Generator & Theory Working Group Chapter for CWP

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1 Introduction

LHC experimental results continue to show excellent agreement with Standard Model predictions driving High Energy Physics into a new era of precision collider physics measurements. Theoretical predictions at the LHC and other colliders require perturbative calculations in Quantum Chromodynamics (QCD), the theory of the strong force that binds quarks and gluons into the colliding protons. As a rough guideline to the required order in the QCD perturbative expansion, leading order (LO) only gets the order of magnitude of the result correct. Next-to-leading order (NLO) gets results accurate to tens of percent. Percent-level precision is possible at next-to-next-to-leading order (NNLO).

Event generators use Monte Carlo methods to calculate the interaction cross-sections of LHC proton-proton collisions, and allow to interpret each unweighted Monte-Carlo sampling point as collision event in the measurement. This feature greatly alleviates a direct comparison between theory and experiment, and it makes event generators a necessity for interpreting measurements and identifying new physics beyond the Standard Model.

The precision of LHC Run 2 analyses already rivals or exceeds the precision of theoretical predictions from NLO perturbative QCD [11, 12]. As the LHC continues to break records in luminosity delivered and the High-Luminosity LHC (HL-LHC) comes online in 2025 experimental precision will continue to improve and the need for larger and larger simulated event samples will increase. The particle multiplicity per event continues to rise as well. These conditions

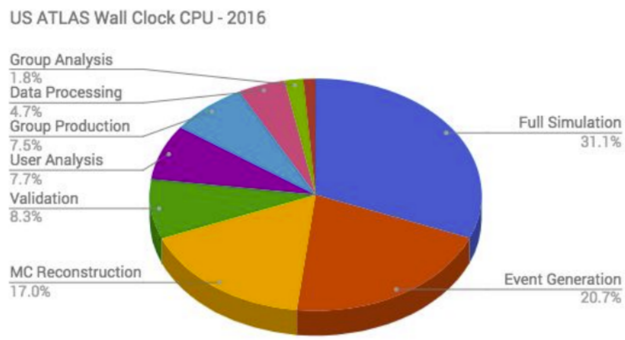

Figure 1: Distribution of job types run by the ATLAS experiment in 2016.

drive an increase in the computing requirements of theoretical calculations and event generators. This chapter addresses plans for mitigating these increases and proposes solutions to ensure theory calculations and event generators are prepared to provide results in LHC Run 4 and beyond.

1.1 Importance of Generators for LHC Experiments

Event generators are the first step in the simulation chain of LHC experiments such as ATLAS and CMS. They calculate parton interaction cross-sections for LHC proton-proton interactions, then generate collision events based on these cross-sections. Figure 1 shows the distribution of work performed by the ATLAS experiment on the grid in 2016 with 20% going to event generation. ATLAS uses approximately 1.5 billion core-hours per year on the Grid and elsewhere. During the Run-1 (Run-2) MC production campaign, ATLAS generated 6.1 (12.5) billion events using 1.6 (91.4) CPU-time per event.

There are two main contributing factors in the difference between Run-1 and Run-2 CPU consumption. During Run-1 the usage of Les Houches event (LHE) files [5, 9] (produced with off-grid resources) was commonplace whereas this has largely been replaced with centralised LHE file production by ATLAS in Run-2. Also, in Run-2 higher precision calculations, for example using NLO merging, are more prevalent and such calculations naturally take up signifacntly more resources.

2 Current Landscape

LHC experiments depend on many different physics event generators and theory calculations for both their similarities and their differences. The fact that theoretical approaches as well as implementations can vary offers an opportunity to validate and cross-check the predictions in a similar way that ATLAS and CMS provide systematic checks of experimental measurements.

The following section reviews some of the more heavily used generators in LHC experiments and some leading edge theory calculations.

2.1 Leading-Order Event Generators

Ever since the first detailed, phenomenological studies of fragmentation by Feynman and Field [60], computer simulations of "events" have played an increasingly important role in understanding and validating the Standard Model. The roots of event generators begin in the attempt to describe the non-perturbative hadronization process. With the acceptance of QCD, the perturbative evolution of partons was added, yielding the parton shower description. The combination of leading order differential cross sections for the simplest Standard Model processes with the parton shower and hadronization model gave a good description of jet and weak boson physics. To understand physics at hadron colliders, models of beam remnant evolution (so-called underlying event models) were developed analogously to the first models of hadronization. The challenging search for the top quark at the Tevatron collider, and the inherent weakness of the parton shower approach in predicting high-p_T jets, led to interfaces with tree-level matrix-element based predictions. By the end of the Tevatron era, precise measurements of the top quark cross section had necessitated the development of consistent NLO + parton shower predictions.

At the start of the LHC era, two of the main event generators had migrated to C++ code (Herwig++ and Pythia8) while a third had started from the beginning in C++ (Sherpa).

In recent years, our ability to make predictions at NLO and NNLO has increased by leaps and bounds. Nonetheless, event generators are still the main workhorses of LHC experiments, for direct physics measurements, but also for the important tasks of estimating trigger rates, occupancy, detector performance, etc. Event generator predictions are used almost exclusively to describe jet physics. Many exotic physics scenarios beyond the Standard Model can also be studied with event generators. However, as a shift has been made to making matrix element based predictions, event generators take on the role of handling the matching/merging of these predictions with the parton shower, underlying event, hadronization, etc. In any event, lowest-order event generators remain a crucial part of high-energy-physics computing. Besides modeling hadronization in general, they are needed for a detailed description of pile-up, minimum bias events, the underlying event, and jet structure and sub-structure.

To give an example, the modeling of hadronization, perturbative QCD and soft QCD effects dominate the uncertainty on the top quark mass derived from data [96] and are a significant part of the uncertainty on the W boson mass [1]. Data-driven pile-up modelling needs to be validated and cross-checked with event generators (see e.g. [45]), theoretical uncertainties on the (sub-)structure of jets need to be assessed by parton showering [17, 112, 26] and the effects of high-jet-multiplicity background and signal events must be modeled using multi-jet-merged calculations [40, 102, 98, 111, 106, 6, 84, 76, 83, 118, 103, 104, 63].

As another example, the simulation of pile-up events with event generators requires detailed models of how the total proton-proton scattering cross section is distributed over phase-space, and how different scattering processes (elastic scattering, diffractive scattering producing rapidity gaps, single- or multi-parton scattering) compete for the available phase space. These processes can yield any number of detectable particles, with rare events containing a very large number of particles. The event generator model of pile-up-like scatterings needs to avoid and bias like the bias that is e.g. introduced by cuts that are necessary to avoid singularities in perturbative scattering calculations. This then means that a simultaneous integration of processes with cross sections differing by many orders of magnitude is necessary. In turn, this requires the generation of very large samples of phase-space points. Currently, high-throughput computing is used to address this problem.

Another computational frontier of leading-order event generators is the generation of perturbative variations that allow to assess the uncertainties of the calculations. This includes both uncertainties in the modelling of the hardest scattering that produces the partonic seeds of jets as well as uncertainties in the evolution of partons into jets of hadrons. Both of these facets have recently seen a move away from schemes to produce individual uncorrelated variations based on high-throughput computation towards producing statistically correlated systematic variations on-the-fly in a single event-generator run [17, 112, 26]. The latter means that automated uncertainty estimates might become amenable to high-performance computing in the near future.

Finally, the omnipresence of matching- and merging approaches to enable an accurate modeling of multi-jet final states (for both signal- and background processes) has shifted much of the computational challenges of modern event-generator calculations to the production of fixed-order multi-parton scattering events. The phase space in which parton-showering is allowed to produce additional partons is severely restricted by matching/merging. Thus, for matched/merged calculations, the efficiency of the calculation is almost directly inherited from the efficiency of the fixed-order (LO, NLO, ...) calculation, such that the bottlenecks described in Section 2.2 impact the event generator calculation as well. An example for the capabilities of modern tree-level event generators is given in Tab 1. Note that a staged approach of pretabulating and storing fixed-order results before showering, as e.g. used in the MadGraph5_aMC@NLO + Pythia or Alpgen + Pythia event-generation chain, can leads to computational overhead since certain pieces of the fixed-order calculation (i.e. splitting histories) have to be reconstructed at shower run-time to guarantee a consistent combination. This overhead can become significant at high parton multiplicity, but may be amendable to speed gains from high-performance computing. The approach of generating fixed-order results and showering simultaneously also suffers from computational challenges, as it leads to increased executable size and the loss of information about the partonic scattering event. It is therefore obvious clear that developments that make fixed-order calculations amenable to high-performance gains alone will not improve the speed and efficiency of matched/merged event generator calculations, Instead, developments in fixed-order parts as well as showers (and how

Process	W^-+0j	W^-+1j	W^-+2j	W^-+3j
RAM Usage	<1MB	<1MB	1MB	2 MB
Initialization time	<1s	<1s	<1s	2s
Startup time	<1s	<1s	<1s	<1s
Integration time	8s	2m 4s	22m 8s	2h 3m
MC uncertainty [%]	0.18	0.14	0.25	0.44

Process	W^-+4j	W^-+5j	W^-+6j	W^-+7j
RAM Usage	23 MB	81 MB	435 MB	1.51 GB
Initialization time	33s	3m 17s	51m 52s	6h 50m
Startup time	<1s	<1s	2s	12s
Integration time	1d 5h	6d 23h	32d 19h	64d 15h
MC uncertainty [%]	0.66	0.78	1.29	2.70

Table 1: Example performance measures for the computation of $pp \to W^- + n$-jets production at $\mathcal{O}(\alpha^2\alpha_s^n)$. The center-of-mass energy is 13 TeV and jets are defined as $p_{T,j} > 30$ GeV, $|y_j| < 4.5$. All partonic channels are included in the calculation, and the CKM matrix is chosen to be diagonal. Numbers are generated on a dual 18-core Intel® Xeon® 2.30GHz CPU. Integration times are cumulative for all MPI ranks in the parallel calculation.

they are used to enable matching/merging) have to go hand-in-hand with the integration of codes to allow for maximal computational gain.

2.2 Next-to-Leading Order Event Generators

Calculations and event simulation at NLO in perturbative QCD are used both for direct comparison with experimental data that are corrected to the parton level, and as an input to particle-level event simulation. At the tree level, calculations have long been performed completely automatically using programs like Alpgen [105], Amegic [99], Comix [73], CompHEP [25], HELAC [95], MadGraph [8] and Whizard [97]. At the next-to-leading order, such a level of automation required two main ingredients: The implementation of known generic methods to perform the subtraction of infrared singularities and the automated computation of one-loop amplitudes.

The calculation of virtual corrections for processes with a large number of hard, light jets in the final state has been one of the focal points in the past decades. The field received a boost from generalized unitarity [21, 20, 22], which is used in this context to determine one-loop amplitudes by decomposing them into known scalar one-loop integrals and rational coefficients determined from on-shell tree amplitudes, plus a rational piece [114, 62, 54, 115, 56, 117, 81]. A large number of programs have been developed that automate these methods [18, 55, 57, 23, 80, 7, 13, 38, 48, 61] based on library computing the scalar integral [58, 128, 75, 116, 129] and that supplement well-established codes based on

process	Virtual	Tree-Level	Subtraction
$pp \to t\bar{t}$	18%	17%	37%
$pp \to t\bar{t}j$	35%	23%	38%
$pp \to t\bar{t}jj$	31%	32%	34%
$pp \to W^+W^-$	10%	20%	48%
$pp \to W^+W^-j$	15%	36%	36%
$pp \to W^+W^-jj$	35%	38%	23%
$pp \to e^+e-$	4%	14%	26%
$pp \to e^+e-j$	3%	51%	34%
$pp \to e^+e-jj$	14%	40%	31%

Table 2: Relative CPU time dedicated to the evaluation of the virtual matrix-element, of the tree-level matrix-element (Born and Real) and of the various subtraction terms. Numbers are computed with MadGraph5_aMC@NLO. The difference between 100% and the sums of virtual, tree-level and subtraction is due to other parts of the code (like generating/writing events, computation of systematics, etc.)

analytic calculations [35, 36, 37] and on improved automated tensor reduction [52, 24, 47, 46, 38, 3]. A completely numerical approach exists [16, 15]. All these developments have brought about the construction of ever faster numerical programs for phenomenological applications. Monte-Carlo methods can be used to reduce the number of loop-evaluations when computing NLO computation [7] allowing to have NLO computations not dominated by loop-computations. An example for the arising timing distribution is shown in Table 2. Despite all these advantages, NLO computations typically require significantly more computing power than their leading-order counterparts. In addition, the numerical methods to evaluate NLO corrections can suffer from numerical instabilities, such that re-evaluation in higher precision arithmetics becomes necessary. In this case the computation can be slowed down significantly.

A major bottleneck is nowadays often found in the computation of real corrections and the corresponding infrared subtraction terms [41, 39]. The subtraction terms consist of color-correlated tree-level matrix elements multiplied by spin-dependent splitting operators, hence the aforementioned programs for leading order calculations are ideally suited for this part of the computation. Correspondingly, infrared subtraction techniques have been implemented in various general-purpose matrix element generators [74, 51, 65, 66, 64]. Their reach is expanded sinificantly by parallel computing [87, 19, 85], and it is expected that this trend will continue in the future.

2.3 NNLO Fixed-Order Calculations

Achieving NNLO precision is an enormously difficult theoretical challenge. Individual contributions to the expansion are separately divergent, necessitating regularization at intermediate stages. It is also an enormous computational challenge.

These theoretical and computational challenges have received significant attention in the community New methods have proven capable of providing the NNLO predictions needed to match the exacting experimental precision. Those which have proven capable of handling the full complexity of $2 \to 2$ scattering with colored final states at the LHC are: antennae subtraction [121]; N-jettiness subtraction [31, 69]; sector-improved residue subtraction [49, 33]. Together these techniques have made possible NNLO predictions for W+jet [31], Z+jet [120, 27], Higgs+jet [29, 30, 43], and $t\bar{t}$ production [50], as well as partial results for di-jet production [122]. We demonstrate the utility of these higher-order calculations using a result for the Z+jet process obtained using N-jettiness subtraction [32]. The figure shows a plot for the H_T distribution in the Z+jet process. This observable provides an important control sample in the search for dark matter at colliders. The data points as measured by the experimental collaborations are shown as points with error bars. Theory predictions at NLO and NNLO are shown as red and blue bands respectively, where the bands denote an estimate of the residual theoretical error. The NLO result falls below the measured data by nearly a factor of two, and fails to properly describe the distribution shape. The NNLO prediction obtains both the correct normalization and shape. More examples and a detailed discussion of the theoretical precision are given in Ref. [32], but the message of this plot is clear: one simply cannot describe this important LHC data without a NNLO prediction.

We discuss the computational aspects and challenges at NNLO using N-jettiness subtraction as an example. The N-jettiness subtraction idea utilizes a novel computational approach that relies critically on parallel high-performance computing (HPC) systems. The N-jettiness subtraction scheme achieves NNLO precision for LHC scattering processes by splitting the necessary integrations over the phase space of the N final-state particles according to a resolution criterion on the N-jettiness event shape variable:

$$\sigma_{\mathrm{NNLO}} = \int d\Omega \left[\frac{\mathrm{d}\sigma_{\mathrm{NNLO}}}{\mathrm{d}\mathcal{T}_N} \theta(\mathcal{T}_N^{cut} - \mathcal{T}_N) + \frac{\mathrm{d}\sigma_{\mathrm{NNLO}}}{\mathrm{d}\mathcal{T}_N} \theta(\mathcal{T}_N - \mathcal{T}_N^{cut}) \right]. \quad (1)$$

The N-jettiness variable $\mathcal{T}_N$ was defined in Ref. [127]. For our purposes we note that it divides the phase space into an 'above-cut' region (the second term in Eq. 1, where $\mathcal{T}_N > \mathcal{T}_N^{cut}$) which can be obtained from a simpler NLO calculation for $N+1$ jets. The 'below-cut' region (the first term in Eq. 1, where $\mathcal{T}_N < \mathcal{T}_N^{cut}$) can be obtained from an all-orders result in the strong coupling constant [126]. A detailed discussion of how this technique is practically implemented was presented in the initial work. The end result is the reduction of the number of required integrations to three: a computationally-simple below-cut integration, and two computationally-intensive above-cut integrations. These integrations typically live in 10-15 dimensions and contain numerous peaks throughout phase space, and are approached with Monte-Carlo techniques such as the VEGAS algorithm [100].

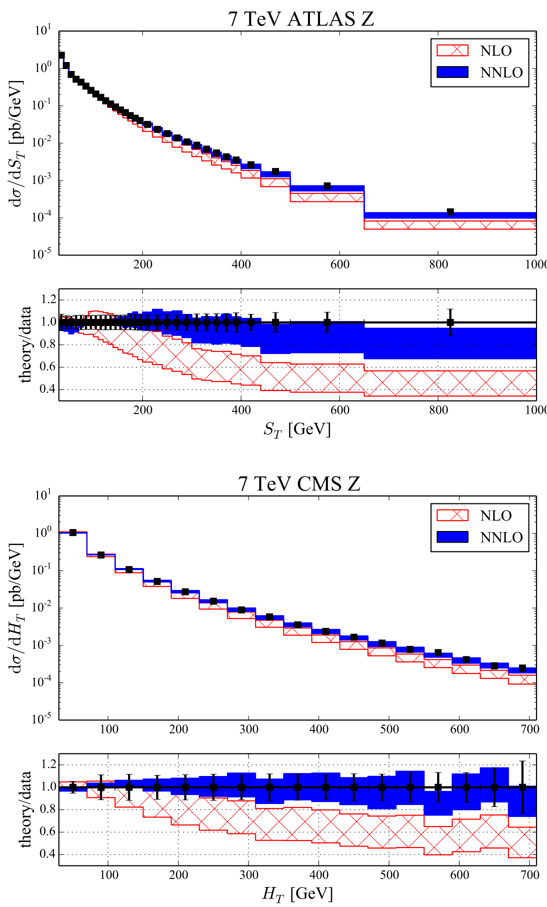

Figure 2: Comparison of the H_T distribution in the Z+jet process measured by ATLAS (left panel) and CMS (right panel) to theoretical predictions at NLO and NNLO. The data points denote the experimental measurements with the reported errors, while the red and blue bands respectively denote the estimated NLO and NNLO theoretical errors.

The primary computational challenge is that each integral in Eq. (1) contains logarithms of the resolution parameter $\mathcal{T}_N^{cut}$ that cancel upon addition of all three terms. Each separate term has up to $\log^4(\mathcal{T}_N^{cut})$ dependence. Since $\mathcal{T}_N^{cut}$ must be taken small for theoretical reasons, we must dig out the residual result from the numerical noise induced by the cancellation between large logarithms in the numerical integration. The figure-of-merit to consider is the degree of cancellation between the above-cut and below-cut integrations. In applications considered so far this ranges from 1 part in 10 to 1 part in 1000. The desired numerical precision on the final result is sub-percent, implying that some of the separate integrals must be computed to 10^{-6} relative accuracy. To reach this target for a Monte Carlo integration with a large number of dimensions requires an enormous number of integrand evaluations. We split these between many threads, which must be coupled in order to use this information to appropriately refine the integration grid. This explains the need for a massively parallel HPC resource.

The N-jettiness subtraction method is a general theoretical framework that can be implemented in publicly available codes for NLO calculations. Several independent codes incorporating N-jettiness subtraction have been successfully run on the Mira supercomputer at the Argonne Leadership Computing Facility (ALCF) [28, 2]. These are written in a combination of Fortran77 and Fortran90. All codes performs a Monte-Carlo integration of multi-dimensional integrands. The many required integrand evaluations are the most computationally expensive part of the code, are parallelized using a hybrid MPI-OpenMP approach. Reasonably good scaling up to the million-thread level is obtained on the Mira supercomputer at the ALCF. As more complex scattering processes are studied, this scaling will become increasingly important.

2.4 Parton Showers at Higher Order

Parton shower algorithms describing QCD and QED multiple radiation have been a central ingredient of simulation programs for particle physics experiments at the energy frontier [130, 34]. Invented about three decades ago, they have undergone tremendous developments since then, with some of the most important steps being the introduction of QCD coherent evolution [131, 107, 108] and the incorporation of process-independent soft-gluon enhacement [42].

About a decade of work has been spent on matching [67, 82, 77, 78, 90, 89] and merging [40, 102, 98, 106, 6, 84, 76, 83, 118, 103, 104, 63] algorithms to include fixed-order higher-order corrections. More recently, the need for improved overall simulations triggered a resurgence of interest in improving parton-shower algorithms themselves. Several new parton showers have been constructed [71, 125, 124, 53, 132, 70, 119, 123, 86], and the possibility of including next-to-leading order corrections into the evolution has been explored [79, 101, 91, 88, 113]. In addition, NLO splitting functions have been recomputed [93, 72], with the aim to improve parton-shower simulations, and the dependence of NLO matching terms on the parton-shower evolution variable has been investigated [92].

While all these developments may lead to theoretically improved simulations rather soon, they also require a significant increase in computation time for the generation of each event. As a simple example, the implementation of next-to-leading order accurate splitting functions in the parton shower effectively turns the previously probabilistic simulation of the parton branching process into a true NLO calculation. The occurrence of negative weights for the splitting kernels is characteristic and leads to additional weight fluctuations in the overall simulation that have to be compensated by a higher number of generated events, while each event also comes at an additional computational cost. This situation is very much alike to fixed-order perturbation theory.

3 Future Strategies

The following techniques will be investigated with the goal of increasing the precision of generators needed for analyses of the HL-LHC while aiming to reduce our computing requirements.

3.1 Scalable Adaptive Monte-Carlo Integrators

As generators move to higher orders in perturbative QCD and the HL-LHC probes higher multiplicity processes, the time needed to integrate the interaction cross-section becomes prohibitively large on a single CPU core. Parallel processing becomes a requirement and being able to scale on a supercomputer enables ever more aggressive analyses.

Existing generators were not developed in the mulit-core age that has become the industry standard in the past five years and therefore parallel processing was added after frameworks had largely been implemented. This leads to meager performance improvements when running in parallel, especially when running in parallel across many compute nodes of a supercomputer. Work has been done to improve scalability of existing generators such as Sherpa and Alpgen [44].

In the case of advanced frameworks such as MadGraph and Sherpa, the architecture of the framework was not designed to take advantage of highly parallel computers and maintain high CPU and memory efficiency. The development of new scalable adaptive Monte-Carlo integrators that can be used by existing frameworks would be a big step toward addressing HL-LHC computing requirements. In the US, the DOE is planning to deploy supercomputers over the next five years that will increase the scientific computing capacity by a factor of 200. Developing algorithms that target these machines will offload computation from Grid resources and will in general lead to the development of better algorithms.

3.2 Reweighting of Event Samples

Re-weighting method consists to attach to a given partonic events a new weight corresponding to a new theory. Those new weights allow to predict accurately (up to statistical precision) all the differential distributions at parton-level and to perform a single detector simulation for all the models under consideration.

Different types of re-weighting exist. First there is the reweighting mentioned in Sec. 2.1, which relates to the estimation of the theoretical uncertainties of a simulation. Second the same techniques can be used to accomodate BSM re-weighting for both LO [68, 14, 94, 109] and NLO event samples, both approximatively [4, 59] and exactly [109].

At LO accuracy the new weight (W_{new}) can be easily obtained from the original one (W_{orig}) by simply multiplying it by the ratio of the matrix-elements estimated on that event for both models (noted respectively $|M_{orig}|^2$ and $|M_{new}|^2$):

$$W_{new} = \frac{|M_{new}|^2}{|M_{orig}|^2} W_{orig}. \tag{2}$$

While at NLO, one needs to track the dependence in the various event and counter-event and reweight by the associated matrix-element.

A few remarks are in order regarding the range of validity of this method. First, even if the method returns the correct weight, it requires that the event sampling related to W_{orig} covers appropriately the phase-space for the new theory. In particular, W_{orig} must be non-zero in all regions where W_{new} is non-vanishing. Though obvious, this requirement is in fact the most important and critical one. In other words, the phase-space where the new theoretical hypothesis contributes should be a subset of the original one. For example, re-weighing can not be used for scanning over different mass values of the final state particles[1], yet it is typically well-suited for probing different types of spin and/or coupling structures.

Second, the parton-level configuration feeder to parton-shower programs not only depends of the four-momenta but also of additional information, which is commonly encoded in the Les Houches Event File (LHEF) [5, 9]. Consequently, re-weighting by an hypothesis that does not preserve such additional information is not accurate. In general, such informations are related to:

- **Helicity:** The helicity state of the external states of a parton-level event is optional in the LHEF convention, yet some programs (e.g. [110]) use this information to decay the heavy state with an approximated spin-correlation matrix. [109, 10] proposes a dedicated re-weihting method in this case to fix such issue.

- **Color-flow:** A second piece of information presented in the LHEF is the color assignment in the large N_c limit. This information is used as the starting point for the dipole emission of the parton shower and therefore determines the result of the QCD evolution and hadronisation. Such information is untouched by the re-weigthing limiting the validity of the method.

[1] For intermediate particle a small variation of the mass –order of the width– is reasonable.

- **Internal resonances:** In presence of on-shell propagators, the associated internal particle is written in the LHEF. This is used by the parton-shower program to guarantee that the associated invariant mass is preserved during the re-shuffling procedure intrinsic to the showering process. Consequently, modifying the mass/width of internal propagator should be done with caution since it can impact the parton-shower behaviour. This information can not be corrected via a re-weighting formula, as it links in a non-trivial way short-distance with long-distance physics.

Even with such limitation the application of such re-weighting will allow to decrease by huge factor the time spent on the generation of BSM samples.

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