Aspects of MC simulations for top quark physics

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Top Quark Physics at the Precision Frontier
Fermilab, 05/15/2019
Observation of Top Quark Production in pp Collisions

Abstract

We establish the existence of the top quark using a 67 pb\(^{-1}\) data sample of pp collisions at \(\sqrt{s} = 1.8\) TeV collected with the Collider Detector at Fermilab (CDF). Employing techniques similar to those we previously published, we observe a signal consistent with \(t\bar{t}\) decay to WWb\(\bar{b}\), but inconsistent with the background prediction by 4.8\(\sigma\). Additional evidence for the top quark is provided by a peak in the reconstructed mass distribution. We measure the top quark mass to be 176 \pm 8(\text{stat.}) \pm 10(\text{sys.}) GeV/c\(^2\), and the \(t\bar{t}\) production cross section to be 6.8\(-2.4\) pb.
Top as a probe of the Higgs sector

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


Top mass

- Extracted from measurements of various observables e.g. $\sigma_{tt}$, $m_{lb}$, $m_{T2}$, ...
- 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
  - ...

![Graph showing top mass distribution with measurements and uncertainties]
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 WW\bar{b}\bar{b}** [Bevilacqua,Czakon,Hammeren,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 WW\bar{b}\bar{b}** [Garzelli,Kardos,Trocsanyi '14], [Jezo,Lindert,Nason,Oleari,Pozzorini '16]
  - **NLO QCD+PS vs. NLO WW\bar{b}\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 $t\bar{t}+\text{jets}$ at NLO

- Renormalization/factorization scale typically used at very high multiplicity: sum of transverse mass $H'_{T,m} = \sum m_\perp$


  - Interpret event in terms of QCD branchings, like in a parton-shower
  - Assign transverse momentum scales $q$ to splittings, evaluate one $\alpha_s$ 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

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

- Various central scales investigated for perturbative convergence
- Best choices observable dependent and given by
  \[ \mu_0 = \begin{cases} 
  \frac{m_T}{2} & \text{for: } p_{T,t}, p_{T,\bar{t}} \text{ and } p_{T,t}/\bar{t} \\
  \frac{H_T}{4} & \text{for: all other distributions}
  \end{cases} \]
- Peculiar behavior of $H'_T,m$ based scale at NNLO
Multi-jet merging for $t\bar{t}+\text{jets}$

- 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 $\mu_R/\mu_F$ variations, central values agree well with LO merged predictions
EW corrections in multi-jet merging

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

\[ pp \rightarrow t\bar{t} + 0, 1, 2, 3, 4 \text{ jets at } 13 \text{ TeV} \]

\[ \frac{d\sigma}{dp_T,t} \text{ [pb GeV}^{-1}] \]

\[ \mu = \mu_{CKKW} \]

\[ pp \rightarrow t\bar{t} (+ \text{ jet}) \text{ at } 8 \text{ TeV} \]

\[ \frac{d\sigma}{dp_T,t} \text{ [pb GeV}^{-1}] \]

Theory / Data
Matching – Processes with intermediate resonances

NLO subtraction methods do not preserve virtuality of possible resonances
IR cancellation takes place highly non-locally → efficiency problem

Problem worsens in POWHEG, as uncontrollable ratios are exponentiated:

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

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

→ Use kinematic proximity to resonance

$$\Pi_{fb} = \frac{P_{fb}}{\sum_{f_b' \in \text{res hists}} P_{f_b'}}$$

$$P_{fb} = \prod_{i \in \text{res}} \frac{M_i^4}{(s_i - M_i^2)^2 + \Gamma_i^2 M_i^2}$$
Matching – $Wt$ vs $tt\bar{t}$

$Wt$ production in the 5F scheme:
- NLO corrections swamped by LO $tt\bar{t}$ decay
- Requires ad-hoc subtraction prescription (DR/DS)

$Wt$ production in the 4F scheme:
- Unified treatment of $Wt$ and $tt\bar{t}$ (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

If top quark mass extracted from kinematical distributions quality of Monte Carlo modeling limits precision

1. Generators of increasing accuracy → NLO \( tt \), NLO production \( \times \) decay, NLO \( W^+ W^- b\bar{b} \)
2. Different parton-shower models → Pythia, Herwig

For a large range of observables good consistency, except PS dependence

- **Py8.2**: \( m_t = 172.500^{+0.784}_{-0.766} \) GeV
- **Hw7.1**: \( m_t = 175.392^{+1.045}_{-1.138} \) GeV

![Graph showing distributions and extracted masses](image)
Top quark mass from $m_{lb}$

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

- Determine top mass from template fit to $m_{lb}^2 = (p_b - \text{jet} + p_l)^2$
- 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 $m_{lb}$

- $m_{lb}^2 > m_t^2 - m_W^2$ 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?

[Heinrich, Maier, Nisius, Schlenk, Winter] arXiv:1312.6659
Top quark mass from $m_{t\bar{b}}$

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

- Investigated jet mass distribution in $e^+e^- \rightarrow t\bar{t}$
- 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 $\lim_{Q_0 \rightarrow 0} m_{CB}(Q_0) = m_{pole}$, 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 $t\bar{t}b\bar{b}$

- 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 $t\bar{t}+\text{HF}$

- **Five-flavor scheme:**
  - Inclusive NLO+PS $t\bar{t}$ sample with HF from parton shower $g \to b\bar{b}$
  - Multi-leg merged $t\bar{t}+\text{jets}$ 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 → 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
  - 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 $\mu_R = (E_T,t E_T,\bar{t} E_T,b E_T,\bar{b})^{1/4}$
  - New benchmark for NLO+PS programs! [Buccioni, Pozzorini, Zoller '19]
Matching $X +\text{jets}$ & $X b\bar{b}$

- **Interpret $X b\bar{b}$ as part of $X jj$**
  1. Cluster to obtain parton shower history
  2. Apply $\alpha_s(\mu^2_R) \to \alpha_s(p_T^2)$ 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 $X b\bar{b}$
       ("direct component")
     - Light Flavour $\to$ keep from $X +\text{jets}$
       ("fragmentation component")
     - Subleading $g \to b\bar{b}$ splittings
       not from $X b\bar{b}$ ME, but $X 4j$ ME+PS

- **Match 5F $\to$ 4F in PDFs and $\alpha_s$**
  1. Use 5F PDF / $\alpha_s$ to be consistent with $X jj$
  2. Use matching coefficients to correct to 4F scheme
     $\to$ Coefficients up to (N)LL generated by (N)LO parton shower!
  3. Reweighting needed only for $\alpha_s$ in hard ME

Can be applied to LO and NLO merging!
Example: $Z+\text{jets} \ & \ Z\bar{b}b$

- Validation with LHC data

### Transverse momentum of $Z$-boson

<table>
<thead>
<tr>
<th>$Q_{\text{cut}}$</th>
<th>ATLAS JHEP07(2013)032</th>
<th>$Z+\text{jets} \oplus Z\bar{b}b$</th>
<th>direct component</th>
<th>fragmentation component</th>
<th>$Z+\text{jets}$</th>
<th>$Z\bar{b}b, 4\text{FS}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$15 \text{ GeV}$</td>
<td>3.55 ± 0.24$_{\text{comb}}$</td>
<td>3.80(5) ± 0.037$_{\text{comb}}$</td>
<td>0.83 ± 0.24$_{\text{comb}}$</td>
<td>0.282(4) ± 0.027$_{\text{comb}}$</td>
<td>0.027 ± 0.033$_{\text{comb}}$</td>
<td>0.022 ± 0.033$_{\text{comb}}$</td>
</tr>
</tbody>
</table>

$Z+\geq 1b$

$Z+\geq 2b$
Matching $t\bar{t}+\text{jets}$ & $t\bar{t}b\bar{b}$

- Combination of $t\bar{t}+0,1\text{jet@NLO}+2,3\text{jets@LO}$ 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!

[Preliminary]

SNEAK PREVIEW: Application to $ttbb$

- Application to fusion of MEPS@NLO $tt + 0,1\text{jet@NLO} + 2,3\text{jets@LO}$ and massive $ttbb@NLO$
- 2-bjet production dominated by direct component, but 1-bjet observables with equal contributions from direct and fragmentation configurations!
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 . . .