# MC simulation of heavy flavor production

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# Overview

- $\blacktriangleright$  This talk: Heavy Flavor  $=t$
- $\triangleright$  Studied intensely, both at fixed order
	- ▶ NNLO QCD [Czakon,Fiedler,Mitov '13], [Czakon,Heymes,Mitov '16]
	- $\triangleright$  NLO QCD / EW in production  $\times$  decay [Bernreuther, Brandenburg, Si '04], [Melnikov,Schulze '09], [Campbell,Ellis '15], [Bernreuther,Si '10]
	- $\blacktriangleright$  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]
	- $\triangleright$  NLO QCD  $t\bar{t}$ +(multi-)jet [Dittmaier,Uwer,Weinzierl '07], [Bevilacqua,Czakon,Papadopoulos,Worek '10], [Maierh¨ofer,Moretti,Pozzorini,Siegert,SH '16]
- $\triangleright$  and in the context of particle-level Monte Carlo
	- ▶ NLO QCD+PS [Frixione,Nason,Webber '03], [Frixione,Nason,Ridolfi '07]
	- $\triangleright$  NLO QCD+PS in production  $\times$  decay [Campbell, Ellis, Nason, Re '15]
	- $\blacktriangleright$  NLO QCD+PS  $WWb\bar{b}$  [Garzelli,Kardos,Trocsanyi '14], [Jezo,Lindert,Nason,Oleari,Pozzorini '16]
	- ▶ NLO QCD+PS  $t\bar{t}$ +(multi-)jet [Kardos,Papadopoulos,Trocsanyi '11], [Alioli,Moch,Uwer '11], [Huang,Luisoni,Sch¨onherr,Winter,SH '13], [Krauss,Maierh¨ofer,Pozzorini,Sch¨onherr,Siegert,SH '14]
- $\triangleright$  Will focus on
	- $\triangleright$  NLO QCD for  $t\bar{t}$ +multi-jets
	- $\triangleright$  Matching to parton shower and (N)LO merging
	- $\blacktriangleright$  Parton shower uncertainties

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# Top-quark pairs – A QCD scale uncertainty study

- $\blacktriangleright$  Renormalization/factorization scale typically used at very high multiplicity: sum of transverse mass  $H_{T,m}=\sum m_\perp$
- $\blacktriangleright$  Has been criticized for being 'too large' and insensitive to dynamics of process
- $\triangleright$  Very different scale defined by MINLO [Hamilton, Nason, Zanderighi] arXiv: 1206.3572
	- $\triangleright$  Interpret event in terms of QCD branchings, like in a parton-shower
	- $\triangleright$  Assign transverse momentum scales q to splittings, evaluate one  $\alpha_s$  at each of these scales
	- $\blacktriangleright$  Multiply with NLL Sudakov factors, subtract first-order expansion
- $\triangleright$  MINLO scale probes detailed dynamics, typically very small  $\rightarrow$  good candidate for comparison to  $H_{T,m}$



#### 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]

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

#### Multiplicative (POWHEG-like)

[Nason '04]

- $\blacktriangleright$  Use matrix-element corrections to replace parton-shower splitting kernel by full real-emission matrix element in first shower branching
- $\triangleright$  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

[Huang, Luisoni, Schönherr, Winter, SH '13]

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

$$
\langle O \rangle = \int d\Phi_B \, \bar{\mathbf{B}}^{(\mathrm{K})} \, \mathcal{F}_{\mathrm{MC}}^{(0)}(\mu_Q^2, O) + \int d\Phi_R \, \mathbf{H}^{(\mathrm{K})} \, \mathcal{F}_{\mathrm{MC}}^{(1)}(t(\Phi_R), O)
$$
  

$$
\bar{\mathbf{B}}^{(\mathrm{K})} = \mathbf{B} + \tilde{\mathbf{V}} + \mathbf{I} + \int d\Phi_1 \left[ \mathbf{S} - \mathbf{B} \mathbf{K} \right] f(\Phi_1), \quad \mathbf{H}^{(\mathrm{K})} = \left[ \mathbf{R} - \mathbf{B} \mathbf{K} \right] f(\Phi_1)
$$

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



[Campbell,Ellis,Nason,Re '15]



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





#### Matching – Processes with intermediate resonances

[Jezo,Nason '15]

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

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

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

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

# Matching –  $Wt$  vs  $t\bar{t}$

[Jezo,Lindert,Oleari,Nason,Pozzorini '16]

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- $\blacktriangleright$  Wt production in the 5F scheme:
	- $\triangleright$  NLO corrections swamped by LO  $t\bar{t}$  decay
	- $\blacktriangleright$  Requires ad-hoc subtraction prescription (DR/DS)
- $\blacktriangleright$  Wt production in the 4F scheme:
	- ► Unified treatment of  $Wt$  and  $t\bar{t}$  (identical at LO)
	- Requires off-shell  $WW b\bar{b}$  calculation
- $\triangleright$  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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- $\triangleright$  Matching of  $t\bar{t}b\bar{b}$  NLO calculations requires special care
- ► Secondary  $b\bar{b}$  pair(s) from  $g \to b\bar{b}$  splitting in PS can have larger invariant mass than primary pair if PS scale high enough  $\rightarrow$  distortion of MC@NLO spectrum compared to NLO





[SH (PhD thesis) '08]

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



# Merging in  $t\bar{t}+$ jets – NLO

- $\triangleright$  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]
- $\triangleright$  Decays & spin correlations at LO
- In Largely reduced  $\mu_{R/F}$  variations, central value agrees well with LO merged prediction





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Light jet transverse momenta

# Parton shower uncertainties - Splitting functions

7 1.083 ± 0.003

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

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

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

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



 $\blacktriangleright$  Also: Effects of massive recoil partners in momentum mapping

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#### Parton shower uncertainties – Shower model

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

 $p_i p_k$  $\frac{p_i p_k}{(p_i p_j)(p_j p_k)} \rightarrow \frac{1}{p_i p_j}$  $p_i p_j$  $p_i p_k$  $\frac{p_ip_k}{(p_i+p_k)p_j}+\frac{1}{p_{k1}}$  $p_k p_j$  $p_i p_k$  $(p_i+p_k)p_j$  $+$  $k$  j i  $k$  j i  $k$  j i

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

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

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

#### Parton shower uncertainties – Shower model  $54.8$   $\overline{64.8}$

[Stoll (Diploma thesis)], [Plätzer (IPPP HF WS '16)]  $[<sub>S</sub>$ 

► Something odd in this model for  $g\to b\bar{b}$  splittings

- $\triangleright$  Not a bug, consistent between generators (Herwig7, Sherpa, ...)
- Simulation results for the design results for various  $(n_1, ..., n_n)$ <br>
Not fixed by a scale choice  $(p_T \text{ vs. } m_{q\bar{q}})$  $\sum_{n=1}^{\infty}$  not the dipole shower in the mass  $\lfloor pt \rfloor$  with  $mqq$
- $\blacktriangleright$  Not a kinematics/ordering effect



# Parton shower uncertainties – Shower model er<br>—

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

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▶ Something odd in this model for  $g \to b \bar b$  splittings

0.15

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



#### Parton shower uncertainties – Kinematics

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

#### Heavy Flavor particularities

 $\blacktriangleright$  Resonance-aware matching for top

#### Major sources of uncertainty

- $\triangleright$  4F vs. 5F scheme in hard process
- $\triangleright$  Splitting kernels and scales in PS
- $\triangleright$  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](http://inspirebeta.net/search?action_search=Search&p=1205.1466) [Huang,Luisoni,Sch¨onherr,Winter,SH] [arXiv:1306.2703](http://inspirebeta.net/search?action_search=Search&p=1306.2703)

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



 $\triangleright$  But inclusive asymmetry is mainly generated by momentum mapping

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

subdominant as  $\Delta_-\langle\Delta_+ \rangle$  ((b) vs. (a)) dominant as  $\Delta_+> \Delta_-$  ((a) vs. (b))

 $P_{-+}/P_{+-}$  - probabilities for  $\Delta y$  to increase / decrease in splitting  $\triangleright$  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