QCD Simulations with Light, Strange and Charm dynamical Quark Flavours: Exploring the chiral limit of QCD

Application for Computing Time on the IBM Blue Gene/P system Jugene, the Juropa system and the apeNEXT parallel machine at the John von Neumann-Institute for Computing

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1 Problem description

The European Twisted Mass collaboration (ETMC) has performed a very successful research program over the last years. To list the already published results, we mention here for the case of simulations with two mass degenerate light quark flavours a detailed analysis of light meson physics [1, 2], the calculations of the nucleon and Δ masses [3, 4], moments of parton distribution functions [5], non-perturbatively obtained renormalisation constants using the RI-MOM [6] and Schrödinger functional [7] schemes, light quark masses and decay constants [8, 9, 10], charm physics [10, 11], B_K [12], meson [13, 14] and nucleon [15] form factors, investigations of the ϵ-regime of chiral perturbation theory [16, 17, 18], study of cut-off effects at tree-level of perturbation theory [19] and non-perturbatively [20, 21], neutral [22] and η' [23] mesons, $\omega - \rho$ mass splitting [24], static light mesons [25], the $\tau_{1/2}$, $\tau_{3/2}$ Isgur-Wise functions [26] and the vacuum polarisation tensor [27]. We also want to mention the exploration of twisted mass fermions at non-vanishing temperature [28, 29]. Further physics projects such as the computation of meson and nucleon scattering lengths, topological aspects or the resonance parameters of the ρ meson are presently being developed and in progress. We show in fig. 1 a comparison between our lattice results from our $N_f = 2$ simulations and the corresponding quantity as can be extracted from experiment. Note that for a number of quantities the lattice errors are already comparable or even smaller than the "experimental" ones.

The project that we shall propose here will deal with a setup of including in addition to the mass degenerate light up- and down-quark flavours also the heavier strange and heavy charm degrees of freedom. This novel situation – which we denote with $N_f = 2+1+1$ setup – has been explored in ref. [30] and first promising results have been presented in ref. [31], see also the discussion below.

For this set-up, which is closer to the physical situation than the $N_f = 2$ situation, our experiences from the $N_f = 2$ simulations are very valuable. One important lesson we could learn from those is that there is one major uncertainty when attempting to provide physical values: our lightest meson masses were about $m_{\mathrm{PS}} \approx 300$ MeV. We therefore had to perform an extrapolation of all our observables to the physical value of $M_\pi = 140$ MeV. Although for the light meson masses and decay constants and the proton mass such an extrapolation seems to be safe and chiral perturbation theory appears to work very well, for other quantities such an extrapolation is problematic:

- In the case of strange baryons, we find that, while ratios of baryon masses extrapolate linearly to the physical point, the masses themselves are difficult to extrapolate. In particular, the applicability of chiral perturbation theory is questionable. Therefore, quark masses should be taken at values where one does not have to rely on chiral perturbation theory. At the same time, chiral perturbation theory itself can be tested then.

- For nucleon form factors, e.g. g_A or moments of parton distribution functions the data are essentially linear in the quark mass but a linear extrapolation overshoots the experimental point significantly. It is thus rather unclear how to reconcile the lattice data with experiment. Thus, it will be crucial to go to lower quark masses to check the approach of the lattice data to the physical values and to see, whether chiral perturbation theory describes this approach correctly.

- For quantities in the strange (and even more in the charm) sector such chiral extrapolations are badly understood.

- For the meson form factors we had to include the NNLO contributions of chiral perturbation theory. Entering a region in quark masses where the NNLO terms become negligible would allow for an important cross-check of our results.

- The extrapolation of the vector (ρ) meson to the physical point is an unexplored problem.

From these observations, we find it necessary to understand the chiral behaviour of physical observables in detail in order to control the systematic errors originating from these extrapolations, which give in fact the largest systematic errors in the analysis of various quantities.

We propose therefore to perform simulations at our so far finest value of the lattice spacing ($a \approx 0.06$fm) with dynamical mass-degenerate up and down as well as strange and charm quarks at their physical value. From our earlier experience, we estimate that at a lattice spacing of $a \approx 0.06$fm we can safely lower the pseudoscalar mass to about $m_{\rm PS} \approx 160$MeV, without being affected by discretisation errors or the phase structure of Wilson lattice QCD. The aim is to have a sequence of meson masses in the range $150 \lesssim m_{\rm PS} \lesssim 400$MeV. Given the very good scaling behaviour of maximally twisted mass fermions, see [20, 21] and fig. 2, at $a \approx 0.06$fm our results will be essentially continuum like such that we can apply, where available, continuum chiral perturbation theory with a negligible error from remaining discretisation effects. It is important to remark at this point that we have performed already simulations at two values of the lattice spacing in the last year with $N_f = 2+1+1$ quark flavours. From these computations we found that lattice spacing artefacts for $m_{\rm PS}$, $f_{\rm PS}$ and $m_{\rm Nucleon}$ are small and show a similar behaviour as in the case of our $N_f = 2$ simulations, see below. In addition, at our target value of the lattice spacing of $a \approx 0.06$ fm we are in the process of tuning the theory to maximal twist. Therefore, the project could start immediately once the necessary computer resources become available. Our planned investigation is not only relevant for the ETM collaboration but for lattice QCD as a whole.

We think that our collaboration is perfectly able to achieve the above goal since it brings together a large amount of different expertise, ranging from code optimisation and algorithm development, theoretical aspects and chiral perturbation theory calculations to physical applications that are directly relevant for ongoing experiments and phenomenological analyses. Thus, we think that ETMC is a very unique collaboration concerning the plethora of physics results that we can achieve and which covers many aspects of QCD and Standard Model phenomenology.

Therefore, we ask for a substantial amount of computer time on the Blue Gene/P, the Juropa and the apeNEXT systems. We emphasize that more than 60 physicists including eleven Ph.D. students from all over Europe are participating in the project and rely on the availability of sufficiently large computer resources.

This project proposal is submitted in the name of the European Twisted Mass Collaboration (ETMC) which comprises 17 institutions in Europe, i.e.

- Cyprus: Univ. of Cyprus,
- France: Univ. of Paris Sud and LPSC Grenoble,
- Germany: Humboldt Univ. zu Berlin, Univ. of Münster, DESY in

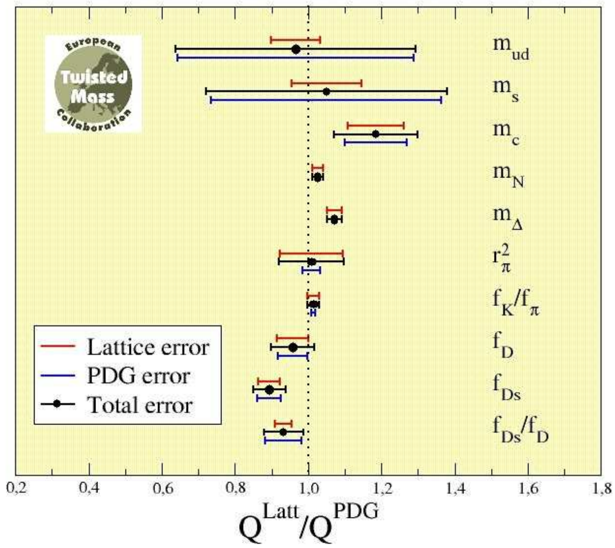


Figure 1: A selection of physics results obtained from twisted mass fermion simulations for $N_f = 2$ flavours of mass-degenerate quarks by the ETMC. We show the ratio of our lattice results in comparison to extractions of these quantities from experiment.

Hamburg and Zeuthen,

- Great Britain: Univ. of Glasgow, Univ. of Liverpool and Univ. of Cambridge
- Italy: Univ. of Rome I, II and III, ECT* Trento,
- Netherlands: Univ. of Groningen,
- Poland: Univ. of Poznan,
- Spain: Univ. of Valencia, Univ. of Barcelona,
- Switzerland: Univ. of Bern.

Twisted Mass Fermions

The Wilson twisted mass fermionic lattice action for two flavours of degenerate quarks reads (in the so-called twisted basis [32] and with fermion

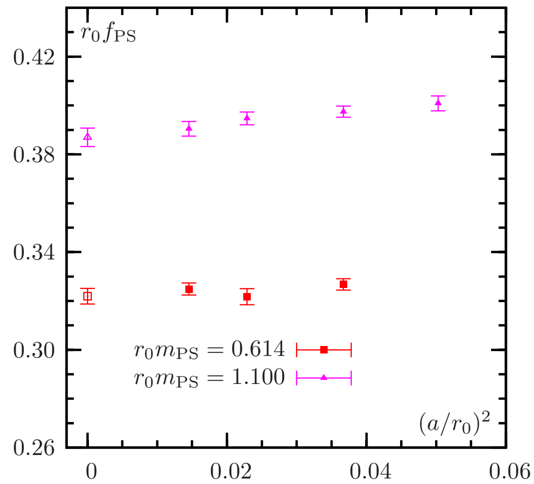


Figure 2: We show the continuum limit scaling of $r_0 f_{\rm PS}$ as a function of $(a/r_0)^2$ at two fixed values of $r_0 m_{\rm PS}$. The data are obtained for our setup of $N_f = 2$ mass degenerate flavours of quarks. Note that in this plot a new lattice spacing of $a \approx 0.05$fm is used, which is a finer lattice spacing than so far published by ETMC. The plot confirms that the (expected) a^2 scaling violations are as small as the previous calculations suggested.

fields with continuum dimensions)

$$\begin{aligned} S_{\rm tm} = a^4 \sum_x \Big\{ & \bar\chi_x \left[m_0 + i\gamma_5\tau_3\mu_l + \frac{4r}{a} \right] \chi_x \\ & + \frac{1}{2a} \sum_{\nu=1}^{4} \bar\chi_x \left[U_{x,\nu}(-r+\gamma_\nu)\chi_{x+\hat\nu} + U^\dagger_{x-\hat\nu,\nu}(-r-\gamma_\nu)\chi_{x-\hat\nu} \right] \Big\} , \end{aligned} \tag{1}$$

where am_0 is the bare untwisted quark mass and $a\mu_l$ the bare twisted mass, τ_3 is the third Pauli matrix acting in flavour space and r is the Wilson parameter, which we set to one in our simulations. Adding the strange and charm fermions can be realized by a mass term of the form:

$$S_h = a^4 \sum_x \bar\chi^h_x \left[m_0 + i\gamma_5\tau_1\mu_\sigma + \tau_3\mu_\delta \right] \chi^h_x \; . \tag{2}$$

Physical values of the strange and the charm quark mass can be achieved in this formulation by suitably tuning the parameters $a\mu_\sigma$ and $a\mu_\delta$ [30, 31]. Note that the bare untwisted quark mass parameter am_0 is the same in the heavy and the light doublet, as indicated by the notation and will be discussed later.

In the gauge sector we consider a general form which includes besides the plaquette term $U^{1\times1}_{x,\mu,\nu}$ also rectangular (1×2) Wilson loops $U^{1\times2}_{x,\mu,\nu}$

$$S_g = \frac{\beta}{3}\sum_x\left(b_0\sum_{\substack{\mu,\nu=1\\1\leq\mu<\nu}}^{4}\{1-\mathrm{Re}\,\mathrm{Tr}(U^{1\times1}_{x,\mu,\nu})\}+b_1\sum_{\substack{\mu,\nu=1\\\mu\neq\nu}}^{4}\{1-\mathrm{Re}\,\mathrm{Tr}(U^{1\times2}_{x,\mu,\nu})\}\right) \quad (3)$$

with β the bare inverse gauge coupling and the normalisation condition $b_0 = 1-8b_1$. Note that at $b_1 = 0$ this action becomes the usual Wilson plaquette gauge action. In our work, we will use the Iwasaki form [33] of the gauge action, i.e. $b_1 = -0.331$.

In twisted mass QCD $\mathcal{O}(a)$ improvement can be obtained by tuning Wilson twisted mass fermions to maximal twist, i.e. by tuning the bare Wilson quark mass am_0 to its critical value am_{crit}. In fact, it was first proved in ref. [34] that parity even (and therefore physical) correlators are free from $\mathcal{O}(a)$ lattice artifacts at maximal twist by using spurionic symmetries of the lattice action. Later on it was realised [35, 36] that a simpler proof is possible based on the parity symmetry of the continuum QCD action and the use of the Symanzik effective theory.

From this latter way of proving $\mathcal{O}(a)$ improvement, it becomes also clear how to define maximal twist: first, choose an operator odd under parity (in the physical basis) which has zero expectation value in the continuum. Second, at non-vanishing value of the lattice spacing tune the expectation value of this operator to zero by adjusting the value of the bare quark mass am_0. This procedure is realised by tuning the hopping parameter $\kappa = 1/(2am+8r)$ such that the so-called PCAC quark mass becomes zero, where the PCAC mass reads

$$m_{\mathrm{PCAC}} = \frac{\sum_{\mathbf{x}}\langle\partial_0 A^a_0(x)P^a(0)\rangle}{2\sum_{\mathbf{x}}\langle P^a(x)P^a(0)\rangle}\,, \qquad a=1,2\,. \quad (4)$$

It is very important to realise that this tuning procedure can be performed by tuning the bare mass term in the light sector only. Choosing for the heavy sector the same value of the bare untwisted quark mass guarantees $\mathcal{O}(a)$ improvement also in the strange-charm sector.

Besides being a theoretically sound formulation of lattice QCD, Wilson twisted mass fermions offer a number of advantages when tuned to maximal twist: (i) tuning of operator-specific improvement-coefficients is avoided, because only one parameter needs to be tuned to realise maximal twist; (ii) the mixing pattern in the renormalisation process is expected to be simplified; (iii) the twisted mass is directly related to the physical quark mass without the need for additive renormalisation; (iv) the twisted mass provides an infra-red regulator helping to overcome possible problems with ergodicity in molecular dynamics based algorithms.

The main drawback of the twisted mass approach is the explicit breaking of parity and isospin symmetry which are only restored when the continuum limit is reached. However, due to $\mathcal{O}(a)$ improvement, this breaking is an $\mathcal{O}(a^2)$ effect as confirmed by simulations performed in the quenched approximation [37, 38]. Furthermore, the simulation results in the $N_f = 2$ set-up indicate that these $\mathcal{O}(a^2)$ effects become large *only* for a particular observable: the neutral pion mass. All other splittings measured so far are zero within errors. This observation can be understood by theoretical considerations [39].

The algorithm we are using is based on a HMC algorithm with mass preconditioning [40, 41] and multiple time scale integration as described in detail in ref. [42].

1.1 Existing results from the $N_f = 2+1+1$ simulations

In this section we shall present some preliminary results from our simulations with $N_f = 2+1+1$ quark flavours. ETMC is presently analysing the existing configurations and hence we can provide here only a first account of our work. We have performed simulations at two β values, $\beta = 1.9$ and $\beta = 1.95$ with several quark masses and several lattice sizes, see table 1.

In fig. 3 we show the results of our tuning to maximal twist. We employed a criterion that the absolute value of the PCAC quark mass as well as its error is less than 10% of the value of the light twisted mass parameter used. As argued in [2] this condition is expected to lead to a very good scaling behaviour of physical quantities. As fig. 3 demonstrates, we have indeed been able to fulfill our tuning condition to the precision we were aiming for.

In fig. 4(a) we show $r_0 m_{\mathrm{PS}}$ as a function of $r_0 \mu_l$ for the two values of β we have used. Note that we plot here the bare quark mass since we do not have the relevant renormalisation constants yet. However, we expect that the renormalisation constants at these two values of β will be close to each other and consider the results in fig. 4(a) as a first indication that lattice spacing artefacts are small.

This indication is strengthened by fig. 4(b) where we show the situation

Table 1: Simulation parameters, volumes, β values and chosen values of the light bare twisted mass $a\mu_l$ and the parameters $a\mu_\sigma$ and $a\mu_\delta$ controlling the mass splitting. For each $a\mu_l$ we tuned to the critical value of the hopping parameter κ_{crit} separately by having $am_{\mathrm{PCAC},l} \approx 0$ demanding that $|am_{\mathrm{PCAC},l}/a\mu_l| \lesssim 0.1$. Each run has about 1000 trajectories for equilibration and at least 5000 trajectories for measurements. The trajectory length has been always set to one.

$L^3 \cdot T$	β	$a\mu_l$	$a\mu_\sigma$	$a\mu_\delta$	κ_{crit}
$20^3 \cdot 48$	1.90	0.004	0.15	0.19	0.163270
$24^3 \cdot 48$	1.90	0.004	0.15	0.19	0.163270
	1.90	0.006	0.15	0.19	0.163265
	1.90	0.008	0.15	0.19	0.163260
	1.90	0.010	0.15	0.19	0.163255
$32^3 \cdot 64$	1.90	0.003	0.15	0.19	0.163272
	1.90	0.004	0.15	0.19	0.163270
	1.90	0.005	0.15	0.19	0.163267
$24^3 \cdot 48$	1.95	0.0085	0.135	0.170	0.1612312
$32^3 \cdot 64$	1.95	0.0035	0.135	0.170	0.161240
	1.95	0.0055	0.135	0.170	0.161236
	1.95	0.0075	0.135	0.170	0.161232

for $r_0 f_{\mathrm{PS}}$ for comparison but now as a function of $(r_0 m_{\mathrm{PS}})^2$ which does not require any renormalisation constant for a comparison. We show in the same graph the corresponding data from our $N_f = 2$ simulations at $\beta = 3.9$ (with a very similar value of the lattice spacing). As a result, we conclude that there is no significant lattice spacing dependence and that the data for $N_f = 2$ and $N_f = 2 + 1 + 1$ agree very nicely.

The corresponding situation for the nucleon mass is shown in fig. 5(a). Again, we find very small differences between the data at the two values of the lattice spacing and also again a good agreement with the results of our $N_f = 2$ simulations. This indicates that also for the nucleon mass the lattice artefacts will be as small as they came out for our $N_f = 2$ analysis.

Finally, we give in fig. 5(b) our results for the Kaon mass. We find that the data for the kaon mass squared show a linear behaviour in the light quark mass. An extrapolation to the physical point reveals that our chosen values for $a\mu_\sigma$ and $a\mu_\delta$ lead to a slight overshooting of the physical Kaon mass at $\beta = 1.9$. At $\beta = 1.95$ the situation is much better and the data seem to extrapolate to the physical value of the Kaon mass. Note that we have taken $r_0 \sim 0.44$fm to estimate the physical Kaon mass value. We are exploring presently the possibility to reweight our configurations to the correct values of $a\mu_\sigma$ and $a\mu_\delta$. Since the expected changes are rather small, we hope that we can avoid additional simulations to reach the physical Kaon mass.

These first results from our $N_f = 2+1+1$ simulations are very promising and encouraging. In fact, we have already started a tuning run for $\beta = 2.1$ to prepare the simulations we want to perform with the next computer time allocation.

Let us end the description of our preparatory work with a few remarks:

1. The analysis of the heavy quark sector and, in particular, the charmed mesons and baryons, turn out to be rather difficult due to flavour mixing effects in the s-c quark pair. We are exploring several strategies to circumvent this issue. Besides an analysis in an unitary setup, we are also using Osterwalder-Seiler fermions in the valence sector. Both approaches can provide very important cross-checks for the results in the heavy quark sector.

2. We have started simulations with $N_f = 4$ mass degenerate, light quarks. This set of simulations ought to be performed at several values of the quark mass and shall enable us to compute the necessary renormalisation constants for our $N_f = 2+1+1$ setup.

3. We have also performed simulations with stout smearing. We found that using one level of stout smearing and a smearing parameter of $\rho = 0.15$ no significant improvement could be obtained. We therefore decided to stay with the conceptually cleaner simulations without smearing. In particular, we have not performed further tests of stout smearing.

4. We are in the process of studying the effects of isospin breaking. From a first analysis at $\beta = 1.9$ the relative pion mass splitting turns out to be larger than what we measured in our $N_f = 2$ simulations at a comparable value of the lattice spacing.

   It is important to remark that from the $N_f = 2$ investigations we found that *only* the neutral pseudo-scalar mass is affected by isospin

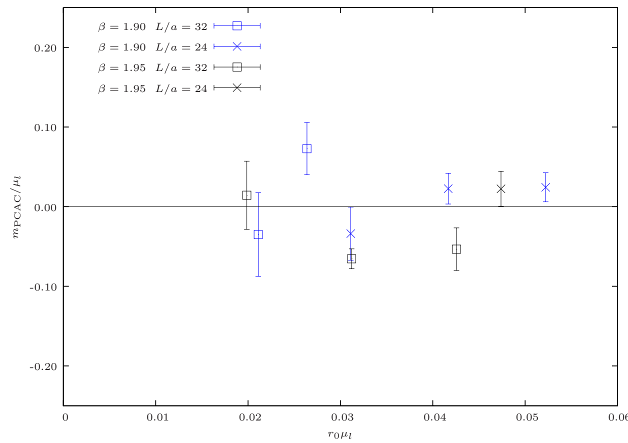


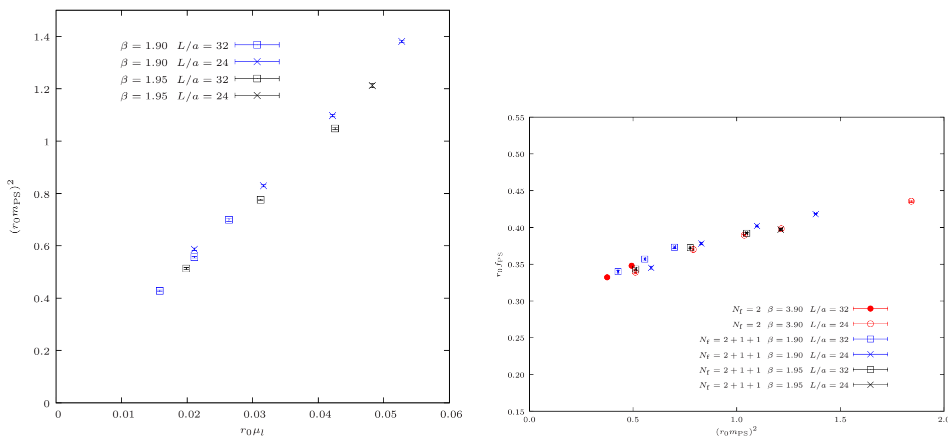
Figure 3: The ratio $R = m_{\rm PCAC}/\mu_l$ for the case of $N_f = 2+1+1$ flavours of quarks as a function of $r_0\mu_l$. This ratio should be less than $|R| = 0.1$ in order to fulfill our criterion for maximal twist. As can be seen, for all simulation points shown and and to be used in our analysis, the condition of maximal twist is satisfied.

breaking. All other observables considered did not suffer from such effects. Nevertheless, it is very important to have the size of the mass splitting also at our second value of $\beta = 1.95$. This analysis is in progress and it is too early to draw definite conclusions at the time of writing this proposal.

Proposed project

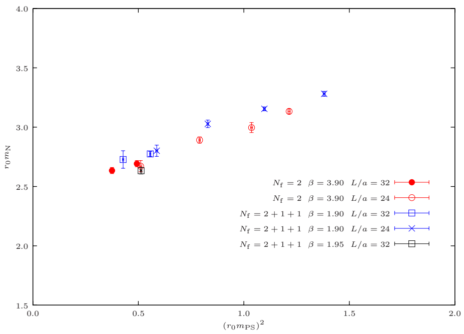
As detailed above, we have already results for the physically realistic case of simulating lattice QCD with mass-degenerate up and down and heavy strange (s) and charm (c) dynamical quark flavours. We use a formulation as described in ref. [43, 44] and the work of refs. [30, 31] clearly showed the feasibility of such simulations.

We also mention that we have two completely independent and optimised simulation programs to cross-check results. One of these programs has been adapted to the BG/P. The efficiency of the code comes out to be about 20% of peak performance and we also see a good scaling behaviour of the code with the number of processors. Hence, our code is well suited to perform

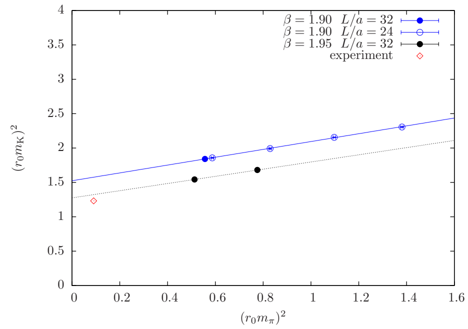


(a) (b)

Figure 4: We show in (a) the pseudo scalar mass as a function of $r_0\mu_l$ from our $N_f = 2+1+1$ simulations. The data are obtained at two values of the lattice spacing. The fact that the results come out very close to each other indicate that there are no big lattice artefacts. Note that for a more precise comparison, the relevant renormalisation factors to obtain the renormalised quark mass would be needed. In (b), the pseudo scalar decay constant is shown as a function of $(r_0 m_{\mathrm{PS}})^2$ and hence no renormalisation factor is needed. We show also data from our $N_f = 2$ simulations. The graph demonstrates that lattice spacing artefacts are small for the case of $N_f = 2+1+1$ flavours, too. It shows a nice agreement with our previous $N_f = 2$ simulations.



(a)



(b)

Figure 5: The nucleon mass (left) and the Kaon mass (right) as a function of $(r_0 m_{\mathrm{PS}})^2$. For the nucleon mass we also show data from our $N_f = 2$ simulations. The Kaon mass shows a rather linear dependence on the quark mass. Note that while at $\beta = 1.95$ our tuning to the physical value of the Kaon mass (diamond in (b)) has been done rather precisely, for $\beta = 1.9$ our data overshoot the physical value. We expect to be able to correct for this mismatch by reweighting in the twisted mass parameters that control the strange-charm quark mass splitting.

large scale simulations on the BG/P.

For certain analysis questions other machines are more appropriate. In particular, all our codes to determine the renormalisation constants in the RI-MOM scheme are written in tao and hence we are bound to the apeNEXT machine to obtain the very important and necessary renormalisation constants. The same holds true for the determination of the meson form factors for which, again, we only have tao codes. Thus such important physical questions as meson form factors or $K_{(l3)}$ decays need the usage of the apeNEXT machines.

In addition, for the final analysis step of many quantities, such as the Sommer scale r_0, static-light physics and many memory intensive contractions the Juropa system is most useful.

2 Description of the aims and of what one wants to learn

With the inclusion of the strange and charm quarks in the simulation as proposed here, for the first time lattice QCD simulations in real physical conditions can be performed. Taking into account also the virtual effects of the charm quark is certainly beneficial for the study of charm physics in a strictly unitary setup and in the study of weak matrix elements because the GIM mechanism is then fully operative. As we have already discussed above, the appropriate choice of the critical mass value to which m_0 is set at any given β from our condition for tuning to maximal twist, guarantees that the cutoff effects brought about by the heavy quark pair in the sea do not harm significantly the observables containing only light valence quarks (see e.g. fig. 4(a) and fig. 4(b)).

Simulations

The goal of the simulations is the generation of configurations staying at $\beta = 2.1$ and driving the quark mass close to the physical point. The linear extent of our lattices of size $L^3 \cdot T$, with $T = 2L$, will be $L \gtrsim 3.0$fm in order to suppress finite size effects. In addition, we will choose parameters such that $m_{\mathrm{PS}}L > 3.5$. Our planned simulations will then be:

- $48^3 \cdot 96$ lattices for 5 quark masses in the range of pseudo scalar masses of $250 < m_{\mathrm{PS}} < 400$ MeV
- $64^3 \cdot 128$ lattices for 3 quark masses in the range of pseudo scalar masses of $180 < m_{\mathrm{PS}} < 250$ MeV
- $96^3 \cdot 192$ lattices for one quark mass with $m_{\mathrm{PS}} \approx 160$ MeV
- Simulations with $N_f = 4$ mass degenerate flavours of quarks.

We emphasize that some of these simulations will be performed on other computers such as the BG/P Babel machine at the Idris supercomputer center in Orsay and the apeNEXT machines in Rome. In particular, this holds true for the $N_f = 4$ simulations needed for obtaining the relevant renormalisation constants. Therefore, we ask only for time of a part of the above simulations at NIC. However, the really challenging simulation on the large $96^3 \cdot 192$ lattice very close to the physical point can only be performed on the NIC system and is hence the main target of this application.

Another point worth stressing is that we shall start the simulations with the $48^3 \cdot 96$ lattices at $\beta = 2.1$. This will allow us to check explicitly for the size of lattice artifacts, which are expected to be small.

Physics program

We list below our physics targets which are to be obtained. With the above setup, we will be able to fully control the extrapolation to realistic pion masses. In particular, we can confront our results with results of various kinds of chiral perturbation theory and check in detail their validity. In turn, the comparison to chiral perturbation theory will allow us to extract the low energy constants of the effective chiral Lagrangian. Our physics targets are:

- a comprehensive meson and baryon spectrum calculation including the full octet and decuplet
- quark masses, including a precise determination of the light, the strange and the charm quark masses
- various meson form factors, including the pion, Kaon and D-meson form factors and decay constants, Isgur-Wise functions and the charge radius of the pion
- the electromagnetic, axial and pseudo scalar nucleon and Delta form factors and the nucleon to Delta transition form factors
- various moments of parton distribution functions and generalized parton distributions for the pion and the nucleon as relevant for deep inelastic scattering experiments and for studying the spin structure of the nucleon
- precise evaluation of low energy constants from chiral fits both, in the p- and ϵ regime of chiral perturbation theory
- meson and nucleon scattering phase shifts which can be determined through finite volume effects of the avoided level crossing
- resonance parameters of the ρ meson or the Δ baryon and other unstable particles in QCD

- the vacuum polarisation tensor which is computed from conserved currents. The results of this investigation are of great importance for the muon $g-2$ experiments and for tests of possible non-perturbative effects to describe the τ-data. In addition, moments of the vacuum polarisation tensor can be directly compared to corresponding results from perturbation theory.

- neutral mesons, which will provide most interesting information on the η' particle

- topological susceptibility, which is a quantity of interest of its own and will provide together with the computation of the η' particle a test of the Witten-Veneziano formula

- static-light mesons crucial for treating B-meson physics on the lattice

- B_K, which is a phenomenologically very interesting quantity and a benchmark observable for lattice calculations. We are planning to evaluate B_K with the twisted mass formulation using the so-called Osterwalder-Seiler formulation of twisted mass quarks

- effects of isospin breaking in the twisted mass approach. The size of these cut-off effects will provide important hints about the size of scaling violations in the twisted mass approach.

- Up to now only the contributions of connected diagrams to many of the above mentioned quantities have been computed. However, it is very important to evaluate also the disconnected contributions, e.g. for the meson and nucleon form factors, the vacuum polarization tensor or the scattering phase shifts. We have in the ETMC developed efficient techniques for the calculation of these quantities which we plan to employ in the evaluation of these disconnected contributions.

- computation of renormalization constants using the RI-MOM as well as the Schrödinger functional schemes.

The techniques and programmes for the broad physics spectrum detailed above are fully developed and tested where possible in the $N_f = 2$ set-up. Hence, the projects can directly be started once the configurations are available. The physics program listed above demands the computation of many propagators and the corresponding contractions. In particular, for computing disconnected diagrams, many inversions have to be performed in order to obtain a a good signal-to-noise ratio. For this analysis, the Juropa and apeNEXT systems are ideally suited. Emphasis is put on the apeNEXT machine since many physical observables such as the meson form factors are available presently solely as tao codes and need to be run on this special architecture. Also all programs to perform the non-perturbative computations of the renormalisation constants in the RI-MOM scheme exist in tao codes. In the long run, we will also implement these very relevant quantities in C codes to be able to calculate them on the large lattices we want to simulate in the future. However, at the moment, we are relying on the tao codes and the apeNEXT machines which can be used up to the $48^3 \cdot 96$ lattices. We therefore ask for computer time also on the apeNEXT machine at NIC.

3 Detailed description of the algorithmic and mathematical numerical methods

The programmes for twisted mass fermions are fully developed and implemented in parallel codes on the IBM Blue Gene/P machine. The code runs also well on cluster architectures and we expect a good performance on the Juropa system. The apeNEXT code for computing propagators is highly optimised and we reach approximately 40% efficiency of peak performance. For the Blue Gene/P code we achieve an efficiency of about 20% of peak performance. The parallelisation strategy is in general domain decomposition using MPI for the IBM-Blue Gene/P machines while for apeNEXT we use the direct remote memory access feature. We remark that already now we are using both machines such that we could obtain reliable performance figures. We checked the scaling of the code explicitly on the Blue Gene/P machine. We found that on the massively parallel Blue Gene/P machines the problem is indeed scalable to a large number of nodes, up to 32768 processors (8 racks) without big performance losses. We are also in the process of improving the I/O performance of our code. Our present tests show that using parallel I/O we see scaling of the I/O performance with the number of I/O nodes (up to hardware and file system limits). We therefore think that I/O will not be a bottleneck for the simulations on the large lattices we are planning.

Our algorithms are state of the art versions of the HMC and PHMC algorithms. We have incorporated improvements such as preconditioning and Hasenbusch's trick as well as a multiple step size integration scheme to accelerate the simulations for both algorithms. We have also developed a complete measurement program with all (mesonic and baryonic) 2-point and also 3-point functions, as well as the baryonic 2-point and 3-point functions including smearing and noise reduction techniques. We refer to ref. [2] for a detailed description of our techniques, which were partly newly developed for the case of twisted mass fermions. We have also tried to implement inexact deflation in our code. However, we did not find an improvement in the performance. Although we are still investigating this question, the straightforward implementation of inexact deflation does not seem to work in our case.

4 Projects and estimated resources required

From our experience from the runs we are already performing on the BG/P machine we find the following performance figures. On one rack of Blue Gene/P we achieve per day about 20 trajectories on a $48^3 \cdot 96$, 7 trajectories on a $64^3 \cdot 128$ lattice and 2.5 trajectories on the $96^3 \cdot 192$ lattice. Given these numbers and the knowledge gained from our scaling tests, we estimate the computer resources detailed below for the next computer time allocation. The project consists of two parts.

(a) $N_f = 2 + 1 + 1$ chiral extrapolation

We aim at a detailed investigation and understanding of the behaviour of physical quantities when approaching the physical value of the pion mass. To this end, we want to start with pseudo scalar masses around $m_{\rm PS} \approx 400$MeV and reach values of $m_{\rm PS} \approx 160$MeV. The simulations shall be performed at one value of the lattice spacing of $a \approx 0.06$fm and with conditions of $L > 3$fm and $m_{\rm PS}L > 3.5$ in order to suppress finite size effects. The chosen value of the lattice spacing will ensure that remaining lattice spacing effects are negligible. As has been discussed above, we believe that a detailed understanding of the chiral limit is mandatory to control the chiral extrapolations.

(b) Analysis

We plan to compute a large number of physical observables. The evaluation of these physical observables is comparable to a quenched approximation computation and hence an order of magnitude less demanding than the dynamical simulations. Although we plan to perform many propagator computations on the BG/P, there are a number of quantities for which the Juropa system is much more appropriate. This concerns the computation of r_0, the computation of the static-light masses and especially the computations of many contractions which need only a smaller, but still significant number of processors and a large memory. Since we are currently developing a parallelised contraction code, the Juropa system is ideally suited for this task.

Finally, we need the apeNEXT system for specialised tasks for which only tao codes exist.

In summary, we ask for the following computer resources at NIC:

11 rack years of the Blue Gene/P machine

- $a = 0.06$fm, 2 quark masses, $48^3 \cdot 96$ lattice: 20 rack months
- $a = 0.06$fm, 1 quark masses, $64^3 \cdot 128$ lattice: 35 rack months
- $a = 0.06$fm, 1 quark mass, $96^3 \cdot 192$ lattice: 65 rack months
- total time for inversions: 12 rack months

apeNEXT machine

- RI-MOM Z-factors and meson form factors: 18 rack months

100 computing node years of the Juropa system.

- These nodes will be used for the computation of the static potential and static-light mesons as well as for those contractions that need a large memory.

Size of the project and quality of the proposers

The problem we address here is highly time consuming and can only be performed on very powerful machines such as the Blue Gene/P, apeNEXT and Juropa machines. The project has the ambitious goal to explore the chiral regime of lattice QCD close to physical values of the pion mass under realistic conditions including the strange and the charm quarks in the simulation. This is one of the most demanding problems in lattice QCD and needs substantial computing resources to be successfully solved. We have formed and established a large European collaboration (ETMC) in which all three universities of Rome, the universities of Glasgow, Liverpool, Valencia, Paris Sud, Groningen, Cyprus, Barcelona, Bern, Berlin, Münster, Poznan and the research centers DESY in Hamburg and Zeuthen, ECT* in Trento and LPSC in Grenoble are involved. Only in this way, we can collect the necessary expertise to realistically achieve the aims of the project. We stress again that without a substantial involvement of NIC and its resources, the project would also not be feasible for our European colleagues alone.

The proposers have extensive experience in high performance computing using vector and nowadays massively parallel supercomputers such as the CRAY T3E, PC-Cluster systems, APE and IBM machines. Our group includes algorithm experts who were involved over many years in developing efficient algorithms for the overlap operator and for dynamical fermion algorithms.

It is clear to the proposers that we ask for a large fraction of computer time on the NIC resources. However, as we emphasised above the machines at NIC in Jülich are crucial to provide the configurations on which the whole ETM collaboration relies. We strengthen again that the NIC part of the resources is a share of an European collaborative effort towards solving QCD.

We also remark that several groups in Germany involved in high performance simulation in lattice QCD have been already integrated into this project, who would have otherwise separately applied for computing time. We point out once more the novelty and the scientific relevance of our program, where for the first time four dynamical quarks are simulated in physical conditions. The complementing expertise of the members of our collaboration and its quality will ensure a successful realization of the proposed simulation program.

Relation to the International Lattice Data Grid

We also want to point out that the configurations will be stored within the ILDG context and will be available to the public after some grace period of a few months after the first publication of our collaboration using these configurations. Such procedure will guarantee the best use of these very costly configurations, giving chance for the exploration of an even broader range of physical observables than the one addressed by our collaboration.

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