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NNLO Matrix-Element Corrections in VINCIA

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We report on a new formalism for parton showers whose fixed-order expansion can be corrected through next-to-next-to-leading order (NNLO) in QCD. It is the first such formalism we are aware of that has no dependence on any auxiliary scales or external resummations and which is fully differential in all of the relevant phase spaces. Since the shower acts as the phase-space generator, the dominant singularity structures are encoded by construction and the method can generate unweighted events with very high efficiency without any significant initialisation time. We argue that the the method should be capable of achieving (at least) NNLO+NNDL accuracy for the shower evolution variable and use hadronic Z decays as a specific example.

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1. Introduction

The presence of infrared (IR) poles in amplitudes with partons that can become soft and/or collinear complicates making precise predictions in theories with massless gauge bosons (such as QED and QCD). Although the resulting IR singularities can be treated consistently and cancel order by order in the relevant gauge coupling(s), they leave a legacy in physical observables in the form of logarithms of scale ratios. If significant scale hierarchies are present in the process or observables at hand, these logarithms counteract the naive coupling-power suppression of higher-order terms. This reduces the effective accuracy of fixed-order calculations for multi-scale problems.

This is a concern for ongoing experimental and phenomenological studies, e.g. at the LHC, where ever-more complex final states are being targeted — and accurately measured — with multiple resolved objects each of which defines an intrinsic scale, and/or for observables sensitive to substructure. It also applies to differential observables that cover a wide range of scales over their domain(s), which are often well described by fixed-order perturbation theory in hard tails while log-enhanced terms affect the bulk/peak of the differential distributions.

To give a schematic example, an NNLO QCD calculation of a cross section with a jet veto would include the following terms:

$$\overbrace{F_0}^{\text{LO}} \ + \ \overbrace{\alpha_s(L^2+L+F_1)}^{\text{NLO}} \ + \ \overbrace{\alpha_s^2(L^4+L^3+L^2+L+F_2)}^{\text{NNLO}} \ , \tag{1}$$

where α_s is the QCD coupling constant, F_i denote non-log terms at each order and L^m in this example represents terms proportional to powers of logs of the jet-veto scale to a scale characteristic of the Born-level hard process. If the scales are such that $\alpha L^2 \sim 1$ then all terms $\alpha_s^n L^{2n}$ would be of order unity, invalidating any fixed-order truncation of the series. For less extreme hierarchies, the consequence is a reduction of the effective relative accuracy of the truncation.

At face value, fixed-order calculations are therefore always most accurate for single-scale problems, while their effective accuracy for processes/observables with scale hierarchies is reduced.

The applicability of perturbation theory can be extended to multi-scale problems by *resumming* the log-enhanced terms to all orders, now using a logarithmic order counting in which a rate like that in eq. (1) is (re)expressed, here shown schematically up to NNLO+N4DL accuracy:

$$\left(\overbrace{F_0}^{\text{LO}} \ + \ \overbrace{\alpha_s F_1}^{\text{NLO}} \ + \ \overbrace{\alpha_s^2 F_2}^{\text{NNLO}}\right) \times \exp\left(\overbrace{-\alpha_s L^2}^{\text{DL}} \ \overbrace{-\alpha_s L \ -\alpha_s^2 L^3}^{\text{NDL}} \ \overbrace{-\alpha_s^2 L^2 \ -\alpha_s^3 L^4}^{\text{NNDL}} \right. \tag{2}$$
$$\left. \underbrace{-\alpha_s^2 L \ -\alpha_s^3 L^3 \ -\alpha_s^4 L^5}_{\text{N3DL}} \ \underbrace{-\alpha_s^3 L^2 \ -\alpha_s^4 L^4 \ -\alpha_s^5 L^6}_{\text{N4DL}}\right) ,$$

where the “double-log” (DL) counting in the exponent here is intended to emphasise that we focus on towers of logs that dominate in kinematical regions in which $\alpha_s L^2 \sim 1$ (as distinct from the widely used N^{n}LL counting which is based on $\alpha_s L \sim 1$). The fixed-order coefficient F_1 is needed both for NLO matching and also for NNDL accuracy, and the coefficient F_2 is required for matching to NNLO and for N4DL accuracy. In shower parlance, exponentials such as the one in eq. (2) are called Sudakov factors; we call them that below.

Several general resummation methods exist, which operate at different levels of inclusiveness; here we focus only on the most exclusive one, parton showers. The requirement of full exclusivity comes at a cost: this is generally the hardest method to reach high formal accuracy with. One might ask why, then, pursue this method, when complementary, more inclusive methods, are available, which can reach better accuracy than showers do? There are at least four strong reasons for this:

1. **Universality.** Given a starting scale, a parton-shower algorithm can be applied to *any* parton configuration. This means that, once a shower algorithm has been defined and encoded in a Monte-Carlo implementation, it can be applied to almost any conceivable process type, within and beyond the SM, with little or no additional manpower. This is the basis of the near-ubiquitous applicability of general-purpose shower Monte Carlos (GPMCs) in HEP.

2. **Efficiency.** Since shower algorithms are based directly on the dominant singularity structures of radiative corrections, they are highly efficient in producing unweighted events in the (Born+ n)-parton phase spaces. This happens by construction, without significant inititalization time. This property also underpins so-called forward-branching phase-space generators [1, 2].

3. **Fully differential final states.** While inclusive resummation methods typically require a separate dedicated calculation for each specific observable, shower algorithms produce fully-differential exclusive final states, on which *any* observable can be evaluated. Thus, one calculation can suffice to make predictions for any number of observables.

4. **The IR cutoff** of the shower algorithm, combined with the fact that all-orders corrections have been included above it, makes it possible to interface the perturbative calculation consistently with explicit and detailed dynamical models of hadronization, such as string or cluster fragmentation. This in turn also enables embedding the calculation within a more complete modelling framework, including detailed simulations of experimental fiducial and efficiency effects, and making the calculation accessible to the full suite of collider-physics phenomenology study tools, again a main reason for the wide use of GPMCs in HEP.

These properties, together with the increasing phenomenological relevance of multi-scale problems in general, make it interesting to embed fixed-order calculations systematically within shower calculations, in a general and efficient way.

Up to NLO accuracy, this is relatively straightforward [3–10]. Beyond NLO, however, there is *ab initio* a problem. At best, current parton showers achieve NLL resummation accuracy [11–14]. Comparing eqs. (1) and (2), we see that the $\alpha_s^2 L^2$ and $\alpha_s^2 L$ pieces in eq. (1) are associated with NNDL and N3DL terms in eq. (2), respectively; these are categorised as NLL and NNLL respectively if one employs "Caesar-style" log counting [15]. This makes it impossible to write down matching equations in which the log-enhanced terms are all on the shower side. To circumvent this issue, previous NNLO matching approaches [16–19] have utilised analytically calculated Sudakov factors to supplement the parton-shower ones. This is probably the best one can do with current showers but does have the drawback that the accuracy in shower-dominated phase-space regions is not improved. There is also the need to calculate separate analytical Sudakov factors. And subtleties associated with the fact that they (and their resummation variables) are not completely identical to their equivalents on the shower side, though this difference can be made at least formally subleading by making suitable resummation-variable and scale choices.

Returning to eqs. (1) and (2), a fully self-contained embedding of an NNLO calculation in a parton-shower framework would appear to require an N3DL accurate shower algorithm (and N3LO calculations, which are also beginning to emerge on the phenomenological scene, would then require N6DL showers). This is not realistic to shoot for, and is also not strictly necessary.

Instead, we aim for a consistent shower that exponentiates the full $O(\alpha_s^2)$ pole structure of the NNLO fixed-order matrix elements. This is sufficient to enable a fully differential matching, where all poles that appear on the fixed-order side also appear on the shower side. If the $O(\alpha_s^3)$ soft anomalous dimension is also included, we argue that the shower Sudakov factor contains all terms required for NNDL accuracy on the shower evolution variable. By construction, the method also exponentiates the N3DL $\alpha_s^2 L$ term, but the other N3DL coefficients are not included. We note that for modest scale hierarchies, characterised by $\alpha_s L^2 < 1$, the relative importance of the $\alpha_s^3 L$ and $\alpha_s^2 L$ cofficients swap places, hence in such regions we would still expect our partial N3DL resummation to represent a systematic improvement over NNDL.

Below, we describe the ingredients that are needed to accomplish this, based on refs. [20–23].

2. Phase-Space Generation and NNLO Matching

In a conventional fixed-order calculation, each of the (Born + m)-parton phase spaces are generated separately. In a shower-style algorithm, instead all events start out as Born-level events, and all higher multiplicities are produced by the shower branching process. The unitarity of the shower generates a Sudakov-weighting of exclusive cross sections, which at each higher multiplicity comes multiplied by the kernel(s) of the relevant branchings. If the shower algorithm is sufficiently tractable, these weights can be expanded and matched to any given fixed order [24]. This has been worked out for final-state antenna showers at both tree level [24–26] and at one loop [20].

Here, we focus on a MEC/POWHEG-style multiplicative matching procedure. For this to work, it is obviously necessary that the shower algorithm is able to populate all of the relevant phase spaces, with no "dead zones". This is not true of conventional strongly-ordered parton showers[1]. E.g., a $p_\perp$-ordering condition will typically cut out part of the (Born + 2)-parton phase space [24].

A path to a robust approach can be found by analysing the propagator structure of the amplitudes that contribute to the regions that are cut out by strong ordering. These phase-space points are characterised by having no strong hierarchy in the propagator virtualities. Intuitively, they should therefore be thought of not as resulting from iterated (ordered) $n \to n+1$ splittings, but as direct (single-scale) $n \to n+2$ splittings. They are also associated with qualitatively different terms in both the fixed-order and logarithmic expansions than the points in the ordered region are; the unordered region only borders on double-unresolved limits of the fixed-order matrix elements, and hence integrals over it should also only contribute to $\alpha_s^2 L^2$ (NNDL) and $\alpha_s^2 L$ (N3DL) coefficients. This is consistent with conventional showers being able to reach up to NDL accuracy without addressing

[1]This can in principle be circumvented by modifying the shower ordering variable (e.g., virtuality-ordering can trivially be seen to cover all of phase space), but at least for LL branching kernels we are discouraged from doing so, for the reasons elaborated on in ref. [24], and it also appears to lead to the wrong resummation structure [20, 21]. Another option was "smooth ordering" [24], but again we believe this would lead to an undesirable resummation structure.

this region, but we suspect it would not be possible to reach accuracy higher than NDL without some form of dedicated treatment of the unordered/double-unresolved region of phase space.

Our solution [21] is to add new "direct" $2 \to 4$ branchings, based on a Sudakov-style 6D phase-space sampler with an $\alpha_s^2/p_\perp^4$ kernel. In a sector-shower context [22, 25], we divide the (Born + 2)-parton phase-space cleanly into an unordered sector to be populated by the direct $2 \to 4$ sampler, and an ordered sector populated by iterated $2 \to 3$ ones. (In a global shower, one would instead sum over $2 \to 3$ and $2 \to 4$ contributions, when formulating the matching conditions.) The specific criterion we use to decide which sector we are in is the following: in an m-parton configuration, find the smallest (colour-ordered) 3-parton $p_\perp$ resolution scale. Tentatively perform that clustering, using antenna kinematics. Now again find the smallest 3-parton $p_\perp$ resolution scale, denoted $\hat{p}_\perp$. If $\hat{p}_\perp > p_\perp$, the $(m \to m-1)$-parton clustering is ordered; otherwise it is unordered.

Unordered Part: to realise the direct $2 \to 4$ sampler, we make use of the iterated (exact) $2 \to 3$ antenna phase-space factorisation, and define a *trial* $2 \to 4$ Sudakov factor as follows:

$$-\ln \hat{\Delta}_{2\to4}(p_{\perp0}^2, p_\perp^2) = \int_0^{p_{\perp0}^2} \mathrm{d}p_{\perp1}^2 \int_{p_\perp^2}^{p_{\perp0}^2} \mathrm{d}p_{\perp2}^2 \; \overbrace{\Theta(p_{\perp2}^2 - p_{\perp1}^2)}^{\text{Unordered: } p_{\perp1}<p_{\perp2}} \int \mathrm{d}y_1 \mathrm{d}y_2 \, \hat{a}_{2\to4} \,, \tag{3}$$

where a simple choice for the trial function $\hat{a}_{2\to4}$ is proportional to $C_A^2\, \alpha_s^2(p_{\perp2}^2)/p_{\perp2}^4$. We then exploit the definition of the unordered region to swap the order of the integrations,

$$\Longrightarrow \quad -\ln \hat{\Delta}_{2\to4}(p_{\perp0}^2, p_\perp^2) \;=\; \int_{p_\perp^2}^{p_{\perp0}^2} \mathrm{d}p_{\perp2}^2 \; \underbrace{\int_0^{p_{\perp2}^2} \mathrm{d}p_{\perp1}^2}_{\text{Unordered:} p_{\perp1}<p_{\perp2}} \int \mathrm{d}y_1 \mathrm{d}y_2 \, \hat{a}_{2\to4} \,. \tag{4}$$

Details of the trial-generation procedure are given in ref. [21]. Unweighted ME-corrected events are generated by accepting trial branchings with a tree-level second-order MEC ratio,

$$P_{2\to4}^{\mathrm{MEC}} \;=\; \frac{|M_{\mathrm{Born}+2}^{(0)}|^2}{\hat{a}_{2\to4}|M_{\mathrm{Born}}^{(0)}|^2} \,, \tag{5}$$

where subscripts denote multiplicities and the superscript indicates relative loop order. For hadronic Z decay, the physical $2 \to 4$ Sudakov factor generated by the matched shower is then:

$$-\ln \Delta_{2\to4}(m_Z^2, p_\perp^2) \;=\; \int_{p_\perp^2}^{m_Z^2} \mathrm{d}p_{\perp2}^2 \int_0^{p_{\perp2}^2} \mathrm{d}p_{\perp1}^2 \int \mathrm{d}y_1 \mathrm{d}y_2 \, \frac{|M_{q\bar{q}gg}^{(0)}|^2}{|M_{q\bar{q}}^{(0)}|^2} \,. \tag{6}$$

After a $2 \to 4$ trial branching is accepted, the pure shower evolution can simply be continued, starting from the $p_\perp$ scale of the accepted $2 \to 4$ branching.

Ordered Part: in the ordered part of the nested phase spaces, the first $2 \to 3$ branching receives a standard first-order (tree-level) MEC, augmented by a second-order (one-loop) correction,

$$P_{2\to3}^{\mathrm{MEC}} \;=\; \overbrace{\frac{|M_{\mathrm{Born}+1}^{(0)}|^2}{\hat{a}_{2\to3}|M_{\mathrm{Born}}^{(0)}|^2}}^{\text{Tree-Level } 2\to3 \text{ MEC}} \overbrace{\left(1 + \tilde{w}_{\mathrm{Born}+1}^{\mathrm{NLO}} - \tilde{w}_{\mathrm{Born}}^{\mathrm{NLO}} - \tilde{w}_{2\to3}^{\mathrm{Sudakov}} - \frac{\alpha_s}{2\pi}\frac{\beta_0}{2}\ln\frac{\mu_{\mathrm{FO}}^2}{\mu_{\mathrm{PS}}^2}\right)}^{\text{One-Loop Corrections}} \,. \tag{7}$$

The one-loop corrections are defined so that the second-order shower expansion will match the NNLO real-virtual coefficient [23]. The fixed-order weights $\tilde{w}^{\rm NLO}_{\rm Born+1}$ and $\tilde{w}^{\rm NLO}_{\rm Born}$ are each IR finite,

$$|M^{(0)}_{\mathrm{Born}+m}|^2\,\tilde{w}^{\rm NLO}_{\mathrm{Born}+m} \;=\; 2\mathrm{Re}\left[M^{(1)}_{\mathrm{Born}+m}M^{(0)*}_{\mathrm{Born}+m}\right] \;+\; \int_0^{\mathrm{p}^2_{\perp\mathrm{m}}} \mathrm{d}\Phi_{+1}\,|M^{(0)}_{\mathrm{Born}+m+1}|^2\,, \tag{8}$$

and $\tilde{w}^{\rm Sudakov}_{2\to3}$ is the first-order expansion of the $2\to3$ shower Sudakov weight [20],

$$\tilde{w}^{\rm Sudakov}_{2\to3} \;=\; -\int_{p^2_\perp}^{p^2_{\perp0}} \mathrm{d}\Phi_{+1}\,\frac{|M^{(0)}_{\mathrm{Born}+1}|^2}{|M^{(0)}_{\mathrm{Born}}|^2}\,. \tag{9}$$

The last term in eq. (7) matches the parton-shower and fixed-order renormalisation-scale choices. The canonical choice for coherent showers is $\mu_R \propto p_\perp$ augmented by the so-called “CMW factor”, $\kappa_{\rm CMW}$ [11], which absorbs the 2-loop cusp anomalous dimension,

$$\mu^2_{\rm PS} = \kappa^2_{\rm CMW}p^2_\perp \;\;,\;\; \kappa^2 = \exp(K/\beta_0) \;\;,\;\; K = \frac{67C_A}{18} - \frac{\pi^2}{6} - \frac{10n_FT_R}{9} \;\;,\;\; \beta_0 = \frac{11C_A - 4T_Rn_F}{3}\,. \tag{10}$$

Putting it all together, the $2\to3$ Sudakov factor for hadronic Z decay becomes:

$$\begin{aligned}-\ln\Delta_{2\to3}(m_Z^2,p_\perp^2) \;=\; & \int_{p^2_\perp}^{m^2_Z} \mathrm{d}p^2_{\perp1}\mathrm{d}y_1 \left(\frac{|M^{(0)}_{q\bar{q}g}|^2}{|M^{(0)}_{q\bar{q}}|^2}\left[1 - \overbrace{\frac{\alpha_s}{\pi}}^{\tilde{w}^{\rm NLO}_{\rm Born}} + \overbrace{\int_{p^2_\perp}^{m^2_Z}\mathrm{d}p'^2_\perp\mathrm{d}y'\,\frac{|M^{(0)}_{q\bar{q}g'}|^2}{|M^{(0)}_{q\bar{q}}|^2}}^{\tilde{w}^{\rm Sudakov}_{2\to3}} \right.\right.\\ & \left.\left. - \frac{\alpha_s}{2\pi}\frac{\beta_0}{2}\ln\frac{m_Z^2}{\kappa^2p^2_{\perp1}}\right] + \underbrace{\frac{2\mathrm{Re}\left[M^{(1)}_{q\bar{q}g}M^{(0)*}_{q\bar{q}g}\right]}{|M^{(0)}_{q\bar{q}}|^2} + \int_0^{\mathrm{p}^2_{\perp1}}\mathrm{d}p^2_{\perp2}\mathrm{d}y_2\,\frac{|M^{(0)}_{q\bar{q}gg}|^2}{|M^{(0)}_{q\bar{q}}|^2}}_{\tilde{w}^{\rm NLO}_{\rm Born+1}}\right)\,.\end{aligned} \tag{11}$$

The combined Sudakov factor for a jet veto at the scale $p_\perp$ is found by multiplying the two Sudakov factors, eqs. (6) and eq. (11). We see that something quite beautiful happens; the integral over ordered 4-parton phase-space points in the last term of eq. (11) combines with that over unordered 4-parton points in eq. (6) to yield a seamless integral over the full 4-parton phase space.

Before analysing the structure of the combined Sudakov factor in more detail, two final aspects must be clarified to define the full NNLO matching. The first is that, after a $2\to3$ trial branching is accepted, the shower evolution continues, starting from the $p_\perp$ scale of the accepted $2\to3$ branching. A tree-level 4-parton ME correction factor is then applied to the next branching, analogous to that used in the unordered region, eq. (5), but here for ordered histories:

$$P^{\rm MEC}_{3\to4} \;=\; \frac{|M^{(0)}_{\mathrm{Born}+2}|^2}{\hat{a}_{3\to4}|M^{(0)}_{\mathrm{Born}+1}|^2}\,. \tag{12}$$

Thus all 4-parton points are corrected to the NNLO matrix element, irrespective of whether they are reached by the direct $2\to4$ generator, or by the iterated $2\to3$ generator.

The second aspect of achieving the NNLO matching is that, since all events start out as Born-level events, the Born-level phase-space weight is augmented by a differential NNLO “K-factor”, which enforces the NNLO normalisation of the total cross section and differential distributions [23].

3. Argument for NNDL Accuracy in the Shower $p_\perp$ Evolution Variable

Let us be a bit more definite about what exactly the combined Sudakov factor corresponds to. Specifically, consider a jet clustering algorithm that corresponds to the inverse of the sector-shower branching algorithm. Since we use dipole-antenna kinematics and ARIADNE $p_\perp$ [27] as our sector-resolution variable, this is known as the ARCLUS algorithm [28], suitably extended to incorporate inverses of our new direct $2 \to 4$ branchings. We call this ARCLUS 2.

For a global shower, this jet algorithm would have to be defined in a stochastic way, to allow for the multiple histories that can contribute to each phase-space point. But since a sector shower is bijective the corresponding inverse algorithm is in our case a conventional deterministic jet clustering algorithm, producing a unique clustering sequence for each event.

The rate of events that will pass an ARCLUS-2 jet veto at a scale $p_\perp$ is:

$$k^{\rm NNLO}\, |M^{(0)}_{\rm Born}|^2\, \Delta_{2\to3}(m_Z^2, p_\perp^2)\, \Delta_{2\to4}(m_Z^2, p_\perp^2)\ . \tag{13}$$

We shall assume that the NNLO matching ensures that $k^{\rm NNLO}$ matches the coefficients F_i in eq. (2).

Before considering the log terms in the Sudakov factors, we first ask whether further shower evolution could in principle lead to violations of the jet veto, e.g., via recoil effects from subsequent branchings. If so, that would invalidate eq. (13). In a global shower setup, this question is nontrivial since at least some of the shower histories would involve scales higher than the veto scale, and because recoils that increase the resolution scale are not explicitly forbidden. In a sector shower setup, however, neither of these complications are present, hence the above equation is exact.

Assuming the order-α_s log terms to be guaranteed by the integral over the tree-level matrix-element ratio, $|M_{q\bar{q}g}|^2/M_{q\bar{q}}|^2$ and the remaining $\alpha_s^2 L^3$ NDL coefficient via the CMW factor, the question of NNDL accuracy on eq. (13) boils down to whether the remaining terms in the combined shower Sudakov produce the correct $\alpha_s^2 L^2$ coefficient in eq. (2). We then rely on extending the CMW prescription to match the 3-loop cusp anomalous dimension to get the $\alpha_s^3 L^4$ piece.

Terms proportional to $\alpha_s^2 L^2$ arise in quite a few places in eqs. (11) and (6). Many of these are analytically tractable, e.g. using the expressions in [20, 29]; the most challenging are the ones from the 4-parton phase space. We have not completed a full analysis of this structure yet and hence are not in a position to *prove* NNDL accuracy. However, since all of the relevant ME poles are clearly exponentiated in eqs. (11) and (6), with the matching to fixed order eliminating double-counting of non-singular coefficients (like α_s/π), we believe there is good reason to expect that the method we have proposed is capable of achieving (at least) NNDL accuracy.

For clarity and completeness, we emphasise that we are only making this statement about an observable that corresponds to the shower-evolution variable itself. We also note that we have here neglected subtleties that arise at subleading colour.

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