Resonance-aware NLOPS matching for off-shell top-pair plus tW production with semileptonic decays

based on <u>2307.15653</u> (in collaboration with T. Jezo, S. Pozzorini)

University of Sussex

Jonas M. Lindert



UK Research and Innovation

HP2 Turin, 10th Sep 2024



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University of Sussex

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NLO+PS predictions for top-pair and Wt production and decay



Jonas M. Lindert

work in collaboration with: T. Ježo, P. Nason, C. Oleari, S. Pozzorini based on [Ježo, Nason; '15] & [Ježo, JML, Nason, Oleari, Pozzorini; '16]

HP2 Buenos Aires, 8th September 2016



The fate of the Universe



- M_t/GeV •top-mass measurements at the LHC via combination of different strategies:
 - total x-section, tt+jet, kinematic reconstruction, kinematic edges,....
- many techniques rely on kinematic information of top decay products
 - ➡ need realistic MC modelling

[ATLAS+CMS; arXiv:2402.08713]



• Also: tt ubiquitous background, QCD laboratory, anomalous coupling, etc....



Top-pair production and decay





@ NLO+PS



Top-pair production and decay

NLO incl. off-shell/non-resonant/ interference effects

q

 \overline{q}



O NLO+PS

bb4l [Jezo, JML, Nason, Oleari, Pozzorini, '16]

Physics features:

- exact non-resonant / off-shell / interference / spin-correlation effects at NLO
- consistent NLO+PS treatment of top resonances, including quantum corrections to top propagators and off-shell top-decay chains thanks to POWHEG-BOX-RES
- unified treatment of top-pair and Wt production with interference at NLO
- access to phase-space regions with **unresolved b-quarks** and/or jet vetoes

What's new? [T. Jezo, JML, S. Pozzorini, <u>2307.15653</u>]

- Consistent inverse-width expansion
- Matrix-element based resonance histories
- Semi-leptonic decays

Resonance-unaware NLOPS matching in POWHEG

► Already at **NLO**:

- FKS (and similar CS) subtraction does not preserve virtuality of intermediate resonances
- Real (R) and Subtraction-term ($S \sim B$) with different virtuality of intermediate resonances $(\Phi_{\rm B}, \Phi_{\rm rad}) \longleftrightarrow \Phi_{\rm R}^{(\alpha)}$ from FKS mappings
- IR cancellation spoiled

 \Rightarrow severe efficiency problem!

- More severe problems at NLO+PS:
 - in POWHEG: $d\sigma = \bar{B}(\Phi_{\rm B}) d\Phi_{\rm B} \left| \Delta(q_{\rm cut}) + \sum_{c \in \mathcal{C}} \Delta(k_{{\rm T},c}) \frac{R_c(\Phi_{{\rm R},c})}{B(\Phi_{\rm B})} d\Phi_{{\rm rad},c} \right|$

Sudakov form-factor generated from uncontrollable R/B ratios:

$$\Delta \left(\Phi_B, p_{\mathrm{T}} \right) = \exp \left\{ -\sum_{\alpha} \int_{k_{\mathrm{T}} > p_{\mathrm{T}}} \frac{R(\Phi_{\mathrm{R}}^{(\alpha)})}{B(\Phi_{\mathrm{B}})} \right\}$$

• also subsequent radiation by the **PS** itself reshuffles internal momenta and does in general not preserve the virtuality of intermediate resonances.

\Rightarrow expect uncontrollable distortion of important kinematic shapes!



Resonance-aware NLOPS matching in POWHEG-RES

Rigorous solution to all these issues within POWHEG-BOX-RES according to []ežo, Nason; '15]

Idea: preserve invariant mass of intermediate resonances at all st

✓ NLO:

- Split phase-space integration into regions dominated by
- within a given resonance history modify FKS mappings, s that they *always* preserve intermediate resonances \Rightarrow R and S~B *always* with same virtuality of intermed \implies IR cancellation restored

✓ NLO+PS:

- R and B related via modified FKS mappings
 - \Rightarrow R/B ratio with fixed virtuality of intermediate resonances
 - \Rightarrow Sudakov form-factor preserves intermediate resonances

√ PS:

- pass information about resonance histories to the shower (via extension of LHE)
- tell **PS to respect intermediate resonances** (available in Pythia8)

tages!

$$\bar{B}_{h}(\Phi_{\rm B}) = \omega_{h}^{(\rm hist)}(\Phi_{\rm B}) \bar{B}(\Phi_{\rm B})$$

$$\omega_{h,c}(\Phi_{\rm R}) = \rho_{h,c}(\Phi_{\rm R}) \left[\sum_{h'\in\mathcal{H}}\sum_{c'\in\mathcal{C}(h')}\rho_{h',c'}(\Phi_{\rm R})\right]$$
such
diate resonances

$$\rho_{h,c}^{(\rm hist)}(\Phi_{\rm R}) = \prod_{r\in\mathcal{R}(h,c)}\frac{M_{r}^{4}}{(q_{\rm R,r}^{2} - M_{r}^{2})^{2} + \Pi}$$
original kinematic proje

$$d\sigma = \sum_{h\in\mathcal{H}}\bar{B}_{h}(\Phi_{\rm B}) d\Phi_{\rm B} \left[\Delta_{h}(q_{\rm cut}) + \sum_{c\in\mathcal{C}(h)}\Delta_{h}(k_{\rm T,c})\frac{R_{h,c}(\Phi_{\rm R,c})}{B_{h}(\Phi_{\rm B})} d\Phi_{\rm rad}\right]$$







Key advantage I: Interplay between top-pair and Wt

 $\eta(t)$

Interference effects between top-pair and Wt production

"'Probing the quantum interference between singly and doubly resonant top-quark production in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector"



Phys. Rev. Lett. 121 (2018) 152002

 $m_{b\ell}^{\text{minimax}} \equiv \min\{\max(m_{b_1\ell_1}, m_{b_2\ell_2}), \max(m_{b_1\ell_2}, m_{b_2\ell_1})\}$

For tT (double-resonant) at LO: $m_{b\ell}^{\rm minimax} < \sqrt{m_t^2 - m_W^2}$

- → sensitivity to off-shell effects/ tt-Wt interference beyond endpoint
- → measure top width [Herwig, Jezo, Nachman, '19]





▶ In traditional approach only hardest radiation is generated by POWHEG:



always the hardest.

- \rightarrow emission off decays are mostly generated by the shower.
- Multiple-radiation scheme:
 - keep hardest overall emission and additionally hardest emission from any of n decaying resonances.



Key advantage II: Multiple-radiation scheme

BUT: for top-pair (or single-top) production and decay, emission from production is almost

introduced in [Campbell, Ellis, Nason, Re; '15]

Consistent inverse-width expansion at NLO
[Jezo, JML, Pozzorini, 2307.15653]
NWA:
$$d\sigma_{prod \times dec} = d\sigma \frac{d\Gamma}{\Gamma}$$
, where $\Gamma = \int_{dcc} d\Gamma$ This hold to all orders!
 $\downarrow_{dec} \qquad for this ensures: \int_{dec} d\sigma_{prod \times dec} = d\sigma$
Naive NLO expansion of NWA: $d\sigma_{NLO} = d\sigma_0 + d\sigma_1$, $d\Gamma_{NLO} = d\Gamma_0 + d\Gamma_1$, $\Gamma_{NLO} = \Gamma_0 + \Gamma_1$
 $\downarrow_{dec} \qquad \int_{dec} d\sigma_{prod \times dec} = d\sigma_0 + d\sigma_1 - d\sigma_1 \frac{\Gamma_1}{\Gamma_{NLO}} \qquad spurious$
Consistent NLO expansion of NWA: $d\sigma_{NLO} = d\sigma_0 + d\sigma_1$, $d\Gamma_{NLO} = d\Gamma_0 + d\Gamma_1$, $\frac{1}{\Gamma_{NLO}} \rightarrow \frac{1}{\Gamma_0} \left(1 - \frac{\Gamma_1}{\Gamma_0}\right)$
 $\downarrow_{dec} \qquad \int_{dec} d\sigma_{prod \times dec} = d\sigma_0 + d\sigma_1$

$$\sigma \frac{d\Gamma}{\Gamma}, \text{ where } \Gamma = \int_{dec} d\Gamma \qquad \text{This hold to all orders!}$$

$$(\downarrow \text{ this ensures: } \int_{dec} d\sigma_{\text{prod}\times\text{dec}} = d\sigma$$

$$\forall A: d\sigma_{\text{NLO}} = d\sigma_0 + d\sigma_1, \qquad d\Gamma_{\text{NLO}} = d\Gamma_0 + d\Gamma_1, \qquad \Gamma_{\text{NLO}} = \Gamma_0 + \Gamma_1$$

$$(\downarrow \int_{dec} d\sigma_{\text{prod}\times\text{dec}}^{\text{NLO}} = d\sigma_0 + d\sigma_1 - d\sigma_1 \frac{\Gamma_1}{\Gamma_{\text{NLO}}} \qquad \text{spurious}$$

$$(Melnikov, Schulze, "O)$$

$$(Melnikov, Schulze, "O)$$

$$(\downarrow f \text{NWA: } d\sigma_{\text{NLO}} = d\sigma_0 + d\sigma_1, \qquad d\Gamma_{\text{NLO}} = d\Gamma_0 + d\Gamma_1, \qquad \frac{1}{\Gamma_{\text{NLO}}} \rightarrow \frac{1}{\Gamma_0} \left(1 - \frac{\Gamma_1}{\Gamma_0}\right)$$

$$(\downarrow f \text{NWA: } d\sigma_{\text{NLO}} = d\sigma_0 + d\sigma_1, \qquad d\Gamma_{\text{NLO}} = d\Gamma_0 + d\Gamma_1, \qquad \frac{1}{\Gamma_{\text{NLO}}} \rightarrow \frac{1}{\Gamma_0} \left(1 - \frac{\Gamma_1}{\Gamma_0}\right)$$

Generalise to multiple resonances:
$$d\sigma_{\text{prod} \times \text{dec}}^{\text{NLO}_{exp}} = \left[d\sigma_0 + \sum_r \left(d\sigma_0 \frac{d\Gamma_{r,1}}{d\Gamma_{r,0}} - d\sigma_0 \frac{\Gamma_{r,1}}{\Gamma_{r,0}} \right) + d\sigma_1 \right] \left(\prod_{r \in \mathcal{R}} \frac{d\Gamma_{r,0}}{\Gamma_{r,0}} \right)$$

$$d\sigma_{\rm spurious} = d\sigma_{\rm prod \times dec}^{\rm NLO} - d\sigma_{\rm prod \times dec}^{\rm NLO_{exp}} = \delta\kappa_{\rm sp}$$

E.g.: $\delta \kappa_{\text{spurious}}^{t\bar{t}+X} \simeq -2 \frac{\mathrm{d}\sigma_1}{\mathrm{d}\sigma_0} \frac{\Gamma_{t,1}}{\Gamma_{t,0}} \simeq +17\% \frac{\mathrm{d}\sigma_1}{\mathrm{d}\sigma_0} \,!$ $_{
m purious}\,{
m d}\sigma_{
m prod imes dec}^{
m LO}$



Start from fNLO in NWA:
$$d\sigma_{\text{prod}\times\text{dec}}^{\text{NLO}_{exp}} = \left[d\sigma_0 + \sum_r \left(d\sigma_0 \frac{d\Gamma_{r,1}}{d\Gamma_{r,0}} - d\sigma_0 \frac{\Gamma_{r,1}}{\Gamma_{r,0}} \right) + d\sigma_1 \right] \left(\prod_{r \in \mathcal{R}} \frac{d\Gamma_{r,0}}{\Gamma_{r,0}} \right)$$

(fNLO for off-shell computation: $d\sigma_{\text{off-shell}}^{\text{NLO}_{exp}} = \left(\prod_{r \in \mathcal{R}} \frac{\Gamma_{r,\text{NLO}}}{\Gamma_{r,0}} \right) \left[d\sigma_{\text{off-shell}}^{\text{NLO}} - \left(\sum_{r \in \mathcal{R}} \frac{\Gamma_{r,1}}{\Gamma_{r,0}} \right) d\sigma_{\text{off-shell}}^{(0)} \right]$
Use $\Gamma_{r,\text{NLO}}$ is $\Gamma_{r,\text{NLO}}$ is $\Gamma_{r,\text{NLO}}$ is $\Gamma_{r,0}$ is

Consistent inverse-width expansion at NLOPS

n ME

Matrix element-based resonance histories

+



*illustration courtesy of T. Jezo





- $P_1 = B_{t\bar{t}}$ $P_2 = B_{tW^+}$
- squared-ME in pole approximation

$$\frac{P_3}{P_3}d\sigma + \frac{P_3}{P_1 + P_2 + P_3}d\sigma$$

 $P_3 = B_{\bar{t}W^-}$

$$_{\rm ME} = |\mathcal{A}_{\bar{t}W^+}|^2 \quad \rho_{tW^-}^{\rm (hist)}(\Phi_{\rm B})|_{\rm ME} = |\mathcal{A}_{tW^-}|^2$$



Matrix element-based resonance histories

		inclusive	2LB	2LB + off-shell
		phase space	cuts	cuts
LHE	OrigH	9.672(4)	4.422(3)	0.1908(6)
LHE	MeH	9.653(3)	4.411(2)	0.1912(4)
LHE	tW fraction	4.31%	3.86%	43.0%
NLOPS	OrigH	9.672(4)	4.419(3)	0.3515(8)
NLOPS	MeH	9.653(3)	4.408(2)	0.3502(5)
NLOPS	tW fraction	4.31%	3.86%	23.3%



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

Different resonance history projectors agree at <1% level!

Matrix element-based resonance histories

Naive
$$\rho_{t\bar{t}}^{(\text{hist})}(\Phi_{\text{B}})\Big|_{\text{naive}} = W_t(p_t)W_t(p_{\bar{t}}) - \rho_{\bar{t}W^{\pm}}^{(\text{hist})}(\Phi_{\text{B}})\Big|_{\text{naive}} = \frac{\chi m_t^2}{E_{\text{T},b}^2}W_t(p_{\bar{t}}) - W_t(p) = \frac{M_t^4}{(p^2 - M_t^2)^2 + \Gamma_t^2 M_t^2}$$

ME-based
$$A_{\text{full}} = A_{t\bar{t}} + A_{\bar{t}W^+} + A_{tW^-} + A_{\text{rem}}$$

$$\mathsf{ME} \quad \frac{\rho_{t\bar{t}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}} = |\mathcal{A}_{t\bar{t}}|^{2}}{\rho_{\bar{t}W^{\pm}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}}} = |\mathcal{A}_{\bar{t}W^{\pm}}|^{2}} \quad \mathsf{ME}' \quad \frac{\rho_{t\bar{t}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}'} = |\mathcal{A}_{\bar{t}W^{\pm}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2}}{\rho_{\bar{t}W^{\pm}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}'}} = |\mathcal{A}_{\bar{t}W^{\pm}}|^{2}, \qquad \mathsf{ME}' \quad \frac{\rho_{t\bar{t}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}''} = |\mathcal{A}_{\bar{t}W^{\pm}}|^{2}, \\ \rho_{\bar{t}W^{\pm}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}'} = |\mathcal{A}_{\bar{t}W^{\pm}}|^{2}, \qquad \mathsf{ME}' \quad \frac{\rho_{t\bar{t}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}''} = |\mathcal{A}_{\bar{t}W^{\pm}}|^{2}, \\ \rho_{\mathrm{rem}}^{(\mathrm{hist})}(\Phi_{\mathrm{B}})\big|_{\mathrm{ME}''} = |\mathcal{A}_{\mathrm{full}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2}, \qquad \mathsf{ME}'' \quad \mathsf{ME}'' \quad \mathsf{ME}'' \quad \mathsf{ME}'' \quad \mathsf{ME}'' \quad \mathsf{ME}'' \quad \mathsf{ME}'' = |\mathcal{A}_{\mathrm{full}}|^{2} - |\mathcal{A}_{\bar{t}W^{\pm}}|^{2} - |\mathcal{A}_{\bar{$$

	naive		matrix-	
	$\chi = 1$	$\chi = 0.1$	ME	
$t\bar{t}$	90.6%	95.3%	94.2%	9
tW	9.4%	4.7%	5.8%	
rem				

Might open the door to **tt vs tW separation**. Similar to "matrix-element methods". ^[Kondo, '88] However, remember: here separation at LO + Real





Semi-leptonic tt

 $pp \rightarrow \ell^{\pm} \nu_{\ell} j j b \bar{b}$

$lpha_{ m S}^n lpha^m$	dominant subprocesses	type	order		
$lpha_{ m S}^4 lpha^2$	$W^{\pm}b\bar{b}$ + 2 jets	V+HF	NNLO		
$lpha_{ m S}^3 lpha^3$	tiny interference				
$lpha_{ m S}^2 lpha^4$	$t\bar{t}+tWb$	$t\bar{t} + tW$	4FNS LO		
	$gq ightarrow tq' \overline{b}$ + 1 jet	t-chanel single-top	4FNS NLO 🔍		
	$q\bar{q}' ightarrow tar{b}$ + 2 jets	s-chanel single-top	NNLO		
	$W^{\pm}Z$ + 2 jets with $Z \rightarrow b\bar{b}$	VV	NNLO		
	$W^{\pm}jj$ + 2 <i>b</i> -jets	VBF	NNLO		
$lpha_{ m S}^1 lpha^5$	tiny interference				
$lpha^6$	$W^{\pm}Zjj$ with $Z ightarrow bar{b}$	VBS	LO		
	$W^{\pm}ZV$ with $Z ightarrow bar{b}, V ightarrow jj$	VVV	LO		
	1	1	1		



 $pp
ightarrow \ell^{\pm} \nu_{\ell} q \bar{q}' b \bar{b}$: [Denner, Pellen; 'I7]



Semi-leptonic tt





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Semi-leptonic tī: bb4l-sl





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Semi-leptonic tī: bb4l-sl









bb4I-sl vs. on-shell top-pair plus single-top





•Large differences between ST-DR and ST-DS in the tail of pTI

• bb4l agrees at O(1%) with ST-DS

bb4I-sl vs. on-shell top-pair plus single-top







- Control of reconstructed top-mass crucial for top-mass measurements

bb4I-sl vs. on-shell top-pair plus single-top

• Significantly smaller shower effects (and MEC) in bb4l-sl compared to hvq+ST



- Precision NLOPS predictions for off-shell tt+Wt crucial for top-mass measurements and backgrounds in searches.
- Resonance-aware matching mandatory
- Inverse-width expansion in off-shell fNLO and NLOPS computations ensures narrow-width limit. Numerical impact can be significant.
- Matrix-element based projectors indicate small remaining systematics in RES method.

- Semi-leptonic tt x decay available in **bb4I-sI** approximation (valid for $|m_{j_1j_2} m_W| < 30 \, \text{GeV}$) percent-level agreement of bb4l-sl with hvq+ST in inclusive phase-space Crucial shape-effects and reduced shower dependency with bb4l-sl

Conclusions

The resonance-aware bb4l generator [Jezo, JML, Nason, Oleari, Pozzorini, '16]

- Full process $pp \rightarrow b\bar{b}e^+\nu_e\mu^-\bar{\nu}_\mu$ with massive b's (**4FS scheme**)
- Implemented in the POWHEG-BOX-RES framework



Physics features:

- exact non-resonant / off-shell / interference / **spin-correlation** effects at NLO
- unified treatment of **top-pair and Wt** production with interference at NLO
- access to phase-space regions with **unresolved b**quarks and/or jet vetoes
- consistent NLO+PS treatment of top resonances, including quantum corrections to top propagators and off-shell top-decay chains

Standard POWHEG matching:

- Standard FKS/CS subtraction does not preserve virtuality of intermediate resonances \rightarrow R and B $(\sim S)$ with different virtualities.
- R/B enters POWHEG matching via generation of radiation and via Sudakov form-factor

 \rightarrow uncontrollable distortions

Resonance-aware POWHEG matching: [lezo, Nason, '15]

- Separate process in resonances histories
- Modified FKS mappings that retain virtualities

