TECHNISCHE UNIVERSITÄT DRESDEN

Fakultät Mathematik und Naturwissenschaften Institut für Kern- und Teilchenphysik

QCD Parton Shower Simulations: How to raise their predictive power

Graduate School Seminar
"Particle and Astro-Particle Physics in the Light of the LHC"

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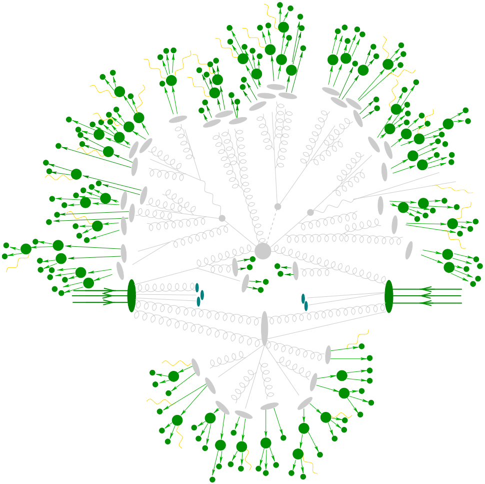
RWTH Aachen, May 2014

Introduction: Monte-Carlo event generators



- We want:
  Simulation of $pp \to$ full hadronised final state
- MC event representation (e.g. $pp \to t\bar{t}H$ 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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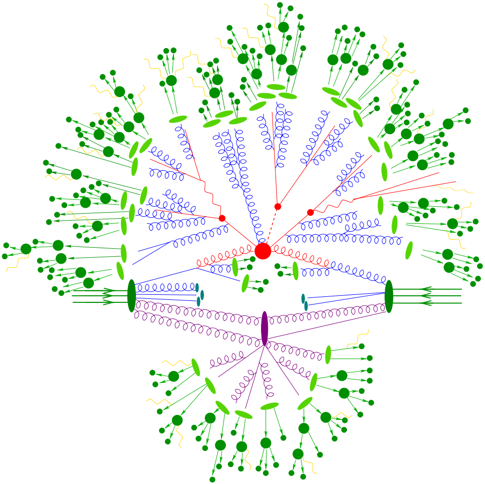

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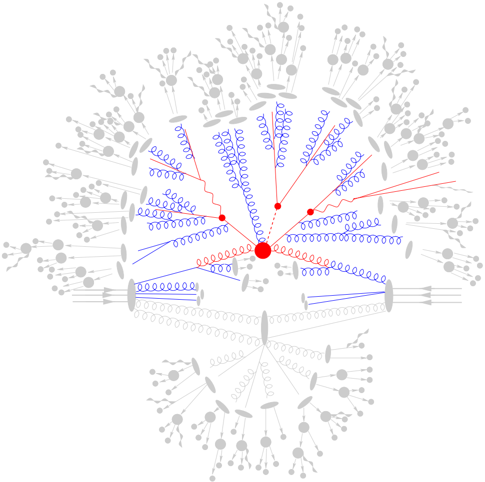

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Outline

- Reminder: QCD perturbation theory
- The parton shower approximation
- Correcting that approximation as far as possible:
  - NLO+PS matching (2002)
  - Tree-level ME+PS merging (2001)
  - ME+PS merging at NLO (2012)

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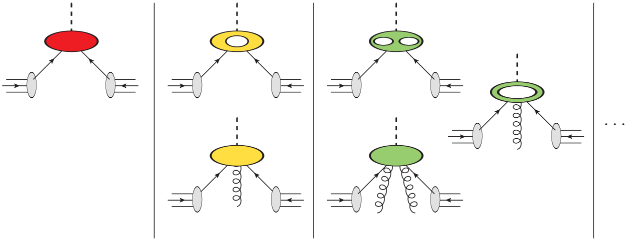
- Cannot solve QCD and calculate e.g. $pp \to t\bar{t}H$ exactly
- But can calculate parts of the perturbative series in α_s:



~ 1 ("LO") $\quad$ $\sim \alpha_s$ ("NLO") $\quad$ $\sim \alpha_s^2$ ("NNLO")

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

From fixed order to resummation

- Predictions for inclusive observables calculable at fixed-order ($\rightsquigarrow$ KLN theorem for cancellation of infrared divergences)
- But if not inclusive $\to$ finite remainders of infrared divergences:

$$\text{logarithms of } \frac{\mu^2_{\text{hard}}}{\mu^2_{\text{cut}}} \text{ with each } \mathcal{O}(\alpha_s)$$

can become large and spoil convergence of perturbative series

Examples:

- Study certain regions of phase space, like $p_\perp^Z \approx 0$ @ DY
- Making predictions for hadron-level final states: confinement at $\mu_{\text{had}} \approx 1$ GeV

$\Rightarrow$ 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

$\to$ Parton Showers!

Universal structure at all orders

- Factorisation of QCD real emission for collinear partons (i, j):

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

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

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- Factorisation of phase space element

$$\mathrm{d}\Phi_{\mathcal{R}} \;\to\; \mathrm{d}\Phi_{\mathcal{B}}\,\mathrm{d}\Phi_1 = \mathrm{d}\Phi_{\mathcal{B}}\;\mathrm{d}t\,\frac{1}{16\pi^2}\,\mathrm{d}z\,\frac{\mathrm{d}\phi}{2\pi}$$

$\Rightarrow$ Combination gives differential branching probability

$$\mathrm{d}\sigma_{ij}^{(\mathrm{PS})} \sim \mathrm{d}t\,\frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}} \sim \frac{\mathrm{d}t}{t}\,\frac{\alpha_s}{2\pi}\,\mathcal{K}_{ij}$$

Resummation of multiple emissions

- $\mathrm{d}\sigma_{ij}^{(\mathrm{PS})}$ is universal and appears for each emission
- How do we get the resummed branching probability according to multiple such emissions?

$\rightarrow$ 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

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

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

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

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

Parton shower branching

- Differential branching probability

$$f(t) \equiv \frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}}$$

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

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

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

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

Parton shower recursion

- Generate next branching "time" t with probability
$$\mathcal{P}(t, t_{\text{previous}}) = f(t) \exp\left(-\int_{t_{\text{previous}}}^t f(t')\mathrm{d}t'\right)$$
- Analytically:
$$t = F^{-1}\left[F(t_{\text{previous}}) + \log(\#_{\text{random}})\right] \text{ with } F(t) = \int_{t_0}^t \mathrm{d}t' f(t')$$
- If integral/its inverse are not known: "Veto algorithm" = extension of hit-or-miss
  - Overestimate $g(t) \geq f(t)$ with known integral $G(t)$ $\rightarrow t = G^{-1}\left[G(t_{\text{previous}}) + \log(\#_{\text{random}})\right]$
  - 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:

$$\mathcal{N}(t) \sim \exp\Big(- \int_0^t \mathrm{d}t' \, f(t') \Big) \quad \to \quad \Delta(t', t'') = \prod_{\{ij\}} \exp\left(- \int_{t'}^{t''} \mathrm{d}t \, \frac{\mathcal{D}_{ij}^{(\mathrm{PS})}}{\mathcal{B}} \right)$$

- 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 $k_\perp^2$, ...
- Starting scale μ_Q^2 (time $t = 0$ in radioactive decay) defined by hard scattering
- Cutoff scale related to hadronisation scale $t_0 \sim \mu_{\mathrm{had}}^2$
- Other variables (z, ϕ) generated directly according to $\mathrm{d}\sigma_{ij}^{(\mathrm{PS})}(t, z, \phi)$

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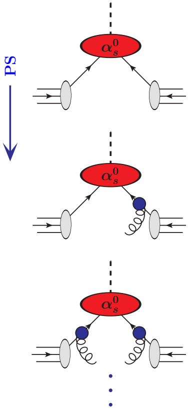
Example: pp $\rightarrow$ h+jets



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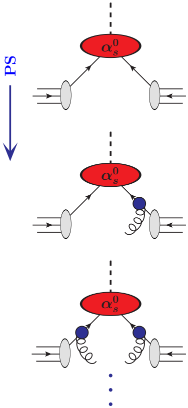

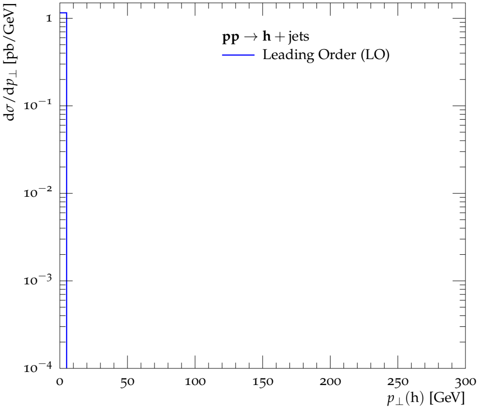

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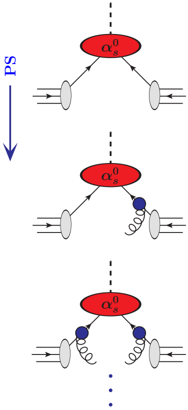

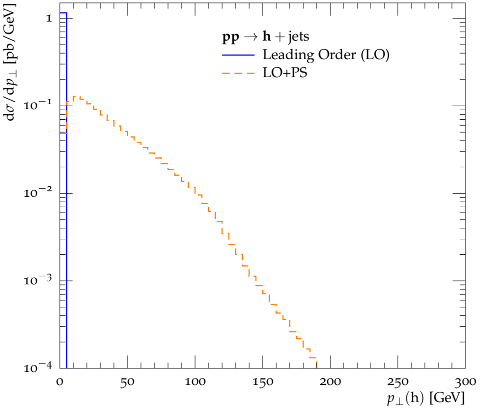

Parton shower improvements: Classification

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, . . .)
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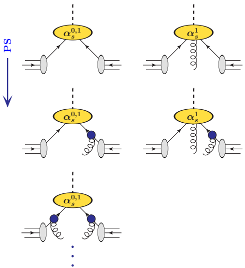
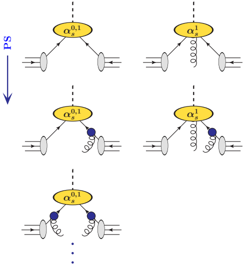


Basic idea

- "double-counting" between emission in real ME and parton shower
- ME is better than PS $\rightarrow$ subtract PS contribution first
- but: shower unitary $\rightarrow$ re-add "integrated" PS contribution with Born kinematics

NLO+PS matching in a nutshell



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

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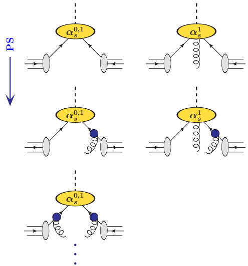

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Additional subtraction

- introduce additional (shower) subtraction terms $\mathcal{D}^{(\mathrm{A})}_{ij}$

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

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

- now apply PS resummation using $\mathcal{D}^{(\mathrm{A})}_{ij}$ as splitting kernels

Master formula for NLO+PS up to first emission

$$\mathrm{d}\sigma^{(\mathrm{NLO+PS})} = \mathrm{d}\Phi_B\, \bar{\mathcal{B}}^{(\mathrm{A})} \Bigg[\underbrace{\Delta^{(\mathrm{A})}(t_0, \mu_Q^2)}_{\text{unresolved}} + \underbrace{\sum_{\{ij\}} \int_{t_0}^{\mu_Q^2} \mathrm{d}t\, \frac{\mathcal{D}_{ij}^{(\mathrm{A})}}{\mathcal{B}} \Delta^{(\mathrm{A})}(t, \mu_Q^2) \Bigg]}_{\text{resolved, singular}}$$

$$+ \; \mathrm{d}\Phi_R \; \underbrace{\Bigg[\mathcal{R} - \sum_{\{ij\}} \mathcal{D}_{ij}^{(\mathrm{A})} \Bigg]}_{\text{resolved, non-singular} \equiv \mathcal{H}^{(\mathrm{A})}}$$

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- To $\mathcal{O}(\alpha_s)$ this reproduces $d\sigma^{(\mathrm{NLO})}$
- Exact choice of $\mathcal{D}_{ij}^{(\mathrm{A})}$ distinguishes MC@NLO vs. POWHEG vs. S-MC@NLO vs. . . .

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

Special cases: MC@NLO vs. S-MC@NLO

MC@NLO

Frixione, Webber (2002)

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

- \+ Shower algorithm for Born-like events easy to implement
- – "Non-singular" piece $\mathcal{R} - \sum_{ij} \mathcal{D}_{ij}^{(\mathrm{A})}$ 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)

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

- \+ "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

$$\mathcal{D}_{ij}^{(\mathrm{A})} \to \rho_{ij}\,\mathcal{R} \qquad \text{where} \qquad \rho_{ij} = \frac{\mathcal{D}_{ij}^{(\mathrm{S})}}{\sum_{mn} \mathcal{D}_{mn}^{(\mathrm{S})}}$$

- $\mathcal{H}$-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

$$\mathcal{D}_{ij}^{(\mathrm{A})}(\Phi_R) \to \rho_{ij}(\Phi_R)\,\left[\mathcal{R}(\Phi_R) - \mathcal{R}^r(\Phi_R)\right] \qquad \text{where} \qquad \rho_{ij} \text{ as above}$$

- 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
  $\mu_F = \mu_R = \frac{1}{2}\mu \ldots 2\mu$

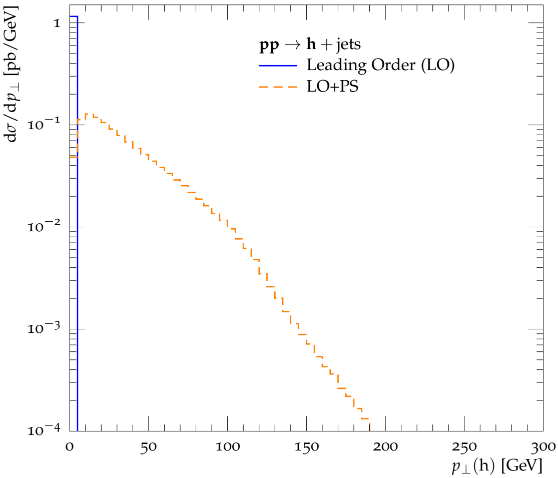
Non-perturbative uncertainties

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

Resummation uncertainties

- Arbitrariness of $\mathcal{D}^{(\mathrm{A})}$ and thus of the exponent in $\Delta^{(\mathrm{A})}$
- 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

Example: pp $\rightarrow$ h+jets



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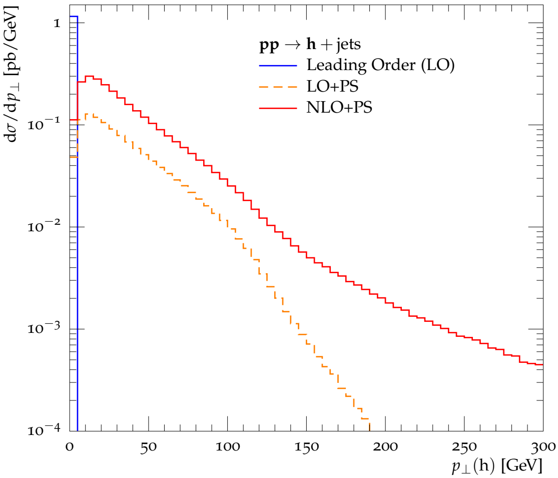

Parton shower improvements: Classification

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, ...)
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Main idea

Phase space slicing for QCD radiation in shower evolution

- Hard emissions $Q_{ij}(z,t) > Q_{\rm cut}$
  - Events rejected $\rightsquigarrow$ Sudakov suppression
  - Compensated by events starting from higher-order ME regularised by $Q_{\rm cut}$

  $\Rightarrow$ Splitting kernels replaced by exact real-emission matrix elements

$$\mathcal{D}_{ij}^{(\rm PS)} \quad \to \quad \mathcal{R}_{ij}$$

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

- Soft/collinear emissions $Q_{ij,k}(z,t) < Q_{\rm cut}$

  $\Rightarrow$ Retained from parton shower $\quad \mathcal{D}_{ij}^{(\rm PS)} = \mathcal{B} \times \left[8\pi\alpha_s \, \frac{1}{2p_ip_j} \, \mathcal{K}_{ij}(p_i,p_j) \right]$

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?

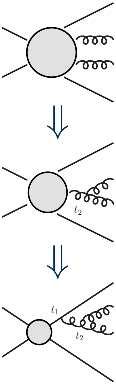
- Need starting scales t for PS evolution
- Have to embed existing emissions into PS evolution

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 probablities
2. Recombine partons using inverted shower kinematics $\rightarrow$ 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

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

Features

- LO weight B for Born-like event
- Unitarity slightly violated due to mismatch of $\Delta^{(\mathrm{PS})}$ and $\mathcal{R}/\mathcal{B}$
  $[\ldots] \approx 1 \Rightarrow$ 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

Features and shortcomings by example

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

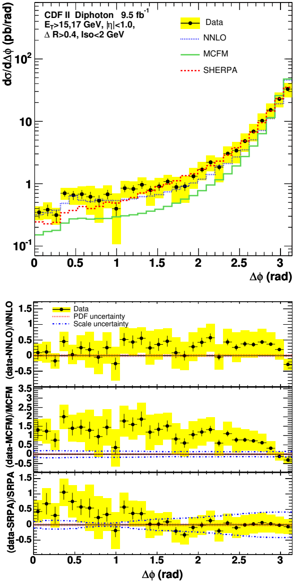
Höche, Schumann, FS (2009)

Conclusions

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

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

Scale variations high $\Rightarrow$ NLO needed



Parton shower improvements: Classification

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, $\ldots$)
- 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, $\ldots$
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$\Downarrow$ $\Downarrow$

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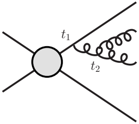
Concepts continued from ME+PS merging at LO

- For each event select jet multiplicity k according to its inclusive NLO cross section
- Reconstruct branching history and nodal scales $t_0 \ldots t_k$
- 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: $k = 1$

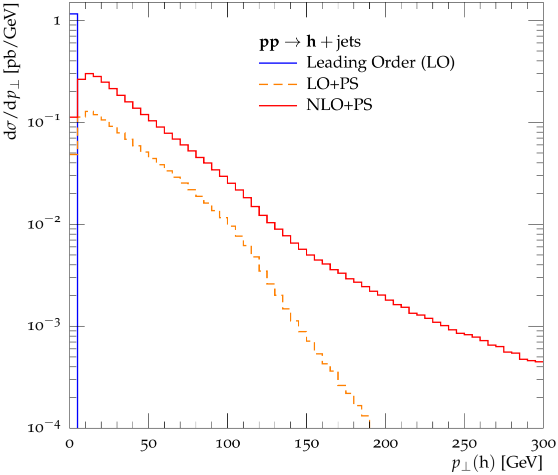


Master formula

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

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

Example: pp $\rightarrow$ h+jets



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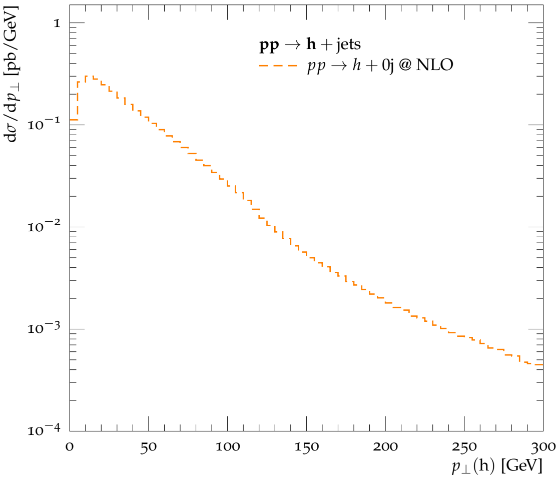

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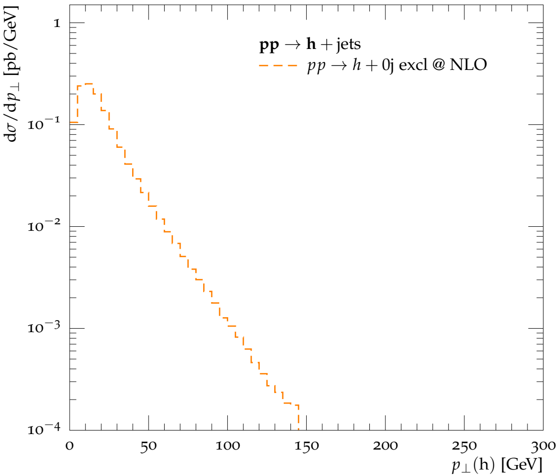

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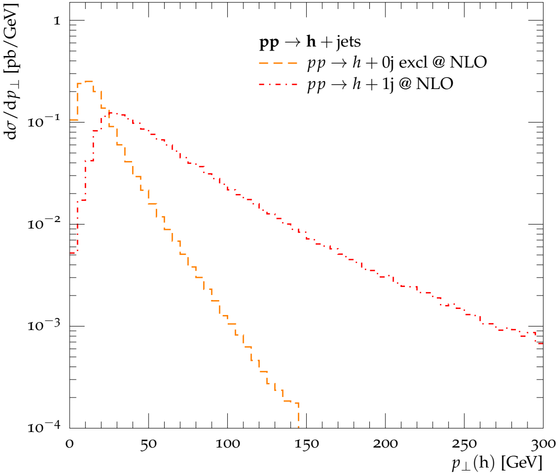

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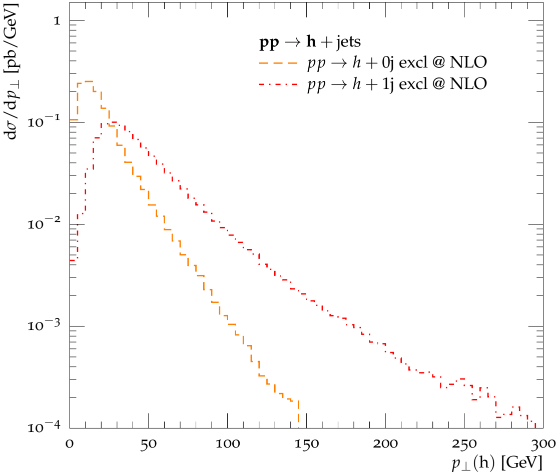
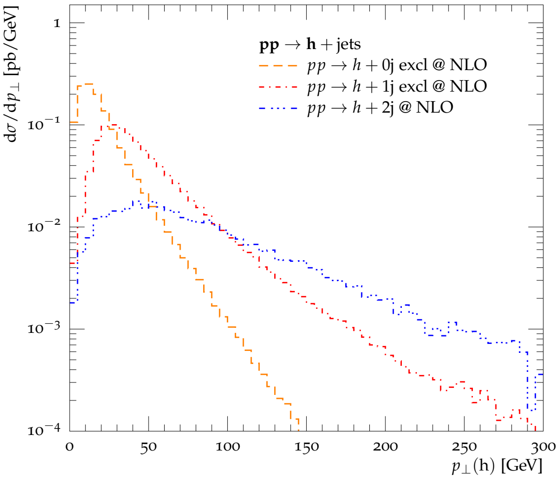


Example: pp $\rightarrow$ h+jets



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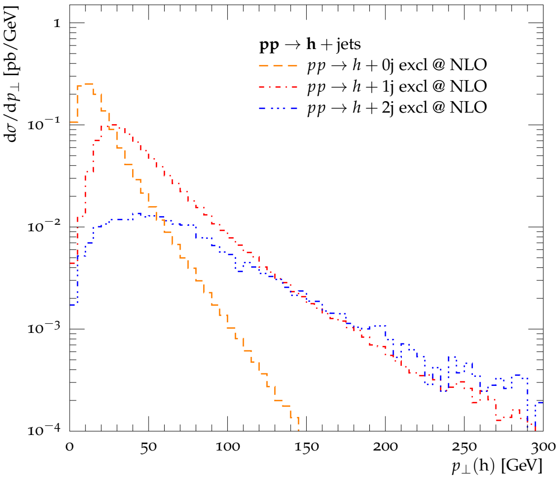

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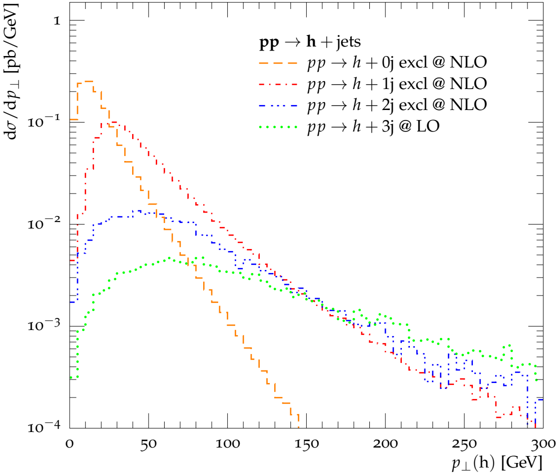

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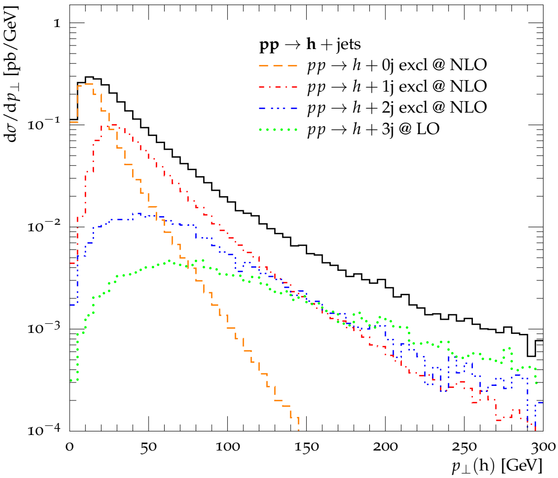

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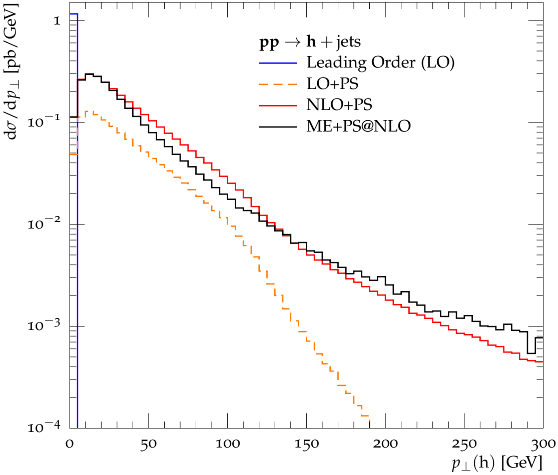
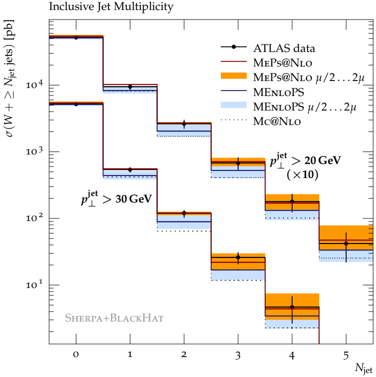
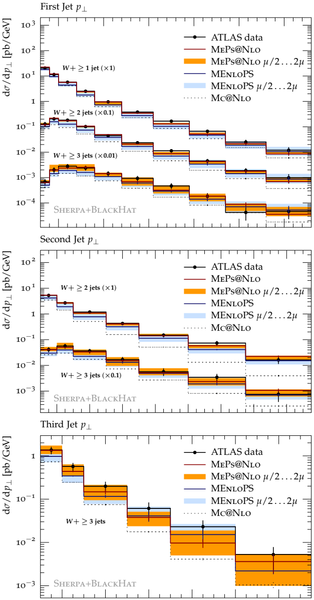


Results for W + jets: Jet multiplicities and $p_\perp$

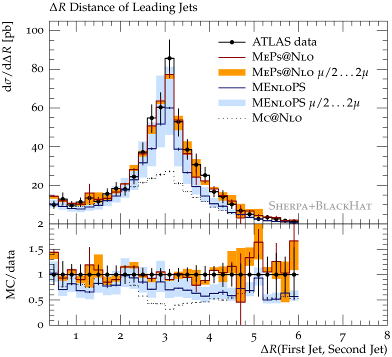
Höche, Krauss, Schönherr, FS (2012)

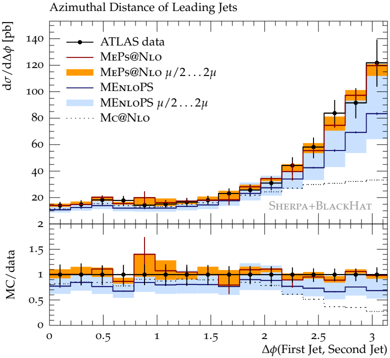




- Comparison to ATLAS measurement Phys.Rev. D85 (2012), 092002
- Significant reduction of ME+PS@NLO scale uncertainties in "NLO" multiplicities
- Improved agreement with data

Results for W + jets: Angular correlations

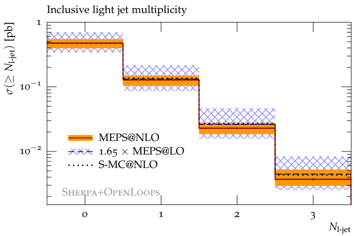


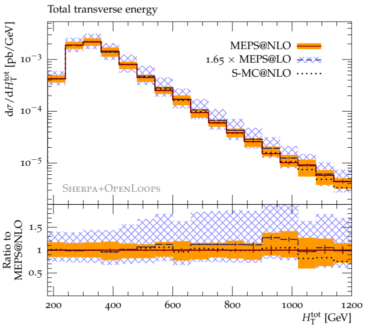


- Pure Mc@Nlo simulation misses correlations between the two leading jets

Results for $t\bar{t}$ + 0,1,2 jets @ NLO

Höche, Krauss, Maierhöfer, Pozzorini, Schönherr, FS (2014)





- Uncertainty reduction from 80% to 25% in 2-jet bin
- Important BSM search selection: high total transverse energy
  $\rightarrow$ major reduction of theoretical uncertainties compared to tree-level merging

Conclusions

NLO+PS matching

- Parton shower on top of NLO prediction (e.g. inclusive W production)
- Objectives: ✓
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$\Downarrow$ $\Downarrow$

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- Objectives: ✓ ✓
  - combine into one inclusive sample
  - preserve NLO accuracy for jet observables

Conclusions

- I’m most certainly out of time by now.
- Nachsitzung?