

Computational challenges for multi-loop collider phenomenology

A Snowmass 2021 white paper

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Precision measurements at the LHC and future colliders require theory predictions with uncertainties at the percent level for many observables. Theory uncertainties due to the perturbative truncation are particularly relevant and must be reduced to fully exploit the physics potential of collider experiments. In recent years the theoretical high energy physics community has made tremendous analytical and numerical advances to address this challenge. In this white paper, we survey state-of-the-art calculations in perturbative quantum field theory for collider phenomenology with a particular focus on the computational requirements at high perturbative orders. We show that these calculations can have specific high-performance-computing (HPC) profiles that should to be taken into account in future HPC resource planning.

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1 Introduction

Already today, a number of measurements at the LHC reach uncertainties at the percent level. Standard candle processes like Z -boson production allow for even better experimental accuracy, down to the per-mille level for normalized kinematic distributions. At future colliders a comparable level of precision is expected for a wider range of observables. For example, for the high-luminosity run at the LHC (HL-LHC) even rare processes like Higgs boson production require theoretical control of cross sections at the level of 1%. For many processes current theoretical uncertainties do not match the anticipated experimental errors.

To fully exploit the physics potential of current and future collider experiments, in particular to unambiguously identify signals of new physics, it is crucial to improve the precision of theoretical predictions.

Theory predictions for hadron collider phenomenology are based on collinear factorization. In this framework predictions are made in terms of parton distribution functions (PDFs) and partonic hard cross sections, and they are expected to be valid up to corrections which are suppressed in the high energy limit. The partonic cross sections are computed in perturbation theory, and within the Standard Model of particle physics (SM) this means an expansion in the strong and the electroweak couplings. A dominant source of uncertainty originates from higher-order terms in these expansions which is the focus of this white paper. Nevertheless, we also note that depending on the observable studied and the kinematic region considered, other sources of uncertainty might dominate, for example due to parametric dependence (on PDFs, couplings, masses), non-perturbative effects (like hadronization, multi-parton interactions, etc.), or the appearance of large logarithms which would need to be resummed.

In this white paper, we focus on current calculational methods and computational challenges necessary to reduce perturbative truncation uncertainties of parton-level predictions. We performed a survey and asked authors of various state-of-the-art *multi-loop* calculations about their computational resources needs. For our survey we received responses that cover 53 scientific publications. This data provides a picture of where current analytic and computational requirements lie, and gives an impression of where the field is moving with respect to resource requirements.

In the following, we first give a brief overview of a related study made during the 2013 Snowmass community planning. In section 2 we highlight state-of-the-art methods for the calculation of Feynman integrals, while in section 3 we discuss multi-loop scattering amplitudes. In section 4 we highlight recent precision cross section calculations. We end with conclusions and an outlook in section 5, where we point out specific computing needs of our community which should be taken into account in future high performance computing (HPC) resource planning.

State-of-the-art at Snowmass 2013. In 2013 a white paper on “Computing for perturbative QCD” [1]¹ presented a survey of computational requirements of then state-of-the-art hadron collider phenomenology. This included benchmarks for high-multiplicity next-to-leading-order (NLO) QCD calculations with up to 6 final-state particles and also benchmarks of early next-to-next-to-leading-order (NNLO) QCD calculations for $2 \rightarrow 1$ and $2 \rightarrow 2$ processes.

Concretely, examples presented included an NLO QCD calculation of $W + 5$ -jet production [3] which required about 600,000 CPU hours with year 2013 hardware. Differential NNLO QCD calculations for $W/Z/H$ production were available [4–6] and benchmarked. Their evaluation took 50,000 core hours (2013), while total inclusive $t\bar{t}$ production [7, 8] took about 1M core hours (2013). Further processes with NNLO QCD corrections included single jet production [9] (85,000 core hours in 2013) and H +jet production [10] (500,000 core hours in 2013) in the gluon-gluon channel. Translating these core hour numbers into node days (100,000 core hours equal about 500 node days assuming 8-core systems from 2013) makes clear that these calculations were only possible due to the use of HPC systems. Nevertheless, apart from these

¹see also the Snowmass QCD working group report [2]

examples, the majority of developments at that time did not rely on larger-scale computing resources.

Compared to state-of-the-art hardware from 2013, current state-of-the-art hardware (2022) has single-threading performance that is better by a factor of four to five. Moreover, due to improvements in multi-core architecture, current single CPU (but multi core) node performance is better by a factor of up to 25-30. For example, this alone means that $2 \rightarrow 1$ NNLO QCD calculations that required a large cluster with hundreds of nodes 10 years ago would now run on a small-size cluster with just a few nodes. Furthermore, algorithmic and theory developments have considerably brought down computational requirements, for example allowing (multi-)boson $2 \rightarrow 1$ and $2 \rightarrow 2$ production at NNLO QCD to be computed within hours on current desktop machines [11].

In 2013 a community goal was envisioned to take advantage of new large-scale computing and to benefit from using new hardware like GPUs and Intel Phi many-core systems. Further, questions regarding the increased role of parallel computing, what could be gained by consolidation of resources, and limitations in the software environment were posed. Also questions about public availability of codes, grade of automation, expandability, versatility (cuts, etc.) and user-friendliness were raised. All of these are important aspects to ensure that the efforts to complete these challenging calculations have the highest impact in the theoretical and experimental communities. These topics continue to be relevant and we will comment on them from today's perspective in this white paper.

Enormous progress has been achieved since the last Snowmass exercise in the field of precision high energy phenomenology. The very challenging calculations from then have become standard and relatively fast, and calculations that then would have appeared as unfeasible have actually been completed, like for example fiducial-level next-to-next-to-next-to-leading-order (N^3LO) QCD calculations for $2 \rightarrow 1$ processes and NNLO QCD calculation for $2 \rightarrow 3$ processes. In the rest of this article we highlight analytical and numerical techniques that have been developed to allow this to happen and discuss challenges for the coming decade in precision QCD phenomenology.

2 Feynman integrals

Feynman or loop integrals are basic building blocks of perturbative quantum field theory (for a recent pedagogical introduction see ref. [12]). They contain key information about the structure of scattering amplitudes and their singularities. This motivates detailed studies of the mathematical representations of Feynman integrals to gain a deep understanding of their analytical properties and (singular) behaviour in particular kinematic limits. For phenomenological purposes, one ultimately wants to numerically evaluate the expressions, such that the error is reliable, the result has sufficient precision and the computation requires acceptable resources. In that context, suitable analytical preparations of the integrals (and amplitudes) can be regarded as effort during the *development* phase, while the actual numerical evaluation of the expressions during the Monte Carlo integration over phase space represent the *production* phase for collider observables. Different methods have been developed which put more or less emphasis on the analytical preparations. Typically, dedicated analytical manipulations are somewhat process specific and more difficult to automate, while numerical techniques allow more flexibility perhaps at the expense of lower efficiency. Below we highlight

recent progress in the development of techniques for the analytic and numerical evaluation of Feynman integrals for collider phenomenology.

The current state-of-the-art in evaluating multi-loop Feynman integrals include two-loop integrals for $2 \rightarrow 2$ processes with internal masses (see e.g. [13–18]), $2 \rightarrow 3$ processes with up to one massive leg (see e.g. [19–28]), three-loop integrals for $2 \rightarrow 2$ processes (see e.g. [29, 30]), and four-loop integrals for $2 \rightarrow 1$ processes (see e.g. [31–38]).

Analytical solutions. In the method of differential equations [39–41], one derives a coupled, first-order, linear system of differential equations for a set of basis or master integrals, where the derivatives are taken with respect to the external kinematic invariants. To achieve this, one needs to determine linear relations between Feynman integrals, usually computed through integration-by-parts reductions. In simpler cases with few physical scales, one can solve the differential equations analytically, where a suitable choice of basis integrals is essential for the successful integration. In particular, the choice of a canonical basis [42] can greatly simplify the construction of a solution and has been used in many calculations in the recent past. The direct integration of parametric representations can also be used to obtain solutions. In the case of linearly reducible integrals [43], the program `HyperInt` [44] allows for an automated approach to obtain results in terms of multiple polylogarithms, see e.g. [45, 46] for applications.

Obtaining analytical solutions typically requires one to study non-standard special mathematical functions in some detail, possibly developing new algorithmic methods for them. Examples for such functions are harmonic polylogarithms [47], multiple polylogarithms [47, 48] and elliptic polylogarithms [49–54]. If a functional basis is chosen with numerical performance in mind, the resulting expressions may allow for precise and fast numerical evaluation using universal libraries, at the order of a second per phase space point for state-of-the-art two-loop amplitudes. Several such universal libraries have been developed for multiple polylogarithms, for example the implementation of ref. [55] in `GiNaC` and the `HandyG` library [56]. More recently, algorithms and tools for iterated integrals related to elliptic Feynman integrals have been developed [57, 58]. A more comprehensive discussion of special functions relevant for collider physics can be found in a recent Snowmass white paper [59]. The above methods usually aim at numerical evaluation through series expansions of the special functions. Alternatively, mapping Chen-iterated integrals to one-fold integral representations were shown to provide good performance through numerical quadrature, see for example the `C++` libraries for $2 \rightarrow 3$ processes in [23, 25].

Numerical methods. In particular for cases with many masses and complicated branch cut structure, an analytical solution suitable for numerical applications may be difficult to obtain, in particular if intricate analytical continuations are required. Numerical methods allow to treat these cases and offer great potential for automation.

A numerical method which has been studied for a long time are integrations of Feynman parametric representations. Due to the presence of divergences when taking the limit $\epsilon \rightarrow 0$ for the dimensional regularization parameter, one cannot simply expand the integrand in ϵ for arbitrary integrals. One way to make the poles in ϵ manifest and to arrive at finite integrals for the ϵ expansion which can be evaluated on the computer is the technique known as sector decomposition [60]. In the past decade, this method has been fully automated for

physical kinematics [61] and the public codes `pySecDec` [62] and `Fiesta` [63] can efficiently exploit quasi-Monte Carlo methods as well as the usage of GPUs, see e.g. [15, 64–67] for applications.

It has also been observed that one can always reduce Feynman integrals in terms of a basis of finite Feynman integrals [15, 45, 68]. In principle, one can straight-forwardly expand these integrals in ϵ and perform the integration numerically. In practice, evaluating such finite integrals with established sector decomposition codes provides better performance than each of these methods alone [69]. Still, obtaining sufficient precision for phenomenological applications can require substantial computation time and the usage of cluster resources. Other numerical approaches include building on established libraries for one-loop integrals to exploit dispersion relations to calculate two-loop integrals with internal masses [70], and using Mellin-Barnes representations to calculate two-loop integrals with several internal masses [71], among other.

A semi-analytic alternative can also be constructed by solving differential equations for master integrals with respect to external invariants numerically using generalized power series. The latter method gained significant popularity in the last few years, since it allows not only for a very generic approach but also for particularly precise and fast evaluations [13, 14, 21, 26, 72–76]. Typical evaluation times are of the order of a minute per phase-space point for two-loop applications. The `DiffExp` program [77] provides a public implementation based on the method of Frobenius. One can combine this method with the direct integration techniques discussed above to fix boundary values in Euclidean phase space points [78].

Another alternative to obtain boundary conditions goes under the name of the auxiliary mass flow method [79–82]. It exploits differential equations with respect to a technical mass parameter introduced in the propagators, and a public implementation of the approach, `AMFlow` [83], has been presented recently. Applications of this method can be found for example in refs. [16–18]. While in the auxiliary mass flow method the required integration-by-parts reductions are more challenging (given the modified propagator structure), it has the advantage that it allows to easily fix boundary values in a generic way.

3 Scattering amplitudes

Scattering amplitudes are at the core of all collider phenomenology predictions. They contain the dynamical information associated with the models used to describe data. At the energies of current high energy colliders, amplitudes are computed perturbatively in the strong and electroweak couplings. Quantitatively reliable predictions at the LHC with uncertainties of $\mathcal{O}(15\text{--}20\%)$ require the inclusion of at least first-order corrections in the strong coupling (NLO QCD), while for precision studies with uncertainties below $\mathcal{O}(7\%)$ it is generally necessary to include second-order or higher corrections in the strong coupling (NNLO QCD) as well as first-order corrections in the electroweak coupling (NLO electroweak).

To obtain these types of predictions for the wide variety of processes of interest at the LHC, a myriad of one-loop, two-loop and three-loop amplitudes are required (also tree-level amplitudes, which can now be computed for essentially arbitrary particle multiplicities with standard tools). Although general calculational methods are available, the complexity of amplitude calculations grows quickly with the number of loops as well as with the number of physical scales such as particle masses and kinematic invariants. As a consequence, large

efforts are required by the high energy theory community to make sure that amplitudes are available for phenomenological applications.

One-loop amplitude calculations in the SM (as well as in theories beyond the SM) can now be completed employing highly automated frameworks. Even for whopping $2 \rightarrow 8$ processes with multiple internal/external massive particles they can be obtained with standard computational resources. This has been the case thanks to the development of highly automated libraries like `Helac-NLO` [84], `MG5_aMC@NLO` [85, 86], `NLOX` [87], `OpenLoops` [88], `Recola` [89], as well as many other public and private tools.

Two- and higher-loop calculations remain challenging, in particular those that are related to many scales. But in the last five years many new calculations have been completed due to several major advances in our understanding of the analytic structure of scattering amplitudes in perturbative quantum field theory. These calculations include for example two-loop amplitudes for $2 \rightarrow 2$ processes with 4 or more scales [15, 17, 46, 65, 67, 90–93], two-loop amplitudes for massless $2 \rightarrow 3$ processes [94–103], two-loop amplitudes for $2 \rightarrow 3$ processes with one external massive particle [24, 104–106], three-loop form factors for $2 \rightarrow 1$ processes with massive particles [107–112], three-loop amplitudes for massless $2 \rightarrow 2$ processes [113–116], and four-loop form factors for $2 \rightarrow 1$ processes [31, 38, 117]. Major progress has been achieved also for the calculation of related quantities, for example the complete five-loop beta function [118, 119] and first results for the four-loop splitting functions [120, 121].

Multiloop amplitude construction. Multi-loop scattering amplitudes are typically decomposed in terms of so-called master integrals and their algebraic coefficients. This decomposition can be achieved by generating Feynman diagrams, applying projectors to them, and using integration-by-parts identities [122] to reduce the resulting integrals to master integrals. It is well known that when considering helicity amplitudes their analytic expressions are considerably simpler than what their Feynman diagrammatic representation would suggest. This simplicity is made even more evident when employing a specially chosen basis of special functions, which reflects the holomorphic structure of the amplitude.

In order to construct an analytic integrand, projector methods have been proposed recently [123–125] that avoid evanescent structures in the calculation of helicity amplitudes in dimensional regularization, which is of particular relevance for higher multiplicities. Techniques based on numerical integrand reduction have also been developed at the multi-loop level [126–129], which build on the success of the one-loop OPP method [130–132]. They allow to efficiently extract integrand coefficients by matching to numerical evaluations. One novel integrand parametrization is that of the *master-surface* decomposition [133] which allows to incorporate the reduction to master integrals directly in the integrand matching procedure. This parametrization was key for pushing the numerical unitarity method [134–136] to the multi-loop level [137–140] where full amplitudes can be computed numerically based on tree-level amplitudes, removing the need of building analytic integrands. Efforts are also underway to extend successful one-loop numerical techniques based on 4-dimensional integrand reduction and recursive techniques for rational term calculations to the two-loop level [141–144].

A core computational bottleneck in the computation of amplitudes is the handling of linear relations between Feynman integrals (integration-by-parts identities). In principle, Laporta’s algorithm [145] provides a general solution to the problem. Currently, several public reduction

codes are available, for example `Fire` [146], `Reduze` [147], `LiteRed` [148], and `Kira` [149]. In practice, one still faces significant practical challenges for state-of-the-art problems due to the large size of the required systems of equations and the complexity of the emerging algebraic coefficients. In recent years, a deeper systematic understanding of the linear relations has been gained through methods from polynomial ideal theory [15, 150–155]. In particular, the computation of syzygies allows to systematically reduce integrals to a set of master integrals without the introduction of many auxiliary integrals.

Choosing suitable master integrals helps to avoid the introduction of spurious denominator factors (singularities) [156, 157], which helps to reduce the algebraic complexity. Pioneering work based on intersection theory [158, 159] raises the question whether such completely new techniques to efficiently perform integral reductions for complicated problems may become available in the future.

Sampling methods and distributed computations. Perhaps one of the most drastic changes in the field regards the wide use of various numerical sampling techniques to construct analytic expressions for multi-loop amplitudes. Since all multi-scale multi-loop amplitudes mentioned above are functions of not too many variables (say up to six variables), one might expect that symbolic results allow for faster evaluation compared to numerical approaches. However, due to the sheer size of the intermediate algebraic expressions, arriving at these results by symbolic manipulations can become very challenging. Instead, numerical or semi-numerical approaches avoid computational complexity at intermediate stages and are better suited for distributed computations.

The use of modular arithmetic (finite fields) in the calculation of integration-by-parts reductions was proposed in ref. [160]. The general idea is to perform computations with different integer samples for the variables in the problem and to reconstruct the symbolic information of interest from many such evaluations. A major advantage of this approach is that intermediate expression swell can be systematically avoided. Soon after it was shown [161] how helicity amplitude coefficients can be reconstructed from finite field samples, treating multivariate rational functions through a carefully crafted nested approach.

Finite field sampling and functional reconstruction techniques like these have become standard for cutting-edge problems in the past few years, and several public [146, 149, 162–164] and private implementations have been developed. These algorithms are rather flexible and can be employed at several stages of the calculations, allowing simplifications to be readily applied before the analytic structures are reconstructed. This includes for example removing lower-loop information by targeting the corresponding “finite remainder”, accessing the amplitude at the special function level by expanding it as a Laurent series in ϵ , precomputing the denominator structure of the rational functions involved, among others. Another numerical approach for extracting analytic expressions but using high-precision floating-point arithmetic together with carefully crafted ansätze was presented in ref. [165] (see applications in ref. [166–168]) and recently extended to an approach closely related to finite fields, based on p -adic numbers [169].

To use an amplitude calculation in a phenomenological application, the corresponding numerical evaluation has to be efficient (in time and memory) and numerically stable over phase space even close to singular regions. The identification of linear relations between rational functions and a suitable representation of the rational functions themselves can help

to reduce the size and numerical stability of the amplitudes. In particular, using multivariate partial fraction decomposition [170, 171] instead of a common-denominator form can help significantly in that regard, see for example ref. [96]. Public implementations of recent algorithms in the `Singular` CAS [172] and in the `MultivariateApart` [173] package can be used for distributed computation of the necessary manipulations in a cluster-friendly way.

These novel techniques have opened the door to perform computer algebraic computations for quantum field theory on HPC systems. These novel methods typically use integer arithmetic rather than floating point arithmetic and, depending on the problem, they may require a significant amount of memory per core. The development of (public) codes for challenging amplitude calculations in a HPC friendly way is an ongoing effort. Currently, in some situations, one may need to resort to implementations that have large memory demands and require run-times that are hard to predict and possibly well beyond available batch limits on a given cluster.

4 Applications in collider phenomenology

Ultimately multi-loop amplitudes and other associated ingredients enter the calculation of cross sections and other observables. To obtain cross sections, degenerate final states at each order in perturbation theory must be summed over. This in turn requires the introduction of a mechanism to regularize and cancel related infrared (IR) divergences, the so-called IR subtraction methods.

IR subtraction methods. Subtraction methods are available that cancel IR singularities locally in phase space, or that are based on a single IR cutoff (slicing) that must be extrapolated to a vanishing cutoff size. In general, the complexity of subtraction methods increases with the number of colored particles until all different singular limits of a given perturbative order are probed and extensions to more particles turn into a combinatoric problem. For example in NNLO three-jet production all double-singular limits are probed among colored particles.

While local subtraction schemes require significant development time, they generally lead to Monte Carlo phase space integrations that are numerically easier to perform. Slicing methods on the other hand are simpler to construct and have the benefit that they can easily re-use lower order components. An example slicing method is the one based on factorization in the q_T variable, which is currently the only technique used to obtain fully differential N³LO results for a color singlet process [174]. If a fully inclusive N³LO calculation is available, also projection to Born (P2B) is a method to perform an efficient and fully differential calculation [175].

Slicing methods are typically based on factorization in a kinematic observable. At NNLO methods are available based on the q_T observable [176–178] for color singlet systems or based on N -jettiness [179–181] for generic processes. With N -jettiness the ingredients are available for NNLO calculations with up to one colored final-state particle. N³LO (three loop) soft [182, 183] and beam functions [184, 185] in q_T factorization allow for fully differential N³LO calculations of colorless final states, see also the Snowmass white paper on “The Path forward to N³LO” [186]. The calculation of power corrections allows for accelerated

calculations using larger slicing cutoffs, see e.g. [187–189]. A different slicing approach at NNLO has been undertaken in ref. [190].

As for local subtraction schemes, Antenna subtractions [191, 192] and sector-improved residue subtraction (STRIPPER) [193–195] have been applied up to two [196–198] and three [199, 200] colored final states in pp collisions. Nested soft collinear subtractions [201] have been applied to deep inelastic scattering (DIS), Higgs production and mixed QCD-EW corrections in Drell-Yan production [202–204], ColorFulNNLO [205] to e^+e^- three-jet production [206] and $H \rightarrow b\bar{b}$ [207], and local analytic subtraction [208] to Drell-Yan production. A recent comprehensive overview of all past processes implemented using the various subtraction schemes is available in ref. [209], table 5. The local subtraction methods differ in the partitioning of phase-space and analyticity of counterterms. Extensions beyond NNLO will be a major undertaking both in phase-space partitioning and integration of triple singular counterterms and one can expect progress on them during the next decade. Overall the current development focus is still at the level of refining, automating and generalizing current methods at NNLO.

The current frontier in multi-loop phenomenology revolves around NNLO QCD corrections for $2 \rightarrow 3$ processes with massless particles, two-loop mixed QCD-EW corrections for $2 \rightarrow 1$ and $2 \rightarrow 2$ processes, corrections to $2 \rightarrow 2$ processes involving two-loop amplitudes with additional internal masses (massive QCD) and fiducial N³LO QCD $2 \rightarrow 1$ processes. For one-loop phenomenology, high-multiplicity processes play a special role as they also consume a considerable amount of resources. In the following we list a few examples of state-of-the-art applications that rely on the advancements presented in this white paper.

$2 \rightarrow 1$ fiducial N³LO. Currently, the upper end of computational resource requirements is consumed by fiducial N³LO calculations. In the q_T subtraction approach, NNLO real emissions need to be determined with high precision in regions close to singularities, resulting in significant computational costs of up to about 10M CPU core hours.

Fiducial Drell-Yan production at N³LO has been computed in ref. [174] using q_T subtractions and using antenna subtractions for the NNLO real emission process. Fiducial Higgs results have been presented at N³LO [210] using P2B and using antenna subtractions for the real emission, reducing resource requirements by an order of magnitude or two compared to slicing. Improved Higgs results that include q_T resummation of fiducial power corrections at the level of N³LO have been presented in ref. [211].

$2 \rightarrow 3$ at NNLO. Phenomenology for $2 \rightarrow 3$ processes at NNLO broadly uses a few hundred thousand up to a million CPU core hours per project, depending on the final state. In this, the real emission is a major factor. While the analytic calculation of the two-loop amplitudes may need substantial computational resources by itself, the numerical evaluation of carefully optimized representations typically does not represent a major challenge. Alternatively, the virtual corrections have been integrated using a pre-computed interpolation grid.

Triphoton production ($\gamma\gamma\gamma$) has been computed within the STRIPPER framework [212]. It has also been studied with q_T subtractions [213], evaluating the two-loop integrals with the `PentagonFunctions++` library [23] using the two-loop matrix elements of ref. [98]. Using STRIPPER, a calculation of 3-jet production at NNLO has been presented [199] using the double-virtual contributions of ref. [101] (see also recent related work in ref. [200]). Using the

same framework also $\gamma\gamma$ +jet production at NNLO has been computed [214] employing the double-virtual contributions of refs. [102, 103]. For the latter process also the gluon-initiated (loop-induced) contributions have been computed including NLO corrections [215] employing the two-loop matrix elements of ref. [216].

$2 \rightarrow 1$ and $2 \rightarrow 2$ with many scales. The computational requirements for $2 \rightarrow 2$ color singlet processes at NNLO without internal masses are much lower, at the order of just a few hundred CPU core hours. However, the demands increase drastically in the presence of jets due to the more complicated singularity structure, in some cases reaching a few hundred thousand CPU core hours, see e.g. refs. [196, 197, 203, 217–219]. Computational demands can also increase due to cuts for otherwise simple processes [220].

The calculational and computational complexity also increases with a larger number of scales, as for example in EW corrections or in QCD with massive quarks. Often such problems are at the frontier of loop-integral complexity. In some cases, such as for the mixed QCD-EW corrections to Drell-Yan processes, analytical representations of two-loop amplitudes with internal masses were still an option [91, 204, 221], rendering the computational demands for phenomenological applications unproblematic. In other cases, numerical approaches are the only available option. The computational demands of the latter are up to a few hundred thousand CPU core hours, while memory requirements are again dominated by the reduction to master integrals and can be especially demanding here, up to 2TB per node for some surveyed calculations.

For example, for H +jet and di-Higgs production the full top-quark mass dependence has been obtained only numerically with sector decomposition [64, 65, 90]. These calculations used around 10,000 hours on GPUs (generation 2012) each for the numerical integration, with a median of two hours (and up to two days) necessary for evaluating one phase space point. These calculations are the only ones in our survey that systematically use GPU resources. Given the development of this type of technology in most planned HPC systems, such applications may increase in the future.

The numerical evaluation of loop integrals through series solutions of differential equations is becoming increasingly popular and has been used in several phenomenological applications already. In ref. [111] the exact top-mass dependence in fully inclusive Higgs production has been calculated this way at NNLO in QCD. The mixed QCD-EW corrections to Drell-Yan production presented in ref. [92] relied on numerical evaluations of the most complicated integrals through series expansions. A further application of the method was the calculation of two-loop non-factorizable NNLO QCD contributions in single-top-quark production [18].

High-multiplicity NLO and NNLO matched to parton showers. State-of-the-art NLO predictions for processes with high multiplicities (see e.g. $t\bar{t}b\bar{b}$ production studies [222–224]) can have computational costs similar to current state-of-the-art NNLO calculations, at the order of 100k–1M CPU core hours.

Resource demands for event generators that include parton shower, hadronization and possibly detector simulation are overall orders of magnitude larger than parton-level predictions. They fall outside the scope of this white paper, see e.g. the Snowmass white paper on event generators [225]. Nevertheless, we would like to mention that meanwhile NNLO calculations are matched to parton showers, and the resource requirements of matched processes reach

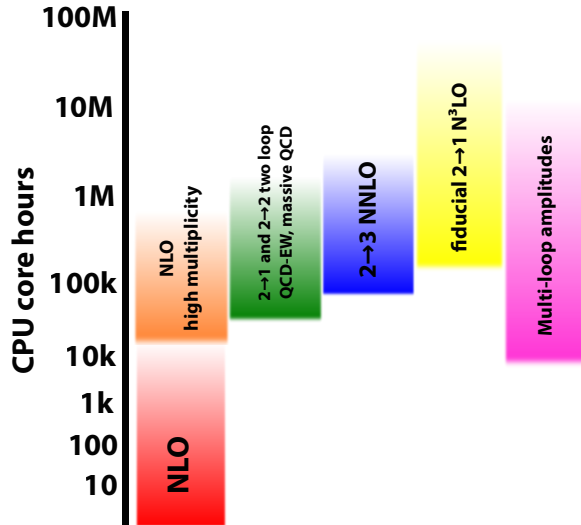


Figure 1: Run-time requirements of recent perturbative calculations for collider phenomenology. Memory requirements ranged up to about 2 TB of RAM per node.

those of more complicated NNLO calculations, at the level of a few hundred thousand CPU core hours, see e.g. refs. [226–229].

5 Conclusions and outlook

During the last ten years tremendous progress on higher-order calculations for collider physics has been achieved. The use of HPC systems for these applications is now both a standard as well as a requirement. With Snowmass 2013, the computational requirements of perturbative calculations were assessed and several questions were posed for discussion in order to efficiently push the boundaries of precision studies [1, 2]. For this Snowmass 2021 white paper we provide an update regarding the current status of the field and give an outlook for the decade ahead.

Use of CPU parallel computing. When comparing previous with current state-of-the-art computations, we notice that node hour requirements are not *vastly* different despite a very significant increase in the complexity of the treated problems. In many cases, theoretical developments lead to much more efficient approaches. In addition, single core performance has increased by a factor of four to five since 2013 and single CPU/node performance has increased by a factor of 25-30 for state-of-the-art hardware. This discrepancy between single core performance and CPU/node performance is a trend that is expected to continue in the future, given that transistors already reach a few nm in size. A consequence of this is that using parallel high performance computing becomes ever more important to benefit from improvements in computing technology.

Parallel computing is used by the community, although mostly in terms of independent jobs and not with inter-process communication using for example MPI. For some cases this is sufficient or advantageous, but in other cases, e.g. large phase-space integrations,

calculations can benefit from efforts in using distributed computations based on MPI or a similar framework.

Use of GPUs. Modern computing paradigms focus more and more on the use of specialized GPUs instead of general purpose CPUs. All new leading DOE clusters like NERSC Perlmutter, Argonne Aurora and Oak Ridge Frontier follow this paradigm and focus on nodes with GPUs. GPUs offer distinct advantages for single instruction multiple thread and multiple data problems that do not require irregular access to large amounts of memory. The use of GPUs is still unclear in our field, since many problems in our field rely on the numerical evaluation or handling of algebraic expressions which are large and/or require irregular memory access patterns. So far, GPUs have found application to cutting-edge problems with the numerical integration of sector decomposed loop integrals. A first step for future applications could include the efficient evaluation of one-loop amplitudes. This would help the huge computational requirements for NLO high-multiplicity evaluations, but also for the real emission integrations for NNLO calculations. Since the efficient use of GPUs is still unclear, future computing for our community will still need to focus on providing CPU resources without attached GPU resources.

Memory and run-times requirements. A number of multi-loop amplitude calculations involving computer algebra are limited by the available memory per core or even per node. In addition, long run-times may be required and break-pointing might not be a good option in practice due the required additional development efforts or the use of proprietary software and external dependencies. We note that both memory and run-time requirements may be intrinsically difficult to predict for such type of problems. Moreover, often a variety of different approaches and codes will be tested or combined, and only limited human resources are available for software development to adapt to the given constraints on the available clusters. Currently, many of these calculations are being performed on local computing resources, partly outside of a larger shared cluster infrastructure to circumvent constraints imposed by general cluster policies. Regarding availability of resources, more high-memory nodes and more flexibility on long job run-times could provide effective help. Through snapshots, virtualization solutions in cluster environments may resolve the tension between such calculational demands and requirements of cluster maintenance.

Machine learning. Machine learning, while being explored, has not made significant impact yet within the research scope presented here at the multi-loop level. Machine learning is being explored for improving traditional optimization and interpolation problems. For example the optimization of phase-space integration has been studied, as well as the fast interpolation of multi-loop hard scattering functions. So far the most promising applications focus on the event generation beyond the parton level, see e.g. the Snowmass white paper on “Machine Learning and LHC Event Generation” [230].

Availability and usability of codes. The public availability of codes and results is a crucial aspect to improve efficiency of the community and to reduce friction in exchanges and comparisons. State-of-the-art multi-loop amplitudes are nowadays provided by many authors in machine-readable format, and increasingly also building blocks like master integrals or even

reduction tables. The level of sophistication of modern tools for tasks like integral reduction or integral evaluation clearly motivates their public availability, such that they can be used by different research groups. Indeed, an increasing number of authors invest the required time to make their codes accessible to others and share them early on. We believe this is an important development which increases productivity in our field, and that attention should be paid to longer-term career perspectives of young researchers engaging in these efforts. Of course, public codes with proper documentation also avoids loss of intellectual achievements if Ph.D. students or postdocs leave the field. Public availability is also relevant for entire cross section calculations to allow for derived work and comparative studies. Currently, a subset of NNLO codes are publicly available.

Codes using proprietary software like Mathematica or Maple are limited by license availability for large deployments on clusters. In practice, such systems may offer distinct advantages as a development platform and are therefore frequently used, both for less resource-critical tasks and for prototyping. While limitations regarding the usage on clusters can eventually be avoided with dedicated implementations not relying on proprietary software, it remains a problem-specific decision whether the expected gains justify this additional effort.

Grade of automation. Nowadays, highly automated codes are available for the computations of NLO corrections, including even electroweak interactions. While 2013 marked the early advent of NNLO calculations, meanwhile a much higher level of sophistication has been achieved by treating also $2 \rightarrow 3$ processes like $pp \rightarrow 3$ jets and lower multiplicity processes with many scales at NNLO. Amplitudes, loop integrals and IR subtractions all pose highly difficult problems that require dedicated efforts for their automation. With current technology we are indeed getting closer to the automation of NNLO calculations – raw ingredients are available for amplitudes, the numerical evaluation of loop integrals and NNLO IR subtractions to high multiplicities. Typically generic numerical methods allow for easier automation, while targeted analytical work can provide particularly efficient implementations. Overall, a lot of consolidation work is still necessary for automated NNLO frameworks, which we expect to take place in the upcoming decade.

Closing remarks. Overall the sample state-of-the-art projects surveyed for this white paper took each 2-5 years of total PhD/postdoc research time. This is a significant time in terms of the average hiring span of PhD students and postdocs and points to the trend for larger collaborations to exploit synergies. Furthermore, each precision calculation (at NNLO or beyond) relies on more than a decade of developments in the IR subtraction frameworks and in the mathematical and algorithmic developments for amplitudes and loop integrals. This motivates a continued effort to provide public and well documented codes for tools and predictions, so that the whole theory and experimental communities can benefit from state-of-the-art advancements.

Today’s typical computational resource requirements for phenomenological predictions are at the order of a few hundred thousand core hours and reach up to about 10M core hours; a distribution of them is sketched in fig. 1. This is in stark contrast to the last Snowmass planning in 2013, where the use of cluster resources was more of an exception rather than standard. The majority of people answering our survey deemed the currently-available resources sufficient for their current projects, although in some cases easier access to suitable cluster resources would have been beneficial. For the next 5-15 years, we expect to see

NNLO predictions for more complex final states, the automation of these calculations, and N³LO predictions for diboson processes. Numerical and semi-numerical methods as well as distributed computing are expected to play an essential role in these efforts. It remains unclear to which degree GPUs can be employed, such that the availability of CPU-oriented cluster resources stays important. Nodes with multiple TB of memory continue to be of high relevance for computer-algebraic components of the calculations. Flexible job run times significantly benefit some developments, and virtualization solutions with snapshot capabilities could enable this in cluster environments.

Acknowledgments. We would like to thank the following people for filling out our survey and providing valuable input on the computational resources of their projects: Samuel Abreu, Bakul Agarwal, Konstantin Asteriadis, Simon Badger, Matteo Becchetti, Marco Bonetti, Federico Buccioni, Luca Buonocore, Fabrizio Caola, Gudrun Heinrich, Alexander Huss, Stephen P. Jones, Stefan Kallweit, Matthias Kerner, Matteo Marcoli, Javier Mazzitelli, Johannes Michel, Sven Moch, Marco Niggetiedt, Costas Papadopoulos, Mathieu Pellen, Rene Poncelet, Jérémie Quarroz, Luca Rottoli, Gabor Somogyi, Qian Song, Vasily Sotnikov, Matthias Steinhauser, Gherardo Vita, Chen-Yu Wang, Stefan Weinzierl, Marius Wiesemann, Malgorzata Worek, Tongzhi Yang and YuJiao Zhu.

The work of Fernando Febres Cordero is supported in part by the United States Department of Energy under grant DE-SC0010102. Andreas von Manteuffel is supported in part by the National Science Foundation under Grant 2013859. Tobias Neumann is supported by the United States Department of Energy under Grant Contract DE-SC0012704.

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