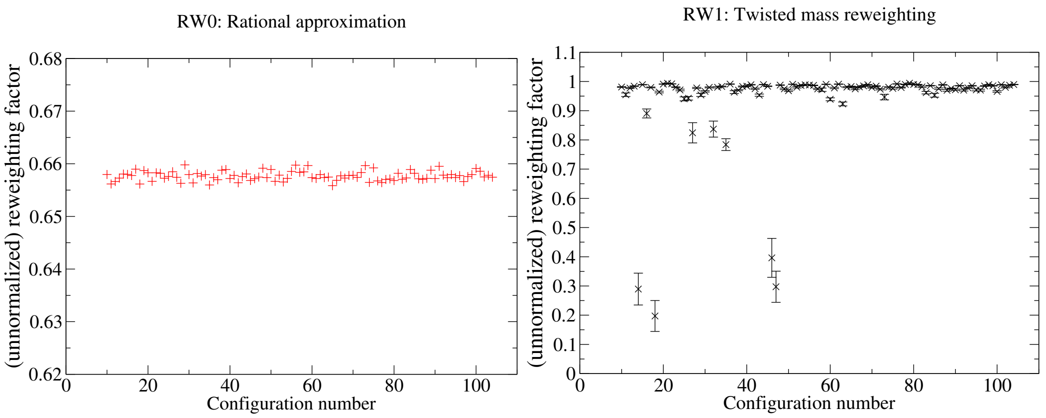

Figure 7: Reweighting factors for a subset of the configuration produced of E250. Fluctuations in the reweighting factor associated with the rational approximation are very mild (left pane; red). The reweighting factor for the twisted mass reweighting (right pane; black) shows larger fluctuations.

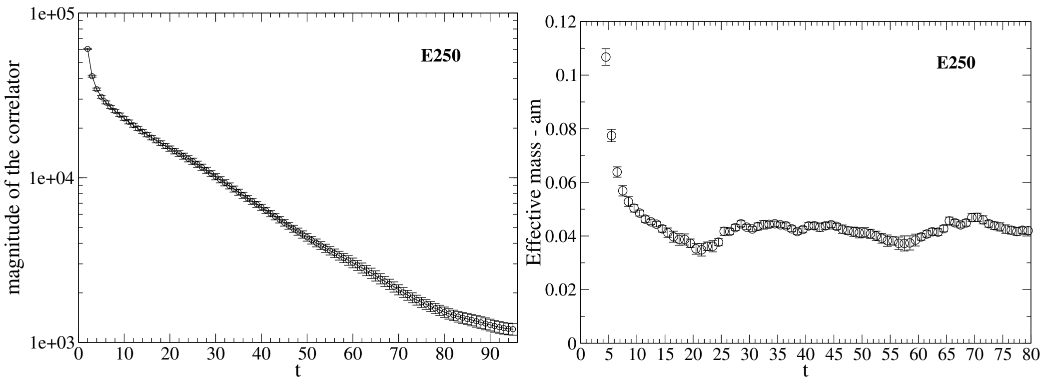

Figure 8: Left pane: Pion correlator from 70 configurations of E250. Right pane: Corresponding effective mass. For details of the correlator construction please refer to the text.

and the periodic boundary conditions by randomly shifting source locations. The current results indicate $m_\pi \approx 130(3)$ MeV, reasonably close to the physical pion in the isospin limit and without electromagnetic contributions [15], with a mass of 134.8(3) MeV.

3.2 Challenges encountered during the thermalization

The initial thermalization runs with $T \times L^3 = 64 \times 48^3 a^4$ proceeded smoothly. The same was the case for runs at intermediate volume, which needed various minor parameter adjustments, such as more frequent updates of the deflation subspace along the MD trajectory. Switching to the large volume with $T \times L^3 = 192 \times 96^3 a^4$, which was an unprecedented lattice size for CLS simulations using the openQCD Software, a change to a large deflation blocksize was needed in order to maintain a manageable size of the little Dirac operator. While the deflation subspace for CLS runs in smaller volumes is typically of order $4^3 \times 8$ we had to use a much larger blocksize ($8 \times 4 \times 8^2$) to achieve a stable run. For this setup the resulting iteration counts are somewhat higher than desirable, as deflation is not as efficient. This indicates that a multigrid setup with 3 levels might be preferable for this lattice volume[2]. Such a setup is currently not possible with openQCD. For even larger lattices further algorithmic improvements or a paradigm shift on how lattice QCD simulations are carried out [16] would be needed.

4 Conclusions and Outlook

The CLS consortium continues its effort to produce a large library of high-quality 2+1 flavor gauge configurations [3, 4]. As part of this effort we started production of an ensemble with lattice spacing $a \approx 0.064$ fm and (close-to) physical light- and strange-quark masses. This ensemble will play a crucial role in reducing systematic uncertainties for ongoing projects within the CLS consortium. Examples of such projects (with a focus on activities by the Mainz group) include calculation of the hadronic contribution to a_μ [17, 18], ongoing baryon structure calculations [19], a program on lattice spectroscopy and scattering [20], and high precision scale setting [14]. While no significant issues were encountered during thermalization, simulations with a large lattice volume, such as E250, might profit from a 3 level multigrid setup not currently available within the openQCD package.

Acknowledgements

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[2] It is currently not clear that this would pay off for E250, as possible run parameters would also be quite limited

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