Precision event generation for top-quark production



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Outline & introduction

review of some recent results
focus mostly on tt, few comments on tt+X

- Fully-differential partonic results: NNLO QCD (prod. and decay), NLO EW corrections known (+ analytic resummation)
- MC event generators (from data to parton-level / background for BSM / measure parameters):
 - stable tops: NLO+PS established, NNLO+PS available, approximated decays
 - full final state (leptons+jets) with QCD corrections: NLO+PS methods available (+ ongoing developments)
 - full assessment of TH uncertainties missing (\rightarrow NLL showers will play crucial role)

tt measurements: status



- TH in this plot: NLO+PS, NNLO, NNLO+PS (and aN3LO)
- scale choice: μ =H_T/4=(m_T(t)+m_T(t))/4 studied in [1606.0350]
- NNLO corrections \rightarrow fix long-standing issue with $\textbf{p}_{T}(t)$

tt (differential) parton-level computations



- NNLO known for prod & decay
- decay: NWA, spin correlations
- NNLO x NNLO x NNLO

Parton-level results: summary

- QCD corrections: clear picture, good perturbative convergence
- different scale choices possible: H_T-like seems to do a good job for distributions
 - insights on hardness vs. kinematics in tt:

[Caola,Dreyer et al. 2101.06068]

- Full NLO EW available [Denner,Pellen '16], possible to validate different approximations.
- Combination of EW and QCD corrections: done for stable top quarks (possible to supplement it with resummation(s))
- Residual uncertainty (size, PDF vs μ) depends on observables

Foundations on which MC developments are based



[ATL-PHYS-PUB-2023-014]

MC event generators: status

- Several NLO+PS generators available: POWHEG BOX, MG5_aMC@NLO, Sherpa, Herwig (through Matchbox).
- Approximations made to include decays and off-shell effects (e.g. ttb_NLO_dec: prod@NLO x decay@NLO)
- Exact MC simulation for decay, offshell effects and interferences:
 bb41 NLO+PS generator
 [Ježo,Lindert et al. '16]
 - NEW: NLOPS matching for off-shell tt+Wt production with semileptonic decays [Ježo,Lindert,Pozzorini '23]
- Multijet merging up to 2 jets @ NLO+PS [MEPS@NLO, FxFx, '12-'13]
- tt NNLO+PS results available

[Mazzitelli,Monni,Nason,ER,Wiesemann,Zanderighi '20-'21]

- NNLO+PS available for b-bar, ongoing work on tt+H [Mazzitelli,Wiesemann,Ratti,Zanderighi '23/Mazzitelli,Wiesemann WIP]

NNLO+PS: goals and accuracy

NNLO accuracy for observables inclusive on radiation. $\left[d\sigma/dy_F \right]$ ▶ NLO(LO) accuracy for F + 1(2) jet observables (in the hard region). $[d\sigma/dp_{T,i_1}]$ appropriate scale choice for each kinematics regime Sudakov resummation from the Parton Shower (PS) $\left[\sigma(p_{T,i} < p_{T,\text{veto}})\right]$ preserve the PS accuracy (leading log - LL) possibly, no merging scale required. methods: reweighted MiNLO' ("NNLOPS") [Hamilton, et al. '12,'13,...], UNNLOPS [Höche,Li,Prestel '14,...] / [Plätzer '12] Geneva [Alioli,Bauer,et al. '13,'15,'16,...], MiNNLO_{PS} Monni,Nason,ER,Wiesemann,Zanderighi '19,...

[Notation: From this point, $X = \sum_{k} \left(\frac{\alpha_{\rm S}}{2\pi} \right)^k [X]^{(k)}$]

top pair-production @ NNLO+PS: MiNNLO (I)

from
$$p_T$$
 resummation, differential cross section for $F+X$ production can be written as:

$$\frac{d\sigma}{dp_T d\Phi_F} = \frac{d}{dp_T} \left\{ \mathcal{L}(\Phi_F, p_T) \exp(-\tilde{S}(p_T)) \right\} + R_{\text{finite}}(p_T)$$

$$\mathcal{L}(\Phi_F, p_T) \ni \{H^{(1)}, H^{(2)}, C^{(1)}, C^{(2)}, (G^{(1)} \cdot G^{(1)})\} = R_{\text{finite}}(p_T) = \frac{d\sigma_{FJ}}{d\Phi_F dp_T} - \frac{d\sigma^{\text{sing}}}{d\Phi_F dp_T}$$
recast it, to match the POWHEG $\bar{B}^{(FJ)}(\Phi_{FJ})$

$$\frac{d\sigma}{d\Phi_F dp_T} = \exp[-\tilde{S}(p_T)] \left\{ D(p_T) + \frac{R_{\text{finite}}(p_T)}{\exp[-\tilde{S}(p_T)]} \right\}$$

$$D(p_T) \equiv -\frac{d\tilde{S}(p_T)}{dp_T} \mathcal{L}(p_T) + \frac{d\mathcal{L}(p_T)}{dp_T} = \tilde{S}(p_T) = \int_{p_T}^Q \frac{dq^2}{q^2} \left[A_f(\alpha_S(q)) \log \frac{Q^2}{q^2} + B_f(\alpha_S(q)) \right]$$

expand the above integrand in power of $\alpha_{\rm S}(p_{\rm T})$, keep the terms that are needed to get NLO^(F) & NNLO^(F) accuracy, when integrating over $p_{\rm T}$

top pair-production @ NNLO+PS: MiNNLO (II)

$$\begin{split} \frac{\mathrm{d}\bar{B}(\Phi_{\mathrm{FJ}})}{\mathrm{d}\Phi_{\mathrm{FJ}}} &= \exp[-\tilde{S}(p_{\mathrm{T}})] \bigg\{ \frac{\alpha_{\mathrm{S}}(p_{\mathrm{T}})}{2\pi} \left[\frac{\mathrm{d}\sigma_{\mathrm{FJ}}}{\mathrm{d}\Phi_{\mathrm{FJ}}} \right]^{(1)} \left(1 + \frac{\alpha_{\mathrm{S}}(p_{\mathrm{T}})}{2\pi} [\tilde{S}(p_{\mathrm{T}})]^{(1)} \right) \\ &+ \left(\frac{\alpha_{\mathrm{S}}(p_{\mathrm{T}})}{2\pi} \right)^{2} \left[\frac{\mathrm{d}\sigma_{\mathrm{FJ}}}{\mathrm{d}\Phi_{\mathrm{FJ}}} \right]^{(2)} + [D(p_{\mathrm{T}})]^{(\geq 3)} F_{\ell}^{\mathrm{corr}}(\Phi_{\mathrm{FJ}}) \bigg\} \\ &+ \left[D(p_{\mathrm{T}}) \right]^{(\geq 3)} = - \frac{\mathrm{d}\tilde{S}(p_{\mathrm{T}})}{\mathrm{d}p_{\mathrm{T}}} \mathcal{L}(p_{\mathrm{T}}) + \frac{\mathrm{d}\mathcal{L}(p_{\mathrm{T}})}{\mathrm{d}p_{\mathrm{T}}} - \frac{\alpha_{\mathrm{S}}(p_{\mathrm{T}})}{2\pi} [D(p_{\mathrm{T}})]^{(1)} - \left(\frac{\alpha_{\mathrm{S}}(p_{\mathrm{T}})}{2\pi} \right)^{2} [D(p_{\mathrm{T}})]^{(2)} \\ &- F_{\ell}^{\mathrm{corr}}(\Phi_{\mathrm{FJ}}) : \text{projection} \rightarrow \text{recover} \left[D(p_{\mathrm{T}}) \right]^{(\geq 3)} \text{ when integrating over } \Phi_{\mathrm{FJ}} \text{ at fixed } (\Phi_{\mathrm{F}}, p_{\mathrm{T}}) \\ &- \frac{\mathrm{The second radiation is generated by the usual POWHEG mechanism.}{\mathrm{d}\sigma = \bar{B}(\Phi_{\mathrm{FJ}}) \mathrm{d}\Phi_{\mathrm{FJ}} \left\{ \Delta_{\mathrm{pwg}}(\Lambda_{\mathrm{pwg}}) + \mathrm{d}\Phi_{\mathrm{rad}}\Delta_{\mathrm{pwg}}(p_{\mathrm{trad}}) \frac{R(\Phi_{\mathrm{FJ}}, \Phi_{\mathrm{rad}})}{B(\Phi_{\mathrm{FJ}})} \right\} \\ &\text{. if emissions are strongly ordered, same emission probabilities as in } k_{t} \text{-ordered shower} \\ &\rightarrow \mathrm{LL} \text{ shower accuracy preserved} \end{split}$$

top pair-production @ NNLO+PS: MiNNLO for tt

Starting point: resummation formula for $t\bar{t}$ transverse momentum. [Catani,Grazzini,Torre '14] Very schematically:

 $\equiv \overline{\mathscr{L}}_i$

$$d\sigma_{\text{res}}^{F} \sim \frac{d}{dp_{T}} \left\{ e^{-S} \operatorname{Tr}(\mathbf{H}\Delta) \left(C \otimes f \right) \left(C \otimes f \right) \right\}$$

$$S = -\int \frac{dq^{2}}{q^{2}} \left[\frac{\alpha_{s}(q)}{2\pi} \left(A^{(1)} \log(M/q) + B^{(1)} \right) + \frac{\alpha_{s}^{2}(q)}{(2\pi)^{2}} \left(A^{(2)} \log(M/q) + B^{(2)} \right) + \dots \right]$$

$$\operatorname{Tr}(\mathbf{H}\Delta) = \langle M | \Delta | M \rangle, \quad \Delta = \mathbf{V}^{\dagger} \mathbf{D} \mathbf{V}, \quad \mathbf{V} = \exp \left\{ -\int \frac{dq^{2}}{q^{2}} \left[\frac{\alpha_{s}(q)}{2\pi} \Gamma_{t}^{(1)} + \frac{\alpha_{s}^{2}(q)}{(2\pi)^{2}} \Gamma_{t}^{(2)} \right] \right\}$$

$$\blacktriangleright \text{ With some approximations (respecting our goal), terms due to soft interference can be rearranged so that the "resummation" can be eventually recasted as:$$

$$d\sigma_{\text{res}}^{F} \sim \frac{d}{dp_{T}} \left\{ \sum_{i \in \text{colours}} e^{-\overline{S}_{i}} \underbrace{c_{i} \overline{H} (\overline{C \otimes f}) (\overline{C \otimes f})}_{= \overline{C} \otimes f} \right\} + \mathcal{O}(\alpha_{\mathrm{S}}^{5})$$

inputs from [Catani, Devoto, Grazzini, Kallweit, Mazzitelli + Sargsyan '19] paper: [Catani, Devoto, Grazzini, Mazzitelli '23].

Each term has the "same structure" as in the color-singlet case!

top pair-production @ NNLO+PS: results I



- nice agreement with NNLO (and with data - both ATLAS and CMS). $\mu_{core} = H_T/4$

- m(tt), 1st bin: finite-width effects + non-relativistic effects + QED

top pair-production @ NNLO+PS: results II



- implemented top-quark decays @ tree level + approximated off-shell effects

- NB: if analysis probes off-shell/non-resonant regions →bb41 NLO+PS should be method of choice

12

ttH production @ NNLO+PS

[Mazzitelli, Wiesemann WIP]



- soft function computation extended (arbitrary kinematics):

- 2-loops using "soft Higgs" approximation

[Devoto,Mazzitelli WIP]

[Catani et al. 2210.07846→talk by S. Devoto] 13

tt / Wt: EXP/TH status



[diagrams from slides by T. Ježo]

- Interference tt/Wt: long-standing issue
- Approximations made (DR/DS) to treat processes separately, with unstable resonances in final state
- DR/DS differences might become an issue in BSM search regions
- bb41 NLOPS generator in POWHEG-BOX-RES: interferences/off-shell effects, top decay at NLO
- resonant-aware methods also in MG5_aMC@NLO



Off-shell tt + tW: status



- each term (Born- and real-like) is attributed to an unique resonance history
 - virtuality-preserving mappings
 - POWHEG radiation can be assigned a resonance \rightarrow (up to) 1 emission per resonance

<u>Off-shell t₹ + tW: status → recent progress</u>

- ьъ41 NLO+PS [1607.04538]: generator available for leptonic decays (used also for TH studies, e.g. [Ferrario Ravasio,Ježo et al. '18])
- <u>NEW:</u> [Ježo,Lindert,Pozzorini 2307.15653]: improvements + semi-leptonic decays
- 1. width effects
- 2. improved resonance histories

Off-shell tt + tW: recent progress

[Ježo,Lindert,Pozzorini 2307.15653]



- last equation: used in new bb41-d1/s1 generators

<u>Off-shell tt + tW: recent progress</u>

[Ježo,Lindert,Pozzorini 2307.15653]

O immediate an encode biotoxic ex	resonance history	production subprocess	- b
2. Improved resonance histories:	$tar{t}$	$pp \to t\bar{t}$	W^+
			\overline{t}
- original bb41 : {tt, Z }	tW^-	$pp \to t W^- \bar{b}$	
- bb41-d1/s1: {tt, tW ⁺ , tW ⁻ }	$\bar{t}W^+$	$pp \to \bar{t} W^+ b$	
ightarrow expect better treatment of "decay" emissions	Z	$pp \rightarrow Z/H + b\bar{b}$	

$$\begin{split} \rho_{t\bar{t}}^{(\rm hist)}(\Phi_{\rm B})\big|_{\rm ME} &= \left|\mathcal{A}_{t\bar{t}}\right|^2,\\ \text{- ME-based projectors:} \quad \left. \rho_{\bar{t}W^+}^{(\rm hist)}(\Phi_{\rm B})\right|_{\rm ME} &= \left|\mathcal{A}_{\bar{t}W^+}\right|^2 \end{split}$$

$$\rho_{tW^{-}}^{(\text{hist})}(\Phi_{\text{B}})\big|_{\text{ME}} = |\mathcal{A}_{tW^{-}}|^2$$

- several variations, new mappings, thorough validation

$$\sigma_{t\bar{t}} = \lim_{\xi_t \to 0} \left(\xi_t^2 \sigma_{\text{bb4l}} \Big|_{\Gamma_t \to \xi_t \Gamma_t} \right)$$



- LHS: resonance histories ambiguities (in off-shell regions*) → negligible after PS
- RHS: even when interference effects large, hvq+wtch-DS ≈ bb41

- naive width $\rightarrow \frac{\sigma_{bb41-s1}}{\sigma_{hvq+ST}}\Big|_{no \ 1/\Gamma_t \text{ expansion}} = 1.074$

*
$$Q_{\text{off-shell}} = \max\left\{|Q_t - m_t|, |Q_{\bar{t}} - m_t|\right\} > 60 \,\text{GeV}^{-19}$$

TH uncertainties in MC generators

Possible TH uncertainties:

- scale variation (hard matrix elements)
- matching uncertainties (e.g. hdamp in POWHEG, hard veto scale in MC@NLO,...)
- change matching scheme / shower [e.g. Matchbox study, 1810.06493]
- other "shower-related" pQCD uncertainties can be probed
- recoil scheme
-
- non-perturbative parameters & tuning
 - possible to include such variations (→<u>certainly not the ultimate</u> solution)
 - within the current paradigms for matching & merging, rethinking needed for some of the above items, once matching to NLL parton showers will be achieved (Panscales, Alaric, FHP,)





1810.06493]

Conclusions

- MC event generators play a role in ~ all EXP analysis
 - data to parton-level, background for BSM, measure parameters
- processes with top quarks: NNLO+PS available (with MiNNLOPS method), approximate decays
- full off-shell final state (leptons+jets): NLO+PS "resonance-aware" methods available

- full assessment of TH uncertainties missing (\rightarrow NLL showers will play crucial role)
- tt+X: once NNLO known (exactly or approximately) \rightarrow NNLO+PS possible

• Other approaches: Geneva for tt....[2111.03632 (0-jettiness resummation)]

Thank you for your attention!

Backup slides

top pair-production @ NNLO+PS: MiNNLO for tt



- diagonalization of $\mathbf{V}_{\mathrm{NLL}} \rightarrow$ recast as sum of "colour-singlet-like" terms

EW corrections: from total cross sections....



- fully exclusive results (2 lep channel)
- NLO EW = $O(\alpha_s^2 \alpha^5)$
- total x-section: EW corrections < 1%
- no uncertainty on EW corrections (but irrelevant for total x-section)



Ch.	$\sigma_{\rm LO}$ [fb]	$\sigma_{\rm NLO \; EW}$ [fb]	δ [%]
gg	2824.2(2)	2834.2(3)	0.35
q ar q	375.29(1)	377.18(6)	0.50
${ m g}q(/ar q)$		0.259(4)	
$\gamma { m g}$		27.930(1)	
$_{\rm pp}$	3199.5(2)	3211.7(3)	0.38

[Denner,Pellen '16]



- corrections ~ 10-15 % (radiative tails (left) / Sudakov logs (right))

- here: no approximations. Possible to study "DP approximations" for tops or Ws.
- scales fixed at top mass (enter in $\alpha_s \& PDFs$)
- TH uncertainties: needed? Uncharted territory: change of scheme (?),...



preferred combination: multiplicative \Rightarrow

- stabilize scale uncertainty of $\Sigma_{\text{NLO EW}} = O(\alpha_s^2 \alpha)$ - $\Sigma_{\text{mixed}} = O(\alpha_s^3 \alpha) \approx \Sigma_{\text{NLO QCD}} \Sigma_{\text{NLO EW}} / \Sigma_{\text{LO QCD}}$ - correct in regime "soft gluon" + "Sudakov log"

top pair-production @ NNLO+PS: results III



- nice agreement with NNLO (and with data - both ATLAS and CMS). μ_{core} = $H_{T}/4$

Resonant-aware NLO+PS: details I

- 1. complete matrix elements for $W^+W^-b\overline{b}$: need to project each partonic subprocess onto all possible "resonance histories":
 - each contribution should be dominated by a single resonance history:

$$B = \sum_{f_b} B_{f_b}, \text{ where } B_{f_b} \equiv \frac{P^{f_b}(\Phi_B)}{\sum_{f'_b} P^{f'_b}(\Phi_B)} B(\Phi_B)$$

 $P^{f_b}(\Phi_B)$ (products of) Breit-Wigner functions \Leftrightarrow resonance history f_b

- for real contributions, split also according to compatible FKS regions
 - \Rightarrow a term R_{α_T} is dominant <u>if</u> the collinear partons of region α_r have the smallest k_T , <u>and</u> the corresponding resonance history is the closest to its mass shell.
- 2. each term (Born-like and real) is attributed to an unique resonance history
 - virtuality-preserving mappings between Φ_B and (Φ_B, Φ_{rad}) can be used
 - POWHEG radiation(s) can now be assigned to a resonance
 - (& other technical but crucial subtleties...)

Resonant-aware NLO+PS: details II

"multiplicative POWHEG": keep multiple emissions before showering

- EI

- by default POWHEG is additive: keeps only the hardest emission
- keep hard radiation and the emissions from all decaying resonances, then merge them into a single radiation phase space with several radiated partons, up to one for each resonance





in the above case, the interface to parton shower becomes more complicated.

TH uncertainties in MC generators: looking ahead

- plots from: [Hamilton et al. 2301.09645]
- thrust in e⁺e⁻: NLO+PS multiplicative matching + NLL shower
- dots: modified splitting function in hard region dashes: μ_{R} scale variation (also in hard matrix elements)
- here matching fulfils NNDL accuracy (i.e. the same accuracy of a NLL resummation matched with NLO)

$$\Sigma(O < e^L) = h_1(\alpha_s L^2) + \sqrt{\alpha_s} h_2(\alpha_s L^2) + \alpha_s h_3(\alpha_s L^2) + \dots$$

