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Research of a Research Group: The Case of the Elementary Particle Physics Group at NIC

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We give a short overview of the activities of the NIC research group elementary particle physics. We then concentrate on two conceptual advances in lattice field theory, the improvement of discretization errors and the usage of finite size effects. An example, structure functions on the lattice, will serve to demonstrate how these concepts work in practical applications. We finally report about the status of the APE machines and the planned installations.

1 Introduction

Elementary particle physics covers a broad range of phenomena like spontaneous symmetry breaking, dynamical mass generation, confinement, asymptotic freedom and phase transitions to name only a few. The physics of these phenomena is often of inherent non-perturbative nature. In such cases the approach of *lattice field theory* can help to understand physical phenomena better and test model predictions. In the lattice approach our usual space-time is made discrete and a non-vanishing value of a lattice spacing a is introduced. In this way physics problems can be made understandable in form of a program code to a computer. This allows for first principle calculations of physical observables having as only input a theoretical model. Of course, the discreteness of the space-time structure is only an approximation to the real world and eventually this systematic error has to be removed through a well-controlled continuum limit where the lattice spacing a is sent to zero.

Lattice field theory has reached a quite mature stage. Many areas of physics are addressed by this approach ranging from 2-dimensional spin systems, the standard model of elementary particle interactions and even investigations of quantum gravity (see the proceedings of the annual lattice symposia[1]). Still, the main activity of the lattice physicists community is the understanding of quantum chromodynamics (QCD), i.e. our model for the strong interactions. This is also reflected in the activities of the NIC research group elementary particle physics where various aspects of QCD are investigated. Topics are

- determination of fundamental parameters of QCD like the coupling strength and quark masses[2,3]
- the recent development of chiral invariant formulations of QCD[4–7]
- structure functions and hadron spectrum of QCD[8,9]
- confinement, monopoles and topology[10]
- high precision studies of lower dimensional spin models[11]

- finite temperature phase transitions[12]

- improvement of algorithms for dynamical quark[13] and chiral invariant fermion simulation[14]

- participation in the array processor experiment (APE), leading to the development of APE computers that are dedicated to QCD applications[15]

It is clear that in this contribution not all the above topics can be covered. I will rather concentrate on a particular example that demonstrates how two new concepts in lattice field theory are incorporated in practical applications. I refer to a few contributions to this symposium where also other topics of the above list are addressed[4,16–18]. Besides the author himself, at the time of this write-up the team that works in the NIC research group on the topics above consist of *S. Capitani* (Postdoc), *T. Chiarappa* (Ph.D. student), *M. Hasenbusch* (Postdoc), *C. Hoelbling* (Postdoc), *R. Horsley* (Postdoc), *T. Kovacs* (EU fellow) *D. Pleiter* (Postdoc), *G. Schierholz* (permanent member), *C. Urbach* (Diploma student) and *I. Wetzorke* (Postdoc).

2 Scary Animals on the Lattice

When working in lattice field theory, two rather scary animals are met: the first is the non-vanishing lattice spacing, the second is the finite volume. If we keep the physical size of the box fixed, say $L = 1\mathrm{fm}$, corresponding to the diameter of the proton, then this physical length is realized by putting N points for a given value of the lattice spacing a such that $L = N \cdot a$. If we start with $a = 0.1\mathrm{fm}$, we would have $N = 10$. Now, if we want to reach the continuum limit, the value of a has to be decreased while L is to be kept fixed. Hence, for $a = 0.01\mathrm{fm}$ we would need $N = 100$, for $a = 0.001\mathrm{fm}$, $N = 1000$ and so on. Since we are working in four space-time dimensions, the number of lattice points to be kept in the computer grows like N^4 in this so-called "naive" continuum limit. Clearly, one runs easily out of computer resources, with respect to available computer power as well as memory.

What is to do? The idea of keeping the value of the lattice spacing finite is not a very good one: severe artifacts of the non-vanishing lattice spacing are detected leading to systematic errors in physical observables that are difficult to control. Also, keeping the physical length smaller than 1fm gives rise to large finite size effects inducing again systematic errors that are hard to control. We seem to end up with a real dilemma forcing us to go the brute force way and just increase the number of lattice points while decreasing a.

However, modern conceptual advances have paved the way to partly circumvent these problems. We nowadays have the tool of the *improvement programme* to at least diminish the effects of a non-vanishing lattice spacing. In addition, we have learnt to actually make use of finite size effects to extract physical information of the infinitely large system. For an example see[4]. In the following we will discuss these concepts a little more detailed (more extended reviews can be found in[19,20]).

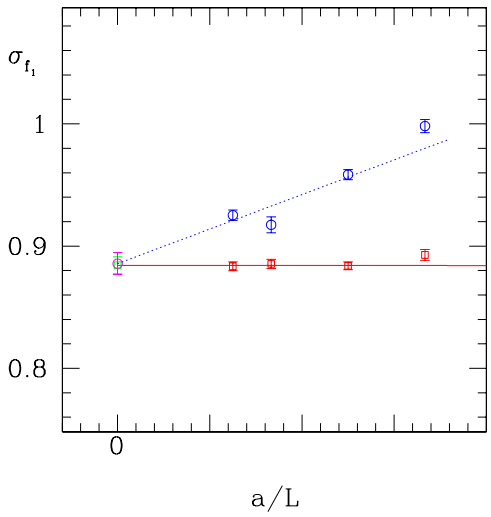

Figure 1. The continuum limit of a step scaling function.

3 Improvement Programme

When physical observables are computed in lattice QCD it is noticed that the dependence of these observables may depend rather strongly on the lattice spacing[22], rendering any continuum extrapolation difficult and costly. The reason for this problem is seen directly from the action of lattice QCD. The standard form is

$$S_{\text{old}} = \underbrace{S_{\text{G}}}_{\text{O}(a^2)} + \underbrace{S_{\text{wilson}}}_{\text{O}(a)} \tag{1}$$

where S_{G} is the pure gluonic part of the action while S_{wilson} is the fermionic part. As indicated in eq. (1), in contrast to the pure gluonic part of the action, the fermions induce a linear dependence on the lattice spacing, resulting in sizable lattice artifacts that are problematic to extrapolate away.

A (part) solution is to add new terms to the action. If all possible symmetries on the lattice and the equations of motion are used, it is found that there is only one more term that can appear at $\text{O}(a)$[21]. The action then reads

$$S_{\text{sw}} = a^5 \sum_x c_{\text{sw}} \bar{\Psi}(x) \frac{i}{4} \hat{F}_{\mu\nu}(x) \Psi(x) \ . \tag{2}$$

The particular form of the new term is not of interest here. What is important, however, is the fact that the parameter c_{sw} is freely tunable. In particular, c_{sw} can be tuned such that the additional term in eq. (2) exactly cancels the $\text{O}(a)$ effects from the original action, eq. (1), thus leaving only errors of $\text{O}(a^2)$ behind.

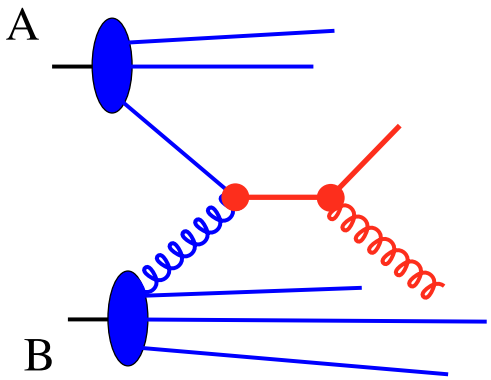

Figure 2. A typical collision of two hadrons.

Figure 1 shows, how this procedure works in practice. A particular physical observable (a step scaling function, see next section) is shown whose physics interpretation is not of importance here. We only remark that first of all this quantity has a well defined continuum limit. Second, we see that the evaluation with the standard fermion action, eq. (1) (dashed line), leads to large lattice artifacts while the use of the improved action (solid line), eq. (2), seems to eliminate these artifacts almost completely. In this way, an acceleration to the continuum limit is achieved and the systematic errors coming from discretization errors are much better controlled.

4 Finite Size Effects and Structure Functions

Let us now come to the second dangerous animal on the lattice, finite size effects. While in the case of discretization errors we could only achieve an improvement in reaching the continuum limit, the situation with finite size effects is completely different: here we "turn around the table" and instead of trying to eliminate finite size effects, we are actually going to use them to extract physical information.

To illustrate this, we will discuss the important field of structure functions. Let us consider a typical particle collision as performed at large accelerators, e.g. at DESY, see figure 2.

Here a hadron A hits a hadron B, a jet is formed and some remnants are left over. We denote by x_{A} a fraction of the momentum of hadron A (and similar of the hadron B). Now, what we want to know is the internal structure of the hadron which is believed to consist of quarks and gluons. Our aim is to know the probability $f_a(x_{\mathrm{A}})$ to find a quark a in the hadron that carries a momentum fraction x_{A} of the hadron A. Similarly, we can ask for the probability function of the quark b and, of course, of the gluons. The complete knowledge of the probability functions $f(x)$ –also called *structure functions*– would give us the desired information about all the internal constituents of the hadron.

Unfortunately, the structure functions are very complicated to compute on the lattice.

However, in experiment, not only the structure functions themselves but also their moments can be determined. The nth moment is defined by

$$M_a^{(n)} = \int_0^1 dx x^{n-1} f_a(x) \ \ , n = 1, 2, \cdots \ . \tag{3}$$

For example, the 2nd moment corresponds to the average momentum $\langle x \rangle$ that is carried by the quark. Knowing all the moments, the complete structure function maybe reconstructed. In practice, it is presumably only possible to compute a few moments on the lattice. Estimates indicate, however, that even with $n \leq 3$ a rather good approximation of the full structure function can be achieved[24]. The advantage of considering moments of structure functions is that these are related to local operators that can be computed with lattice techniques using standard methods[8].

The scattering process of figure 2 is a quantum process. This means that the simple picture of figure 2 is not what actually occurs in nature. Rather, many quantum fluctuations disturb the picture and a steady generation and annihilation of virtual quark-antiquark pairs and gluons take place. This leads to the phenomenon that the moments depend on the energy scale μ at which the collision process is observed since the probability of generating virtual quarks and gluons depends on the energy. Therefore,

$$M_a^{(n)} = M_a^{(n)}(\mu) \ . \tag{4}$$

In quantum field theory we speak of a *scale dependent renormalization* of the moment.

In practice this means that we have to evaluate a moment not as a single number but as a function of the energy scale μ. The energies we have to consider reach from the inverse W-mass to the confinement scale, while at the same time we should eliminate the discretization and the finite volume errors:

$$a \ll \underbrace{0.001\mathrm{fm}}_{1/\mathrm{M_W}} - \underbrace{1\mathrm{fm}}_{\mathrm{conf.scale}} \ll L \ . \tag{5}$$

Clearly, covering all the distances of eq. (5) in a single lattice would lead to a totally unrealistic number of lattice points.

The way out of this problem comes in two steps. In the first step we identify the scale with the inverse box length, $\mu = 1/L$, thus using the finite box length as a probe for the physics taking place at this scale. In the second step, we break the problem into many smaller steps each of which can be evaluated with moderate computer resources.

Let us be a bit more concrete and focus on the expectation value of the average momentum, $\langle x \rangle(\mu_0)$, assuming that we know this expectation value at a certain energy scale μ_0. This scale will be chosen such that $\langle x \rangle(\mu_0)$ is easily accessible for lattice computations. Then the expectation value at a different scale μ is obtained by applying the so-called step scaling function $\sigma(\mu/\mu_0)$, i.e.

$$\langle x \rangle(\mu) = \sigma(\mu/\mu_0) \cdot \langle x \rangle(\mu_0) \ . \tag{6}$$

The step scaling function describes the full scale evolution of the a scale dependent quantity of interest. Note that different observables need a different step scaling function. A very important property of the step scaling function is that it can be split into several steps. Identifying the scale $\mu = 1/L$, this means that (choosing steps of size 2)

$$\sigma(L_0/L) = \sigma(2L_0/L_0) \cdot \sigma(4L_0/2L_0) \cdot \ldots \cdot \sigma(2L/L) \ . \tag{7}$$

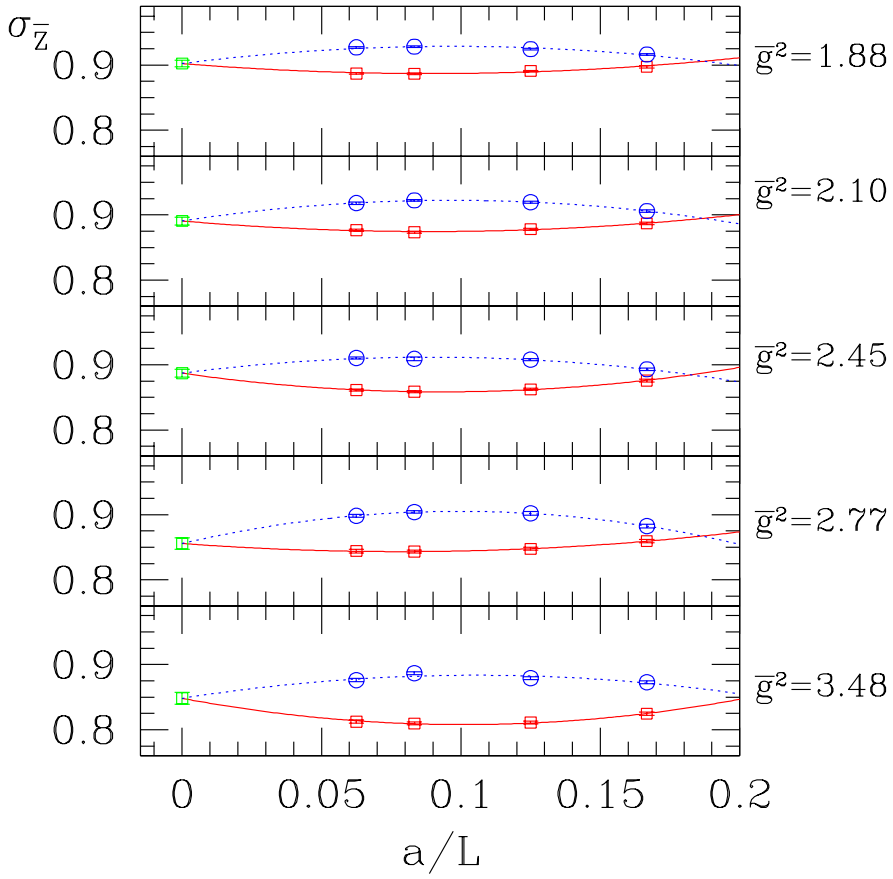

Figure 3. The continuum limit of the lattice step scaling function for two ways of discretizing fermions on the lattice.

The aim in the end is to have the step scaling function, eq.(7), and the running of $\langle x \rangle(\mu)$ non-perturbatively. It is exactly at this point that we depart from our continuous space-time structure and introduce a discrete lattice with non-vanishing lattice spacing a allowing us to resort to numerical simulations. Of course, in the end the discretization error has to be removed in a well-controlled continuum limit. As an important side remark we note that $\sigma(2L/L)$ has indeed a well-defined continuum limit such that the whole procedure makes sense.

On the lattice we introduce the lattice step scaling function

$$\Sigma(a) = \sigma(2L/L, a) \; . \tag{8}$$

$\Sigma(a)$ is the quantity that we want to (and can) compute with lattice methods. The contin-

uum step scaling function is then reached through

$$\sigma = \lim_{a\to 0} \Sigma(a)\Big|_{\mu^{-1}=L \text{ fixed}} \quad . \tag{9}$$

An important remark is that in the $a \to 0$ limit the physical scale L is kept fixed. This can be achieved by fixing the value of the renormalized gauge coupling $\bar{g}$.

We show in figure 3 the approach to the continuum limit of $\Sigma(a)$, eq.(8), for two ways of discretizing fermions on the lattice, once with standard fermions (dashed lines) using the action of eq.(1) and the non-perturbatively improved action (full lines) of eq. (2). It is reassuring that both Σ's extrapolate to the same continuum step scaling function showing the universality of the continuum limit. The individual graphs are obtained at fixed values of the running coupling $\bar{g}$ corresponding to a fixed scale $1/L$.

Figure 3 demonstrates that the approach to the continuum limit of the lattice step scaling function is well controlled. At this point we then have the behaviour of the non-perturbatively evaluated step scaling function *in the continuum* and can safely forget that we ever worked on the lattice. In a very similar fashion, also matrix elements themselves, like $\langle x \rangle(\mu_0)$ can be computed at a reference scale μ_0 in the continuum limit (see ref.[8]). What we have achieved then are results in the continuum theory from fully non-perturbative calculations – which is nothing else but the goal of lattice calculations. The price we have to pay for such a result is –besides having to use powerful computers– that we end up with statistical errors and not with an analytical prediction. But, with increasing computer power these errors can eventually be rendered as small as required by the precision of the experimental data.

Let us discuss shortly, the result of the above described computation for the average momentum in a pion at a scale of $\mu = 2.4\text{GeV}$. One result that is interesting for lattice physicists is that there can be rather large discretization errors. Changing the lattice spacing from about $a = 0.1\text{fm}$ to zero, we find

$$\langle x \rangle(a = 0.093\text{fm}) = 0.30 \to \langle x \rangle(a = 0) = 0.20 \; . \tag{10}$$

This means that discretization errors can lead to about 50% systematic errors and demonstrates that a controlled continuum limit is mandatory. Another result that is interesting for the theoretical physicist is that the effects of a non-perturbative renormalization procedure can be at the order of 10% to 15% as compared to perturbative results.

Finally, the result that interests everybody is the comparison to experiment:

$$\begin{aligned} \langle x \rangle^{\text{experiment}}(\mu = 2.4\text{GeV}) &= 0.23(2) \\ \langle x \rangle^{\text{quenched}}_{\overline{\text{MS}}}(\mu = 2.4\text{GeV}) &= 0.30(3) \; . \end{aligned} \tag{11}$$

We indicated in eq. (11) that the theoretical values are obtained in the commonly used $\overline{\text{MS}}$ scheme and in the quenched approximation, where the internal generation of (virtual) quarks inside the hadron is neglected. The still somewhat large error of both the experimental and the theoretical results saves us from really claiming a discrepancy. Of course, we do not have a very safe control about the systematic error of using the quenched approximation and it will be very interesting to repeat the calculation presented here in the full theory with dynamical quarks. As a final comment we mention that the main result of a computation outlined above are *renormalization group invariant* (RGI) quantities. The reason is that RGI quantities can be used directly in other regularization schemes used e.g.

in perturbation theory. We give the definition of the RGI matrixelement and the result from the lattice in appendix A for the interested reader.

5 Machines

Concepts like the improvement of discretization errors or the usage of finite size effects as described above are certainly very important. Nevertheless, without powerful supercomputers such physics projects would not be able to perform. Now, the numerical problem that is in the heart of applications in QCD is fortunately rather simple: roughly –and somewhat over-simplified– speaking one needs mainly complex normal operations, $a + b * c$, and a communication between only nearest neighbours on the lattice. This simple structure makes it possible to design and develop special purpose machines that are highly efficient for lattice QCD calculations.

The NIC research group is involved in these developments, in particular in the APE (Array Processor Experiment) machines. APE computers are custom made and have a long history already with a first machine installed in Italy around 1985. The first machine used in the high energy physics community in Germany was the APE100. This machine appeared to be extremely successful. It is a massively parallel SIMD machine with a fast interconnecting network. APE100 ran very stable in practice and became the workhorse for many groups performing lattice gauge theory simulations.

The APEmille computer is the successor of APE100 and hence already the third generation of APE machines. It is based on a 3-dimensional mesh of nodes connected by a synchronous communication network, linking nearest neighbours of nodes. We give its specification in table 1.

Peak performance	528 MFlops/proc
Clock frequency	66 MHz
FP registers	512 (32-bit)
Data memory	32 MByte/proc
Communication BW	66 MByte/s/direction
I/O BW per master	6 MByte/s
Power consumption	28 W/GFlops
Price	2.5 Euro/MFlops peak

Table 1. *Key parameters of APEmille:*

Power consumption of APEmille systems is very low (less than 30 W/GFlops) and the footprint of a two-crate rack is about $0.7m^2$. For these reasons, APEmille machines are simply air cooled and do not need complex infrastructure.

At present, several APEmille installations exist Europe wide at various places (Rome I,II, DESY/NIC Zeuthen, Pisa, Milano, Bari, Paris Sud, Bielefeld, Swansea and INFN-LNGS). In the near future all planned installations will be finished and an integrated peak performance of about 2 Teraflops will be reached. Typical applications reach an efficiency of 32% - 47% depending on the distribution of the lattice onto the mesh of nodes. The stability of the existing APEmille platforms as is experienced today strongly indicates that

APEmille has the potential to become the workhorse to the lattice physicists in Europe in the next years – as APE100 was in the past.

But, this is not the end of the story. A follow-up machine, apeNEXT is being envisaged and actually already quite far in its developing stage. Major differences to earlier APE machines are that apeNEXT runs in 64-bit precision while its predecessors had only 32-bit words. It is a SPMD machine and runs asynchronously giving new challenges to the APE collaboration. Details of the architecture can be found in[15] where also the present status of apeNEXT is described. The final installations (intended for 2003) will achieve 2-3Tflops for a stand alone system with price/performance ratio of 0.5Euro/Mflop (peak). These parameters will then meet the requirements formulated by an ECFA panel[25] for the performance needs of lattice field theory in the next years.

6 Conclusion

Lattice calculations benefit from

- conceptual theoretical developments like improving discretization errors and using finite size effects,
- improvements of the algorithms employed,
- further and further increase of available computer power as it is provided by centers like NIC, housing commercial supercomputers and custom made machines like APE.

It is the interplay between all these three areas that furthers the precision of lattice field theory computations to a stage where direct contact to experiment will be achieved. If the progress in lattice field theory we have observed in the last years can be maintained in the coming years, lattice field theory will certainly be a major player in analyzing and interpreting experimental data coming from future accelerators. The NIC research group works in all the three areas of theoretical, algorithmic and machine developments and we hope that we can contribute to the ambitious aim mentioned above.

Appendix A

Let us discuss here a theoretical point that is meant to be for the experts. The step scaling function of the main text is –in the perturbative regime– of course nothing else but the Callen-Symanzik function. This allows to define renormalization group invariant quantities if the scale μ is sent to large enough values

$$\langle x \rangle^{\rm ren}_{\rm INV} = O^{\rm ren}_{\rm SF}(\mu) \cdot f^{\rm SF}(\bar{g}^2(\mu)) \tag{12}$$

with

$$f^{\rm SF}(\bar{g}^2(\mu)) = (\bar{g}^2(\mu))^{-\gamma_0/2b_0} \exp\left\{ -\int_0^{\bar{g}(\mu)} dg \left[\frac{\gamma(g)}{\beta(g)} - \frac{\gamma_0}{b_0 g} \right] \right\} \tag{13}$$

where g is the coupling strength, $\gamma(g)$ is the anomalous dimension function, $\beta(g)$ is the β-function and SF stands for the *Schrödinger functional* renormalization scheme[23] that

is particularly suitable for lattice calculations. Now, in perturbative computations in the continuum theory schemes different from the Schrödinger functional one are used. The renomalization group invariant quantities now help to make contact to these schemes used in the continuum theory:

$$\begin{aligned} \langle x \rangle^{\overline{\rm MS}} &= O^{\rm ren}_{\rm INV} / f^{\overline{\rm MS}}(\bar{g}^2(\mu)) \\ \langle x \rangle^{\rm my\ preferred} &= O^{\rm ren}_{\rm INV} / f^{\rm my\ preferred}(\bar{g}^2(\mu)) \end{aligned} \tag{14}$$

where $\overline{\rm MS}$ stands for a standard schme, often used in perturbative calculations and my preferred is self-explanatory. From these considerations it should become clear that the computation of the RGI quantities are the most important ones to come out from the non-perturbative lattice calculations.

For completeness, we will give the value of the RGI matrixelement as obtained form the numerical simulations discussed in the main text, i.e. $O^{\rm ren}_{\rm INV} = 0.222(24)$.

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