

Status and outlook of SM QCD predictions

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I review the status of QCD predictions for SM processes at the LHC and emphasize the need for further improvements in the theoretical description of hard hadron collisions.

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The main focus of two largest multipurpose LHC experiments, ATLAS and CMS, is the study of very hard collisions between protons, i.e. collisions where protons exchange large momentum and disintegrate. These types of collisions are interesting for two reasons. On the one hand, when they occur, so much energy is packed into a tiny space-time volume, that production of the heaviest particles of the Standard Model – top quarks, W, Z and Higgs bosons becomes possible. Moreover, the probability to excite the yet-unknown particles from the vacuum, or to observe interactions caused by unknown heavy degrees of freedom in such events is significantly higher than in events that are less violent. Hence, if we are interested in exploring properties of the heaviest particles in the SM, or in searching for extensions of the Standard Model with additional heavy particles, such events are the place to look at.

On the other hand, thanks to the phenomenon of asymptotic freedom in QCD, hard collisions can be described, with the great level of confidence and with high precision, in terms of quarks and gluons – even though they originate from collisions of two protons and are observed in multi-hadron final states. In contrast to hadrons, quarks and gluons do appear in the Lagrangian of the Standard Model, which means that we can describe outcomes of hadron collisions with large momentum transfers from *first principles, using a framework that is systematically improvable*.

Since by now QCD in the perturbative regime is rather well understood, its main role in the context of collider physics is to facilitate thorough studies of the Standard Model and, hopefully, the discovery of New Physics. This is an extremely important role to play since, without reliable QCD predictions, one will still be in the dark about interpretations of every single measurement of any hard process at the LHC.

Perhaps, the best observable to illustrate this point is the Higgs production cross section in gluon fusion where the theoretical prediction changes by nearly a factor of two when one goes from the leading to the highest available order in perturbative QCD [1]. If the QCD corrections to this process were not computed, we will be, most likely, discussing the fifty percent discrepancy in the observed Higgs production rate and inventing exotic models to address it, instead of celebrating the success of the Standard Model. A similar conclusion follows from across-the-board comparison of many experimental measurements and theoretical predictions which all show a remarkable consistency.

Advances in the LHC physics have been shaping the development of QCD as a perturbative quantum field theory and kept QCD practitioners on their toes. This can be easily seen by comparing two so-called wishlists which every two years are compiled by enthusiasts of perturbative QCD computations from experimental and theoretical communities [2], see Fig. 1. The list has expanded dramatically and if 20 years ago, next-to-leading order QCD predictions for complex final-state processes were desired, now predictions through third and even fourth order in the perturbative expansion in QCD are sometimes considered necessary.

Making predictions at such high orders in a theory as complex as QCD and for processes as diverse as what you see in Fig. 1, is impossible using the methodology that Feynman, t'Hooft and Veltman taught us. Instead, one needs to go beyond that, discover and develop new theoretical methods which in some cases require a radical departure from the established ones. Appreciation of this fact defined one of the main avenues along which perturbative QCD has been developing during the recent years.

Although we have witnessed a tremendous progress with understanding perturbative QCD in the past decades, we should not forget that we deal with a real-world problem where phenomena

Higher order cross sections: The first wishlist
An experimenter's wishlist

Run II Monte Carlo Workshop

Single Boson	Diboson	Triboson	Heavy Flavour
$W + \leq 5j$	$WW + \leq 5j$	$WWW + \leq 3j$	$t\bar{t} + \leq 3j$
$W + b\bar{b} \leq 3j$	$W + b\bar{b} + \leq 3j$	$WWW + b\bar{b} + \leq 3j$	$t\bar{t} + \gamma + \leq 2j$
$W + c\bar{c} \leq 3j$	$W + c\bar{c} + \leq 3j$	$WWW + \gamma\gamma + \leq 3j$	$t\bar{t} + W + \leq 2j$
$Z + \leq 5j$	$ZZ + \leq 5j$	$Z\gamma\gamma + \leq 3j$	$t\bar{t} + Z + \leq 2j$
$Z + b\bar{b} + \leq 3j$	$ZZ + b\bar{b} + \leq 3j$	$ZZZ + \leq 3j$	$t\bar{t} + H + \leq 2j$
$Z + c\bar{c} + \leq 3j$	$ZZ + c\bar{c} + \leq 3j$	$WZZ + \leq 3j$	$t\bar{b} \leq 2j$
$\gamma + \leq 5j$	$\gamma\gamma + \leq 5j$	$ZZZ + \leq 3j$	$b\bar{b} + \leq 3j$
$\gamma + b\bar{b} \leq 3j$	$\gamma\gamma + b\bar{b} \leq 3j$		single top
$\gamma + c\bar{c} \leq 3j$	$\gamma\gamma + c\bar{c} \leq 3j$		
	$WZ + \leq 5j$		
	$WZ + b\bar{b} \leq 3j$		
	$WZ + c\bar{c} \leq 3j$		
	$W\gamma + \leq 3j$		
	$Z\gamma + \leq 3j$		

circa 20 years ago, NLO calculations are requested

Wishlist, the 2022 edition

process	known	desired
$pp \rightarrow t\bar{t}$	NNLO _{QCD} + NLO _{EW} (w/o decays) NLO _{QCD} + NLO _{EW} (off-shell effects) NNLO _{QCD} (w/ decays)	N ³ LO _{QCD}
$pp \rightarrow t\bar{t} + j$	NLO _{QCD} (off-shell effects) NLO _{EW} (w/o decays)	NNLO _{QCD} + NLO _{EW} (sys)
$pp \rightarrow t\bar{t} + 2j$	NLO _{QCD} (w/o decays)	NLO _{QCD} (w/ decays)
$pp \rightarrow V$	N ³ LO _{QCD} N ^(1,1) LO _{QCD} ⊗EW NLO _{EW}	N ³ LO _{QCD} + N ^(1,1) LO _{QCD} ⊗EW N ² LO _{EW}
$pp \rightarrow VV'$	NNLO _{QCD} (w/o decays) + NLO _{EW} (gg channel)	NLO _{QCD} (gg channel, w/ massive loops) N ^(1,1) LO _{QCD} ⊗EW
$pp \rightarrow V + j$	NLO _{QCD} + NLO _{EW}	hadronic decays
$p\bar{p} \rightarrow t\bar{t}$	NLO _{QCD} + NLO _{EW} (QCD component) NLO _{QCD} + NLO _{EW} (EW component)	NNLO _{QCD}
$pp \rightarrow 2 \text{ jets}$	NNLO _{QCD} NLO _{QCD} + NLO _{EW}	N ³ LO _{QCD} + NLO _{EW}
$pp \rightarrow 3 \text{ jets}$	NNLO _{QCD} + NLO _{EW}	

and many many more...

Huss, Huston, Jones, Pellen

Figure 1: The two wish lists, separated by a twenty-year interval, see Refs. [2, 3] for further details.

that we want to describe start and end with hadrons. As the result, improving theoretical description of such events requires us to address two very different type of challenges.

The first one is technical. We would like to continue improving our ability to compute partonic cross sections for complex processes. This is a multi-facet problem that involves calculation of virtual loop amplitudes, development of subtraction schemes for real-emission contributions, understanding how to perform phase-space integrations efficiently and so on.

The second problem is of a more conceptual nature; it is related to the fact that in order to describe hard processes fully, we need to control transitions from two protons to quarks and gluons, and a transition from quarks and gluons back to hadrons in a controllable and, ideally, improvable way. These steps are currently addressed with parton distribution functions and parton showers, but there is hardly a systematic way to improve on these descriptions.

To make the next step in addressing this problem, one needs to develop a systematic approach for describing hard scattering processes at the LHC at the level of *power corrections*, i.e. non-perturbative effects that are suppressed by ratios of a non-perturbative QCD scale Λ_{QCD} and the hard scale that exists in a particular process, for example a mass of a heavy color-charged particle or a transverse momentum of a jet.

Current theoretical understanding of power corrections is such that they cannot be computed from first principles. Moreover, one cannot even predict with confidence the degree of their suppression for arbitrary processes and observables! Indeed, one can write a general formula for a hard scattering cross section

$$d\sigma_{\text{hadr}} = \sum_{ij} \int dx_i dx_j f_i(x_i) f_j(x_j) d\sigma_{ij}^{\text{part}}(x_i, x_j) \left(1 + O\left(\frac{\Lambda_{\text{QCD}}^n}{Q^n}\right) \right), \quad (1)$$

indicating that power corrections scale as $(\Lambda_{\text{QCD}}/Q)^n$ where n is unknown. Whether or not these corrections are relevant for the LHC physics depends on the power n ; for $n > 1$, they are basically irrelevant but if $n = 1$, they may become relevant once the perturbative expansion in QCD reaches

N3LO or if ultra-precise observables such as e.g. the mass of the top quark and the value of the strong coupling constant are discussed. Precision quoted by the experimental collaborations for these two observables reached the level where understanding of power corrections becomes worthwhile. Again, it is useful to reiterate that the degree of suppression, i.e. the exponent n in Eq. (1), cannot be predicted currently for arbitrary observables and processes.

Let us start with the discussion of the technical progress with perturbative computations. Basically, for any perturbative computation where the goal is to compute $O(\alpha_s^k)$ correction to a particular LHC process with N -partons in the final state, one needs to account for k -loop correction to $f_1 f_2 \rightarrow N$ process, $(k-1)$ -loop correction to $f_1 f_2 \rightarrow N+1$ process, $(k-2)$ -loop correction to $f_1 f_2 \rightarrow N+2$ process and, eventually, a Born-process for $f_1 f_2 \rightarrow N+k$ tree-level process. Each of these contributions exhibits explicit or implicit infra-red and collinear divergences, and only their sum is finite. Hence, to produce a result for a partonic cross section that can be used in phenomenological studies, one needs 1) to figure out a way to compute loop amplitudes; 2) to understand how to integrate individually divergent contributions over partonic phase space and 3) to implement this procedure in an efficient numerical code.

Computation of loop amplitudes presents an interesting problem because it is extremely well-posed. Indeed, for any process and to any loop order, we can draw Feynman diagrams and construct rational functions in momentum space that we need to integrate to assign a numerical value to a particular diagram, needed to describe its contribution to a probability amplitude. The problem of loop calculations is really a problem of finding a way to compute complicated, potentially divergent integrals of rational functions of momenta in Minkowski space.

Although this problem sounds simple, solving it in full generality proved to be very difficult. However, attempts to do this for many years were a source of interesting ideas, which became important elements of the current theoretical toolbox. Many of these ideas are of a mathematical nature, some are sophisticated and some are not, but all are battle-tested and important.

They include the celebrated integration-by-parts technology [4], the idea that Feynman integrals are linear combinations of basis (master) integrals, local generalized unitarity [5–10] (see Ref. [11] for a review of amplitude-based methods), which is the incarnation of the old bootstrap idea in a perturbative setting, differential equations for master integrals, canonical bases for differential equations [12], solutions of large systems of linear equations using numerical reconstruction techniques [13], mathematics of very special functions such as generalized polylogarithms and elliptic functions (see [14, 15] for a review and further references).

A special place in these developments is occupied by very natural attempts to construct a robust numerical framework for computing Feynman integrals. There are several ideas about how this can be done, that range from direct integrations over loop momenta [16, 17] or over Feynman parameters [18] after isolating singular contributions to the integrand in some way, to numerical solutions of the differential equations that Feynman integrals satisfy [19, 20].

I believe that the importance of robust numerical methods will keep increasing as we move forward, but I also think that we are still quite far away from even imagining how the ultimate solution to the problem of loop integrations in perturbative QCD will eventually look like, and that new ideas are needed here.

On the other side of the spectrum, there are real emission contributions whose integration over partonic phase spaces is accomplished with the help of the so-called “subtraction-” and “slicing”

methods [21–33]. As the names suggest, the crux of these methods is the isolation of a singular contribution to the integral either by subtracting it away or by slicing the phase space. This can be done in many different way, and a choice of how to do this defines a particular scheme. Integrated subtraction or slicing terms then produce infra-red divergencies that cancel with similar divergencies in loop contributions. Although many NNLO QCD computations have been performed by now, such cancellations were always established on a case-by-case basis.

A new development of the past few years, is that extensions of available subtraction and slicing methods for NNLO QCD computations appeared, where such cancellations are demonstrated *analytically for arbitrary processes at colliders* [32, 34–36]. These developments bring us one step closer to the formulation of an "ultimate" subtraction scheme at NNLO which, hopefully, will be amenable to an efficient automation and to the construction of general purpose codes that can compute NNLO real emission contributions to *arbitrary* collider processes with the minimal amount of the process-specific input.

In summary, a highly developed theory of partonic collisions exists that can be used to describe hard collider processes with complicated final states in perturbative QCD. This theory is based on the expansion of partonic cross sections in powers of the strong coupling constant α_s and subsequent convolution of these predictions with parton showers. Leading and next-to-leading order computations are a done deal in the sense that many such computations can be performed in a completely automated fashion [37, 38]. Perhaps, the only point still worth emphasizing is the fact that a *fully realistic treatment of unstable particles has been achieved in NLO QCD computations*. In fact, one does not talk about production of, say, top quarks and W -bosons anymore, but rather about production of final states that are made up of their decay products and one includes all diagrams, both resonant and non-resonant, in theoretical predictions (see e.g. [39] for a recent example). This may sound simple, but it is not, and a possibility to do that implies high maturity of theoretical methods on which such computations are based.

At NNLO, the limiting factor at this point are virtual amplitudes and the efficiency of numerical implementations. The next frontier for the virtual amplitudes are $2 \rightarrow 3$ processes with a few massive particles in the final state [40–42]. At N3LO, cross sections are known for $2 \rightarrow 1$ processes [43]. Slicing schemes for dealing with the production of color-less final states at this order are available. The current frontier for virtual corrections are three-loop $2 \rightarrow 2$ amplitudes with one massive external particle, such as $V + j$ or $H + j$ [44, 45].

Before moving on to the discussion of the conceptual problem of power corrections that I mentioned earlier, I would like to discuss a few examples which show how progress with higher-order computations in QCD helps to address tangible phenomenological problems in collider physics.

A unique measurement that the LHC experiments can perform is the observation of the running of the strong coupling constant at the highest available energies, i.e. at around 1 TeV. One way to do this is to study the so-called shape variables in dependence of the transverse collision energy. NNLO computations of shape variables in 3-jet events at the LHC have been recently completed [46]; this calculation employs very complex two-loop amplitudes and integrals [47, 48] computed using modern methods that I briefly described earlier, and a particular subtraction scheme that is capable of handling computations of such complexity [26–28].

The ATLAS collaboration employed these results to extract the value of the strong coupling constant using the so-called azimuthal transverse energy-energy correlations and obtained a precise result which is fully compatible with the world average [49]. The NNLO QCD computation helped to reduce the uncertainty of the strong coupling constant extracted in this way by about a factor of 3.

While this result tells us in no uncertain terms that the strong coupling constant at the highest energies that are currently available runs as expected in the Standard Model, this computation is also quite remarkable for another reason since it uses an enormous amount of computational resources. This fact is a testimonial to the need for better algorithms if NNLO QCD calculations for even higher multiplicity processes are ever to be performed.

My second example concerns the determination of the Higgs boson width at the LHC. It is well-understood by now that one can determine the Higgs width indirectly, by comparing 4-lepton events at the Higgs resonance, and 4-lepton events with the invariant mass significantly higher than the mass of the Higgs boson. Both CMS and ATLAS have measured the Higgs width in this way, and the results are close to the expected SM value with the uncertainty of about 70 percent. To put this into a perspective – these results beat the pre-LHC expectations for the precision with which determination of Γ_H at the LHC is possible by about a factor $O(200)$, so it is quite a spectacular achievement.

One of the things that goes into this result is the theoretical estimate of the irreducible background, $gg \rightarrow ZZ$, where two Z 's are produced directly through a loop of quarks, and the interference of this process with the process where Z 's are produced in a decay of a highly off-shell Higgs boson. The NLO QCD corrections (two-loop contributions) to $gg \rightarrow ZZ$ are known since a long time, but only in the case when quarks in the loop are massless [50, 51]; in the case where top quarks propagate in the loop, the computation becomes so difficult that it was only done in an approximate way [52, 53]. Because of this since the first measurements of the Higgs width at the LHC there was always the nagging feeling that there might be a tiny chance that this irreducible background was not estimated in the right way.

All this has changed now since as of earlier this year, the computation of the top loop contribution to $gg \rightarrow ZZ$ has been completed [35]. The computation relied on sophisticated techniques for loop computations that are an interesting blend of advanced analytic and numeric methods. The result confirms earlier approximate estimates of the irreducible background, giving us full confidence that the theoretical foundation for the extraction of the Higgs boson width from the off-shell production at the LHC is quite solid.

My next example is the determination of the strong coupling constant α_s from the transverse momentum distribution of Z bosons. There are many reasons that make it difficult to determine α_s at the LHC with a competitive $O(1\%)$ precision, but it was realized by the authors of Ref. [54] that the Z -boson transverse momentum distribution is the place to look at. Following this suggestion, the ATLAS collaboration recently measured the strong coupling constant [55] and obtained a very precise result in excellent agreement with the world average value.

I would like to emphasize that the extraction of α_s reported in the ATLAS paper [55] relies either directly or indirectly on a huge body of theoretical work since providing a theoretical prediction for the Z -boson transverse momentum distribution with $O(1\%)$ precision is highly non-trivial. The

current prediction includes – a N3LO result for the Z-boson production cross section and rapidity distributions, NNLO QCD and one-loop electroweak corrections to the production of Z boson in an association with a jet, extremely advanced resummation of logarithms of the ratio of Z-boson transverse momentum to its mass and some other things (see [56] and references therein).

My last example concerns the determination of the W-mass at the LHC from the lepton transverse momentum spectrum and the so-called mixed QCD electroweak corrections (see [57] and references therein). These corrections are definitely tiny. However, to understand why they might be important for the W-mass determination, we should recall that one tunes models that describe Z-production at the LHC to agree with data and then uses these models to describe W production arguing that from the QCD point of view the two processes are very similar. Because of this, all effects that distinguish between Z and W production, even the tiny ones, become very important, and electroweak corrections as well as mixed QCD-electroweak corrections are examples of such effects.

To estimate how important these effects are, one compares first moments of the charged lepton transverse momentum distributions in Z and W cases and assumes that the correlation between moments and masses of vector bosons is the same. Electroweak corrections affect this correlations in different ways, and we can estimate the shift in the W mass that needs to be applied to account for this [57]. The resulting shifts in the W mass are found to be below $O(15)$ MeV; the precise value strongly depends on the interplay of the selection criteria that are applied to leptons in Z and W production, including acceptance intervals for the charged lepton transverse momentum and rapidity. Although these estimates are unlikely to survive realistic experimental simulations, I think they are interesting as they allow us to see a potential impact of a very complex computation on an observable that is measured in a rather complicated way.

Let me now turn to the discussion of the problem of power corrections that I called a “conceptual problem” earlier in this talk. This is a conceptual problem because, as of today, we do not know much about these non-perturbative effects in collider observables.

Currently, they are described by parton showers and hadronization models, but it is fair to say that sooner or later the standard approach where partonic calculations are pushed to higher and higher orders and the fact that hadrons collide and are observed is not critically assessed on the theoretical side will not be a valid approach anymore. One can already see this in *ultra-precise* measurements at the LHC, such as the top quark mass measurement, where lack of understanding of power-suppressed effects causes debates about their interpretation [58, 59].

One may wonder why non-perturbative effects are discussed in the talk which is centered around perturbative physics. The reason is that since it proved to be very difficult to describe non-perturbative effects at colliders from first principles, an old idea that one may learn something about non-perturbative physics from QCD perturbation theory, came back into the focus recently.

For example, a recent discussion of interdependencies between perturbative evolution of parton showers, and aspects of hadronization models is a clear example of this [60]. Another way to think about this problem is to notice that Feynman integrals run over all momenta, including soft ones, so that we can use them to estimate the sensitivity of a particular observable to soft physics. In some sense, the famous Kinoshita-Lee-Naunberg (KLN) theorem [61, 62], as well as the idea of

renormalons and their connection to QCD where gluons are given a tiny mass λ can be understood from this perspective (see e.g. Ref. [63] for an introduction to renormalons). Indeed, the KLN theorem states that in properly defined observables the *logarithmic* sensitivity to infrared physics is absent, and renormalons probe the $O(\lambda)$ sensitivity of such observables.

Let me summarize how this works. We consider QCD where gluons are given a mass and compute cross sections and observables in this theory, study the limit when the gluons mass λ goes to zero and determine a term that is linear in λ . We then use the renormalon model to translate such a term to $O(\Lambda_{\text{QCD}})$ power correction; this translation is universal and allows one to correlate the magnitude of non-perturbative contributions between different observables.

An interesting fact that was appreciated only recently, is that all calculations required to do that can be performed without much effort for a broad class of processes [64]. Indeed, the origin of linear $O(\lambda)$ contributions can be traced to very specific kinematic configurations, as well as particular limits of amplitudes and observables. Hence, they can be computed in a process-independent way using the so-called Burnett-Low-Kroll theorem [65, 66], as well as momenta redefinitions of final state particles that allow us to factorize all $O(\lambda)$ contributions from amplitudes, phase-spaces and observables in a universal way [67]. The limitation of this approach at this point is that it is intrinsically Abelian, since it is difficult to give a mass to a gauge boson of a non-Abelian gauge theory without breaking gauge invariance.

Nevertheless, one can learn quite a few things by employing this approach to study power corrections. For example, one can show that it is *not possible* to determine the top quark *pole* mass from the $t\bar{t}$ production cross section with the precision higher than Λ_{QCD} . However, the so-called short-distance top quark masses (see e.g. [59] and references therein) can be extracted from this quantity with very high precision [68]. This result is, perhaps, not too surprising because of what was learned in B -physics, but it is for the first time that these expectations are supported by an explicit computation in the context of an important collider physics process.

Furthermore, one can show that the most basic distributions in the top quark pair production processes *do* receive linear power corrections whose relation to the hadronization models in parton showers is, at best, unclear [68]. This point makes the whole idea of ultra-precise determination of the top quark mass from complex kinematic distributions questionable simply because non-perturbative corrections that would affect such distributions are unknown. One can also show that polarization observables and spin correlations in top quark production processes receive linear power corrections and that, in general, lepton kinematic distributions from top decays are also affected [69]. It is to be noted that these analyses employ stable top quarks whereas the width of the top quark should, in principle, further screen the infra-red sensitivity. How exactly this works is unknown at the moment, but it is an interesting question to pursue further.

Finally, one can show that linear power corrections in 3-jet and 2-jet contributions to shape variables in e^+e^- annihilation are different [70], in variance to the standard assumptions employed in the previous extractions of the strong coupling constant α_s from this observable. Whether this leads to significant shifts in the fitted values of α_s from shape variables, is currently being debated [71, 72].

To conclude, perturbative QCD plays an extremely important role in the current studies of the high-energy frontier of particle physics. It provides a solid theoretical framework to describe hard hadron collisions and enables interpretation of the results of the LHC measurements in terms

of parameters that appear in the Lagrangian of the SM or of its possible extensions. Continuous progress in perturbative QCD allows us to describe processes of greater complexity with higher and higher precision, which then translates into a more reliable and realistic phenomenology.

Finally, an important conceptual issue with the theory of hadron collisions is a need for a better understanding of non-perturbative, power-suppressed effects from first principles. These effects are small, but they are becoming relevant for ultra-precise measurements at colliders, such as the top quark mass or the strong coupling constant determinations. An interesting development here is the resurrection of the old idea that one can learn about non-perturbative effects by studying certain aspects of perturbative computations.

In general, the impressive successes of the *perturbative approach* to the description of hadron collisions, emphasize the need for a systematic understanding of non-perturbative power corrections to hadron collider processes. Without it, meaningful improvements in ultra-precise determinations of physical parameters (the top quarks mass, the strong coupling constant etc.) may not be possible, in spite of being statistically achievable.

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