



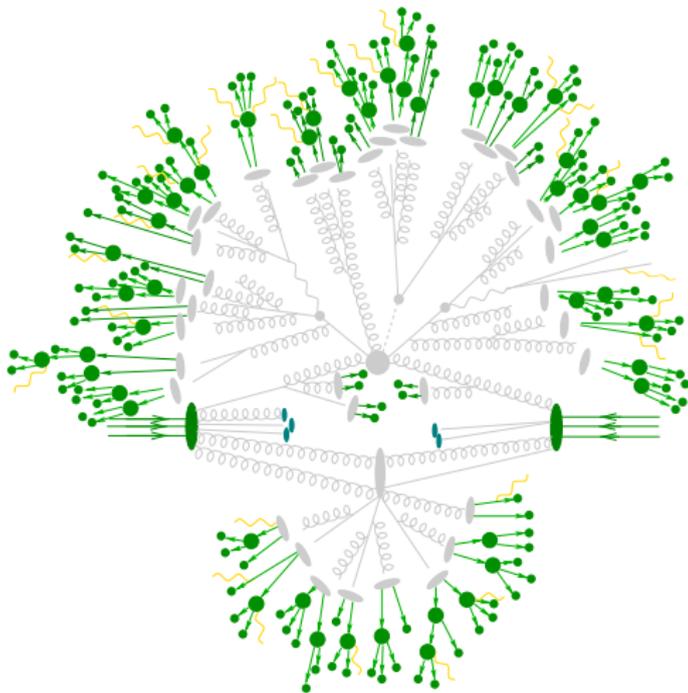
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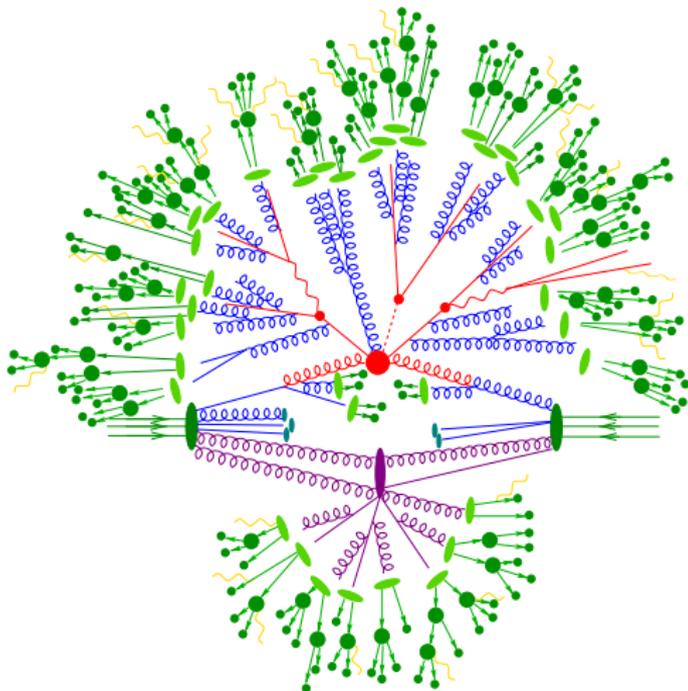
CONSTRUCTING AND IMPROVING QCD PARTON SHOWER SIMULATIONS

Frank Siegert

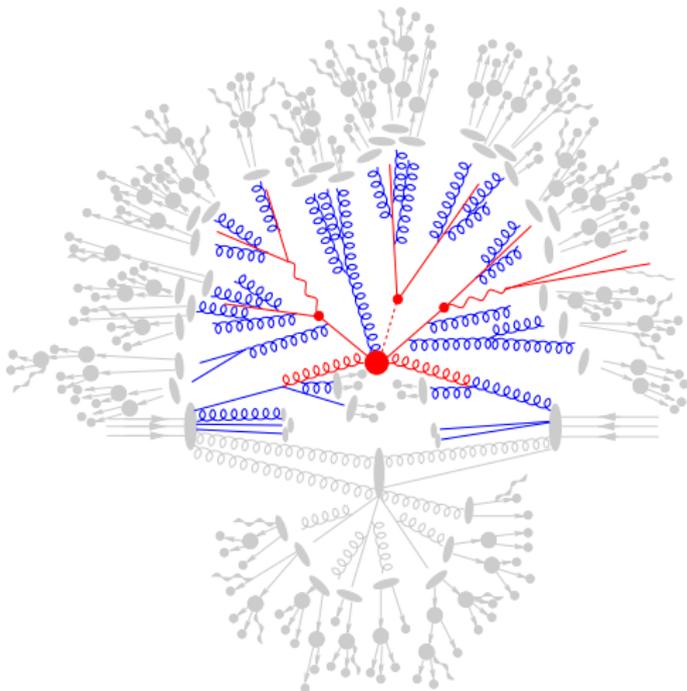
IKTP-Seminar, TU Dresden, January 2014



- We want:
Simulation of $pp \rightarrow$ full hadronised final state
- MC event representation for $pp \rightarrow t\bar{t}H$ event
- We know from first principles:
 - Hard scattering at fixed order in perturbation theory (Matrix Element)
 - Approximate resummation of QCD corrections to all orders (Parton Shower)
- Missing bits:
Hadronisation/Underlying event (ignored here)



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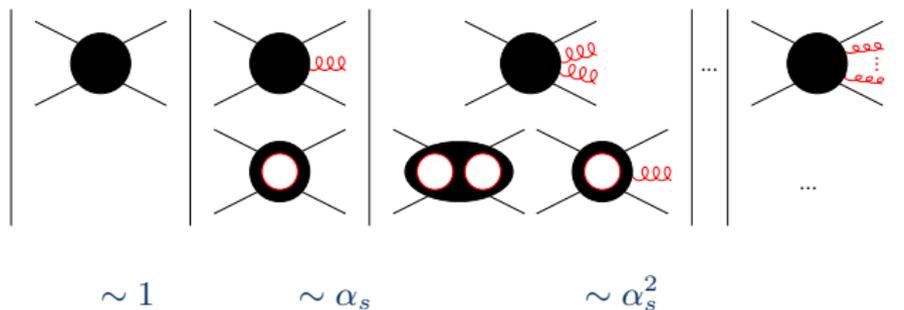


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Outline

- Reminder: QCD perturbation theory
- The parton shower approximation
- Correcting that approximation as far as possible:
 - NLO+PS (2002)
 - Tree-level ME+PS merging (2001)
 - MENLOPS (2010)
 - ME+PS merging at NLO (2012)
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- Cannot solve QCD and calculate e.g. $pp \rightarrow t\bar{t}H$ exactly
- But can calculate parts of the perturbative series in α_s :



- Exact calculations possible up to $\mathcal{O}(\alpha_s^2)$ for some processes
- $\alpha_s^2 \approx 1\% \Rightarrow$ high enough precision, right?
- Why is that not always true?

- Predictions for **inclusive** observables calculable at fixed-order (\rightsquigarrow KLN theorem)
- But what if **not inclusive** enough, e.g.:
 - Study certain regions of phase space, like $p_{\perp}^Z \rightarrow 0 @ DY$
 - Making predictions for hadron-level final states: confinement at $\mu_{\text{had}} \approx 1 \text{ GeV}$

\Rightarrow Finite remainders of infrared divergences:

logarithms of $\frac{\mu_{\text{hard}}^2}{\mu_{\text{res}}^2}$ with each $\mathcal{O}(\alpha_s)$

are large and spoil convergence of perturbative series

- Need to resum the series to all orders
 - Problem: We are not smart enough for that.
 - Workaround: **Resum only the logarithmically enhanced terms in the series**
- Parton showers resum these terms in their evolution of a parton ensemble between μ_{hard}^2 and μ_{had}^2

How?

Let's start simple: one emission, no resummation

- Universal factorisation of QCD real emission ME for collinear parton pair (i, j) :

$$\mathcal{R} \rightarrow \mathcal{D}_{ij}^{(\text{PS})} = \mathcal{B} \times \left[\frac{1}{2p_i p_j} 8\pi\alpha_s \mathcal{K}_{ij}(p_i, p_j) \right]$$

- \mathcal{B} = Born matrix element
- \mathcal{K}_{ij} splitting kernel for branching $(ij) \rightarrow i + j$
Specific form depends on factorisation scheme (DGLAP, Catani-Seymour, Antenna, ...)
- Massless propagator $\frac{1}{2p_i p_j}$
(Later: Evolution variable of shower $t \sim 2p_i p_j$, e.g. k_{\perp} , angle, ...)

- Radiative phase space factorises as well:

$$d\Phi_{\mathcal{R}} = d\Phi_{\mathcal{B}} d\Phi_1 = d\Phi_{\mathcal{B}} dt \frac{1}{16\pi^2} dz \frac{d\phi}{2\pi}$$

(ignoring z and ϕ dependence from here on, because they are "trivial", not related to large logs)

- Combined with radiative part of the factorised ME

(Jacobian/symmetry factor/PDFs ignored)

$$d\sigma_{ij}^{(\text{PS})} \sim dt \mathcal{D}_{ij}^{(\text{PS})} \sim \frac{dt}{t} \frac{\alpha_s}{2\pi} \mathcal{K}_{ij} \quad \text{Differential branching probability}$$

Evolution with respect to t

- $d\sigma_{ij}^{(\text{PS})} \sim dt \mathcal{D}_{ij}^{(\text{PS})}$ is universal and appears for each emission
- How do we get the resummed branching probability according to multiple such emissions?
 → Analogy to evolution of ensemble of radioactive nuclei:
 Survival probability at time t_1 depends on decay/survival at times $t < t_1$

Radioactive decay

- Constant differential decay probability

$$f(t) = \text{const} \equiv \lambda$$

- Survival probability $\mathcal{N}(t)$

$$-\frac{d\mathcal{N}}{dt} = \lambda \mathcal{N}(t)$$

$$\Rightarrow \mathcal{N}(t) \sim \exp(-\lambda t)$$

Parton shower branching

- Differential branching probability

$$f(t) \equiv \mathcal{D}_{ij}^{(\text{PS})}$$

- Survival probability $\mathcal{N}(t)$

$$-\frac{d\mathcal{N}}{dt} = f(t) \mathcal{N}(t)$$

$$\Rightarrow \mathcal{N}(t) \sim \exp\left(-\int_0^t dt' f(t')\right)$$

Radioactive decay

- Survival probability $\mathcal{N}(t)$

$$\mathcal{N}(t) \sim \exp(-\lambda t)$$

- Resummed decay probability $\mathcal{P}(t)$

$$\mathcal{P}(t) = f(t) \mathcal{N}(t) \sim \lambda \exp(-\lambda t)$$

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- Resummed branching probability $\mathcal{P}(t)$

$$\mathcal{P}(t) = f(t) \mathcal{N}(t) \sim f(t) \exp\left(-\int_0^t dt' f(t')\right)$$

Parton shower recursion

- Generate next branching “time” t (after t_{previous}) with probability

$$\mathcal{P}(t, t_{\text{previous}}) = f(t) \exp\left(-\int_{t_{\text{previous}}}^t f(t') dt'\right)$$

- Analytically:

$$t = F^{-1} [F(t_{\text{previous}}) + \log(\#\text{random})] \text{ with } F(t) = \int_{t_0}^t dt' f(t')$$

- If integral/its inverse are not known: “Veto algorithm” = extension of hit-or-miss

- Overestimate $g(t) \geq f(t)$ with known integral $G(t)$
 $\rightarrow t = G^{-1} [G(t_{\text{previous}}) + \log(\#\text{random})]$
- Accept t with probability $\frac{f(t)}{g(t)}$ using hit-or-miss

Summary of main parton shower ingredients

- “Sudakov form factor” \equiv Survival probability of parton ensemble between two scales:

$$\mathcal{N}(t) \sim \exp\left(-\int_0^t dt' f(t')\right) \rightarrow \Delta(t', t'') = \prod_{\{ij\}} \exp\left(-\int_{t'}^{t''} dt \mathcal{D}_{ij}^{(\text{PS})}\right)$$

- Evolution variable t : not time, but scale of collinearity from hard to soft
 $t \sim 2p_i p_j \sim$ e.g. angle θ , virtuality Q^2 , relative transverse momentum k_{\perp}^2, \dots
- Starting scale μ_Q^2 (time $t = 0$ in radioactive decay) defined by hard scattering
- Cutoff scale related to hadronisation scale $t_0 \sim \mu_{\text{had}}^2$
- Other variables (z, ϕ) generated directly according to $d\sigma_{ij}^{(\text{PS})}(t, z, \phi)$

\Rightarrow **Differential cross section** (up to first emission)

$$d\sigma = d\Phi_B \mathcal{B} \left[\underbrace{\Delta^{(\text{PS})}(t_0, \mu_Q^2)}_{\text{unresolved}} + \underbrace{\sum_{\{ij\}} \int_{t_0}^{\mu_Q^2} dt \frac{d\sigma_{ij}^{(\text{PS})}}{dt} \Delta^{(\text{PS})}(t, \mu_Q^2)}_{\text{resolved}} \right]$$

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NLO+PS matching

- Parton shower on top of **NLO** prediction (e.g. inclusive W production)
- Objectives:
 - avoid double counting in real emission
 - preserve inclusive NLO accuracy



ME+PS@LO merging

- Multiple LO+PS simulations for processes of different jet multi (e.g. W , Wj , Wjj , ...)
- Objectives:
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Combination: ME+PS@NLO

- **Multiple NLO+PS** simulations for processes of different jet multiplicity e.g. W , Wj , Wjj , ...
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Reminder + Notation: Subtraction method

- Contributions to NLO cross section: \mathcal{B} orn, \mathcal{V} irtual and \mathcal{R} eal emission
- \mathcal{V} and \mathcal{R} divergent in separate phase space integrations
 \Rightarrow Subtraction terms \mathcal{D} and their integrated form \mathcal{I} for NLO cross section:

$$d\sigma^{(\text{NLO})} = d\Phi_B \left[\mathcal{B} + \tilde{\mathcal{V}} + \sum_{\{ij\}} \mathcal{I}_{(ij)}^{(\text{S})} \right] + d\Phi_R \left[\mathcal{R} - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\text{S})} \right]$$

Idea of NLO+PS matching

- Applying PS resummation to LO event was “simple” ✓
- Apply the same separately for \mathcal{B} and \mathcal{V} and \mathcal{R} at NLO?

\Rightarrow double counting

- Instead: additional subtraction terms $\mathcal{D}_{ij}^{(\text{A})}$

$$d\sigma^{(\text{NLO sub})} = d\Phi_B \tilde{\mathcal{B}}^{(\text{A})} + d\Phi_R \left[\mathcal{R} - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\text{A})} \right]$$

$$\text{with } \tilde{\mathcal{B}}^{(\text{A})} = \mathcal{B} + \tilde{\mathcal{V}} + \sum_{\{ij\}} \mathcal{I}_{(ij)}^{(\text{S})} + \sum_{\{ij\}} \int dt \left[\mathcal{D}_{ij}^{(\text{A})} - \mathcal{D}_{ij}^{(\text{S})} \right]$$

Master formula for NLO+PS up to first emission

$$\begin{aligned}
 d\sigma^{(\text{NLO+PS})} = & d\Phi_B \bar{\mathcal{B}}^{(A)} \left[\underbrace{\Delta^{(A)}(t_0, \mu_Q^2)}_{\text{unresolved}} + \underbrace{\sum_{\{ij\}} \int_{t_0}^{\mu_Q^2} dt \frac{\mathcal{D}_{ij}^{(A)}}{\mathcal{B}} \Delta^{(A)}(t, \mu_Q^2)}_{\text{resolved, singular}} \right] \\
 & + d\Phi_R \left[\underbrace{\mathcal{R} - \sum_{\{ij\}} \mathcal{D}_{ij}^{(A)}}_{\text{resolved, non-singular} \equiv \mathcal{H}^{(A)}} \right]
 \end{aligned}$$

- To $\mathcal{O}(\alpha_s)$ this reproduces $d\sigma^{(\text{NLO})}$
- Event generation: $\bar{\mathcal{B}}^{(A)}$ or $\mathcal{H}^{(A)}$ seed event according to their XS
 - First line (“S-event”): from one-step PS with $\Delta^{(A)}$
 \Rightarrow emission (resolved, singular) or no emission (unresolved) above t_0
 - Second line (“H-event”): kept as-is \rightarrow resolved, non-singular term
- Resolved cases: Subsequent emissions can be generated by ordinary PS
- Exact choice of $\mathcal{D}_{ij}^{(A)}$ will specify MC@NLO vs. S-MC@NLO vs. POWHEG ...

Mc@NLO

Frixione, Webber (2002)

 $\mathcal{D}^{(A)} = \text{PS splitting kernels}$

- + Shower algorithm for Born-like events easy to implement
- "Non-singular" piece $\mathcal{R} - \sum_{ij} \mathcal{D}_{ij}^{(A)}$ is actually **singular**:
 - Collinear divergences subtracted by splitting kernels ✓
 - Remaining soft divergences as they appear in non-trivial processes at sub-leading N_c ✗

Workaround: \mathcal{G} -function dampens soft limit in non-singular piece
 \Leftrightarrow Loss of formal NLO accuracy
 (but heuristically only small impact)

S-Mc@NLO

Höche, Krauss, Schönherr, FS (2011)

 $\mathcal{D}^{(A)} = \text{Subtraction terms } \mathcal{D}^{(S)}$

- + "Non-singular" piece fully free of divergences
- Splitting kernels in shower algorithm become **negative**

Solution: Weighted $N_C = 3$ one-step PS based on subtraction terms

\Downarrow
 Used in SHERPA

Original POWHEG

- Choose additional subtraction terms as

$$\mathcal{D}_{ij}^{(A)} \rightarrow \rho_{ij} \mathcal{R} \quad \text{where} \quad \rho_{ij} = \frac{\mathcal{D}_{ij}^{(S)}}{\sum_{mn} \mathcal{D}_{mn}^{(S)}}$$

- \mathcal{H} -term vanishes \Rightarrow No negative weighted events
- Similar to PS with ME-correction for 1st emission (e.g. Herwig, Pythia)

Mixed scheme

- Subtract arbitrary regular piece from \mathcal{R} and generate separately as \mathbb{H} -events

$$\mathcal{D}_{ij}^{(A)}(\Phi_R) \rightarrow \rho_{ij}(\Phi_R) [\mathcal{R}(\Phi_R) - \mathcal{R}^r(\Phi_R)] \quad \text{where} \quad \rho_{ij} \text{ as above}$$

- Tuning of \mathcal{R}^r to reduce exponentiation of arbitrary terms
- Allows to generate the non-singular cases of \mathcal{R} without underlying \mathcal{B}

Perturbative uncertainties

- Unknown higher-order corrections
- Estimated by scale variations

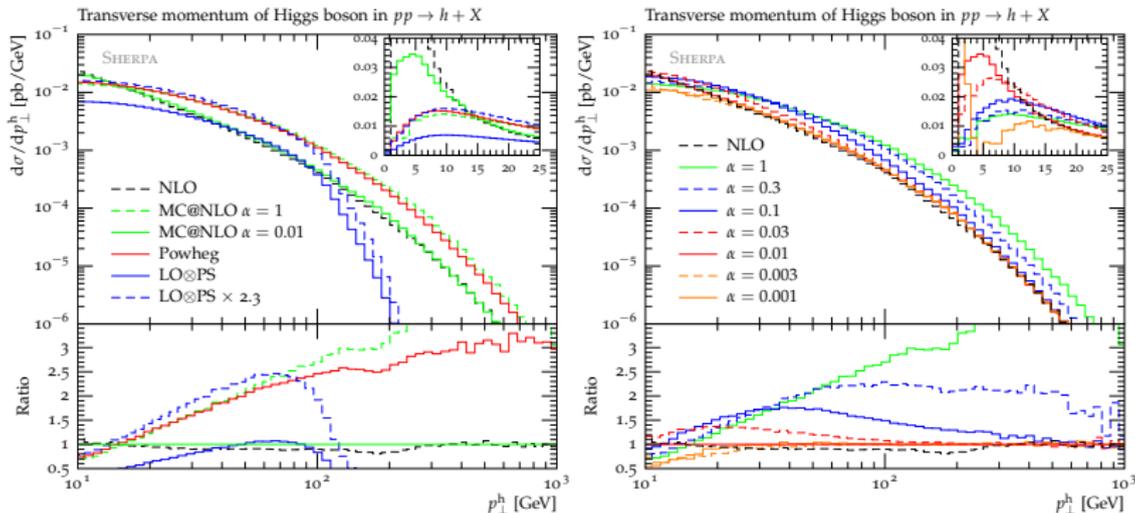
$$\mu_F = \mu_R = \frac{1}{2}\mu \dots 2\mu$$

Non-perturbative uncertainties

- Model uncertainties in hadronisation, hadron decays, multiple parton interactions
- Estimated by variation of parameters/models within tuned ranges

Exponentiation uncertainties

- Arbitrariness of $\mathcal{D}^{(A)}$ and thus of the exponent in $\Delta^{(A)}$
- Estimated by:
 - Variations of μ_Q^2 in MC@NLO
 - (Variation of \mathcal{R}^r in POWHEG)
- Reduced by merging with NLO for higher parton multiplicities \rightsquigarrow later

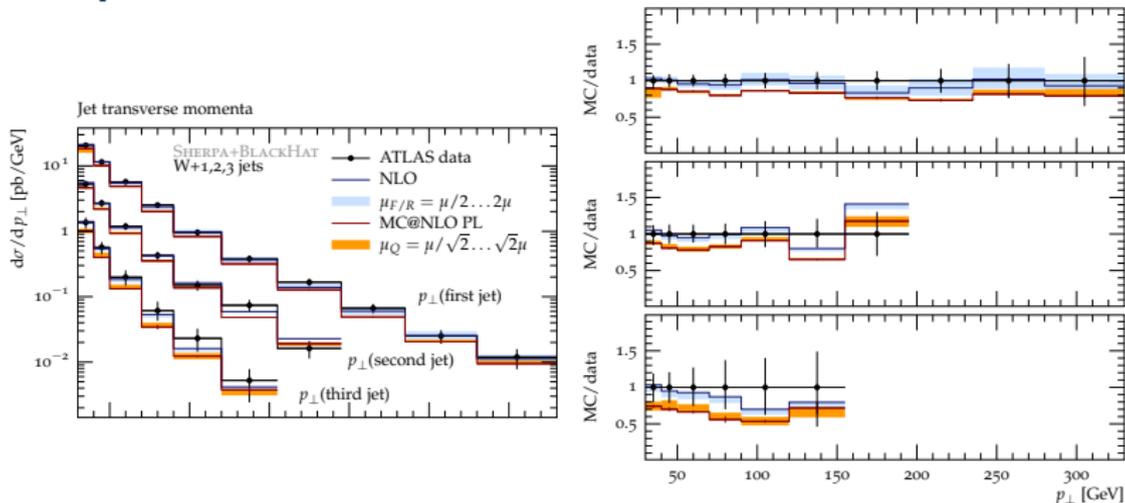


For demonstration purposes

- Strong sensitivity to exponentiation especially at large p_{\perp}^h
- POWHEG and completely unrestricted MC@NLO similar
- Decrease exponentiation of non-singular pieces using (unphysical) dipole α :
 $\alpha_{\text{cut}} \lesssim 0.01$ recovers NLO behaviour

Proper physical assessment of variation:
Dipole restriction at (and variation of) resummation scale μ_Q

Comparison to ATLAS data



ATLAS measurement (arXiv:1201.1276)
SHERPA+BLACKHAT NLO+PS predictions (arXiv:1201.5882)

NLO+PS matching

- Parton shower on top of NLO prediction (e.g. inclusive W production)
- Objectives: 
 - avoid double counting in real emission
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ME+PS@LO merging

- Multiple LO+PS simulations for processes of different jet multiplicity (e.g. W, Wj, Wjj, \dots)
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Main idea

Phase space slicing for QCD radiation in shower evolution

- **Hard emissions** $Q_{ij}(z, t) > Q_{\text{cut}}$
 - Events rejected
 - Compensated by events starting from higher-order ME regularised by Q_{cut}
- ⇒ Splitting kernels replaced by exact real-emission matrix elements

$$\mathcal{D}_{ij}^{(\text{PS})} \rightarrow \mathcal{R}_{ij}$$

(But Sudakov form factors $\Delta^{(\text{PS})}$ remain unchanged)

- **Soft/collinear emissions** $Q_{ij,k}(z, t) < Q_{\text{cut}}$
 - ⇒ Retained from parton shower $\mathcal{D}_{ij}^{(\text{PS})} = \mathcal{B} \times \left[\frac{1}{2p_i p_j} 8\pi\alpha_s \mathcal{K}_{ij}(p_i, p_j) \right]$

Note

Boundary determined by “jet criterion” $Q_{ij,k}$

- Has to identify soft/collinear divergences in MEs, like jet algorithm
- Otherwise arbitrary

Translate ME event into shower language

Why?

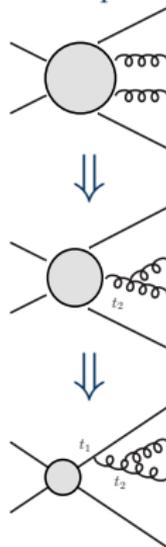
- Need starting scales t for PS evolution
- Have to embed existing emissions into PS evolution

Problem: ME only gives final state, no history

Solution: Backward-clustering (running the shower reversed), similar to jet algorithm:

- 1 Select last splitting according to shower probabilities
- 2 Recombine partons using inverted shower kinematics
→ N-1 particles + splitting variables for one node
- 3 Reweight $\alpha_s(\mu^2) \rightarrow \alpha_s(p_{\perp}^2)$
- 4 Repeat 1 - 3 until core process ($2 \rightarrow 2$)

Example:



Truncated shower

- Shower each (external and intermediate!) line between determined scales
- “Boundary” scales: resummation scale μ_Q^2 and shower cut-off t_0

Cross section up to first emission in ME+PS

$$\begin{aligned}
 d\sigma = d\Phi_B \mathcal{B} & \left[\underbrace{\Delta^{(\text{PS})}(t_0, \mu_Q^2)}_{\text{unresolved}} + \sum_{\{ij\}} \int_{t_0}^{\mu_Q^2} dt \Delta^{(\text{PS})}(t, \mu^2) \right. \\
 & \times \left. \left(\underbrace{\frac{\mathcal{D}_{ij}^{(\text{PS})}}{\mathcal{B}} \Theta(Q_{\text{cut}} - Q_{ij})}_{\text{resolved, PS domain}} + \underbrace{\frac{\mathcal{R}_{ij}}{\mathcal{B}} \Theta(Q_{ij} - Q_{\text{cut}})}_{\text{resolved, ME domain}} \right) \right]
 \end{aligned}$$

Features

- LO weight \mathcal{B} for Born-like event
- Unitarity slightly violated due to mismatch of $\Delta^{(\text{PS})}$ and \mathcal{R}/\mathcal{B}
 $[\dots] \approx 1 \Rightarrow$ LO cross section only approximately preserved
- Unresolved emissions as in parton shower approach
- Resolved emissions now sliced into PS and ME domain
- Only for one emission here, but possible up to high number of emissions

Example

Diphoton production at Tevatron

- Measured by CDF [Phys.Rev.Lett. 110 \(2013\) 101801](#)
- Isolated hard photons
- Azimuthal angle between the diphoton pair

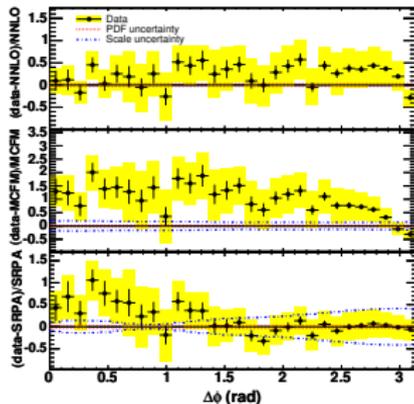
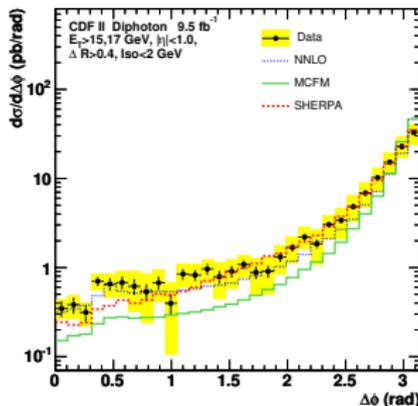
ME+PS simulation using SHERPA vs. (N)NLO

Conclusions

Shapes described very well even for this non-trivial process/observable for both:

- Hard region, e.g. $\Delta\Phi_{\gamma\gamma} \rightarrow 0$
- Soft region, e.g. $\Delta\Phi_{\gamma\gamma} \rightarrow \pi$

Scale variations high \Rightarrow NLO needed



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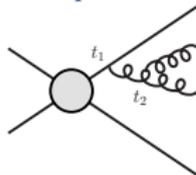
Concepts continued from ME+PS merging at LO

- For each event select jet multiplicity k according to its inclusive NLO cross section
- Reconstruct branching history and nodal scales $t_0 \dots t_k$
- Truncated vetoed parton shower, but with peculiarities (cf. below)

Differences for NLO merging

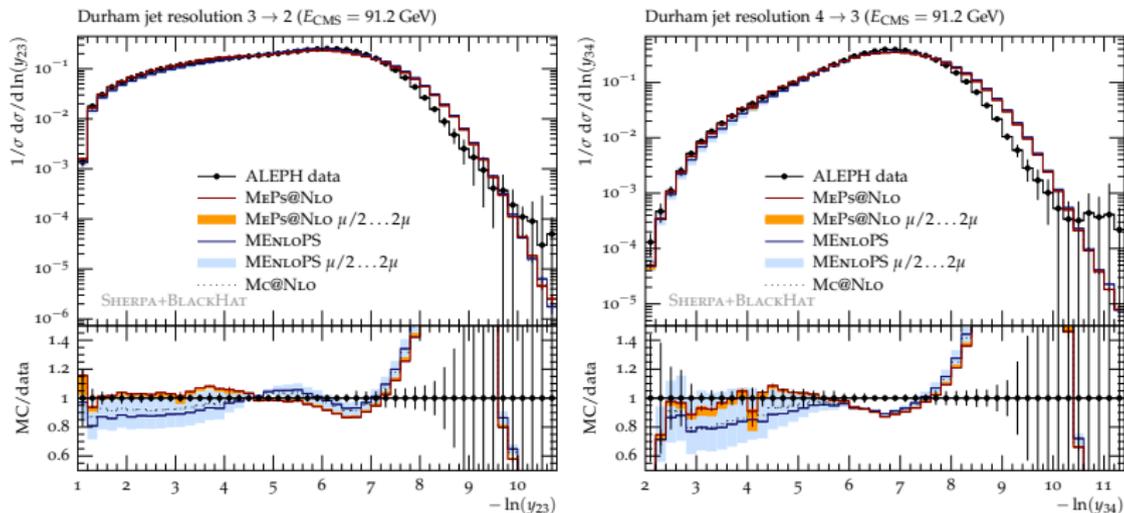
- For each event select type (\mathbb{S} or \mathbb{H}) according to absolute XS
 \Rightarrow Shower then runs differently
- \mathbb{S} event:
 - 1 Generate MC@NLO emission at t_{k+1}
 - 2 Truncated “NLO-vetoed” shower between t_0 and t_k :
 First hard emission is only ignored, no event veto
 - 3 Continue with vetoed parton shower
- \mathbb{H} event:
 (Truncated) vetoed parton shower as in tree-level ME+PS

Example: $k = 1$

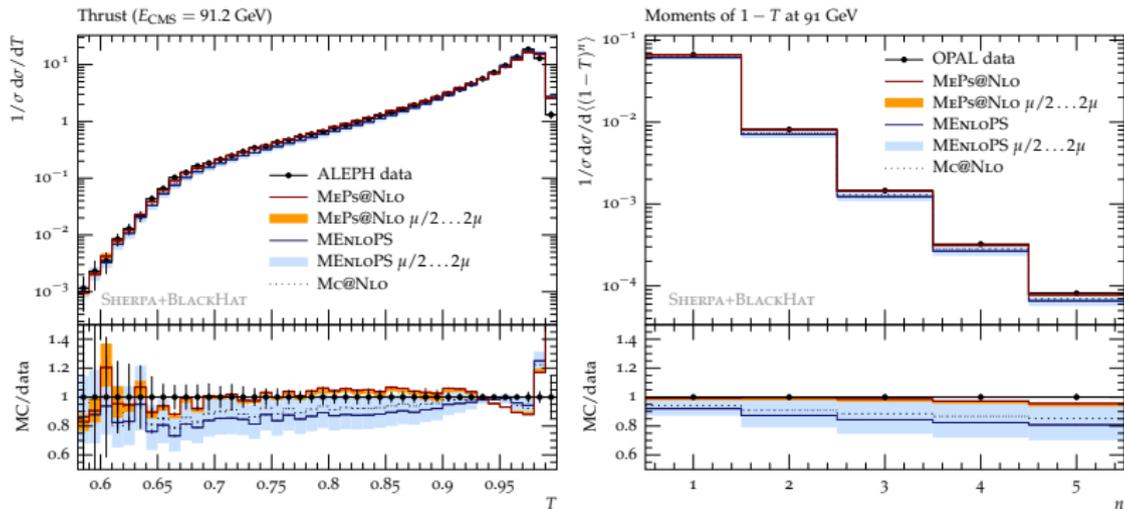


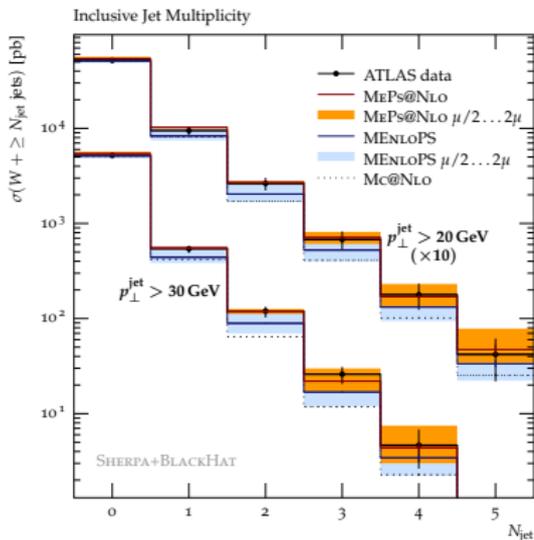
ME+PS@NLO prediction for combining NLO+PS samples of multiplicities n and $n + 1$

$$\begin{aligned}
 d\sigma = & d\Phi_n \bar{B}_n^{(A)} \left[\Delta_n^{(A)}(t_c, \mu_Q^2) + \int_{t_c}^{\mu_Q^2} d\Phi_1 \frac{D_n^{(A)}}{B_n} \Delta_n^{(A)}(t_{n+1}, \mu_Q^2) \Theta(Q_{\text{cut}} - Q_{n+1}) \right] \\
 & + d\Phi_{n+1} H_n^{(A)} \Delta_n^{(\text{PS})}(t_{n+1}, \mu_Q^2) \Theta(Q_{\text{cut}} - Q_{n+1}) \\
 & + d\Phi_{n+1} \bar{B}_{n+1}^{(A)} \underbrace{\left(1 + \frac{B_{n+1}}{\bar{B}_{n+1}^{(A)}} \int_{t_{n+1}}^{\mu_Q^2} d\Phi_1 K_n \right)}_{\text{MC counterterm} \rightarrow \text{NLO-vetoed shower}} \Delta_n^{(\text{PS})}(t_{n+1}, \mu_Q^2) \Theta(Q_{n+1} - Q_{\text{cut}}) \\
 & \times \left[\Delta_{n+1}^{(A)}(t_c, t_{n+1}) + \int_{t_c}^{t_{n+1}} d\Phi_1 \frac{D_{n+1}^{(A)}}{B_{n+1}} \Delta_{n+1}^{(A)}(t_{n+2}, t_{n+1}) \right] \\
 & + d\Phi_{n+2} H_{n+1}^{(A)} \Delta_{n+1}^{(\text{PS})}(t_{n+2}, t_{n+1}) \Delta_n^{(\text{PS})}(t_{n+1}, \mu_Q^2) \Theta(Q_{n+1} - Q_{\text{cut}}) + \dots
 \end{aligned}$$

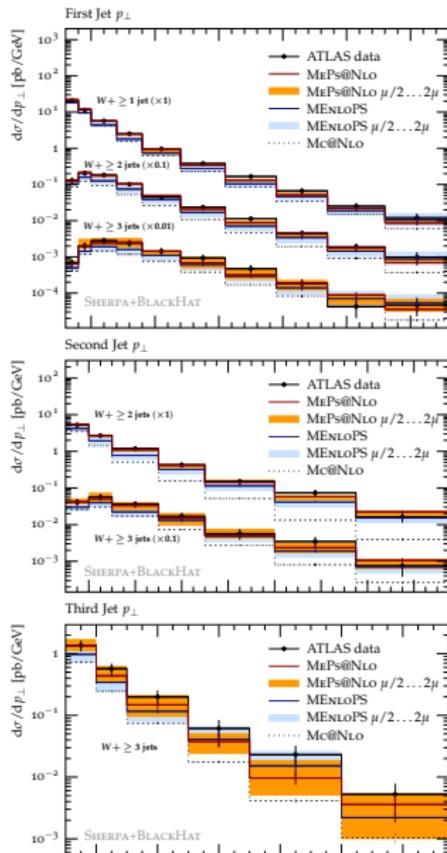


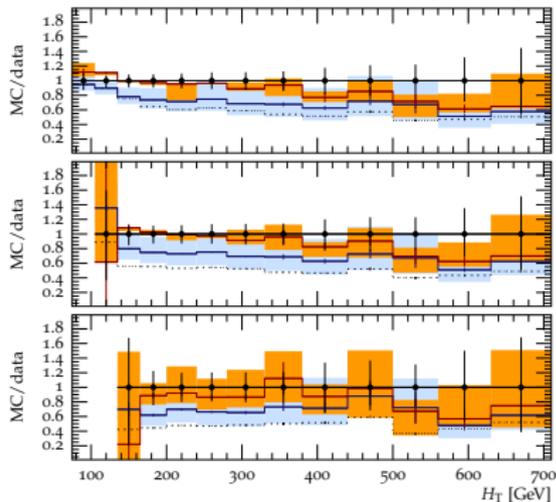
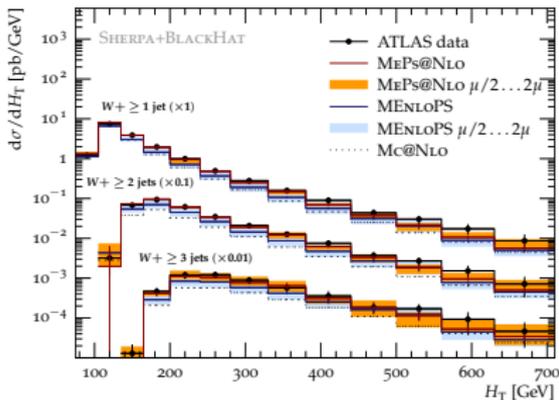
- Significant reduction of ME+PS@NLO scale uncertainties in perturbative region
- Improved agreement with experimental data





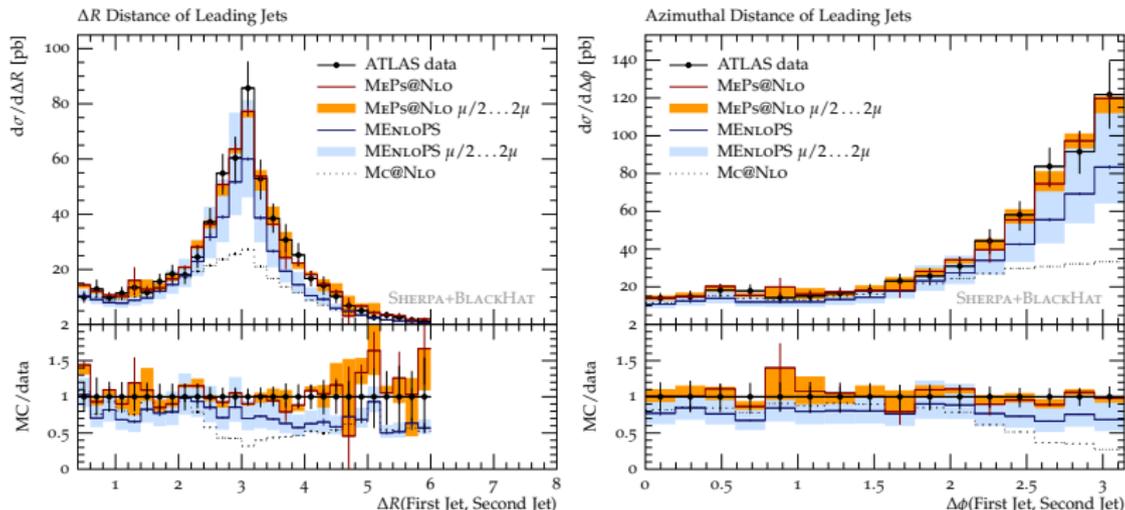
- Comparison to ATLAS measurement [Phys.Rev. D85 \(2012\), 092002](#)
- Significant reduction of ME+PS@NLO scale uncertainties in “NLO” multiplicities
- Improved agreement with data





H_T and related observables are sensitive to many jet multiplicities simultaneously

- Need ME+PS@NLO for precise description
- High H_T region affected by higher multiplicities \Rightarrow Larger scale uncertainty



- Pure Mc@NLO simulation misses correlations between the two leading jets

NLO+PS matching

- Parton shower on top of NLO prediction (e.g. inclusive W production)
- Objectives: 
 - avoid double counting in real emission
 - preserve inclusive NLO accuracy



ME+PS@LO merging

- Multiple LO+PS simulations for processes of different jet multi (e.g. W, Wj, Wjj, \dots)
- Objectives: 
 - combine into one inclusive sample by making them exclusive
 - preserve resummation accuracy



Combination: ME+PS@NLO

- Multiple NLO+PS simulations for processes of different jet multiplicity e.g. W, Wj, Wjj, \dots
- Objectives: 
 - combine into one inclusive sample
 - preserve NLO accuracy for jet observables

Summary

- I'm most certainly out of time by now.

Outlook

- Nachsitzung