Aspects of MC simulations for top quark physics

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Top Quark Physics at the Precision Frontier

Fermilab, 05/15/2019

Fermilab's special relationship with the top quark

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Observation of Top Quark Production in $\bar{p}p$ Collisions

Abstract

We establish the existence of the top quark using a 67 pb^{-1} data sam
of $\bar{p}p$ collisions at $\sqrt{s} = 1.8$ TeV collected with the Collider Detector at F
milab (CDF). Employing techniques similar to those we previously publish
we observe a signal consistent with $t\bar{t}$ decay to $WWb\bar{b}$, but inconsistent w
the background prediction by 4.8σ. Additional evidence for the top quark
provided by a peak in the reconstructed mass distribution. We measure t
top quark mass to be $176 \pm 8(\text{stat.}) \pm 10(\text{sys.})$ GeV/c^2, and the $t\bar{t}$ producti
cross section to be $6.8^{+3.6}_{-2.4}$ pb.

Observation of the Top Quark

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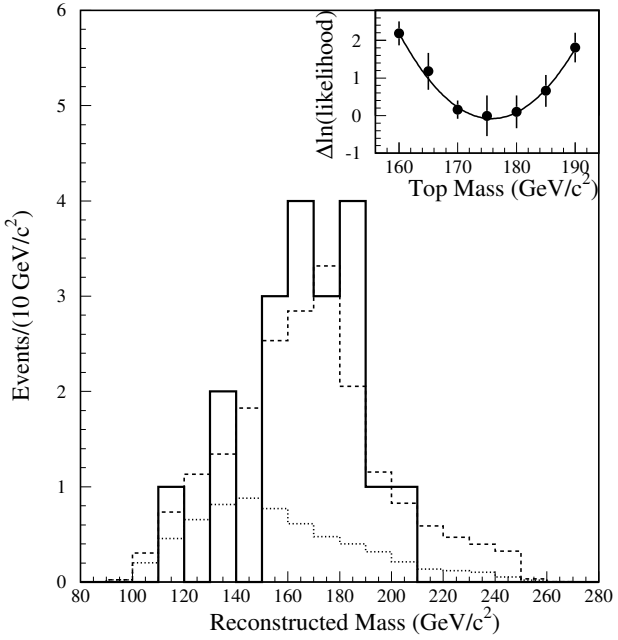
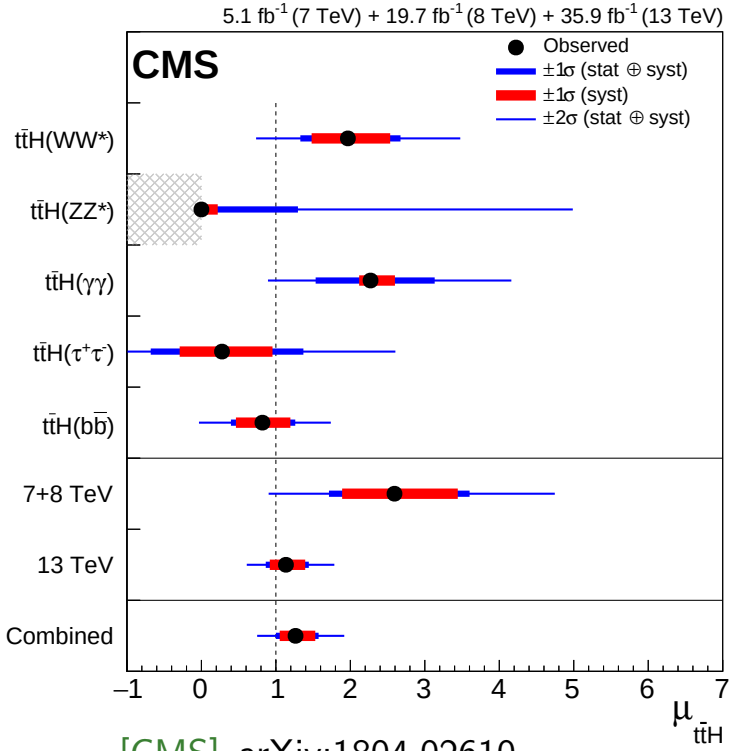
y,[23] T. Fahland,[4] M. Fatyga,[3]
Ferbel,[35] G. Finocchiaro,[38]
M. Fortner,[28] K.C. Frame,[23]

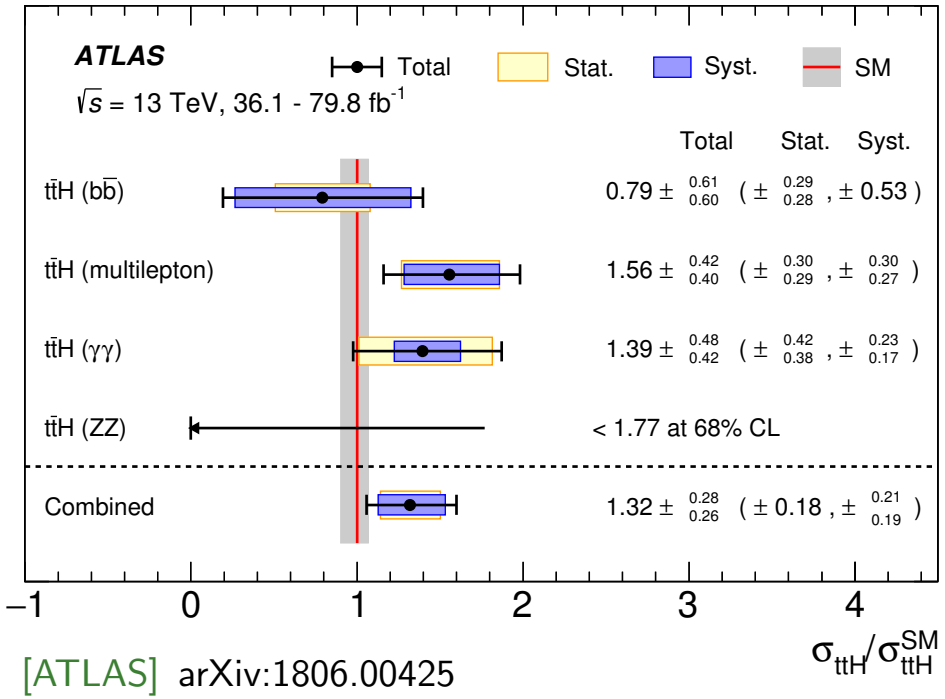


Top as a probe of the Higgs sector

- First direct evidence of Yukawa interactions
- Responsible for stability of EW vacuum?



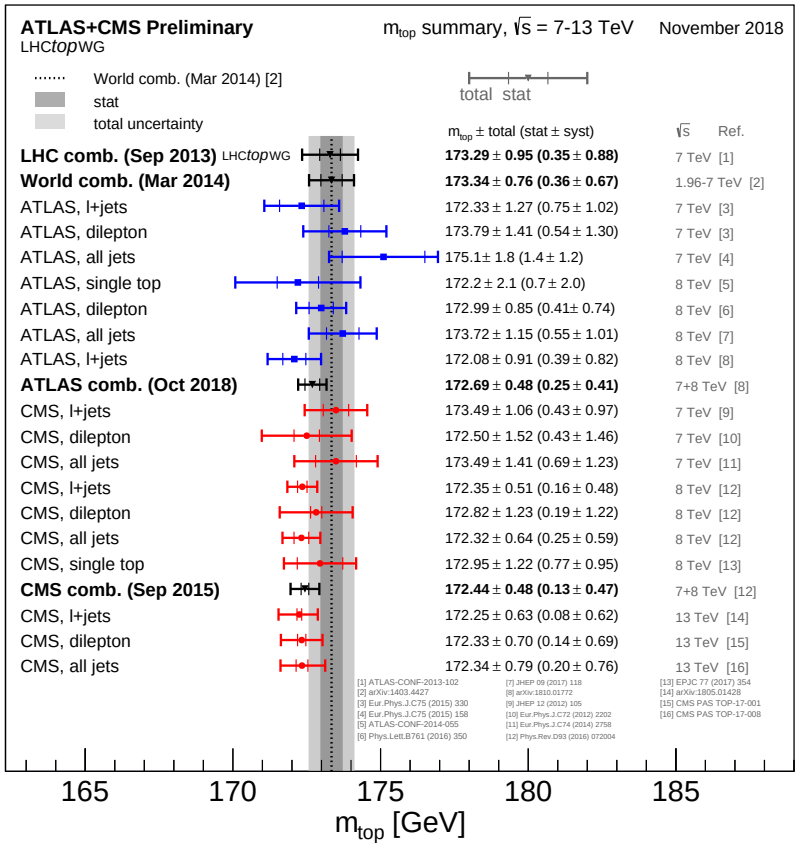
[CMS] arXiv:1804.02610



[ATLAS] arXiv:1806.00425

Top mass

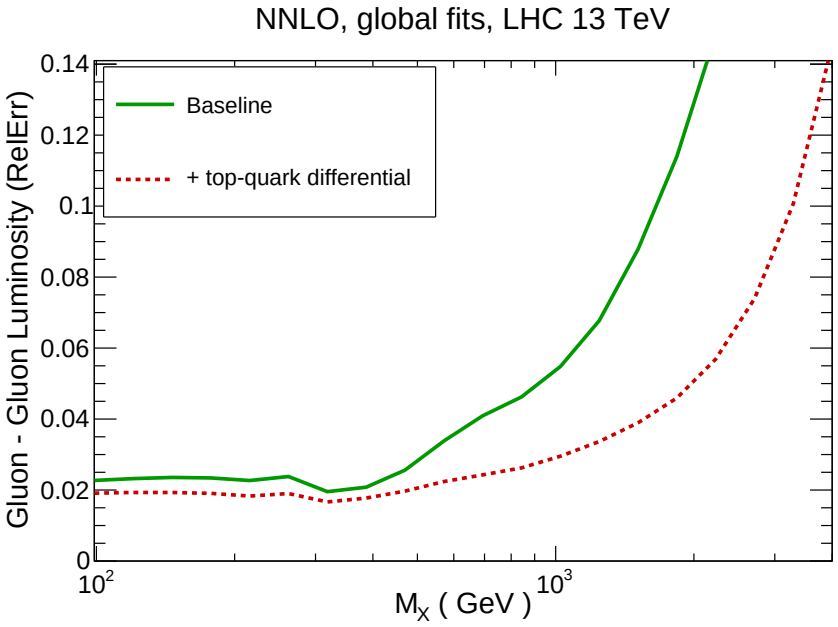
- Extracted from measurements of various observables e.g. $\sigma_{t\bar{t}}$, m_{lb}, m_{T2}, ...
- Complex hadronic & leptonic final states, often with extra jets
- Subtle theoretical issues
  - Top reconstruction
  - Radiative corrections
  - Off-shell effects
  - Color reconnection
  - MC mass vs. pole mass
  - ...

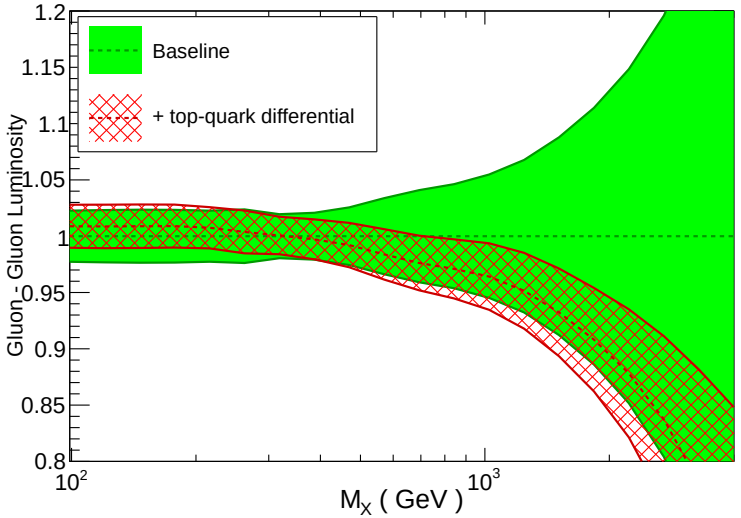


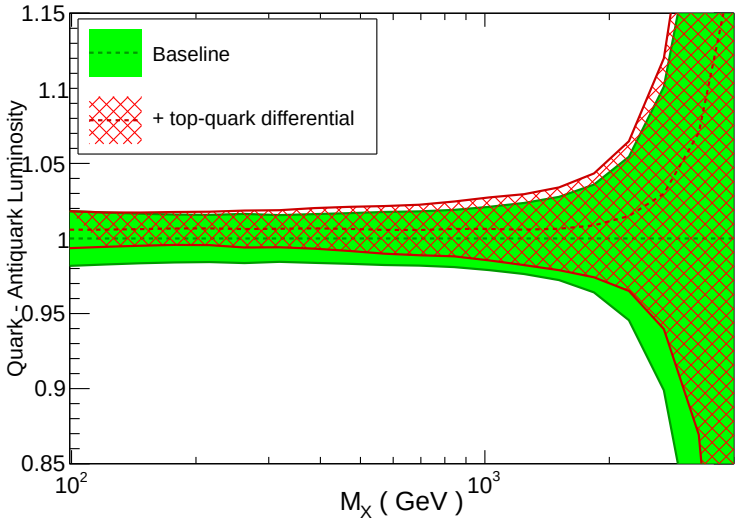
Top as a constraint on PDF fits

[Czakon,Hartland,Mitov,Nocera,Rojo] arXiv:1611.08609

- Pin down large-x gluon with the help of top-quark differential distributions





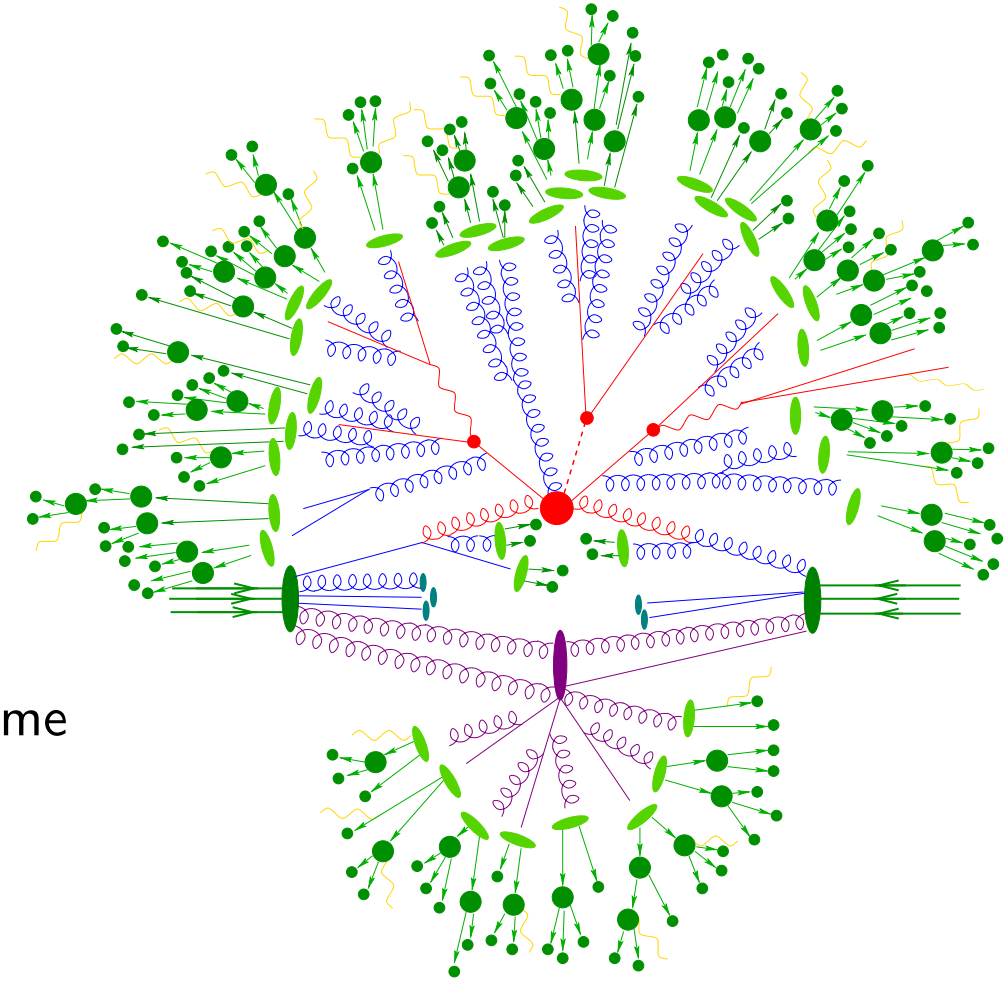


Top quark (pair) production

- Studied intensely, both at fixed order
  - NNLO QCD [Czakon,Fiedler,Mitov '13], [Czakon,Heymes,Mitov '16] [Catani,Devoto,Grazzini,Kallweit,Mazzitelli,Sargsyan '19]
  - NNLO QCD in production $\times$ decay [Gao,Papanastasiou '17] [Behring,Czakon,Mitov,Papanastasiou,Poncelet '19]
  - NNLO QCD + NLO EW [Czakon,Heymes,Mitov,Pagani,Tsinikos,Zaro '17]
  - NLO QCD / EW in production $\times$ decay [Bernreuther,Brandenburg,Si '04], [Melnikov,Schulze '09], [Campbell,Ellis '15], [Bernreuther,Si '10]
  - NLO QCD / EW $WWb\bar{b}$ [Bevilacqua,Czakon,vanHameren,Papadopoulos,Worek '11], [Denner,Dittmaier,Kallweit,Pozzorini '11+'12], [Heinrich,Maier,Nisius,Schlenk,Winter '14], [Frederix '14], [Cascioli,Kallweit,Maierhöfer,Pozzorini '14], [Denner,Pellen '16]
  - NLO QCD $t\bar{t}$+(multi-)jet [Dittmaier,Uwer,Weinzierl '07], [Bevilacqua,Czakon,Papadopoulos,Worek '10], [Maierhöfer,Moretti,Pozzorini,Siegert,SH '16]
  - ...
- and in the context of particle-level Monte Carlo
  - NLO QCD+PS [Frixione,Nason,Webber '03], [Frixione,Nason,Ridolfi '07]
  - NLO QCD+PS in production $\times$ decay [Campbell,Ellis,Nason,Re '15]
  - NLO QCD+PS $WWb\bar{b}$ [Garzelli,Kardos,Trocsanyi '14], [Jezo,Lindert,Nason,Oleari,Pozzorini '16]
  - NLO QCD+PS vs. NLO $WWb\bar{b}$ [Heinrich,Maier,Nisius,Schlenk,Schulze,Scyboz,Winter '17]
  - NLO QCD+PS $t\bar{t}$+(multi-)jet [Kardos,Papadopoulos,Trocsanyi '11], [Alioli,Moch,Uwer '11], [Huang,Luisoni,Schönherr,Winter,SH '13], [Krauss,Maierhöfer,Pozzorini,Schönherr,Siegert,SH '14]
  - ...

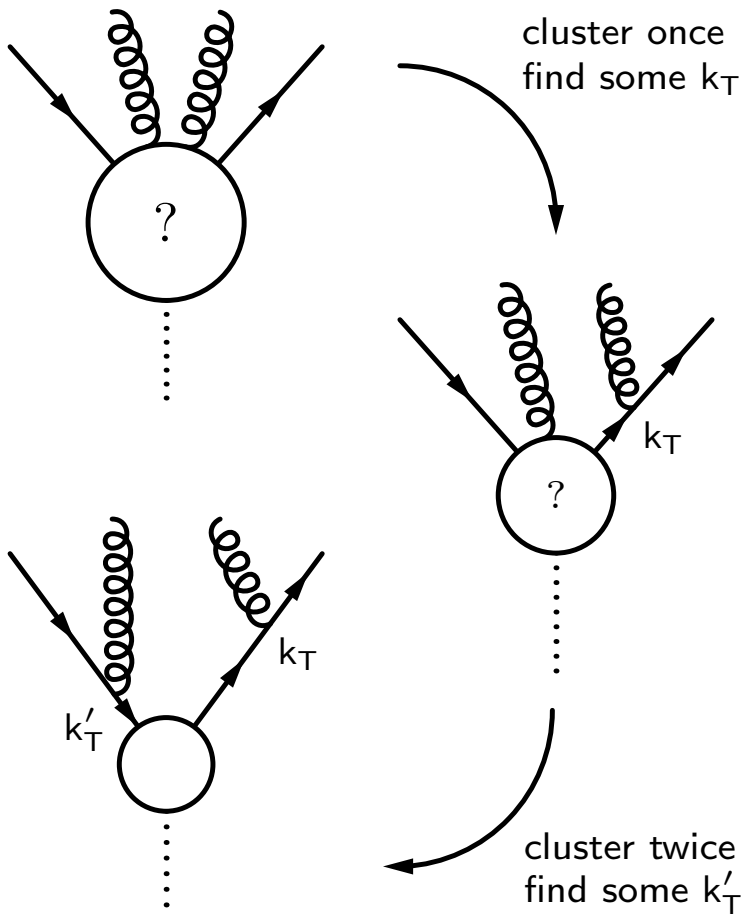
Outline of this talk

- Stability of fixed-order & particle-level predictions
- Impact of parton shower on top mass measurement
- $t\bar{t}b\bar{b}$ four vs. five flavor & variable flavor number scheme



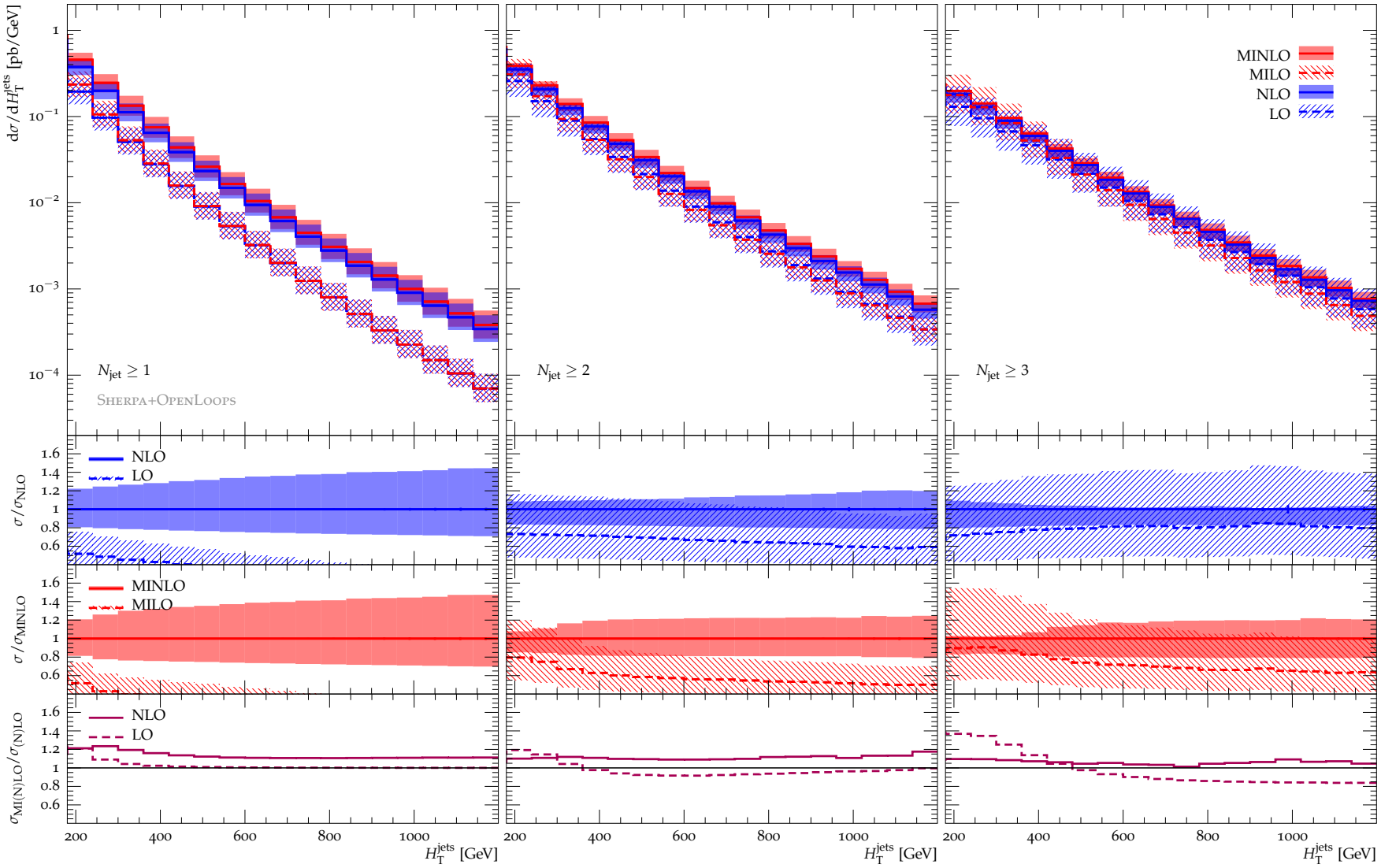
Scale uncertainties in $t\bar{t}$+jets at NLO

- Renormalization/factorization scale typically used at very high multiplicity: sum of transverse mass $H'_{T,m} = \sum m_\perp$
- Very different scale in resummation [Hamilton,Nason,Zanderighi] arXiv:1206.3572
  - Interpret event in terms of QCD branchings, like in a parton-shower
  - Assign transverse momentum scales q to splittings, evaluate one α_s at each of these scales
  - Multiply with NLL Sudakov factors, subtract first-order expansion
- MINLO scale probes detailed dynamics, typically very small $\rightarrow$ good candidate for comparison to $H'_{T,m}$



Scale uncertainties in $t\bar{t}$+jets at NLO

[Maierhöfer,Moretti,Pozzorini,Siegert,SH] arXiv:1607.06934



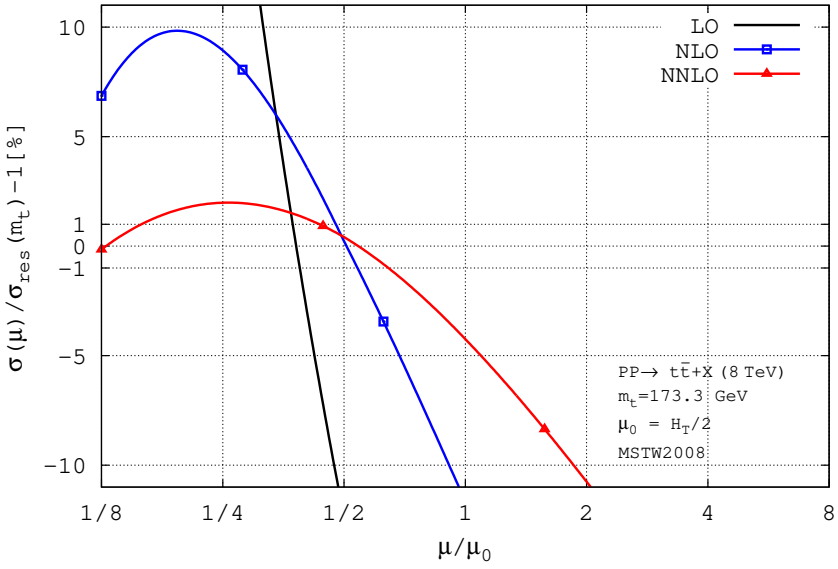
Scale uncertainties in $t\bar{t}$ at NNLO

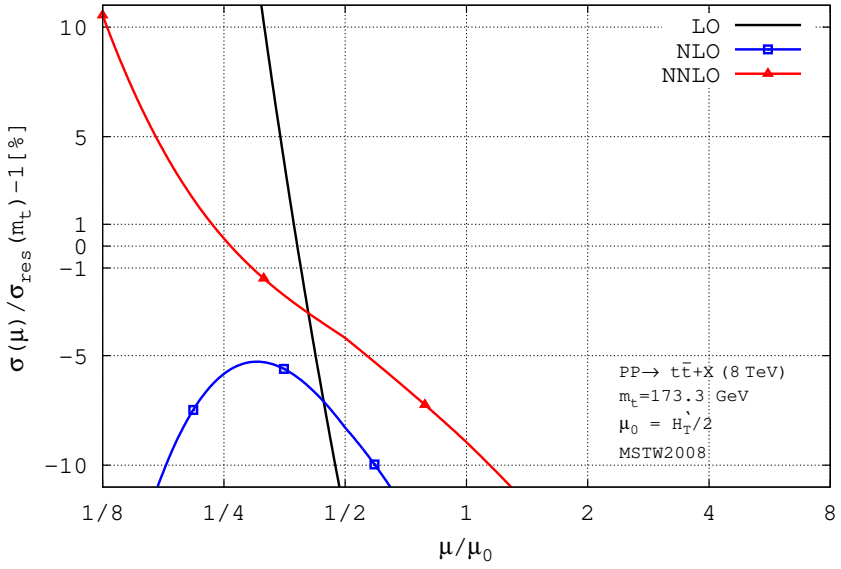
[Czakon,Heymes,Mitov] arXiv:1606.03350

- Various central scales investigated for perturbative convergence
- Best choices observable dependent and given by

$$\mu_0 = \begin{cases} \frac{m_T}{2} & \text{for :} \quad p_{T,t},\ p_{T,\bar{t}} \text{ and } p_{T,t/\bar{t}} \\ \frac{H_T}{4} & \text{for :} \quad \text{all other distributions} \end{cases}$$

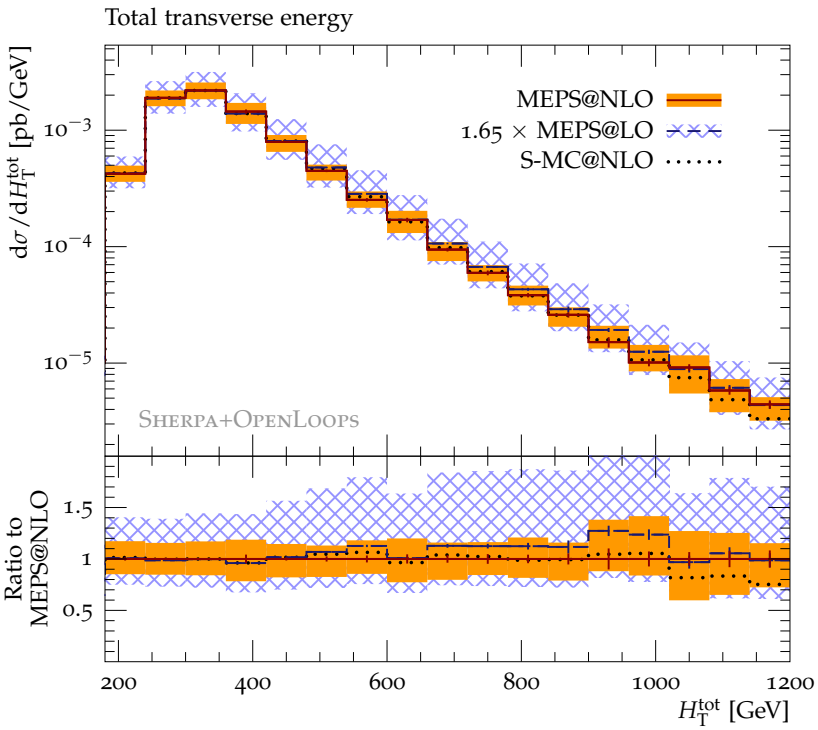
- Peculiar behavior of $H'_{T,m}$ based scale at NNLO

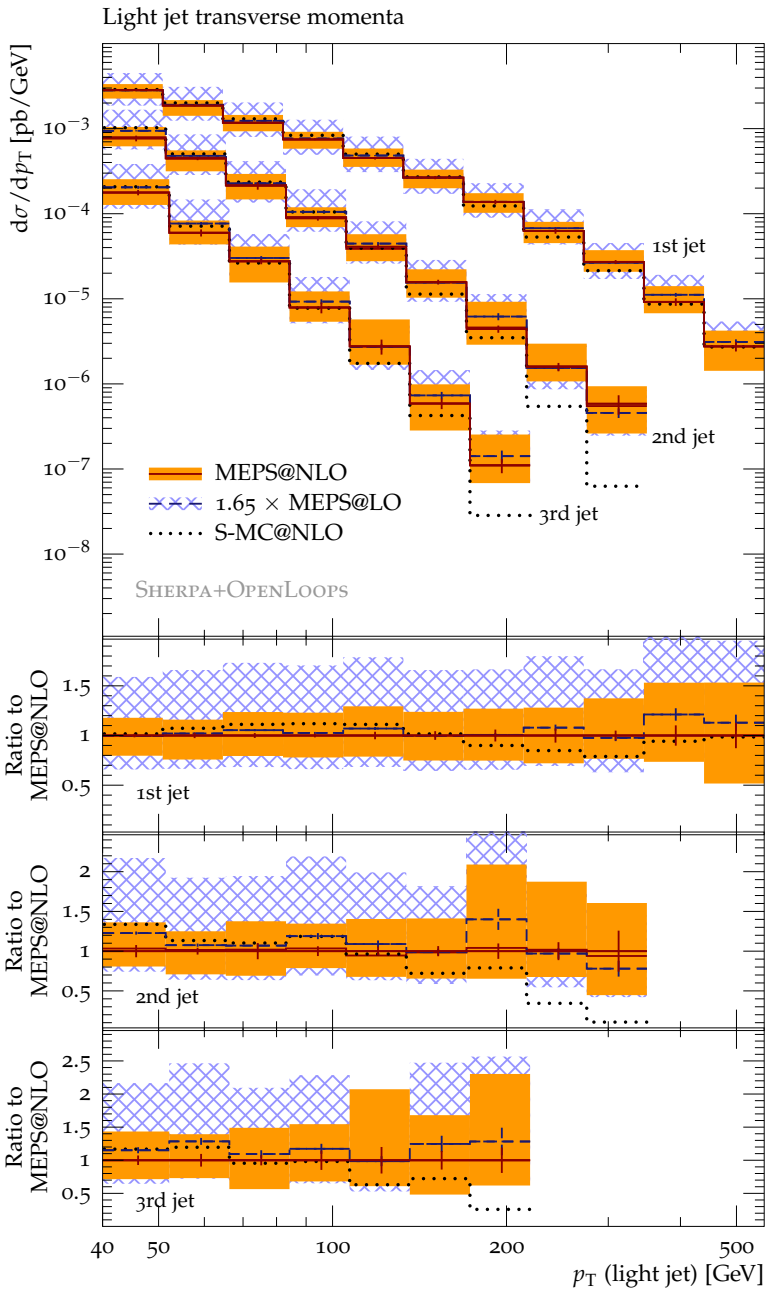




Multi-jet merging for $t\bar{t}$+jets

- NLO-matched & merged simulations available up to $t\bar{t}$+2j [Frederix,Frixione '12], [Krauss,Maierhöfer,Pozzorini,Schönherr,Siegert,SH '14]
- Decays & spin correlations at LO
- Largely reduced $\mu_{R/F}$ variations, central values agree well with LO merged predictions

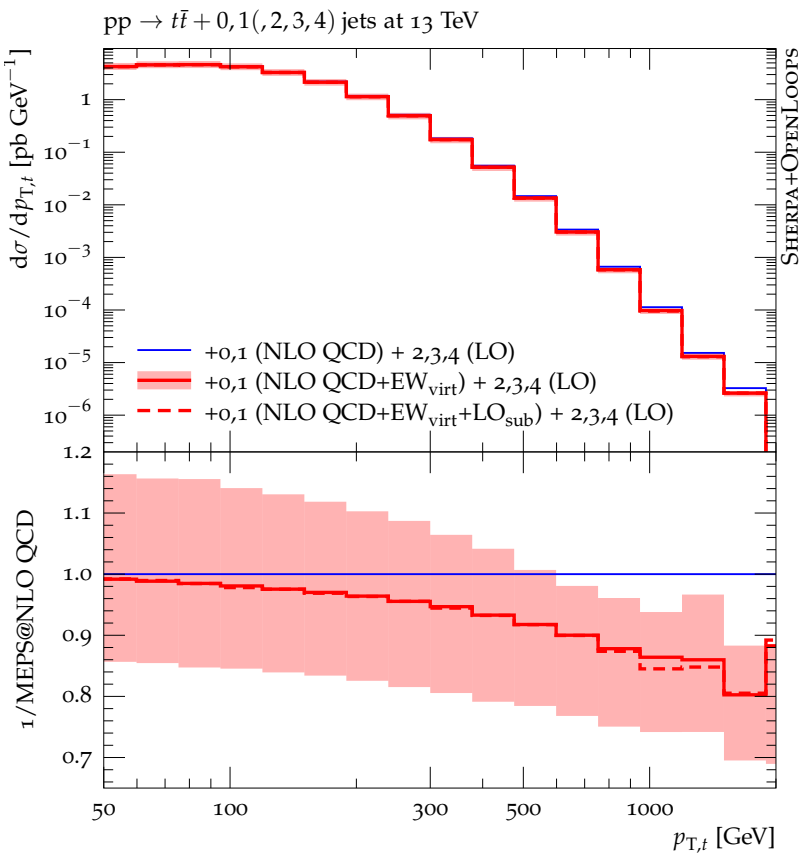


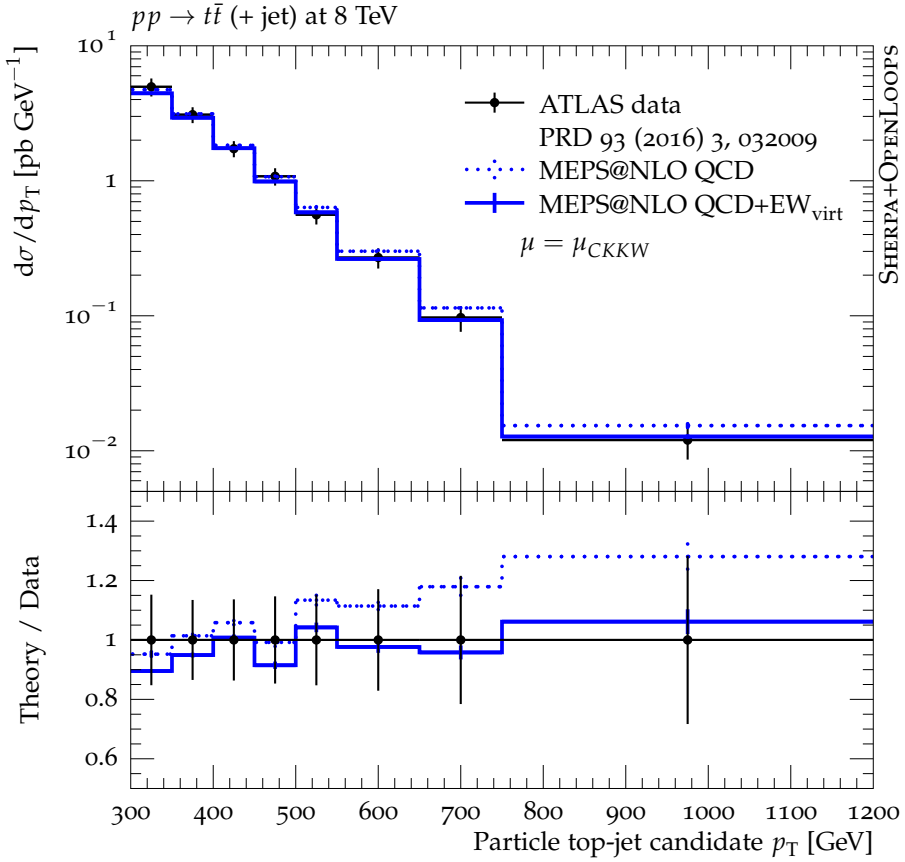


EW corrections in multi-jet merging

[Kallweit,Lindert,Maierhöfer,Pozzorini,Schönherr] arXiv:1511.08692
[Gütschow,Lindert,Schönherr] arXiv:1803.00950

- EW virtual corrections & integrated subtraction can be included in merging
- Real corrections recovered to a good accuracy by parton shower or YFS





Matching – Processes with intermediate resonances

[Jezo,Nason] arXiv:1509.09071

- NLO subtraction methods do not preserve virtuality of possible resonances
  IR cancellation takes place highly non-locally $\rightarrow$ efficiency problem
- Problem worsens in POWHEG, as uncontrollable ratios are exponentiated:

$$\Delta(\Phi_B, p_T) = \exp\left\{ -\sum_\alpha \int \mathrm{d}\Phi_1 \frac{\mathrm{R}(\Phi_R^{(\alpha)})}{\mathrm{B}(\Phi_B)} \Theta(p_T - k_T) \right\}$$

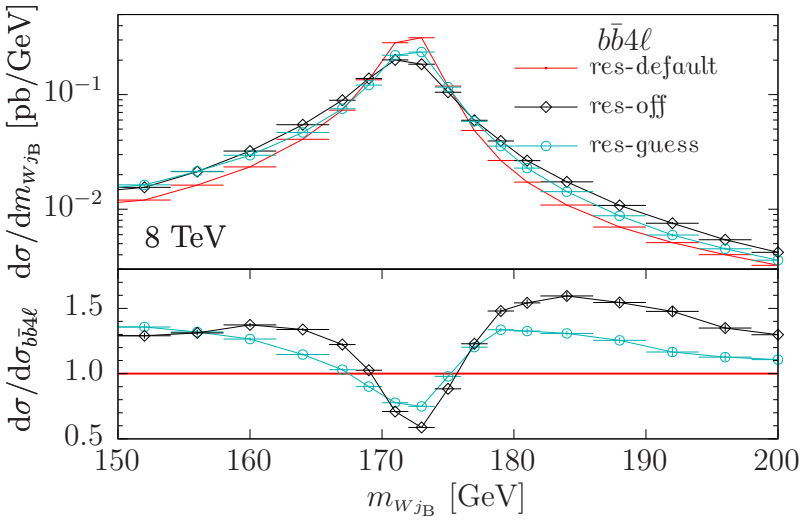
- Proposed solution:
  - Partition phase space such that each region corresponds to a unique resonance history
  - Within each region modify subtraction mappings such that resonance mass is preserved
- Assignment of resonance histories requires algorithm
  $\rightarrow$ Use kinematic proximity to resonance

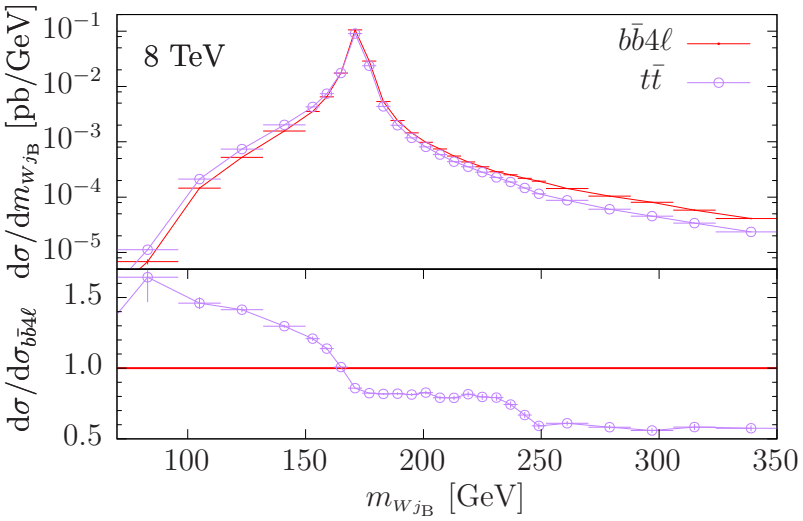
$$\Pi_{f_b} = \frac{P_{f_b}}{\sum_{f_b' \in \text{res hists}} P_{f_b'}} \,, \quad P_{f_b} = \prod_{i \in \text{ress}} \frac{M_i^4}{(s_i - M_i^2)^2 + \Gamma_i^2 M_i^2}$$

Matching – Wt vs $t\bar{t}$

[Jezo,Lindert,Oleari,Nason,Pozzorini] arXiv:1607.04538

- Wt production in the 5F scheme:
  - NLO corrections swamped by LO $t\bar{t}$ decay
  - Requires ad-hoc subtraction prescription (DR/DS)
- Wt production in the 4F scheme:
  - Unified treatment of Wt and $t\bar{t}$ (identical at LO)
  - Requires off-shell $WWb\bar{b}$ calculation
- Sizable differences compared to resonance-unaware matching and to narrow-width approach [Frixione,Nason,Ridolfi] arXiv:0707.3088

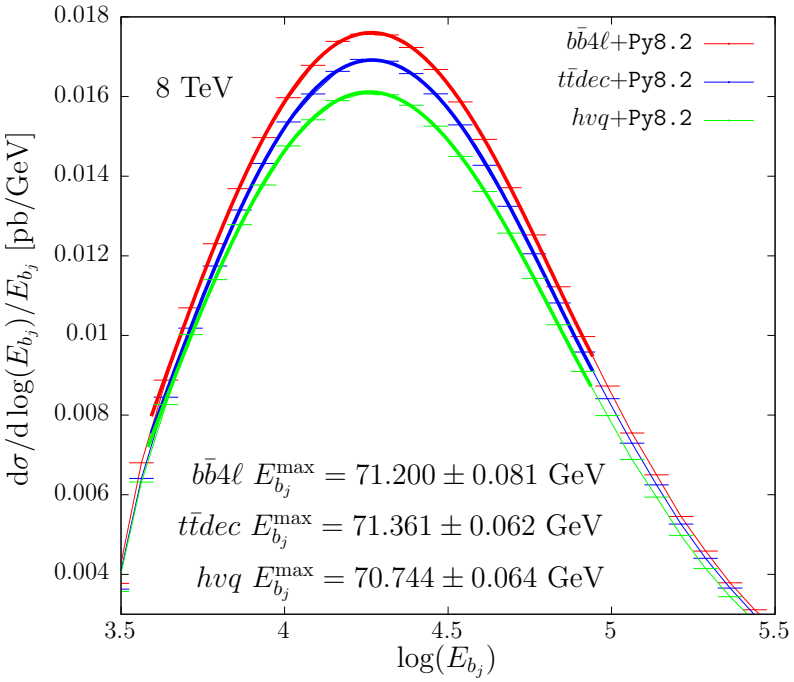


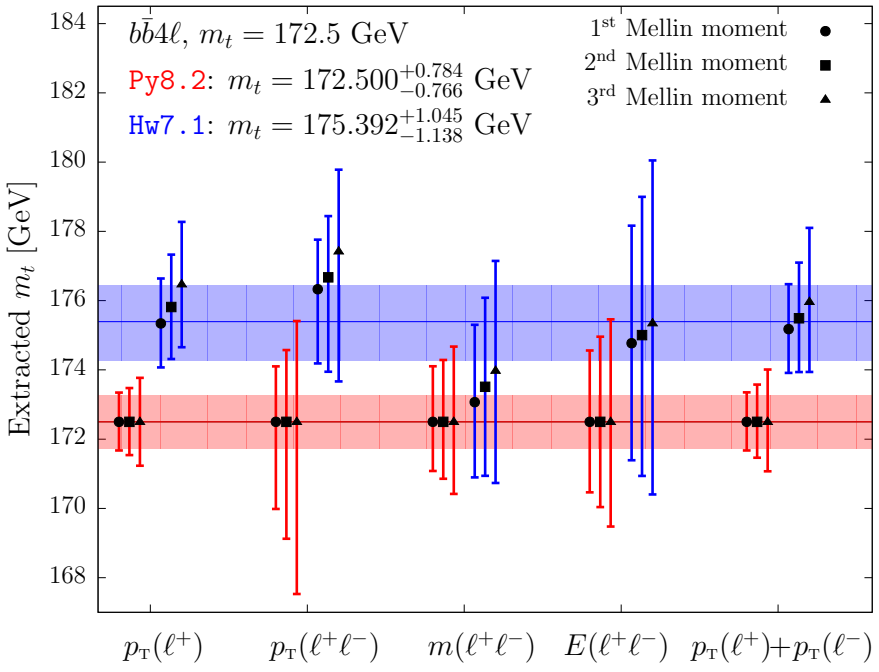


Top quark mass from kinematical distributions

[Ravasio,Jezo,Nason,Oleari] arXiv:1801.03944

- If top quark mass extracted from kinematical distributions quality of Monte Carlo modeling limits precision
  1. Generators of increasing accuracy $\rightarrow$ NLO $t\bar{t}$, NLO production $\times$ decay, NLO $W^+W^-b\bar{b}$
  2. Different parton-shower models $\rightarrow$ Pythia, Herwig
- For a large range of observables good consistency, except PS dependence

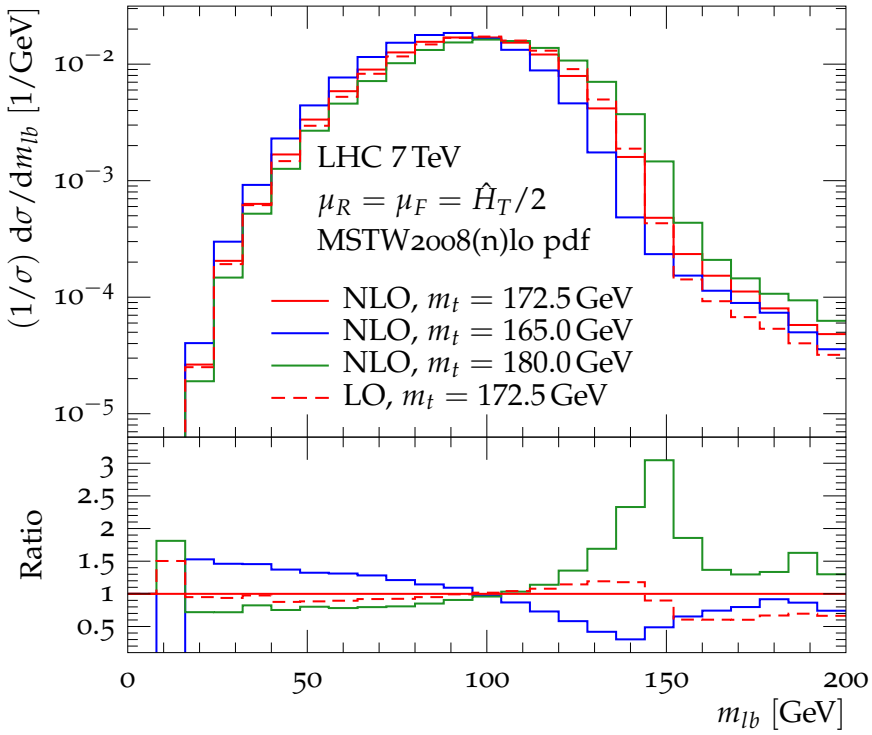


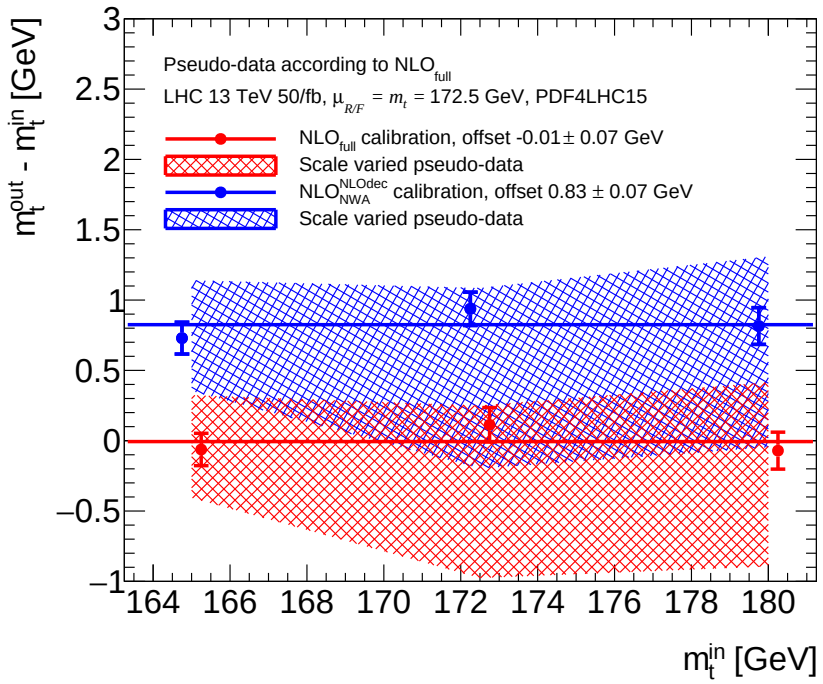


Top quark mass from m_{lb}

[Heinrich,Maier,Nisius,Schlenk,Winter] arXiv:1312.6659
[Heinrich,Maier,Nisius,Schlenk,Schulze,Scyboz,Winter] arXiv:1709.08615

- Determine top mass from template fit to $m_{lb}^2 = (p_{b-\mathrm{jet}} + p_l)^2$
- ATLAS-CONF-2013-077: use lepton b-jet pairing minimizing $\sum m_{lb}$
- Theory uncertainty estimated to 0.8 GeV at $\sqrt{s}$ =7 TeV
- Improve using NLO QCD $W^+W^-b\bar{b}$ from GoSam+Sherpa

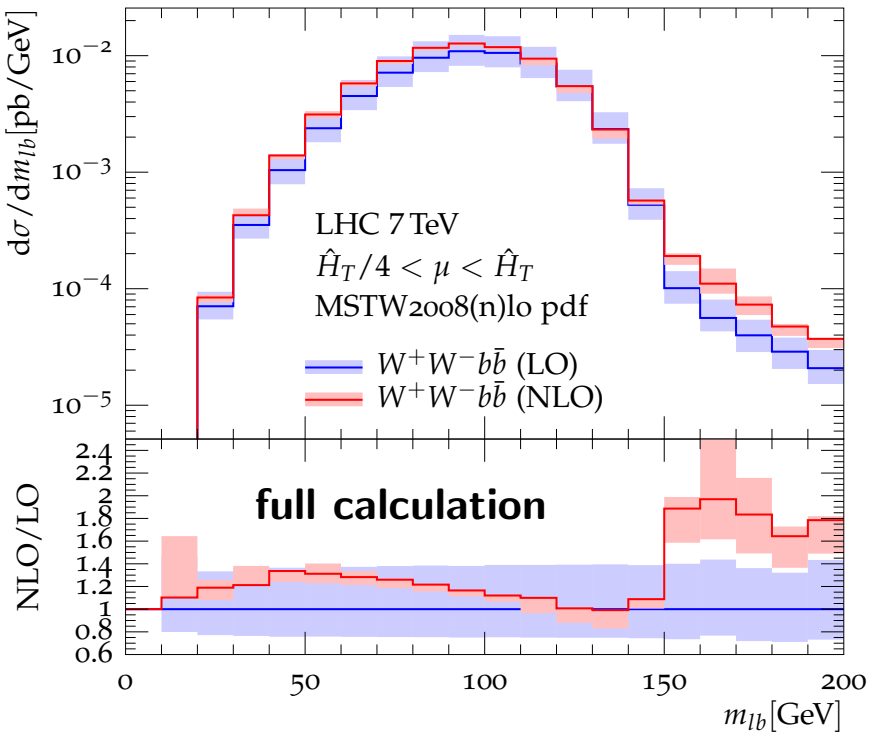


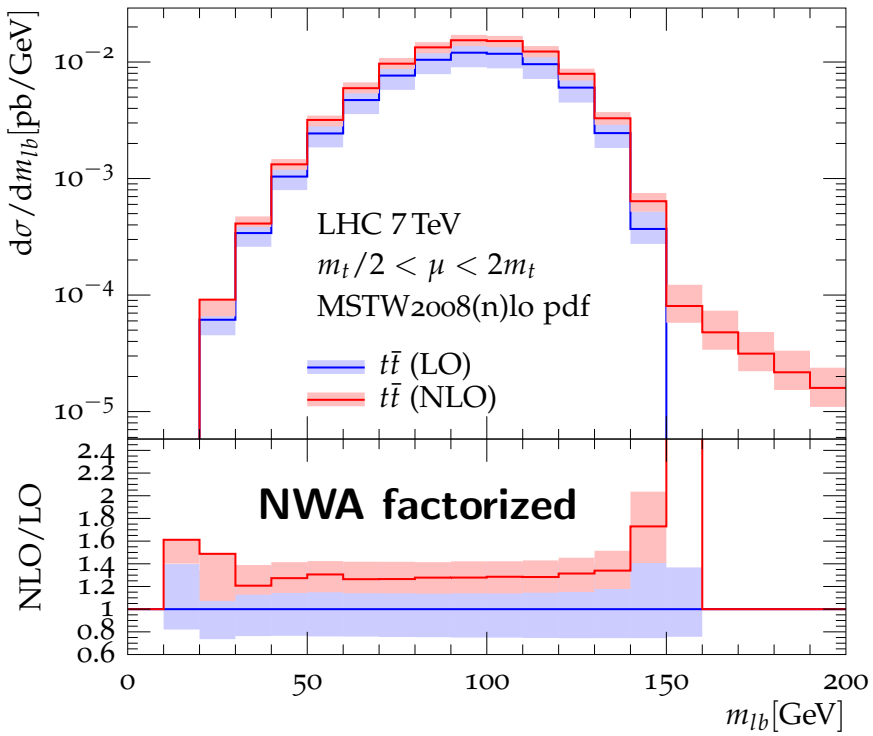


Top quark mass from m_{lb}

[Heinrich,Maier,Nisius,Schlenk,Winter] arXiv:1312.6659

- $m_{lb}^2 > m_t^2 - m_W^2$ kinematically forbidden in NWA at LO
- NLO corrections flat with symmetric bands in NWA
- Significant changes in shapes & uncertainty bands at NLO in $W^+W^-b\bar{b}$
  Driven by radiative corrections or non-factorizing contributions?

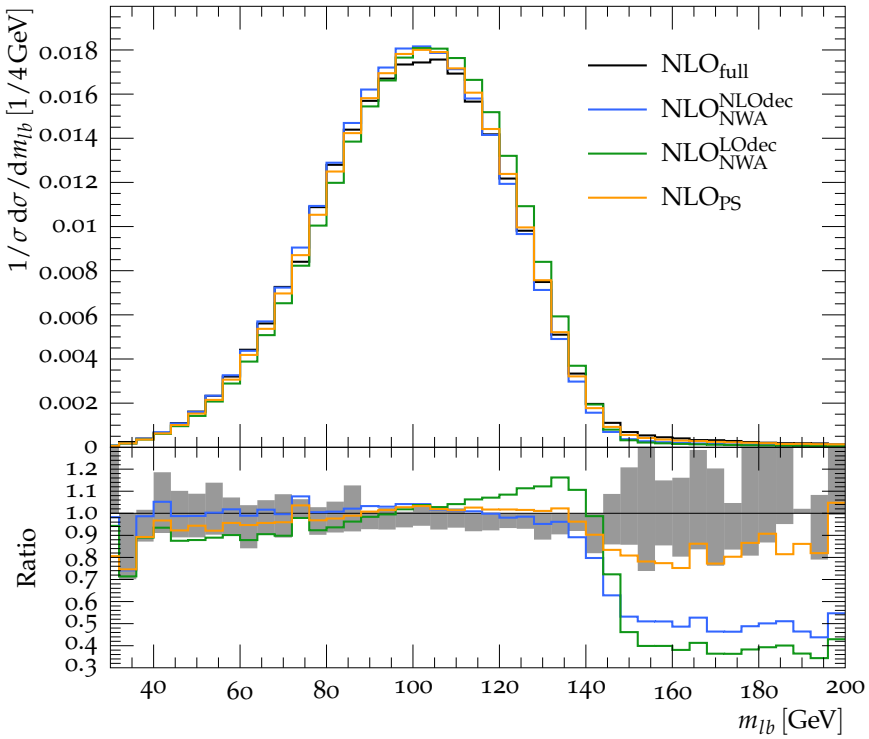


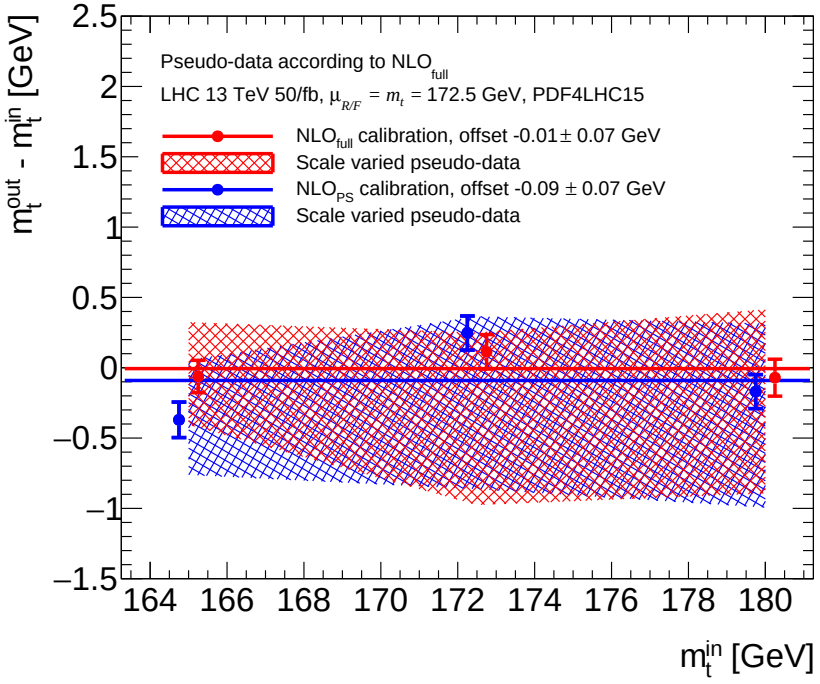


Top quark mass from m_{lb}

[Heinrich,Maier,Nisius,Schlenk,Schulze,Scyboz,Winter] arXiv:1709.08615

- Accidental agreement between NLO $W^+W^-b\bar{b}$ and NLO+PS (Sherpa)
  Maybe not completely accidental? NLO+PS has BW distribution!





Parton shower cutoff and the top-quark mass

[Hoang,Plätzer,Samitz] arXiv:1807.06617

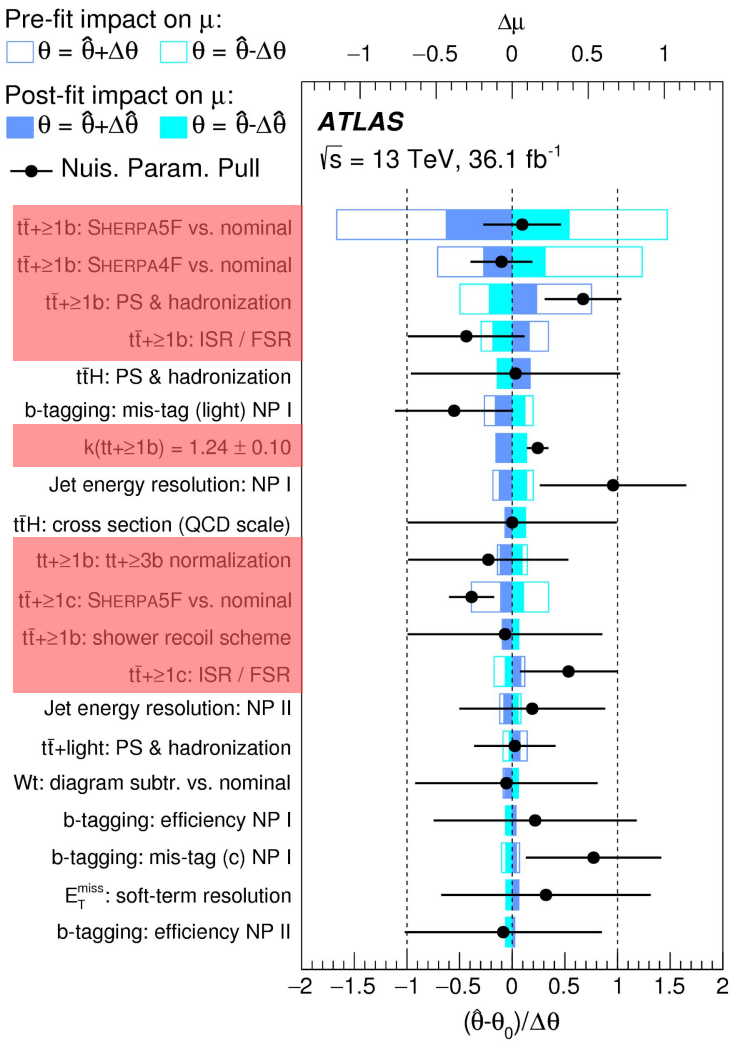
- Investigated jet mass distribution in $e^+e^- \to t\bar{t}$
- Established relation between pole mass, m_{pole}, and coherent branching mass, $m_{CB}(Q_0)$, which depends on the parton-shower cutoff Q_0
- Comparison between coherent branching formalism and SCET shows $\lim_{Q_0 \to 0} m_{CB}(Q_0) = m_{pole}$, both for massless and massive quarks
- Pole mass and coherent branching mass related for finite Q_0 by

$$m_{CB}(Q_0) = m_{pole} - \frac{2}{3}\alpha_s(Q_0)Q_0 + \mathcal{O}(\alpha_s^2)$$

Status of $t\bar{t}b\bar{b}$

[F.Siegert SM@LHC '19]

- ATLAS and CMS $t\bar{t}H(b\bar{b})$ analyses rely on MC modelling for irreducible $t\bar{t}b\bar{b}$ BG
- Largest sources of uncertainty on extracted signal strength related to $t\bar{t}$+HF modeling!
- What can be improved?
  - ATLAS & CMS: relied on NLO+PS $t\bar{t}$ so far! More accurate theory with NLO $t\bar{t}b\bar{b}$ used only to reweight HF fractions (ATLAS) or cross-checks (CMS)
  - Theory: Large perturbative $t\bar{t}b\bar{b}$ uncertainties even increased by NLO+PS algorithms
  - Both: More rigorous combination of inclusive $t\bar{t}$+jets and $t\bar{t}b\bar{b}$ predictions.



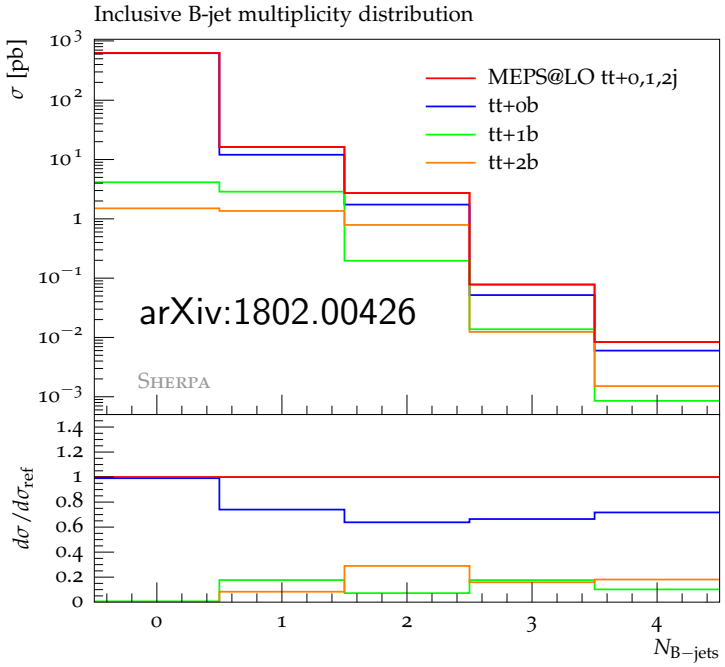
Status of $t\bar{t}b\bar{b}$

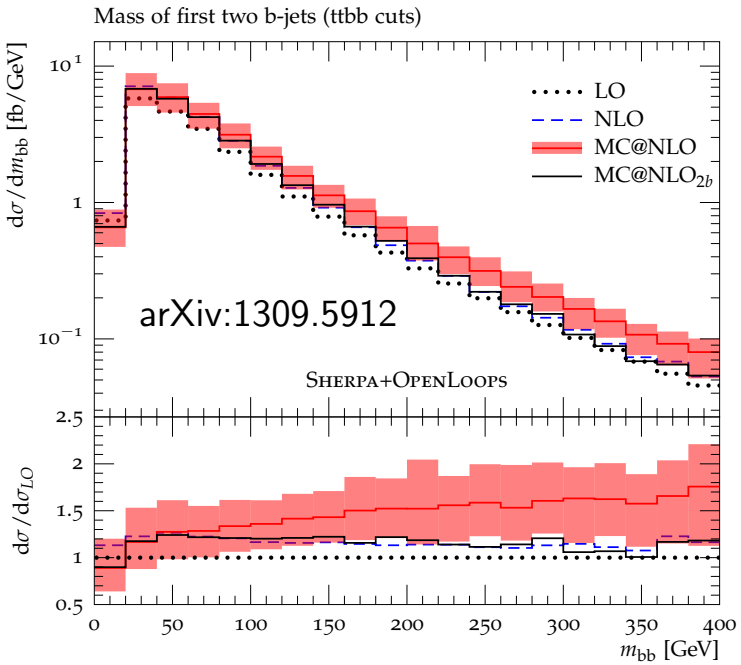
Traditional MC simulation approaches to $t\bar{t}$+HF

- **Five-flavor scheme**:
  - Inclusive NLO+PS $t\bar{t}$ sample with HF from parton shower $g \to b\bar{b}$
  - Multi-leg merged $t\bar{t}$+jets sample with HF from higher-order MEs (hard b) or parton shower $g \to b\bar{b}$ (soft/coll b)

  Surprising feature:
  - Jet production described by hard MEs, but b-jets not always from b-MEs!
  - soft/collinear $g \to b\bar{b}$ from PS can transform light jets into b-jets
- **Four-flavor scheme**:
  - NLO+PS $t\bar{t}b\bar{b}$ using matrix elements with massive b-quarks

  Surprising feature:
  - Secondary $b\bar{b}$ from $g \to b\bar{b}$ in PS can convert light jet into b-jet $\to$ even interpretation changes

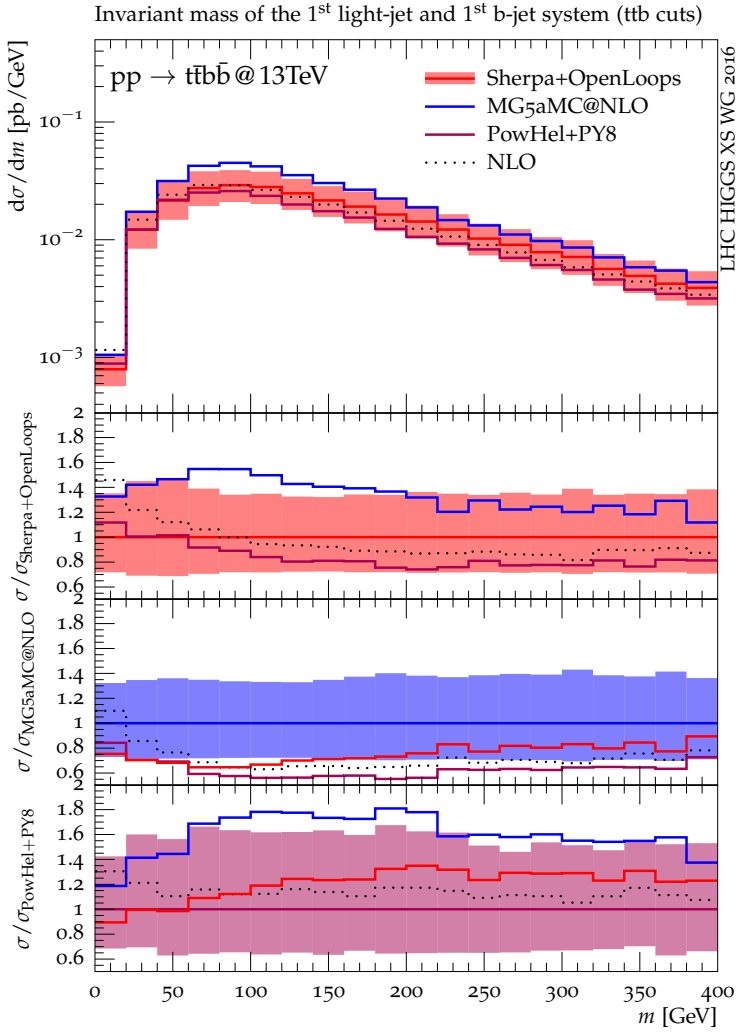




Status of $t\bar{t}b\bar{b}$

- Several tools on the market
  - Sherpa + OpenLoops [Cascioli,Maierhöfer, Moretti,Pozzorini,Siegert] arXiv:1309.5912
  - PowHel + Pythia/Herwig [Bevilacqua,Garzelli,Kardos] arXiv:1709.06915
  - PowhegBox + OpenLoops + Pythia/Herwig [Jezo,Lindert,Moretti,Pozzorini] arXiv:1802.00426
  - MG5_aMC + Pythia/Herwig
  - Herwig7 + OpenLoops
- History of out-of-the-box comparisons:
  - Large discrepancies
  - Due in part to pQCD uncertainties
  - But also beyond: Parton Shower, NLO+PS matching algorithm
- Ongoing: Tuned comparison
- Fixed-order studies of $t\bar{t}b\bar{b}j$ at NLO show stabilization of K-factor for $\mu_R = (E_{T,t}E_{T,\bar{t}}E_{T,b}E_{T,\bar{b}})^{1/4}$
  $\rightarrow$ New benchmark for NLO+PS programs! [Buccioni,Pozzorini,Zoller '19]

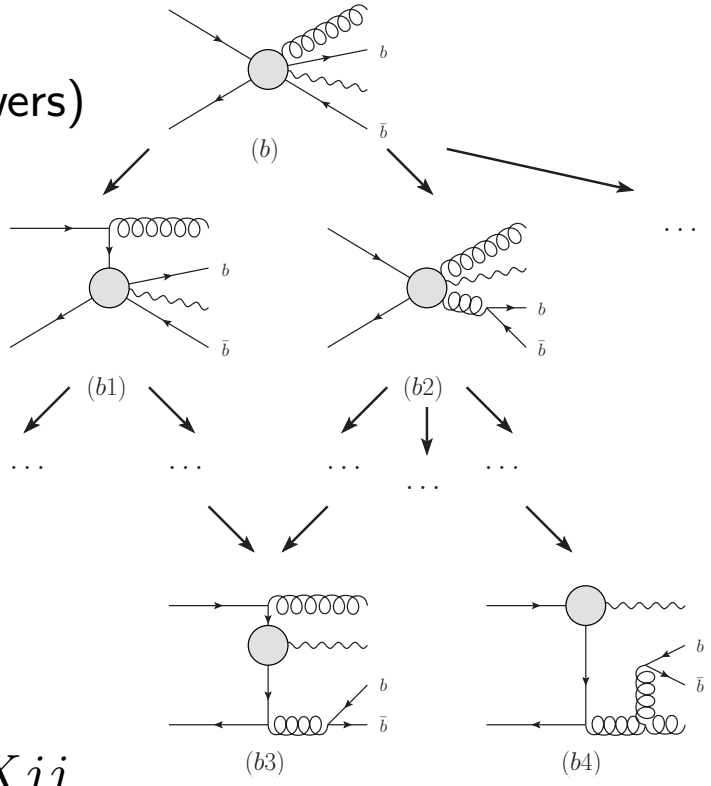
[HXSWG] arXiv:1610.07922



Matching X+jets & $Xb\bar{b}$

[Krause,Siegert,SH] arXiv:1904.09382

- **Interpret $Xb\bar{b}$ as part of Xjj**
  1. Cluster to obtain parton shower history
  2. Apply $\alpha_s(\mu_R^2) \to \alpha_s(p_T^2)$ reweighting
  3. Apply Sudakov factors $\Delta(t, t')$ (trial showers)
- **Remove double-counting**
  1. Cluster PS-level event using inverse PS
  2. Look at leading two emissions
     - Heavy Flavour $\to$ keep from $Xb\bar{b}$ ("direct component")
     - Light Flavour $\to$ keep from X+jets ("fragmentation component")
     - Subleading $g \to b\bar{b}$ splittings not from $Xb\bar{b}$ ME, but $X4j$ ME+PS
- **Match 5F$\to$4F in PDFs and α_s**
  1. Use 5F PDF / α_s to be consistent with Xjj
  2. Use matching coefficients to correct to 4F scheme
     [Buza,Matiounine,Smith,van Neerven] hep-ph/9612398, [Forte,Napoletano,Ubiali] arXiv:1607.00389
     $\to$ Coefficients up to (N)LL generated by (N)LO parton shower!
  3. Reweighting needed only for α_s in hard ME

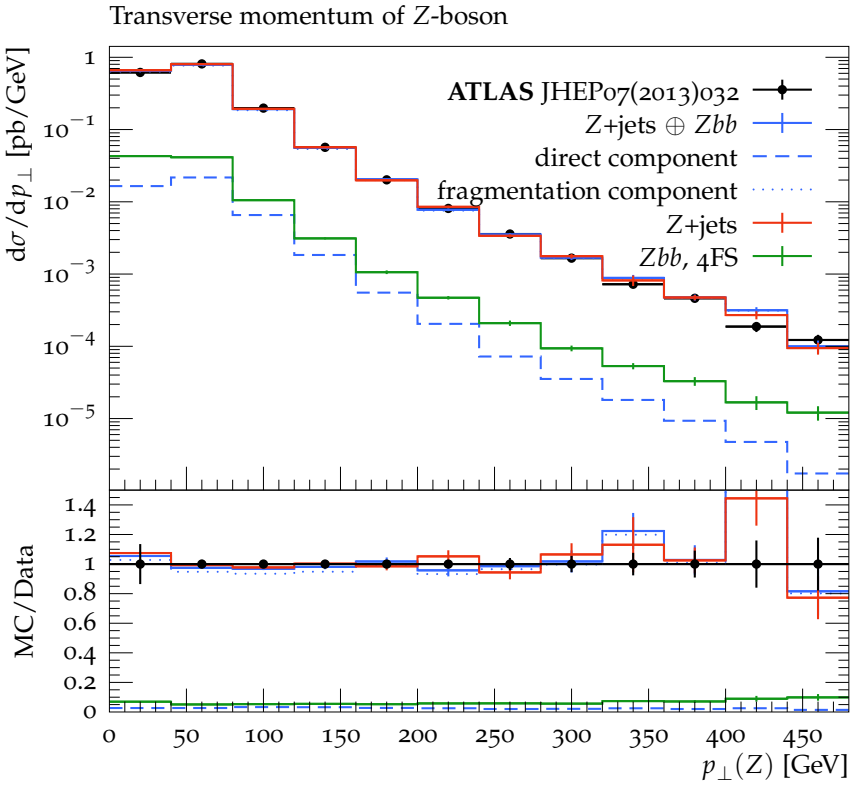


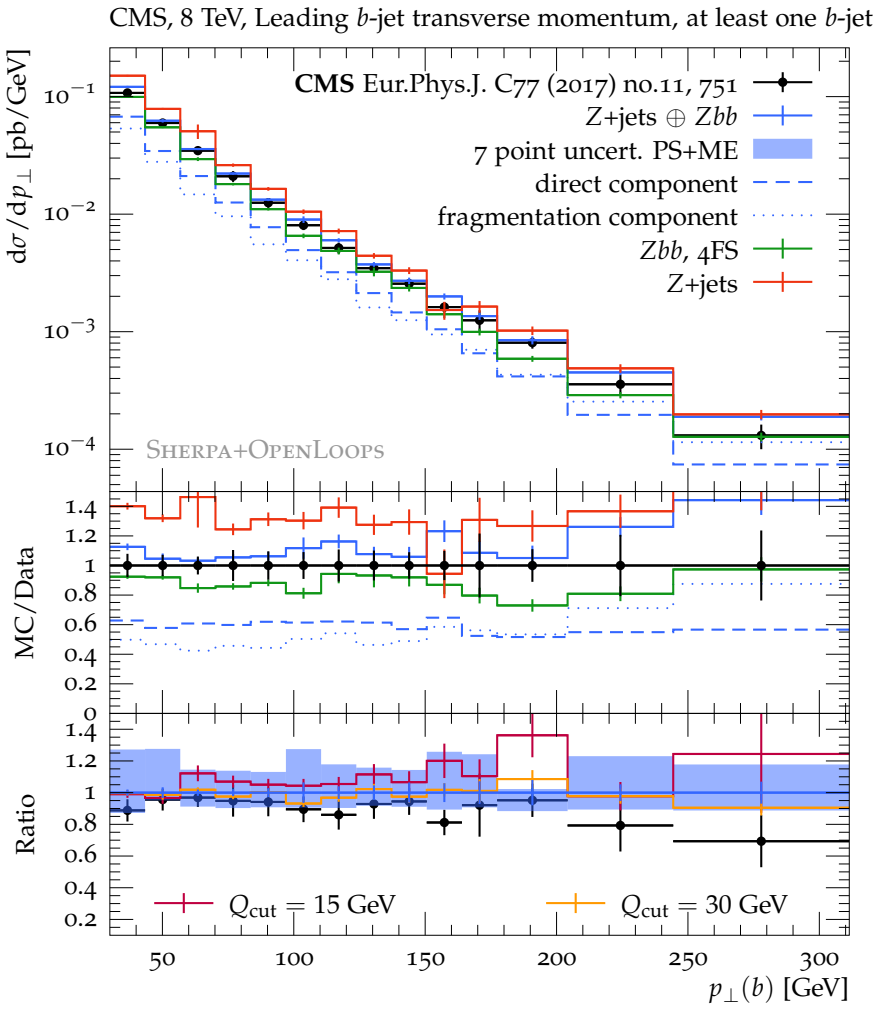
Can be applied to LO and NLO merging!

Example: Z+jets & $Zb\bar{b}$

- Validation with LHC data

[Krause,Siegert,SH] arXiv:1904.09382





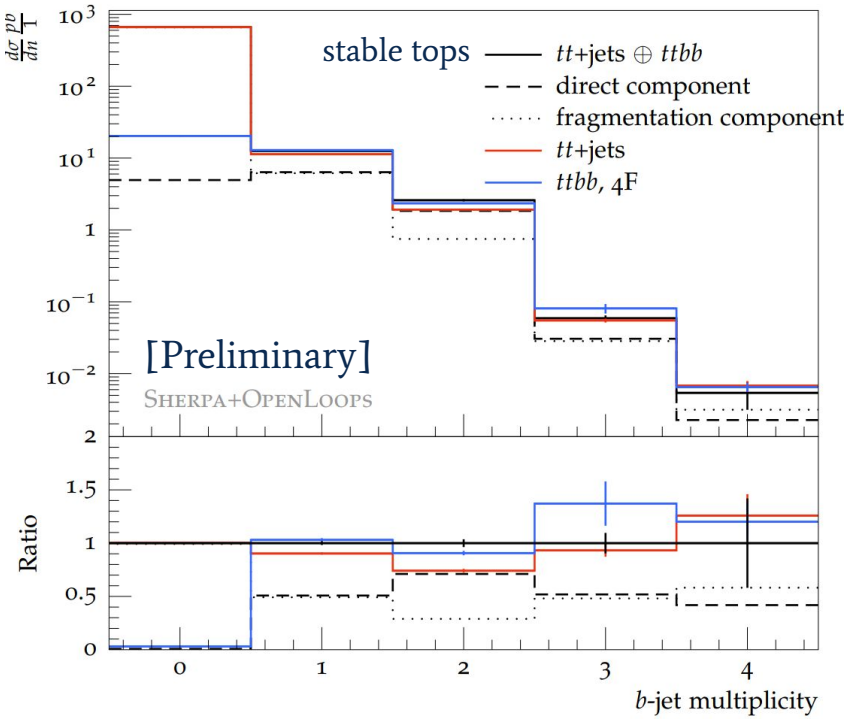
	Data [pb]	**Fusing** [pb]
$Z+\geq 1b$	$3.55 \pm 0.24_{\text{comb}}$	$3.80(5) \pm$ 0.83 0.33
$Z+\geq 2b$	$0.331 \pm 0.037_{\text{comb}}$	$0.282(4) \pm$ 0.027 0.022

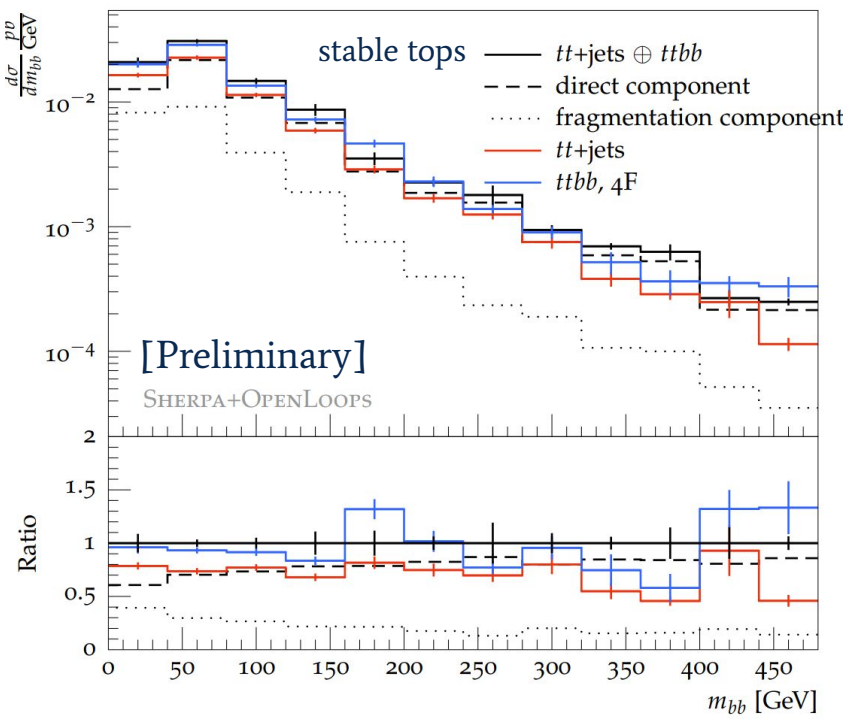
Matching $t\bar{t}$+jets & $t\bar{t}b\bar{b}$

[Katzy,Krause,Pollard,Siegert] in preparation

- Combination of $t\bar{t}$+0,1j@NLO+2,3j@LO and massive $t\bar{t}b\bar{b}$@NLO
- 2-bjet production dominated by direct component, but 1-bjet observables with equal contributions from direct and fragmentation configurations!

[F.Siegert SM@LHC '19]





Summary

Active research directly related to tops:

- Matching for resonant processes
  production, production $\times$ decay, full final state
- Relation between MC masses and pole mass
- 4F vs. 5F scheme and VFNS
- Phenomenology ...

Other topics of current interest:

- Full color parton showers
- Extension of parton showers to NLO
- Benchmarking of parton showers with resummation
- Phenomenology ...