



## QCD at NNLO and beyond

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### Abstract

In this contribution we review the status of higher-order QCD computations, focussing on recent progress in next-to-next-to-leading order and beyond. After a short review of the basics underlying higher-order computations in QCD, we focus on progress for the computation of multi-loop integrals as well as for the subtraction of real-emission singularities. In each case, we report on advances in both of these two fields and discuss milestones achieved using these new techniques.

*Keywords:* QCD, NNLO, NNNLO, polylogarithms.

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### 1. Introduction

The amazing performance of the LHC experiments at CERN has inaugurated a new era of precision physics at hadron colliders. In particular, the measurements of the properties of the Higgs boson by the CMS and ATLAS experiments are already now a major achievement in precision experimental physics, and the experimental uncertainties are expected to be further reduced in the upcoming second run of the LHC experiments. In order to exploit the data for this upcoming run to the fullest, theoretical predictions at an unprecedented level of precision for a large variety of processes, including precision predictions for fully differential distributions will be required. This poses a serious challenge to the current state-of-the-art of theory predictions for hadron colliders.

It is well-known that leading order (LO) predictions for QCD observables are plagued by large uncertainties, coming from missing higher-order corrections. This often results in a strong dependence of the predictions on the renormalisation and factorisation scales, and moreover in many cases, including the case of Higgs production in gluon fusion, perturbative higher-order corrections can be large and may completely invalidate the

LO approximation. Over the last few years, a lot of progress has been made in the context of next-to-leading order (NLO) computations, which have by now been almost completely automated (for a review see [1]). Unfortunately, a similar level of automation is currently out of reach for computations at next-to-next-to-leading order (NNLO) and beyond. There are various reasons for this: First, the multi-loop integrals coming from the integration over the momenta of additional virtual particles usually lead to very complicated classes of special functions, most of which are only poorly understood at best. In particular, these functions have a complicated branch cut structure, and the imaginary parts (which describe the threshold when intermediate virtual particles go on shell) need to be carefully extracted. Second, the multi-loop integrals need to be combined with the corresponding contributions coming from the emission of additional partons in the final state. Indeed, loop integrals in general have infrared singularities that cancel against similar divergences coming from the integration over the phase space for the emission of additional unresolved (i.e., soft or collinear) partons in the process. Combining these two contributions in order to obtain a finite result can be a real challenge, and no completely

general and efficient method to do so is known beyond NLO.

Despite these difficulties, a lot of progress has been made in recent years regarding the the computation of NNLO corrections for two-to-two processes, and even first steps towards inclusive results at next-to-next-to-next-to-leading order (N<sup>3</sup>LO) have been taken. This progress is, on the one hand, due to a deeper understanding of the mathematics underlying large classes of multi-loop integrals, and, on the other hand, to progress in combining two-loop amplitudes with real-emission contributions. The aim of this contribution is to review these new directions and techniques and to summarise recent milestones.

## 2. Multiple polylogarithms and iterated integrals

The last couple of years have seen a lot of progress regarding the computation of multi-loop integrals depending on many scales. This progress is mostly rooted in a deeper understanding of the mathematics underlying the class of special functions appearing in the computation of multi-loop integrals. Indeed, large classes of loop integrals can be expressed through ordinary logarithms and the so-called classical polylogarithms, defined by

$$\log z = \int_1^z \frac{dt}{t} \quad \text{and} \quad \text{Li}_n(z) = \int_0^z \frac{dt}{t} \text{Li}_{n-1}(t), \quad (1)$$

with  $\text{Li}_1(z) = -\log(1-z)$ . Note that this class of functions contains  $\zeta$ -values, i.e., the Riemann  $\zeta$  function evaluated at integer values, as a special case

$$\zeta_n = \sum_{k=1}^{\infty} \frac{1}{k^n} = \text{Li}_n(1), \quad (2)$$

and for even values we have

$$\zeta_{2n} = \frac{(-1)^{n+1} B_{2n} (2\pi)^{2n}}{2(2n)!}, \quad (3)$$

where  $B_{2n}$  denote the Bernoulli numbers.

While these functions are sufficient to write down all one-loop amplitudes in four dimensions, it is well known that starting from two loops generalisations of these functions appear, see, e.g., ref. [2, 3, 4]. Most of the generalisations that physicists have introduced are special instances known in the mathematical literature as *multiple polylogarithms*, defined recursively by [5, 6]

$$G(a_1, \dots, a_n; z) = \int_0^z \frac{dt}{t - a_1} G(a_2, \dots, a_n; t). \quad (4)$$

In the case where all the  $a_i$ 's are zero, the integral (4) is divergent, and we define instead

$$G(\underbrace{0, \dots, 0}_{n \text{ times}}; z) = \frac{1}{n!} \log^n z. \quad (5)$$

The number  $n$  of integrations is called the *weight* of the multiple polylogarithm. Note that the ordinary logarithm and the classical polylogarithms are just special cases of multiple polylogarithms,

$$G(0; z) = \log z \quad \text{and} \quad G(\underbrace{0, \dots, 0}_{(n-1) \text{ times}}; 1; z) = -\text{Li}_n(z). \quad (6)$$

The ordinary logarithm then has weight one and the classical polylogarithms  $\text{Li}_n(z)$  and  $\zeta_n$  have weight  $n$ , and a product of two objects of weight  $n_1$  and  $n_2$  has weight  $n_1 + n_2$ .

Multiple polylogarithms have been in active field of research in number theory over the last decades, and there are many unexpected algebraic structures governing the properties of these functions. In particular, multiple polylogarithms form a so-called *Hopf algebra* [5, 6]. More precisely, we denote by  $\mathcal{H}$  the  $\mathbb{Q}$ -algebra spanned by all multiple polylogarithms, where multiplication is just given by the multiplication of functions. In addition,  $\mathcal{H}$  can be equipped with a co-associative coproduct, i.e., a linear map  $\Delta : \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}$  which preserves the multiplication,

$$\Delta(a \cdot b) = \Delta(a) \cdot \Delta(b). \quad (7)$$

The general definition of the coproduct for generic multiple polylogarithms is rather involved, so we content ourselves to give only the coproduct in the case of the classical polylogarithms,

$$\Delta(\log z) = 1 \otimes \log x + \log x \otimes 1, \quad (8)$$

$$\Delta(\text{Li}_n(z)) = 1 \otimes \text{Li}_n(z) + \sum_{k=1}^n \text{Li}_{n-k}(z) \otimes \frac{\log^k z}{k!}. \quad (9)$$

Note that the coproduct respects the weight of the polylogarithms, i.e., the sums of the weights of the two factors in the tensor product equals the weight of the original function. It is therefore natural to introduce functions that project onto the different weight components, e.g.,

$$\Delta(\text{Li}_n(z)) = \sum_{k=0}^n \Delta_{n-k,k}(\text{Li}_n(z)), \quad (10)$$

with

$$\Delta_{n-k,k}(\text{Li}_n(z)) = \begin{cases} 1 \otimes \text{Li}_n(z), & \text{if } k = n, \\ \text{Li}_{n-k}(z) \otimes \frac{\log^k z}{k!}, & \text{if } k \neq n. \end{cases} \quad (11)$$

Let us briefly discuss how these algebraic concepts are useful in the context of higher-order computations. One of the bottlenecks when computing Feynman integrals computations is that the special functions involved (e.g., the multiple polylogarithms), satisfy many complicated functional equations among themselves. Indeed, analytic results for multi-loop computations often lead to very long and complicated expressions. The question if this result can be simplified therefore naturally arises. Furthermore, it is well known that loop integrals have branch cuts, and functional equations are needed to extract the imaginary parts of the integrals before the functions can be evaluated numerically.

It turns out that the additional algebraic structure carried by multiple polylogarithms can shed light on these problems. Indeed, one of the main consequences of the Hopf algebra structure is that, at least conjecturally, *all* functional equations among multiple polylogarithms can be constructed recursively via the coproduct [7]. Indeed, we can iterate the coproduct to a map

$$\mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H} \rightarrow \dots \quad (12)$$

and co-associativity implies that this iteration is unique. As a consequence, every multiple polylogarithms can be decomposed into a tensor product of polylogarithms of weight one, i.e., ordinary logarithms, for which all functional equations are known. This maximal iteration of the coproduct is equivalent to what is known as the *symbol* in the literature [8, 9, 10, 11, 12, 13]

Let us illustrate this on an example, and let us consider the expression

$$X = \text{Li}_2(1-z) + \log z \log(1-z). \quad (13)$$

We may ask the question whether it is possible to combine these two terms in some way, i.e., whether there is a functional equation that allows us to simplify this expression. Note that  $X$  has uniform weight two, i.e., both terms have the same weight. We can decompose this expression into two factors of weight one by acting with the coproduct. Using eqs. (7 - 11), we find

$$\begin{aligned} \Delta_{1,1}(X) &= \text{Li}_1(1-z) \otimes \log(1-z) \\ &\quad + [\log z \otimes \log(1-z) + \log(1-z) \otimes \log z] \\ &= \log(1-z) \otimes \log z \\ &= \Delta_{1,1}(-\text{Li}_2(z)). \end{aligned} \quad (14)$$

Thus, we see that we must have

$$X = -\text{Li}_2(z) + c, \quad (15)$$

where  $c$  is annihilated by  $\Delta_{1,1}$ . Substituting  $z = 1$  in eq. (13) and (15), we find  $c = \zeta_2$ , and indeed  $\zeta_2$  is in

the kernel of  $\Delta_{1,1}$ . In other words, we have obtained a functional equation among dilogarithms via purely Hopf-algebraic means. While this particular functional equation is of course trivial and well-known in the literature, the same strategy can be applied to more general classes of multiple polylogarithms for which no functional equations can be found in the literature.

Functional equations can play an important role when computing multi-loop amplitudes. Let us illustrate this by discussing some examples. The first time the algebraic concepts we have introduced were applied to physics was not in the context of QCD, but in the context of the  $\mathcal{N} = 4$  Super Yang-Mills (SYM) theory in ref. [12], where the symbol was used to simplify the result of ref. [14, 15] for the two-loop six-point amplitude in  $\mathcal{N} = 4$  SYM to a single line of classical polylogarithms. This simplicity was completely hidden by the results for the individual Feynman diagrams, which are individually complicated combination of multiple polylogarithms, and it is only in the sum over all diagrams that these simplifications occur. By now these techniques have also found their way into QCD computations, and in particular they have been used to simplify the analytic expressions for the two-loop amplitudes for a Higgs boson plus three partons [16, 17, 7], light-quark contributions to top-pair production [18] as well as diboson production at two loops [19, 20]. Moreover, these techniques played a crucial role in the context of the  $\text{N}^3\text{LO}$  corrections to the inclusive Higgs cross section at threshold. This will be reviewed in Section 4.

From the previous discussion it is clear that the concept of weight plays a special role when discussing multiple polylogarithms, and thus loop integrals. It is therefore natural to ask whether the weight of the transcendental functions entering a loop amplitude has a special meaning. While it is known that certain special quantum field theories like the  $\mathcal{N} = 4$  Super Yang-Mills theory are indeed characterised by the fact that the multiple polylogarithms entering an  $\ell$ -loop amplitude all have weight  $2\ell$ , the same statement is false for more realistic theories like QCD. It was recently conjectured that it is always possible to choose the set of basis integrals appearing in a given amplitude (the so-called *master integrals*) in such a way that they have uniform weight order by order in the  $\epsilon$ -expansion in dimensional regularisation [21]. It is well-known that the master integrals satisfy systems of linear differential equations [22, 23, 24]. As differentiation lowers the number of integrations in eq. (4) by one, it follows that a basis of master integrals of uniform weight must satisfy a particularly simple system of differential equations. More precisely, if  $\vec{I}$  denotes the vector of all master integrals, then  $\vec{I}$  satisfies

a differential equation of the type [21]

$$d\vec{I} = \epsilon \left( \sum_i A_i d \log R_i \right) \vec{I}, \quad (16)$$

where  $A_i$  are constant matrices and  $R_i$  are rational functions. The system (16) is a special instance of the so-called Knizhnik-Zamolodchikov equation, which has been extensively studied in number theory. In particular, it is very simple to write down the solution to eq. (16) in terms of iterated integrals, similar to the definition of the multiple polylogarithms (4), to arbitrary order in the dimensional regulator  $\epsilon$ . This new approach to differential equations for loop integrals has led to a plethora of new analytic results, including the results for all two-loop four-point integrals relevant to the computation of the two-loop amplitude for the production of a pair of vector bosons with two different virtualities [25, 26, 27].

Computing NNLO corrections to physical observables does not only require the computation of two-loop amplitudes, but the latter must be consistently combined with the corresponding tree-level and one-loop amplitude for the emission of up to two additional partons in the final. This step will be discussed in the next section.

### 3. Infrared subtraction at NNLO

A physical observable computed at NNLO in perturbative QCD receives contributions from three different sources. Indeed, besides the loop corrections to the hard scattering process, there are contributions with additional unresolved partons in the final which contribute at the same order in the perturbative expansion. At NNLO, we have to consider the following three contributions:

1. The purely virtual corrections, i.e., the genuine two-loop corrections to the process.
2. The mixed real-virtual corrections, i.e., the contributions from the emission of one additional parton at one loop.
3. The doubly-real corrections, i.e., the tree-level contributions from the emission of two additional partons in the final state.

In general, each of these contributions is individually divergent, and the divergencies cancel in the sum, leaving behind the finite NNLO corrections to the observable. Nonetheless, it is not straightforward to combine

the three different contributions, because of the different origins of the infrared divergencies in each contribution. Indeed, while all the infrared poles from the virtual corrections arise explicitly from the loop integrations, the singularities from the real corrections are implicit and are only generated when integrating over the phase space of soft and / or collinear massless partons. Since every contribution involves a different number of final-state particles, and thus different phase spaces, it is not easy to combine them before phase-space integration.

The main strategy to combine the real and virtual contributions consists in the construction of explicit counterterms that can be subtracted from the real-emission contributions to render them finite. These counterterms should possess the same singularity structure as the real contributions, while still be simple enough that they can be added back in integrated form to cancel the explicit infrared poles from the virtual contributions. Moreover, they should be independent of the underlying hard scattering process, to avoid that the process of finding the correct counterterms has to be redone from scratch for each process.

The existence of counterterms that have the desired properties relies by the fact that the infrared poles from the emission of soft and collinear partons are universal and process-independent. For example, if we consider the tree-level production of a heavy colourless state  $X$  in association with two massless partons, then in the limit where the two partons are collinear to one of the incoming parton the amplitude factorises schematically as

$$\mathcal{A}_{2 \rightarrow X+2} \sim \text{Split}_{1 \rightarrow 3} \mathcal{A}_{2 \rightarrow X}, \quad (17)$$

where  $\text{Split}_{1 \rightarrow 3}$  denotes the so-called splitting function and captures the divergence in the amplitude when three partons become collinear. Note that the splitting function is independent of the underlying hard process (the production of the heavy colourless state  $X$ ). We can therefore compute the splitting function once and for all from a given process, and then reuse the same function to define the counterterms to regulate the infrared singularities arising from more general processes.

While the general strategy is quite clear, and the structure of the infrared singularities at NNLO was investigated already more than a decade ago (see, e.g., ref. [28, 29, 30]), a completely generic subtraction scheme for infrared singularities at NNLO is still lacking at the moment.

A lot of progress in this direction has been made over the last couple of years, and various different approaches have been developed to subtract infrared singularities at NNLO [31, 32, 33, 34]. Each of these

approaches comes with its own set of strengths and weaknesses, but they all rely on the factorisation of soft and collinear singularities to construct counterterms for the real emission contributions. While until a couple of years ago only very few NNLO results were available, the development of these new subtraction schemes has recently led to a revolution in the field. By now it is possible to obtain QCD prediction at NNLO accuracy for very large classes of two-to-two processes, provided that the two-loop corrections are available. Recent milestones in NNLO computations for hadron colliders include the NNLO computations for the cross section for the production of a pair of top quarks [35], single-top production (in the form factor approximation) [36], photon-pair [37, 38],  $ZZ$  [39] and  $WW$  [40] production, as well as the production of a Higgs boson in association with a jet [41, 42]. Results for the production of two jets at NNLO are also already available [43, 44, 45, 46, 47]. These results illustrate the maturity reached by the aforementioned techniques, and it is fair to say that NNLO will eventually be the new standard for two-to-two processes at the LHC.

#### 4. Towards QCD at $N^3$ LO

In some cases the knowledge of the NNLO corrections is not sufficient to reach reliable theory predictions. A prominent example of this type is the inclusive production of a Higgs boson at the LHC. Indeed, the main production mechanism at the LHC is the gluon fusion channel, and it has been known for a long time already that NLO corrections to the gluon fusion cross section are large [48, 49, 50, 51], making one wonder whether the perturbative series actually converges. Including NNLO QCD effects [52, 53, 54], as well as finite top-mass effect and NLO electroweak correction allows one to reduce the remaining uncertainty to about 5-10%. This level of uncertainty is challenged already now by the experimental uncertainty, making it clear that even higher-order QCD corrections, i.e., next-to-next-to-next-to-leading order ( $N^3$ LO) corrections will be required for the next phase of the LHC.

Various approximate results for the gluon-fusion cross section at  $N^3$ LO are available [55, 56]. These approximate results rely on the knowledge of various universal logarithms that are dominant for specific values of the partonic center-of-mass energy, combined with experience from the lower orders. The validity of these approximations at  $N^3$ LO can, however, only be confirmed by a full computation of the gluon-fusion cross section at this order in perturbative QCD.

Similar to the NNLO case discussed in the previous section, a complete  $N^3$ LO computation receives contributions from three different sources, corresponding to the emission of up to three additional partons at this order in the perturbative expansion:

1. **Triple-virtual:** The three-loop corrections to the production of a Higgs boson in gluon fusion. This contribution corresponds to the QCD form factor computed in ref. [57, 58].
2. **Double-virtual-real:** The emission of one additional parton at two loops, interfered with the leading-order matrix element for  $H + \text{jet}$ . The corresponding two-loop matrix element was computed in ref. [16].
3. **Real-virtual squared:** The contribution from the square of the one-loop amplitude for the production of an additional jet in the final state.
4. **Double-real-virtual:** The interference of the one-loop matrix element for the production of a Higgs boson plus two partons with the corresponding tree-level amplitude.
5. **Triple-real:** The square of the tree-level amplitude for  $H + \text{three jets}$ .

The full computation of the gluon-fusion cross section at  $N^3$ LO requires the computation of thousands of Feynman diagrams, and, besides the QCD form factor, only the real-virtual-squared contribution is known for arbitrary values of the partonic center-of-mass energy so far [59, 60].

Fortunately, the steep fall of the parton density functions with the energy suggests that the cross section can be well approximated by an expansion close to threshold. This expansion, which is controlled by the single parameter  $z = m_H^2/\hat{s}$ , where  $\hat{s} = x_1 x_2 s$  denotes the partonic centre-of-mass energy, was shown produce reliable results already at NNLO [53, 61, 62]. The cross section close to threshold can be written as

$$\hat{\sigma}_{ij}(s, z) = \delta_{ig} \delta_{jg} \hat{\sigma}_{gg}^{SV} + \sum_{k=0}^{\infty} (1-z)^k \hat{\sigma}_{ij}^{(k)}. \quad (18)$$

Recently the computation of the leading term in the threshold expansion at  $N^3$ LO, the so-called *soft-virtual* term  $\hat{\sigma}_{gg}^{SV}$  was completed [63, 64, 65, 66, 67]. We stress that only non-vanishing for the gluon initial state and contains the entirety of the three-loop corrections to inclusive Higgs production in gluon fusion, as well as the correction coming from the emission of additional soft gluons in the final state. This contribution obviously represents a the first step towards the full computation

of the  $N^3$ LO correction to the Higgs boson cross section.

We stress that the techniques from modern number theory reviewed in Section 2 have played a crucial role in the computation of the  $N^3$ LO corrections to Higgs production at threshold. Indeed, the integration over the phase space of the additional final state partons requires the computation of phase-space integrals which are beyond reach for conventional techniques. The integrations over the phase space often involves of complicated rational functions and (in the case of virtual corrections) multiple polylogarithms depending on the angles between the emitted particles. Standard integration techniques quickly reach their limits in these cases. It is, however, possible to use the number-theoretical tools described in Section 2 to construct algorithms to perform all the required integrations [68].

We conclude this section by giving a brief account on the validity of approximate  $N^3$ LO cross section. Even though the computation of the soft-virtual approximation is complete, it would be premature to draw strong phenomenological conclusions. Indeed, whenever we truncate a series expansion, an ambiguity is introduced which can be quantified by multiplying the result by an arbitrary function  $g(z)$  with  $\lim_{z \rightarrow 1} g(z) = 1$ . Indeed, it is easy to see that

$$\sum_{i,j} \int dx_1 dx_2 [f_i(x_1) f_j(x_2) z g(z)] \times \left[ \frac{\hat{\sigma}_{ij}(m_H^2, x_1, x_2, s)}{z g(z)} \right]_{\text{threshold}}, \quad (19)$$

has the same formal accuracy in the soft-virtual approximation, as long as we make sure that  $g(z)$  approaches 1 in the soft limit. Despite the fact that formal accuracy is the same in the soft limit, the numerical impact on the cross section can be quite sizeable, and a detailed analysis of the numerical impact of different choices for  $g(z)$  was presented in ref. [69]. Note that this ambiguity was already known at NNLO, where it was shown that the soft-virtual approximation underestimates the full NNLO cross section by a large amount. At the same time, it was observed a posteriori that choosing  $g(z) = z$  at NNLO leads to a very good approximation to the full NNLO result. In particular, this choice reproduces correctly the leading logarithmic behaviour of the first subleading term,  $\hat{\sigma}_0$ , in the soft expansion (18). Whether the same choice leads to a good approximation also at  $N^3$ LO currently still remains an open question that can most likely only be resolved once more terms in the threshold expansion, or ideally the full answer for the cross section, are known.

## 5. Conclusion

In this contribution we have reported on the status of QCD computations for the LHC at NNLO and beyond. We have focused mostly on recent developments in the field and have reviewed milestones in higher-order computations that could be achieved using these new techniques.

In a first part, we have reviewed recent progress in the computation of multi-loop integrals. The computation of these integrals has for a long time been a serious bottleneck, and is still one of the main obstacles when trying to perform computations at higher order. Inspired from developments in the  $N = 4$  Super Yang-Mills theory, a lot of progress was made in recent years regarding the understanding of the mathematics underlying multiple polylogarithms, a certain type of special functions which frequently appears in this context. Based on this advances, it was now possible to obtain analytic for multi-loop integrals that were considered beyond reach only a few years ago, both for computations at NNLO and  $N^3$ LO.

In a second part we have reviewed how to combine two-loop amplitudes with the corresponding real-emission contributions to obtain finite NNLO predictions. Several techniques to combine the purely virtual corrections with the real emission at NNLO have reached maturity in recent years. Combined with the aforementioned advances in multi-loop computations, we have entered a new era of QCD computations, where NNLO corrections might become the new standard at least for two-to-two processes.

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