Interplay between IR-Improved DGLAP-CS Theory and NLO ME Matched Parton Shower MC Precision

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Abstract
We present the current status of the application of our approach of exact amplitude-based resummation in quantum field theory to precision QCD calculations, by realistic MC event generator methods, as needed for precision LHC physics. In this ongoing program of research, we discuss recent results as they relate to the interplay of the attendant IR-Improved DGLAP-CS theory of one of us and the precision of exact NLO matrix-element matched parton shower MC’s in the Herwig6.5 environment in relation to recent LHC experimental observations. There continues to be reason for optimism in the attendant comparison of theory and experiment.

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1 Introduction

With the recent announcement [1] of an Englert-Brout-Higgs (EBH) [2] candidate boson after the start-up and successful running of the LHC for 2.5 years, the era of precision QCD, by which we mean predictions for QCD processes at the total precision tag of 1% or better, is squarely upon us. The attendant need for exact, amplitude-based resummation of large higher order effects is now more paramount, given the expected role of precision comparison between theory and experiment in determining the detailed properties of the newly discovered EBH boson candidate. Three of us (B.F.L.W, S.K.M, S.A.Y) have argued elsewhere [3, 4] that such resummation allows one to have better than 1% theoretical precision as a realistic goal in such comparisons, so that one can indeed distinguish new physics (NP) from higher order SM processes and can distinguish different models of new physics from one another as well. In what follows, we present the status of this approach to precision QCD for the LHC in connection with its attendant IR-improved DGLAP-CS [5, 6] theory [7, 8] realization via HERWIRI1.031 [9] in the HERWIG6.5 [10] environment in interplay with NLO exact, matrix element matched parton shower MC precision issues. We will employ the MC@NLO [11] methodology to realize the attendant exact, NLO matrix element matched parton shower MC realizations for both HERWIRI1.031 and HERWIG6.5 in our corresponding comparisons with recent LHC data that we present herein.

The discussion will therefore be seen to continue the strategy of building on existing platforms to develop and realize a path toward precision QCD for the physics of the LHC. We exhibit explicitly a union of the new IR-improved DGLAP-CS theory and the MC@NLO realization of exact NLO matrix element (ME) matched parton shower MC theory. As our ultimate goal is a provable precision tag on our theoretical predictions, we note that we are also pursuing the implementation [12] of the new IR-improved DGLAP-CS theory for HERWIG++ [13], HERWIRI++, for PYTHIA8 [14] and for SHERPA [15], as well as the corresponding NLO ME/parton shower matching realizations in the POWHEG [16] framework. For, one of the strongest cross checks on theoretical precision is the difference between two independent realizations of the attendant theoretical calculation. Such cross checks will appear elsewhere [12].

In order to expose properly the interplay between the NLO ME matched parton shower MC precision and the new IR-improved DGLAP-CS theory, we set the stage in the next section by showing how the latter theory follows naturally in the effort to obtain a provable precision from our approach [1] to precision LHC physics. In the interest of completeness, we review this latter approach, which is an amplitude-based QED⊗QCD(≡ QCD⊗QED) exact resummation theory [4] realized by MC methods, in the next section as well. We then turn in Section 3 to the applications to the recent data on single heavy gauge boson production at the LHC from the perspective of the analysis in Refs. [9] of the analogous processes at the Tevatron, where we will focus in this paper on the single Z/γ* production and decay to lepton pairs for definiteness. The other heavy gauge boson processes will be taken up elsewhere [12]. Section 4 contains our summary remarks.
2 Recapitulation

The starting point for what we discuss here may be taken as the fully differential representation

$$d\sigma = \sum_{i,j} \int dx_1 dx_2 F_i(x_1) F_j(x_2) d\hat{\sigma}_{\text{res}}(x_1 x_2 s)$$  \hspace{1cm} (1)

of a hard LHC scattering process using a standard notation so that the \{\(F_j\)\} and \(d\hat{\sigma}_{\text{res}}\) are the respective parton densities and reduced hard differential cross section where we indicate the latter has been resummed for all large EW and QCD higher order corrections in a manner consistent with achieving a total precision tag of 1% or better for the total theoretical precision of \(d\sigma\). The key theoretical issue for precision QCD for the LHC is then the proof of the correctness of the value of the total theoretical precision \(\Delta\sigma_{\text{th}}\) of (1). This precision can be represented as follows:

$$\Delta\sigma_{\text{th}} = \Delta F \oplus \Delta\hat{\sigma}_{\text{res}}$$  \hspace{1cm} (2)

where \(\Delta A\) is the contribution of the uncertainty on the quantity \(A\) to \(\Delta\sigma_{\text{th}}\). In order to validate the application of a given theoretical prediction to precision experimental observations, for the discussion of the signals and the backgrounds for both Standard Model(SM) and new physics (NP) studies, and more specifically for the overall normalization of the cross sections in such studies, the proof of the correctness of the value of the total theoretical precision \(\Delta\sigma_{\text{th}}\) is essential. If a calculation with an unknown value of \(\Delta\sigma_{\text{th}}\) is used for the attendant studies, the NP can be missed. This point simply cannot be emphasized too much.

In the interest of completeness here, we note that, by our definition, \(\Delta\sigma_{\text{th}}\) is the total theoretical uncertainty that comes from the physical precision contribution and the technical precision contribution \cite{17}: the physical precision contribution, \(\Delta\sigma_{\text{th}}^{\text{phys}}\), arises from such sources as missing graphs, approximations to graphs, truncations,....; the technical precision contribution, \(\Delta\sigma_{\text{th}}^{\text{tech}}\), arises from such sources as bugs in codes, numerical rounding errors, convergence issues, etc. The total theoretical error is then given by

$$\Delta\sigma_{\text{th}} = \Delta\sigma_{\text{th}}^{\text{phys}} \oplus \Delta\sigma_{\text{th}}^{\text{tech}}.$$  \hspace{1cm} (3)

The desired value for \(\Delta\sigma_{\text{th}}\), which depends on the specific requirements of the observations, as a general rule, should fulfill \(\Delta\sigma_{\text{th}} \leq f \Delta\sigma_{\text{expt}}\), where \(\Delta\sigma_{\text{expt}}\) is the respective experimental error and \(f \lesssim \frac{1}{2}\). This would assure that the theoretical uncertainty does not significantly adversely affect the analysis of the data for physics studies.

In order to realize such precision in a provable way, we have developed the QCD \(\otimes\) QED resummation theory in Refs. \cite{4} for the reduced cross section in (1) and for the resummation of the evolution of the parton densities therein as well. In the interest of completeness and also because the theory in Refs. \cite{4} is not widely known, we recapitulate it here briefly. Specifically, for both the resummation of the reduced cross section and that of the evolution of the parton densities, the master formula may be identified as

\footnote{Here, we discuss the situation in which the two errors in (2) are independent for definiteness; (2) has to be modified accordingly when they are not.}
\[ d\bar{\sigma}_{\text{res}} = e^{\text{SUM}_{\text{IR}}(\text{QCED})} \sum_{n,m=0}^{\infty} \frac{1}{n!m!} \int \prod_{j_1=1}^{n} \frac{d^3k_{j_1}}{k_{j_1}} \prod_{j_2=1}^{m} \frac{d^3k'_{j_2}}{k'_{j_2}} \int \frac{d^4y}{(2\pi)^4} e^{iy\cdot(p_1+q_1-p_2-q_2-\sum k_{j_1}-\sum k'_{j_2})} + D_{\text{QCED}} \]

\[ \bar{\beta}_{n,m}(k_1, \ldots, k_n; k'_1, \ldots, k'_m) \frac{d^4p_2 d^4q_2}{p_2^0 q_2^0}, \]  

(4)

where \( d\bar{\sigma}_{\text{res}} \) is either the reduced cross section \( \hat{\bar{\sigma}}_{\text{res}} \) or the differential rate associated to a DGLAP-CS \([5,6]\) kernel involved in the evolution of the \( \{F_j\} \) and where the new (YFS-style \([18]\)) non-Abelian residuals \( \tilde{\bar{\beta}}_{n,m}(k_1, \ldots, k_n; k'_1, \ldots, k'_m) \) have \( n \) hard gluons and \( m \) hard photons and we show the final state with two hard final partons with momenta \( p_2, q_2 \) specified for a generic \( 2f \) final state for definiteness. The infrared functions \( \text{SUM}_{\text{IR}}(\text{QCED}), D_{\text{QCED}} \) are defined in Refs. \([4,7,8]\). This simultaneous resummation of QED and QCD large IR effects is exact.

We stress that in Refs. \([7,9]\) the methods we employ for resummation of the QCD theory have been shown to be fully consistent with the methods in Refs. \([19,20]\). What is shown in Refs. \([7,9]\) is that the methods in Refs. \([19,20]\) give approximations to our hard gluon residuals \( \hat{\bar{\beta}}_n \); for, the methods in Refs. \([19,20]\), unlike the master formula in \([4]\), are not exact results. Specifically, the threshold-resummation methods in Refs. \([19]\), using the result that, for any function \( f(z) \),

\[ \left| \int_0^1 dz z^{n-1} f(z) \right| \leq \left( \frac{1}{n} \right) \max_{z \in [0,1]} |f(z)|, \]

drop non-singular contributions to the cross section at \( z \to 1 \) in resumming the logs in \( n \)-Mellin space. The SCET theory in Refs. \([20]\) drops terms of \( \mathcal{O}(\lambda) \) at the level of the amplitude, where \( \lambda = \sqrt{\Lambda/Q} \) for a process with the hard scale \( Q \) with \( \Lambda \sim 3\text{GeV} \) so that, for \( Q \sim 100\text{GeV} \), we have \( \lambda \simeq 5.5\% \). From the known equivalence of the two approaches, the errors in the threshold resummation must be similar. Evidently, we can only use these approaches as a guide to our new non-Abelian residuals as we develop results for the sub-1% precision regime.

We want to stress that, as it is explained in Refs. \([4]\), the new non-Abelian residuals \( \tilde{\bar{\beta}}_{m,n} \) allow rigorous shower/ME matching via their shower subtracted analogs:

\[ \tilde{\bar{\beta}}_{m,n} \rightarrow \tilde{\beta}_{m,n} \]  

(5)

where the \( \tilde{\bar{\beta}}_{m,n} \) have had all effects in the showers associated to the \( \{F_j\} \) removed from them. This naturally brings us to the attendant evolution of the \( \{F_j\} \); for, in order to have a strict control on the theoretical precision in \([1]\), we need both the resummation of the reduced cross section and that of the latter evolution.

When the QCD restriction of the formula in \([1]\) is applied to the calculation of the kernels, \( P_{AB} \), in the DGLAP-CS theory itself, we get an improvement of the IR limit of these kernels, an IR-improved DGLAP-CS theory \([7,8]\) in which large IR effects are
resummed for the kernels themselves. The resulting new resummed kernels, $P_{AB}^{\text{exp}}$ are given in Ref. [7–9] and are reproduced here for completeness:

\begin{align*}
P_{qq}^{\text{exp}}(z) &= C_F F_{YFS}(\gamma_q) e^{\frac{1}{2} \delta_q \left[ 1 + \frac{z^2}{1-z}(1-z)^{\gamma_q} - f_q(\gamma_q)\delta(1-z) \right]}, \\
P_{Gq}^{\text{exp}}(z) &= C_F F_{YFS}(\gamma_q) e^{\frac{1}{2} \delta_q \left[ \frac{1 + (1-z)^2}{z} \right] z^{\gamma_q}}, \\
P_{GG}^{\text{exp}}(z) &= 2C_G F_{YFS}(\gamma_G) e^{\frac{1}{2} \delta_G \left[ \frac{1}{z} \right] z^{\gamma_G} + \frac{z}{1-z}(1-z)^{\gamma_G}} \\
&\quad + \frac{1}{2}(z^{1+\gamma_G}(1-z) + z(1-z)^{1+\gamma_G}) - f_G(\gamma_G)\delta(1-z)} \\
P_{qG}^{\text{exp}}(z) &= F_{YFS}(\gamma_G) e^{\frac{1}{2} \delta_G \left[ \frac{1}{2} \right] z^2(1-z)^{\gamma_G} + (1-z)^2 z^{\gamma_G}}, \tag{6}
\end{align*}

where the superscript "exp" indicates that the kernel has been resummed as predicted by Eq. (4) when it is restricted to QCD alone, where the YFS [18] infrared factor is given by $F_{YFS}(a) = e^{-C_Ea}/\Gamma(1+a)$ where $C_E$ is Euler’s constant and where we refer the reader to Refs. [7, 8] for the detailed definitions of the respective resummation functions $\gamma_A, \delta_A, f_A, A = q, G$. $C_F(C_G)$ is the quadratic Casimir invariant for the quark(gluon) color representation respectively. These new kernels yield a new resummed scheme for the parton density functions (PDF’s) and the reduced cross section:

$F_j, \tilde{\sigma} \to F_j', \tilde{\sigma}'$ for $P_{Gq}(z) \to P_{Gq}^{\text{exp}}(z)$, etc.,

with the same value for $\sigma$ in (1) with improved MC stability as discussed in Refs. [9] – there is no need for an IR cut-off 'k0' parameter in the attendant parton shower MC based on the new kernels. We point-out that, while the degrees of freedom below the IR cut-offs in the usual showers are dropped in those showers, in the showers in HERWIRI1.031, as one can see from (4), these degrees of freedom are integrated over and included in the calculation in the process of generating the Gribov-Lipatov exponents $\gamma_A$ in (6). We note also that the new kernels agree with the usual kernels at $O(\alpha_s)$ as the differences between them start in $O(\alpha_s^2)$. This means the the NLO matching formulas in the MC@NLO and POWHEG frameworks apply directly to the new kernels for exact NLO ME/shower matching.

For completeness, we feature in Fig. 2 the basic physical idea underlying the new kernels as it was already discussed by Bloch and Nordsieck [23]: an accelerated charge generates a coherent state of very soft massless quanta of the respective gauge field so that one cannot know which of the infinity of possible states one has made in the splitting process $q(1) \to q(1-z) + G \otimes G_1 \cdots \otimes G_\ell, \ell = 0, \cdots, \infty$ illustrated in Fig. 2. The new kernels take this effect into account by resumming the terms $O\left((\alpha_s \ln(\frac{q^2}{\Lambda^2}) \ln(1-z))^n\right)$

\footnote{The improvement in Eq. (6) should be distinguished from the resummation in parton density evolution for the "z → 0" Regge regime – see for example Ref. [21,22]. This latter improvement must also be taken into account for precision LHC predictions.}
when $z \to 1$ is the IR limit. As one can see in (7) and (11), when the usual kernels are used these terms are generated order-by-order in the solution for the cross section $\sigma$ in (1) and our resumming them enhances the convergence of the representation in (1) for a given order of exactness in the input perturbative components therein. We now turn to the illustration of this last remark in the context of the comparison of NLO parton shower/matrix element matched predictions to recent LHC data.

### 3 Interplay of NLO Shower/ME Precision and IR-Improved DGLAP-CS Theory

The new MC HERWIR1.031 [9] gives the first realization of the new IR-improved kernels in the HERWIG6.5 [11] environment. Here, we compare it with HERWIG6.510, both with and without the MC@NLO [11] exact $O(\alpha_s)$ correction to illustrate the interplay between the attendant precision in NLO ME matched parton shower MC’s and the new IR-improvement for the kernels where we use the new LHC data for our baseline for the comparison.

More precisely, for the single $Z/\gamma^*$ production at the LHC, we show in Fig. 2 in panel (a) the comparison between the MC predictions and the CMS rapidity data [25] and in panel (b) the analogous comparison with the ATLAS $P_T$ data, where the rapidity data are the combined $e^+e^- - \mu^+-\mu^-$ results and the $p_T$ data are those for the bare $e^+e^-$ case, as these are the data that correspond to the theoretical framework of our simulations – we do not as yet have complete realization of all the corrections involved in the other ATLAS data in Ref. [26]. These results should be viewed from the perspective of our analysis in Ref. [9] of the FNAL data on the single $Z/\gamma^*$ production in $p\bar{p}$ collisions at 1.96 TeV.

Specifically, in Fig. 11 of the second paper in Ref. [9], we showed that, when the intrinsic rms $P_T$ parameter PTRMS is set to 0 in HERWIG6.5, the simulations for MC@NLO/HERWIG6.510 give a good fit to the CDF rapidity distribution data [28] therein but they do not give a satisfactory fit to the D0 $p_T$ distribution data [29] therein whereas the results for MC@NLO/HERWIR1.031 give good fits to both sets of data.
Figure 2: Comparison with LHC data: (a), CMS rapidity data on \((Z/\gamma^*)\) production to \(e^+e^-, \mu^+\mu^-\) pairs, the circular dots are the data, the green(blue) lines are HERWIG6.510(HERWIRI1.031); (b), ATLAS \(p_T\) spectrum data on \((Z/\gamma^*)\) production to (bare) \(e^+e^-\) pairs, the circular dots are the data, the blue(green) lines are HERWIRI1.031(HERWIG6.510). In both (a) and (b) the blue(green) squares are MC@NLO/HERWIRI1.031(HERWIG6.510(PTRMS = 2.2GeV)). In (b), the green triangles are MC@NLO/HERWIG6.510(PTRMS = 0). These are otherwise untuned theoretical results.

with the PTRMS = 0. Here PTRMS corresponds to an intrinsic Gaussian distribution in \(p_T\). The authors of HERWIG [27] have emphasized that to get good fits to both sets of data, one may set PTRMS \(\approx 2\) GeV. Thus, in analyzing the new LHC data, we have set PTRMS = 2.2GeV in our HERWIG6.510 simulations while we continue to set PRTMS=0 in our HERWIRI simulations.

Turning now with this perspective to the results in Fig. 2 we see a confirmation of the finding of the HERWIG authors. To get a good fit to both the CMS rapidity data and the ATLAS \(p_T\) data, one needs to set PTRMS \(\approx 2\) GeV [30] in the MC@NLO/HERWIG6510 simulations. We again see that at LHC one gets a good fit to the data for both the rapidity and the \(p_T\) spectra in the MC@NLO/HERWIRI1.031 simulations with PTRMS = 0. In quantitative terms, the \(\chi^2/\text{d.o.f.}\) for the rapidity data and \(p_T\) data are (.72,.72)((.70,1.37)) for the MC@NLO/HERWIRI1.031(MC@NLO/HERWIG 6510(PTRMS=2.2GeV)) simulations. For the MC@NLO/HERWIG6510(PTRMS=0) simulations the corresponding results are (.70,2.23).

Thus, we see that the usual DGLAP-CS kernels require the introduction of an intrinsic...
Gaussian spread in $p_T$ inside the proton to reproduce the LHC data on the $p_T$ distribution of the $Z/\gamma^*$ in the pp collisions whereas the IR-improved kernels give in fact a better fit to the data without the introduction of such a hard intrinsic component to the proton’s constituents. This PTRMS is entirely ad hoc; it is in contradiction with the results of all successful models of the proton wave-function [31]. More importantly, it contradicts the known experimental observation of precocious Bjorken scaling [32, 33], where the SLAC-MIT experiments show that Bjorken scaling occurs already at $Q^2 = 1_+ \text{ GeV}^2$ for $Q^2 = -q^2$ with $q$ the 4-momentum transfer from the electron to the proton in the famous deep inelastic electron-proton scattering process whereas, if the proton constituents really had a Gaussian intrinsic $p_T$ distribution with PTRMS $\approx 2 \text{GeV}$, these observations would not be possible. What can now say is that the ad hoc PTRMS $\approx 2.2 \text{GeV}$ value is really just a phenomenological representation of the more fundamental dynamics realized by the IR-improved DGLAP-CS theory. This raises the question of whether it is possible to tell the difference between the two representations of the data in Fig. 2.

Physically, one expects that more detailed observations should be able to distinguish the two. Specifically, we show in Fig. 3 the MC@NLO/HERWIG1.031 (blue squares) and MC@NLO/HERWIG6510 (PTRMS=2.2GeV) (green squares) predictions for the $Z/\gamma^*$ mass spectrum when the decay lepton pairs are required to satisfy the LHC type requirement that their transverse momenta $\{p_\ell^T, p_{\bar{\ell}}^T\}$ exceed 20 GeV. We see that the high precision data such as the LHC ATLAS and CMS experiments will have (each already has over $5 \times 10^6$ lepton pairs) will allow one to distinguish between the two sets of theoretical predictions, as the peaks differ by 2.2% for example. Of course, other such detailed observations may also reveal the differences between the two descriptions of parton shower

![Figure 3: Normalized vector boson mass spectrum at the LHC for $p_T(\text{lepton}) > 20 \text{ GeV}$.](image-url)
physics and we will pursue these elsewhere \[12\]. We await the release of the entire data sets from ATLAS and CMS.

4 Conclusions

We have shown that the realization of IR-improved DGLAP-CS theory in HERWIRI1.031, when used in the MC@NLO/HERWIRI1.031 exact $O(\alpha_s)$ ME matched parton shower framework, affords one the opportunity to explain, on an event-by-event basis, both the rapidity and the $p_T$ spectra of the $Z/\gamma^*$ in pp collisions in the recent LHC data from CMS and ATLAS, respectively, without the need of an ad hoc intrinsic Gaussian $p_T$ distribution with rms value of $\text{PTRMS} \approx 2$ GeV in the proton’s wave function. We argue that this can be interpreted as providing a rigorous basis for the phenomenological correctness of such ad hoc distributions insofar as describing these data using the usual unimproved DGLAP-CS showers is concerned and we have proposed that other distributions such as the invariant mass distribution with the appropriate cuts be used to differentiate between the fundamental description of the parton shower physics in MC@NLO/HERWIRI1.031 and these phenomenological representations in MC@NLO/HERWIG6510. We have emphasized that the precociousness of Bjorken scaling argues against the fundamental correctness of the ad hoc ansatz with $\text{PTRMS} \approx 2$ GeV, as do the successful models \[31\] of the proton’s wave function. We have the added bonus that the fundamental description in MC@NLO/HERWIRI1.031 can be systematically improved to the NNLO parton shower/ME matched level which we anticipate is a key ingredient in achieving the sub-1% precision tag for such processes as single heavy gauge boson production at the LHC. Evidently, the use of ad hoc models would compromise any discussion of the theoretical precision relative to what one could achieve from the fundamental representation of the corresponding physics via IR-improved DGLAP-CS theory as it is realized in HERWIRI1.031 when employed in MC@NLO/HERWIRI1.031 simulations. We are pursuing additional cross checks of the latter simulations against the LHC data.

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