MC simulation of heavy flavor production

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Overview

- This talk: Heavy Flavor = t
- Studied intensely, both at fixed order
 - ► NNLO QCD [Czakon,Fiedler,Mitov '13], [Czakon,Heymes,Mitov '16]
 - NLO QCD / EW in production × decay [Bernreuther,Brandenburg,Si '04], [Melnikov,Schulze '09], [Campbell,Ellis '15], [Bernreuther,Si '10]
 - ► NLO QCD / EW WWbb [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 tt+(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 × decay [Campbell,Ellis,Nason,Re '15]
 - ▶ NLO QCD+PS WWbb [Garzelli,Kardos,Trocsanyi '14], [Jezo,Lindert,Nason,Oleari,Pozzorini '16]
 - NLO QCD+PS tt+(multi-)jet [Kardos,Papadopoulos,Trocsanyi '11], [Alioli,Moch,Uwer '11], [Huang,Luisoni,Schönherr,Winter,SH '13], [Krauss,Maierhöfer,Pozzorini,Schönherr,Siegert,SH '14]
- Will focus on
 - NLO QCD for $t\bar{t}$ +multi-jets
 - Matching to parton shower and (N)LO merging
 - Parton shower uncertainties

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Top-quark pairs – A QCD scale uncertainty study

- ► Renormalization/factorization scale typically used at very high multiplicity: sum of transverse mass $H_{T,m} = \sum m_{\perp}$
- Has been criticized for being 'too large' and insensitive to dynamics of process
- Very different scale defined by MINLO [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 $H_{T,m}$



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Top-quark pairs – A QCD scale uncertainty study

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[Maierhöfer, Moretti, Pozzorini, Siegert, SH '16]



Two possible ways to match NLO calculations and parton showers

Additive (MC@NLO-like)

[Frixione,Webber '02]

- Use parton-shower splitting kernel as NLO subtraction term
- Multiply LO event weight by Born-local K-factor including integrated subtraction term and virtual corrections
- Add hard remainder function consisting of subtracted real-emission correction

Multiplicative (POWHEG-like)

[Nason '04]

- Use matrix-element corrections to replace parton-shower splitting kernel by full real-emission matrix element in first shower branching
- Multiply LO event weight by Born-local NLO K-factor (integrated over real corrections that can be mapped to Born according to PS kinematics)

Both cases: Beware of sub-leading color, spin correlations & off-shell effects!

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Matching – Full vs leading color



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 Standard MC@NLO: Soft-gluon kinematics ignored by fading out real-emission correction to account for leading color MC subtraction terms

$$\begin{split} \langle O \rangle &= \int \mathrm{d}\Phi_B \,\bar{\mathrm{B}}^{(\mathrm{K})} \,\mathcal{F}_{\mathrm{MC}}^{(0)}(\mu_Q^2,O) + \int \mathrm{d}\Phi_R \,\mathrm{H}^{(\mathrm{K})} \,\mathcal{F}_{\mathrm{MC}}^{(1)}(t(\Phi_R),O) \\ \bar{\mathrm{B}}^{(\mathrm{K})} &= \mathrm{B} + \tilde{\mathrm{V}} + \mathrm{I} + \int \mathrm{d}\Phi_1 \left[\,\mathrm{S} - \mathrm{B}\,\mathrm{K}\,\right] f(\Phi_1) \;, \quad \mathrm{H}^{(\mathrm{K})} = \left[\,\mathrm{R} - \mathrm{B}\,\mathrm{K}\,\right] f(\Phi_1) \end{split}$$

► Appropriate for sufficiently inclusive observables, problematic e.g. for *A*_{*FB*} Similar issues could arise in other observables that break PS unitarity



Matching – Production vs decay





- Moderate differences compared to LO decays & no spin correlations
- Sizable differences for varying shower parameters (removing decay ME correction in Pythia improves agreement)





[Campbell, Ellis, Nason, Re '15]

Matching – Processes with intermediate resonances

[Jezo,Nason '15]

- ► 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:

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

- 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 → 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 '16]

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- ► *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 '07]



[Cascioli, Maierhöfer, Moretti, Pozzorini, Siegert '13]

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- Matching of $t\bar{t}b\bar{b}$ NLO calculations requires special care
- ► Secondary bb̄ pair(s) from g → bb̄ splitting in PS can have larger invariant mass than primary pair if PS scale high enough → distortion of MC@NLO spectrum compared to NLO

	ttb	${\rm ttbb}(m_{bb}>100)$
$\sigma_{LO}[fb]$	$2644^{+71\%}_{-38\%}{}^{+14\%}_{-11\%}$	$123.4^{+63\%}_{-35\%}{}^{+17\%}_{-13\%}$
$\sigma_{NLO}[fb]$	$3296^{+34\%}_{-25\%}{}^{+5.6\%}_{-4.2\%}$	$141.8^{+26\%}_{-22\%}{}^{+6.5\%}_{-4.6\%}$
σ_{NLO}/σ_{LO}	1.25	1.15
$\sigma_{MC}[fb]$	$3313^{+32\%}_{-25\%}{}^{+3.9\%}_{-2.9\%}$	$181.0^{+20\%}_{-20\%}{}^{+8.1\%}_{-6.0\%}$
σ_{MC}/σ_{NLO}	1.01	1.28
$\sigma^{2b}_{MC}[fb]$	3299	146
$\sigma^{2b}_{MC}/\sigma_{NLO}$	1.00	1.03



[SH (PhD thesis) '08]

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- ► ME+PS merging possible in top production and decay independently
- Effect of merging in decay negligible for most jet observables



Merging in $t\bar{t}$ +jets – NLO

- NLO-Matched & merged simulations now up to $t\bar{t}+2j$ (+ any jets at LO) [Frederix, Frixione '12], [Krauss, Maierhöfer, Pozzorini, Schönherr, Siegert, SH '14]
- Decays & spin correlations at LO
- Largely reduced $\mu_{R/F}$ variations, central value agrees well with LO merged prediction





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Ratio to MEPS@NLO

Ratio to MEPS@NLO

Ratio to MEPS@NLO

Parton shower uncertainties – Splitting functions

- Splitting functions for heavy flavor ambiguous
- Example: FSR $g \rightarrow Q\bar{Q}$ in Pythia8 [Jimenez (Masters Thesis) LU-TP 14-15]

•
$$w_1 = \beta \left[1 - 2z(1-z) \right]$$
, $\beta = \sqrt{1 - 4m_Q^2/Q^2}$

•
$$w_2 = \beta \left[1 - 2z(1-z)(1-8m_Q^2/Q^2) \right]$$

•
$$w_4 \to \text{full } \gamma^* \to Q\bar{Q} \text{ ME correction}$$



Also: Effects of massive recoil partners in momentum mapping

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Parton shower uncertainties - Shower model

- ► Old angular ordered / vetoed parton showers do not fill full phase space Dipole showers lack parton interpretation → prefer alternative to both
- ► Can preserve parton picture by partial fractioning soft eikonal ↔ soft enhanced part of splitting function [Catani,Seymour '96]



 "Spectator"-dependent kernels, singular in soft-collinear region only → capture dominant coherence effects (3-parton correlations)

$$\frac{1}{1-z} \to \frac{1-z}{(1-z)^2 + \kappa^2} \qquad \kappa^2 = \frac{k_{\perp}^2}{Q^2}$$

For correct soft evolution, ordering variable must be identical at both "dipole ends" (→ recover soft eikonal at integrand level)

Parton shower uncertainties - Shower model

[Stoll (Diploma thesis)], [Plätzer (IPPP HF WS '16)]

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• Something odd in this model for $g \rightarrow b\bar{b}$ splittings

- ▶ Not a bug, consistent between generators (Herwig7, Sherpa, ...)
- Not fixed by a scale choice $(p_T \text{ vs. } m_{q\bar{q}})$
- Not a kinematics/ordering effect



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Parton shower uncertainties – Kinematics

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- ► Two mapping schemes for IF dipoles → local [Catani,Seymour '96] and global [Plätzer,Gieseke '09], [Schumann,Siegert,SH '09]
- Negligible impact e.g. on q_T -spectrum of Drell-Yan lepton pairs
- ► Less well investigated in more exclusive observables and heavy flavor

Heavy Flavor particularities

Resonance-aware matching for top

Major sources of uncertainty

- ▶ 4F vs. 5F scheme in hard process
- Splitting kernels and scales in PS
- Shower model (partons vs dipoles)

All of them under constant investigation

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A_{FB} from a parton shower viewpoint

[Skands,Webber,Winter] arXiv:1205.1466 [Huang,Luisoni,Schönherr,Winter,SH] arXiv:1306.2703

- ▶ Parton-shower unitarity broken by splitting of emission phase space
- ▶ Events with $\Delta y_{t\bar{t}} > 0$ have fewer phase space for radiation



But inclusive asymmetry is mainly generated by momentum mapping

$$\Delta \sigma_{+-} = -2 \int \underbrace{\mathrm{d}\sigma_{LO}|_{\Delta y>0}(1-\Delta_{+})P_{+-}}_{\text{subdominant as }\Delta_{-} < \Delta_{+} \ (\text{(b) vs. (a)})} + 2 \int \underbrace{\mathrm{d}\sigma_{LO}|_{\Delta y<0}(1-\Delta_{-})P_{-+}}_{\text{dominant as }\Delta_{+} > \Delta_{-} \ (\text{(a) vs. (b)})}$$

 P_{-+}/P_{+-} - probabilities for Δy to increase / decrease in splitting Dipole showers generate positive rapidity shift in each emission

$$\Delta y_t = \frac{1}{2} \ln \left(1 + \frac{p_q p_g}{p_q p_t} \left(\frac{1-z}{z} + \frac{m_t^2}{p_q p_t} \right) \frac{\tilde{p}_q^+}{\tilde{p}_t^+} \right) > 0$$

Similar finding for any dipole-like recoil scheme \rightarrow positive asymmetry