Table of Contents

Rivet analysis and standard setup for the comparison of tt+b-jets simulations at NLO

This is the final setup for tt+b-jets simulations (last changes: Sept 24, 2015). Please read everything very carefully before you start the simulations.

An extended Rivet analysis for ttbb production and a new Rivet analysis for the case of top decays as well as a proposal for ttbb MC comparison in the presence of top decays are documented here

Recent changes include:

- list of ATLAS, CMS and theory contact persons that will perform/compare the simulations
- Sherpa, OpenLoops, MG5_aMC@NLO and Pythia versions to be used
- Pythia and Sherpa patches
- detailed instructions and runcards for simulations with Sherpa+OpenLoops and MG5_aMC@NLO
- theory motivated shower settings for consistent comparison of Pythia and Sherpa simulations

First steps

- perform fixed-order LO runs+analysis and share results (for a trivial sanity check)
- same for NLO fixed-order
- move to NLO+PS simulations and share mid statistics results for first assessment before moving to higher statistics

Simulation setup

General goals and motivations (see original proposal for more details)

- precisely defined framework for consistent comparison of different MC simulations (no direct comparison against data)
- omit some layers of MC simulations (see below) to get more transparent picture of QCD mechanism of tt+b-jet production
- simulations done by the MC authors (or under their guidance)
- relevant runcards, Rivet analysis, results will be public
- results will also serve as benchmarks for validation of future tt+HF simulations in ATLAS and CMS
- choice of input parameters, scales, PDFs etc. should be as consistent as possible across the different tools and not necessarily tuned to data: the main aim is a theoretically consistent comparison of the different tools. The optimal choice of parameters for comparing against data will be discussed at a subsequent stage of the study.

Process and heavy flavor treatment

	value	comments
process	pp->ttbb	
collider energy	13 TeV	
flavor scheme	4F scheme	Mb>0 in matrix elements (MEs) and shower
PDFs	NNPDF3.0 4F set with alphaS(MZ)=0.118 (NNPDF30_nlo_as_0118_nf_4)	at variance wit the original proposal (CT10) we now recommend a more recent PDF set. Note that now (July 2015) ATLAS is using CT10 while CMS is using NNPDF3.0
alphaS	from 4F PDFs	requires b-quark loops in 1-loop MEs!! (see below); Note that, for technical reasons, Pythia/Sherpa will use a 5F/4F alphaS beyond the 1st emission
b-quark loops	zero-momentum subtraction (see below)	
t-quark loops	idem	
Mb	4.75 GeV	**Same value should be used in matrix elements and shower!**
Mt	172.5 GeV	At variance with original proposal (173.3 GeV from Tevatron-LHC combination, 1403.4427) we now recommed the value of 172.5!GeV, which is still used in ATLAS and CMS (July 2015). This is consistent with the recent HXSWG recommendation.

Comments:

- NLO PDFs should be used for NLO and LO predictions as well
- Note that to consistently restore b-quark contributions to the alphaS running (to NLO accuracy), b-quark loops have to be included in the MEs and renormalised via zero-momentum subtraction and not in the MSbar scheme. Also top-quark loop contributions to aplhaS need to be renormalised via zero-momentum subtraction in the 4F scheme.

Simulations, tools, runcards and contact persons within TH, ATLAS and CMS

Tools and recommended versions	Sherpa2.1.1+OpenLoops1.2.3	MG5_aMC@NLO 2.3.2 +Pythia8.2.1.0	Powhel+Pythia8.2.1.0

Simulations	SMC@NLO and fixed-order NLO	MC@NLO and fixed-order NLO	NLOPS and fixed-order NLO
Instructions	Sherpa2.1.1+OpenLoops instructions	MG5_aMC@NLO instructions	
Runcards	LO (v1) with Sherpa2.1.1: Run21_ttbjets_LO1.dat NLO (v1) with Sherpa2.1.1: Run21_ttbjets_NLO1.dat !SMC@LO (v1) with Sherpa2.1.1: Run21_ttbjets_SMC1.dat		
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CMS contacts	Marco Harrendorf <marco.harrendorf@cern.ch>	Chris Neu <chris.neu@virginia.edu>, Evan Wolfe <emw5gx@virginia.edu>	
comments	Sherpa2.2.0 is presently under validation and could be used only at a later stage of this study		new Mb>0 simulation recommended but not available yet. A massless simulation requires the technical generation cuts specified below
Requires patches	This Sherpa2.1.1patch (nnpdf_comp.patch) fixes a compatibility issue with 4F NNPDFs. This Sherpa2.1.1 patch (local_psi_itmin.patch) allows one to strongly improve grid optimisation. Both modifications will be implemented in Sherpa 2.2.	This Pythia8 patch (BeamParticle.cc), which will enter the next Pythia 8 release, fixes a compatibility issue with NNPDF/LHAPDF6	

Generation cuts

- **No generation cuts** should be applied in the 4F scheme (full b-quark phase space accessible)
- **Powhel/Powheg** authors are encouraged to provide a NLO+PS implementation with Mb>0. Alternatively they can provide predictions with Mb=0 using the technical generation cuts M_bb>2*xi*Mb and pT_b>xi*Mb, and varying the parameter xi in the range [0.5,1].

Scale choice

scale	scale1	scale2

renormalisation	<ET>_geom (as defined below)	The alternative proposal of using HT/2 was discarded based on the arguments reported here
factorisation	HT/2	
resummation	HT/2	

Comments:

- the proposed (CKKW inspired) renormalisation scale choice is the one of ArXiv:1309.5912; <ET>_geom is the geometric average of the transverse energy of the top, anti-top, bottom and anti-bottom quarks defined **at parton level (in terms b-quarks and not of b-jets)**;
- at variance with 1309.5912, for the factorisation and resummation scales we choose HT/2, where HT is defined at parton level as the sum of the transverse energies, ET=Sqrt(M^2+pT^2), of all final-state partons: top, anti-top, bottom, anti-bottom plus possibly one additional final-state parton at NLO.
- the standard choice of resummation scale (muQ) in MG5_aMC@NLO is based on a smearing procedure with a distribution f1*ECM<muQ<f2*ECM with f1=0.1, f2=1.0, ECM=partonic Born CM energy. The distribution is strongly peaked at (f1+f2)/2. This procedure is reasonably close to the proposed choice muQ=HT/2. However an exact implementation of muQ=HT/2 in MG5_aMC@NLO would allow for a more consistent comparison.
- in the case of Powhel, to achieve a qualitative consistency with the above choice of resummation scale, the h_damp parameter should be set equal to HT/2. It should be possible to set such a dynamical h_damp factor my adapting the Bornzerodamp.f routine. Alternatively a fixed factor h_damp=Mt could be used.

Scale and PDF variations

Idea: we start with standard factor-2 variations around a default scale choice. Alternative dynamic scales will be considered at a later stage

- (muR,muF) rescaling factors: (0.5,0.5), (0.5,1),(1,0.5),(1,1),(1,2),(2,1),(2,2).
- Resummation scale: in MG5_aMC@NLO+Pythia and Sherpa+OpenLoops the resummation scale (shower starting scale) should be varied up and down by a factor 2, while keeping (muR,muF) fixed. Similar factor-2 variations should be applied to the shower starting scale and to h_damp in Powheg.
- PDF variations: they represent a negligible source of uncertainty (wrt the ~30% variation dominated by muR) and we will consider them only in a later stage of this study. But if desired, they can be evaluated starting from the first generation runs.

ttbb simulations and analyses should be performed at the following (idealised) level

	on/off	comments
parton shower	on	
hadronisation	off	see comments and technical study below
UE	off	
top decays	off	in order to focus on the QCD mechanism of b-jet production

Hadronisation effects in Pythia8 vs Sherpa2.1

A preliminary LO+PS study has been performed in order to check if turning off hadronisation might bias the comparison of simulations based on different showers. The results indicate that, as far as b-jet observables are concerned, hadronisation effects in Pythia8 and Sherpa2.1 are moderate and reasonably similar. This suggests that neglecting hadronisation effects should not bias the comparison in a problematic way.

Parton shower tune and alphaS running

- since parton-shower tunes and PDFs are intimately connected it is not trivial to identify a common PDF set that is optimal for all parton showers. For the first phase of this study the NNPDF3.0 will be adopted, keeping in mind that this choice might bias the comparison of the different showers.

- The 4F evolution of alphaS and the value of alphaS(MZ)=alphaS_4F(MZ) as provided by the PDFs should be used both in the matrix elements and in the parton shower, at least at the level of the first emission.
  For the subsequent emissions, the parton shower can use also the five-flavour scheme and a corresponding alphaS_5F(MZ) value. In any case one should not use alphaS_4F(MZ) in combination with 5F-running.
- In general, Sherpa and Pythia adopt different tunings for the ISR and FSR factors (x_ISR,x_FSR) applied to the parton-shower alphaS-scale, alphaS(x*kT^2). The possibility of an additional Catani-Marchesini-Webber (CMW) rescaling factor for the resummation of subleading logarithms is another possible source of differences between Pythia and Sherpa. For a more consistent comparison we recommend to switch off such "tunings" and to synchronise the the alphaS evolution as indicated in the following table:

Tool	extra shower settings	x_ISR	x_FSR	CMW	alphaS running
Sherpa+OpenLoops		1.0	1.0	off	2-loops
MG5_aCM@NLO+Pythia8		1.0	1.0	off	2-loops
Powhel+Pythia8		1.0	1.0	off	2-loops

The above settings are implemented in the Sherpa runcards (see links above). For Pythia they can be implemented as follows in Pythia8 command file:

```
SpaceShower:alphaSuseCMW = off
TimeShower:alphaSuseCMW = off

SpaceShower:alphaSvalue = 0.118
TimeShower:alphaSvalue = 0.118

SpaceShower:renormMultFac = 1.0 # (x_ISR)
TimeShower:renormMultFac = 1.0 # (x_FSR)

SpaceShower:factorMultFac = 1.0 # (x_ISR)
TimeShower:factorMultFac = 1.0 # (x_FSR)

SpaceShower:alphaSorder = 2
TimeShower:alphaSorder = 2
```

Note that these settings neither correspond to the Sherpa default nor to the Pythia default settings. Moreover they are not expected to provide an optimal description of data. They are aimed at a consistent comparison of the two showers, where simple parametric differences are avoided, and the remaining deviations can be attributed to intrinsic shower features, such as the parametrisation of the shower evolution variables.

Analysis

b-jet definition and event categorisation

	value	comment	status
Jet algorithm	anti-kT, R=0.4, full 4-momentum recombination	only light- and b-jets with eta<2.5 are considered	
b-jet	a jet containing one or more b-quarks among its constituents	**no pT-threshold for b-quarks inside b-jets**	
Nb	# of b-jets with pT>25 GeV and eta<2.5 (no top decays here!)	to be used for event categorisation	

Comments:

- to be considered/discussed: an additional analysis including hadronisation and a corresponding particle-level definition of b-jets. This requires a precise definition of b-jet tagging at particle level. Comparing parton- an particle-level analyses would allow one to clarify if hadronisation has a significant impact on the production of tt+b-jets or not.

Observables

The following observables should be analysed for two subsamples with Nb>=1 and Nb>=2. Notation: t1/t2 =1st/2nd top-quark; b1/b2 =1st/2nd b-jet; j1=1st non-b jet

- integrated Nb>=1 and Nb>=2 cross sections
- pT in [0,400] GeV for j1,b1,b2,b1b2,t1,t2,ttbar
- eta in [-4,4] for j1,b1,b2,b1b2,t1,t2,ttbar
- M(i,j) in [0,400] GeV for (j1,b1), (j1,b2), (b1,b2)
- DeltaR(i,j) in [0,5]for (j1,b1), (j1,b2), (b1,b2)

Format and public Rivet implementation:

- 20 bins per histogram
- Here one can find a public Rivet implementation of the above analysis (hxswg_ttbjets_part_v1.cc and hxswg_ttbjets_part_v1.plot files), as well as an example of the resulting plots (for a LO+PS simulation). Note that the original hxswg_ttbjets_part_v1 implementation was upgraded to an equivalent hxswg_ttbjets_part_v1b version that fixes compatibility issues with Rivet >2.2.1.
- to facilitate the comparison we recommend to exchange results in YODA format

Aspects that might be postponed to a 2nd stage of the comparison or included from the beginning

- more b-jet categories or observables that are sensitive to g->bb splittings inside jets

Mailing lists

Blue=Contact persons for simulations (see table above); Black=other interested people

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