ACOT & co..

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Abstract

This work is motivated by two developments in the field of QCD factorisation approaches and calculations. One of the two is the development of the ACOT prescriptons of how to consistently introduce the factorisation in case of non-negligible masses of the colliding partons (e.g. heavy quarks)[6, 7]. The second development was the consistent prescription developed by Collins et al. *of how to merge non-perturbative (parton-shower) calculations with the leading order perturbative pQCD calculations on the level of Monte-Carlo simulations [9, 10, 11, 12], which has been shown to reproduce the NLO* $\overline{\mathrm{MS}}$ *result for a set of processes. The aim of this work is to combine the two developments in a consistent way, which would enable one to adequately model processes involving heavy incoming quarks (e.g. bottom quarks) which play an important role in the calculations leading to experimental predictions and feasibility studies in the LHC environment.*

Key Words:
PACS:

1 Introduction

2 Theoretical overview

The QCD-based parton model is based on the factorisation theorems [1, 2, 3, 4, 5] according to which the squared amplitude for a process $\mathrm{A,B} \to \mathrm{X}$ can be decomposed into a 'hard' and 'soft'(or alternatively denoted 'short time' and 'long time') parts:

$$|\mathcal{M}_{AB\to X}|^2 = \sum_{a,b} f_{a/A} \otimes H_{ab\to X} \otimes f_{b/B} = \sum_{a,b} \int \frac{d\xi_a}{\xi_a} \int \frac{d\xi_b}{\xi_b} f_{a/A}(\xi_a,\mu_F)\, f_{b/B}(\xi_b,\mu_F)\, H_{ab\to X}(\xi_a,\xi_b,\mu_F\ldots), \quad (1)$$

with $\mathrm{a,b}$ as the parton labels which have to be summed over, $\mathrm{H(ab \to X)}$ denoting the hard ('short time') part of the squared amplitude and the soft contributions are absorbed into the parton distribution functions $\mathrm{f_{i/I}(\xi_i,\mu_F)}$ with μ_F being the (factorisation) scale at which the two parts were separated[1]. Subsequently, in the language of perturbative QCD and Feynman diagrams, the above theorem states that the collinear (mass) singularities have to be isolated/subtracted from the process amplitudes and absorbed in the parton distribution functions [3, 4, 5, 6, 7]; all other singularities (UV, soft IR) appearing in the perturbative calculation should be dealt with using the usual regularisation and renormalisation procedures. It has to be stressed at this point that the renormalisation scheme used in subtracting the UV singularities in turn dictates the precise form of the evolution (DGLAP) equations of the parton distribution functions [1, 3]

$$\frac{d}{d\ln\mu_F^2} f_{i/I}(z,\mu_F) = \frac{\alpha_s(\mu_F)}{2\pi} \sum_j \int_z^1 \frac{d\xi}{\xi} P_{j\to i}(\frac{z}{\xi},\alpha_s(\mu_F))\, f_{j/I}(\xi,\mu_F), \quad (2)$$

where $\mathrm{P_{j\to i}}$ denote the usual DGLAP evolution kernels and I describes either a parton or a hadron, which has to be taken into account in the full cross-section calculation.

[1] In case all partons are considered massless the flux factor in the partonic cross-section expression is $\hat{\mathrm{s}} = \xi_\mathrm{a}\xi_\mathrm{b}(2\mathrm{s})$ with $(2s)$ being the hadronic flux and the Eq. 1 results in the common expression $\sigma_{\mathrm{AB\to X}} = \int \mathrm{d}\xi_\mathrm{a} \int \mathrm{d}\xi_\mathrm{b} \mathrm{f_{a/A}}(\xi_\mathrm{a},\mu_\mathrm{F})\, \mathrm{f_{b/B}}(\xi_\mathrm{b},\mu_\mathrm{F})\, \sigma^{\mathrm{hard}}_{\mathrm{ab\to X}}(\hat{\mathrm{s}},\mu_\mathrm{F})$

An elegant way of isolating the mass singularities in perturbative calculations is found by observing that the pQCD squared amplitude $|\mathcal{M}_{\mathrm{ab}\to\mathrm{X}}|^2$ involving initial state partons a, b is subject to the same factorisation theorem:

$$|\mathcal{M}_{ab\to X}|^2 = \sum_{c,d} f_{c/a} \otimes H_{cd\to X} \otimes f_{d/b}, \tag{3}$$

with the $\mathrm{f_{i/j}}$ representing the distribution functions of the parton i inside the parton j. The above equation must hold to any order in perturbation theory in order for the factorisation theorem to be valid. Consequently, since the $|\mathcal{M}_{ab\to X}|^2$ can be calculated to any order by using the Feynman rules and the prescriptions for calculating the $\mathrm{f_{i/j}}$ to high orders in α_s are also well established [1, 21, 22] one can use the procedure of [5, 6, 7] to extract the $H_{cd\to X}$ to the chosen order.

The procedure is derived from the fact that at zero-th order in α_s:

$$f^{(0)}_{i/j}(\xi) = \delta^i_j \delta(\xi - 1) \tag{4}$$

and thus at this order:

$$|\mathcal{M}^{(0)}_{ab\to X}|^2 = H^{(0)}_{ab\to X}. \tag{5}$$

Subsequently, at first order in α_s:

$$f_{i/j}(\xi) = f^{(0)}_{i/j}(\xi) + f^{(1)}_{i/j}(\xi), \tag{6}$$

and thus at this order:

$$|\mathcal{M}^{(1)}_{ab\to X}|^2 = H^{(1)}_{ab\to X} + \sum_c f^{(1)}_{c/a} \otimes H^{(0)}_{cb\to X} + \sum_d H^{(0)}_{ad\to X} \otimes f^{(1)}_{d/b}, \tag{7}$$

where formally the virtuality μ^2 of the particles c or d (which is in turn proportional to the $(p_T)^2$ of the particles $\bar{c}$ or $\bar{d}$, see Fig. **1**) is used as the factorisation measure with the limit μ^2_{F}: The hard part $\mathrm{H}^{(1)}_{\mathrm{ab}\to\mathrm{X}}$ includes the cases $\mu^2 \geq \mu^2_{\mathrm{F}}$ and the soft one the cases $\mu^2 \leq \mu^2_{\mathrm{F}}$. Note that in the above equation the phase space integral over $\bar{c}/\bar{d}$ particles has already been performed (resulting in the convolution integral) and thus the phase space integration over the final state particles (when performed) for the soft part formally involves one less particle.

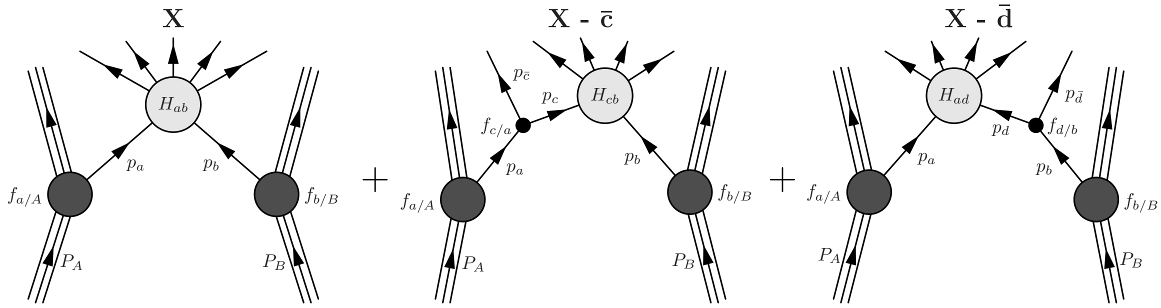

Fig. 1: The diagrammatic representation of the method applied in isolating the soft (collinear) terms in propagators corresponding to virtual particles $\mathrm{p_c}$ and/or $\mathrm{p_d}$ when calculating the $|\mathcal{M}^{(1)}_{ab\to X}|^2$. Note that in factorisation theorem the particles incoming into the hard part of the probability amplitude are considered to be on-shell.

The above equation can be inverted to give:

$$H^{(1)}_{ab\to X} = |\mathcal{M}^{(1)}_{ab\to X}|^2 - \sum_c f^{(1)}_{c/a} \otimes |\mathcal{M}^{(0)}_{cb\to X}|^2 - \sum_d |\mathcal{M}^{(0)}_{ad\to X}|^2 \otimes f^{(1)}_{d/b} \tag{8}$$

and analogous steps can be repeated at subsequent orders. It should be emphasised that the presence of the subtraction terms in the above Eq. 8 effectively means the prevention of the 'double counting' when performing the perturbative cross-section calculation since the collinear effects included in the $|\mathcal{M}^{(1)}_{\mathrm{ab}\to\mathrm{X}}|^2$ are already re-summed in the parton distribution functions $\mathrm{f_{a/A}}$ of the initial hadrons.

When inserting the perturbative expansion of $H_{ab\to X} = H^{(0)}_{ab\to X} + H^{(1)}_{ab\to X}$ given by Eq. 5 and Eq. 8 into the cross-section expression (Eq. 1) one thus obtains the formula:

$$|\mathcal{M}_{AB\to X}|^2 = |\mathcal{M}^{(0)}_{AB\to X}|^2 + |\mathcal{M}^{(1)}_{AB\to X}|^2 - |\mathcal{M}_{AB\to X}|^2_{\mathrm{s}}, \tag{9}$$

with the subtraction terms given by:

$$|\mathcal{M}_{AB\to X}|^2_{\mathrm{s}} = \sum_{a,b} f_{a/A} \otimes \sum_c f^{(1)}_{c/a} \otimes H^{(0)}_{cb\to X} \otimes f_{b/B} + \sum_{a,b} f_{a/A} \otimes \sum_d H^{(0)}_{ad\to X} \otimes f^{(1)}_{d/b} \otimes f_{b/B}. \tag{10}$$

For further discussion on the 'double counting' issues it is illuminating to calculate the $f_{i/j}$ at scale μ_F up to the order of α_s. One starts by writing down the perturbative expansion of the evolution kernels in the DGLAP equations:

$$P_{j\to i}(\xi, \alpha_s(\mu_F)) \ = P^{(0)}_{j\to i}(\xi) + \left(\frac{\alpha_s(\mu_F)}{2\pi}\right) P^{(1)}_{j\to i}(\xi) + \ldots \tag{11}$$

and observing that the evolution increases the order of $\mathrm{f}^{(\mathrm{n})}_{\mathrm{i/j}}$ by one. This can explicitly be seen by inserting the zero-th order $\mathrm{f}^{(0)}_{\mathrm{i/j}}$ of Eq. 4 into the Eq. 2, and increasing the factorisation scale from the lowest kinematic limit (mass m of the particle i) to the scale μ_F, i.e. integrating over the range $[\mathrm{m}^2, \mu_{\mathrm{F}}^2]$ and keeping only the terms up to the order of α_s:

$$f_{i/j}(\xi, \mu_F) = f^{(0)}_{i/j}(\xi) + \frac{\alpha_s(\mu_F)}{2\pi} P^{(0)}_{j\to i}(\xi) \ln\left(\frac{\mu_F^2}{m^2}\right). \tag{12}$$

The above expression matches the perturbative expansion given by Eq. 6 with the second term identified as the $\mathrm{f}^{(1)}_{\mathrm{i/j}}$ parton distribution function.

While the expression of Eq. 9 can subsequently be used for estimating the total cross-section of a given process one should take further steps when dealing with the estimation of the differential cross-sections or (equivalently) Monte-Carlo simulation. In terms of Monte-Carlo simulation the DGLAP parton evolution, re-summed in the parton density functions $f_{i/I}$ (c.f. Eq. 2), is made explicit by evolving the factorisation scale from its initial value μ_0 to the lowest kinematic limit (or an imposed cutoff). Identifying the evolving factorisation scale with the virtuality μ^2 of the incoming particle c the probability that the particle c will be un-resolved into a particle a (or equivalently, that a particle a will branch and produce the particle c and an additional spectator particle) is given by the Sudakov term (see e.g. [15]):

$$S_a = \exp\left\{ -\int_{\mu^2}^{\mu_0^2} \frac{d\mu'^2}{\mu'^2} \frac{\alpha_s(\mu'^2)}{2\pi} \times \sum_c \int_{\xi_c}^{1} \frac{dz}{z} P_{a\to c}(z) \frac{f_{a/I}(\frac{\xi_c}{z}, \mu'^2)}{f_{c/I}(\xi_c, \mu'^2)} \right\}. \tag{13}$$

At each evolution step (branching) the number of particles is thus increased by one and its contribution to the differential cross-section in terms of α_s is also increased by one. The described procedure is commonly known as (initial state) *parton showering*.

The (next-to-leading order) subtraction terms of Equation 10 thus compensate for the first branching in the backward evolution of the incoming partons participating in the (leading order) term $H^{(0)}_{ab\to X}$. Note that in order to match the subtraction terms in Eq. 8 with the first–order matrix element the fraction ξ_{c} (or equivalently ξ_{d}) of the evolved parton is kept constant and the virtuality is in fact *decreased* corresponding to a 'backward' evolution in time from the starting point of virtuality μ_0^2 of $\mathrm{H}^{(0)}_{\mathrm{ab}\to\mathrm{X}}$. to the virtuality μ^2 of $\mathrm{H}^{(1)}_{\mathrm{ab}\to\mathrm{X}}$ (c.f. Figure **1**). Writing the expressions of Equation 10 in differential form in μ^2 one thus gets for the first term:

$$|\mathcal{M}_{AB\to X}|^2_{\mathrm{s}} = \frac{d\mu^2}{\mu^2} \sum_{a,b,c} \int \frac{d\xi_a}{\xi_a} \int \frac{d\xi_b}{\xi_b} \int \frac{d\xi_c}{\xi_c} f_{a/A}(\xi_a, \mu_0^2) \frac{\alpha_s(\mu_0^2)}{2\pi} P^{(0)}_{a\to c}\left(\frac{\xi_c}{\xi_a}\right) H^{(0)}_{cb\to X}(\xi_c, \xi_b)\, f_{b/B}(\xi_b, \mu_0^2) + \ldots \tag{14}$$

and an equivalent expression can be obtained for the second term of Eq. 10. Using again the Eq. 5, multiplying by the flux factor $1/2\sqrt{\lambda(s, m_A^2, m_B^2)}$, given by the Lorentz invariant function:

$$\lambda(s, m_1^2, m_2^2) = (s - (m_1 + m_2)^2)(s - (m_1 - m_2)^2) \tag{15}$$

and integrating over the final state n-particle phase space denoted by $\int \mathrm{d}\Phi_{\mathrm{X}}$, one obtains the first subtraction term:

$$\frac{d\sigma_{s1}^{(0)}(AB \to X)}{d\xi_a d\xi_b d\mu^2 d\xi_c d\phi} = \tag{16}$$
$$\sum_{a,b,c} \frac{\theta(\mu_0^2 - \mu^2)}{2\sqrt{\lambda(s, m_A^2, m_B^2)}\xi_c\xi_b} \frac{\alpha_s(\mu_0^2)}{4\pi^2\, \mu^2} \frac{1}{\xi_a} f_{a/A}(\xi_a, \mu_0^2)\, P_{a\to c}^{(0)} \left(\frac{\xi_c}{\xi_a}\right) f_{b/B}(\xi_b, \mu_0^2) \int |\mathcal{M}_{cb\to X}^{(0)}|^2(\xi_c, \xi_b) d\Phi_{X-\bar{c}}$$

and equivalently also the second subtraction term by appropriate replacements $a \to b$ and $c \to d$.
The two derived equations correspond to the expressions obtained by Chen,Collins *et al.* [9, 10, 11, 12], derived by the Sudakov exponent expansion.

In addition to writing the cross-sections in differential form the integration over an angle ϕ was introduced, where the angle ϕ represents the azimuthal angle of the spectator particle $\bar{\mathrm{c}}$ or $\bar{\mathrm{d}}$ and is in effect a dummy quantity which nevertheless has to be sampled in a Monte–Carlo simulation procedure. The notation $\mathrm{d}\Phi_{\mathrm{X}-\bar{\mathrm{d}}}$ denotes that the final space integral does not contain the spectator particles $\bar{\mathrm{c}}$ or $\bar{\mathrm{d}}$ since they are already accounted for in the $(\mathrm{d}\xi/\xi)\mathrm{d}\mu^2\mathrm{d}\phi$ differential (see e.g. [1]). In contrast the first order matrix element of Equation 8 is integrated over the full phase space X:

$$\frac{d\sigma^{(1)}(AB \to X)}{dx_a dx_b} = \tag{17}$$
$$\sum_{a,b} \frac{1}{2\sqrt{\lambda(s, m_A^2, m_B^2)}x_a x_b} f_{a/A}(x_a, \mu_0^2)\, f_{b/B}(x_b, \mu_0^2) \int |\mathcal{M}_{ab\to X}^{(1)}|^2(x_a, x_b) d\Phi_X\ ,$$

whereby the outstanding issue is the kinematic translation between $\mathrm{n}-1$ $(\mathrm{X}-\bar{\mathrm{c}})$ and n (X) particle kinematics; one should also not implicitly equate the variables $\xi_{\mathrm{a,b}}$ and $\mathrm{x_{a,b}}$, since e.g. in Eq. 16 the $\xi_{\mathrm{c,b}}$ imply that the incoming particles c and b are on shell in the matrix element calculation while in Eq. 17 in contrast the particle a (as the 'parent' of particle c) is the on-shell one.

The mapping of the kinematic quantities between between the expressions of order α_{S} (i.e. the pQCD derived expression of Eq. 18 and the (showering) subtraction terms of Eq. 17) needs a consistent and possibly a formally correct definition. In order to achieve this the prescription developed by Collins *et al.* of how to merge non-perturbative (parton-shower) calculations with the leading order perturbative pQCD calculations on the level of Monte-Carlo simulations [9, 10, 11, 12] was implemented, which has been explicitly shown to reproduce the NLO $\overline{\mathrm{MS}}$ result for a set of processes.

Another outstanding issue is that in case of heavy quarks participating as the initial state partons the (commonly used) approximation of treating the incoming particles as massless can lead to a significant error. This fact, as well as the the solution in terms of consistent treatment of the kinematics in terms of light-cone variables, has been demonstrated in the ACOT prescriptons of how to consistently introduce the factorisation in case of non-negligible masses of the colliding partons (e.g. heavy quarks)[6, 7]. The ACOT prescription has in this paper been introduced in the formalism of Monte-Carlo simulation by modifying the prescription of Collins *et al.* accordingly.

In the Monte–Carlo generation steps one thus has to produce two classes of events; one class is derived from the leading order process with one branching produced by Sudakov parton showering and the second class are events produced from the next-to-leading order hard process calculation (i.e. the pQCD calculation with the appropriate subtraction terms).

3 Kinematic Issues

3.1 Phase-Space Transformation

The aim of this section is to derive generic expressions of how to translate the kinematics from the 'hard' to the 'soft' (or showering) n-particle system, i.e. split the 'hard' n-particle phase space involving heavy quarks into $\mathrm{n}-1$ 'hard' $\oplus 1$ 'soft' particle phase space in order to perform appropriate MC simulation (c.f. Figure **2**). As already stated the existing prescriptions deal either with massive particles [6, 7] on the level of integrated cross-sections or with explicit Monte-Carlo algorithms involving light ($\sim$ massless) particles (e.g. [25, 15, 11, 13, 14]) while no generic combination of the two algorithms has so far been published. In order to accommodate the particle masses it is convenient to work in light-front coordinates $p^\mu = (p^+, \vec{p}^T, p^-)$ where $\mathrm{p}^\pm = \frac{1}{\sqrt{2}}(\mathrm{p}^0 \pm \mathrm{p}^3)$ and the remaining two coordinates are considered 'transverse' $\vec{p}^T$. The kinematic prescription of relating the hard n-particle kinematics to the soft $\mathrm{n}-1$ case is as follows:

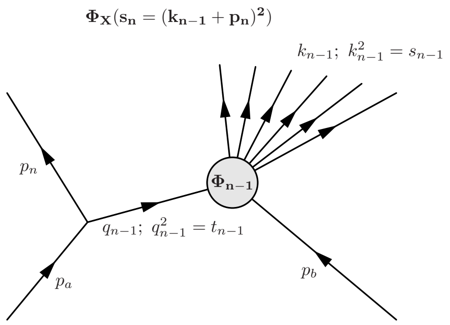

Fig. 2: The diagrammatic representation of the method applied in translating a t-channel (space-like) split going from n to $n-1$ particle phase space.

1. Hadron A is moving in the z direction and hadron B in the $-$z direction, carrying momenta $\mathrm{P_A}$ and $\mathrm{P_B}$ with the centre-of-mass energy $\sqrt{\mathrm{s}}$, whereby one can neglect the hadron masses at LHC energies.
2. The incoming partons with momenta $\mathrm{p_a}$ and $\mathrm{p_b}$ have the momentum fractions $\mathrm{p_a^+} = \mathrm{x_a P_A^+}$ and $\mathrm{p_b^-} = \mathrm{x_b P_B^-}$ relative to the parent hadrons and the centre-of-mass energy $\sqrt{s_n}$.
3. The split propagator (i.e. particle c) virtuality $p_c^2 = (p_a - p_{\bar{c}})^2 = t_{n-1}$ (c.f. Fig. **2**) gives the μ^2 value from $t_{n-1} - m_{\bar{c}}^2 = -\mu^2$. (c.f. Eq. 16).
4. The scale correspondence is given by $\mathrm{s_{n-1}} = \mu_0^2$ (c.f. Eq. 16).
5. All incoming and outgoing particles (partons) are on mass shell.
6. The splitting parameter of the evolution kernel is $\mathrm{z} = \frac{\xi_c}{\xi_a}$ (already used in Eq. 16).
7. The rapidity $\mathrm{y} = \frac{1}{2}\ln\left(\frac{\mathrm{k_{n-1}^+}}{\mathrm{k_{n-1}^-}}\right)$ of the subsystem (c.f. Figure **2**) is preserved in the translation.

In order to further relate the n and n$-$1 particle phase space for hard and soft interpretation one can use the recursive t-channel splitting relation [16, 18]:

$$\Phi_n(s_n, m_1, m_2, \ldots, m_n) = \tag{18}$$
$$= \int\limits_{(\sum_{i=1}^{n-1} m_i)^2}^{(\sqrt{s_n}-m_n)^2} \frac{ds_{n-1}}{4\sqrt{\lambda(s_n, m_a^2, m_b^2)}} \int\limits_0^{2\pi} d\varphi_n^* \int\limits_{t_{n-1}^-}^{t_{n-1}^+} dt_{n-1}\, \Phi_{n-1}(s_{n-1}, m_1, m_2, \ldots, m_{n-1}),$$

where $\varphi_\mathrm{n}^* \equiv \phi$ of Eq. 16 and the limits $t_{n-1}^{\pm}$ are given by analytic, albeit complex expressions [16, 18]. Using the above relation one can e.g. introduce the $\mathrm{X} - \bar{\mathrm{c}}$ particle phase space split into Equation 17 by identifying $\mathrm{p_{\bar{c}}} \equiv \mathrm{p_n}$:

$$\frac{d\sigma^{(1)}(AB \to X)}{dx_a dx_b dt_{n-1} ds_{n-1} d\varphi^*} = \tag{19}$$
$$\sum_{a,b} \frac{1}{2\sqrt{\lambda(s, m_A^2, m_B^2)} x_a x_b} f_{a/A}(x_a, s_{n-1})\, f_{b/B}(x_b, s_{n-1}) \int |\mathcal{M}_{ab\to X}^{(1)}|^2 (x_a, x_b) \frac{1}{4\sqrt{\lambda(s_n, m_a^2, m_b^2)}} d\Phi_{X-\bar{c}}\ ,$$

Using the translation prescriptions introduced above the remaining unresolved requirement is to relate the variables $\xi_\mathrm{a}, \xi_\mathrm{c}, \xi_\mathrm{b}$ with the variables x_a, x_b, s_{n-1}. The requirement (**2**) in the list gives the equivalence $\xi_\mathrm{a} \equiv \mathrm{x_a}$ since both particles in question are incoming partons originating in hadron A. The remaining relations between $\xi_\mathrm{c}, \xi_\mathrm{b}$ and x_b, s_{n-1} are then given by energy and rapidity conservation requirements. The derived relations are explicitly listed in Appendix A.

Combining all the derived rules for kinematic translation one finally obtains a transformation of Eq. 16:

$$\frac{d\sigma_{s1}^{(0)}(AB \to X)}{dx_a dx_b dt_{n-1} ds_{n-1} d\varphi^*} = \mathcal{J}\frac{(\xi_c, \xi_b)}{(s_{n-1}, x_b)}\ \frac{d\sigma_{s1}^{(0)}(AB \to X)}{d\xi_a d\xi_b d\mu^2 d\xi_c d\phi}\Bigg|_{\xi_a \to x_a,\, \mu^2 \to -(t_{n-1} - m_{\bar{c}}^2),\, \phi \to \varphi^*,\, (\xi_c, \xi_b) \to (s_{n-1}, x_b)}, \tag{20}$$

where $\mathcal{J}\frac{(\bar{\tau},\bar{y})}{(s_{n-1},x_b)}$ is the Jacobian of the transformation derived in the Appendix A.

An issue which deserves special consideration is the prescribed substitution $t_{n-1} - m_{\bar{c}}^2 = -\mu^2$, where the split particle virtuality μ^2 is the propagator virtuality shifted by the spectator mass $m_{\bar{c}}^2$. This prescription differs from the one of Collins [9], where the relation is directly $t_{n-1} = -\mu^2$ and the spectator (propagator) mass shift is omitted. The reason for this modification becomes transparent when one considers that the phase space limits $[t_{n-1}^-, t_{n-1}^+]$ of the t_{n-1} parameter are functions of s_n and invariant masses of the objects (particles) participating in a t-channel split of Equation 18 [16, 18] and thus do not match the simple limits $[m_{\bar{c}}^2, s_{n-1}]$ of the virtuality μ^2 in the equation 16. Indeed, studies have shown that the presence of the cutoff $\theta(s_{n-1} + t_{n-1})$ does not provide a sufficient solution since it only sets the upper integration limit to $t_{n-1}^+ \to -s_{n-1}$ while the lower limit t_{n-1}^- can in certain instances be even smaller than $m_{\bar{c}}^2$. The condition of reproducing a logarithmic term of the collinear singularity $\ln\left(\frac{\mu_F^2}{m^2}\right)$ (Eq. 12) with $\mu_F^2 = \mu_0^2 = s_{n-1}$:

$$\int\limits_{t_{n-1}^-}^{t_{n-1}^+} \frac{\theta(s_{n-1} + t_{n-1})}{t_{n-1}} dt_{n-1} = \ln\left(\frac{-s_{n-1}}{t_{n-1}^-}\right) \neq \ln\left(\frac{s_{n-1}}{m_{\bar{c}}^2}\right) \tag{21}$$

is thus not satisfied in when prescribing $t_{n-1} = -\mu^2$. In order to resolve this issue one needs to go back to the basics of the factorisation procedure, where the actual collinear singularity (i.e. the corresponding logarithmic term) is isolated from the (integrated) hard process cross-section (for a nice example with massive particles see e.g. [7]) and these logarithmic terms match with the required collinear logarithm $\ln\left(\frac{\mu_F^2}{m^2}\right)$ only in the high s_n (hard centre-of-mass) limit. The logarithmic collinear terms can subsequently be traced back to the propagator integral:

$$\int\limits_{t_{n-1}^-}^{t_{n-1}^+} \frac{dt_{n-1}}{t_{n-1} - m_{\bar{c}}^2} = \ln\left(\frac{t_{n-1}^+ - m_{\bar{c}}^2}{t_{n-1}^- - m_{\bar{c}}^2}\right) \xrightarrow{s_n \to \infty} \ln\left(\frac{s_{n-1}}{m_{\bar{c}}^2}\right). \tag{22}$$

The expression of Eq. 22 is indeed found to match the logarithmic terms of [7] exactly[2]. In order to reproduce the collinear cutoff one thus has to put $-\mu^2 = t_{n-1} - m_{\bar{c}}^2$ which, combined with the factorisation cutoff $\theta(\mu_F^2 - \mu^2) = \theta(s_{n-1} - \mu^2)$, indeed reproduces the required logarithm in the high s_n limit:

$$\int\limits_{-(t_{n-1}^- - m_{\bar{c}}^2)}^{-(t_{n-1}^+ - m_{\bar{c}}^2)} \frac{\theta(s_{n-1} - \mu^2)}{\mu^2} d\mu^2 = \ln\left(\frac{s_{n-1}}{-(t_{n-1}^- - m_{\bar{c}}^2)}\right) \xrightarrow{s_n \to \infty} \ln\left(\frac{s_{n-1}}{m_{\bar{c}}^2}\right). \tag{23}$$

[2]Specifically the expressions of Eq. 17, page 14, whereby one has to write down the explicit expressions for the limits on t_{n-1} and set the mass of the incoming particle corresponding to the incoming gluon to zero in order to reproduce the kinematical topology of the process studied in [7].

3.2 Monte-Carlo Generation Steps

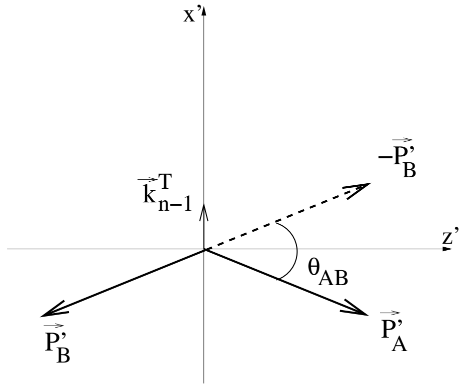

Fig. 3: The definition of the reference Collins-Soper frame as the rest frame of the subsystem $\mathrm{s_{n-1}}$ with the transverse component $\vec{k}^T_{n-1}$ oriented in the $x' - axis$ direction.

In order to simulate a full Monte–Carlo event the generation steps are thus as follows:

1. Generate the particle momenta and corresponding phase space weight for the n-particle final state X and compute the full weight corresponding to the process of Eq. 17.
2. Re-calculate the kinematic quantities of the $\mathrm{n} \rightarrow (\mathrm{n}-1) \oplus 1$ transformation as described above.
3. Boost the whole system into the Collins-Soper frame [2] of the $\mathrm{n}-1$ subsystem, i.e. the s_{n-1} centre of mass frame where the angle between the boosted hadron momenta P'_A or $-P'_B$ and z'-axis is now $\tan(\frac{1}{2}\theta_{AB}) = |\vec{k}^T_{n-1}|/\sqrt{s_{n-1}} = |\vec{p}^T_{\bar{c}}|/\sqrt{s_{n-1}}$ (c.f. Fig. **3**). In other words, this transformation manifestly puts the transverse contribution due to the induced virtuality into the hadron momenta directed perpendicularly to the z'-axis. One can thus eliminate this virtuality by shifting the hadron momenta to the z'-axis while preserving the centre-of mass energy s_{n-1}.
4. The $n-1$ (hard) system corresponding to the Eq. 16 is then achieved by eliminating the particle $\bar{c}$ and boosting the remaining particles in the z-axis direction with the boost value of:
$$\beta = \frac{\xi_c(\xi_c\xi_b s + m_b^2) - \xi_b(\xi_c\xi_b s + m_c^2)}{\xi_c(\xi_c\xi_b s + m_b^2) + \xi_b(\xi_c\xi_b s + m_c^2)} \tag{24}$$
in order to restore the sub-system rapidity y.
5. Since boosts do not change the phase space weight the necessary modification consists of multiplying the phase space weight by:
$$4\sqrt{\lambda(s_n, m_a^2, m_b^2)}\theta(s_{n-1} + t_{n-1})\mathcal{J}\frac{(\xi_c, \xi_b)}{(s_{n-1}, x_b)} \tag{25}$$
and then obtaining the first subtraction weight by putting the reconstructed momenta into the Eq. 16.
6. An analogous procedure can be repeated to obtain the alternate kinematic configuration (with the parton evolution of the other incoming particle) and the second subtraction weight.
7. The final weight, after performing both subtractions is then passed to the event unweighing procedure.

As Chen, Collins*et al.* pointed out, [9, 10, 11, 12], the described procedure of subtraction is not equivalent to the standard subtraction schemes (e.g. $\overline{\mathrm{MS}}$) used to obtain the cross-sections for specific processes (see e.g. [23, 19]) and hence the data-fitted parton distribution functions with the corresponding evolution kernels (for example the widely used CTEQ5 PDF-s [26]). The relation between the procedure applied derived by Chen, Collins*et al.* for the massless case and (with inclusion of parton masses) applied above states that the correspondence between the $\overline{\mathrm{MS}}$ scheme and the applied JCC scheme is given by relatively simple relations; an example for the expression of the quark i distribution function involves a convolution of the gluon g distribution function and the $\mathrm{g} \to \mathrm{i}\bar{\mathrm{i}}$ splitting kernel $\mathrm{P}_{\mathrm{g}\to\mathrm{i}\bar{\mathrm{i}}}(\mathrm{z})$:

$$\begin{aligned} z\, f_{i/I}^{\mathrm{JCC}}(z,\mu^2) &= z\, f_{i/I}^{\overline{\mathrm{MS}}}(z,\mu^2) \\ &+ \frac{\alpha_s(\mu^2)}{2\pi}\int_z^1 d\xi \frac{z}{\xi} f_{g/I}^{\overline{\mathrm{MS}}}(\xi,\mu^2)\left[P_{g\to i\bar{i}}(\frac{z}{\xi})\ln\left(1-\frac{z}{\xi}\right)+\frac{z}{\xi}\left(1-\frac{z}{\xi}\right)\right] \\ &+ \mathcal{O}(\text{first-order quark terms}) + \mathcal{O}(\alpha_s^2) \end{aligned} \tag{26}$$

These new distributions can in a reasonably straightforward manner be obtained by numerical integration.

In order to complement the subtracted process one also has to generate a parton-shower evolved zero-th order process with $(\mathrm{n}-1)$ particles in the participating in the hard process and an additonal particle added by 'soft' evolution of the incoming particles. Since one is interested in the heavy initial state quarks this subsequently means that one has to 'unresolve' one of the initial quarks back to a gluon, whereby an additional (anti) quark is added. The procedure to achieve this is straightforward [9, 10, 11, 12] and complementary to the procedure described above, i.e. one has to perform the following steps in the Monte-Carlo algorithm:

1. Generate the particles corresponding to the $(\mathrm{n}-1)$ phase space topology, along with the momentum fractions ξ_c and ξ_b of the incoming particles in the sense of light-front components. Consequently, the invariant mass of the hard system is s_{n-1} and the rapidity y is given by Equation 31.
2. Generate a virtuality μ^2 of the incoming heavy quark c, a longitudinal splitting fraction z for the branching of gluon a into the $c\bar{c}$ pair and an azimuthal angle ϕ of the branching system. All the values are sampled from the Sudakov-type distribution:

$$S_a = \exp\left\{-\int_{\mu^2}^{\mu_0^2}\frac{d\mu'^2}{\mu'^2}\frac{\alpha_s(\mu'^2)}{2\pi}\times\int_{\xi_c}^1\frac{dz}{z}P_{a\to c}(z)\frac{f_{a/I}(\frac{\xi_c}{z},\mu'^2)}{f_{c/I}(\xi_c,\mu'^2)}\right\}. \tag{27}$$

   In case there are two quarks in the initial state that can evolve back to gluon and give the contribution of the same order (like e.g. $\mathrm{b}\bar{\mathrm{b}} \to \mathrm{Z}^0$ process) both virtualities are sampled and the quark with the higher one is chosen to evolve.

Subsequently, the four-momenta of the participating particles are reconstructed with the requirement that the subsystem invariant mass s_{n-1} and the rapidity y are preserved; the construction is of course identical to the one used in the $\mathrm{n} \to (\mathrm{n}-1)\oplus 1$ transformation given in Section 3.1. A point to stress is that a kinematic limitation arises on the allowed $\mathrm{x_a}$ and thus $\mathrm{z} = \frac{\xi_c}{\mathrm{x_a}}$ values due to the requirement $|\vec{p}_{\bar{c}}^{\,T}|^2 \geq 0$. The latter condition gives the minimal value of the invariant mass of the n-particle system $\mathrm{s_n} = \mathrm{x_a x_b s} + \mathrm{m_b^2}$ (taking into account that one of the incoming particles is a gluon, $m_a = 0$) with:

$$(x_a x_b s)_{\min} = \frac{(m_c^2+\mu^2)}{2}\left(\frac{(s_{n-1}+\mu^2-m_b^2)}{\mu^2}+\sqrt{\frac{(s_{n-1}+\mu^2-m_b^2)^2}{\mu^4}+\frac{4m_b^2}{\mu^2}}\right), \tag{28}$$

which combines with the rapidity y conservation requirement into:

$$x_a^2 \geq \frac{(x_a x_b s)_{\min}^2\left((x_a x_b s)_{\min}-(m_c^2+\mu^2)\right)}{s\left[(s_{n-1}+\mu^2)e^{-2y}\,(x_a x_b s)_{\min}-m_b^2(m_c^2+\mu^2)\right]}. \tag{29}$$

In the massless limit the above expression translates back into the requirement $x_a \geq \xi_a$ or equivalently $z \leq 1$. In practice (i.e. Monte-Carlo generation) this thus means that a certain fraction of generated topologies have to be rejected and/or re-generated until the above conditions are met (or equivalently, that the z (or $\mathrm{x_a}$) sampling limits have to be shifted to prevent this from happening).

4 Examples of the Algorithm Implementation

Two examples of the procedure described in this paper have been developed: The associated Z^0b production process and the single top production process, both expected to be observed at the LHC. The processess were implemented in the AcerMC 3.0 Monte-Carlo generator [17]. Due to the subtraction terms a fraction of event candidates achieve negative sampling weights and unweighted events are produced with weight values of ± 1 using the standard unweighing procedures.

4.1 Associated Drell-Yan and b-quark Production

The (Drell-Yan) lepton pair production associated with one or more heavy quarks represents the irreducible background component in the Higgs boson searches at the LHC and is also of importance in several detector calibration studies.

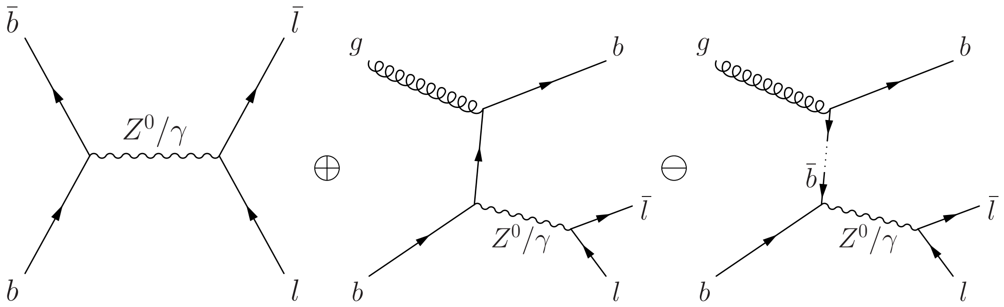

Fig. 4: Representative Feynman diagrams for the Drell-Yan with associated b-quark production process for (from left to right): Order $\alpha_s^{(0)}$, order $\alpha_s^{(1)}$ and order $\alpha_s^{(1)}$ subtraction term.

Table 1: The process cross-sections for the leading order process $b\bar{b} \to Z \to \mu^+\mu^-$, next-to-leading order process $gb \to Zb \to \mu^+\mu^- b$ and the subtraction process $(g \to b\bar{b})b \to Zb \to \mu^+\mu^- b$ in the LHC environment (proton-proton collisions at $\sqrt{s}$ = 14 TeV) are listed. The b-quark mass is set to $m_b = 4.8$ GeV and the factorisation and renormalisation scales are set to the Z^0 invariant mass squared. In addition, the order $\alpha_s^{(2)}$ $gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$ process cross-section is shown for comparison. The cross-sections are given for the LO CTEQ5L [26] and the derivedJCC PDFs. In the Monte-Carlo procedure the next-to-leading process weights are combined with the subtraction weights on the event-by-event basis as described in the text.

Process	$\sigma_{\mathrm{CTEQ5L},\mu_0=\mathrm{m_Z}}$ [pb]	σJCC, $\mu_0 = \mathrm{m_Z}$) [pb]
$b\bar{b} \to Z \to \mu^+\mu^-$	57.9	39.9
$gb \to Zb \to \mu^+\mu^- b$	72.1	60.0
$(g \to b\bar{b})b \to Zb \to \mu^+\mu^- b$	73.3	60.9
Σ	56.7	39.0
$gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$	22.8	22.8

In the given case both incoming particles can be evolved back to gluons at the same order in $\alpha_s^{(1)}$ therefore when performing the showering both particle virtualities are sampled and the higher one is chosen as explained in the previous section; the other virtuality is kept on-shell in order to match the developed subtraction procedure.

The cross-sections obtained for the leading order process $b\bar{b} \to Z \to \mu^+\mu^-$, next-to-leading order process $gb \to Zb \to \mu^+\mu^- b$ and the subtraction process $(g \to b\bar{b})b \to Zb \to \mu^+\mu^- b$ in the LHC environment (proton-proton collisions at $\sqrt{s}$ = 14 TeV) are given in the Table **1**, both for leading order PDF (CTEQ5L [26] was used) and the PDF-s evolved according to the

Collins prescription (c.f. Equation 27, labelled JCC), along with the cross-section for the order $\alpha_s^{(2)}$ $gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$ process. Separate cross-section contributions for the next-to-leading order process and the subtraction term are given for convenience; in the Monte-Carlo procedure developed in this paper the events are generated according to the differential cross-section corresponding to the 'hard' order $\alpha_s^{(1)}$ process, i.e. the next-to-leading calculation with the subtraction terms subtracted on an event-by-event basis.

The differential distributions of the virtuality μ and the transverse momentum (p_T) distribution of the b-quark with the highest p_T of the two (produced either in the hard process or in the subsequent Sudakov showering) are shown in Figure **5**, whereby also the p_T distribution of the b-quark with the highest p_T from the order $\alpha_s^{(2)}$ $gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$ process is shown.

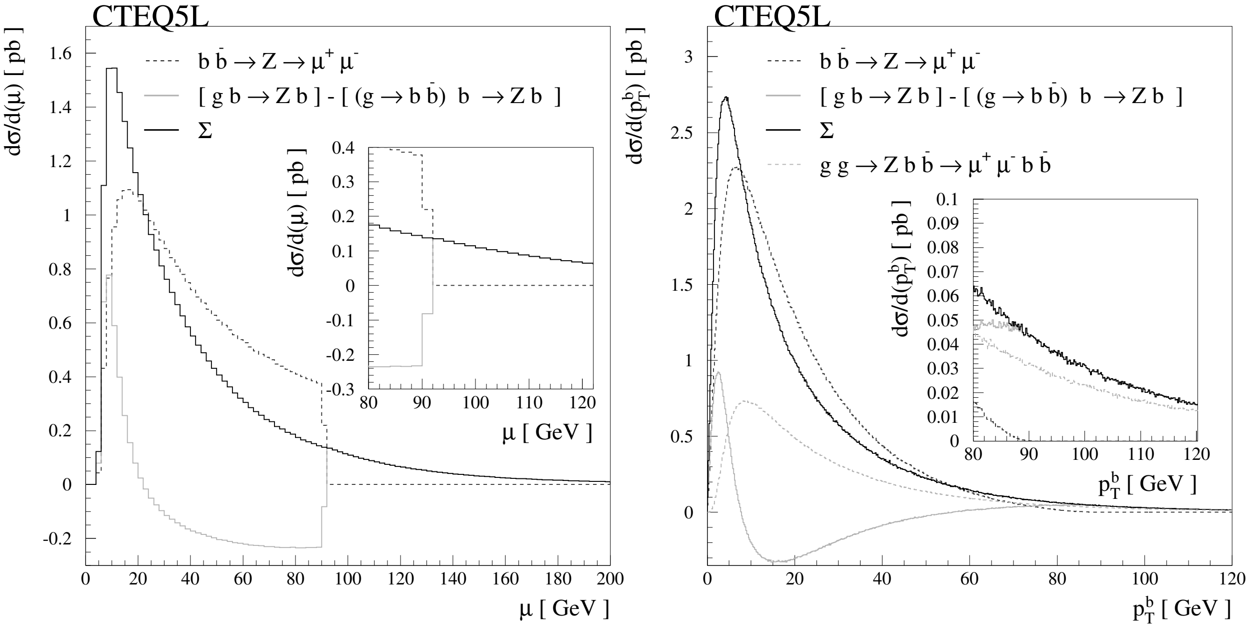

Fig. 5: The differential distributions of the virtuality μ and the transverse momentum (p_T) distribution of the b-quark with the higher virtuality (produced either in the hard process or in the subsequent Sudakov showering) are shown for the calculations using the LO CTEQ5L parton density functions. The next-to-leading order process entries contain the subtraction terms as calculated on event-by event basis.

In the results in Fig. **5** one can again observe a smooth distribution of the virtuality μ over the full kinematic range as the result of the implemented matching procedure. It is manifest that the cutoff on the b-quark virtuality μ and the resulting subtraction contribution do not map to the p_T distribution in a simple way. An interesting result is that the order $\alpha_s^{(2)}$ $gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$ process p_T distribution of the b-quark seems to be quite close to the result of the merging procedure in the high kinematic range as one could indeed expect if the perturbative calculations are to be consistent in the perturbative regime. In the low p_T region the $gg \to Zb\bar{b} \to \mu^+\mu^- b\bar{b}$ process undershoots the expected distribution of the merged $\alpha_s^{(0)} \oplus \alpha_s^{(1)}$ processes which is to be expected since in this case the non-perturbative contributions prevail. One has to keep in mind when comparing the two results results that in the derived $\alpha_s^{(1)}$ calculation the other incoming b-quark is still effectively on-shell, i.e. its virtuality and branchings are obtained solely from the Sudakov showering, where as in the $\alpha_s^{(2)}$ process both incoming b-quarks are treated as propagators in the full perturbative calculation. A further improvement would certainly be to repeat and extend the procedures derived in this paper to include the full order $\alpha_s^{(2)}$ calculation.

From the results one can observe that the use of JCC evolved PDF-s significantly reduces the cross-section of the leading-order process with respect to the values obtained using the CTEQ5L [26] PDFs and to a lesser extent the cross-sections of the next-to-leading and the subtraction contribution, since the latter two include only one b-quark and one gluon in the initial state and are thus less affected by the change in the b-quark PDF evolution.

4.2 Single top Production Process

The single top production mechaninsm is of importance at the LHC since it provides a clean signal for top quark and W boson polarisation studies.

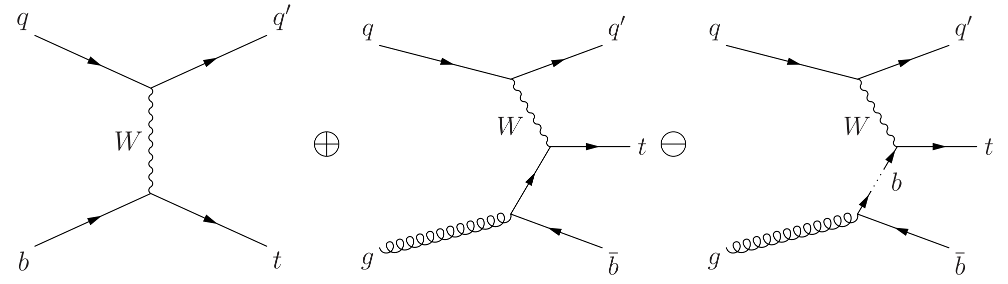

Fig. 6: Representative Feynman diagrams for the single top production process for (from left to right): Order $\alpha_s^{(0)}$, order $\alpha_s^{(1)}$ and order $\alpha_s^{(1)}$ subtraction term.

The cross-sections obtained for the leading order process $bq \to tq'$, next-to-leading order process $gq \to tq'\bar{b}$ and the subtraction process $(g \to b\bar{b})q \to tq'\bar{b}$ (and charge conjugates) in the LHC environment (proton-proton collisions at $\sqrt{\mathrm{s}}$ = 14 TeV) are given in the Table **2**, both for leading order PDF (CTEQ5L [26] was used) and the PDF-s evolved according to the Collins prescription (c.f. Equation 27, labelled JCC) for the scale choices $\mu_0 = \mathrm{m_t}$ and $\mu_0 = 60$ GeV. The differential distributions of the virtuality μ and the transverse momentum (p_T) distribution of the b-quark (produced either in the hard process or in the subsequent Sudakov showering) are shown in Figures **7** and **8**. Separate cross-section contributions are given for convenience; in the Monte-Carlo procedure developed in this paper the $gq \to tq'\bar{b}$ events are generated according to the differential cross-section corresponding to the 'hard' order $\alpha_s^{(1)}$ process, i.e. the next-to-leading calculation with the subtraction terms subtracted on an event-by-event basis.

Table 2: The process cross-sections for the leading order process $bq \to tq'$, next-to-leading order process $gq \to tq'\bar{b}$ and the subtraction process $(g \to b\bar{b})q \to tq'\bar{b}$ (including the charge conjugates) in the LHC environment (proton-proton collisions at $\sqrt{\mathrm{s}}$ = 14 TeV) are listed. These inclusive cross-sections include all top (and $W^{\pm}$) decay channels, the b-quark mass is set to $m_b = 4.8$ GeV and top-quark mass to $m_t = 175$ GeV with the factorisation and renormalisation scales set to the top mass values $\mu_0 = \mathrm{m_t}$ and $\mu_0 = 60$ GeV. The cross-sections are given for the LO CTEQ5L and JCC PDFs. In the Monte-Carlo procedure the next-to-leading process weights are combined with the subtraction weights on the event-by-event basis as described in the text.

Process	$\sigma_{\mathrm{CTEQ5L},\mu_0=\mathrm{m_t}}$ [pb]	$\sigma_{\mathrm{JCC},\mu_0=\mathrm{m_t}}$ [pb]	$\sigma_{\mathrm{CTEQ5L},\mu_0=60\ \mathrm{GeV}}$ [pb]	$\sigma_{\mathrm{JCC},\mu_0=60\ \mathrm{GeV}}$ [pb]
$bq \to tq'$	222.2	187.8	178.1	138.7
$gq \to tq'\bar{b}$	156.2	154.2	188.2	184.4
$(g \to b\bar{b})q \to tq'\bar{b}$	140.1	138.2	102.8	100.5
Σ	238.3	203.8	263.5	222.6

From the results in Fig. **7** and Fig. **8** one can observe that the applied procedure produces a very good match of the processes in the combined distribution of the b-quark virtuality μ resulting in a smooth (almost seamless) transition in the vicinity of the cutoff. As one can also observe the cutoff on the b-quark virtuality μ and the resulting subtraction contribution do not map to the p_T distribution in a trivial manner; hence one can surmise that the simple gluing methods of the processes based on p_T distribution cuts most probably give erroneous predictions.

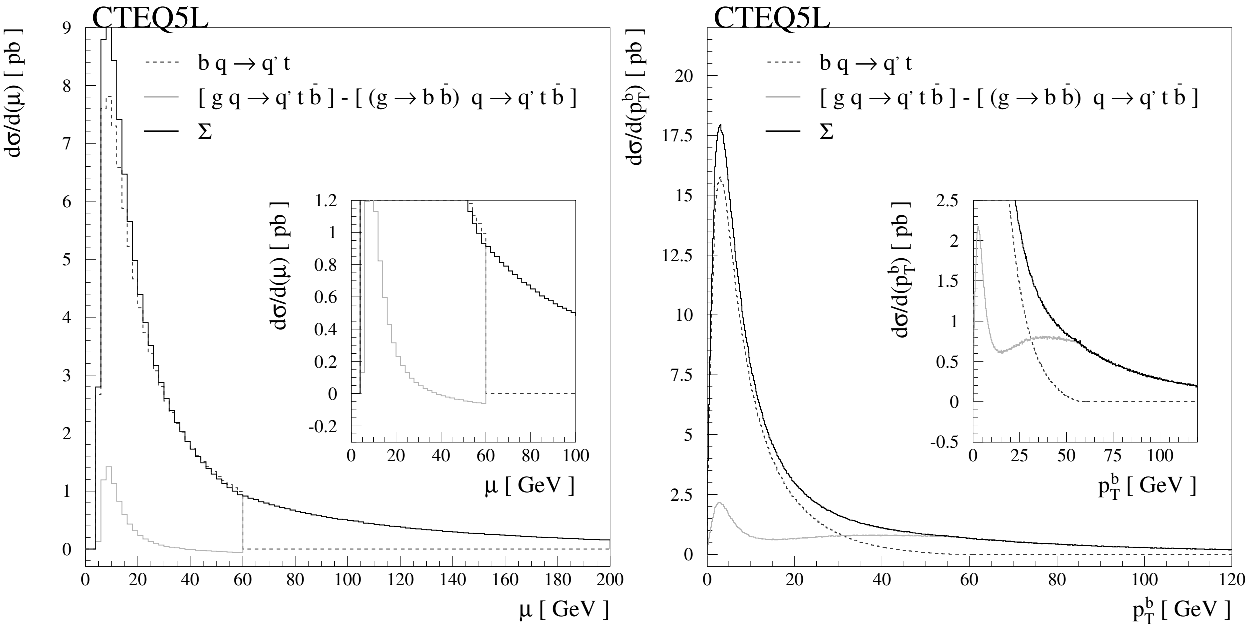

Fig. 7: The differential distributions of the virtuality μ and the transverse momentum (p_T) distribution of the b-quark (produced either in the hard process or in the subsequent Sudakov showering) are shown for the calculations using the LO CTEQ5L PDFs and the showering (factorisation) scale set to $\mu_0 = 60$ GeV. The next-to-leading order process entries contain the subtraction terms as calculated on event-by event basis.

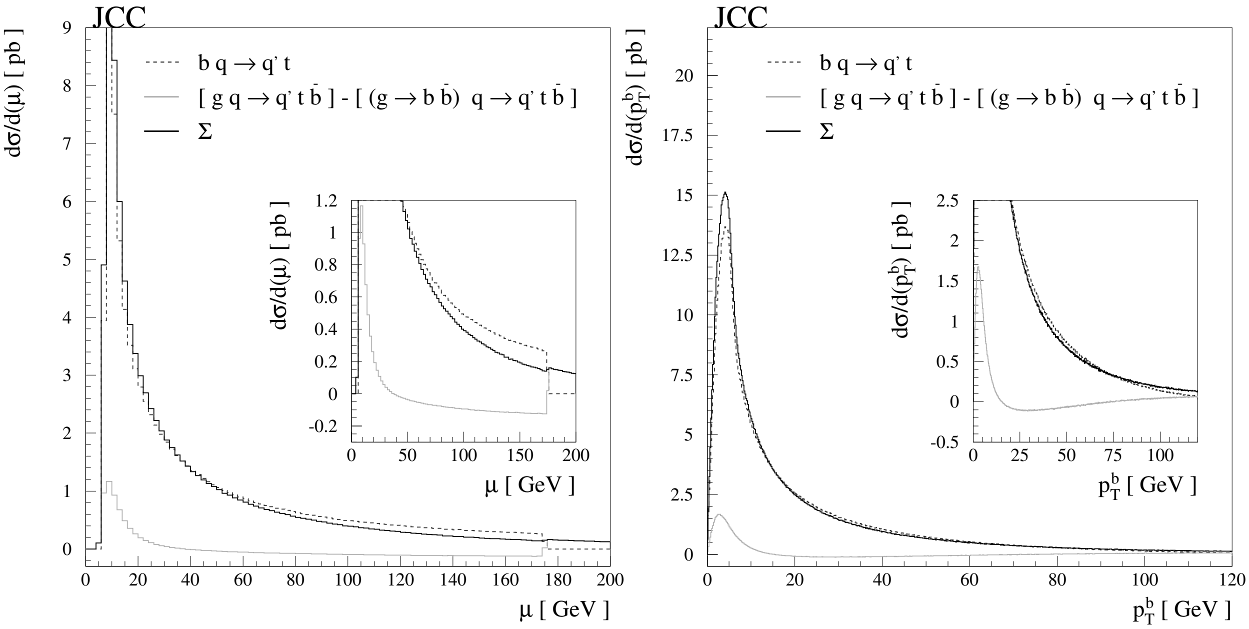

Fig. 8: The differential distributions of the virtuality μ and the transverse momentum (p_T) distribution of the b-quark (produced either in the hard process or in the subsequent Sudakov showering) are shown for the calculations using the JCC PDFs and the showering (factorisation) scale set to $\mu_0 = \mathrm{m_t}$. The next-to-leading order process entries contain the subtraction terms as calculated on event-by event basis.

One of the interesting results is also that the use of JCC evolved PDF-s significantly reduces the cross-section of the $bq \to tq'$ process with respect to the values obtained using the CTEQ5L PDFs and to a lesser extent the cross-sections of the $gq \to tq'\bar{b}$ and the subtraction contribution, since the latter two contain only the light quarks and gluons which are less (or in case of gluons not at all) affected by the change in PDF evolution compared to the b-quark PDF.

A somewhat cruder method of merging different order processes has for the single top production already been implemented a while ago in the program ONETOP[27]; the results from the two methods are compatible within the differences of the methods used in both implementations. It is instructive to inquire where the differences between the two procedures originate. Specifically, in ONETOP the subtraction term is higher than the cross-section of the $(2 \to 3)$ $gq \to tq'\bar{b}$ process; from the Fig. 3.6 in [27] the subtraction cross-section of the process $(g \to b\bar{b})q \to tq'\bar{b}$ is of the order of about 190 pb compared to the 140 pb one gets using the procedures described in this paper. The difference originates in part in the massless approximation of the participating particles implemented in ONETOP and can be traced back to the fact that the subtraction term in ONETOP (as given in Appendix D in [27]) is calculated from the *integrated* parton density function correction (the first-order term in Eq. 12 of this paper) coupled to the zero-th order $bq \to tq'$ cross-section, i.e. the virtuality is already integrated over into the $\log \frac{\mu^2}{m_b^2}$. Contrariwise, in the present work the procedure is more complex and requires identifying the virtuality of the $2 \to 3$ process in the massive calculation. In addition, in ONETOP the spectator energy fraction is kept unchanged whereas in the new procedure only the rapidity constraint is used instead. The ONETOP calculation using the integrated PDF correction has been repeated as a sanity check and gives the hence derived subtraction term with the value of about 185 pb which is deemed to be consistent with the ONETOP results.

5 Conclusion

to be written.

A Kinematic relations

The requirement (**2**) in the list of Subsection 3.1 gives the equivalence $\xi_\mathrm{a} \equiv \mathrm{x_a}$. The remaining relations between $\xi_\mathrm{c}, \xi_\mathrm{b}$ and x_b, s_{n-1} are then given by energy and rapidity conservation requirements and are thus given by the conditions:

$$s_{n-1} = (p_c + p_b)^2 = m_c^2 + m_b^2 + 2(p_c^+ p_b^- + p_c^- p_b^+) = m_c^2 + m_b^2 + \xi_c \xi_b s + \frac{m_c^2 m_b^2}{\xi_c \xi_b s} \tag{30}$$

where $p_c = (p_c^+, \vec{0}^T, p_c^-) = (\xi_c P_A^+, \vec{0}^T, \frac{m_c^2}{2\xi_c P_A^+})$ and $p_b = (p_b^+, \vec{0}^T, p_b^-) = (\frac{m_b^2}{2\xi_b P_B^-}, \vec{0}^T, \xi_b P_B^-)$ and:

$$y = \frac{1}{2}\ln\left(\frac{k_{n-1}^+}{k_{n-1}^-}\right) = \frac{1}{2}\ln\left(\frac{\xi_c}{\xi_b}\right) + \frac{1}{2}\ln\left(\frac{\xi_c\xi_b s + m_b^2}{\xi_c\xi_b s + m_c^2}\right) \tag{31}$$

with:

$$\frac{k_{n-1}^+}{k_{n-1}^-} = \left(\frac{1+\beta}{1-\beta}\right)\left(\frac{k_{n-1}^{+*}}{k_{n-1}^{-*}}\right) \qquad \left(\frac{1+\beta}{1-\beta}\right) = \frac{x_a(x_a x_b s + m_b^2)}{x_b(x_a x_b s + m_a^2)} \tag{32}$$

and:

$$k_{n-1}^{\pm\star} = \frac{1}{\sqrt{2}}\left[\frac{s_n + s_{n-1} - m_{\bar{c}}^2}{2\sqrt{s_n}} \mp \frac{t_{n-1} - m_b^2 - s_{n-1} + 2\left(\frac{s_n + m_b^2 - m_a^2}{2\sqrt{s_n}}\right)\left(\frac{s_n + s_{n-1} - m_{\bar{c}}^2}{2\sqrt{s_n}}\right)}{2\left(\frac{\sqrt{\lambda(s_n, m_a^2, m_b^2)}}{2\sqrt{s_n}}\right)}\right] \tag{33}$$

which can be inverted to give the expressions for ξ_c and ξ_b as functions of $s_n, x_b, \ldots$ A further simplification in derivation can be achieved by introducing another set of variables $\bar{\tau} = \xi_c \cdot \xi_b$ and $\bar{y} = 1/2\ln(\xi_c/\xi_b)$ with the Jacobian of the transformation $\mathcal{J}\frac{(\xi_c,\xi_b)}{(\bar{\tau},\bar{y})} = 1$ and subsequently:

$$\bar{\tau} = \frac{1}{2s}\left\{\left(s_{n-1} - (m_c^2 + m_b^2)\right) + \sqrt{\lambda(s_{n-1}, m_c^2, m_b^2)}\right\}, \tag{34}$$

$$\bar{y} = \frac{1}{2}\ln\left(\frac{k_{n-1}^+}{k_{n-1}^-}\right) - \frac{1}{2}\ln\left(\frac{\bar{\tau}s + m_b^2}{\bar{\tau}s + m_c^2}\right). \tag{35}$$

As one can observe the $\bar{\tau}$ is only a function of s_{n-1} so the only remaining term to compute in the Jacobian of the transformation $\mathcal{J}\frac{(\bar{\tau},\bar{y})}{(s_{n-1},x_b)}$ is $d\bar{y}/dx_b$:

$$\mathcal{J}\frac{(\bar{\tau},\bar{y})}{(s_{n-1},x_b)} = \left|\frac{d\bar{\tau}}{ds_{n-1}}\right| \cdot \left|\frac{d\bar{y}}{dx_b}\right| = \mathcal{F}(s_n, s_{n-1}, t_{n-1}, x_a, x_b, m_a, m_b, m_{\bar{c}}) \tag{36}$$

with $\mathcal{F}$ being a lengthy function of the listed parameters and therefore omitted. In the massless approximation the above expression reduces to:

$$\mathcal{J}\frac{(\xi_c,\xi_b)}{(s_{n-1},x_b)}_{m\to 0} = \left|\frac{x_a}{2(x_a x_b s + t_{n-1})} + \frac{1}{2x_b s}\right| \tag{37}$$

which is in agreement with the expressions derived by Chen, Collins *et al.* [9, 10, 11, 12]. Analogous expressions can trivially be obtained also for the split of the other parton.

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