WHAT CAN WE LEARN ABOUT QUARKS, GLUONS AND PROTON'S INTERNAL STRUCTURE FROM SUPERCOMPUTER SIMULATIONS?*

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In this paper, I discuss contemporary research on constituents of the nucleon, making up atomic nuclei and giving mass to almost entire visible matter. These constituents, quarks and gluons, interact strongly and this interaction is described by quantum chromodynamics (QCD), one of the pillars of the Standard Model of elementary particles. QCD is much more complicated than *e.g.*, quantum electrodynamics and several aspects can be investigated from first principles only via numerical calculations, by formulating it on a discretized spacetime grid, the lattice. The huge complexity of the problem causes it to require advanced tools and computing power offered by the world's most powerful supercomputers. I discuss how QCD is formulated on the lattice such that it can be tackled on such machines, what we have learned so far and what are the directions of on-going and future research on nucleon structure from the lattice QCD.

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1. Introduction

Quantum chromodynamics (QCD) is the accepted theory of the strong interaction, one of the four fundamental interactions in nature. The strong interaction is responsible for several essential features of the world, most notably for binding nucleons into atomic nuclei and, at an even more fundamental level, for binding quarks and gluons into nucleons and other hadrons. Nucleons, *i.e.*, protons and neutrons, are responsible for over 99% of the mass of the visible Universe and their mass comes almost exclusively from the strong interaction. The masses of quarks sum up to only around 10 MeV out of the approx. 940 MeV rest mass of the nucleon and the remainder of the nucleon mass comes from the dynamical QCD interactions between quarks and gluons.

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QCD is formally similar to the prototype quantum field theory describing the electromagnetic interaction, quantum electrodynamics (QED). They are both gauge field theories, with fundamental fermions interacting via exchange of gauge bosons, gluons or photons, respectively. The crucial difference between QCD and QED, however, comes from the structure of the gauge group, SU(3) *vs.* U(1). The former is non-Abelian and this leads to a crucial new feature of QCD with respect to QED — the self-interaction of gauge bosons. This has far-reaching consequences, in particular, it causes a strong dependence of the interaction coupling on the energy scale, the so-called running. While for QED, the coupling constant, called the fine structure constant, is almost unchanged over several order of magnitudes of energy, $\alpha \approx 1/137$, in QCD the coupling runs from $\alpha_s = \mathcal{O}(0.118)$ at the Z boson mass scale (≈ 91 GeV) up to $\mathcal{O}(1)$ at low energies, of the order of 200–300 MeV. QCD at high energy evinces the celebrated property of asymptotic freedom [1, 2], *i.e.*, the asymptotic weakening of the interaction strength with increasing energy. On the other hand, at low energies, confinement sets in and quarks and gluons are strongly bound together into hadrons. The coupling strength values of QED and QCD have immediate methodological consequences. The smallness of the fine structure constant implies that perturbation theory (PT) is valid for all energy scales relevant to current phenomenology. In turn, PT can work in QCD only at relatively large energies, more than at least 2 GeV. For lower energies, non-perturbative methods are needed. These can take the form of phenomenological models, which have had several successes in describing various features of the strong interaction. However, for a truly first-principle description, there is basically no alternative to the lattice approach. It was first proposed in 1974 by Wilson [3], who showed how to quantize a gauge field theory on a discrete lattice, preserving exactly the gauge invariance.

In the remainder of the paper, I will discuss the lattice formulation of QCD and its features in Sec. 2. In Sec. 3, I will briefly report the recent progress in lattice hadron structure computations, with special attention to computations of the x-dependence of partonic distributions. Section 4 will summarize and shortly discuss future prospects for this field.

2. Lattice QCD (LQCD)

2.1. Generalities of the lattice approach

QCD as a part of the Standard Model is formulated in continuous four-dimensional Minkowski spacetime. In the path integral formalism, observables are expressed as functional integrals over all possible fermionic and gluonic field configurations. To be amenable to numerics, these formally infinite-dimensional integrals need to be regularized and this is achieved by

discretization on a spacetime grid. However, one more step is necessary to perform numerical computations. The Minkowski spacetime integrals are weighted with a highly oscillatory factor $\exp(iS)$, where S is the QCD action. These factors effectively prohibit numerical probing, and the unavoidable remedy is to change the signature of spacetime from Minkowski to Euclidean, by performing the so-called Wick rotation. In this way, the time becomes imaginary and the exponential factor in the path integral takes the form of $\exp(-S)$, formally a Boltzmann factor of a statistical–mechanical system. For a wide class of observables, the Euclidean expectation values coincide with Minkowski ones. However, notable exceptions are quantities involving the real time that become practically inaccessible in the Euclidean LQCD. In particular, this involves observables defined on the light cone, relevant for investigating partonic structure of hadrons. A way of overcoming this limitation will be discussed in the next section.

The key property in Wilson's formulation [3] is that gauge invariance is preserved at a finite lattice spacing. This is achieved by taking the link variables to be SU(3) group-valued, instead of algebra-valued. In this way, there are two types of gauge-invariant objects on the lattice — quark fields connected by a path of gauge links or closed paths of gauge links (Wilson loops). The QCD action is constructed from such gauge-invariant objects and the QCD partition function, as well as any observable, can be expressed as a finite-dimensional path integral and evaluated numerically. The lattice provides regularization both in the ultraviolet (UV) and in the infrared (IR), with UV and IR regulators provided by the finite lattice spacing and the finite volume.

The typical number of lattice sites in an LQCD simulation is 32–128 in each direction. Thus, even though observables evaluated in LQCD are finite-dimensional, having four spacetime directions, the integral has 10^7–10^9 dimensions. Clearly, such an integral can only be evaluated with stochastic methods, in particular variants of Monte Carlo (MC) sampling. In MC methods, one generates a Markov chain of field configurations. In principle, both gluon and fermion fields need to be sampled. However, the former are analytically integrated out, yielding a determinant involving gauge fields. Thus, the MC Markov chain consists of a sequence of gauge fields only. Even so, the configuration space is inaccessibly large and it is essential to only generate gauge fields that are relevant at a given set of simulation parameters. This is called importance sampling and in practice allows to evaluate observables with typically between 100 and 10000 independent field configurations. Over the years, several MC algorithms have been thoroughly investigated from the point of view of their suitability for LQCD. The simplest algorithms, such as the Metropolis algorithm, cannot be effective for LQCD, since they involve only local updates of field variables. The method that is currently

most commonly used in LQCD is the so-called Hybrid Monte Carlo (HMC) algorithm [4]. It combines a molecular dynamics (MD) evolution with a Metropolis accept–reject step. One introduces fictitious momenta conjugate to field variables and constructs a Hamiltonian governing the evolution of the system in MD time. Simulating this evolution requires solving a system of first-order differential equations (Hamilton's equations). To sample the path integral faithfully, one needs to accurately solve these equations. In order to do it with a practically large step size (to make sure that the field configurations are sufficiently far away from each other and can be considered independent), the additional Metropolis step is introduced. The HMC algorithm has been subject to many refinements over the years and also optimized for the different ways one can discretize the continuum fields. It is important to note that MC simulations are restricted to cases where a probability measure can be defined to probe the relevant distribution. Luckily, this is the case for QCD at zero baryon density. In the case of a non-zero chemical potential, this is no longer true. For small baryon densities, there are rather straightforward ways of taming this sign problem, but the problem becomes severe at larger chemical potentials. There are large efforts in the community to find methods that can overcome this issue, for a review see *e.g.*, Ref. [5].

For more details about the lattice formulation of QCD and other gauge theories, we refer to the excellent textbooks [6–8].

2.2. Brief history of LQCD

LQCD simulations are one of the most demanding areas of science in terms of the required computational power. The insufficient computing power was a major hindrance in the early years after Wilson's proposal and it was initially believed that it may take 30–40 years before they become practical. However, already in 1980, Creutz reported first simulations [9], not yet of QCD, but of a simpler SU(2) gauge theory without fermions (so-called pure gauge SU(2) theory). Working with lattices consisting of 4–10 sites in each direction, Creutz managed to show numerical evidence for both confinement and asymptotic freedom in this theory. Soon afterwards, this work was extended to the SU(3) group and with increasing computational power several aspects of QCD could be explored. This was still for the pure gauge theory case, also called the quenched approximation, which amounts to the lack of dynamics of quark–antiquark pairs. This dynamics is encoded in the determinant resulting from analytical integration of the fermion fields and the computing power of the 1980s and 1990s was yet not enough to tackle this determinant. The quenched approximation is uncontrolled, in the sense that it is not possible to reach the unquenched results

without actually simulating the determinant. Nevertheless, it was commonly believed that this approximation is not too severe and amounts to numerical effects of the order of 10% in most observables. This was seen *e.g.*, in the computations of the hadron spectrum that yielded particle masses in reasonable agreement with the ones found experimentally or differing by just a few percent. With further increasing computer power and algorithmic developments, the inclusion of the fermionic determinant was possible towards the end of the 1990s and an era of so-called dynamical simulations began. At first, basically during the entire 2000s decade, dynamical light quarks were included at heavier than physical masses. Since the simulation cost strongly depends on the quark masses, first dynamical simulations included light quarks corresponding to pion masses typically in the range from 300 to 600 MeV. Results at the physical quark masses could then be obtained by an extrapolation in the light-quark mass, guided by chiral perturbation theory [10]. In the next decade, dynamical simulations at physical quark masses were started (at the so-called physical point). This again resulted from the increasing computing power, but a crucial ingredient were also algorithmic improvements. Actually, without these algorithmic improvements, even today physical point simulations would be prohibitively expensive. The algorithms of 2000 s exhibited very bad scaling with decreasing pion mass and the improvement of this scaling was essential.

2.3. Systematic effects in LQCD computations

As of today, LQCD has become a mature field allowing for reliable quantitative investigation of many aspects of QCD. Its main strength is the possibility to control all conceivable systematic effects. We shortly discuss them here point by point.

2.3.1. Discretization of the action and cut-off effects

An obvious systematic effect comes from the fact that simulations are necessarily performed at a non-zero lattice spacing. Thus, lattice results are always subject to discretization effects. Nevertheless, this uncertainty can be fully controlled by performing simulations at a few values of the lattice spacing, preferably at least three. The leading cut-off effects depend on the used discretization of fermionic and gluonic fields. For the latter, three main discretizations are used (Wilson plaquette, tree-level Symanzik improved and Iwasaki actions) and they all exhibit leading cut-off effects at $\mathcal{O}(a^2)$, with practical differences between them being not very large. In the fermionic sector, in turn, several conceptually different discretizations are used. The naive discretization of the covariant derivative leads to the so-called doubling problem — instead of *e.g.*, 2 desired fermion flavors, one

simulates 2^d of them, with d being the dimensionality of spacetime. Thus, it is mandatory to remove the doubler modes. The original way proposed by Wilson [3] consists in adding a second-derivative term to the fermionic action. This so-called Wilson term gives a large mass to the doubler modes, thus quenching their dynamics at a finite lattice spacing and decoupling them altogether in the continuum limit. The price to pay for removing doublers is that the Wilson term, being effectively a mass term, explicitly breaks chiral symmetry. The latter is restored in the continuum limit and in the zero quark mass limit, but at a finite lattice spacing gives rise to leading cut-off effects at $\mathcal{O}(a)$. Two main improvements of Wilson fermions are commonly used. One of them is to add a specific term (clover term) to the fermionic action. This results in the $\mathcal{O}(a)$-improvement of the action, but observables need to be separately improved by adding further improvement coefficients. Another way to improve Wilson fermions is to add the so-called twisted mass term [11]. By tuning just one parameter in the action, one can then obtain automatic $\mathcal{O}(a)$-improvement of physical observables. The twisted mass fermionic action is used by the Extended Twisted Mass Collaboration (ETMC), whose results on the nucleon structure will be shortly discussed in the next section. Both clover and twisted mass fermions explicitly break chiral symmetry by the inclusion of the Wilson term. Ways of preserving chiral symmetry have been proposed [12, 13] and used to some extent, but they are significantly more computer-time expensive. Apart from Wilson-type and overlap fermions, other popular discretizations are Kogut–Susskind (staggered) fermions [14] and domain wall fermions [15]. All of the mentioned fermionic discretizations, apart from unimproved Wilson quarks, exhibit $\mathcal{O}(a^2)$ scaling towards the continuum limit. Given their different advantages and disadvantages, they may be more or less suitable for certain applications, but in general, allow different groups to cross-check one another's results — the results at a finite lattice spacing may differ, but after taking the continuum limit (and eliminating other sources of systematic effects, see below), they should agree, *i.e.*, correspond to the desired continuum theory of QCD. In practice, the continuum extrapolations are performed using 3–5 values of the lattice spacing, ranging from 0.04–0.06 fm to 0.1–0.15 fm. Larger lattice spacings cannot be usually used, since higher-order cut-off effects may become dominating and the extrapolation may become unreliable.

2.3.2. Finite volume effects (FVE)

Lattice simulations are, obviously, also performed in a finite volume. The size of FVE is usually related to the mass of the lightest particle in the spectrum — the pion. The relevant finite size parameter is the product of the pion mass, m_π, and the lattice extent, L, and FVE are exponentially

suppressed by a factor proportional to $\exp(-m_\pi L)$. Thus, they become of $\mathcal{O}(1\%)$ if $m_\pi L \gtrsim 4$. Nevertheless, even if $m_\pi L$ is rather large, it is good practice to explicitly check for the size of FVE by performing computations at 2 or 3 physical lattice extents.

2.3.3. Values of quark masses and the number of active quark flavors

As discussed above, for many years simulations have been performed at non-physical values of the quark masses, in particular of light quarks. In this way, making contact to real-world QCD required an extrapolation to the physical point or to the chiral limit. For many quantities, such an extrapolation could be guided by analytical predictions obtained in the framework of chiral perturbation theory [10]. Still, such an analytical guidance is not possible or reliable for certain observables and thus, it is preferable to avoid the chiral extrapolation by simulating directly at the physical point. Concerning heavier quarks, their influence on the dynamics of the sea is limited. For most observables, the difference of results obtained with only 2 lightest active flavors and with dynamical strange quarks is smaller than the typical statistical and systematic precision. Nevertheless, since inclusion of the strange and charm quarks is technically and computationally not very demanding, it is preferred to include these quarks in the simulations. These heavier quarks are usually taken at their physical mass values.

2.3.4. Isospin breaking

In most LQCD applications, the two lightest quarks are taken as degenerate. This approximation is well-justified if the overall precision of the calculation is much worse than the expected effects of different masses and electric charges of the up and down quarks *e.g.*, $\mathcal{O}(0.2\%)$ for the mass difference between the proton and the neutron. In applications discussed in the next section, where the currently aimed precision is at the few percent level, the light quarks can be safely assumed to be degenerate. However, there exist LQCD computations where the total error becomes of the order of expected isospin breaking effects. Taking them into account is feasible, but highly non-trivial, since the quarks not only need to have different masses, but also electromagnetic corrections resulting from their different electric charges have to be incorporated.

2.3.5. Renormalization

The lattice provides IR and UV regularizations, ensuring finite results are obtained in numerical calculations. However, for several observables, renormalization of bare lattice results is needed. The most common renormalization scheme in phenomenology is the minimal subtraction scheme of

dimensional regularization. Obviously, this scheme cannot be directly used on the lattice, which is limited to an integer number of dimensions. Instead, several non-perturbative renormalization schemes have been proposed for the lattice. The most popular are variants of the regularization-independent momentum subtraction scheme (RI-MOM) [16]. In this momentum-space scheme, one computes amputated vertex functions of the operator that is to be renormalized and comparing them to their tree-level values gives the renormalization factor of the operator. Other non-perturbative schemes that have been used on the lattice are the Schrödinger functional [17] and the coordinate space method [18]. Since it is usually desirable that the final results are given in the $\overline{\text{MS}}$ scheme, a necessary ingredient is the conversion between the intermediate scheme and $\overline{\text{MS}}$. The matching factor can be computed in continuum perturbation theory. Note that this may lead to truncation effects as an additional source of systematics in the final result and that they need to be quantified and controlled.

2.3.6. Other systematic effects

Apart from the effects mentioned above, other ones usually can be named. Naturally, they depend on the quantity of interest and may be significant in some observables and totally negligible in others. Moreover, the influence of systematics depends also on the desired precision — studies aiming at per mille precision need to take into account sources of systematic effects that can be safely ignored in analyses aiming at 10% or 20%. It is worth to emphasize that the key feature of LQCD is that, in principle, all systematics can be controlled. In some cases, this may require spending very large computational resources, which is also usually required to have small statistical errors. However, after this is done, one has the unique opportunity of having an *ab initio* result, a direct first-principle prediction from the QCD Lagrangian.

3. Nucleon structure from LQCD

One of the research areas where LQCD has provided valuable insights is the internal structure of hadrons, in particular of the nucleon. In particular, one of standard LQCD applications have for many years been computations of nucleon charges, electromagnetic form factors, quark momentum fractions and other moments of parton distribution functions (PDFs) and generalized parton distributions (GPDs) [19]. These quantities can also be used to conclude about the decomposition of the nucleon spin into contributions from quark angular momentum, quark spin and gluon angular momentum, see Ref. [20] for a state-of-the-art computation. In general, the lattice calculation of such observables requires the evaluation of the so-

called quark-connected and disconnected diagrams. The latter are much more noisy and require significantly larger computational resources and special techniques. Hence, the best precision is obtained for flavor non-singlet quantities, such as the combination u–d, in which the disconnected contributions cancel for degenerate light quarks. To obtain individual contributions of different quark flavors, computations of disconnected insertions are unavoidable. Nevertheless, there has been much progress in this area recently and reliable extractions are already available.

A relatively new area in lattice hadron structure is to calculate the full x-dependence of PDFs. For many years, it has been considered impossible, since PDFs are defined on the light cone and, as we have mentioned above, LQCD works in Euclidean spacetime that is unable to probe light-cone correlations. In principle, one can compute several moments of PDFs that are given as matrix elements of local operators and reconstruct the PDFs from these moments. However, it is, in practice, impossible to go beyond the third moment. Higher moments suffer from very unfavorable signal-to-noise ratio and moreover, inevitable power-divergent mixings with lower-dimensional operators appear. Thus, the lattice can offer reliable results basically for the lowest 2 moments, which is clearly not enough to reconstruct the full distributions. Proposals how to access the full x-dependence were put up, but not much progress was achieved until the seminal proposal of Ji in 2013 [21] to compute so-called quasi-distributions, in which one probes spatial correlations between boosted nucleon states. Such quasi-distributions can be shown to share the same IR properties as their light-cone counterparts and thus, if the nucleon boost is large enough, can be perturbatively matched to them to account for the difference in the UV region [22]. Ji's proposal has been subject to intense theoretical and numerical studies, see Refs. [23–28] for efforts by the ETMC and Ref. [29] for a broad review of the community efforts for the quasi-distribution approach, as well as alternative approaches to PDFs from the lattice.

As an example of these lattice investigations, we show the PDFs obtained by ETMC in a recent effort [26–28]. Simulations have been performed using twisted mass fermions and Iwasaki gluons on a single ensemble of gauge field configurations with a lattice spacing of $a \approx 0.094$ fm and lattice volume $48^3 \times 96$, with 2 dynamical light quarks of physical masses. Bare matrix elements were obtained for all 3 cases of PDFs (unpolarized, longitudinally polarized (helicity) and transversely polarized (transversity)), for the flavor non-singlet u–d combination. They were subject to non-perturbative renormalization in the RI-MOM scheme and matched to light-cone distributions. The influence of matching is illustrated in the upper left plot of Fig. 1. As can be seen, the quasi-distribution at the nucleon boost of $10\pi/L \approx 1.4$ GeV is yet far away from the typical shape of PDFs. Apart from the matching,

the effect of nucleon mass corrections is also shown that turns out to be negligible at this level of precision. In the upper right plot of Fig. 1, a comparison to selected phenomenological distributions is shown. Likewise, the lower plots illustrate such comparisons for helicity and transversity PDFs. For the polarized PDFs, we observe agreement with the phenomenological determinations for a range of x values. Unpolarized PDFs qualitatively follow the light-cone PDFs, but no quantitative agreement is seen yet. The reason for this is simple to explain according to the discussion of the previous section. Our computation has been performed with only one ensemble of configurations, in particular at a single lattice spacing, and is, hence, subject to systematic effects that are not yet quantified. The good agreement at the qualitative level is promising and is a milestone in lattice computations of PDFs. However, significantly more work is needed to investigate the systematics and large computational resources will be needed for this, *e.g.*, to perform the simulations at finer lattice spacings and extrapolate out cut-off effects. The current work in progress indeed suggests that discretization effects are responsible for a large part of the difference between the lattice-extracted distributions in Fig. 1 and the phenomenological ones. Thus, full

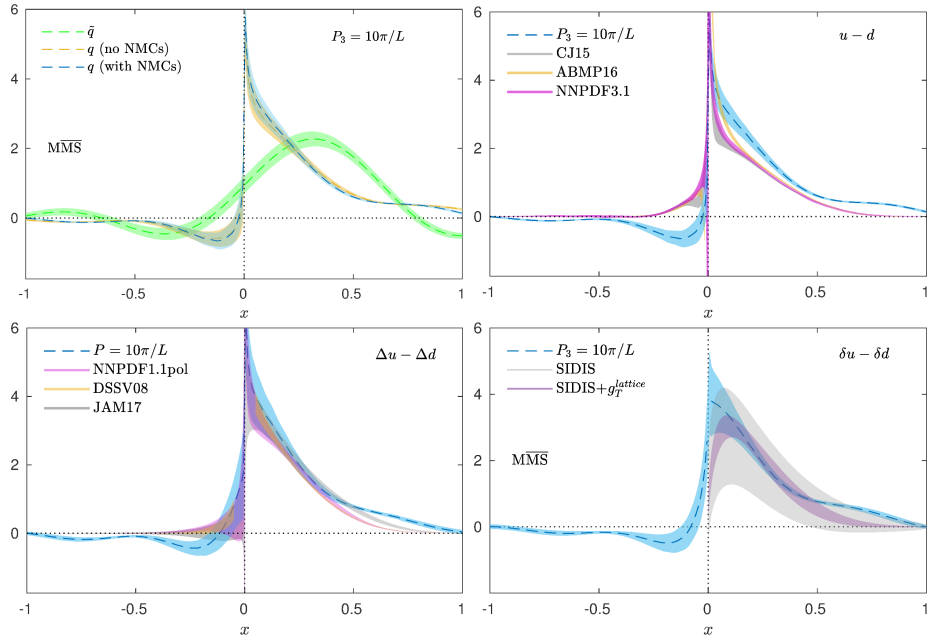

Fig. 1. Upper left: unpolarized quasi-PDF ($\tilde{q}$) and PDF after matching (q) and nucleon mass corrections (NMCs). Upper right: unpolarized PDF from the lattice compared to selected phenomenological distributions. Lower left/right: the same for helicity/transversity PDFs. Source: Ref. [28], article published under the terms of the Creative Commons Attribution 4.0 International license.

quantitative comparisons with phenomenology will only be possible after careful investigation of all sources of systematics that are relevant at this level of precision. It is interesting to note that, as of now, the statistical precision that can be obtained on the lattice for the transversity PDF is much better than the one obtained in global fits. The latter can be improved by including a lattice determination of the tensor charge, as illustrated in the lower right plot of Fig. 1, but it is conceivable that, having fully quantified lattice systematics, the most accurate determinations of transversity PDFs will come in the future from the lattice. In general, it is also plausible that the lattice can help in constraining also the better-known unpolarized and helicity PDFs, at least in some regions of x. For a recent investigation of the possible impact of lattice on PDFs extractions, see Ref. [30]. Apart from computations of PDFs, lattice is starting to extract also the x-dependence of GPDs, see Ref. [31] for first exploratory results for the nucleon. Proposals how to handle transverse momentum-dependent distributions (TMDs) have also been put up. With access to these quantities, prospects for a deeper understanding of nucleon structure in the next years are becoming a reality.

4. Summary

The lattice QCD has achieved enormous progress since the seminal proposal of Wilson more than 45 years ago. The progress can be attributed to a comparable extent to both the huge development of computers and the improvement of simulation algorithms and computational methods. This has led to reliable first-principle investigations of different aspects of QCD. For some of them, LQCD has already entered a precision era, with calculations aiming at per-mille level total uncertainty. However, there are also more difficult computations, such as the ones probing the internal structure of the nucleon. Many of these are still at the exploratory level and new quantities are being calculated, which were not so long ago thought to be practically inaccessible. We have exemplified this thread of research with the recent computation of the x-dependence of PDFs by the ETM Collaboration. Finally, there are some observables where no viable lattice methods exist for QCD, such as quantities at a large baryon chemical potential that encounter the sign problem in MC simulations or real-time dynamics that cannot be accessed in Euclidean spacetime. Thus, the future progress in LQCD will concentrate on increasing precision of on-going computations, but also on looking for further algorithmic improvements and on devising new methods that can help to investigate aspects of QCD not attainable so far. The constantly increasing computing power will help as well.

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