QCD Simulations with Light, Strange and Charm dynamical Quark Flavors: Continuum QCD results at light quark masses

Application for Computing Time on the Blue Gene/P, IBM-P690 and apeNEXT Parallel Machines at the John von Neumann-Institute for Computing

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1 Problem description

This project proposal is submitted in the name of the European Twisted Mass Collaboration (ETMC) which comprises 16 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 Hamburg and Zeuthen,
- Great Britain: Univ. of Glasgow and Univ. of Liverpool,
- Italy Univ. of Rome I, II and III, ECT* Trento,
- Netherlands: Univ. of Groningen,
- Poland, Univ. of Poznan,
- Spain: Univ. of Valencia,
- Switzerland: Univ. of Bern.

This collaboration brings together a large amount of different expertise, ranging from code optimization and algorithm development, theoretical aspects and chiral perturbation theory calculations to physical applications that are directly relevant for ongoing experiments and phenomenological analyses. To list the already published results, we mention here our first account of meson physics [1], the calculations of the nucleon and Δ masses [2, 3], moments of parton distribution functions [4], non-perturbatively obtained renormalisation constants using the RI-MOM scheme [5], light quark masses and decay constants [6, 7], charm physics [8], meson form factors [9], exploration of the ϵ-regime of chiral perturbation theory [10], study of cut-off effects at tree-level of perturbation theory [11] and non-perturbatively [12], neutral mesons [13], overlap fermions on twisted mass sea quarks [14, 15] and twisted mass fermions at non-vanishing temperature [16]. Further physics projects such

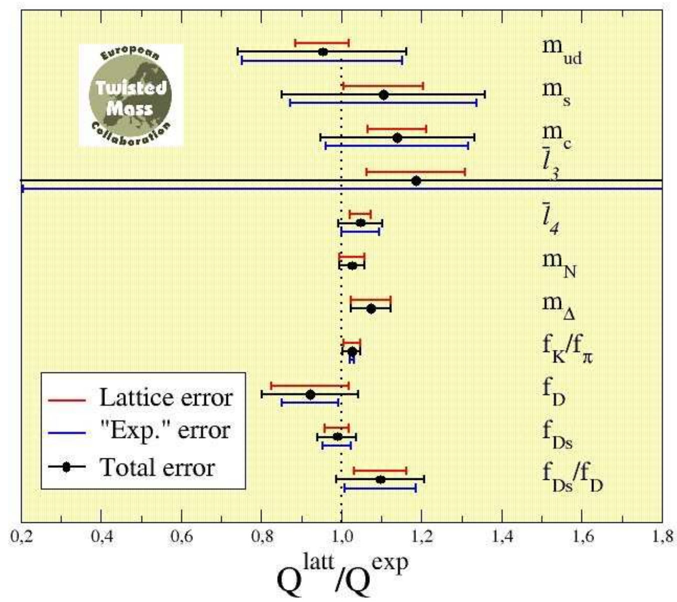


Figure 1: A selection of physics results obtained from twisted mass fermion simulations for $N_f = 2$ flavours of mass-degenerate quarks by the ETMC. We show our lattice results in comparison to experimental measurements.

as the computation of meson and nucleon scatterings lengths, topological aspects, heavy-light mesons and the vacuum polarization tensor are presently being developed and in progress. We show in fig. 1 a comparison between our lattice results and the corresponding quantity taken from experiment. Note that for a number of quantities the lattice errors are already comparable or even smaller than the experimental ones. We point out that a number of technical details of the simulations, which have been indispensable for reaching our precise results, have been published in [17].

Thus, we think that the ETMC is a very much unique collaboration concerning the plethora of physics results that we can achieve and which covers many aspects of QCD. Furthermore, in our $N_f = 2$ simulations we have proved that the twisted mass formulation of lattice QCD is a sound and successful way of performing non-perturbative computations. In particular, we could show that with this formulation the continuum limit and the extrapolation to the physical point can be obtained in a completely reliable way. We will provide below a number of examples for the success of twisted mass simulations.

ETMC is asking NIC to play the role of the major computer platform for further simulations with maximally twisted mass fermions which will include, for the first time in lattice QCD, dynamical strange and charm quark degrees of freedom.

The major goal of this ETMC project is to repeat the complete $N_f = 2$ physics programme with including the strange and the charm quark dynamically. In particular, we want to obtain these results in the continuum limit. We find it important to also understand the quark mass dependence of the physical quantities we want to address. Aiming at pseudo scalar masses in the range $250 < m_{\rm PS} < 450$MeV we can use chiral perturbation theory as a tool to extrapolate to the physical point, as we have demonstrated in our previous $N_f = 2$ simulations. We ask therefore for a substantial amount of computer time on the BG/P, the IBM-P690 and the apeNEXT systems. We emphasize that more than 50 physicists from all over Europe are participating in the project and rely on the availability of sufficient computer resources.

Twisted Mass Fermions

The Wilson twisted mass fermionic lattice action for two flavours of degenerate quarks reads (in the so called twisted basis [18] and with fermion fields with continuum dimensions)

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

where am_0 is the bare untwisted quark mass and $a\mu_q$ 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 (omitting the kinetic part of the heavy fermions):

$$S_h = \sum_x \bar{\chi}_x \left[i\gamma_5\tau_1\mu_\sigma + \tau_3\mu_\delta \right] \chi_x \ . \tag{2}$$

Physical values of the strange and the charm quark mass can be achieved in this formulation by suitably tuning the parameters μ_σ and μ_δ [19].

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 $U^{1\times2}_{x,\mu,\nu}$

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

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 twisted mass QCD $\mathcal{O}(a)$ improvement can be obtained by tuning Wilson twisted mass fermions to maximal twist. In fact, it was first proved in Ref. [20] 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 [21, 22] 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 a zero expectation value in the continuum. Second, at a 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 equivalent to tuning the so-called PCAC mass to zero, where the PCAC mass is

$$m_{\mathrm{PCAC}} = \frac{\sum_{\mathbf{x}} \langle \partial_0 A_0^a(x) P^a(0)\rangle}{2\sum_{\mathbf{x}} \langle P^a(x) P^a(0)\rangle}\,, \qquad a = 1,2\,. \tag{4}$$

It is very important to realize that this tuning to maximal twist can be done 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) in this case automatic $\mathcal{O}(a)$ improvement is obtained by tuning only one parameter, the bare untwisted quark mass, while avoiding additional tuning of operator-specific improvement-coefficients; (ii) the mixing pattern in the renormalisation process can be significantly 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 [23, 24]. Furthermore, theoretical considerations indicate that these $\mathcal{O}(a^2)$ effects become large *only* for the particular observable of the neutral pion mass [25]. This expectation is confirmed by results from numerical simulations for observables which possibly are affected by flavour breaking effects: all other splittings measured so far are zero within errors.

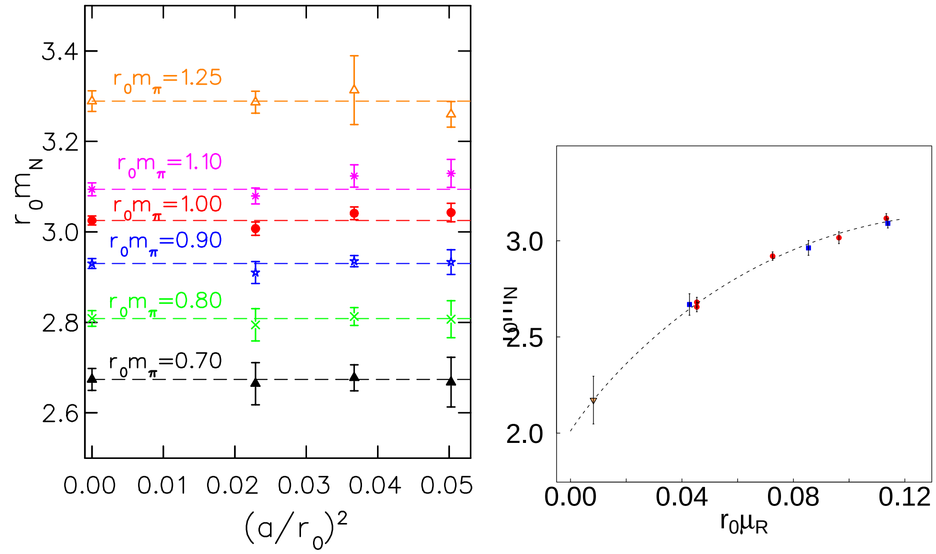
The algorithm we are using is based on a HMC algorithm with mass preconditioning [26, 27] and multiple time scale integration as described in detail in Ref. [28].

1.1 Results from the $N_f = 2$ simulations

In this section we shall present some results from our previous simulations with $N_f = 2$ mass degenerate quark flavours. These results will be the motivation for the $N_f = 2 + 1 + 1$ flavour simulations proposed here and demonstrate the precision that can be obtained using twisted mass fermions.

As a first test of dynamical twisted mass fermions, we analyzed the scaling behaviour in the lattice spacing for various quantities. We show in fig. 2(a) a continuum extrapolation of the nucleon mass at fixed values of the pseudo scalar meson mass. As can be seen, the cut-off effects are only tiny and show basically no lattice artefacts allowing for a controlled continuum limit extrapolation within statistical errors.

Thus we are in a position to compute the quark mass dependence of the nucleon mass *in the continuum* and fit the data to the appropriate expressions from chiral perturbation theory (we refer the reader to ref. [3] for a detailed description). In fig. 2(b) we show a chiral perturbation theory fit to our very precise data for the nucleon mass. We see that the data can be fitted very well. In particular, the extracted value of the nucleon mass at the physical point (which is not included in the fit) is completely consistent with the experimentally measured value. Thus we have here a lattice determination



(a) (b)

Figure 2: We show in (a) the continuum limit of the nucleon mass at various fixed values of the pseudo scalar mass. For the nucleon mass the cut-off effects come out to be tiny and fully compatible with the expected $\mathcal{O}(a)$ improvement. We show in (b) the mass dependence of the nucleon mass together with a chiral perturbation theory fit. The plot includes results from two values of the lattice spacing (circles $a \sim 0.07$ fm, squares $a \sim 0.09$ fm. We emphasize that the nucleon mass as extrapolated to the physical point (denoted by the downward triangle) is *not* included in the fit.

of the nucleon *at the physical point* and in the continuum limit providing thus a real first principles calculation of the nucleon mass in lattice QCD with two dynamical quark flavours.

The very good scaling behaviour of the nucleon mass is confirmed by results in the meson sector. We show in fig. 3(a) the quality of the continuum extrapolation of our lattice results for $f_{\rm PS}$ evaluated at fixed $r_0 m_{\rm PS}$. Clearly, the cut-off effects are not only compatible with the anticipated $\mathcal{O}(a)$-improvement, but even the higher order cut-off effects seem to be tiny again. These findings suggest that using continuum fit formulae from chiral perturbation theory is justified. Indeed, we find that when including lattice artefacts in the chiral perturbation theory fit formulae, the corresponding fit coefficients are compatible with zero.

We fit therefore the appropriate ($N_f = 2$) χPT formulae [29, 30]

$$m_{\rm PS}^2(L) = 2B_0\mu \left[1 + \frac{1}{2}\xi\tilde{g}_1(\lambda)\right]^2 \left[1 + \xi \log(2B_0\mu/\Lambda_3^2)\right] , \qquad (5)$$

$$f_{\rm PS}(L) = F \left[1 - 2\xi\tilde{g}_1(\lambda)\right] \left[1 - 2\xi \log(2B_0\mu/\Lambda_4^2)\right] , \qquad (6)$$

to our raw data for $m_{\rm PS}$ and $f_{\rm PS}$ simultaneously. Here

$$\xi = 2B_0\mu/(4\pi F)^2 , \qquad \lambda = \sqrt{2B_0\mu L^2} . \qquad (7)$$

The finite size correction function $\tilde{g}_1(\lambda)$ was first computed by Gasser and Leutwyler in Ref. [29] and has been extended in Ref. [30] from which we take our notation (except that our normalisation of f_π is 130.7 MeV). In Eqs. (5) and (6) NNLO χPT corrections are assumed to be negligible. The formulae above depend on four unknown parameters, B_0, F, Λ_3 and Λ_4, which will be determined by the fit. For our two smallest masses we found the effect of finite size corrections to be 0.5% and 0.2% for the pseudo scalar mass and 2.2% and 0.9% for the pseudo scalar decay constant, respectively. For our larger masses the finite size corrections are negligible.

For our lightest four μ-values, we find an excellent fit to our data on $f_{\rm PS}$, see fig. 3(b). A similarly good fit can also be obtained for the pseudo scalar mass, see refs. [1, 31]. The fitted values of the four parameters are

$$\begin{aligned} 2aB_0 &= 4.99(6) , \\ aF &= 0.0534(6) , \\ \log(a^2\Lambda_3^2) &= -1.93(10) , \\ \log(a^2\Lambda_4^2) &= -1.06(4) . \end{aligned} \qquad (8)$$

Our results for the low energy constants compare nicely to other determinations (for a review see Ref. [32]) but gives these low energy constants with a very high (presumably world record) precision.

From the above results, we were able to extract the scalar and tensor scattering lengths of the pion using Roy equations

$$a_{00} = 0.220 \pm 0.002 \qquad (9)$$

$$a_{20} = -0.0449 \pm 0.0003 . \qquad (10)$$

To the best of our knowledge, these are so far the most precise determinations of a_{00} and a_{20} from lattice computations. From these values, also the pion radius can be estimated [33],

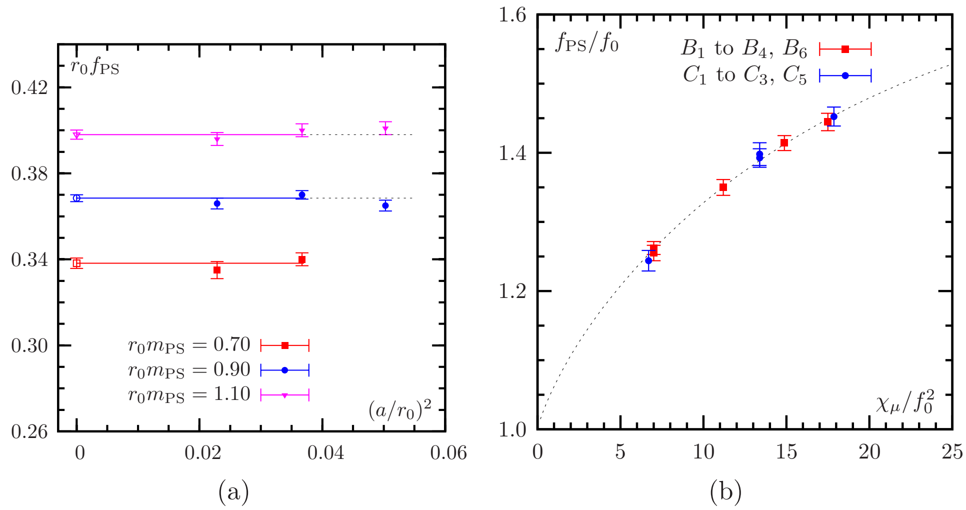


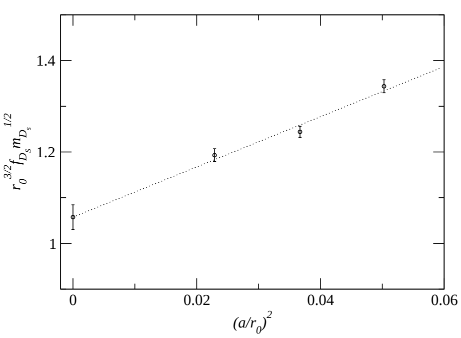
Figure 3: In (a) we show $r_0 f_{\rm PS}$ as a function of $(a/r_0)^2$. The graph demonstrates the smallness of lattice artefacts which turn out to be negligible. In (b) we show a chiral perturbation theory fit of $f_{\rm PS}/f_0$ to the chiral perturbation theory formula of eq. (6) which provides an excellent description of the data.

$$< r^2 >= 0.637(26) \mathrm{fm}^2 \tag{11}$$

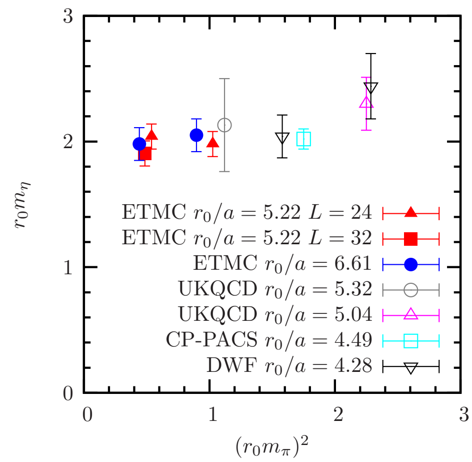
which compares again nicely with estimates from chiral perturbation theory by Colangelo, Gasser and Leutwyler: $< r^2 >= 0.61(4) \mathrm{fm}^2$.

In fig. 4(a) we show as an example of our charm physics results the quantity $f_{D_s}\sqrt{m_{D_s}}$ as a function of the lattice spacing squared. The nice linear behaviour in a^2 demonstrates again the $\mathcal{O}(a^2)$ improvement. As another quantity we consider in fig. 4(b) the masses of the η_2 particle which is the analogue of the η' particle in the case of $N_f = 2$. We compare our results to other data that are available in the literature. As can be seen, with twisted mass fermions we are able to obtain this notably difficult to compute quantity with a very good precision. Furthermore, with twisted mass fermions we can compute the mass of the η_2 at much smaller quark masses than has been done with other lattice QCD formulations, see ref. [34] for details.

As mentioned in the introduction, the ETMC is computing many more physical observables on the configurations obtained with $N_f = 2$ quark flavours and the results presented here are just a selection of those.



(a)



(b)

Figure 4: In the left graph we show the continuum limit behaviour of $f_{D_s}\sqrt{m_{D_s}}$. We observe a nice linear scaling in a^2 demonstrating the $\mathcal{O}(a)$ improvement. The right graph shows the analogue of the η' mass for $N_f = 2$ quark flavours. We also compare to other determinations demonstrating that with twisted mass fermions substantially smaller quark masses can be reached.

In summary, we believe that therefore the $N_f = 2$ simulations with maximally twisted mass Wilson fermions have been very successful.

- The ETMC has demonstrated that lattice artefacts are very small with twisted mass fermions at maximal twist.
- With this approach very precise results can be obtained at pseudo scalar masses of 300MeV and even below as presently ongoing and so far unpublished simulations show.
- Thus with maximally twisted mass fermions, a controlled continuum limit can be obtained and the mass dependence of physical quantities can be determined. Having small quark masses available, chiral perturbation theory turns out to be a reliable tool to perform extrapolations to the physical point.

Proposed project

On the basis of the success in the two-flavor case described above in detail, we have been motivated to extend the lattice twisted mass simulation program to the physically realistic case of also including the strange (s) and charm (c) dynamical quark flavours. We use a formulation as described in ref. [35]. This setup has been already tested by us in ref. [19], where the feasibility of such simulation was clearly demonstrated.

We have started already dynamical simulations with dynamical up, down, strange and charm quarks with the purpose of tuning parameters of our action. This part of the work is more demanding from the computational point of view than in the two-flavor theory, since it also requires the tuning of two additional parameters related to the s and c quark masses. We have successfully completed all these non-trivial tuning by now. At present, for a value of the twisted quark mass corresponding to a pion mass $M_{\rm PS} \simeq 300$ MeV, we have achieved the following goals: we have found a suitable formulation in the gauge sector, the Iwasaki action widely applied for large-scale simulations by the Japanese lattice collaborations; the β-value corresponding to a lattice spacing of $a \approx 0.09$ fm; the critical untwisted quark mass which is necessary to obtain automatic $\mathcal{O}(a)$-improvement; the values of the parameters in the s-c split-doublet ensuring reproduction of the expected hierarchy in the hadron spectrum. We show in fig. 5 the results of the tuning to maximal

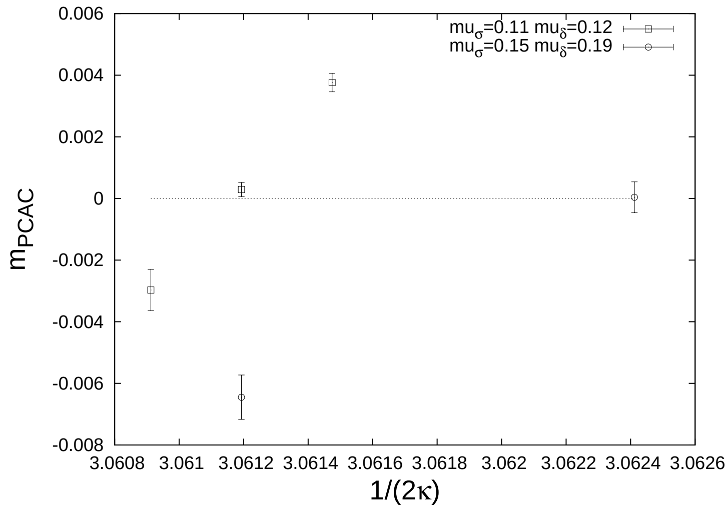


Figure 5: We show the PCAC quark mass $am_{\rm PCAC}$ as a function of $1/2\kappa$ for two different mass splittings in the heavy (s,c) doublet, $a\mu_\sigma = 0.11, a\mu_\delta = 0.12$ and $a\mu_\sigma = 0.15, a\mu_\delta = 0.19$, respectively. The figure demonstrates that we have successfully tuned the theory to maximal twist at two values of the mass splitting. We remark that the larger splitting with $a\mu_\sigma = 0.15$ and $a\mu_\delta = 0.19$ corresponds to physical values of the strange and charm quark masses.

twist as we have obtained so far. Note that despite the fact that $a\mu_\delta = 0.19$ is larger than $a\mu_\sigma = 0.15$ the renormalized quark masses are still positive, since at maximal twist $m_{s,c} \sim \mu_\sigma \mp Z_P/Z_S\mu_\delta$ and the ratio of renormalization constants comes out to be $Z_P/Z_S \approx 0.65$.

We also stress that we have two completely independent and optimized simulation programs to cross-check results. One of these programs has been adapted to the BG/P and we perform already simulations there. The efficiency of the code comes out to be about 20% and we also see a good scaling behaviour of the code with the number of processors. Thus, we think that our code is suitable to perform large scale simulations on the BG/P.

We also want to emphasize that for certain analysis questions other machines are more appropriate. In particular, all our codes to determine the renormalization 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 renormalization 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 quantities as the Isgur-Wise function, and the scalar form factor 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 IBM Regatta machine is most useful.

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

Since now, in addition to the light u and d flavours, also the strange and charm quarks are taken into account, this will provide for the first time lattice QCD simulations in real physical conditions.

Simulations

The goal of the simulations is the generation of configurations at 3 values of the lattice spacing and 5 values of the quark mass at each value of the lattice spacing. The linear extent of our lattices of size $L^3 \cdot T$, with $T = 2L$, will be $L > 2.4$ fm in order to suppress finite size effects. In particular, the simulations should be performed at

- 5 pseudo scalar masses corresponding to a range of $250 < m_{\mathrm{PS}} < 450$ MeV
- 3 lattice spacings covering $0.05\mathrm{fm} < a < 0.1\mathrm{fm}$
- lattice size $L^3 \cdot T$ with $T = 2L$ and $L > 2.4\mathrm{fm}$

Physics program

We list below our physics targets which are to be obtained *in the continuum limit* and *at the physical point* for which we want to use chiral perturbation theory as an extrapolation tool.

- 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, the Isgur-Wise function 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 for the pion and the nucleon as relevant for deep inelastic scattering experiments
- 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 and other unstable particles in QCD
- the vacuum polarization 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 polarization tensor can be directly compared to corresponding results from perturbation theory.
- neutral mesons, which will provide most interesting information on the η' particle
- various disconnected diagrams relevant for e.g. the vacuum polarization tensor mentioned above, the nucleon sigma term, the scattering phase shifts and many other quantities
- topological susceptibility, which is a quantity of its own interest 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 itself 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.

We emphasize that the techniques and programmes for the broad physics spectrum detailed above are fully developed and the projects can directly be started once the configurations are available.

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-P690 and IBM Blue Gene/P. The apeNEXT code for computing propagators is highly optimized and we reach around 40% efficiency of peak performance. For the Blue Gene/P code we achieve an efficiency of about 20%. A similar performance figure of about 12% we reach for the IBM Regatta system. The parallelization strategy is in general domain decomposition with using MPI for the IBM-P690 and IBM-Blue Gene/P machines while for apeNEXT we use the direct remote memory access feature. We remark that already now we are using all three machines such that we could obtain reliable performance figures. We also demonstrated that on the IBM-P690 our problem is scalable up to 128 nodes. On the massively parallel apeNEXT and Blue Gene/P machines the problem is scalable to even larger number of nodes, up to 32768 processors (8 racks) without big performance losses.

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 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. [17] for a detailed description of our techniques which were partly newly developed for the case of twisted mass fermions.

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 about 200 configurations per day on the $24^3 \cdot 48$, about 80 configurations on the $32^3 \cdot 64$ lattices and 15 configurations on a $48^3 \cdot 96$ lattice. Given these numbers, we estimate the computer resources detailed here for the next computer time allocation. The project consists of two parts.

$N_f = 2 + 1 + 1$ continuum physics

We aim at continuum results at the physical point. Our method will be to use chiral perturbation theory to extrapolate to the value of the pseudo scalar mass of $m_\pi = 140$MeV. We have demonstrated that this can be achieved when precise data at 5 quark masses corresponding to a range of $250 < m_{\mathrm{PS}} < 450$ MeV are available. Given the proved smallness of lattice artefacts with the maximally twisted mass fermion action, a reliable continuum limit can be achieved by having 3 values of the lattice spacing covering $0.05\text{fm} < a < 0.1\text{fm}$. Finite size effects can be controlled, as we also have shown, by using volumes with linear spatial extension of $L > 2.4$fm. The time extent should be twice the spatial extent in order to be able to extract physical observables in a reliable way. Thus, we are aiming at 15 simulation points.

Analysis

As discussed above, 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 Jump 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 a large memory. We are thinking here in particular at all kind of 3-point functions. We consider therefore the IBM-Regatta at NIC as an ideally suited machine for this purpose. We estimate that we need 5 nodes of the Jump machine in order to perform the memory intensive computation of the various physical quantities we are aiming at.

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

6 rack years of the Blue Gene/P machine

- $a = 0.100$ fm, 5 quark masses, $24^3 \cdot 48$ lattice: 4 rack months
- $a = 0.075$ fm, 5 quark masses, $32^3 \cdot 64$ lattice: 10 rack months
- $a = 0.050$ fm, 5 quark masses, $48^3 \cdot 96$ lattice: 54 rack months
- total time for inversions: 4 rack months

apeNEXT machine

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

5 computing node years of the IBM-P690 machine.

- 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 IBM-P690 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 successful. We have searched and established a large European collaboration (ETMC) in which all three universities of Rome, the universities of Glasgow, Liverpool, Valencia, Paris Sud, Groningen, Cyprus, Bern, Münster 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 emphasized above the machines at NIC in Jülich are crucial to provide the configurations on which the whole ETM collaboration relies. We strengthen also 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 doing high performance simulation in lattice QCD have been already integrated into this project, who would have otherwise separately applied for computing time. We stress 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 a broader range of physical observables than the one addressed by our collaboration.

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