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Monte Carlo tools for top physics

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Summary. — I review recent developments in Monte Carlo tools for top physics at hadron colliders, with particular attention to the interfacing of next-to-leading order results with shower Monte Carlo.

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Monte Carlo event generators are essential tools for physics studies at the Tevatron and at the LHC. In the case of top production, cross section measurements rely on the generators ability to model the production phenomenon, in order to estimate the effect of acceptance cuts on the top sample. In top mass measurements, we rely on Monte Carlo generators for estimating how mass sensitive observables depend upon the top mass. It is clear that the precision that we achieve in the simulation of the production and decay process should be reflected in the error on the measured mass. At the LHC, $t\bar{t}$ production is a background to Higgs and to several new physics searches. Here again, Monte Carlo generators are used for background estimates.

The basic simulation tools for top production processes are the all-purpose shower Monte Carlo Generators, like `PYTHIA` [1, 2], `HERWIG` [3, 4] and `HERWIG++` [5]. These generators use leading-order matrix elements for the basic production processes. Further radiation, including the production of extra jets, is generated using the collinear approximation, and, to a limited extent, the soft approximation. Thus, for example, in the case of $t\bar{t}$ production, jets at small angle with respect to the collision axis are well described, and, to a lesser extent, soft jets. So, we should expect a fair description of relatively small p_T jets in the forward and backward region; we should be more suspicious of soft jets in the central region, and we should not trust at all the description of the production of jets with large transverse momentum.

Since the top quark decays before hadronization, the angular distribution of its decay products are correlated with the whole kinematics of the event. Some Shower Monte Carlo programs (`HERWIG++`, for example), include methods to treat these spin correlations correctly at leading order.

1. – Matrix elements and parton showers

The very basic accuracy reached by standard MC tools contrasts with the existence of methods to compute very high multiplicity processes at the parton level, and with the existence of several next-to-leading results relevant for top physics. In recent years, considerable theoretical progress has taken place for the inclusion of these higher-order processes in the framework of Shower Monte Carlo generators. On one side, methods for interfacing high multiplicity, tree level matrix element calculations with shower Monte Carlo programs (ME+PS) have become available [6], following the work of ref. [7]. Using these methods, one can easily prepare samples of events for a given basic process, including a relatively large number of associated jets. Thus, for example, in $t\bar{t}$ production (a process of order α_S^2), corrections of order α_S^3, α_S^4, etc., are added, although only at the tree level (*i.e.* not including virtual loops). These higher-order effects amount to the addition of processes with a higher number of final state partons, all computed at the tree level. Several collaborations provide these ME+PS generators [8-11]. Most of them are meant to be interfaced to standard parton shower generators, like Herwig and Pythia. The SHERPA Monte Carlo [8] provides instead its own showering and hadronization mechanism, thus constituting a full standalone generator with ME+PS capabilities. Spin correlations in decays are also easily included, and furthermore, within the same framework one can generate extra jet produced in the decay process (in case the decay involves coloured particles). An example along these lines is given in fig. 14 of ref. [12].

2. – NLO and parton showers

The first proposal for merging NLO results and parton showers is the MC@NLO one, of ref. [13]. Subsequently, the POWHEG method has been proposed [14]. Other proposals have appeared in the literature [15-18]; however, at present, only MC@NLO and POWHEG have reached a mature enough stage to be useful for everyday collider physics needs. In the following I will illustrate the basics of approaches along the lines of MC@NLO or POWHEG.

The basic concept of NLO+PS is better clarified by considering the example of a process with a single massless coloured parton involved (one can think, for example, of top decay, assuming the W to be stable and neglecting the b mass). In a Shower Monte Carlo, the radiation of a final state light parton is generated with an algorithm that resums all leading log corrections to the Born process. The hardest emission in a shower Monte Carlo is well described by the following formula [14]:

$$\mathrm{d}\sigma = B(\Phi_B)\mathrm{d}\Phi_B \left[\Delta_{t_0}^{\mathrm{MC}}(\Phi_B) + \Delta_t^{\mathrm{MC}}(\Phi_B)\frac{R^{\mathrm{MC}}(\Phi)}{B(\Phi_B)}\mathrm{d}\Phi_r^{\mathrm{MC}}\right], \tag{1}$$

where t is the radiation transverse momentum, t_0 is the minimum allowed value for t (typically of the order of a hadronic scale), $B(\Phi_B)\mathrm{d}\Phi_B$ is the Born differential cross section, and $R^{\mathrm{MC}}\mathrm{d}\Phi_B\Phi_r$ is the real radiation differential cross section in the Monte Carlo (MC from now on) approximation. It is assumed that the full phase space Φ including radiation is parametrized in terms of the Born phase space Φ_B and the radiation phase space Φ_r, *i.e.* $\Phi = \Phi(\Phi_B, \Phi_r)$. We refer to Φ_B as the underlying Born configuration associated with Φ. In typical MC's, the radiation phase space is determined by three variables characterizing the collinear splitting process, like, for example, the splitting angle, the momentum fraction and the azimuth. The radiation transverse momentum t is a function of Φ_B and Φ_r. It can be defined as the momentum component of the radiated parton orthogonal to the momentum of the radiating parton. The MC Sudakov form factor

$$\Delta_{t_l}^{\mathrm{MC}}(\Phi_B) = \exp\left[-\int_{t>t_l} \frac{R^{\mathrm{MC}}(\Phi)}{B(\Phi_B)} \mathrm{d}\Phi_r^{\mathrm{MC}}\right] \tag{2}$$

represents the probability for not having radiation harder than t_l.

The basic idea in NLO+PS is to improve formula (1) in such a way that NLO accuracy is reached. One replaces formula (1) with the following one:

$$\mathrm{d}\sigma = \bar{B}(\Phi_B)\mathrm{d}\Phi_B \left[\Delta_{t_0}^{s}(\Phi_B) + \Delta_{t}^{s}(\Phi_B)\frac{R^s(\Phi)}{B(\Phi_B)}\mathrm{d}\Phi_r^{\mathrm{MC}}\right] + [R(\Phi) - R^s(\Phi)]\mathrm{d}\Phi, \tag{3}$$

where Φ is the full phase space, with $\mathrm{d}\Phi = \mathrm{d}\Phi_B \mathrm{d}\Phi_r$, and R is the exact radiation cross section. We have also defined

$$\bar{B}(\Phi_B) = B(\Phi_B) + \left[V(\Phi_B) + \int R^s(\Phi)\mathrm{d}\Phi_r\right], \tag{4}$$

where V is the virtual NLO correction to the Born process. Notice that soft and collinear singularities in V cancel against those arising from the integral of R^s in the square bracket of eq. (4). The Sudakov form factor is now

$$\Delta_{t_l}^{\mathrm{s}}(\Phi_B) = \exp\left[-\int_{t>t_l} \frac{R^{\mathrm{s}}(\Phi)}{B(\Phi_B)}\mathrm{d}\Phi_r\right]. \tag{5}$$

Both POWHEG and MC@NLO implement formula (3), although the two methods are in practice very different.

In POWHEG, we require that $R \to R^s$ in the soft and collinear limit, and that $R^s \leq R$, so that the last contribution in the square bracket of eq. (3) is non-negative. The choice $R^s = R$ is also possible, and it is quite common.

The phase space factorization in the POWHEG formula needs not to match that of any shower Monte Carlo. One only requires that in the soft and collinear limit the full phase space Φ is related to the Born phase space Φ_B in the correct way, *i.e.* they are identical in the soft limit once the soft particle is removed, and they are identical in the collinear limit once the collinear particles are merged. The POWHEG formula (3) can be viewed as an improvement of the Monte Carlo formula (1), such that the Born cross section is replaced with an NLO inclusive cross section, and high transverse momentum radiation is corrected so that it becomes exact at large angles. In fact, for large t the Sudakov form factor becomes 1, and the POWHEG cross section reduces to

$$\mathrm{d}\sigma = \bar{B} \times \frac{R^s}{B}\mathrm{d}\Phi + [R - R^s]\mathrm{d}\Phi \approx R\mathrm{d}\Phi, \tag{6}$$

since $\bar{B}/B = 1 + \mathcal{O}(\alpha_s)$. At small t the POWHEG formula becomes equal to that of a standard shower MC, up to higher-order terms. However, since by construction

$$\Delta_{t_0}^{\mathrm{s}} + \int \theta(t - t_0)\, \Delta_t^{\mathrm{s}} \frac{R^s(\Phi)}{B(\Phi_B)}\mathrm{d}\Phi_r^{\mathrm{MC}} = 1 \tag{7}$$

the POWHEG formula maintains NLO accuracy for integrated (*i.e.* inclusive) quantities.

Formula (3) also describes the radiation of the hardest parton in MC@NLO, provided R^s is identified with the shower Monte Carlo (*i.e.* HERWIG's) approximation of the real emission cross section. In fact, in MC@NLO two types of events are generated, called $\mathcal{S}$ and $\mathcal{H}$ events. $\mathcal{S}$ events correspond to the term proportional to $\bar{B}$. In MC@NLO the corresponding underlying Born kinematics is generated with a probability $\bar{B}(\Phi_B)\mathrm{d}\Phi_B$, while the hardest radiation kinematics is generated by the HERWIG shower algorithm. It was demonstrated in ref. [14] that the hardest radiation in HERWIG corresponds to the factor in square bracket multiplying $\bar{B}$ in eq. (3). The $\mathcal{H}$ events correspond instead to the $R - R^s$ term in eq. (3). However, since R^s is now given by the HERWIG shower algorithm, there is no guarantee that the difference $R - R^s$ should be positive, and this is why negative weighted events are an essential feature of MC@NLO. Notice also that it is not guaranteed that the difference $R - R^s$ vanishes in the soft limit. Shower Monte Carlo's like HERWIG, in fact, have only limited accuracy in the description of soft radiation. So, in MC@NLO a matching procedure is adopted in the soft limit, that effectively cuts off the divergence that would arise if formula (3) was used as is.

The fact that both in MC@NLO and POWHEG the hardest radiation can be described by a similar formula has allowed a better understanding of the agreement and discrepancies between the two approaches. First of all, one understands why most distributions compare very well in the two schemes (see, for example, [19-22]). A first area of discrepancy has emerged following the work of ref. [23]. In $t\bar{t}$ production, a dip in the rapidity distribution of the hardest jet of MC@NLO was found, that is not present neither in ALPGEN nor in POWHEG. It was shown later [21, 24] that this dip is a feature of MC@NLO that is present in several processes. The origin of this dip has been clarified in several papers [25, 26], and will not be further discussed here. I simply stress that these differences are well understood, so that we do have a fair understanding of the similarities and the differences of the two methods.

3. – Available NLO generators for top production

While for ME+PS generators, given the matrix element, an ME+PS implementation requires essentially no further work, in the case of NLO+PS the available generators lag behind the available NLO calculations for top production. NLO+PS generators exist for $t\bar{t}$, single top, tW and even tH (top in association with a charged hoggs) do exist. However, in all cases spin correlations are only included witht the approximate method of ref. [27]. Furthermore, top decays always involve coloured particles in the final state, and yet, NLO radiative corrections to the decays are not included in the available shower programs, in spite of the fact that NLO calculations that include full spin correlations and NLO corrections to the decay are available [28], and that there are indications that final state NLO corrections may affect top mass measurements [29]. Notice also that NLO corrections to the production of a $t\bar{t}$ pair in association with a jet is also available [30], and that NLO corrections to $t\bar{t}$ production in association with two jets have also been presented at this conference [31].

The status of NLO+PS generators for top production can be summarized as follows. Top pair production is implemented in both MC@NLO and POWHEG [32, 20]. Single top production (s and t channel processes) is also implemented in both codes [33, 22]. Single top production in association with a W is available in MC@NLO [34], and is in preparation in POWHEG [35]. Top production in association with a charged Higgs is available in MC@NLO [36] and is in progress in POWHEG. In all implementations, spin correlations are treated in an approximate way, along the lines of ref. [27]. In refs. [20] and [22],

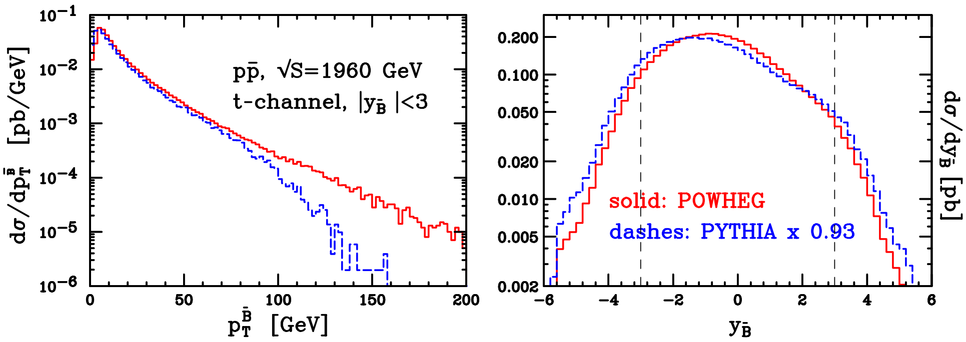

Fig. 1. – Transverse momentum (left) and rapidity (right) of the $\bar{B}$ meson in single top production: POWHEG and PYTHIA compared.

an extensive comparison between MC@NLO and POWHEG results was performed. In the case of $t\bar{t}$ production, a remarkable agreement was found among the two methods. The only area of discrepancy has to do with the rapidity distribution of the hardest jet, which was mentioned earlier. Even better agreement was found in single top production on most distribution, although, it must be said good agreement was found also with PYTHIA, suitably rescaled with a constant K-factor. In figs. 1 and 2 we show comparisons between POWHEG, PYTHIA and MC@NLO for some distributions that do display some noticeable differences.

First of all, we see that the transverse momentum of the $\bar{B}$ is much softer in PYTHIA than in POWHEG. This is to be expected. In t-channel single top production, in the primary partonic process a b quark coming from the hadron structure function converts into a t quark. The associated $\bar{b}$ quark is generated by the backward evolution shower of the MC. It is thus described accurately only in the collinear limit (*i.e.* for small transverse momenta) and it is not surprising that it fails at large transverse momentum. On the other hand, in POWHEG, when the $\bar{b}$ has large transverse momentum it is generated as the hardest radiation, and thus it has full tree level accuracy.

We also notice a considerable difference in the rapidity distribution of the $\bar{B}$ meson when HERWIG rather than PYTHIA is used for subsequent showering. This problem is

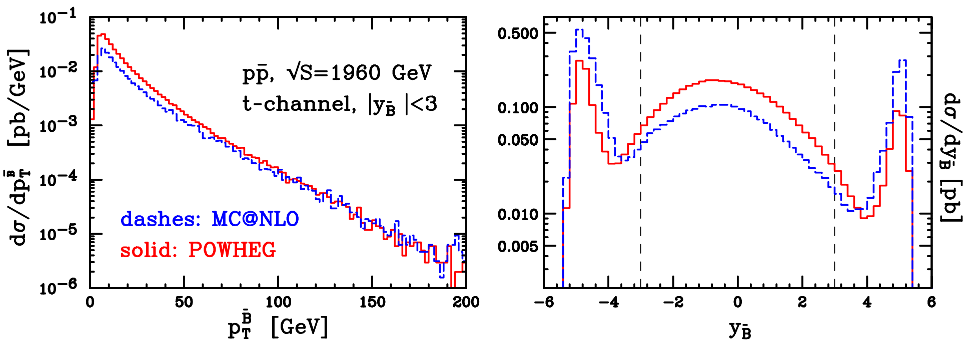

Fig. 2. – Transverse momentum (left) and rapidity (right) of the $\bar{B}$ meson in single top production: POWHEG and MC@NLO compared.

inherited from a known HERWIG problem, in the build up of backward evolution when heavy flavours are involved. Of course, in POWHEG an accurate tree-level correction comes into play when the hardest radiation is associated with the formation of the $b\bar{b}$ pair. However, the hardest radiation may also be simply a radiated gluon from an incoming b quark, so that the initial formation of the $b\bar{b}$ pair takes place earlier in the shower development. Thus, for at least part of the event, it is HERWIG that determines the formation of the heavy flavoured pair. In MC@NLO this problem is even more present, since in this case it is HERWIG that generates a large fraction of the hardest radiation (in the so called $\mathcal{S}$ events). The problem is not present in POWHEG interfaced to PYTHIA.

4. – Merging ME+PS and NLO+PS approaches

Given the fact that ME+PS and NLO+PS cover complementary aspects of the production process, the natural question arises: can they be merged? This is undoubtedly a difficult problem. There are several proposals in the literature [15-17]. At present, none of these methods has achieved useful results for hadron collider physics. In ref. [37], a practical approach to this problem has been pursued, and proven in the framework of W production and $t\bar{t}$ production.

In order to illustrate the findings of ref. [37], let us focus upon our simple example, of $t \to Wb$, treating the b quark as massless and the W as stable. In this framework we just have a single jet to worry about. In a standard Shower approach, the b quark will undergo collinear splitting recursively, according to the shower algorithm. We will have a final state of several light partons. Appliying a k_T clustering algorithm to the final state, we will basically reconstruct the skeleton of the splitting process. In the ME+PS approach, we also apply a clustering algorithm to the final state partons, that are computed in this case using exact tree level matrix elements. We thus reconstruct a shower skeleton, and, according to the CKKW approach, we modify the tree level ME cross section by substituting each power of the coupling constant with one running coupling for each skeleton vertex, and by supplying Sudakov form factor to each intermediate line of the skeleton. The initial line of the skeleton is always the b quark from t decay, and the first skeleton vertex will be given by the b radiating a gluon. Thus, in the ME+PS case we can associate with each final state configuration a hardest radiation configuration Φ, corresponding to the skeleton kinematics up to the first splitting in the reconstructed skeleton. Given the hardest radiation configuration, we can associate with it an underlying Born configuration Φ_B, using the same definition that we adopt in a NLO+PS approach to this decay problem. It has been demonstrated in ref. [37], that in order to achieve NLO accuracy in the ME+PS result (*i.e.* the same accuracy that a NLO+PS generator would achieve) one should reweight the ME+PS result with a $K(\Phi_B)$ factor, *i.e.* with a K-factor dependent upon the underlying Born. A detailed discussion of this point is given in ref. [37]. Here I will only give a brief argument to support this conclusion. If we sum over all possible final states of the ME+PS result keeping fixed the underlying Born configuration Φ_B, we will get a result that equals the Born cross section, up to a factor $\tilde{K}(\Phi_B) = 1 + \tilde{k}_1(\Phi_B)\alpha_s + \mathcal{O}(\alpha_s^2)$ that embodies the effect of higher-order emission included in the ME+PS approach. In other words, the ME+PS cross section, differential in the underlying Born kinematics, differs from the Born cross section by subleading terms in the coupling constant. On the other hand, also the NLO cross section, differential in the underlying Born kinematics, differs from the Born cross section by a NLO factor $\bar{K}(\Phi_B) = 1 + \bar{k}_1(\Phi_B)\alpha_s + \mathcal{O}(\alpha_s^2)$. It is clear now that, in order to get the correct NLO result from the ME+PS generator, we should supply a factor $K(\Phi_B) = \bar{K}(\Phi_B)/\tilde{K}(\Phi_B)$.

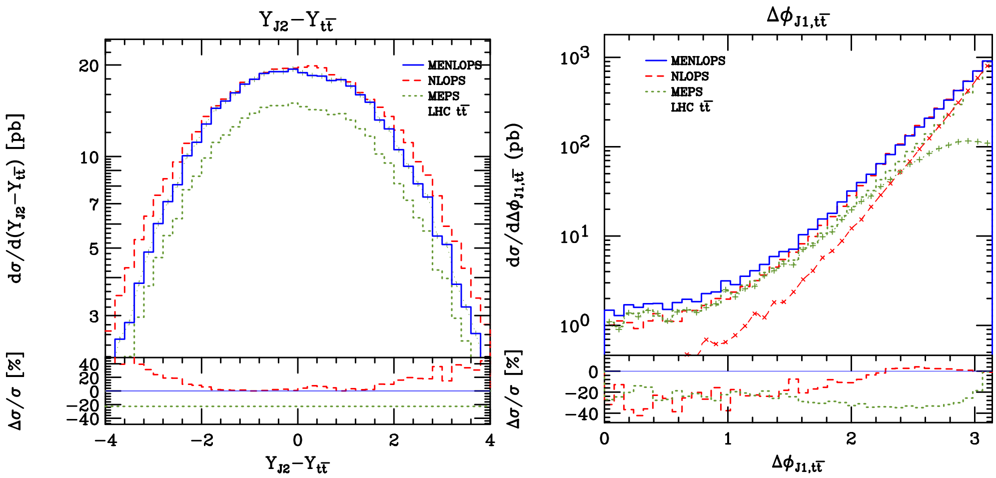

Fig. 3. – Left: rapidity of the second hardest jet relative to the $t\bar{t}$ system. Right: azimuthal distance of the hardest jet with respect to the direction of the $t\bar{t}$ system.

The effective computation of the $K(\Phi_B)$ factor is a difficult task, mainly becaus $\bar{K}$ is hard to compute. In ref. [37], a simple recipe is suggested that, although it does not give a theoretically satisfactory solution of the NLO+PS and ME+PS merging problem, gives nevertheless a satisfactory solution in practice. It is a recipe for merging event samples obtained with a ME+PS approach and with POWHEG. The recipe is represented by the following equation:

$$\mathrm{d}\sigma = \mathrm{d}\sigma_{\mathrm{PW}}(0) + \frac{\sigma_{\mathrm{ME}}(1)}{\sigma_{\mathrm{ME}}(\geq 1)}\,\frac{\sigma_{\mathrm{PW}}(\geq 1)}{\sigma_{\mathrm{PW}}(1)}\,\mathrm{d}\sigma_{\mathrm{PW}}(1) + \frac{\sigma_{\mathrm{PW}}}{\sigma_{\mathrm{ME}}}\,\mathrm{d}\sigma_{\mathrm{ME}}(\geq 2). \tag{8}$$

The arguments (j) and $(\geq j)$ represent the subsample in the matrix element (ME) or POWHEG (PW) samples containing exactly J or at least J jets. The construction of the sample is summarized by the following rules: i) events with no jets are always taken from the POWHEG sample; ii) events with one jet are also taken from the POWHEG sample. However, their cross section is reweighted, in such a way that the ratio of events with at least one jet, relative to those with one jet, agrees with the ME+PS result; iii) Events with at least two jets are always taken from the ME+PS sample. However, their cross section is reweighted with a K factor that is equal to the POWHEG rate for at least one jet relative to the corresponding ME+PS rate. In the $t\bar{t}$ study of ref. [37], the NLO+PS sample is generated using POWHEG, and the ME+PS sample is generated with Madgraph [10] interfaced to virtuality ordered PYTHIA. A 20 GeV generation cut was used, and the scale used to count jets in the ME+PSNLO+PS merging (menlops from now on) was 30 GeV. Few highlights of the results are given in the figures below. Several quantities are plotted and studied in the original paper [37]. Here I only report two plots, that represent well how the method works. In fig. 3, on the left panel, the rapidity of the second hardest jet relative to the $t\bar{t}$ system is displayed. There we see that the menlops result matches in shape the prediction of the ME+PS rather than POWHEG. This is as desired, since in the POWHEG sample the second hardest jet is generated by the Shower Monte Carlo in the collinear approximation. On the right plot, the azimuthal distance of the hardest jet with respect to the direction of the $t\bar{t}$ pair is displayed. In this case, the NLO+PS contribution dominates the large angular separations (corresponding to the hardest jet being back-to-back to the $t\bar{t}$ pair), while away from the back-to-back region, the ME+PS result dominates. This is again as desired, since the region away from the back-to-back configuration is dominated by the radiation of a relatively hard second jet.

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