Status of Single-Top Generators

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CERN theory group

CMS Single-Top Workshop, Napels, 19-20 December, 2013

NLO IS THE NEW STANDARD

- NLO calculations are completely automated
- (almost) as easy to use as LO
- The only public code that can generate unweighted events at NLO in QCD consistently matched to the parton shower is MadGraph5_aMC@NLO
- These should be(come) the new standard tools; uncertainties reduced compared to LO MC predictions

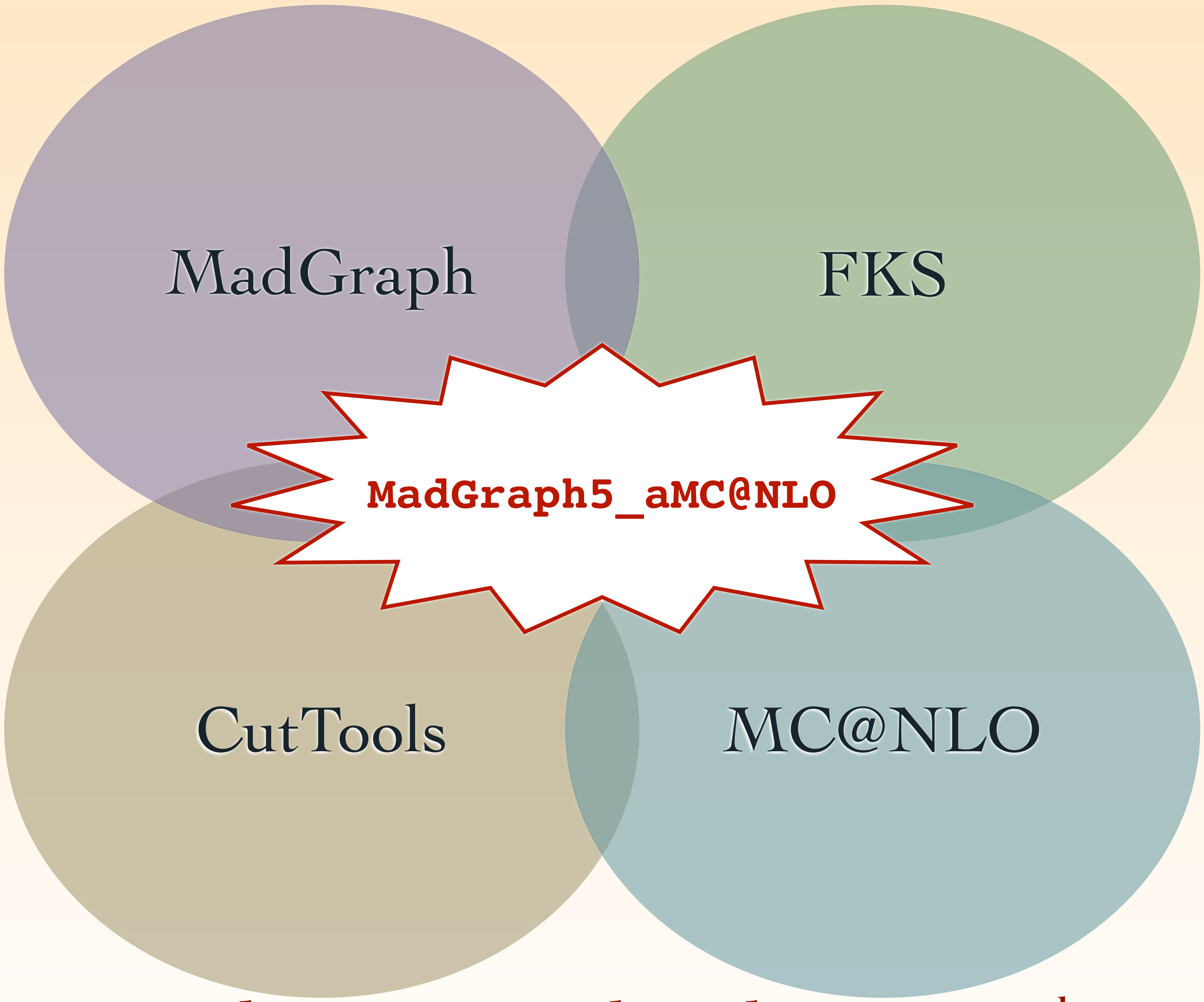
New code released

- MadGraph5 and aMC@NLO have joined forces. Last Monday's release of the code contains both MadGraph5 and aMC@NLO and is therefore called:

MadGraph5_aMC@NLO

- It has all the current features of MadGraph5 and aMC@NLO, in addition to some new ones

MadGraph5_aMC@NLO joint venture



Non-beta version released on Dec. 16th

(NLO) features

- All the tree-level/LO functionalities in the SM and BSM of MadGraph5
- Fully automatic computation of NLO corrections in QCD (loop, real, counterterms) for any SM process
- Fully automatic event generation at the NLO, matched to Pythia8, Herwig++, Herwig6, Pythia6(Q2), Pythia6(pt, ISR only) according to the MC@NLO formalism
- Very significant improvements in speed and efficiency wrt the beta version of aMC@NLO, leading basically to the possibility of computing at NLO in QCD any SM process up to 2 -> 4 at the Born level
- Automatic computation of scale and pdf uncertainties at NLO and MC@NLO level at no extra computational cost
- Support of the LHE format v3.0 with reweighting information for uncertainties as well as for parameter scanning
- A much more flexible and complete user interface, including an easy-to-use analysis framework for fixed-order NLO computations
- Semi-automation of the FxFx multi-parton merging at NLO with HERWIG6

Speed improvements

Madgraph5 2.0.0beta3

```
Summary:
Process p p > t t~ [QCD]
Run at p-p collider (4000 + 4000 GeV)
Total cross-section: 1.770e+02 +- 1.7e+00 pb
Ren. and fac. scale uncertainty: +13.5% -13.0%
Number of events generated: 10000
Parton shower to be used: HERWIG6
Fraction of negative weights: 0.16
Total running time : 12m 12s

DEBUG:
Number of loop ME evaluations: 168120
```

Madgraph5_aMC@NLO

```
Summary:
Process p p > t t~ [QCD]
Run at p-p collider (4000 + 4000 GeV)
Total cross-section: 1.765e+02 +- 9.2e-01 pb
Ren. and fac. scale uncertainty: +12.2% -12.3%
Number of events generated: 10000
Parton shower to be used: HERWIG6
Fraction of negative weights: 0.16
Total running time : 1m 35s

DEBUG:
Number of loop ME evaluations (by MadLoop): 6967
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N.A.

MadGraph5_aMC@NLO

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```

```
Summary:
Process p p > t b t~ b~ [QCD]
Run at p-p collider (4000 + 4000 GeV)
Total cross-section: 2.671e+00 +- 1.2e-02 pb
Ren. and fac. scale uncertainty: +39.1% -27.8%
Number of events generated: 200000
Parton shower to be used: HERWIG6
Fraction of negative weights: 0.29
Total running time : 17h 0m
Sequential running time : ~ 6 days

DEBUG:
   Number of loop ME evaluations (by MadLoop): 367802
```

4 flavour, no cuts

MadGraph5_aMC@NLO example

	LO	NLO
Start the python interface	./bin/mg5	./bin/mg5
Generate a process	generate p p > t t~ w+	generate p p > t t~ w+ [QCD]
write the process to disk	output MY_TTW_PROC	output MY_TTW_NLOPROC
start the event generation	launch unweighted events	launch unweighted events up to a sign
Accuracy	LO + PS	NLO + PS

Which processes can I generate at NLO?

- Any SM process you are interested in...
  - The only thing to keep in mind is that NLO processes are a lot more complicated than the corresponding LO process (so, do not try to do ttbar+3jets @ NLO...)

Which processes can I generate at NLO?

- p p > t t~ [QCD]
- p p > t t~ j [QCD]
- p p > t t~ h [QCD]
- p p > t t~ z [QCD]
- p p > t t~ t t~ [QCD]
- p p > t t~ w+ a [QCD]
- p p > t t~ b b~ [QCD]
- ...

- p p > t b~ [QCD]
- p p > t j $$ w+ [QCD]
- p p > t b~ j $$ w+ [QCD]
- p p > t b~ h $$ w+ [QCD]
- p p > t j z $$ w+ [QCD]
- p p > t j a $$ w+ [QCD]
- ...

- All possible with aMC@NLO on a multi-core desktop machine

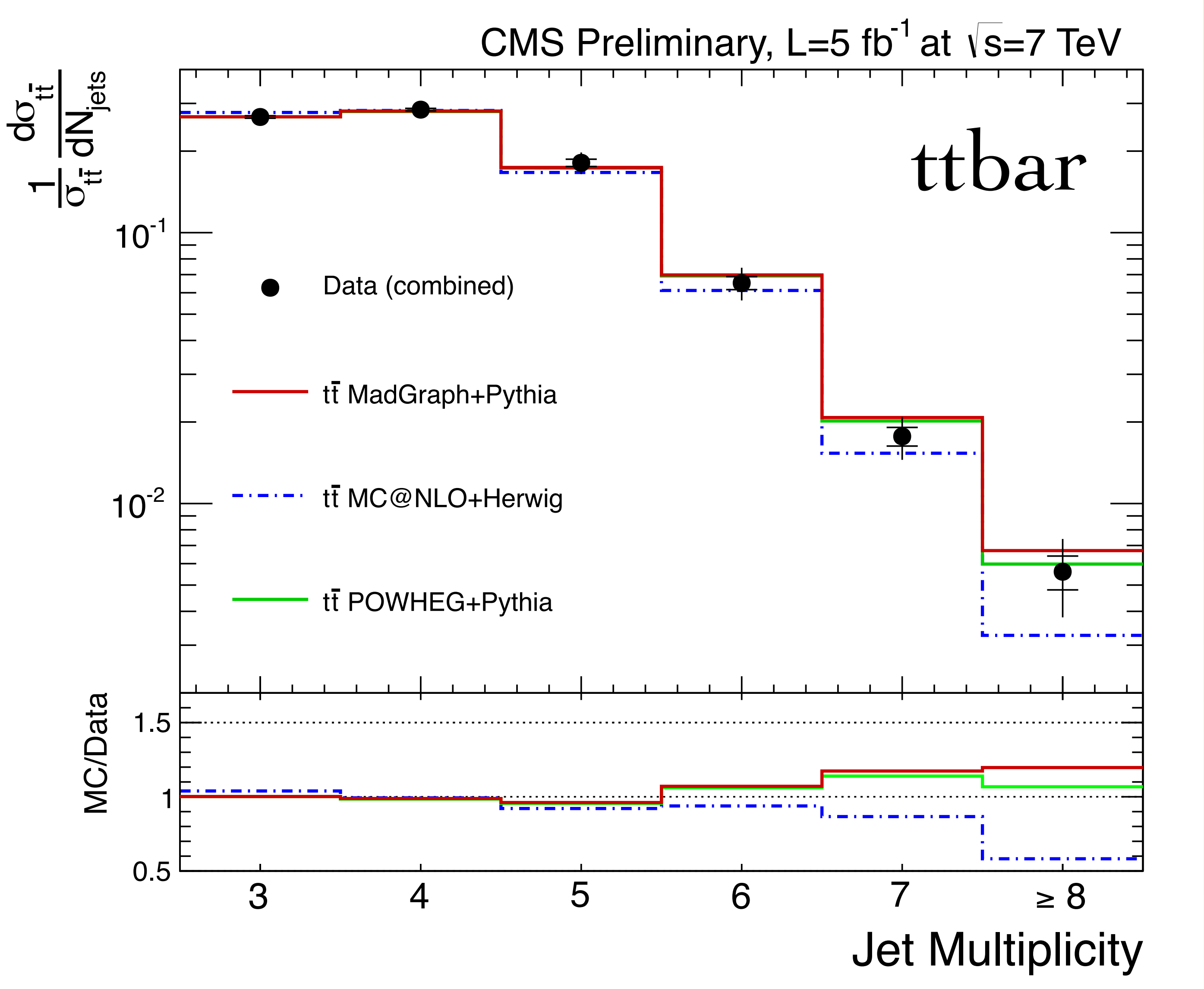
  "$$ w+" means to forbid W^+-bosons to appear in the s-channel; in general not gauge invariant, so use with extreme care

Further subtlety

- There is another class of processes for which QCD NLO corrections cannot simply be included
- In general, QCD NLO corrections to an EW process are of the same order as EW NLO corrections to a QCD process
  - In general, one cannot disentangle them and both need to be included for consistency
  - But NLO EW corrections are usually not available; at least not in the codes that aim for full automation of NLO+PS
    - although, implementation in MadGraph5_aMC@NLO has started
- Possibly a problem for single top production because it is an EW process, but there is no equivalent QCD process so it's okay in most cases (we'll see an example later where some tricks were needed)

When to use NLO+PS

- It makes only sense to NLO corrections if the observable is sensitive to those corrections.
- Otherwise it is just a waste of time and one might as well use stand-alone Pythia or Herwig

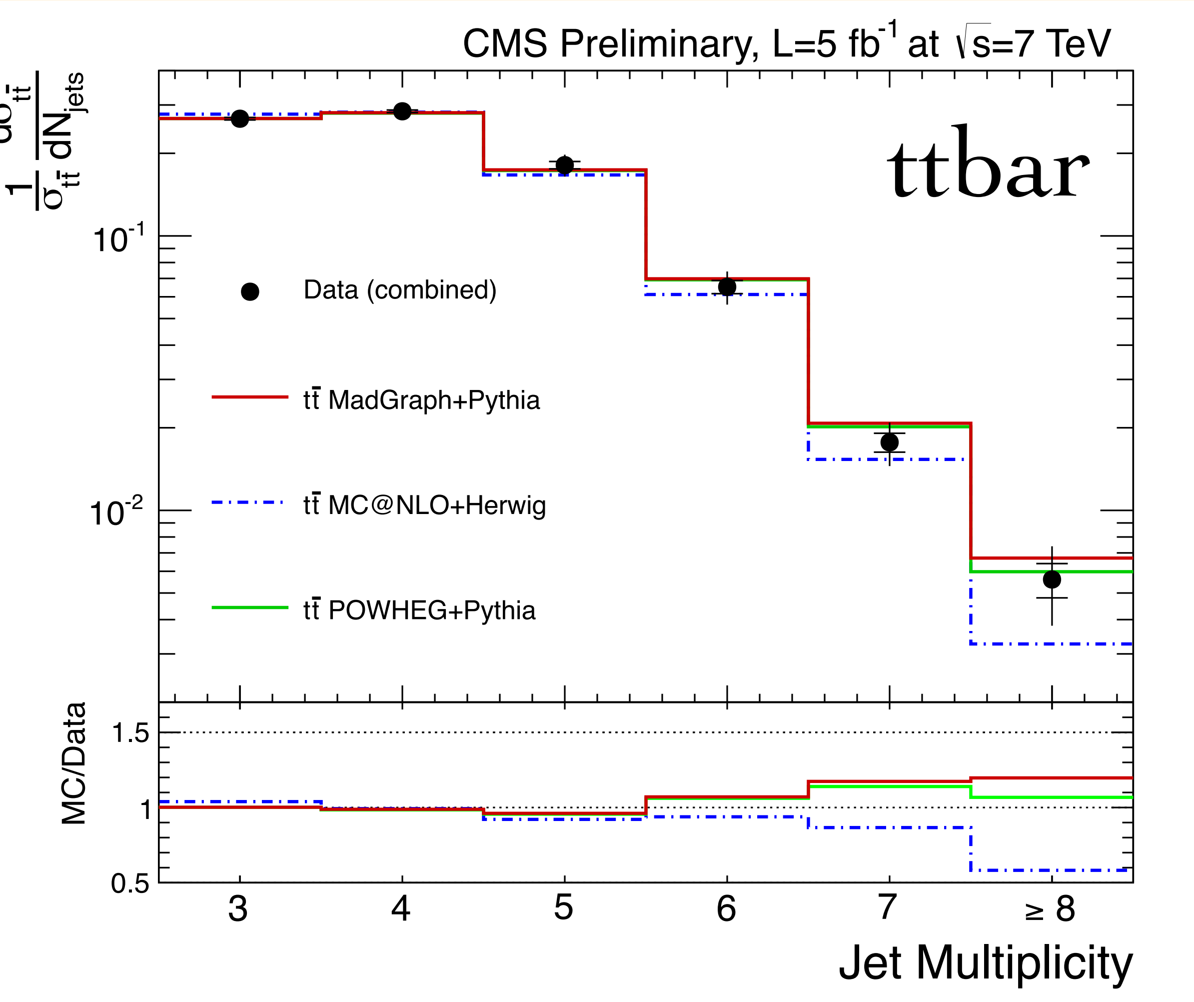


Uncertainty estimates

- For observables that have NLO precision, the theory/generator uncertainties can be estimated by
  - Independent renormalisation and factorisation scale variations
  - PDF error sets (preferably following the PDF4LHC agreement)
  - Matching an NLO computation to at least 2 different parton showers
  - These PDF and scale variations can be obtained via reweighting in MG5_aMC@NLO and POWHEG, not yet possible in Sherpa.
- For observables that do not have NLO precision, further uncertainties are coming from the shower starting scale ("Power" or "Wimpy" shower). Currently these cannot be approximated with the (a)MC@NLO program, but not really relevant because why use an NLO+PS computation for these observables in the first place?
  They can be estimated more correctly in the NLO Sherpa program.

NLO corrections to higher Multiplicities

- For this example/observable there is a straight-forward way of also getting (some of) the higher multiplicity bins at NLO accuracy:



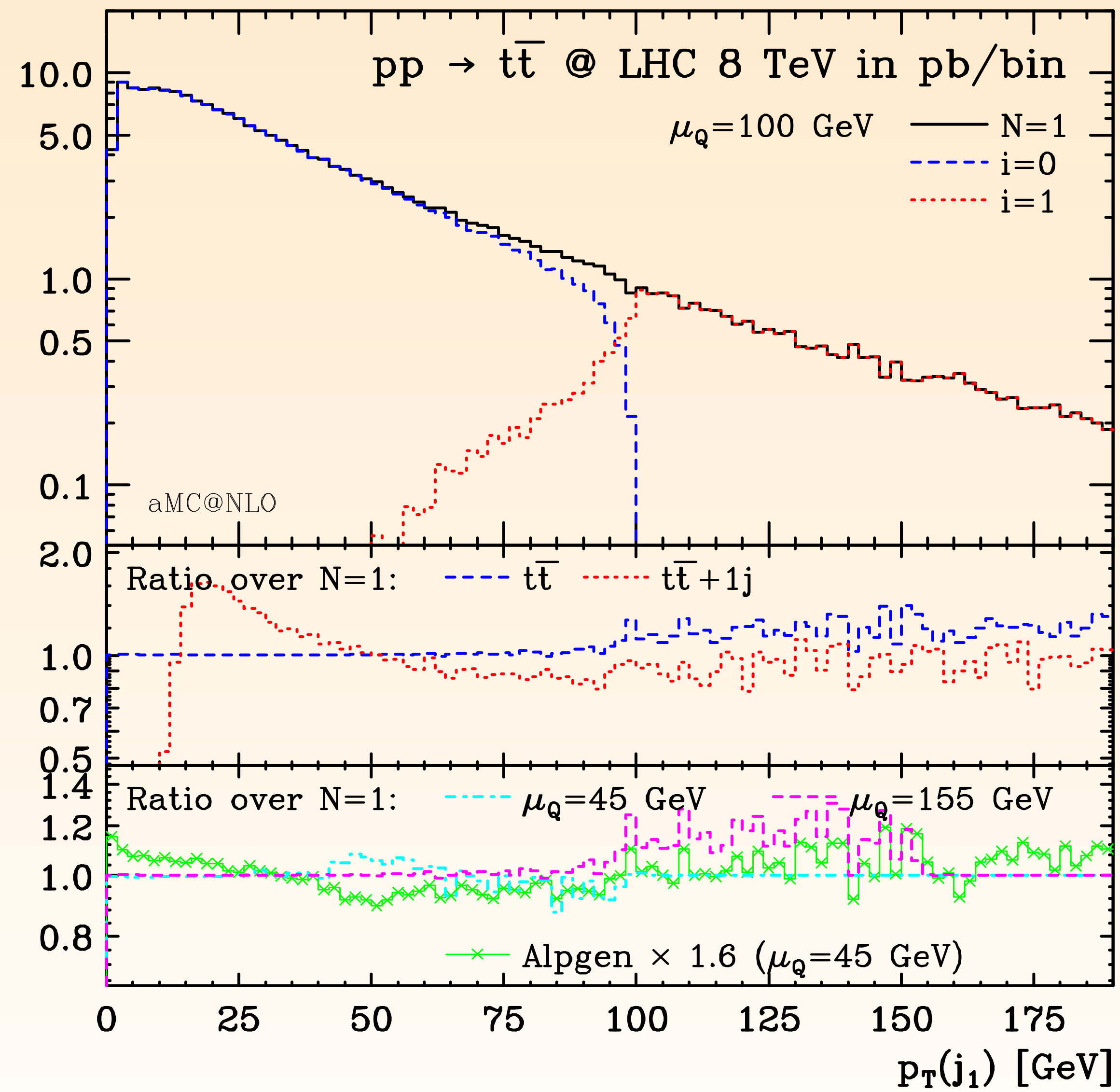
- Compute NLO corrections to ttbar+jet or ttbar+2jets and match that calculation to the shower.
- This requires a generation cut, otherwise the process diverges, and it should be check that the final results are independent from the generation cut
- This will also work for single top+jets or any other processes

Single-top + jet

- Single-top + jet production is not straight-forward
  - QCD and EW corrections do no longer completely factorize
  - Need to include loops with W-boson as propagator
  - Not a pure QCD correction, so not (yet) possible with MadGraph5_aMC@NLO in a completely automated way

Extending NLO accuracy over more than one multiplicity

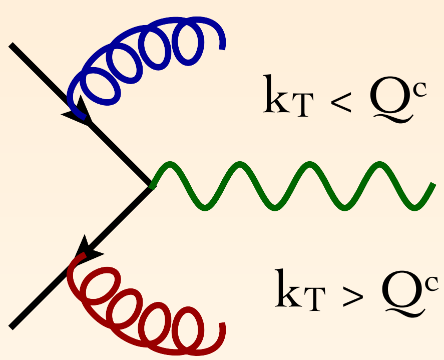
- Using a special procedure ('FxFx' or 'MEPS@NLO' or 'MINLO' or 'UNLOPS' or 'some other acronym') NLO accuracy can be extended over more than one multiplicity.
- **This only works for processes that do not have matrix element jets at the lowest multiplicity Born matrix elements**
  (ttbar is okay, single top isn't)



Merging ME with PS: LO case

CKKW and MLM

- Use tree-level matrix elements of various multiplicities to generate hard radiation, and the parton shower for the collinear and soft: at LO this has been solved ~10 years ago
- Double counting no problem: we simply throw events away when the matrix-element partons are too soft, or when the parton shower generates too hard radiation
- Applying the matrix-element cut is easy: during phase-space integration, we only generate events with partons above the matching scale



- For the cut on the shower, there are two methods. Throwing events away after showering is not very efficient, although it is working ("MLM method")
- Instead we can also multiply the Born matrix elements by suitable product of Sudakov factors (i.e. the no-emission probabilities) $\Delta(Q^{max}, Q^c)$ and start the shower at the scale Q^c ("CKKW method"):
- For a given multiplicity we have $\sigma_{n,\mathrm{excl}}^{\mathrm{LO}} = B_n \Theta(k_{T,n} - Q^c) \Delta_n(Q_{\mathrm{max}}, Q^c)$

Merging at NLO

- To make a LO prediction exclusive in the number of jets, we need to multiply it by a Sudakov damping factor; this is CKKW method:

$$\sigma_{n,\text{excl}}^{\text{LO}} = B_n \Theta(k_{T,n} - Q^c) \Delta_n(Q_{\text{max}}, Q^c)$$

  This makes the prediction exclusive at leading logarithmic accuracy

- Similarly we can make an NLO prediction exclusive at leading logarithm

$$\sigma_{n,\text{excl, LL}}^{\text{NLO}} = \left\{ B_n + V_n + \int d\Phi_1 \, R_{n+1} \right\} \Theta(k_{T,n} - Q^c) \Delta_n(Q_{\text{max}}, Q^c)$$

- We can improve here and use the real-emission matrix elements instead of just the Sudakov:

$$\sigma_{n,\text{excl, LL}}^{\text{NLO}} = \left\{ B_n + V_n + \int_0^{Q^c} d\Phi_1 \, R_{n+1} - B_n \Delta_n^{(1)}(Q_{\text{max}}, Q^c) \right\} \Theta(k_{T,n} - Q^c) \Delta_n(Q_{\text{max}}, Q^c)$$

Exclusive MC@NLO

- Converting the NLO exclusive predictions in the number of jets to the **MadGraph5_aMC@NLO event generation** is straight-forward:

$$\mathbb{S}\text{-events:} \qquad \left\{ B_n + V_n + \int_0^{Q^c} d\Phi_1 \, \mathrm{MC} - B_n \Delta_n^{(1)}(Q_{\mathrm{max}}, Q^c) \right\}$$
$$\Theta(k_{T,n}^B - Q^c)\Delta_n(Q_{\mathrm{max}}^B, Q^c)$$

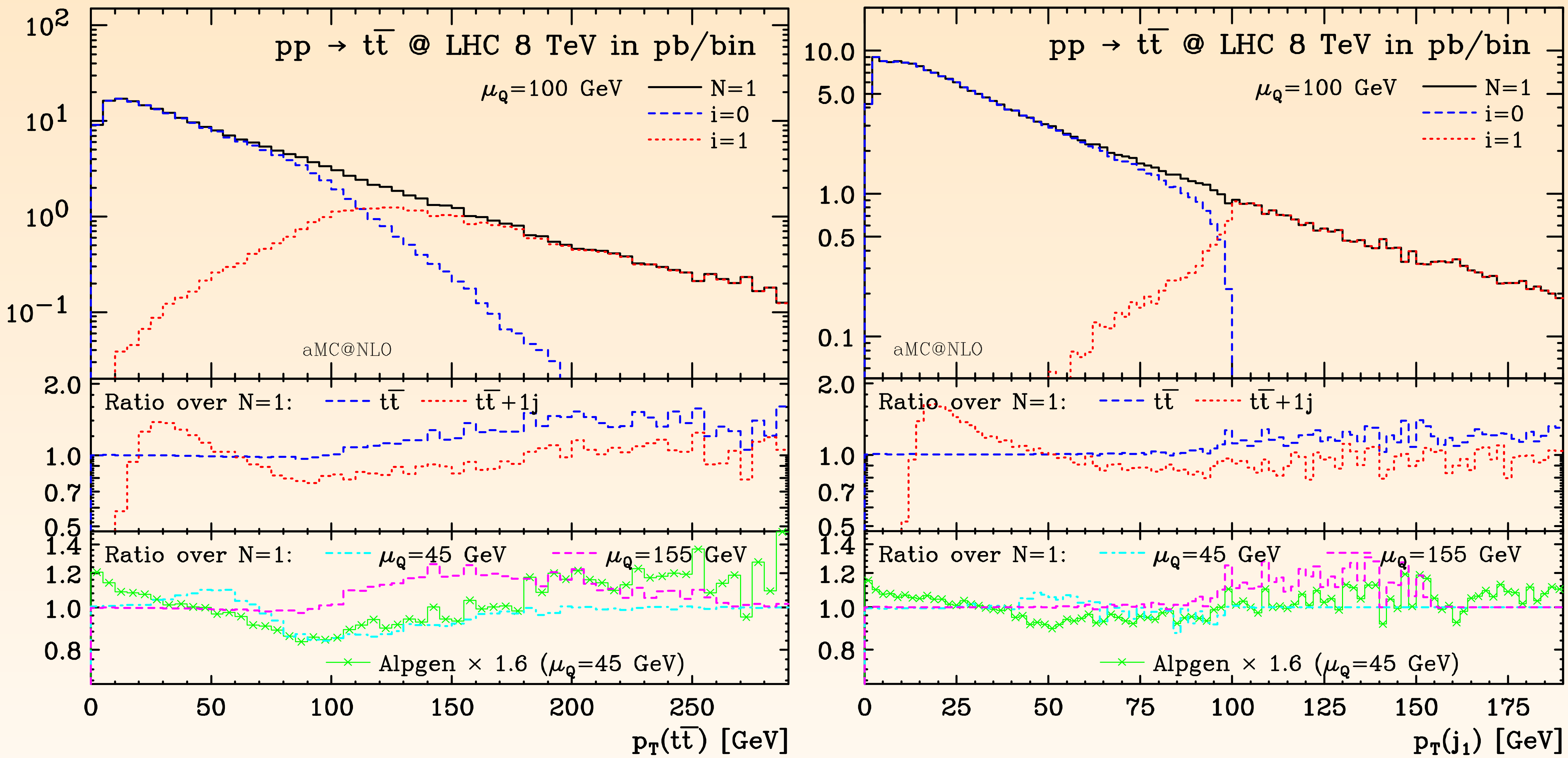
$$\mathbb{H}\text{-events:} \qquad \left\{ R_{n+1}\Theta(k_{T,n}^R - Q^c) - \mathrm{MC}\,\Theta(k_{T,n}^B - Q^c) \right\}$$
$$\Theta(Q^c - k_{T,n+1}^R)\Delta_n(Q_{\mathrm{max}}^R, Q^c)$$

- **Merging in Sherpa works very similarly**

- It is not clear how the MiNLO description in POWHEG ("merging without merging scale") can be extended to processes with more than 3 colored particle (like ttbar production)

FxFx merging at NLO with aMC@NLO

RF & Frixione arXiv:1209.6251

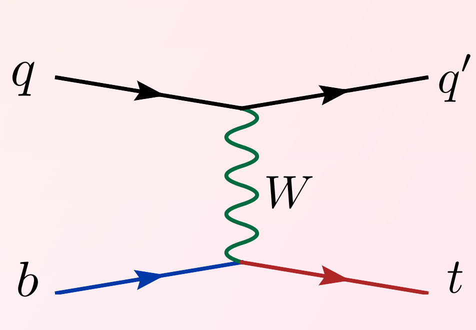
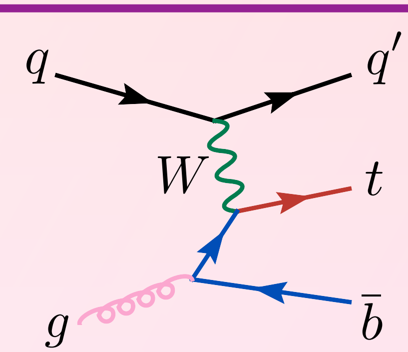
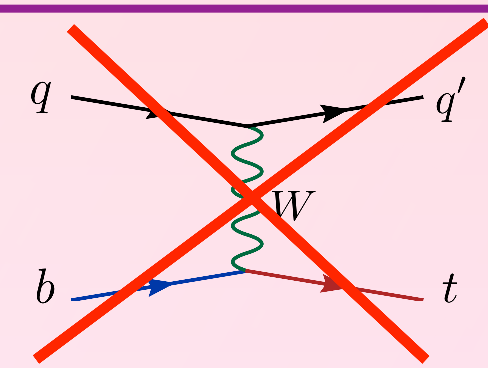
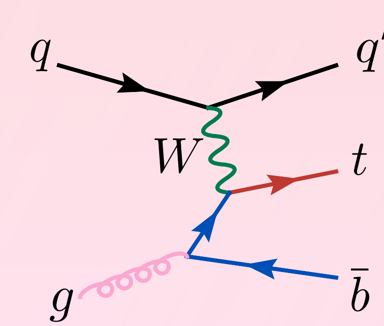


- Agreement with ttbar+0j at MC@NLO and ttbar+1j at MC@NLO in their respective regions of phase-space
- Smooth matching in between
- Small dependence on matching scale

FxFx merging

- Semi-automated in MadGraph5_aMC@NLO for HERWIG6; Pythia8 to come soon (with a higher level of automation)
  See http://amcatnlo.cern.ch/FxFx_merging.html for details
- Inclusion of the NLO ttbar+2j possible, although at the limit of what is currently possible with the MadGraph5_aMC@NLO code
- W+0,1,2,3 jets @NLO also possible
- Unfortunately, single top not (yet), because of the light jet at the lowest-multiplicity Born

4- & 5-flavor schemes

2 ways of making predictions	
5 flavour scheme	**4 flavour scheme**
massless b	massive b
PDF includes initial state b quarks	No b quarks in PDF
$\mathrm{Log}[m_b/\mu_F]$ resummed in PDF	Finite terms correctly included
Simpler calculation	More involved prediction
 leading order  (contribution to) NLO	 Does not exist  (part of) leading order
Descriptions are equivalent when including all orders in perturbation theory	

Uncertainties

- Estimate of the theory uncertainty:
  - independent variation of renormalization and factorization scales by a factor 2
  - 44 eigenvector CTEQ6.6 PDF's
  - Top mass: 172 ± 1.7 GeV (sorry, it's a bit of an old table!)
  - Bottom mass: 4.5 ± 0.2 GeV
- Uncertainties from scales slightly larger in 4F (as expected)
- Other sources are comparable in size
- Don't forget the uncertainty from the bottom quark mass uncertainty!

$\sigma^{\mathrm{NLO}}_{\mathrm{t-ch}}(t+\bar{t})$	$2 \to 2$ (pb)					$2 \to 3$ (pb)				
Tevatron Run II	1.96	$^{+0.05}_{-0.01}$	$^{+0.20}_{-0.16}$	$^{+0.06}_{-0.06}$	$^{+0.05}_{-0.05}$	1.87	$^{+0.16}_{-0.21}$	$^{+0.18}_{-0.15}$	$^{+0.06}_{-0.06}$	$^{+0.04}_{-0.04}$
LHC (7 TeV)	62.6	$^{+1.1}_{-0.5}$	$^{+1.4}_{-1.6}$	$^{+1.1}_{-1.1}$	$^{+1.1}_{-1.1}$	59.4	$^{+2.1}_{-3.4}$	$^{+1.4}_{-1.4}$	$^{+1.0}_{-1.0}$	$^{+1.3}_{-1.2}$
LHC (14 TeV)	244	$^{+5}_{-4}$	$^{+5}_{-6}$	$^{+3}_{-3}$	$^{+4}_{-4}$	234	$^{+7}_{-9}$	$^{+5}_{-5}$	$^{+3}_{-3}$	$^{+4}_{-4}$

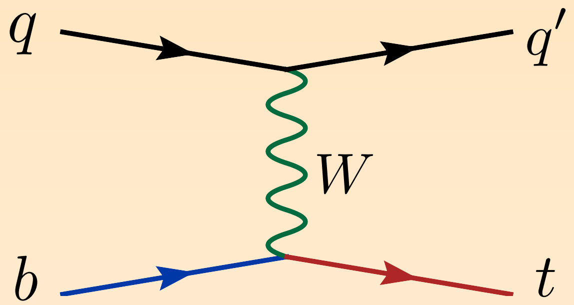
Fac. & Ren. scale

PDF

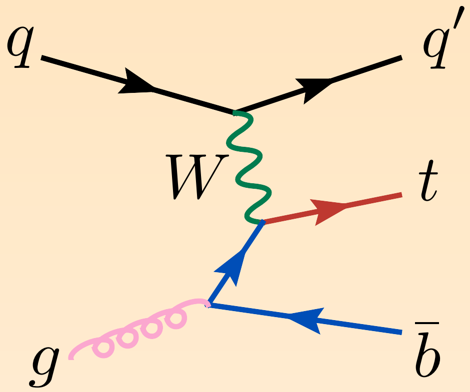
top mass

b mass

T-CHANNEL SINGLE TOP PRODUCTION



5-flavor scheme: “2 ➞ 2”

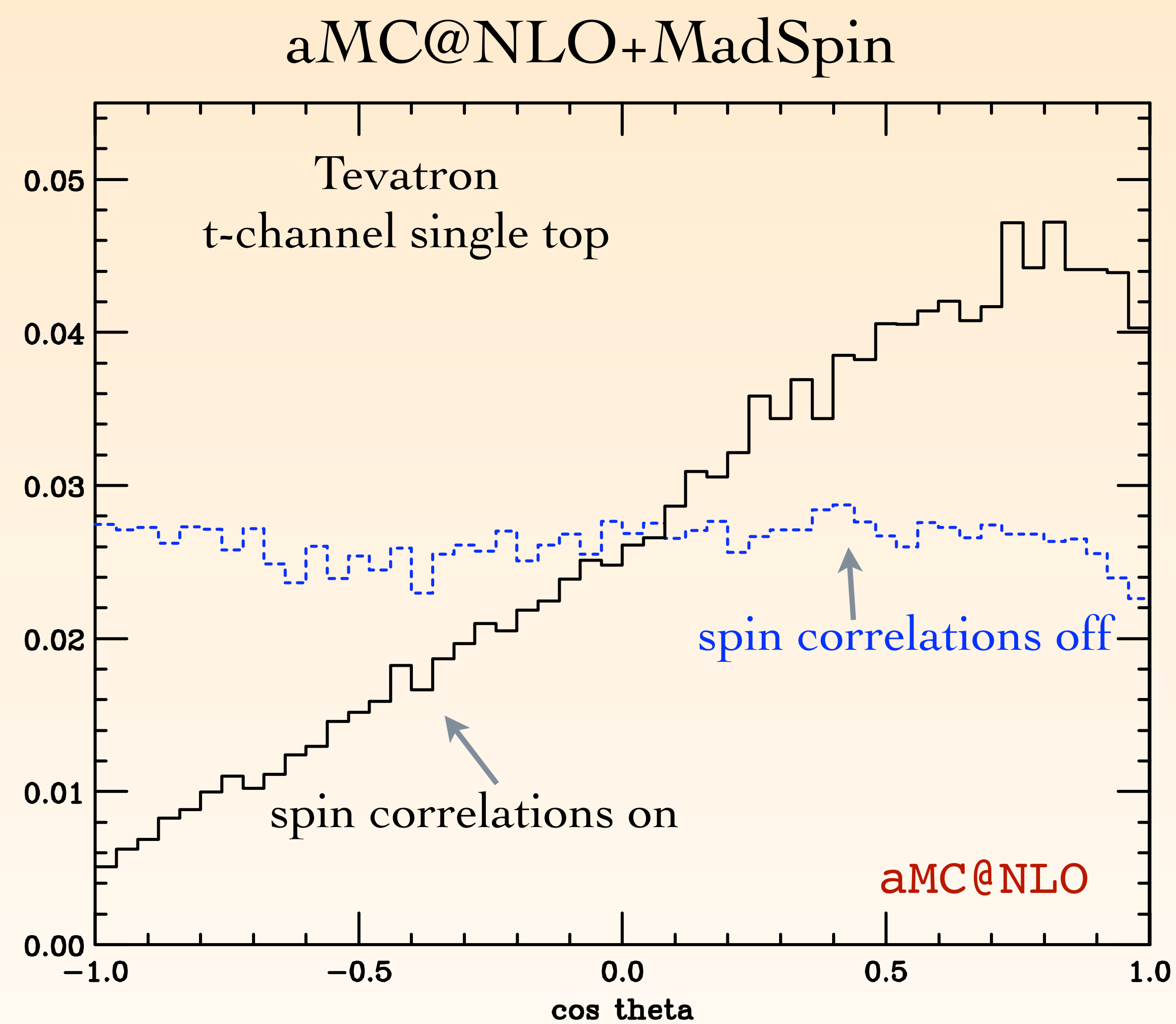


4-flavor scheme: “2 ➞ 3”

- Not (yet) known how to do this merging at NLO for single top processes: jets at the Born need special treatment
- Best available option for t-channel single top is the 4-Flavor scheme at NLO, matched to parton shower, but normalized to the inclusive NLO 5F scheme calculation
  - All kinematics of the top, the light jet and **the “spectator b-quark”** are NLO correct because of the 4 flavour scheme
- Recently, a detailed comparison between POWHEG and aMC@NLO appeared [RF, Re, Torrielli arXiv:1207.5391]
- Spin correlations can be included using MadSpin (which can also be used for POWHEG events, after some trivial changes in the header of the event file)

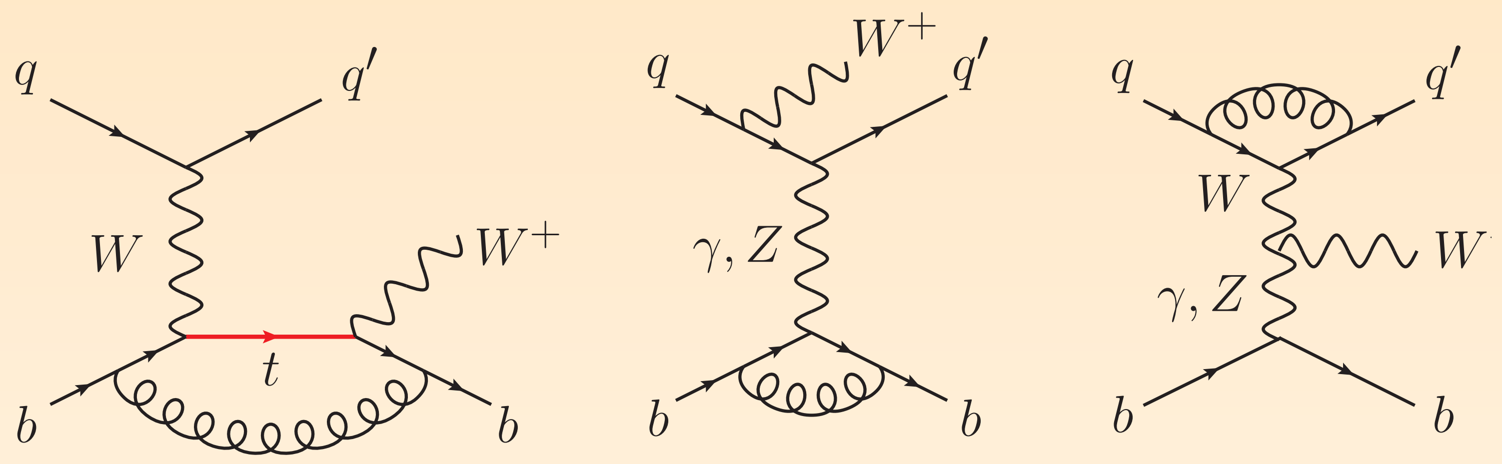
Spin correlations: MadSpin

- In MadGraph5_aMC@NLO, spin correlations can be included using MadSpin
  - Uses only tree-level information
  - Includes some off-shell effects
- Also POWHEG events can be decayed with MadSpin this way (when not directly available in POWHEG, i.e. single top 4 flavour), although some MadGraph-style information should be added to the header of the event file to tell MadSpin the process definition and all that.



[Artoisenet, RF, Mattelaer, Rietkerk '12]

Off-shell single top

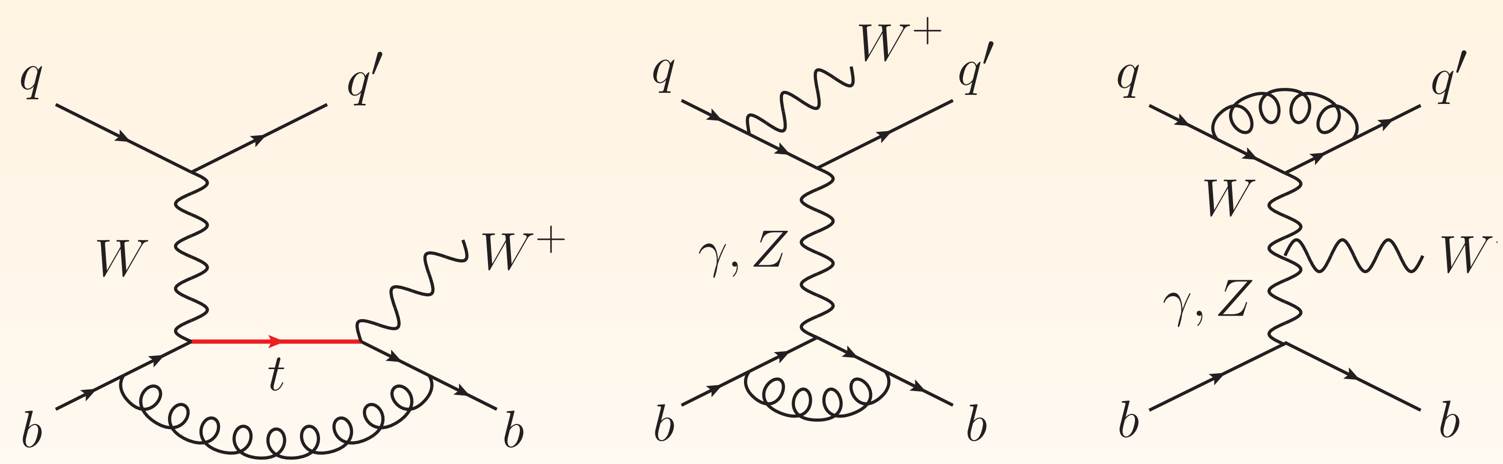


- To include the full NLO spin correlations, as well as all the all off-shell effects, the complete set of diagrams are needed
- Not really possible for single top in the 4 flavour scheme, because of the EW nature of the single top process, QCD corrections mix with the EW corrections to a corresponding QCD process

Process definition

Papanastasiou, RF, Frixione, Hirschi, Maltoni arXiv:1305.7088

- Particular care needed in process definition: $p\,p \to W^+\,J_b\,J_{\mathrm{light}} + X$
  - Single top production is EW process. In general QCD corrections to an EW process cannot be disentangled from EW corrections to a QCD process
    - Need to use diagonal CKM matrix (at least for the 3rd generation) to prevent interference from QCD Born with EW Born. Only possible for 5F scheme calculations, not possible in the 4F scheme.
  - Setting V_{tb}=1 also allows for separation of t and s-channel contributions (which results in easier comparison with literature)
  - With decays, the process is not finite: need a cut on the b-jet
    - s-channel could be included in our approach bur requires that J_b does not include two b quarks



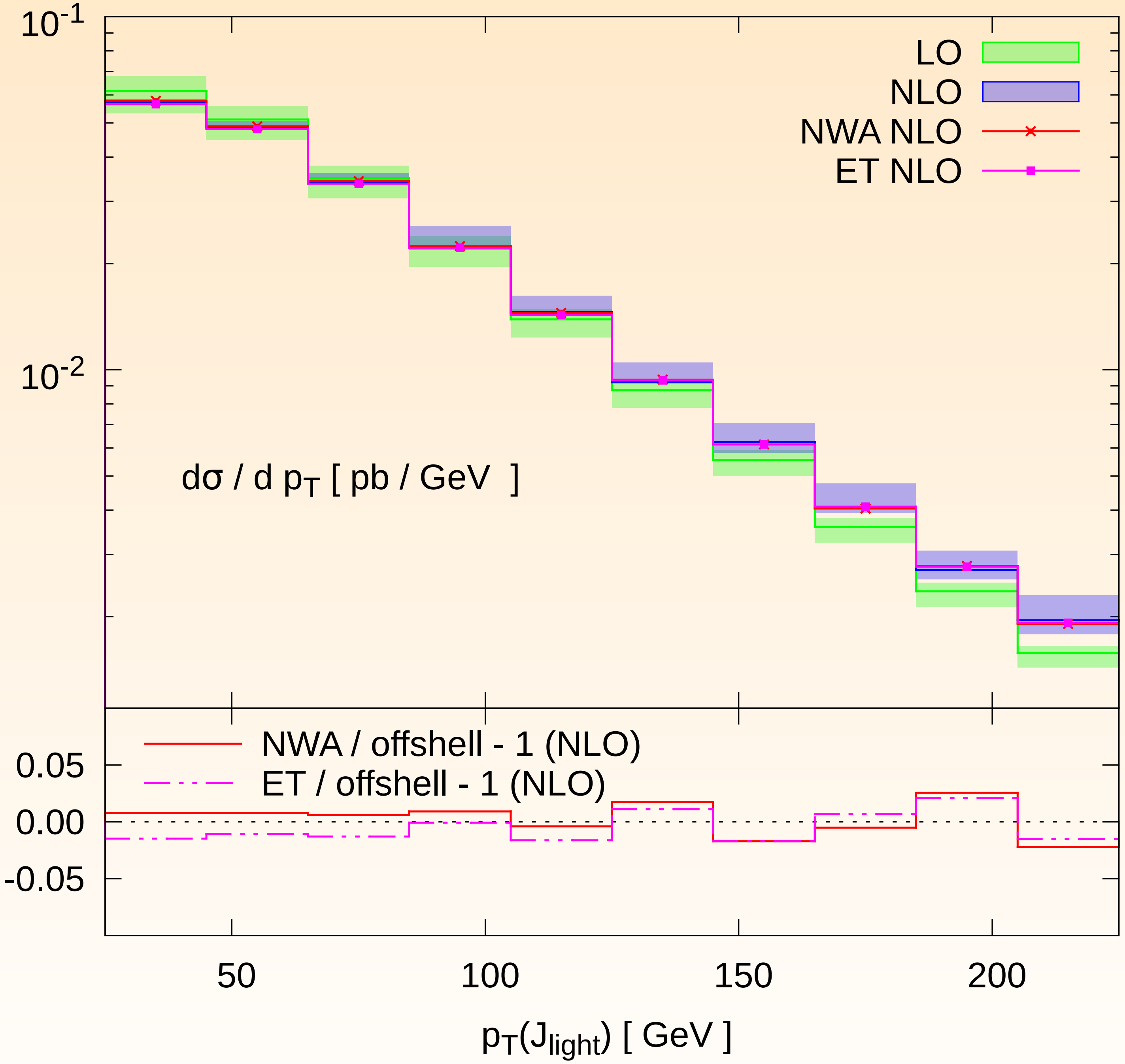
- With V_{tb}=1, the NLO corrections to the t-channel process are finite and well defined, provided that J_b has a non-zero transverse momentum

Comparing to other approximations

- Comparing the complex mass scheme (full calculation to)
  - NWA (narrow width approximation)
    - as implemented in MCFM [Campbell, Ellis, Tramontano, '04]
    - on-shell top quark, NLO top decay, NLO spin correlations
  - ET (effective theory expansion)
    - [Falgari, Mellor, Signer, '10]
    - resonant top decay, but dominant finite width effects included

Comparison between approximations

Papanastasiou, RF, Frixione, Hirschi, Maltoni arXiv:1305.7088

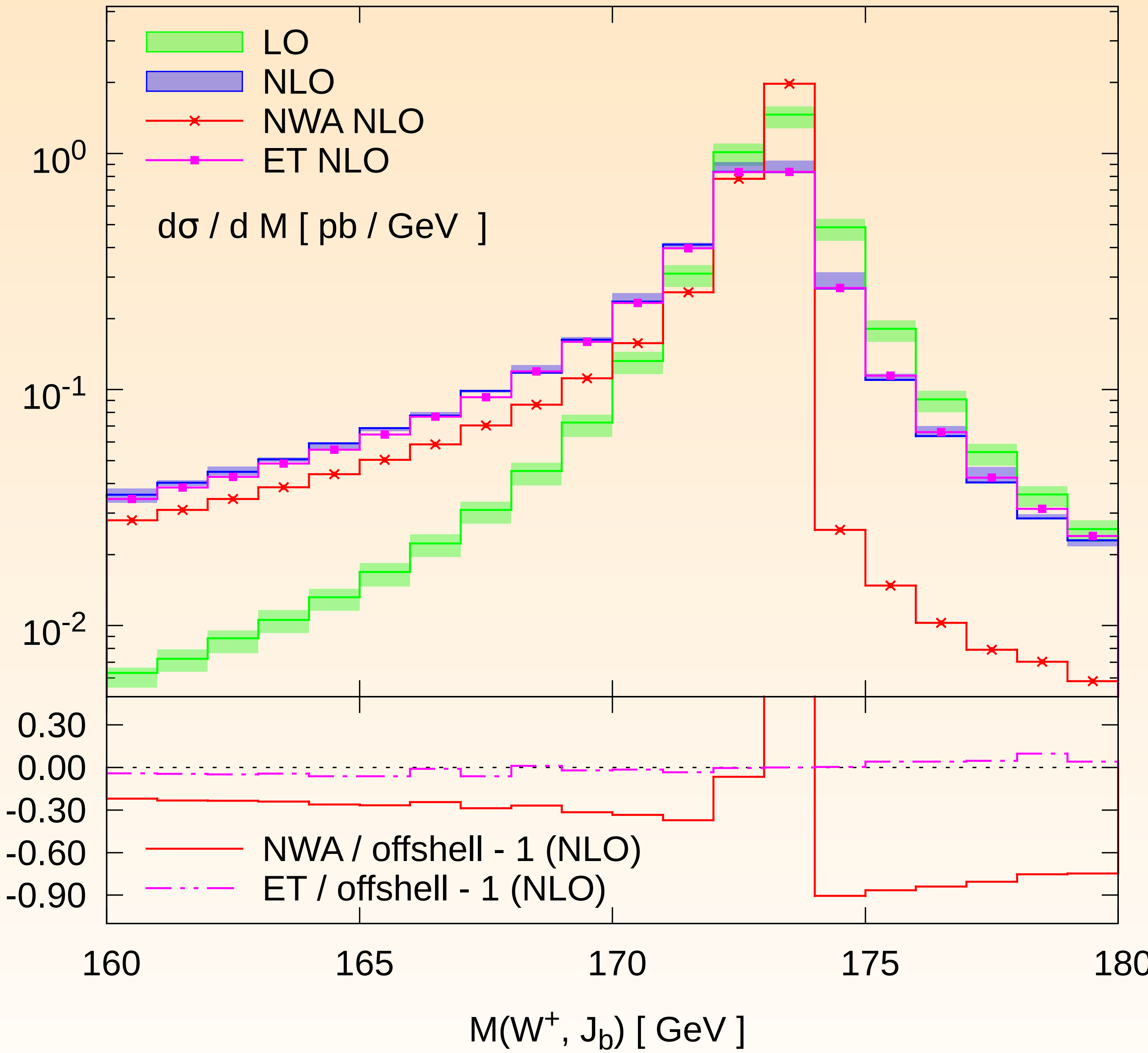


- Comparison of LO, NLO, NLO in the narrow width approximation (NWA) [MCFM] and the effective theory (ET) approach [Falgari, Mellor, Signer arXiv:1007.0893; + Giannuzzi arXiv: 1102.5267] that includes the leading contributions beyond the NWA
- For observables that are integrated over the top resonance peak, differences between NWA, ET and full NLO are rather small:
  - No visible effects in shape of the transverse momentum of the light jet

"TOP INVARIANT MASS": $M(W^+,J_B)$

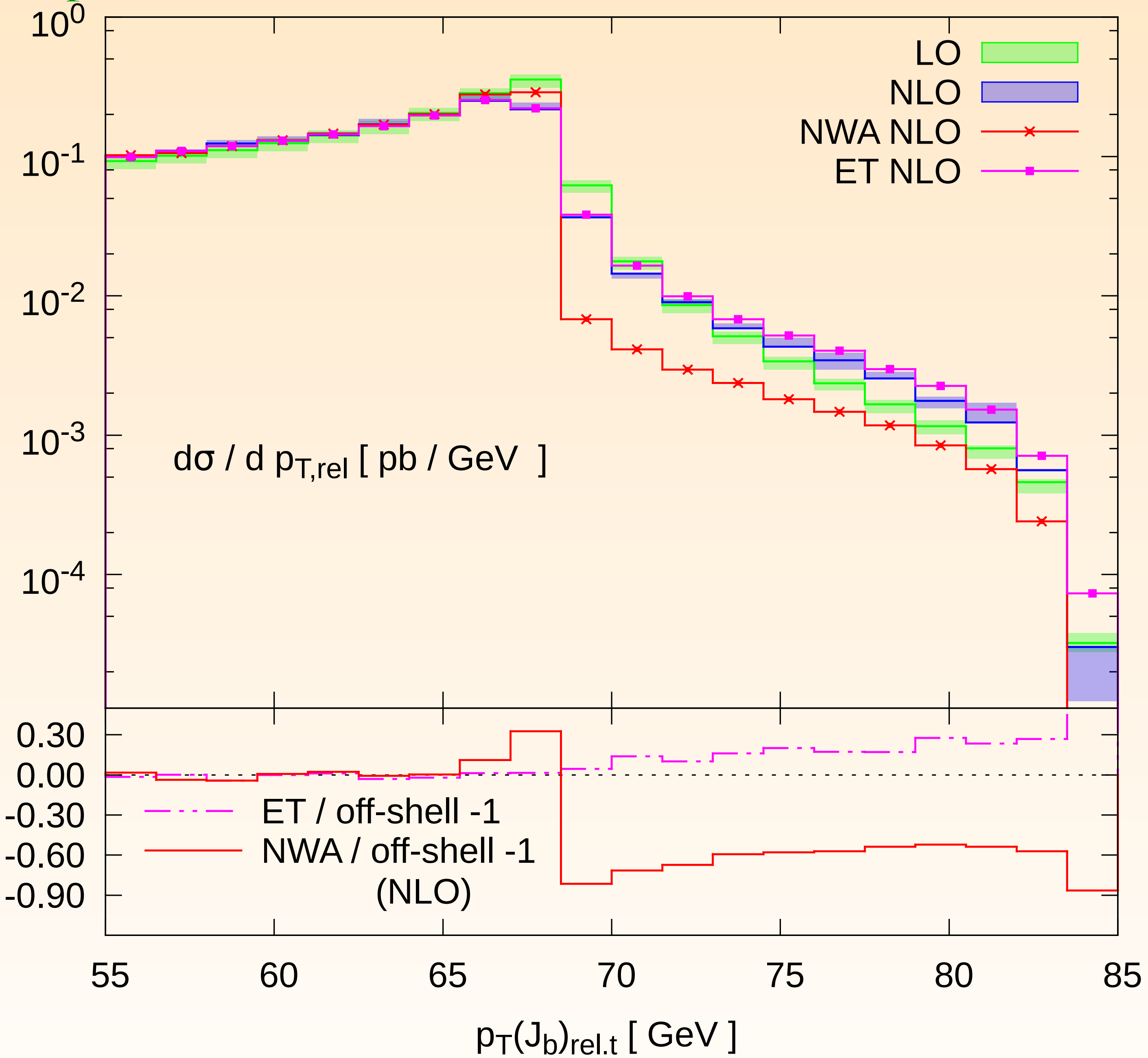
Papanastasiou, RF, Frixione, Hirschi, Maltoni arXiv:1305.7088

- Invariant mass of the W-boson and the b-jet
- LO prediction greatly undershoots the NLO results below the peak: no radiation from the b-jet
  - Including parton shower should get most of this right
- Above peak, NWA undershoots by a long way: no off-shell effects are included
- Effective theory approach results in an excellent description over the whole range plotted here



Relative $p_T(J_B)$ to the (reconstructed) top quark direction

Papanastasiou, RF, Frixione, Hirschi, Maltoni arXiv:1305.7088



- At LO with on-shell top quarks, this distribution has a kinematic cut-off at $p_T(J_b)=(m_t^2-m_W^2)/(2m_t)$
- In the NWA this cut-off largely remains
- Again ET approach does a very good job, apart in the far tail. This is a sign that subleading Γ_t contributions become important

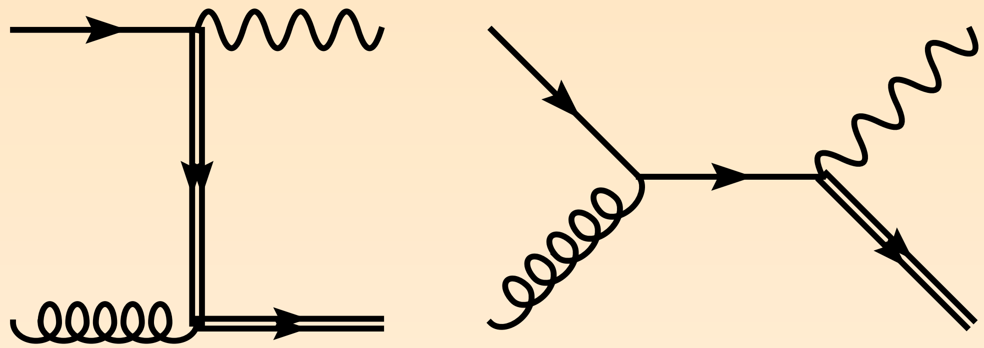
Narrow width approximation

- Most observables are well-described by the NWA
- However, always keep this approximation in mind: care must be taken when observables as $M(W^+,J_b)$ or $p_T(J_b)_{rel,t}$ are used (e.g. in template fitting).
- Effective theory approach does an excellent job close to the resonance, but will ultimately fail as well
  - Excellent for top quarks as signals
  - When top quarks are background, and on-shell contributions are removed with cuts, relative enhancement of non-resonant contributions

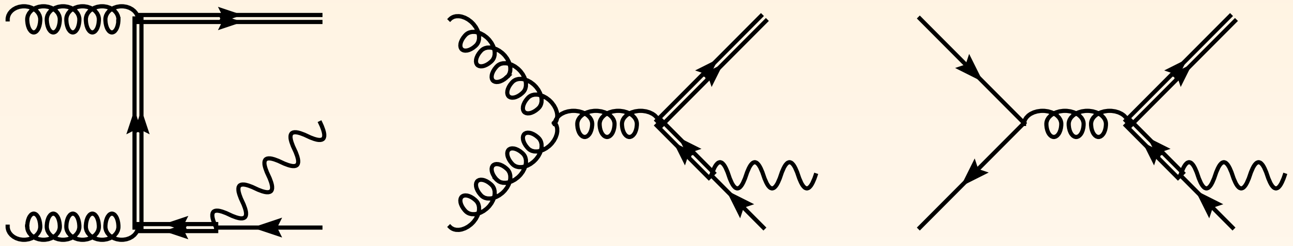
Adding parton shower

- For processes with intermediate top quark resonances it is not straight-forward to include parton shower effects
- Possible double counting from radiation from those top quarks and real-emission corrections. In the default MC@NLO scheme this double counting is not subtracted
- Possibly simple solution with excellent approximation is to forbid the parton shower to include radiation from the top quarks
- Under investigation...

Wt-channel



- Biggest issues in single top modeling are coming from the W-boson associated single top channel
- At NLO, the real-emission diagrams have a contribution from top pair production

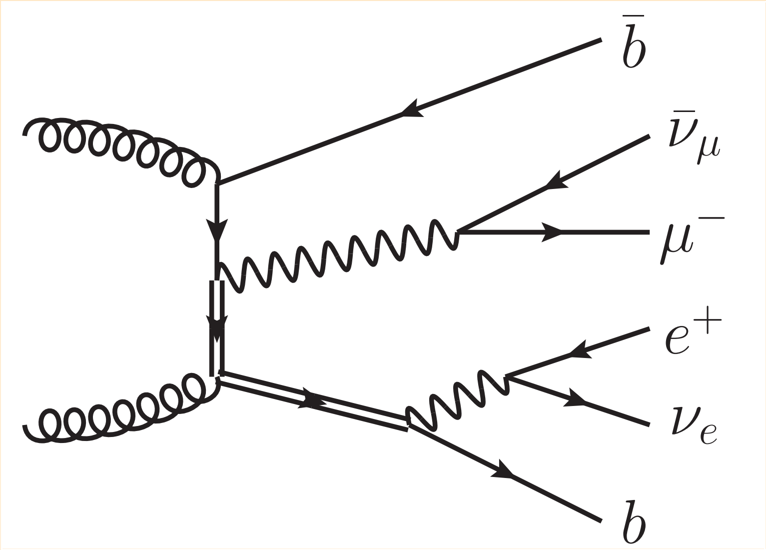


- "Perturbation theory breaks down": the full NLO corrections to Wt production are much larger than the Born, because they receive a contribution from LO top pair production
- DR/DS scheme has been developed to remove/subtract them

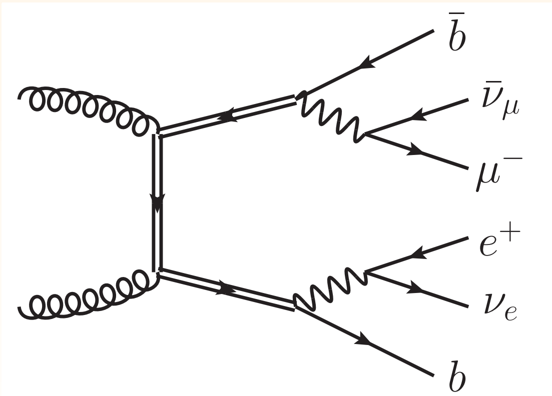
DR/DS scheme

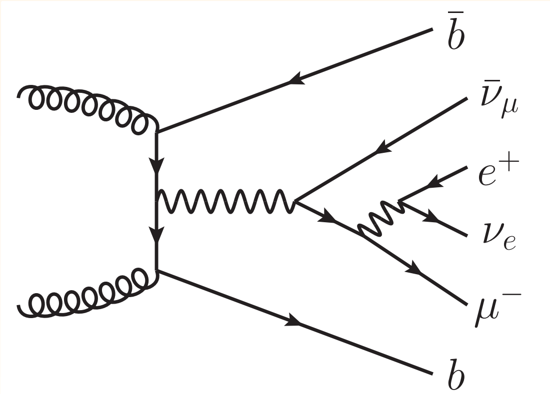
- Remove double resonant (ttbar-like) contributions at the level of amplitude (DR) or matrix elements (DS)
- Difference is the interference between Wt and ttbar production
- Both descriptions are formally not gauge invariant
- Wt with DR/DS available in MC@NLO and POWHEG
- Not available in MadGraph5_aMC@NLO (not so easy to automate), i.e. not worth it for Wt production only...
  - Wt is the only example in the SM where this is needed, but many BSM processes have the same problems
  - When BSM can be done in an automated way, this is something that we'll start thinking about more carefully

4-FLAVOUR WT-CHANNEL



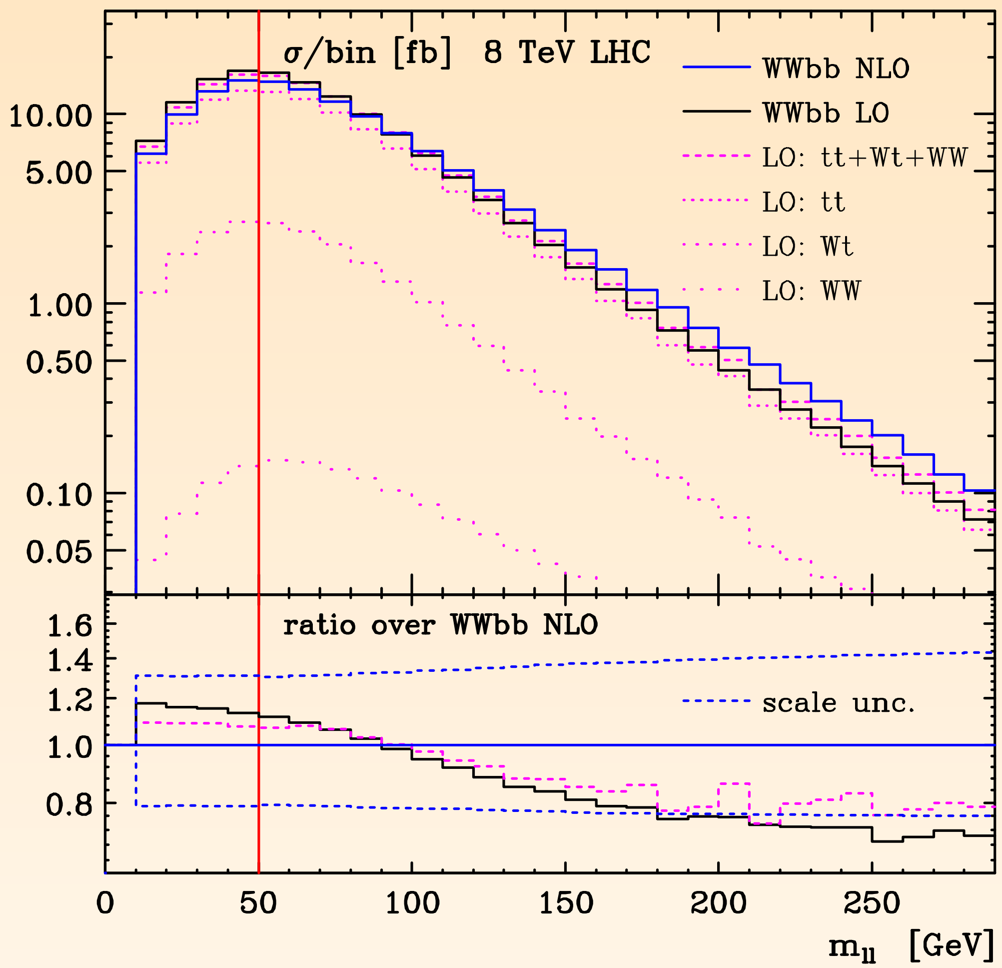
- In the 4-flavour scheme, the problem is even more severe
- Already at LO Wt and ttbar interfere, but no "break down of perturbation theory"
- However the solution is much simpler: compute the NLO corrections to this process and one captures
  - No longer a separate definition of Wt and ttbar production
  - Single and double and non-resonant contributions included at NLO
  - All interferences included
  - All off-shell effects included
  - Technical challenge

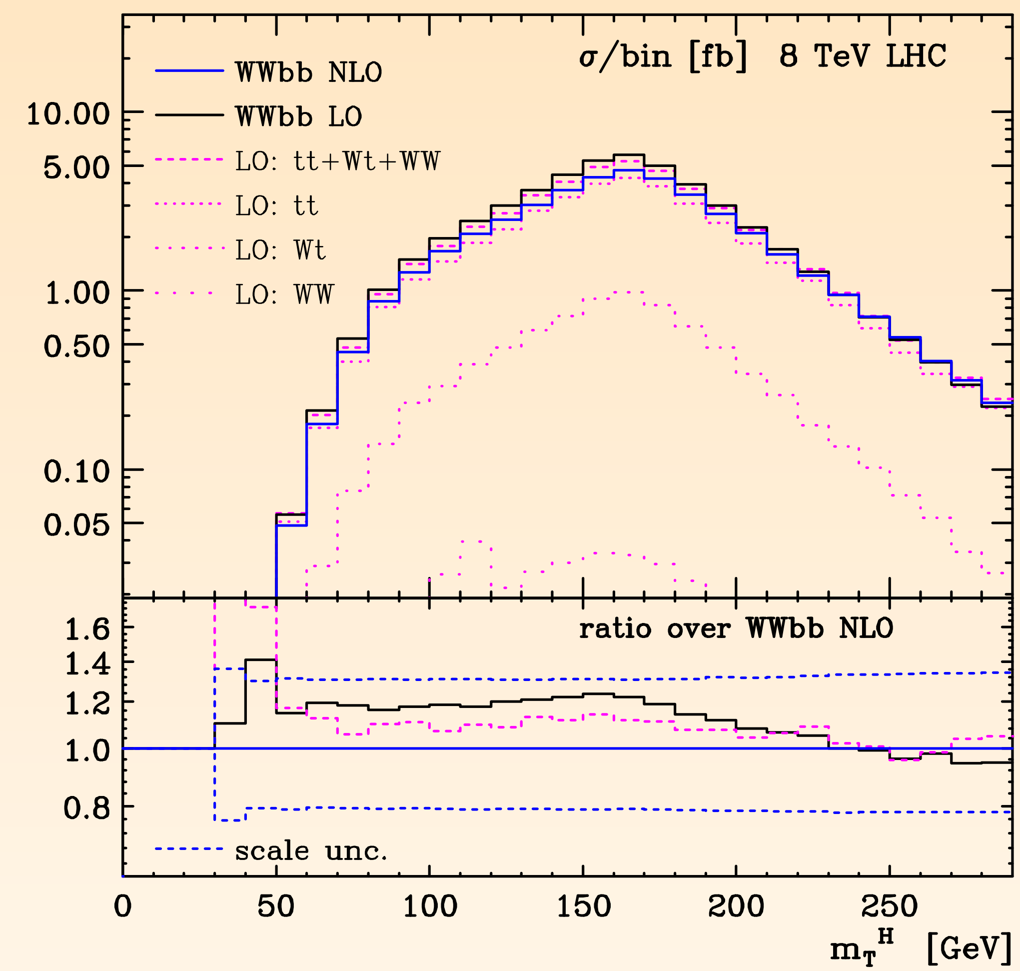




WWbb at NLO

RF arXiv:1311.4893



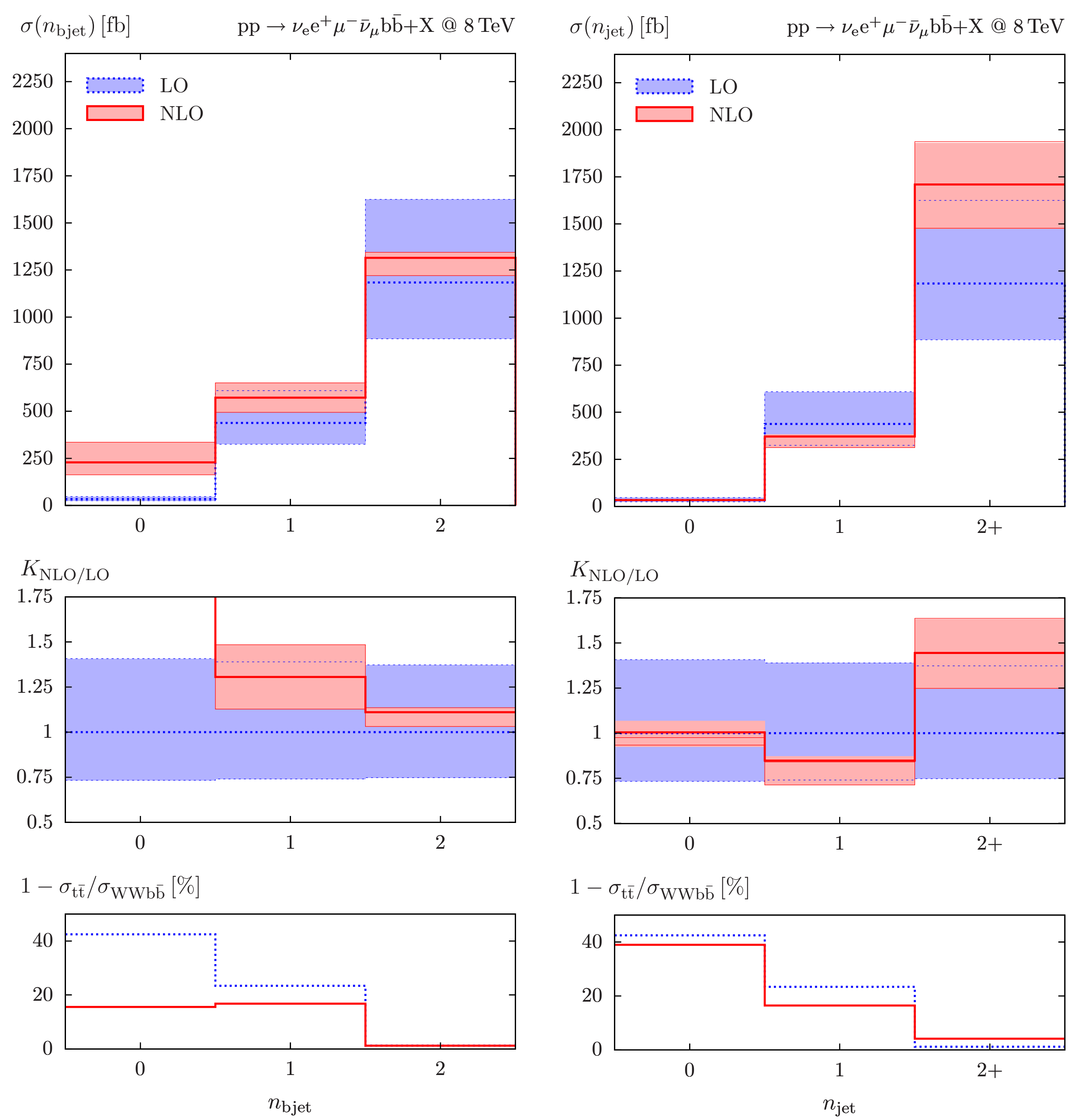


- This has recently been achieved and applied to the H -> WW* measurement channel in the one-jet bin, requiring a single jet
- Long list of cuts to suppress backgrounds
- For these observables, NLO scale dependence remains large

Independent calculation by the Zurich group

Cascioli, Kallweit, Maierhöfer & Pozzorini, arXiv: 1312.0546

Multiplicity of (b)jets with $p_{\mathrm{T}} \geq 30\,\mathrm{GeV}$



First "off-shell" insights into **exclusive 0- and 1-(b)jet bins** of the combined process $\mathrm{t\bar{t}} + \mathrm{tW}$

bjet multiplicity

- large K factors in 0-bjet and 1-bjet bins due to light-jet emission,
- tW contribution to 0-bjet and 1-bjet bins reduced at NLO.

(generic) jet multiplicity

- reduced K factors in the lower jet-multiplicity bins,
- relative contribution from tW stays quite constant when going from LO to NLO.

$|V_{tb}|$ from single top

$$|V_{tb} f_{L_V}| = \sqrt{\frac{\sigma_{t\text{-ch.}}}{\sigma^{th}_{t\text{-ch.}}}}$$

=1 in the SM

$|V_{tb}|$=1 assumed

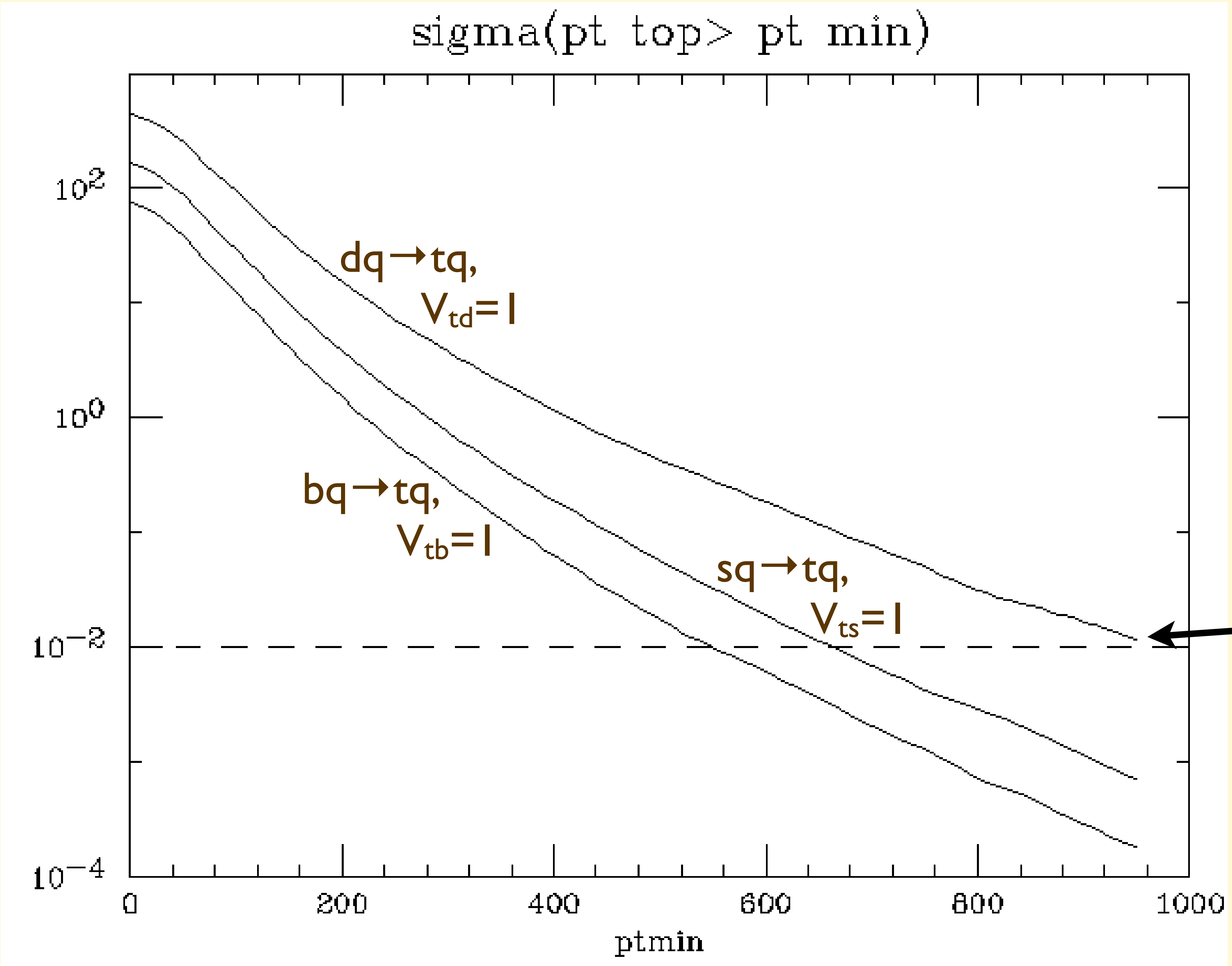
- $|V_{tb}|$ from cross section: determined assuming $B(t\to Wb)\cong 1$
  - 7 TeV: $|V_{tb}| = 1.020 \pm 0.046(\text{exp}) \pm 0.017(\text{th})$ (t-ch. 4.8%)
    $|V_{tb}| = 1.01^{+0.16}_{-0.13}(\text{exp})^{+0.03}_{-0.04}(\text{th})$ (tW-ch., 14.8%)
  - 8 TeV: $|V_{tb}| = 0.96 \pm 0.08(\text{exp}) \pm 0.02(\text{th})$ (t-ch. 8.6%)
    $|V_{tb}| = 1.03 \pm 0.12(\text{exp}) \pm 0.04(\text{th})$ (tW-ch. 12.3%)
- As comparison, from $B(t\to Wb)/B(t\to Wq)$ in tt~:
  $|V_{tb}|=1.011^{+0.018}_{-0.017}$ (stat.+syst) (tt~ 1.7%) [TOP-12-035]
- By dropping the $B(t\to Wb)=1$ assumption single top may reach competitive precision with tt~: $|V_{tb}| \sim (\sigma_{t\text{-ch.}}/\sigma_{t\text{-ch.}}^{th})^{1/4}$
- Corrections from $|V_{ts}|$, $|V_{td}|$ terms should be applied properly
  - Work in progress: may be a topic for the TOPLHCWG

CMS single-top workshop, Naples, 19-12-2013

Luca Lista

17

Single top production, what for ?



Set direct limit on $|V_{td}|^2 \sim 0.01$

Slide by MLM, ERCminiworkshop, Dec. 2013

Conclusions

- Automation of NLO QCD corrections done; should be(come) the new standard
  - But not always:
    - be careful when trying NLO QCD corrections to an EW process
- For single top, use NLO 4-flavour, but normalise to the total 5-flavour rate
- Non-resonant contributions are being included at fixed order NLO (not yet with inclusion of the parton shower as well, but that should be soon)
- First results at NLO without separating Wt & ttbar have been presented. This amounts to computing the NLO corrections to the full WWbb
  - Attaching the shower underway