Improved Wilson QCD simulations at light quark masses

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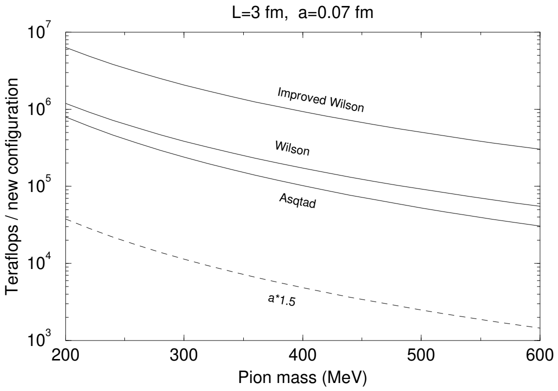
We present preliminary results from UKQCD simulations at light quark masses using two flavours of non-pertubatively improved Wilson fermions. We report on the performance of the standard HMC algorithm at these quark masses where $m_\pi/m_\rho < 0.5$ in comparison with simulations using improved staggered quarks.

1. SIMULATION PERFORMANCE

Since 1997, UKQCD has been conducting dynamical fermion simulations on a Cray T3E machine using typically 128 processors (35 Gflops sustained). This has permitted production studies on lattices up to $16^3 \times 32$ and m_π/m_ρ down to around 0.60 [1]. Study groups within the collaboration are now planning physics programmes for the advent of the QCDOC multi-Teraflops machine which is expected to be our main resource from 2003 onwards. Actions and algorithmic performance are key concerns.

1.1. HMC performance

The next figure shows estimates of the work (in Teraflops) required to obtain a 'new' configuration using three of the main methods currently available.



The data for the plot was mostly taken from that provided last year at LAT01 for the session on algorithm performance [2]. The top curve corresponds to the UKQCD 'clover-Wilson' estimate:

$$\frac{\text{Gflops}}{\text{config}} = 0.157\left(\frac{L}{a}\right)^{3.41}\left(\frac{T}{a}\right)^{1.14}\left(\frac{1}{am_\pi}\right)^{2.77}. \quad (1)$$

The accompanying curves correspond to Wilson fermions as measured by the SESAM collaboration [3] and the Asqtad MILC code ('order a^2 tadpole' improved staggered fermions using the R-algorithm [4]). The dashed curve corresponds to the Asqtad data but where the lattice spacing has been increased by 50%. The Asqtad scaling curve was taken from the performance data in [5]. We performed an independent check by carrying out Asqtad simulations with 2 flavours on the same size lattice and machine used to produce the UKQCD data. For this comparison, a 'new configuration' amounts to 20 MD trajectories for the Wilson and clover HMC runs and 6 for the Asqtad runs. These numbers are based on using at least twice the measured integrated plaquette autocorrelation time in each case. The motivation for the extra comparison of Wilson at lattice spacing a with Asqtad at spacing $1.5a$ is the observation that the improvement for the latter is much greater ($\mathcal{O}(a^2\alpha_s)$) than for Wilson at a given spacing a. Since the work scales like a^{-8} this contributes very significantly to the saving in work at fixed physical lattice size and m_π.

The Wilson/SESAM simulation [3] appears to be 8 times faster than the improved Wilson/UKQCD one. Detailed comparison shows

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that a factor of 3.4 comes from solver iterations (better preconditioning and solver algorithm and better underlying condition number); a factor of 1.8 from larger MD step size (higher acceptance, physics); a factor of 1.3 from the numerical overhead of the clover term. These naive comparisons do not take into account other factors such as relative scaling behaviour and accessibility and efficiency of measurement operators.

1.2. HMC stability

These HMC runs are expected to be susceptible to instabilities (occasional large ΔH values and zero acceptance) when the fermion force term gets too large [6]. We have observed this effect directly on the clover-Wilson run at $\kappa = 0.1358$ where we find it necessary to use a step size of 1/400. When the step size is this, or smaller, we find that 64 bit for our field storage and matrix-vector manipulations is required so as to avoid a dramatic loss of acceptance due to rounding errors. This is so even though we always use full 64-bit arithmetic and sophisticated summing techniques in the global summing of our ΔH (energy difference) calculations.

1.3. Run parameters

The main parameters of the new light quark run are shown in the following table. In physical units, $L \approx 1.5 fm$ and $m_\pi \approx 430$ Mev before extrapolation.

(β, κ)	(5.2, .1358)
trajectories/hour	3
no. trajectories	2440
no. configs	122
$\tau_{AC}^{\rm int}$(plaquette)	6.9(6)
r_0/a	5.3(5)
a (using $r_0 = 0.49$ fm)	0.0925(9) fm
am_{PS}	0.207(5)
m_{PS}/m_V	0.43(2)
$m_{PS}L$	3.3(1)

The integrated autocorrelation time for the plaquette follows the previously observed trend that it *decreases* with decreasing quark mass. For comparison, $\tau_{AC}^{\rm int}$=16(3) at $\kappa = .1350$ where $m_{PS}/m_V \approx 0.7$. Although not expected, this trend can be accommodated in simple models [1].

The ratio 'm_π/m_ρ' is below the threshold for the continuum decay $\rho \to \pi\pi$ but not for decay on this size of lattice. We are using maximum entropy methods [7] to look for evidence of decay of the lattice state at the relevant energy.

2. MEASUREMENTS

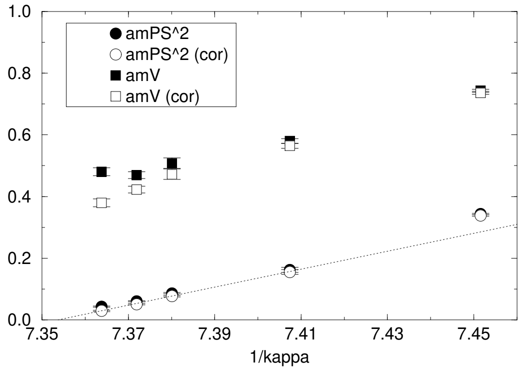
2.1. Hadron masses and finite size effects

Since $m_\pi L = 3.3(1)$ (significantly below 5) we anticipate finite size effects. For small and intermediate size boxes there is evidence [8] that hadron mass corrections follow a power law (L^{-3}) rather than exponential ($\exp(-L/L_0)$) size dependence. A simple phenomenological model for this might be

$$\frac{\delta m_h}{m_h} = \frac{c_h}{(m_\pi L)^3}\,. \tag{2}$$

The dimensionless parameter c_h is presumably related to the form factor of the hadron h.

The figure below shows a compilation (from UKQCD and QCDSF [9]) of pseudoscalar and vector masses (fixed $\beta = 5.2$ and $\kappa_s = \kappa_v$). The filled points are the raw masses extracted from multi-channel fits.



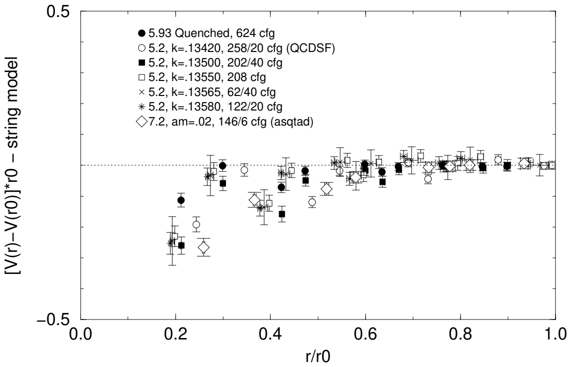
Aside from the point at very heavy quark mass ($\kappa = 0.1342$), the m_{PS} data (filled circles) are well fitted by lowest order chiral PT (linear in $1/\kappa$).

We have estimated $c_\pi \approx 6$ and $c_\rho \approx 7$ from the finite size (FS) effects reported by the JLQCD Collaboration, who used the same action (clover-Wilson) [10] on a variety of lattice sizes. We have checked that the corrections implied by these values are consistent with the FS effects which UKQCD has previously measured using a slightly different action [11]. Using this model to 'correct' the measured values, we get the open points shown in the figure.

The FS-corrected pseudoscalar points are still well fitted by a straight line and yield $\kappa_{crit} = 0.135978(9)(55)$. The first error is statistical and the second systematic - estimated by including the heaviest quark point in a quadratic fit. Taking the above FS corrections for the pseudoscalar and vector into account we estimate $m_{PS}/m_V \approx 0.45$ for the lightest quark simulation.

2.2. Static potential

The next figure shows the difference of the measured static potential from the universal bosonic string model for all UKQCD data sets at fixed $\beta = 5.2$ [1] including this latest run (stars) at $\kappa = 0.1358$ and a QCDSF set at $\kappa = 0.1340$ [9].



Also shown is the corresponding result from a modest run we have made using the MILC Collaboration's code at $a \approx 0.130$ fm [4]. Violations of rotational symmetry are marked for $r < 0.7r_0 \approx 0.35$ fm for all these coarse lattices. Although the improved staggered fermion measurements (Asqtad) are at a coarser lattice spacing, they show smaller violations of rotational symmetry than the clover-Wilson data. This is presumably due to the significantly improved gluonic action. The Asqtad data (at $m_{PS}/m_V \approx 0.50$) show a greater effect of the running coupling in the Coulomb term at short distances than the corresponding clover-Wilson data (lower at short distances). Within the fixed β clover-Wilson set there is no very clear trend with decreasing quark mass. The corresponding plot for clover-Wilson data at fixed lattice spacing [1] shows more clearly the effect of the running coupling.

3. CONCLUSIONS

We have analysed data from more than 2200 trajectories of a clover-improved Wilson simulation at $m_q/m_s \approx 0.3$. We have estimated finite volume corrections to meson masses. Light quark masses are accessible using clover-improved Wilson fermions and standard HMC but simulations are slow and can suffer from instabilities. Improved staggered fermions appear to offer a more efficient route to configurations with light dynamical quarks, but physics measurements are in general more complicated.

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