DESY Summer Student Report

Comparison of NLO MC Generators for Top Pair Production

Jason Mansour*

Supervisors: Marcello Barisonzi, Ulrich Husemann

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1 Introduction

With the LHC getting started and the first data to be taken soon, precise predictions of the expected measurements are required. In my task, I will compare different Monte Carlo event generators which are supposed to simulate top pair production and decay with next-to-leading-order precision.

2 Monte Carlo methods in QCD

Monte Carlo (MC) is the general term for various numerical methods using random number generators, hence the name. These methods are widely in use to do calculations that would be otherwise intractable or very hard. One example is to perform an integral numerically not by discretizing it, and risking problems such as numeric artifacts, but by using a random number generator to eventually fill the area under the integrand and approximating the result (See for instance [1]). This is used in particle physics to calculate the complicated integrals resulting from the Feynman diagrams of perturbation theory.

Once one has calculated the differential probability densities or cross sections for a given process with regard to all interesting observables, such as angle and momentum of the final state particles, one can use these to dice random events. This simulation of particle physics processes is called MC event generation.

2.1 Factorisation of the QCD cross section

Due to the properties of quark confinement and asymptotic freedom in QCD, it is not possible to calculate a cross section of a hadron-hadron process in the perturbative framework. However, one can separate the problem into three parts, which can each be dealt with by special methods:

1. Which partons contribute with which momentum fraction x to the collision is governed by the parton distribution functions (PDFs) $f_a(x)$, where a can either indicate valence quarks, sea quarks, or gluons. PDFs have been measured for the proton in detail especially at the HERA electron-proton-collider.

*jd.mansour@gmail.com

2. Hard scattering can be calculated perturbatively due to asymptotic freedom in QCD, given that the transferred momentum Q^2 is high enough for α_s to be in the perturbative regime.

3. Quarks and gluons produced in hard scattering, as well as remnants of the initial hadron, now undergo the process of showering. Due to radiation of further gluons, decays and hadronisation, the partons form cascades. Given a suitable algorithm, one can identify jets among these cascades. This lower-energetic phase of the reaction cannot be calculated using perturbation theory, however there exist phenomenological models which work quite well, for example the Lund sting model implemented in PYTHIA [2], or the cluster model used in HERWIG [3].

The differential cross section for the collision of two hadrons H_1 and H_2 with momenta p_1 and p_2 respectively can be written as follows:

$$d\sigma(p_1, p_2) = \sum_{a,b} \iint dx_1 dx_2 \cdot f_a^{H_1}(x_1) f_b^{H_2}(x_2) \cdot d\hat{\sigma}_{ab}(x_1 p_1, x_2 p_2)\,. \qquad (1)$$

Here $f_a^{H_i}$ denotes the PDF for the hadron H_i, and $d\hat{\sigma}_{ab}(x_1 p_1, x_2 p_2)$ is the partonic cross section with the partons a and b in the initial state. This will be expanded in a power series in α_s. The so called factorisation theorem ensures that the factored form of the cross section in (1) remains valid for all orders of α_s (see for instance [4]).

3 Monte Carlo in next-to-leading order

Until recently, most Monte Carlo generators have performed the "hard" part of the reaction in leading order (LO), that is just including tree-level diagrams with two vertices, which give terms of order α_s^2.

One way to consider next-to-leading order (NLO) effects is then to calculate the total NLO cross section by other means than MC, and then scaling the LO distributions to the NLO cross section. While this may be a valid approximation for some processes, it is clear that there are effects which cannot be included this way.

For example, consider the process $gg \to t\bar{t}$ (gg-fusion). According to the LO matrix elements, the top and antitop are emitted back-to-back. The inclusion of final state gluon radiation in NLO allows for a percentage of the momentum to be carried away, so that the angle between t and $\bar{t}$ drops below $180°$. While the showering process after LO also handles gluon radiation in the final state, it doesn't manage to create the same angular distribution that NLO MC gives.

It is expected that the $t\bar{t}$ cross section will be measureable at LHC with an uncertainty of about 5% [5]. In this case a comparable accuracy will be needed for the theoretical predictions. This requires at least NLO, if not even NNLO (next-to-next-to leading order) calculations.

3.1 Difficulties

The NLO Feynman diagrams can be divided into two types, those with additional virtual particles that form loops or vertex corrections, and those with extra ($n > 2$) outgoing particles. In traditional (LO) Monte Carlo, only $2 \to 2$ hard processes were calculated perturbatively, and $2 \to n$ configurations were achieved through parton showering. In NLO, we would like to use the same showering algorithms, but now we have $2 \to 3$ processes already in the perturbative part. In this case, using the showering algorithms naively would lead to an overestimation of parton radiation, which is called overcounting. Two strategies to avoid this shall be mentioned in the following:

- The **MC@NLO** algorithm by Frixione and Webber [6] implements all NLO matrix elements in a straightforward way. To deal with overcounting, simply speaking, the extra partons from the hard interaction are matched to partons from showering, and it is determined when there will be overcounting. For these cases, counterevents with negative weights are generated, which cancel the wrong events out. The number of negative weight events is about 10%-15% of the total event count. In spite of the negative weights, for a sufficient number of events all cross sections will be finite and positive. However, one has to calculate slightly more events to get the same statistics in the end.

  The matching calculations have to be done once for each process and for a specific showering algorithm. Because of this, at the moment MC@NLO can only be used with HERWIG for showering.

- The newer **POWHEG** approach by Frixione, Nason and Oleari [7] tries to avoid the problem of overcounting and the negative weights, by doing the most energetic parton emission first, and letting the showering algorithm continue from there. POWHEG can be used in principle with any showering tool which supports the Les Houche interface [8].

4 Comparing two Distributions

For my task I have to compare various setups of Monte Carlo generators and find out if their results are equivalent, or if there are significant differences. The generators produce (after the showering part) a number of events that contain information about the incoming and outgoing particles, as well as of intermediate (decayed) states. This data is referred to as **MC truth**, as opposed to data which has gone through a detector simulation and reconstruction, and therefore has uncertainties from measurements and reconstruction algorithms.

From the MC truth, observables of certain particles (e.g. the transverse momentum p_T of the top quarks) are extracted and filled into histograms. In the limit of a small bin size and large statistics, these histograms can be interpreted as differential cross sections (say $d\sigma/dp_T$). My task is then to compare two histograms and decide if they are in agreement.

Statistically speaking: One has two measured distributions x_i and y_i, where $i = 1 \ldots N$. The **null hypothesis** H_0 is the assumption that these datasets have been drawn randomly from the same underlying distribution $d\sigma/dx$. One would like to be able to disprove this hypothesis by finding significant differences between the two empirical distributions. Note that this can only be done on statistical grounds, and one cannot *prove* that two given distributions *have to* come from a different source. One can just give a statistical measure whether to reject the assumption of similarity (H_0) or not. It is unavoidable to sometimes make a mistake here:

- The **error of the first kind** occurs when one rejects the null hypothesis (and says the histograms are "different"), although they do come from the same underlying distribution.
- The **error of the second kind** on the other hand is not to reject H_0, although the two datasets have different sources.

When one has a number of histograms drawn statistically from the same theoretical distribution, using a certain criterion for rejection, the probability to make a mistake of the first kind is denoted by α. The **confidence level** (CL) is defined as $1 - \alpha$. A higher CL reduces the chance of an error of the first kind, at the cost of lowering the rejection power of the test. Typical values for the confidence level are for example 90%, 95%, 99%. (See also any textbook on statistical methods, for example [1]).

Note that while it is possible to reject H_0 at a certain CL, one can in principle not prove the null hypothesis. Imagine two theoretical distributions in $x \in [0, 1]$, with their mean values differing just by $\Delta\bar{x} = 10^{-6}$ or less. A tremendous amount of statistics would be necessary to see this deviation. This also plays a role in my analysis, as the (theoretical) distributions from two different MC generators will very likely *not* be the *same*, but for all practical purposes they should be indiscernible, which will be the H_0 in the following.

4.1 Kolmogorow-Smirnov-Test

The Kolmogorov-Smirnov-Test (KS) can be either be used to compare a set of measurements x_i with a given distribution function $f(x)$ or, as in our case, to compare two measured distributions x_i and y_j. First, the **empirical cumulative distribution function** (CDF) $F_n(x)$ is constructed from the measurements. This function starts at zero for $x < \min(x_i)$. It makes a step of height $1/N$ each time x passes a data point x_i, so that it reaches $F_n(x) = 1$ when $x \geq \max(x_i)$ (Figure 1, left). In the same way one constructs $G_m(x)$ from the y_j. When dealing with binned data, the "integral" of the histogram, that is the sum of all bin contents up to the bin containing x, given by $F(x) = \sum_{x_i \leq x} f(x_i)$, takes the role of $F_n(x)$.

The maximum distance between the two functions $F_n(x)$ and $G_m(x)$ then defines the Kolmogorov distance $D_{n,m}$:

$$D_{n,m} := \sup_x \{|F_n(x) - G_m(x)|\}\,. \tag{2}$$

In the case of comparison with a function $f(x)$ its integral $F(x)$ takes the role of the second CDF, and the Kolmogorov distance is given by:

$$D_n := \sup_x \{|F_n(x) - F(x)|\}\,. \tag{3}$$

The important insight by Kolmogorov was that, if the null hypothesis is true, as the number of data points n approaches infinity, the Kolmogorov distance D_n approaches zero. Furthermore, the quantity $\sqrt{n} \cdot D_n$ should be distributed

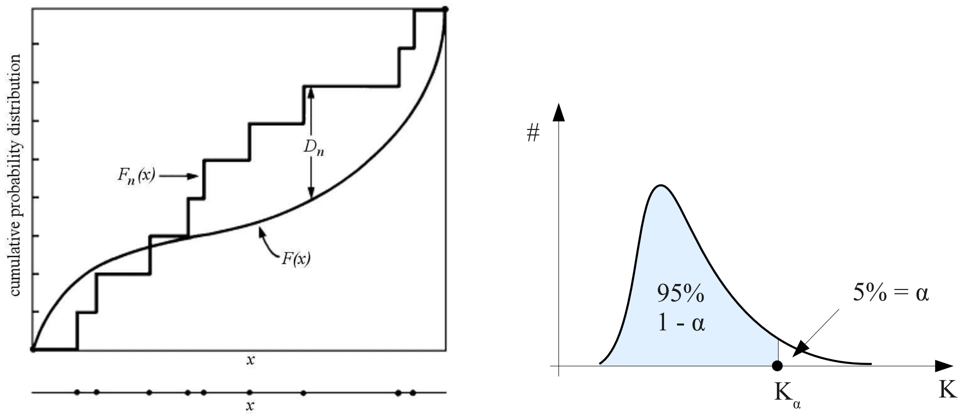

Figure 1: Left: Illustration of the empirical cumulative distribution function (CDF) and the Kolmogorov distance D_n. From: Numerical Recipes in C++ [9]. Right: Sketch of the Kolmogorov distribution, showing the confidence level $1-\alpha$ and the critical value K_α.

according to the so called Kolmogorov distribution K. Likewise, in the case of comparing two empirical distributions, n is replaced by n', which is defined as:

$$n' := \frac{n \cdot m}{n+m}\,.$$

Now one would like to use this information to construct a test for H_0. The idea is to pick a critical value K_α so that if $\sqrt{n} \cdot D_n > K_\alpha$, one rejects the hypothesis of similarity. To get K_α, one chooses a confidence level, say $1-\alpha = 95\%$, and then finds the position K_α in the Kolmogorov distribution, so that only the fraction α of the area enclosed by the curve lies beyond it (Figure 1, right). Now the probability for an error of the first kind is α.

While this way one has a test that allows rejection at a given CL, there is another well known approach which I use for my analysis. Given a certain value of $\sqrt{n} \cdot D_n$ for a pair of distributions, I'm asking for the highest possible CL (the lowest α) at which one could still say that they are different. The CDF (the integral up to K_α) of the Kolmogorov distribution is given by:

$$P(K \leq K_\alpha) = 1 - 2\sum_{j=1}^{\infty}(-1)^{j-1}\mathrm{e}^{-2j^2K_\alpha^2} = 1 - \alpha\,. \qquad (4)$$

Plugging in $\sqrt{n} \cdot D_n$ as the critical value K_α, this gives the maximum CL $1-\alpha$. A lower value of α signifies more strongly that the two distributions are different.

4.1.1 Pseudoexperiments approach

A different approach to the Kolmogorov test uses so called pseudoexperiments. Again, we would like to compare two empirical distributions A and B, where A contains n values. We interpret the histogram of A as a probability density, and dice n random numbers accordingly. The result is a histogram A_1, which is in form similar to the original one, but with the fillings of its bins Poisson-distributed around those of A. This is repeated a large number of times, say $N = 1000$ times, to create the pseudoexperiment histograms A_1 to A_N. Then the Kolmogorov distance between A and each of the A_n, as well as between

A and B is calculated. The question is, how many pseudoexperiments have a larger ($\hat{=}$ worse) KS-distance to A than B does? This percentage α_{pseudo} is then a measure of the dissimilarity of A and B.

Note that the pseudoexperiments test is not completely equivalent with the method shown above. Due to the random nature of the histograms to be tested it is always possible that A is not a typical representative of the underlying distribution, but a exceptionally deviant one. It is not tested if A and B could stem from the same distribution, but rather if B could be a variation of A. If one equates α_{pseudo} to the above α, one underestimates for this reason the error of the first kind. However, in the case of large statistics ($\hat{=}$ low relative errors) for A – the limiting case being the knowledge of the theoretical distribution — the pseudoexperiments result should approach the analytical result. For this reason, it is more suited for comparing e.g. one large body of Monte Carlo data A with some small amounts of measured data B, than comparing several medium-sized datasets as in my task.

In general, the pseudoexperiments approach has the advantage of its simple probabilistic interpretation. It can be used even in cases where the expected distribution of the test quantity is not known analytically.

4.2 χ^2-Test

Another widely used test which is to be used on binned data is called the chi-square-test. Usually it serves as a goodness-of-fit test, comparing a histogram to a fitted curve, but it can also be used to compare two histograms.

The test is simple: For every bin, the squared distance between the two histograms is taken, normalized, and summed up. This gives us the χ^2 value:

$$\chi^2 := \sum_{i=1}^{N} \frac{(x_i - y_i)^2}{x_i + y_i} \tag{5}$$

Besides this, we need the number of **degrees of freedom**, NDF. That is in this case the number of bins minus the number of constraints applied to the distributions. As the number of events is fixed, usually NDF $= N - 1$. In the case that for one bin x_i and y_i are both zero, one cannot compute the fraction and omits it from the sum, while the NDF is reduced by one.

In the case that H_0 is fulfilled (i.e. the histograms come from the same source), the quantity χ^2 follows the so called chi-square distribution, which depends on the NDF. Now with the knowledge of the expected distribution, one can proceed as above and calculate the maximum CL $= 1 - \alpha$, at which two given histograms can be said to be different.

4.2.1 Improvements to the Chi-Square Test

The accuracy of the χ^2-test suffers if many bins are not filled sufficiently. This is for two reasons: On the one hand, the relative error of a bin $\sqrt{N}/N$ decreases with the filling N, on the other hand, due to the expression $x_i + y_i$ in the denominator in (5), barely filled bins have a much higher weight. Therefore, it is recommended to choose a binning such that there are at least 10 entries in each bin (see [9]). This can be done by joining adjacent bins together if one of them contains fewer then 10 entries (and reducing the NDF by one each time).

Another improvement is to weight the terms in (5) according to their errors. For the necessary modifications, see [9]. I am using both improvements in my analysis.

4.3 Runs Test

While the χ^2-Test only looks at the absolute difference $|x_i - y_i|$ between the two histograms, it discards the sign. This leads to the idea to construct a test based solely on the sign instead. Such a test should be complementary to the χ^2 test in the sense that the former delivers information the latter does not, and vice versa.

The test works as follows: One takes the difference $x_i - y_i$ for each pair of bins, and notes a $+$, $-$ or 0, depending on the sign of the difference. Several consecutive pluses or minuses together are called a **run**. One counts the total number of $+$, $-$ and the number of runs r. Runs of zeros are thereby not counted, a zero only serves to stop a previous run.

Under the assumption of H_0, r should be normal distributed. Using combinatorics it is possible to calculate, for a given n_+ and n_-, an expectation value μ and a variance σ^2 for r. With $n = n_+ + n_-$ one has:

$$\mu(r) = \frac{2n_+n_-}{n} + 1 \qquad \text{and} \qquad \sigma^2(r) = \frac{(\mu-1)(\mu-2)}{n-1}\,. \tag{6}$$

Using r as a test statistic, one can then test H_0 as usual, or calculate a critical value of α for a pair of histograms.

5 Setup

For my comparisons, I am looking at simulated events of top pair production from proton-proton collisions ($pp \to t\bar{t}+X$) at a center-of-mass energy of 10 TeV. This is the energy planned to be reached during the first data taking with the LHC in 2008. The events are preselected in a certain way: While the top quarks decay almost always into a W^+ boson and a bottom quark, the W can either decay leptonically ($W^+ \to \ell^+ + \nu_\ell$) or hadronically. The generated samples contain no all-hadronic events, i.e. at least one $W^\pm$ has to decay into leptons. The top mass is assumed to be 172.5 GeV, with a width of $\Gamma = 1.42$ GeV.

The samples, each containing 10000 events, are produced by following generators & showering tools:

- MC@NLO v3.1 and v3.31 with HERWIG
- POWHEG v1.0 with HERWIG
- POWHEG v1.0 with PYTHIA

(In the last two cases I am using the same output file of POWHEG for both HERWIG and PYTHIA.) This allows me to do three comparisons:

1. MC@NLO v3.1 vs. MC@NLO v.3.31
2. Both MC generators using HERWIG: MC@NLO vs. POWHEG
3. Both showering algorithms using POWHEG: HERWIG vs. PYTHIA

In the MC truth I am identifying the $t/\bar{t}$, the $W^{\pm}$ and $b/\bar{b}$, and the leptons from the W decay. I am looking at the following observables:

- For $t/\bar{t}$, $W^{\pm}$, $b/\bar{b}$ and $\ell^{\pm}$:
  - Transverse momentum p_T, Pseudorapidity η, Polar angle ϕ.
- For $W^{\pm}$ additionally:
  - $\cos(\theta^*)$, defined as the angle between the lepton and the (parent) top, in the rest frame of the W. This gives information on the helicity of the W boson in top decays [10]. One expects a mixture of about 70% left-polarized and 30% longitudinal polarized W-bosons.
- For t & $\bar{t}$ together:
  - Combined p_T (vectorial as well as scalar sum $|p_T(t)| + |p_T(\bar{t})|$),
  - The angle between their momentum vectors,
  - $\Delta R = \sqrt{\Delta\eta^2 + \Delta\phi^2}$ as a measure of distance in η-ϕ-space,
  - Rapidity difference Δy.

Each observable is filled into histograms, which are then compared using the KS, the χ^2 and the runs test, as well as visually.

6 Results

While there have been no obvious, large differences in any of the histograms I've compared, I did find some statistical relevant deviations. My results are summarized in Table 1.

- In the comparison of MC@NLO v3.1 with v3.31, there are only small deviations in the top p_T distributions (Figure 2). It is quite possible that these are just the statistical error of the first kind. One would have to repeat the comparison with more data to exclude that possibility.
- In the second comparison, MC@NLO vs. POWHEG, the top p_T distributions show differences as well, however also the p_T of the b-quarks and leptons is affected. One also sees differences in the angular distributions (Figure 3).
- The results of comparing HERWIG vs. PYTHIA look similar (Figure 5), however in this case there are no big deviations in the angular observables (considering a failed runs test alone not significant). This is expected, since the events generated by POWHEG in the MC step were reused for both showering tools, and the main contribution to the shape of the angular distributions comes from the simulation of the hard process.

6.1 Conclusions about the tests used

I have tried several variations of each test mentioned above. This lead to te following results:

	MC@NLO 3.1 / 3.31			MC@NLO / POWHEG			HERWIG vs. PYTHIA		
Measurement, α →	KS	χ²	Run	KS	χ²	Run	KS	χ²	Run
t/tbar pT	0,14	**0,01**	1,00	**0,01**	**0,05**	0,46	**0,00**	**0,01**	0,41
t/tbar pT sum (scalar)	0,57	0,45	0,12	0,15	0,40	0,57	**0,00**	0,33	**0,00**
t/tbar pT sum (log x)	0,17	**0,03**	0,71	**0,06**	0,19	0,69	0,11	0,32	0,19
t/tbar pT sum	0,63	**0,06**	0,13	0,18	**0,01**	**0,06**	0,14	**0,01**	0,73
t/tbar Δy	0,70	0,50	1,00	0,31	0,39	1,00	0,91	1,00	1,00
t/tbar ΔR	0,92	0,52	0,53	**0,03**	0,15	1,00	0,99	0,56	1,00
t/tbar angle	0,71	0,10	0,68	**0,01**	**0,00**	0,51	0,47	0,92	0,13
W pT	0,91	0,89	**0,09**	0,30	0,85	0,25	**0,00**	**0,07**	**0,00**
W eta	0,83	0,36	0,52	0,87	0,91	0,83	1,00	1,00	**0,03**
W phi	0,54	0,97	0,46	0,31	0,82	0,41	1,00	1,00	0,31
b/bbar pT	0,70	0,17	0,35	**0,08**	**0,01**	0,88	**0,00**	0,28	0,14
b/bbar eta	0,37	0,89	0,55	0,86	0,48	0,33	1,00	1,00	**0,03**
b/bbar phi	0,45	0,92	0,27	0,44	0,91	0,65	1,00	1,00	**0,03**
lepton pT	0,24	0,55	0,18	0,94	0,83	**0,02**	0,18	0,83	0,77
cos θ*	0,62	0,55	0,24	0,55	**0,09**	0,63	1,00	1,00	**0,00**

Table 1: Results of all the tests. In the first column, MC@NLO version 3.1 is compared with 3.31, in the second column MC@NLO and POWHEG, both using HERWIG for showering, are compared. The third column shows the comparison of HERWIG VS. PYTHIA using the same POWHEG events.

- The Kolmogorov-Smirnov test provided by `TH1::KolmogorovTest()` in ROOT behaves for my purposes identical to the algorithm listed in Numerical Recipes [9].
- Simple tests suggest that the KS test with pseudoexperiments works as expected. I compared a large number of histograms which were drawn from the same random distribution (top p_T data generated by MC@NLO). The Kolmogorov distances of the random histograms to the original were following approximately a Kolmogorov distribution.
- The runs rest is as expected not very powerful. Also I suspect some error in my implementation, as it sometimes gives an exceptionally low α when the two histograms are clearly in agreement. (See Table 1, second column, lepton p_T, and third column, $b/\bar{b}$ η and *phi*, and $\cos\theta^*$.)
- However, the run test can give information when the χ^2 test is insensitive. An example is in Table 1, third column, the first two rows (p_T and p_T scalar sum). The corresponding histograms are shown in Figure 5.

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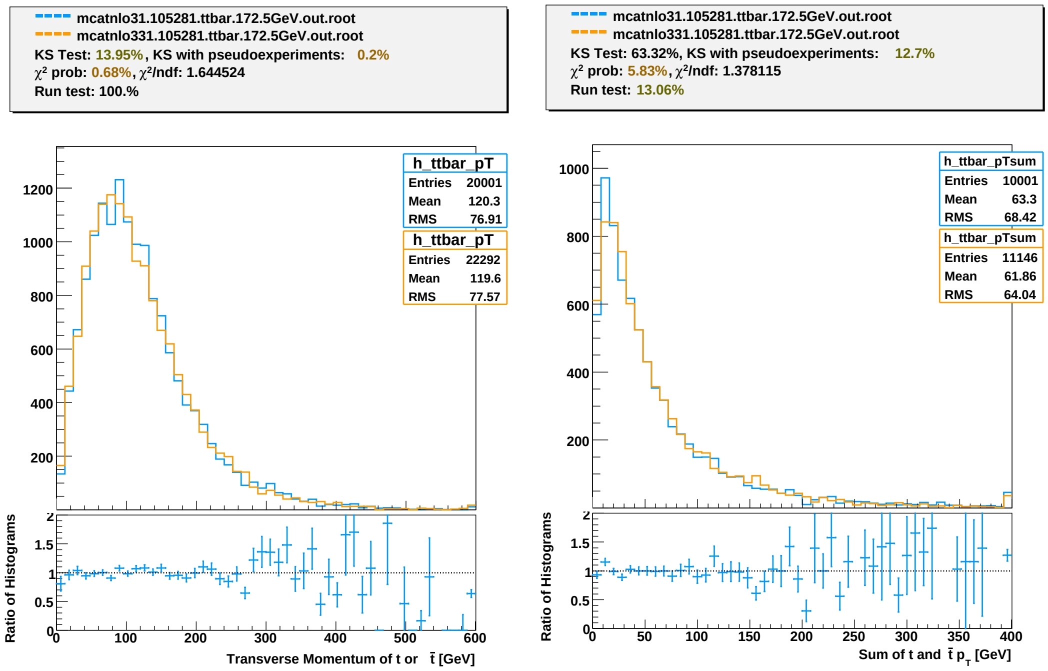

Figure 2: Comparison 1 (MC@NLO v3.1 vs. v3.31). Left: Transverse momentum of $t/\bar{t}$. Right: Absolute value of the vectorial sum of $p_T(t)$ and $p_T(\bar{t})$.

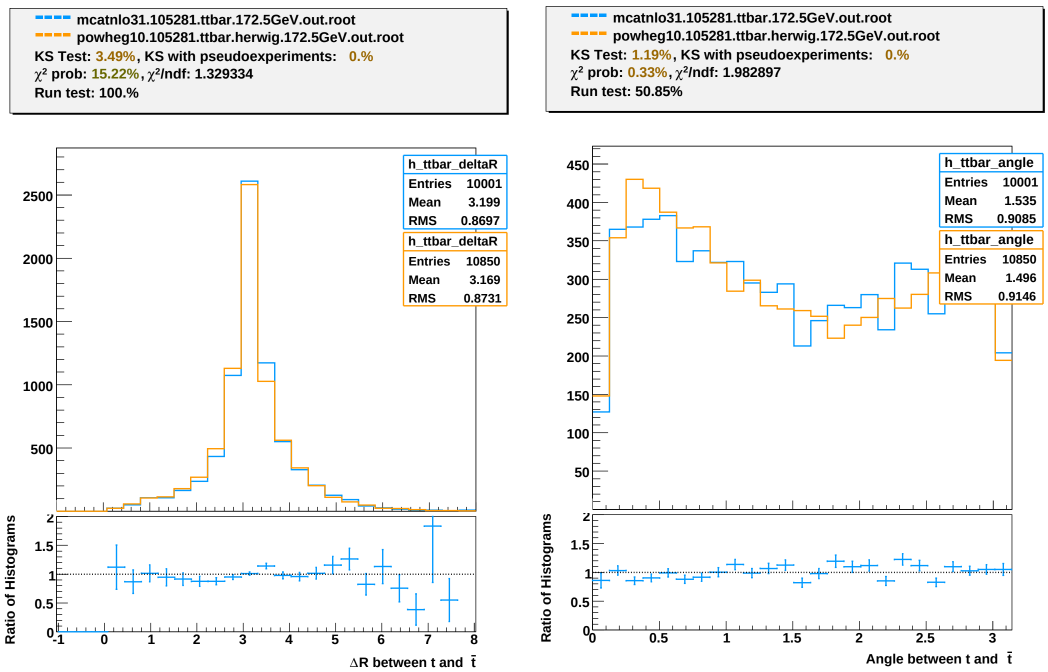

Figure 3: Comparison 2 (MC@NLO vs. POWHEG). Left: $\Delta R = \sqrt{\Delta\eta^2 + \Delta\phi}$. The distribution from POWHEG is clearly shifted to the left. Right: Angle between the momentum vectors of t and $\bar{t}$.

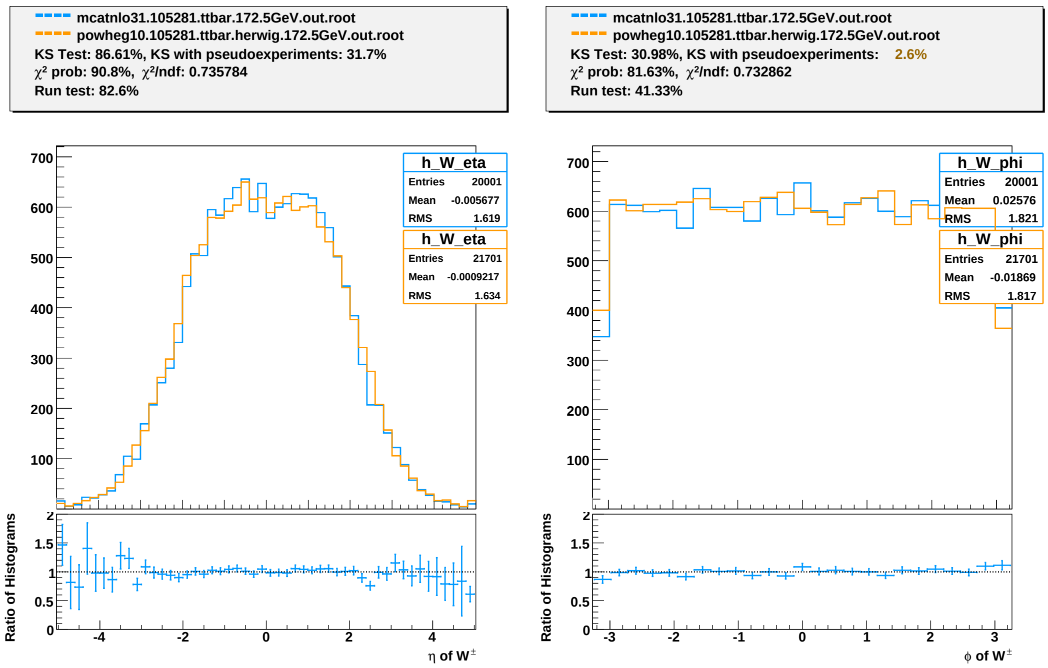

Figure 4: Comparison 2 (MC@NLO vs. POWHEG). Pseudorapidity η (left) and polar angle ϕ (right) of the $W^{\pm}$ bosons.

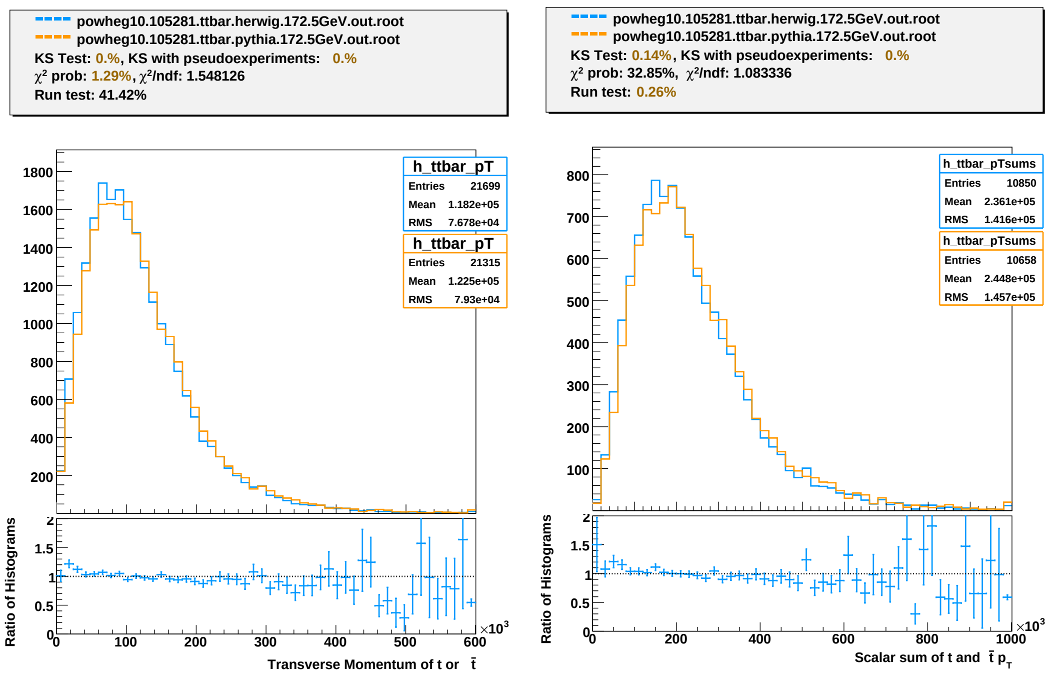

Figure 5: Comparison 3 (HERWIG vs. PYTHIA), showing the transverse momentum p_T of the t and $\bar{t}$ each (left) and their scalar sum (right).

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