Parton distributions and lattice QCD calculations

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Abstract

The detailed understanding of the internal structure of nucleons is an active research field with important phenomenological implications in high-energy, nuclear and astroparticle physics. There exist two main approaches to determine the parton distribution functions (PDFs) of the proton that quantify how its momentum and spin are divided among its quark and gluon constituents. The first is global QCD analysis, which exploits that fact that hard-scattering cross sections can be factorized into short-distance matrix elements computable in perturbation theory and long-distance dynamics encoded in the PDFs. The second approach is based on the nonperturbative computation of PDFs and their moments from their first-principles operator definitions using lattice QCD. Motivated by the recent progress in these two approaches to determining proton structure, in this white-paper we present a systematic overview of the lattice QCD calculations of PDF-related quantities, as well as a state-of-the-art evaluation from global analysis. Following a review of progress in global QCD fits and lattice-QCD calculations, we present benchmark quantities that can be used to validate present and future lattice-QCD calculations of proton structure. We then we quantify how lattice-QCD calculations could be used to improve unpolarized and polarized global PDF fits, assessing as well the implications of these improvements for collider phenomenology. The ultimate aim of this report is to establish a common language between the two communities to to maximize and foster mutual interactions and cross-talk.

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1 Introduction and Motivation

The detailed understanding of the internal structure of protons is an active research field with important phenomenological implications in a wide variety of fields such as high-energy, nuclear physics and astroparticle physics. There are two main methods to quantify how the momentum and spin of nucleons are divided among its constituents, the quarks and gluons. The first is global QCD analysis, which exploits that fact that hard-scattering cross sections can be factorized into short-distance matrix elements, which can be calculated in perturbation theory, and long-distance dynamics encoded in the so-called parton distribution functions (PDFs). By combining a variety of experimental data on hard-scattering processes with state-of-the-art perturbative calculations by means of a robust statistical methodology, it is possible to achieve a reasonably precise determination of these nonperturbative PDFs for unpolarized and polarized nucleons. In this context, several collaborations provide regular updates of phenomenological PDF determinations, both in the unpolarized [1–6] and in the polarized [7,8] cases.

Alternatively, one can compute quantities related to PDFs directly from QCD using the non-perturbative formulation known as lattice QCD. This method introduces an ultraviolet cutoff and allows the direct computation of the QCD path integral in discretized finite-volume Euclidean spacetime. To connect to experimental observations, a continuum-limit extrapolation is necessary to remove the cutoff dependence. Finite-volume effects can also be removed by suitable extrapolation. Lattice-QCD calculations require minimal external input. One needs to set the hadronic scale $\Lambda_{\rm QCD}$ as well as the quark masses. For calculations relevant to low-energy hadron structure, we only need to set the up, down and strange quark masses, which is usually done using the pion and kaon masses as an external input. The overall hadronic scale can be set using well determined baryon masses such as that of the Ω baryon. Many QCD quantities can be

predicted by lattice QCD, including many quantities that are challenging to obtain from experiments. In its early days, lattice-QCD progress on PDFs was limited by available computational resources, with most results concentrating on the first couple moments of non-singlet PDFs at relatively heavy quark masses. In recent years, multiple collaborations work on computations at the physical pion mass, eliminating this way one of the biggest systematic uncertainties: extrapolation in quark masses. In addition, notoriously difficult quantities, gluon contributions and flavor-singlet nucleon matrix elements, have now been calculated as well. Recently, there are also developments in overcoming the limitations in computing the first few moments [9–11] and even making direct calculations of the Bjorken-x dependence of PDFs using large-momentum effective theory (LaMET) [12], computing quasi-PDFs within nucleons having finite momentum boost [13–16].

Recently, there has been very significant progress in our understanding of the polarized and unpolarized partonic structure of the nucleon from both the global PDF fitting and lattice-QCD communities. In the first case, the availability of a wealth of high-precision collider measurements from HERA, the Tevatron and the LHC, together with that of the corresponding NNLO QCD and NLO electroweak perturbative calculations, are pushing the accuracy frontier and leading to improved PDFs with reduced uncertainties.

A paradigmatic illustration of this progress is provided by the gluon PDF, which has been affected by rather large uncertainties due to the limited experimental information, but is known nowadays rather more precisely from small to large-x thanks to the inclusion in the PDF fit of novel processes such as D-meson production [17], the transverse momentum of Z bosons and top-quark pair differential distributions [18]. In the case of lattice-QCD calculations, recent progress has been driven both by better systematic control (physical pion mass, excited-state contamination) for the calculated traditional quantities such as nucleon matrix elements (moments of the PDFs) as well as the development of novel strategies to compute directly the x dependence of PDFs by means of the introduction of quasi-PDFs. These developments imply that, for the first time, it is possible to provide information on the PDF shape of specific flavour combinations, both for quarks and for antiquarks.

Despite these rather important developments, the cross-talk between the two communities has been so far very limited. This situation led some of us to organize the first edition of the "Parton Distributions and Lattice Calculations in the LHC Era" workshop (PDFLattice2017), which took place in Balliol College (Oxford) during the 22nd, 23rd and 24th of March 2017. The scope of this workshop was to create a common ground for the discussions between the two communities, ensuring that we spoke the same language, and starting to consider in a quantitative way how lattice-QCD calculations could be used to improve global PDF fits, and conversely, how PDF fits can be exploited to benchmark lattice calculations. Some of the questions that we proposed ourselves to address during the workshop included:

- What information from PDF fits is relevant to constrain, test or validate lattice calculations?
- What PDF-related quantities are most urgent to compute in lattice QCD in terms of phenomenological relevance?
- What information does lattice QCD provide on the shape (Bjorken-x dependence) of the PDFs? Which specific PDF moments, and up to which order can be computed?
- How do we systematically and consistently quantify the systematic errors in these lattice calculations?

- What accuracy do we need from lattice quantities in order to have a significant impact on global PDF fits?
- To what extent do available lattice results agree with the results of global PDF fits? Is there a tension between global PDF fits, PDF fits based on reduced datasets, and PDF calculations from the lattice?
- What is the ultimate accuracy that can be expected from lattice calculations 5 years from now? What is the ultimate constraining power of lattice calculations on PDFs?

This white paper represents the effort of the two communities to address most of the above questions, following a very fruitful discussion and interactions that took place during the PDFLattice2017 workshop and the discussions in the subsequent weeks. It does not represent our final word, but rather a motivation to encourage further interactions between the two communities.

The outline of this document is as follows: In Sec. 2 we present an overview of the global QCD fit and lattice-QCD methods for the evaluation of polarized and unpolarized parton distributions. Then in Sec. 3 we summarize state-of-the-art benchmark calculations between the most recent available lattice QCD calculations and global PDF fits, both in terms of moments and of x-space PDFs by means of quasi-PDFs. In Sec. 4 we quantify the impact that upcoming lattice calculations could have on unpolarized and polarized PDFs and estimate the impact of these improvements on collider phenomenology. Finally, in Sec. 5 we summarize our studies and discuss the outlook for future interactions between the global QCD fit and lattice-QCD communities.

2 Theory overview

It is specially important that we make sure that we use a consistent notation both in the lattice sections and in the global PDF fitting versions.

2.1 Lattice QCD

- 2.1.1 General intro to lattice QCD
- 2.1.2 PDF moments in lattice QCD
- 2.1.3 *x*-dependent calculations

Where we review quasi-PDFs etc

2.2 Global PDF fits

Collinear unpolarized and polarized PDF analysis.

2.2.1 Unpolarized PDFs

HEADINGS: this is just for editing; we'll remove in the final.

INTRO: We express the collinear unpolarized PDFs as $f_i(x,\mu)$ where the index i represents the parton flavor $i = \{g, u, \bar{u}, d, \bar{d}, s, \bar{s}, ...\}$, x is the fractional momentum carried by the parton, and μ is the factorization (energy) scale.¹ The PDF is a scheme-dependent quantity, and we

¹We could add an additional index to specify the particular hadron (proton, neutron, pion, nuclei, ...); as we mainly refer to the proton in this work, we will omit such a designation unless necessary.

typically work in the \overline{MS} scheme; when this is convoluted with an appropriate hard cross section (Wilson coefficient), we obtain a scheme-independent physical observable.

X-DEPENDENCE: The x-dependence of the PDFs must be deduced by comparing with experimental data in a global fit. For this purpose, we often parameterize the x-dependence of the PDFs in the generic form:

$$f_i(x,\mu) \sim x^a (1-x)^b C(x)$$
 (1)

Here, the x^a term controls the small-x behavior, the $(1-x)^b$ term controls the large-x behavior, and C(x) represents the remaining x-dependence. The a exponent is negative and generally in the range -1 to -2; thus, the PDFs diverge as $1/x^{-1.5}$ for small x and the number of soft partons is infinite. The a exponent must be larger than -2 or the momentum sum rule will diverge. The b exponent is positive, and this ensures the PDF goes to zero as $x \to 1$.

NUMBER SUM RULES: There are a few constraints we can impose on the x-dependence of the PDFs at this point. Since the proton has the quantum numbers of two up quarks and one down quark, we have the following quark number sum rules given in terms of first moments:

$$\int_{0}^{1} dx \ [u(x,\mu) - \bar{u}(x,\mu)] = \langle 1 \rangle_{u^{-}} = 2$$

$$\int_{0}^{1} dx \ [d(x,\mu) - \bar{d}(x,\mu)] = \langle 1 \rangle_{d^{-}} = 1$$

$$\int_{0}^{1} dx \ [s(x,\mu) - \bar{s}(x,\mu)] = \langle 1 \rangle_{s^{-}} = 0$$

with similar results for the heavy quarks: $\langle 1 \rangle_{c^-} = \langle 1 \rangle_{b^-} = \langle 1 \rangle_{t^-} = 0$.

MOMENTUM SUM RULE: The fractional momentum carried by each parton flavor is given by the second moments:

$$\int_0^1 dx \ x \ [u(x,\mu)] = \langle x \rangle_u$$

$$\int_0^1 dx \ x \ [u(x,\mu) + \bar{u}(x,\mu)] = \langle x \rangle_{u^+} \ .$$

Here, $\langle x \rangle_u$ is the fractional momentum carried by the up-quark, $\langle x \rangle_{u^+}$ is the fractional momentum carried by the up-quark and anti-up-quark. Since the total momentum of the proton must equal the momentum of its constituents, we have the momentum sum rule constraint:

$$1 = \langle x \rangle_a + \langle x \rangle_{u^+} + \langle x \rangle_{d^+} + \langle x \rangle_{s^+} + \langle x \rangle_{c^+} + \langle x \rangle_{b^+} + \langle x \rangle_{t^+} + \dots$$

where the "..." represents any other partonic components (such as a photon).

 μ -DEPENDENCE: The μ -dependence of the PDFs is given by the DGLAP evolution equation [?,?,?]

$$\frac{\partial}{\partial \ln \mu^2} f_i(x,\mu) = \sum_{j=a,a,\bar{a}} P_{ij}(x) \otimes f_j(x,\mu) .$$

Here, the logarithmic derivative of the PDF is determined by a convolution of the PDFs with the DGLAP kernel $P_{ij}(x)$ which can be computed perturbatively in powers of $\alpha_s(\mu)$; $P_{ij}(x)$ is known to NNLO.² When performing the global fit to the data, we use the DGLAP equations to combine data from different μ scales when constraining the PDFs.

²The DGLAP (Dokshitzer–Gribov–Lipatov–Altarelli–Parisi) evolution can be modified by $\ln(1/x)$ terms at small-x, and this is characterized by the BFLK (Balitsky-FadinKuraev-Lipatov) equations. [?,?,?] Additionally, at large-x and small μ scale the above framework can receive corrections from non-factorizeable higher-twist (HT) corrections.

$x\rangle_u - \langle x\rangle_d$	Central Value	PDF error	Shift
NNPDF3.0	0.136	2.4%	-
CT14	0.140	3.4%	+2.5%
MMHT14	0.134	2.6%	-1.5%
ABMP16	0.150	1.9%	+10%

Table 1: Benchmark for $\langle x \rangle_u - \langle x \rangle_d$... at $Q=5~{\rm GeV}$

2.2.2 Polarized PDFs

3 Benchmarks

In this section we present updated benchmarks between the most recent available lattice-QCD calculations and global PDF fits, both in terms of moments and of x-space PDFs by means of quasi-PDFs.

3.1 Moments

Here, we provide a systematic comparison between existing lattice-QCD results and PDF fitting calculations for a number of moments both for unpolarized and for polarized PDFs. We provide both summary tables and overview comparison plots.

3.1.1 Unpolarized parton distributions

The moments that we will compare are the following:

• Second moment of $u^+ - d^+$, defined as:

$$\langle x \rangle_{u^+ - d^+} \equiv \int_0^1 dx \, x \, \left[u(x, \mu) + \bar{u}(x, \mu) - d(x, \mu) - \bar{d}(x, \mu) \, . \right]$$
 (2)

• Third moment of $u^- - d^-$, defined as:

$$\langle x^2 \rangle_{u^- - d^-} \equiv \int_0^1 dx \, x^2 \, \left[u(x, \mu) - \bar{u}(x, \mu) - d(x, \mu) + \bar{d}(x, \mu) \, . \right]$$
 (3)

In all the cases, μ should be identified with the QCD factorization scale, the scale that separates long-distance from short-distance dynamics in perturbative factorization. Note that it is customary in PDF fits to assume $\mu = \mu_F = \mu_R$, though in principle the two scales could have different values.

FIO: added sample tables copied from presentations; if the format is OK we can replace/update with the real benchmarks.

3.1.2 Polarized parton distributions

Next we repeat the same exercise, now for the moments of polarized parton distributions.

$x\rangle_u - \langle x\rangle_d$	Central Value	PDF error	Shift
NNPDF3.0	0.102	2.4%	-
CT14	0.104	3.2%	+2.4%
MMHT14	0.101	2.6%	-1.5%
ABMP16	0.113	1.9%	+11%

Table 2: Benchmark for $\langle x \rangle_u - \langle x \rangle_d$... at $Q=100~{\rm GeV}$

$\boxed{\langle x \rangle_{\bar{u}} - \langle x \rangle_{\bar{d}}}$	Central Value	PDF error	Shift
NNPDF3.0	-0.0038	51%	-
CT14	-0.0055	25%	+43%
MMHT14	-0.0060	14%	+57%
ABMP16	-0.0059	11%	+54%

Table 3: Benchmark for $\langle x \rangle_{\bar{u}} - \langle x \rangle_{\bar{d}} \dots$ at $Q=5~{\rm GeV}$

3.2 x-space dependent PDFs

Next we present a number of benchmark comparisons for PDFs at the level of their Bjorken-x dependence.

4 Improving PDF Fits with Lattice Calculations

In this section we quantify the impact of future lattice-QCD calculations in global unpolarized and polarized PDF fits. We use two types of publicly available tools to quantify this impact: for Monte-Carlo sets, the Bayesian reweighting method [19,20] and for Hessian sets, the Hessian profiling method. We consider various assumptions, from pessimistic to optimistic, and then attempt to study what would be the PDF uncertainty reduction in a number of phenomenologically important cross-sections for unpolarized processes at the LHC and for polarized processes at the LHC. In the case of the LHC, potentially important processes include high-mass BSM particle production, Higgs cross sections and the W mass measurement.

5 Outlook

A brief summary of what we have learned from this report and the outlook for future interactions between the lattice-QCD and PDF fitting communities.

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$\langle x \rangle_{s^+}$	Central Value	PDF error	Shift
NNPDF3.0	0.46	6%	-
CT14	0.43	18%	-7%
MMHT14	0.43	16%	-7%
ABMP16	0.47	3%	+2%

Table 4: Benchmark for $\langle x \rangle_{s^+}$... at Q = 5 GeV

$ \frac{\langle x \rangle_{s^+}}{\langle x \rangle_{\bar{u}} - \langle x \rangle_{\bar{d}}} $	Central Value	PDF error	Shift
NNPDF3.0	0.64	8%	-
CT14	0.62	21%	-3%
MMHT14	0.59	19%	-7%
ABMP16	0.66	4%	4%

Table 5: Benchmark for $\langle x \rangle_{s^+} / [\langle x \rangle_{\bar{u}} - \langle x \rangle_{\bar{d}}] \dots$ at Q = 5 GeV

"PDF4BSM - Parton Distributions in the Higgs Boson Era. E. R. N. acknowledges financial support from the UK STFC Rutherford Grant ST/M003787/1.

A Conventional notation

In this appendix, we summarise the convention adopted in this paper to denote moments of relevant unpolarised and longitudinally polarised PDF combinations. We restrict to quantities which can be presently computed in lattice QCD, although those used for benchmarks in Sec. 3 are only a subset of them, specifically: the first moment of the total unpolarised $u^+ - d^+$ PDFs; the second moment of the valence unpolarised $u^- - d^-$ PDFs; the zeroth moment of the total polarised $\Delta u^+ - \Delta d^+$ PDFs; and the first moment of the valence polarised $\Delta u^- - \Delta d^-$ PDFs. We use the shorthand notation $(\Delta)q^{\pm} = (\Delta)q \pm (\Delta)\bar{q}, \ q = u, d, s, c$. In the equations below, μ should be identified with the QCD factorisation scale, and Q^2 should be identified with the characteristic scale of a given hard-scattering process.

The following notation has been agreed by the two communities during the workshop. Its usage is then recommended in any future work whenever PDF moments are referred to.

- Unpolarised moments
 - 1. The first moment of the total $u^+ d^+$ PDFs

$$\langle x \rangle_{u^+ - d^+}(\mu^2) \big|_{\mu^2 = Q^2} = \int_0^1 dx \, x \, \big\{ u(x, Q^2) + \bar{u}(x, Q^2) - d(x, Q^2) - \bar{d}(x, Q^2) \big\} \tag{4}$$

2. The second moment of the valence $u^- - d^-$ PDFs

$$\langle x^2 \rangle_{u^- - d^-}(\mu^2) \big|_{\mu^2 = Q^2} = \int_0^1 dx \, x^2 \left\{ u(x, Q^2) - \bar{u}(x, Q^2) - d(x, Q^2) + \bar{d}(x, Q^2) \right\} \tag{5}$$

3. The first moment of the individual quark q^+ total PDFs

$$\langle x \rangle_{q^+=u^+,d^+,s^+,c^+}(\mu^2) \big|_{\mu^2=Q^2} = \int_0^1 dx \, x \, \{q(x,Q^2) + \bar{q}(x,Q^2)\}$$
 (6)

4. The second moment of the individual quark q^- valence PDFs

$$\langle x^2 \rangle_{q^- = u^-, d^-, s^-, c^-}(\mu^2) \big|_{\mu^2 = Q^2} = \int_0^1 dx \, x^2 \left\{ q(x, Q^2) - \bar{q}(x, Q^2) \right\}$$
 (7)

5. The first moment of the gluon PDF

$$\langle x \rangle_g(\mu^2) \big|_{\mu^2 = Q^2} = \int_0^1 dx \, x \, g(x, Q^2)$$
 (8)

- Longitudinally polarised moments
 - 1. The zeroth moment of the total $u^+ d^+$ PDFs

$$\langle 1 \rangle_{\Delta u^+ - \Delta d^+}(\mu^2) \big|_{\mu^2 = Q^2} = \int_0^1 dx \left\{ \Delta u(x, Q^2) + \Delta \bar{u}(x, Q^2) - \Delta d(x, Q^2) - \Delta \bar{d}(x, Q^2) \right\}$$
(9)

2. The first moment of the valence $u^- - d^-$ PDFs

$$\langle x \rangle_{\Delta u^{-} - \Delta d^{-}}(\mu^{2}) \big|_{\mu^{2} = Q^{2}} = \int_{0}^{1} dx \, x \, \left\{ \Delta u(x, Q^{2}) - \Delta \bar{u}(x, Q^{2}) - \Delta d(x, Q^{2}) + \Delta \bar{d}(x, Q^{2}) \right\}$$

$$(10)$$

3. The zeroth moment of the individual quark q^+ total PDFs

$$\langle 1 \rangle_{q^{+} = \Delta u^{+}, \Delta d^{+}, \Delta s^{+}, \Delta c^{+}}(\mu^{2}) \big|_{\mu^{2} = Q^{2}} = \int_{0}^{1} dx \left\{ \Delta q(x, Q^{2}) + \Delta \bar{q}(x, Q^{2}) \right\}$$
(11)

4. The first moment of the individual quark q^- valence PDFs

$$\langle x \rangle_{\Delta q^- = \Delta u^-, \Delta d^-, \Delta s^-, \Delta c^-}(\mu^2) \big|_{\mu^2 = Q^2} = \int_0^1 dx \, x \, \{ \Delta q(x, Q^2) - \Delta \bar{q}(x, Q^2) \}$$
 (12)

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