

CASCADE3: A Monte Carlo event generator based on TMDs Physics and Manual

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Abstract

The CASCADE3 Monte Carlo event generator based on Transverse Momentum Dependent (TMD) parton densities is described. Hard processes which are generated in collinear factorization with LO multileg or NLO parton level generators are extended by adding transverse momenta to the initial partons according to TMD densities and applying dedicated TMD parton showers and hadronization. Processes with off-shell kinematics within k_t -factorization, either internally implemented or from external packages via LHE files, can be processed for parton showering and hadronization. The initial state parton shower is tied to the TMD parton distribution, with all parameters fixed by the TMD distribution.

1 Introduction

The simulation of processes for high energy hadron colliders has been improved significantly in the past years by automation of next-to-leading order (NLO) calculations and matching of the hard processes to parton shower Monte Carlo event generators which also include a simulation of hadronization. Among those automated tools are the MADGRAPH5_aMC@NLO [1] generator based on the MC@NLO [2–5] method or the POWHEG [6,7] generator for the calculation of the hard process. The results from these packages are then combined with either the HERWIG [8] or PYTHIA [9] packages for parton showering and hadronization. Different jet multiplicities can be combined at the matrix element level and then merged with special procedures, like the MLM merging [10] for LO processes, the FxFx [11] or MiNLO method [12]

for merging at NLO, among others. While the approaches of matching and merging matrix element calculations and parton showers are very successful, two ingredients important for high energy collisions are not (fully) treated: the matrix elements are calculated with collinear dynamics and the inclusion of initial state parton showers results in a net transverse momentum of the hard process; the special treatment of high energy effects (small x) is not included.

The CASCADE3 Monte Carlo event generator, developed originally for small x processes based on high-energy factorization [13] and the CCFM [14–17] evolution equation, has been extended to cover the full kinematic range (not only small x) by applying the Parton Branching (PB) method and the corresponding PB Transverse Momentum Dependent (TMD) parton densities [18, 19]. The initial state evolution is fully described and determined by the TMD density, as it was in the case of the CCFM gluon density, but now available for all flavor species, including quarks, gluons and photons at small and large x and any scale μ . For a general overview of TMD parton densities, see Ref. [20].

With the developments in determination of PB TMDs [18, 19], it is natural to develop a scheme, where the initial parton shower follows as close as possible the TMD parton density and where either collinear (on-shell) or k_t -dependent (off-shell) hard process calculations can be included at LO or NLO. In order to be flexible and to use the latest developments in automated matrix element calculations of hard process at higher order in the strong coupling α_s , events available in the Les Houches Event (LHE) file format [21], which contains all the information of the hard process including the color structure, can be further processed for parton shower and hadronization in CASCADE3.

In this report we describe the new developments in CASCADE3 for a full PB-TMD parton shower and the matching of TMD parton densities to collinear hard process calculations. We also mention features of the small x mode of CASCADE3.

2 The hard process

The cross section for the scattering process of two hadrons A and B can be written in collinear factorization as a convolution of the partonic cross section of partons a and b : $a + b \rightarrow X$ and the densities $f_{a,b}(x, \mu)$ of partons a (b) inside the hadrons A (B):

$$\sigma(A + B \rightarrow Y) = \int dx_a \int dx_b f_a(x_a, \mu) f_b(x_b, \mu) \sigma(a + b \rightarrow X), \quad (1)$$

where $x_a(x_b)$ are the fractions of the longitudinal momenta of hadrons A, B carried by the partons $a(b)$, $\sigma(a + b \rightarrow X)$ is the partonic cross section, and μ is the factorization scale of the process. The final state Y contains the partonic final state X and the recoils from the parton evolution and hadron remnants.

In CASCADE3 we extend collinear factorization to include transverse momenta in the initial state, either by adding a transverse momentum to an on-shell process, as described in detail in section Section 2.1, or by using off-shell processes directly, as described in Section 2.1.

2.1 On-shell processes

The hard processes in collinear factorization (with on-shell initial partons, without transverse momenta) can be calculated by standard automated methods like MADGRAPH5_aMC@NLO [1] for multileg processes at LO or NLO accuracy. The matrix element processes are calculated with collinear parton densities (PDF), as provided by LHAPDF [22].

We extend the factorization formula given in eq.(1) by replacing the collinear parton densities $f(x, \mu)$ by TMD densities $\mathcal{A}(x, k_t, \mu)$ with k_t being the transverse momentum of the interacting parton, and integrating over the transverse momenta.

However, when the hard process is to be combined with a TMD parton density, as described later, the integral over k_t of the TMD density must agree with the collinear (k_t -integrated) density; this feature is guaranteed by construction for the PB-TMDs (also available as integrated PDFs in LHAPDF format).

In a LO partonic calculation the TMD or the parton shower can be included respecting energy momentum conservation, as described below. In an NLO calculation based on the MC@NLO method [2–5] the contribution from collinear and soft partons is subtracted, as this is added later with the parton shower. For the use with PB TMDs, the HERWIG 6 subtraction terms are best suited as the angular ordering conditions coincide with those applied in the PB-method. The PB TMDs play the same role as a parton shower does, in the sense that a finite transverse momentum is created as a result of the parton evolution [23,24].

When transverse momenta of the initial partons from TMDs are to be included to the hard scattering process, which was originally calculated under the assumption of collinear initial partons, care has to be taken that energy and momentum are still conserved. When the initial state partons have transverse momenta, they also acquire virtual masses. The procedure adopted in CASCADE3 is the following: for each initial parton, a transverse momentum is assigned according to the TMD density, and the parton-parton system is boosted to its center-of-mass frame and rotated such that only the longitudinal and energy components are non-zero. The energy and longitudinal component of the initial momenta $p_{a,b}$ are recalculated taking into account the virtual masses $Q_a^2 = k_{t,a}^2$ and $Q_b^2 = k_{t,b}^2$ [25]:

$$E_{a,b} = \frac{1}{2\sqrt{\hat{s}}} (\hat{s} \pm (Q_b^2 - Q_a^2)) \quad (2)$$

$$p_{z\ a,b} = \pm \frac{1}{2\sqrt{\hat{s}}} \sqrt{(\hat{s} + Q_a^2 + Q_b^2)^2 - 4Q_a^2 Q_b^2} \quad (3)$$

with $\hat{s} = (p_a + p_b)^2$ with $p_a(p_b)$ being the four-momenta of the interacting partons a and b . The partonic system is then rotated and boosted back to the overall center-of-mass system of the colliding particles. By this procedure, the parton-parton mass $\sqrt{\hat{s}}$ is exactly conserved, the rapidity of the partonic system is approximately restored, depending on the transverse momenta.

In Fig. 1 a comparison of the Drell-Yan (DY) mass, transverse momentum and rapidity is shown for an NLO calculation of DY production in pp collisions at $\sqrt{s} = 13$ TeV in the

mass range $30 < m_{DY} < 2000$ GeV. The curve labelled NLO(LHE) is the calculation of MADGRAPH5_aMC@NLO with the subtraction terms, the curve NLO(LHE+TMD) is the prediction after the transverse momentum is included according to the procedure described above. In the p_T spectrum one can clearly see the effect of including transverse momenta from the TMD distribution. The DY mass distribution is not changed, and the rapidity distribution is almost exactly reproduced, only at large rapidities small differences are observed.

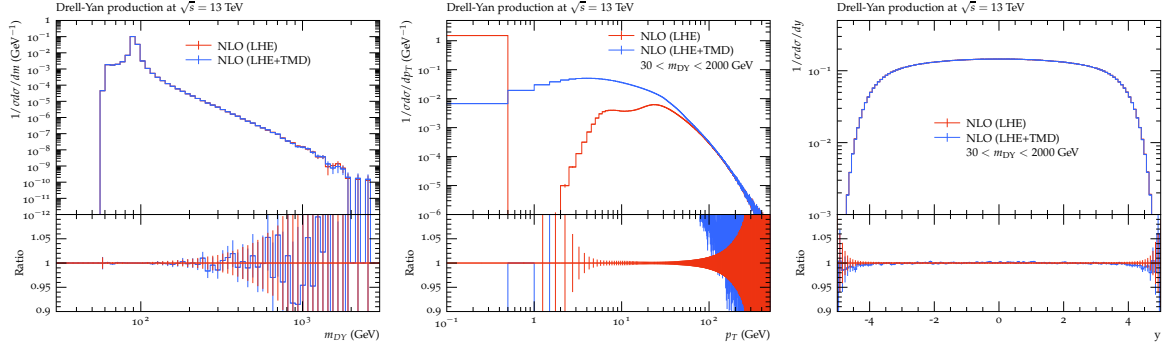


Figure 1: Distributions of Drell-Yan mass, transverse momentum and rapidity for $pp \rightarrow DY + X$ at $\sqrt{s} = 13$ TeV. The hard process is calculated with MADGRAPH5_aMC@NLO. NLO(LHE) is the prediction including subtraction terms, NLO(LHE+TMD) includes transverse momenta of the interacting partons according to the description in the text.

The transverse momenta k_t are generated according to the TMD density $\mathcal{A}(x, k_t, \mu)$, at the original longitudinal momentum fraction x and the hard process scale μ . In a LO calculation, the full range of k_t is available, but in an NLO calculation via the MC@NLO method, a *shower scale* defines the boundary between parton shower and real emissions from the matrix element, limiting the transverse momentum k_t . Technically the factorization scale μ is calculated within CASCADE3 (see parameter `lhesc`) as it is not directly accessible from the LHE file, while the *shower scale* is given by `SCALUP`. The *shower scale* guarantees that the TMD and later the parton shower does not generate transverse momenta which would violate the collinear factorization ansatz.

The advantage of using TMDs for the complete process is that the kinematics are fixed, independent of simulating explicitly the radiation history from the parton shower. For inclusive processes, for example inclusive Drell-Yan processes, the details of the hadronic final state generated by a parton shower do not matter, and only the net effect of the transverse momentum distribution is essential. However, for processes which involve jets, the details of the parton shower becomes also important. The parton shower, as described below, follows very closely the transverse momentum distribution of the TMD and thus does not change any kinematic distribution after the transverse momentum of the initial partons are included.

All hard processes, which are available in MADGRAPH5_aMC@NLO can be used within CASCADE3. The treatment of multijet merging is described in Section 8.

2.2 Off-shell processes

In a region of phase space, where the longitudinal momentum fractions x become very small, the transverse momentum of the partons cannot be neglected and has to be included already at the matrix element level, leading to so-called *off-shell* processes.

In off-shell processes a natural suppression at large k_t [26] (with $k_t > \mu$) is obtained, shown explicitly in Fig. 2, where the matrix element for $g^* g^* \rightarrow QQ$, with Q being a heavy quark, is considered. The process is integrated over the final state phase space [27]:

$$\tilde{\sigma}(k_t) = \int \frac{dx_2}{x_2} d\phi_{1,2} \text{dLips} |ME|^2 (1-x_2)^5 \quad (4)$$

with dLips being the Lorentz-invariant phase space of the final state, ME is the matrix-element for the process and $\phi_{1,2}$ is the azimuthal angle between the two initial partons. A simple scale and k_t independent gluon density $xG(x) = (1-x)^5$ is included to suppress large x contributions. In Fig. 2 we show $\tilde{\sigma}(k_t)$ normalized to its on-shell value $\tilde{\sigma}(0)$ at $\sqrt{s} = 13000$ GeV as a function of the transverse momentum of the incoming gluon $k_{t,2}$ for different values of x_1 , which are chosen such that the ratio $k_{t,1}/\sqrt{s}$ is kept constant.

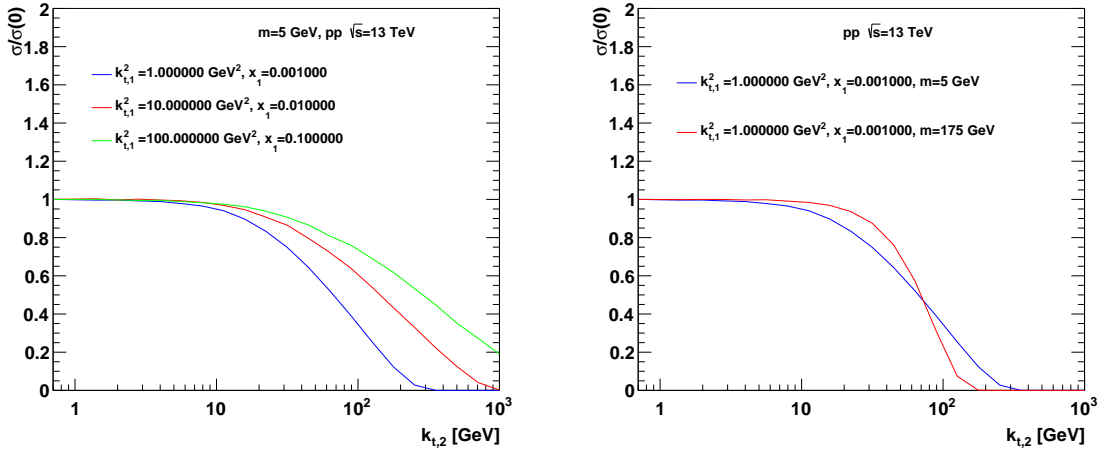


Figure 2: The reduced cross section $\tilde{\sigma}(k_t)/\tilde{\sigma}(0)$ as a function of the transverse momentum $k_{t,2}$ of the incoming gluon at $\sqrt{s} = 13000$ GeV. (Left) for different values of $k_{t,1}$ and x_1 , (right) for different heavy flavor masses and fixed values of $k_{t,1}$ and x_1 .

In Fig. 2 (left) predictions are shown for bottom quarks with mass $m = 5$ GeV and different $k_{t,1}$, in Fig. 2 (right) a comparison is made for different heavy quark masses. Using off-shell matrix elements a suppression at large transverse momenta of the initial partons is obtained, depending on the heavy flavor mass and the transverse momentum. In a collinear approach, with implicit integration over transverse momenta of the initial state partons, the

transverse momenta are limited by a theta function at the factorization scale, while off-shell matrix elements give a smooth transition to a high k_t tail.

When using off-shell processes, BFKL or CCFM type parton densities should be used to cover the full available phase space in transverse momentum, which can lead to k_t 's, larger than the transverse momentum of any of the partons of the hard process [28]. Until now, only gluon densities obtained from CCFM [14–17] or BFKL [29–31] are available, thus limiting the advantages of using off-shell matrix elements to gluon induced processes.

Several processes with off-shell matrix elements are implemented in CASCADE3 as listed in Tab. 1, and described in detail in [32]. However, many more processes are accessible via the automated matrix element calculators for off-shell processes, KATIE [33] and PEGASUS [34]. The events from the hard process are then read with the CASCADE3 package via LHE files. For processes generated with KATIE or PEGASUS no further corrections need to be performed and the event can be directly passed to the showering procedure, described in the next section.

Lepto(photo)production	process	I PRO	Reference
	$\gamma^* g^* \rightarrow q\bar{q}$	10	[35]
	$\gamma^* g^* \rightarrow Q\bar{Q}$	11	[35]
	$\gamma^* g^* \rightarrow J/\psi g$	2	[36–39]
Hadroproduction			
	$g^* g^* \rightarrow q\bar{q}$	10	[35]
	$g^* g^* \rightarrow Q\bar{Q}$	11	[35]
	$g^* g^* \rightarrow J/\psi g$	2	[39]
	$g^* g^* \rightarrow \Upsilon g$	2	[39]
	$g^* g^* \rightarrow \chi_c$	3	[39]
	$g^* g^* \rightarrow \chi_b$	3	[39]
	$g^* g^* \rightarrow J/\psi J/\psi$	21	[40]
	$g^* g^* \rightarrow h^0$	102	[41]
	$g^* g^* \rightarrow ZQ\bar{Q}$	504	[42,43]
	$g^* g^* \rightarrow Zq\bar{q}$	503	[42,43]
	$g^* g^* \rightarrow Wq_i Q_j$	514	[42,43]
	$g^* g^* \rightarrow Wq_i q_j$	513	[42,43]
	$qg^* \rightarrow Zq$	501	[44]
	$qg^* \rightarrow Wq$	511	[44]
	$qg^* \rightarrow qg$	10	[45]
	$gg^* \rightarrow gg$	10	[45]

Table 1: Processes included in CASCADE3. Q stands for heavy quarks, q for light quarks.

3 Initial State Parton Shower based on TMDs

The parton shower, which is described here, follows consistently the parton evolution of the TMDs. By this we mean that the splitting functions P_{ab} , the order and the scale in α_s as well as kinematic restrictions are identical to both the parton shower and the evolution of the parton densities (for NLO PB TMD densities, the NLO DGLAP splitting functions together with NLO α_s is applied, while for the LO TMD densities the corresponding LO splitting functions and LO α_s is used).

3.1 From PB TMD evolution to TMD Parton Shower

The PB method describes the TMD parton density as (cf eq.(2.43) in Ref. [18]):

$$x\mathcal{A}_a(x, k_t^2, \mu^2) = \Delta_a(\mu^2) x\mathcal{A}_a(x, k_t^2, \mu_0^2) + \sum_b \int \frac{dq'^2}{q'^2} \frac{d\phi}{2\pi} \frac{\Delta_a(\mu^2)}{\Delta_a(q'^2)} \Theta(\mu^2 - q'^2) \Theta(q'^2 - \mu_0^2) \\ \times \int_x^{z_M} dz P_{ab}^{(R)}(\alpha_s(f(q'^2)), z) \frac{x}{z} \mathcal{A}_b\left(\frac{x}{z}, k_t'^2, q'^2\right), \quad (5)$$

with $z_M < 1$ defining resolvable branchings, $k_t' = |\mathbf{k} + (1 - z)\mathbf{q}'|$ and $\mathbf{q}' = \mathbf{q}_c/(1 - z)$ being the rescaled transverse momentum vector of the emitted parton (see Fig 3) and ϕ being the azimuthal angle between \mathbf{q}' and \mathbf{k} . The argument in α_s is in general a function of the evolution scale μ'^2 , from higher order calculations the transverse momentum of the emitted parton is preferred as the scale. The real emission branching probability is denoted by $P_{ab}^{(R)}(\alpha_s(f(\mu'^2)))$ including α_s as described in Ref. [18] (in the following we omit α_s for easier reading in the argument of $P_{ab}^{(R)}$). The Sudakov form factor is given by:

$$\Delta_a(z_M, \mu^2, \mu_0^2) = \exp \left(- \sum_b \int_{\mu_0^2}^{\mu^2} \frac{dq'^2}{q'^2} \int_0^{z_M} dz z P_{ba}^{(R)} \right). \quad (6)$$

Dividing eq.(5) by $\Delta_a(\mu^2)$, differentiation wrt dq'^2 gives the differential form of the evolution equation describing the probability for resolving a parton with transverse momentum \mathbf{k}' and momentum fraction x/z into a parton with momentum fraction x and emitting another parton \mathbf{q}' during a small decrease of μ :

$$q^2 \frac{d}{dq^2} \left(\frac{x\mathcal{A}_a(x, k_t^2, q^2)}{\Delta_a(q^2)} \right) = \sum_b \int_x^{z_M} dz \frac{d\phi}{2\pi} P_{ab}^{(R)} \frac{x}{z} \frac{\mathcal{A}_b\left(\frac{x}{z}, k_t'^2, q^2\right)}{\Delta_a(q^2)} \quad (7)$$

The normalized probability is then given by:

$$\frac{\Delta_a(q^2)}{x\mathcal{A}_a(x, k_t^2, q^2)} d \left(\frac{x\mathcal{A}_a(x, k_t^2, q^2)}{\Delta_a(q^2)} \right) = \sum_b \frac{dq^2}{q^2} \int_x^{z_M} dz \frac{d\phi}{2\pi} P_{ab}^{(R)} \frac{\frac{x}{z} \mathcal{A}_b\left(\frac{x}{z}, k_t'^2, q^2\right)}{x\mathcal{A}_a(x, k_t^2, q^2)} \quad (8)$$

187 This equation can be integrated between μ_{i-1}^2 and μ^2 to give the no-branching probability
 188 (Sudakov form factor) for the backward evolution Δ_{bw} :¹

$$\begin{aligned} \log \Delta_{bw}(x, \mu, \mu_{i-1}) &= \log \left(\frac{\Delta_a(\mu^2)}{\Delta_a(\mu_{i-1}^2)} \frac{x \mathcal{A}_a(x, k_t^2, \mu_{i-1}^2)}{x \mathcal{A}_a(x, k_t^2, \mu^2)} \right) \\ &= - \sum_b \int_{\mu_{i-1}^2}^{\mu^2} \frac{dq'^2}{q'^2} \frac{d\phi}{2\pi} \int_x^{z_M} dz P_{ab}^{(R)} \frac{x' \mathcal{A}_b(x', k_t'^2, q'^2)}{x \mathcal{A}_a(x, k_t^2, q'^2)}, \end{aligned} \quad (9)$$

189 with $x' = x/z$. This Sudakov form factor is very similar to the Sudakov form factor in
 190 ordinary parton shower approaches, with the difference that for the PB TMD shower the
 191 ratio PB TMD densities $\frac{x' \mathcal{A}_b(x', k_t'^2, \mu'^2)}{x \mathcal{A}_a(x, k_t^2, \mu'^2)}$ is applied, which includes a dependence on k_t .

192 In eq.(9) a relation between the Sudakov form factor Δ_a used in the evolution equation
 193 and the Sudakov form factor Δ_{bw} used for the backward evolution of the parton shower is
 194 made explicit. A similar relation was also studied in Refs. [46,47]. The PB approach allows a
 195 consistent formulation of the parton shower with the PB TMDs, since in both Sudakov form
 196 factors, Δ_a and Δ_{bw} the same value of z_M is used.

197 The splitting functions $P_{ab}^{(R)}$ contain the coupling:

$$P_{ab}(\alpha_s, z) = \sum_{n=1}^{\infty} \left(\frac{\alpha_s(f(\mu'^2))}{2\pi} \right)^n P_{ab}^{(n-1)}(z), \quad (10)$$

198 where the scale $f(\mu'^2)$ depends on the ordering condition as discussed later (see eq.(11)).

199 3.2 Backward Evolution for initial state TMD Parton Shower

200 A backward evolution method, as now common in Monte Carlo event generators, is ap-
 201 plied for the initial state parton shower, evolving from the large scale of the matrix-element
 202 process backwards down to the scale of the incoming hadron. However, in contrast to the
 203 conventional parton shower, which generates transverse momenta of the initial state partons
 204 during the backward evolution, the transverse momenta of the initial partons of the hard
 205 scattering process is fixed by the TMD and the parton shower does not change the kinemat-
 206 ics. The transverse momenta during the backward cascade follow the behavior of the TMD.
 207 The hard scattering process is obtained as described in section 2. The backward evolution
 208 of the initial state parton shower follows very closely the description in [32, 48, 49], which is
 209 based on Ref. [25].

210 The evolution scale μ is calculated from the hard scattering process, as described in Sec-
 211 tion 2. In case of on-shell matrix elements at NLO, the transverse momentum of the hardest
 212 parton in the parton shower evolution is limited by the *shower-scale*, as described in Sec-
 213 tion 2.1.

¹In equation Eq.(9) ordering in μ is assumed. However, if angular ordering is applied, as in CCFM [14–17], then the ratio of parton densities would change to $\frac{x' \mathcal{A}_b(x', k_t'^2, \mu'^2/z)}{x \mathcal{A}_a(x, k_t^2, \mu'^2)}$ as discussed in [32].

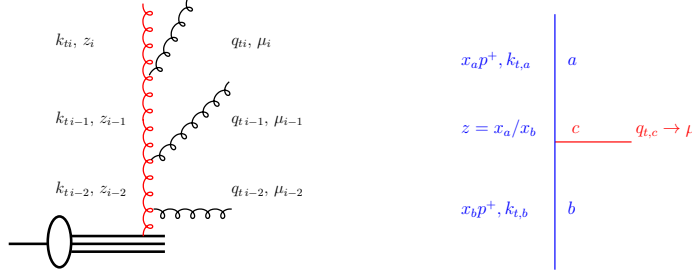


Figure 3: Left: Schematic view of a parton branching process. Right: Branching process $b \rightarrow a + c$.

Starting at the hard scale $\mu = \mu_i$, the parton shower algorithm searches for the next scale μ_{i-1} at which a resolvable branching occurs (see Fig. 3 left). This scale μ_{i-1} is selected from the Sudakov form factor Δ_{bw} as given in eq.(9) (see also [32]). In the parton shower language, the selection of the next branching comes from solving the $R = \Delta_{bw}(x, \mu_i, \mu_{i-1})$ for μ_{i-1} using uniformly distributed random numbers R for given x and μ_i . However, to solve the integrals in Eq.(9) numerically for every branching would be too time consuming, instead the veto-algorithm [25,50] is applied.

The splitting function P_{ab} as well as the argument $f(\mu')$ in the calculation of α_s is chosen exactly as used in the evolution of the parton density. In a parton shower one treats “resolvable” branchings, defined via a cut in $z < z_M$ in the splitting function to avoid the singular behavior of the terms $\frac{1}{1-z}$, and branchings with $z > z_M$ are regarded as “non-resolvable” and are treated similarly as virtual corrections: they are included in the Sudakov form factor Δ_{bw} . The branching splitting variable z_{i-1} is obtained from the splitting functions following the standard methods (see Eq.(2.37) in [18]).

The calculation of the transverse momentum k_t is sketched in Fig. 3 (right). The transverse momentum $q_{t,c}$ can be calculated in case of angular ordering (where the scale μ of each branching is associated with the angle of the emission) in terms of the angle Θ of the emitted parton wrt the beam directions $q_{t,c} = (1 - z)E_b \sin \Theta$:

$$\mathbf{q}_c^2 = (1 - z)^2 \mu'^2. \quad (11)$$

Once the transverse momentum of the emitted parton \mathbf{q}_c is known, the transverse momentum of the propagating parton can be calculated from

$$\mathbf{k}_b = \mathbf{k}_a + \mathbf{q}_c \quad (12)$$

with a uniformly distributed azimuthal angle ϕ assumed for the vector components of \mathbf{k} and \mathbf{q} . The generation of the parton momenta is performed in the center-of-mass frame of the collision (in contrast to conventional parton showers, which are generated in different partonic frames).

The whole procedure is iterated until one reaches a scale $\mu_{i-1} < q_0$ with q_0 being a cut-off parameter, which can be chosen to be the starting evolution scale of the TMD. It is of advantage to continue the parton shower evolution to lower scales $q_0 \sim \Lambda_{qcd} \sim 0.3$ GeV.

The final transverse momentum of the propagating parton \mathbf{k} is the sum of all transverse momenta \mathbf{q}_c (see Fig. 3 right):

$$\mathbf{k} = - \sum_c \mathbf{q}_c . \quad (13)$$

The PB TMD parton shower is selected with `PartonEvolution=2` (or `ICCF=2`).

3.3 CCFM parton evolution and parton shower

The CCFM parton evolution and corresponding parton shower follows a similar approach as described in the previous section and in detail also in Refs. [32,48,49,51]. The main difference to the PB-TMD shower are the splitting functions with the non-Sudakov form factor Δ_{ns} and the allowed phase space for emission. The original CCFM splitting function $\tilde{P}_g(z, q, k_t)$ for branching $g \rightarrow gg$ is given by²:

$$\tilde{P}_g(z, q, k_t) = \frac{\bar{\alpha}_s(q(1-z))}{1-z} + \frac{\bar{\alpha}_s(k_t)}{z} \Delta_{ns}(z, q, k_t), \quad (14)$$

where the non-Sudakov form factor Δ_{ns} is defined as:

$$\log \Delta_{ns} = -\bar{\alpha}_s(k_t) \int_0^1 \frac{dz'}{z'} \int \frac{dq^2}{q^2} \Theta(k_t - q) \Theta(q - z' q_t), \quad (15)$$

with $q_t = \sqrt{\mathbf{q}_t^2}$ defined in Eq.(11) and k_t being defined in Eq.(12).

The CCFM parton shower is selected with `ICCF=1` (`PartonEvolution=1`).³

4 The TMD parton densities

In the previous versions of CASCADE3 the TMD densities were part of the program. With the development of TMDLIB [52,53] there is easy access to all available TMDs, including parton densities for photons (as well as Z, W and H densities, if available).

These parton densities can be selected via `PartonDensity` with a value > 100000 . For example the TMDs from the parton branching method [18, 19] are selected via `PartonDensity=102100` (`102200`) for PB-NLO-HERAI+II-2018-set1 (set2).

Please note, that the features of the TMD parton shower are only fully available for the PB-TMD sets and the CCFM shower clearly needs CCFM parton densities (like for instance [54]).

²Finite terms are neglected as they are not obtained in CCFM at the leading infrared accuracy (cf p.72 in [16]).

³A one loop parton shower (DGLAP like) with $\Delta_{ns} = 1$, one loop α_s and strict ordering in q can be selected with `ICCF=0`.

5 Final state parton showers

The final state parton shower uses the parton shower routine `PYSHOW` of `PYTHIA`. Leptons in the final state, coming for example from Drell-Yan decays, can radiate photons, which are also treated in the final state parton shower. Here the method from `PYADSH` of `PYTHIA` is applied, with the scale for the QED shower being fixed at the virtuality of the decaying particle (for example the mass of the Z-boson).

The default scale for the QCD final state shower is $\mu^2 = 2 \cdot (m_{1\perp}^2 + m_{2\perp}^2)$ (`ScaleTimeShower=1`), with $m_{1(2)\perp}$ being the transverse mass of the hard parton 1(2). Other choices are possible: $\mu^2 = \hat{s}$ (`ScaleTimeShower=2`) and $\mu^2 = 2 \cdot (m_1^2 + m_2^2)$ (`ScaleTimeShower=3`). In addition a scale factor can be applied: `ScaleFactorFinalShower` $\times \mu^2$ (default: `ScaleFactorFinalShower=1`).

6 Hadronization

The hadronization (fragmentation of the partons in color systems) is done exclusively by `PYTHIA`. Hadronization (fragmentation) is switched off by `Hadronization = 0` (or `NFRA = 0` for the older steering cards). All parameters of the hadronization model can be changed via the steering cards.

7 Uncertainties

Uncertainties of QCD calculations mainly arise from missing higher order corrections, which are estimated by varying the factorization and renormalization scales up and down by typically a factor of 2. The scale variations are performed when calculating the matrix elements and are stored as additional weights in the LHE file, which are then passed directly to the `HEPMC` [55] output file for further processing.

The uncertainties coming from the PDFs can also be calculated as additional weight factors during the matrix element calculation. However, when using TMDs, additional uncertainties arise from the transverse momentum distribution of the TMD. The PB-TMDs come with uncertainties from the experimental uncertainties as well as from model uncertainties, as discussed in Ref. [56]. These uncertainties can be treated and applied as additional weight factors with the parameter `Uncertainty_TMD=1`.

8 Multi-jet merging

Showered multijet matrix element calculations can be merged using the prescription discussed in Ref. [57]. The merging performance is controlled by the three parameters `Rclus`, `Etclus`, `Etaclmax`. Final-state partons with pseudorapidity $\eta < \text{Etaclmax}$ present in the event record after the shower step but before hadronization are passed to the merging machinery if `Imerge = 1`. Partons are clustered using the kt-jet algorithm with a cone radius `Rclus` and matched to the PB evolved matrix element partons if the distance between the

parton and the jet $R < 1.5 \times R_{\text{clus}}$. The hardness of the reconstructed jets is controlled by its minimum transverse energy $E_{t\text{clus}}$ (merging scale).

The number of light flavor partons is defined by the `NqmaxMerge` parameter. Heavy flavor partons and their corresponding radiation are not passed to the merging algorithm. All jet multiplicities are treated in exclusive mode except for the highest multiplicity `MaxJetsMerge` which is treated in inclusive mode.

9 Program description

In CASCADE3 all variables are declared as `Double Precision`. With CASCADE3 the source of PYTHIA 6.428 is included to avoid difficulties in linking.

9.1 Random Numbers

CASCADE3 uses the RANLUX random number generator, with luxury level `LUX = 4`. The random number seed can be set via the environment variable `CASEED`, the default value is `CASEED=12345`.

9.2 Event Output

When HEPMC is included, generated events are written out in HEPMC [55] format for further processing. The environment variable `HEPMCOUT` is used to specify the file name, by default this variable is set to `HEPMCOUT=/dev/null`.

The HEPMC events can be further processed, for example with Rivet [58].

9.3 Input parameters

The input parameters are steered via steering files. The new format of steering is discussed in Section 9.3.1 and should be used when reading LHE files, while the other format, which is appropriate for the internal off-shell processes, is discussed in Section 9.3.2.

9.3.1 Input parameters - new format

Examples for steering files are under `$install_path/share/cascade/LHE`.

```
&CASCADE_input
NrEvents = -1           ! Nr of events to process
Process_Id = -1         ! Read LHE file
Hadronisation = 0       ! Hadronisation (on =1, off = 0)
SpaceShower = 1         ! Space-like Parton Shower
SpaceShowerOrderAlphas=2 ! Order alphas in Space Shower
TimeShower = 1          ! Time-like Parton Shower
ScaleTimeShower = 4     ! Scale choice for Time-like Shower
!                       1: 2 (m^2_1t+m^2_2t)
!                       2: shat
!                       3: 2 (m^2_1+m^2_2)
```

```

333 !                                     4: 2*scalup (from lhe file)
334 !ScaleFactorFinalShower = 1.         ! scale factor for Final State Parton Shower
335 PartonEvolution = 2                 ! type of parton evolution in Space-like Shower
336 !                                     1: CCFM
337 !                                     2: full all flavor TMD evolution
338 ! EnergyShareRemnant = 4             ! energy sharing in proton remnant
339 !                                     1: (a+1)(1-z)**a, <z>=1/(a+2)=1/3
340 !                                     2: (a+1)(1-z)**a, <z>=1/(a+2)=mq/(mq+mQ)
341 !                                     3: N/(z(1-1/z-c/(1-z))**2), c=(mq/mQ)**2
342 !                                     4: PYZDIS: KFL1=1
343 ! Remnant = 0                       ! =0 no remnant treatment
344 PartonDensity = 102200               ! use TMDlib: PB-TMDNLO-set2
345 ! PartonDensity = 102100            ! use TMDlib: PB-TMDNLO-set1
346 ! TMDDensityPath= './share'         ! Path to TMD density for internal files
347 Uncertainty_TMD = 0                 ! calculate and store uncertainty TMD pdfs
348 lheInput='MCatNLO-example.lhe'      ! LHE input file
349 lheHasOnShellPartons = 1            ! = 0 LHE file has off-shell parton configuration
350 lheReweightTMD = 0                 ! Reweight with new TMD given in PartonDensity
351 lheScale = 2                       ! Scale definition for TMD
352 !                                     0: use scalup
353 !                                     1: use shat
354 !                                     2: use 1/2 Sum pt^2 of final parton/particles
355 !                                     3: use shat for Born and 1/2 Sum pt^2 of final parton(particle)
356 !                                     4: use shat for Born and max pt of most forward/backward
357 !                                     parton(particle)
358 lheNBornpart = 2                   ! Nr of hard partons (particles) (Born process)
359 ScaleFactorMatchingScale = 2.       ! Scale factor for matching scale when including TMDs
360 ! lheWeightId = 0                  ! use weight Id = ... as weight for LHE file
361 &End
362
363
364 &PYTHIA6_input
365 P6_I tune = 370                     ! Retune of Perugia 2011 w CTEQ6L1 (Oct 2012)
366 ! P6_MSTJ(41) = 1                 ! (D = 2) type of branchings allowed in shower.
367 !                                     1: only QCD
368 !                                     2: QCD and photons off quarks and leptons
369 P6_MSTJ(45) = 4                   ! Nr of flavors in final state shower: g->qqbar
370 P6_PMAS(4,1)= 1.6                 ! charm mass
371 P6_PMAS(5,1)= 4.75                ! bottom mass
372 P6_MSTJ(48) = 1                   ! (D=0), 0=no max. angle, 1=max angle def. in PARJ(85)
373 ! P6_MSTU(111) = 1                ! = 0 : alpha_s is fixed, =1 first order; =2 2nd order;
374 ! P6_PARU(112) = 0.2              ! lambda QCD
375 P6_MSTU(112)= 4                   ! nr of flavours wrt lambda_QCD
376 P6_MSTU(113)=                     ! min nr of flavours for alphas
377 P6_MSTU(114)= 5                   ! max nr of flavours for alphas
378 &End

```

379 9.3.2 Input parameters - off-shell processes

380 Examples for steering files are under \$install_path/share/cascade/PP.

```

381 * OLD STEERING FOR CASCADE
382 *
383 * number of events to be generated
384 *
385 NEVENT 100
386 *
387 * ++++++ Kinematic parameters ++++++
388 *
389 'PBE1'      1    0   -7000.    ! Beam energy
390 'KBE1'      1    0    2212     ! -11: positron, 22: photon 2212: proton
391 'IRE1'      1    0     1       ! 0: beam 1 has no structure
392 *                               ! 1: beam 1 has structure
393 'PBE2'      1    0    7000.    ! Beam energy
394 'KBE2'      1    0    2212     ! 11: electron, 22: photon 2212: proton
395 'IRE2'      1    0     1       ! 0: beam 3 has no structure
396 *                               ! 1: beam 2 has structure
397 'NFLA'      1    0     4       ! (D=5) nr of flavours used in str.fct
398 * ++++++ Hard subprocess selection ++++++
399 'IPRO'      1    0     2       ! (D=1)
400 *                               ! 2: J/psi g
401 *                               ! 3: chi_c
402 'I23S'      1    0     0       ! (D=0) select 2S or 3S state
403 'IPOL'      1    0     0       ! (D=0) VM->11 (polarization study)
404 'IHFL'      1    0     4       ! (D=4) produced flavour for IPRO=11
405 *                               ! 4: charm
406 *                               ! 5: bottom
407 'PTCU'      1    0     1.      ! (D=0) p_t **2 cut for process
408 * ++++++ Parton shower and fragmentation ++++++
409 'NFRA'      1    0     1       ! (D=1) Fragmentation on=1 off=0
410 'IFPS'      1    0     3       ! (D=3) Parton shower
411 *                               ! 0: off
412 *                               ! 1: initial state PS
413 *                               ! 2: final state PS
414 *                               ! 3: initial and final state PS
415 'IFIN'      1    0     1       ! (D=1) scale switch for FPS
416 *                               ! 1: 2(m^2_1t+m^2_2t)
417 *                               ! 2: shat
418 *                               ! 3: 2(m^2_1+m^2_2)
419 'SCAF'      1    0     1.      ! (D=1) scale factor for FPS
420 'ITIM'      1    0     0       ! 0: timelike partons may not shower
421 *                               ! 1: timelike partons may shower
422 'ICCF'      1    0     1       ! (D=1) Evolution equation
423 *                               ! 0: DGLAP
424 *                               ! 1: CCFM
425 *                               ! 2: PB TMD evolution
426 * ++++++ Structure functions and scales ++++++
427 'IRAM'      1    0     0       ! (D=0) Running of alpha_em(Q2)
428 *                               ! 0: fixed
429 *                               ! 1: running
430 'IRAS'      1    0     1       ! (D=1) Running of alpha_s(MU2)
431 *                               ! 0: fixed alpha_s=0.3

```

```

432 *                                ! 1: running
433 'IQ2S'      1      0      3      ! (D=1) Scale MU2 of alpha_s
434 *                                ! 1: MU2= 4*m**2 (only for heavy quarks)
435 *                                ! 2: MU2 = shat(only for heavy quarks)
436 *                                ! 3: MU2= 4*m**2 + pt**2
437 *                                ! 4: MU2 = Q2
438 *                                ! 5: MU2 = Q2 + pt**2
439 *                                ! 6: MU2 = k_t**2
440 'SCAL'      1      0      1.0    ! scale factor for renormalisation scale
441 'SCAF'      1      0      1.0    ! scale factor for factorisation scale*
442 *'IGLU'     1      0      1201   ! (D=1010)Unintegrated gluon density
443 *                                ! > 10000 use TMDlib (i.e. 101201 for JH-2013-set1)
444 *                                ! 1201: CCFM set JH-2013-set1 (1201 - 1213)
445 *                                ! 1301: CCFM set JH-2013-set2 (1301 - 1313)
446 *                                ! 1001: CCFM J2003 set 1
447 *                                ! 1002: CCFM J2003 set 2
448 *                                ! 1003: CCFM J2003 set 3
449 *                                ! 1010: CCFM set A0
450 *                                ! 1011: CCFM set A0+
451 *                                ! 1012: CCFM set A0-
452 *                                ! 1013: CCFM set A1
453 *                                ! 1020: CCFM set B0
454 *                                ! 1021: CCFM set B0+
455 *                                ! 1022: CCFM set B0-
456 *                                ! 1023: CCFM set B1
457 *                                ! 1: CCFM old set JS2001
458 *                                ! 2: derivative of collinear gluon (GRV)
459 *                                ! 3: Bluemlein
460 *                                ! 4: KMS
461 *                                ! 5: GBW (saturation model)
462 *                                ! 6: KMR
463 *                                ! 7: Ryskin,Shabelski
464 * ++++++ BASES/SPRING Integration procedure ++++++
465 'NCAL'      1      0      50000   ! (D=20000) Nr of calls per iteration for bases
466 'ACC1'      1      0      1.0     ! (D=1) relative prec.(%) for grid optimisation
467 'ACC2'      1      0      0.5     ! (0.5) relative prec.(%) for integration
468 * ++++++
469 *'INTE'     1      0      0        ! Interaction type (D=0)
470 *                                ! = 0 electromagnetic interaction
471 *'KT1 '     1      0      0.44    ! (D=0.0) intrinsic kt for beam 1
472 *'KT2 '     1      0      0.44    ! (D=0.0) intrinsic kt for beam 2
473 *'KTRE'     1      0      0.35    ! (D=0.35) primordial kt when non-trivial
474 *                                ! target remnant is split into two particles
475 * Les Houches Accord Interface
476 'ILHA'      1      0      0        ! (D=10) Les Houches Accord
477 *                                ! = 0 use internal CASCADE
478 *                                ! = 1 write event file
479 *                                ! = 10 call PYTHIA for final state PS and remnant frag
480 * path for updf files
481 * 'UPDF'     './share'

```

10 Program Installation

CASCADE3 now follows the standard AUTOMAKE convention. To install the program, do the following

```
1) Get the source
tar xvfz cascade-XXXX.tar.gz
cd cascade-XXXX

2) Generate the Makefiles (do not use shared libraries)
./configure --disable-shared --prefix=install-path --with-lhapdf="lhpdflib_path"
--with-tmdlib="TMDlib_path" --with-hepmc="hepmc_path"

with (as example):
lhpdflib_path=/Users/jung/MCgenerators/lhapdf/6.2.1/local
TMDlib_path=/Users/jung/jung/cvs/TMDlib/TMDlib2/local
hepmc_path=/Users/jung/MCgenerators/hepmc/HepMC-2.06.09/local

3) Compile the binary
make

4) Install the executable and PDF files
make install

4) The executable is in bin
run it with:
export CASEED=1242425
export HEPMCOUT=outfile.hepmc

cd $install-path/bin
./cascade < $install-path/share/cascade/LHE/steering-DY-MCatNLO.txt
```


11 Program Summary

Title of Program: CASCADE3 3.0.2-beta15

Computer for which the program is designed and others on which it is operable: any with standard Fortran 77 (gfortran)

Programming Language used: FORTRAN 77

High-speed storage required: No

Separate documentation available: No

Keywords: QCD, TMD parton distributions.

Method of solution: Since measurements involve complex cuts and multi-particle final states, the ideal tool for any theoretical description of the data is a Monte Carlo event generator which generates initial state parton showers according to Transverse Momentum Dependent (TMD) parton densities, in a backward evolution, which follows the evolution equation as used for the determination of the TMD.

Restrictions on the complexity of the problem: Any LHE file (with on-shell or off-shell) initial state partons can be processed.

Other Program used: PYTHIA (version > 6.4) for final state parton shower and hadronization, BASES/SPRING 5.1 for integration (both supplied with the program package), TMDLIB as a library for TMD parton densities.

Download of the program: <http://www.desy.de/~jung/cascade>

Unusual features of the program: None

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