THEORY CHALLENGES IN QCD PREDICTIONS

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This talk focuses on the state of the art of QCD predictions for collider physics and the challenges faced in improving theoretical predictions to match the precision of current and future runs of the Large Hadron Collider.

1 Overview

Quantum Chromodynamics (QCD), the theory of strong interactions, is celebrating its 50th anniversary in 2023 [1] and represents one of the milestones of modern physics [2,3]. By calculating the scale-dependence of strong interactions and elucidating their different nature at low and high energies, QCD has explained the weakness of strong interactions at the high energies probed at colliders (up to hundreds of GeV) while justifying the existence of only bound states of quarks and gluons at energy scales below a few hundreds MeV.

Because of the overarching nature of QCD, QCD studies address a very broad spectrum of problems, from the precision calculation of QCD effects in the perturbative regime explored by high-energy collider experiments all the way to the exploration of hadronic matter probed in low-energy experiments and new states of matter probed in nuclear reactions. It would be impossible to make justice to the field in its entirety within a single talk. Since results from probing the non-perturbative regime of strong interactions and the effects of QCD at low-energy will be covered in other talks during this symposium [4], here I will focus on the state of the art of QCD predictions for high-energy particle physics, namely collider experiments. In this context, I will focus on QCD at the Large Hadron Collider (LHC) with attention to both the testing of perturbative QCD (pQCD) per se and the impact of QCD corrections on some of the most crucial LHC physics measurements. Complementary talks on the state-of-the-art of α_s determination and on jet physics were also presented during this symposium [5].

After having discovered the Higgs boson two years into its running, the LHC in Run 3 is now exploring new energy scales and testing the Standard Model (SM) of particle physics with higher precision. After a major upgrade, starting with Run 4 the so called high-luminosity LHC (HL-LHC) will provide a 20-fold improved integrated luminosity compared to the one accumulated by the end of Run 2 and test SM predictions to an unprecedented percent-level

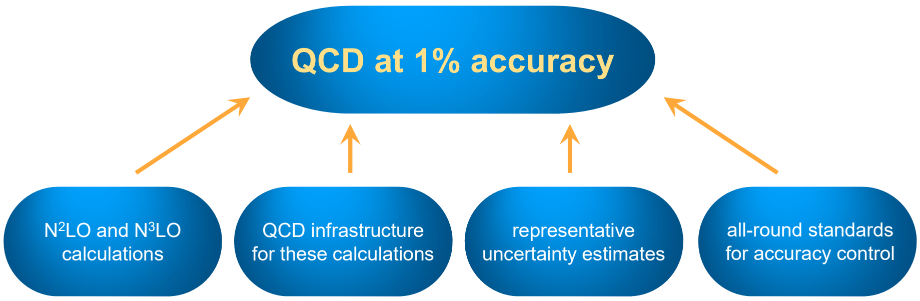


Figure 1 – The many ingredients of QCD predictions at percent level, from the QCD topical group's report of the Snowmass 2021 Energy Frontier [7].

precision. Measurements of couplings (such as α_s or electroweak and Higgs-boson couplings), masses (such as M_W, m_t, or M_H), and a multitude of particle observables will develop the potential to discriminate new physics effects from SM backgrounds through either indirect or direct evidence. Global fit of the SM can unveil tensions [6], subsectors of the SM (top-quark observables, Higgs observables, flavor-observables) can harbor anomalies, searches for exotic signatures can raise red flags. In all cases, it is crucial for the accuracy of theoretical predictions to match the experimental precision and enable a meaningful comparison that could discriminate new physics from SM predictions.

As illustrated in Fig. 1, bringing the precision of theoretical predictions to percent level requires acting on multiple fronts, from improving the precision of the hard core parton-level cross sections to reducing the uncertainty introduced by parton distribution functions (PDF), parton-shower event generators, and hadronization algorithms. It also entails adapting theoretical tools to experimental measurements and proposing well-defined standards for the assessment of theoretical systematics.

At all levels, QCD plays a major role and huge progress has been made in recent years to push the accuracy of QCD calculations to higher precision. In the following section I will review some recent theoretical achievements and illustrate by highlights the many components necessary to deliver state-of-the-art theoretical results and control the residual theoretical uncertainty.

This talk is by no means supposed to be a review of everything that has been achieved in the field of precision QCD calculations. It has its origin in the belief that the physics potential of the LHC greatly depends on enabling and successfully executing a broad precision phenomenology program, within which improving QCD theoretical predictions plays a major role, and will give examples to illustrate that. For percent level precision, combined QCD and electroweak (EW) effects also become mandatory and are nowadays broadly studied, although not specifically the focus of this talk.

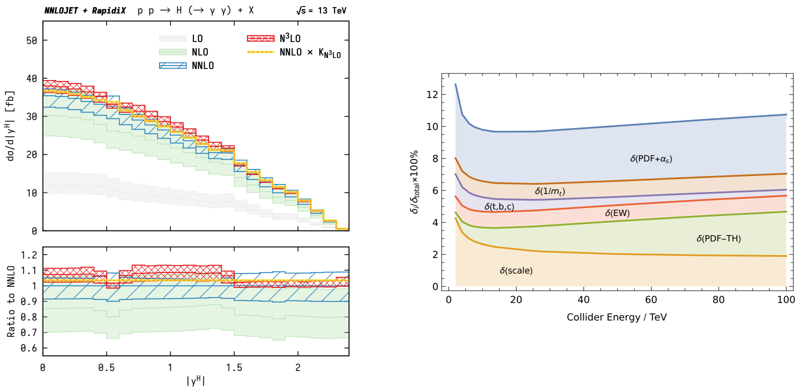
2 QCD for percent-level collider phenomenology

The LHC has certainly performed beyond expectations and projections for the HL-LHC show not only that a broad spectrum of observables will be measured at percent level but also, and most importantly, that the remaining systematic uncertainty will often mainly be of theoretical origin. Depending on the nature of the process and of the observables being measured, the main source of theoretical uncertainty can sometimes come from approximations and missing orders in the calculation of QCD (and EW) corrections to parton-level predictions of the corresponding processes, in the PDF and in parton-shower event generators. In general, adding higher-order QCD and EW corrections reduces the dependence on unphysical scales (renormalization and factorization), includes all possible partonic channels, and better describes the first steps of QCD radiation. Other times, the challenge can be to more faithfully model processes with high multiplicity in order to match the complexity of LHC events in the fiducial volumes chosen by specific experimental analyses, since QCD effects can depend on those. In the following I will discuss a few examples of recent calculations that have advanced the status of QCD predictions for LHC physics in different ways.

In recent years a monumental theoretical effort has been done to push the order of pQCD calculations beyond next-to-leading order (NLO) and next-to-leading logarithms (NLL), and complementing them with QCD+EW mixed corrections at NLO in the full SM. In a trade between perturbative order and multiplicity, $2 \to 1$ processes are now know at N^{3}LO in fixed-order QCD, some with available public code, and progress has been made towards N^{3}LO for $2 \to 2$ processes as well. At N^{2}LO, the focus has been on $2 \to 3$ processes, with particular attention recently on multiple-scale processes such as the production of top-quark pairs with EW gauge bosons and the Higgs boson ($t\bar{t} + X$). NLO QCD+EW corrections have become available for higher multiplicity processes generated by the decay signatures of $2 \to 2$ and $2 \to 3$ processes and have allowed to assess the value of high-multiplicity calculations to better model LHC events. In most cases results that also resum beyond NLL corrections have been obtained. A broad picture of the present and future of higher-order calculations for collider observables can be reviewed in a recent publication submitted to the Snowmass 2021 archive [8].

The case of $2 \to 1$ processes that have been calculated at N^{3}LO QCD, namely Higgs-boson production in gluon-gluon fusion ($gg \to H$) [9,10,11] as well as neutral-current (NC) ($pp \to \gamma^*, Z$) [12,13] and charged-current (CC) ($pp \to W^\pm$) [14] Drell-Yan production (DY), offers a vivid example to illustrate how pQCD effects are so crucial to precision at colliders. In Fig. 2 we see the incremental precision achieved by pushing to N^{3}LO QCD and a breakdown of the residual theoretical uncertainties as presented in Ref. [15]. It is thanks to the precise knowledge of QCD effects that other uncertainties, from unknown EW orders, or quark-mass expansions, PDFs, and more could be estimated and improved upon. Indeed, recently the exact dependence on m_t has been calculated [16] (removing the uncertainty from the $1/m_t$ expansion), and mixed NLO QCD+EW corrections have also been obtained [17], reducing the uncertainty due to EW corrections to 0.26%. Residual uncertainties from matching to NNLO PDFs is being addressed by the progress made in the calculation of N^{3}LO PDF, for which 4-loops splitting functions have been recently provided in Ref. [18], and NC and CC DY process, a crucial input to PDF fits, have been calculated at N^{3}LO QCD [12,14]. A first set of approximate N^{3}LO PDF has also recently appeared [19] based on the N^{3}LO approximation of structure functions and DGLAP evolution, and where use has been made of all available knowledge to constrain PDF parameterizations, including both exact, resummed, and approximate estimates of N^{3}LO results. It has been noticed that the effect on $gg \to H$ decreases the enhancement induced by N^{3}LO corrections in the partonic rate, therefore suggesting that previous uncertainties based on N^{2}LO PDF may have been underestimated.

Among the processes used to constrain PDF fits, NC and CC DY processes are particularly relevant and represent a case in point to appreciate the importance of conquering pQCD predictions to higher order. First of all, as illustrated in Fig. 3, including N^{3}LO QCD corrections has stabilized the cross sections at high momentum transfer (Q) but it has also highlighted some tensions between N^{2}LO and N^{3}LO predictions at lower Q (see l.h.s. plot in Fig. 3) which introduces a previously not known element of uncertainty in PDF fits for which DY is an important input. Indeed, such tension seem to be addressed by the use of approximate N^{3}LO PDF [19] which confirms the potential of substantially reducing theoretical uncertainties in the future when both partonic rates and PDF will be available at the same order. A dedicated study made possible by the N^{3}LO calculation of both DY and VH production has been recently presented [20] where it has been also emphasized how different patterns observed in CC versus NC DY cannot be ignored for precision measurements, since the introduced bias can be sizable at percent level. This is particularly important for Q around M_W since this region plays a crucial role in the determination of M_W itself, both directly through CC DY measurements and indirectly since NC



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\begin{array}{rclll}
\delta(\text{theory}) & = & {}^{+0.13pb}_{-1.20pb} & \binom{+0.28\%}{-2.50\%} & \delta(\text{scale}) \\
& + & \pm 0.56pb & (\pm 1.16\%) & \delta(\text{PDF-TH}) \\
& + & \pm 0.49pb & (\pm 1.00\%) & \delta(\text{EWK}) \\
& + & \pm 0.41pb & (\pm 0.85\%) & \delta(\text{t,b,c}) \\
& + & \pm 0.49pb & (\pm 1.00\%) & \delta(1/m_t) \\
& = & {}^{+2.08pb}_{-3.16pb} & \binom{+4.28\%}{-6.5\%}\,, & \\
\delta(\text{PDF}) & = & \pm 0.89\text{pb} & (\pm 1.85\%)\,, & \\
\delta(\alpha_S) & = & {}^{+1.25pb}_{-1.26pb} & \binom{+2.59\%}{-2.62\%}\,. &
\end{array}
$$

Figure 2 – The l.h.s. plot shows the incremental improvement of theoretical predictions for the $gg \to H$ rapidity distribution from LO to N^{3}LO, from Ref. [11]. The central and r.h.s. pictures give a breakdown of the residual theoretical uncertainties at the time of the first N^{3}LO calculation of $gg \to H$, from Ref. [15]. Subsequent improvements are discussed in the text.

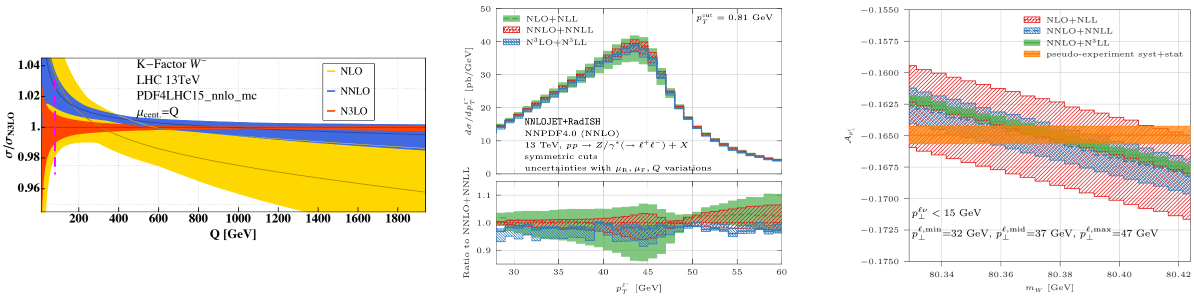

Figure 3 – The l.h.s. plot shows the CC DY total cross section as a function of the virtuality Q of the produced W at N^{3}LO QCD (from Ref. [14]) while the central plot presents results for the differential distribution of the lepton p_T in NC DY production at N^{3}LO+N^{3}LL (from Ref. [13]), including theoretical uncertainty bands. The r.h.s. plot represents the expected uncertainty on the Jacobian peak asymmetry of the lepton p_T spectrum in CC DY production at N^{2}LO+NNLL (from Ref. [22]).

DY measurements are used for normalization. Given the current discrepancies between Tevatron (namely CDF) and LHC measurements and the tension that the value of M_W can generate in EW precision fits [21,6], and since M_W is measured by fitting templates distributions, reducing the uncertainty of theoretical predictions for DY production in this region is crucial. It is estimated that requiring an error on M_W of about 100 MeV implies controlling the shape of the Jacobian peak in template distributions with 1-2% uncertainties. Hence, aiming at determining M_W with a 10 MeV error, as auspicable to fully exploit the constraining power of EW fits, demands a theoretical accuracy on template distributions at the permille level. As illustrated in the central plot [13] of Fig. 3 and discussed in Ref. [22], this is very challenging if not excluded even when N^{3}LO+N^{3}LL QCD effects are included, due to various sources of systematic uncertainty, and has prompted the study of new observables derived from the kinematic features of the W decay products that could improve the determination of M_W to the needed level of precision. This is for instance the case of an observable that encodes the asymmetry of the Jacobian peak in the lepton-p_T distribution which, thanks to its remarkable pQCD properties of stability and accuracy, promises to achieve a measurement of M_W at the permille level [22].

Moving on to processes with higher multiplicity and several mass scales, one of the major recent achievements in QCD results for LHC phenomenology has been the calculation of N^{2}LO QCD corrections for the on-shell associated production of EW gauge boson and Higgs boson with heavy quarks. Results that calculate the 2-loop virtual corrections in the soft H/W approximation have been presented for both $t\bar{t}H$ [23] and $t\bar{t}W$ [24]. They confirm a clear stabilization of the inclusive cross section as illustrated in the left and central plots of Fig. 4. The impact of both

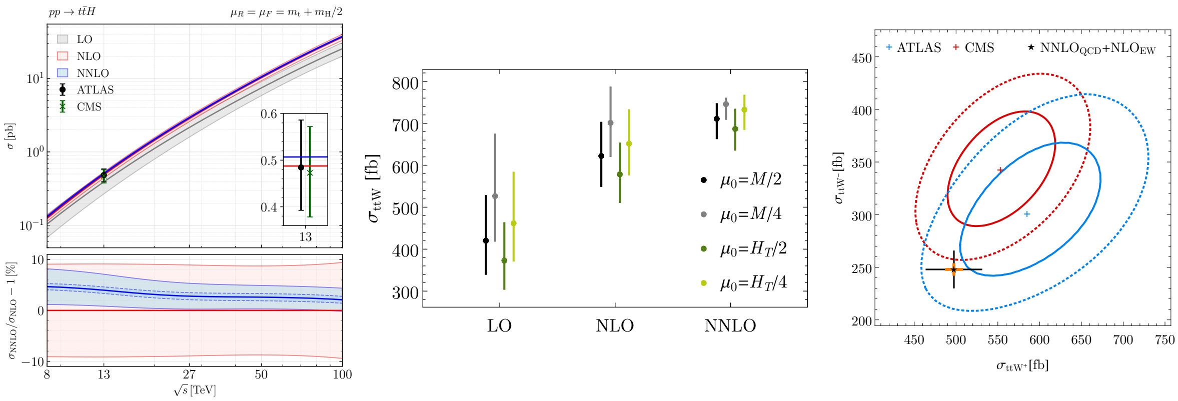

Figure 4 – The l.h.s. and central plots show the impact of N^{2}LO QCD corrections on the cross section for $t\bar{t}H$ (from Ref. [23]) and $t\bar{t}W$ (from Ref.[24]) respectively, while the r.h.s. plots shows the comparison between the state-of-the-art N^{2}LO QCD+NLO EW theoretical predictions and the most recent measurements of $t\bar{t}W^{\pm}$ by ATLAS and CMS (from Ref. [24]).

calculations in reducing the current theoretical uncertainty to about 3%, well in the realm of the precision expected on top-quark couplings from the HL-LHC, is clear. In the particular case of $t\bar{t}W$ these results have furthermore reduced the tension between theoretical predictions and experimental measurements. The current N^{2}LO+NLO EW predictions agree with experimental results within 2σ, showing a stronger tension with CMS than ATLAS results and pointing more to a tension between experiments than not between theory and experiments. Meanwhile, the exact calculation of the 2-loop virtual component of the N^{2}LO QCD cross sections is advancing and partial results have been appearing in recent months [25,26,27,28], pointing to a steady theoretical push to complete the N^{2}LO calculation of these processes.

At the same time, prompted by the importance of these processes in measuring top-quark couplings and by the residual large systematics induced by event modeling in the corresponding experimental analyses, theorists have been considering how to improve the theoretical description of $t\bar{t}+X$ events. In particular, they have been exploring the effect of calculating at NLO QCD the fully decayed processes as opposed to approximating such signatures with the corresponding $t\bar{t}+X$ on-shell process matched to the top-quark and X-boson decays via a narrow-width approximation (NWA). While the calculation in a NWA includes only double resonant effects, the calculation of the fully decayed process includes also single-resonant and non-resonant effects (globally denoted as *off-shell effects*), on top of accounting for the full spin-correlation of production and decay at the corresponding perturbative order (NLO QCD in this case). Several calculations have extended on-shell predictions for $t\bar{t}+X$ processes to consider their fully decayed signatures at NLO QCD and NLO QCD+EW [29,30,31,32,33,34,35]. Off-shell effects have been shown to mainly affect tails and end points of kinematic distributions where, however, direct and indirect signals of new physics are most likely expected and therefore very accurate templates of SM predictions will be necessary. This is therefore a case in which pushing the perturbative order beyond NLO is less relevant, but having control on the shape of events at high multiplicity will be very beneficial. In all cases, the effect of matching the NLO on-shell (for $t\bar{t}H$ and $t\bar{t}W$) or partially off-shell (for $t\bar{t}Z$) calculation to parton-shower event generators has also been studied and found to affect the modeling of final states richer in hadronic activity in regions that are often complementary to where off-shell effects are more relevant and very much depend on the fiducial volume considered. Examples of off-shell studies for $t\bar{t}W$ and $t\bar{t}Z$ are given in Fig. 5 where the effects of parton-shower matching are also illustrated. Interfacing the fully decayed processes to parton-shower is the ultimate goal. Although technically possible, it can be computationally very onerous and will have to be carefully studied in the future. Meanwhile, from a comparison of all available studies, recommendation have been proposed to provide the experiments with differential results that would include both parton-shower and

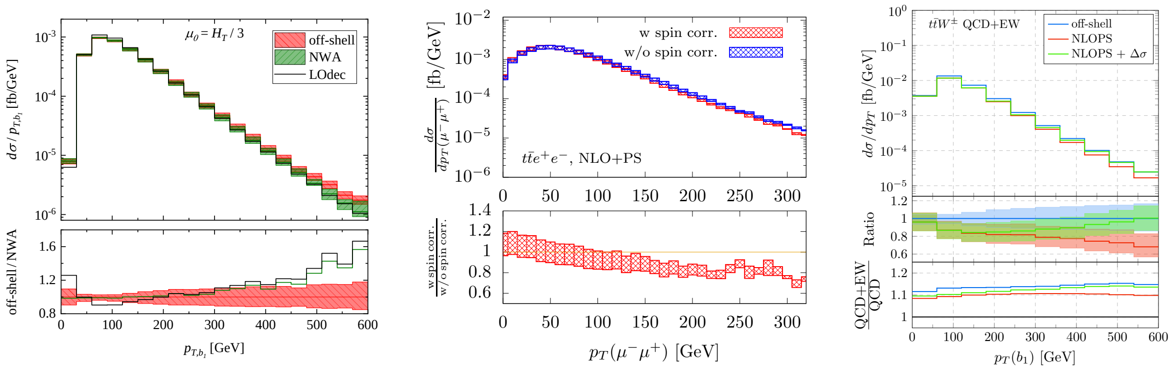

Figure 5 – The l.h.s. and central plots illustrate the impact of off-shell and spin correlation effects in calculating fully or partially decayed signatures for $t\bar{t}W$ (l.h.s., from Ref. [31]) and $t\bar{t}Z$ (center, from Ref. [33]) at NLO QCD. The r.h.s. plot shows a combined study of off-shell fixed-order and parton-shower effects in the case of fully leptonic signatures of $tbartW$ (from Ref. [36]).

off-shell effects [36], some of which have been implemented in recent experimental analyses [37].

Major improvement in controlling QCD effects in collider observables will also come from better parton-shower event generators, the crucial ingredient to reproduce the complexity of collider events. Standard parton-shower are leading logarithmic (LL) and this is becoming a limitation that is being addressed by several groups working on next-to-leading logarithmic (NLL) parton-shower event generators [38].

Finally, one of the main assumptions in calculating hadronic rates is factorization, according to which rates can be calculated as the convolution of partonic rates with PDF modulus non-perturbative QCD effects that scale as $(\Lambda_{\rm QCD}/Q)^p$ for Q the scale of the considered physics process and p some integer power. Establishing the validity of such picture is very important when percent precision is the game. So far we do not have a general theory to address this problem but only specific process-dependent calculations. In particular it has been established that such effects rescale with $p < 1$ for Z transverse-momentum distributions and for the more general case of observables that are inclusive with respect to QCD radiation [39,40,41]. Further theoretical investigation in this direction will be both fundamental and of direct phenomenological relevance.

3 Outlook

QCD is a mature theory that still offers plenty of conceptual challenges. In this talk we have only focused on aspects of QCD theoretical predictions for collider physics and how they can raise to the challenge of enabling LHC phenomenology at percent accuracy.

At such level of accuracy, understanding the multiple components of QCD predictions becomes crucial to interpret precision measurements as well as direct searches of new physics. Interpreting the complexity of LHC events with HL-LHC precision will be challenging and will require diversity of approches. Theoretical developments during the last few years have deeply changed traditional approaches to QCD calculations and given results that were unimaginable only a decade ago, giving us confidence that challenges can be met.

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