

# Monte Carlo efficiency via negative weight reduction in Herwig



JAGIELLONIAN UNIVERSITY  
IN KRAKÓW

**James Whitehead**  
CHEP 2024, Kraków

23 Oct 2024



# Problem statement

**compute cost** = cost per CPU-hour

  × CPU hours per event

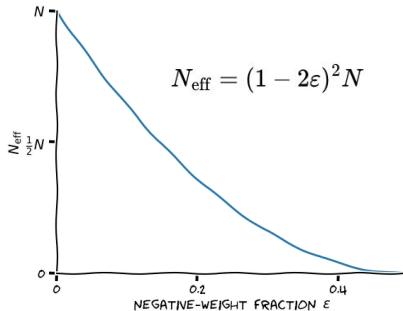
  × number of events

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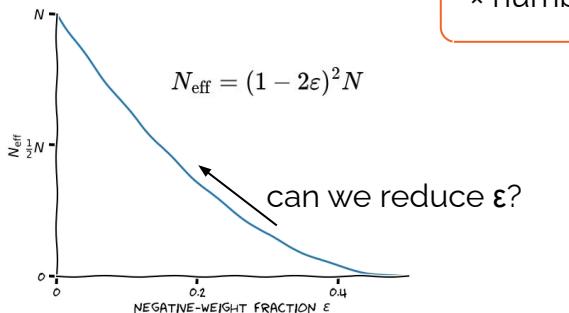
# Big picture

MC generation:

**compute cost** = cost per CPU-hour

× CPU hours per event

× number of events





# I. Theory recap

**NLO parton shower matching** is a key workhorse for LHC phenomenology

- **NLO fixed-order**  
extra loop, extra leg
- **parton-shower algorithms**  
iterative splittings approximate missing MEs
- **angular-ordered or dipole?**  
Herwig's two native showers
- **NLO matching**  
...best of both worlds?

# Anatomy of NLO

perturbative expansion:  
(‘loops and legs’)

$$d\hat{\sigma}_{ab \rightarrow X} = \left(\frac{\alpha_s}{2\pi}\right)^m d\hat{\sigma}_{ab}^{\text{LO}} + \left(\frac{\alpha_s}{2\pi}\right)^{m+1} d\hat{\sigma}_{ab}^{\text{NLO}} + \left(\frac{\alpha_s}{2\pi}\right)^{m+2} d\hat{\sigma}_{ab}^{\text{NNLO}} + \mathcal{O}(\alpha_s^{m+3})$$

subtraction terms  $d\hat{\sigma}_{\text{NLO}}^S$   
provided by Catani-Seymour dipoles  
(automated in H7 **Matchbox** module)

A general algorithm for calculating jet cross  
sections in NLO QCD<sup>★</sup>

$$\begin{aligned} \int d\hat{\sigma}^{\text{NLO}} &= \int d\Phi_{n+1} d\hat{\sigma}^R + \int d\Phi_n d\hat{\sigma}^V \\ &\equiv \int d\Phi_{n+1} \underbrace{[d\hat{\sigma}^R - d\hat{\sigma}_{\text{NLO}}^S]}_{\text{finite by universality}} \\ &\quad + \underbrace{\int d\Phi_n \left[ d\hat{\sigma}^V + \int d\Phi_1 d\hat{\sigma}_{\text{NLO}}^S \right]}_{\text{finite by KLN}} \end{aligned}$$

S. Catani<sup>a</sup>, M.H. Seymour<sup>b</sup>

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I-50125 Florence, Italy

<sup>b</sup> Theory Division, CERN, CH-1211 Geneva 23, Switzerland

# Theoretical parton showers

differential splitting probability (type ‘ $\alpha$ ’):  $P_m^{(\alpha)}(\Phi_{+1}^{(\alpha)})$

Sudakov factor (no-emission probability):  $\Delta|_t^{t_1} = \prod_j \Delta_j|_t^{t_1}$

$$\Delta_i|_t^{t_1} = \exp \left[ - \int_t^{t_1} dt' P_i(t') \right]$$

Iterative operator:

$$\text{PS}[\mathcal{O}](\Phi_m) = \Delta|_{t_0}^{t_1(\Phi_m)}(\Phi_m) \mathcal{O}(\Phi_m)$$

$$+ \sum_{(\alpha)} d\Phi_{+1}^{(\alpha)} \Theta \left[ t_0 < t(\Phi_{m+1}^{(\alpha)}) < t_1(\Phi_m) \right] \left( \frac{\alpha_s(\mu^{(\alpha)}(\Phi_{m+1}^{(\alpha)}))}{2\pi} P_m^{(\alpha)}(\Phi_{+1}^{(\alpha)}) \right) \Delta|_{t(\Phi_{m+1}^{(\alpha)})}^{t_1(\Phi_m)}(\Phi_m) \text{PS}[\mathcal{O}](\Phi_{m+1}^{(\alpha)})$$

NB: unitary!

# Theoretical Practical parton showers

Choose:

1. emission kernels  $P_m^{(\alpha)}(\Phi_{+1}^{(\alpha)})$
2. phase-space mappings  $\Phi_m(p_1, p_2) \xrightarrow{\Phi_{+1}} \Phi_{m+1}^{(\alpha)}$
3. evolution variable  $t(\Phi_{m+1}^{(\alpha)})$
4. starting scale  $t_1(\Phi_m)$ , cut-off scale  $t_0$
5. renormalisation scales  $\mu^{(\alpha)}(\Phi_{m+1}^{(\alpha)})$

$$\text{PS}[\mathcal{O}](\Phi_m) = \Delta|_{t_0}^{t_1(\Phi_m)}(\Phi_m) \mathcal{O}(\Phi_m)$$

$$+ \sum_{(\alpha)} d\Phi_{+1}^{(\alpha)} \Theta[t_0 < t(\Phi_{m+1}^{(\alpha)}) < t_1(\Phi_m)] \left( \frac{\alpha_s(\mu^{(\alpha)}(\Phi_{m+1}^{(\alpha)}))}{2\pi} P_m^{(\alpha)}(\Phi_{+1}^{(\alpha)}) \right) \Delta|_{t(\Phi_{m+1}^{(\alpha)})}^{t_1(\Phi_m)}(\Phi_m) \text{PS}[\mathcal{O}](\Phi_{m+1}^{(\alpha)})$$

# NLO parton shower matching

**parton showers** allow predictions for **exclusive, high-multiplicity** final-states

**NLO fixed order** is limited to a **single** extra resolved emission

→ NLO ‘matching’ combines both

**non-trivial**

- can't spoil hard-won NLO accuracy: need control over  $O(\alpha_s)$  terms
- can't spoil parton shower logarithmic accuracy
- in particular: avoid double-counting where the shower generates an approximation to the real ME



## II. NLO matching

Herwig's **Matchbox** module supports both major general-purpose NLO matching methods

→ **MC@NLO**

'subtractive' matching

→ **Powheg**

'multiplicative' matching; modifies shower

Coming soon (H7.4) for colour-singlet final states:

→ **KrkNLO**

'multiplicative' matching; modifies PDF factorisation scheme



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Frixione & Webber  
[arXiv: [0204244](#)]

Nason [arXiv: [0409146](#)]

Coming soon (H7.4) for colour-singlet final states:

→ **KrkNLO**

'multiplicative' matching; modifies PDF factorisation scheme

Jadach et al. [arXiv: [1503.06849](#)]

# MC@NLO

Main idea:

- shower subtracted real-phasespace events  
('H'-events)
- separately, shower born-phasespace events  
('S'-events)

$$\begin{aligned}
 & d\phi_m u(\phi_m) \Theta_{\text{cut}}[\phi_m] \left[ \left\{ B(\phi_m) + V(\phi_m) + \sum_{\alpha} \left[ I^{(\alpha)}(\phi_m) + dx(P+K)^{(\alpha)}(x; \phi_m) \right] \right\} \right. \\
 & \quad + \sum_{\alpha} dq^{(\alpha)} \left\{ \Theta_R^{(\alpha)} [\Phi_{m+1}^{(\alpha)}(\phi_m, q)] R(\Phi_{m+1}^{(\alpha)}(\phi_m, q)) \left[ \frac{w^{(\alpha)}(\Phi_{m+1}^{(\alpha)}(\phi_m; q))}{\sum_{\beta} w^{(\beta)}(\Phi_{m+1}^{(\beta)}(\phi_m; q))} \right] \Theta_{\mu_s}^{(\alpha)} - D^{(\alpha)} (\Phi_{m+1}^{(\alpha)}(\phi_m; q)) \right\} \\
 & \quad + \sum_{\alpha} dq^{(\alpha)} \left\{ \Theta_{\text{PS}}^{(\alpha)} [\Phi_{m+1}^{(\alpha)}(\phi_m; q)] \text{PS}^{(\alpha)}(\Phi_{m+1}^{(\alpha)}(\phi_m; q)) \Theta_{\mu_s}^{(\alpha)} \right\} \\
 & \quad \left. + \sum_{\alpha} dq^{(\alpha)} \left\{ M_{\text{bridge}}^{(\alpha)}(\Phi_{m+1}^{(\alpha)}(\phi_m; q)) (1 - \Theta_{\mu_s}^{(\alpha)}) \right\} \right] \\
 & + d\phi_{m+1} u(\phi_{m+1}) \left[ R(\phi_{m+1}) \Theta_{\text{cut}}[\phi_{m+1}] \right. \\
 & \quad - \sum_{\alpha} \left\{ \Theta_R^{(\alpha)} [\phi_{m+1}] R(\phi_{m+1}) \left[ \frac{w^{(\alpha)}(\phi_{m+1})}{\sum_{\beta} w^{(\beta)}(\phi_{m+1})} \right] \Theta_{\mu_s}^{(\alpha)} \right\} \Theta_{\text{cut}} [\Phi_m^{(\alpha)}(\phi_{m+1})] \\
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 \end{aligned}$$

# MC@NLO

Main idea:

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(‘H’-events)
- separately, shower born-phasespace events  
(‘S’-events)

over-subtractions cause negative weights

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 & + d\phi_{m+1} u(\phi_{m+1}) \\
 & \quad \left[ R(\phi_{m+1}) \Theta_{\text{cut}}[\phi_{m+1}] \right. \\
 & \quad - \sum_{\alpha} \left\{ \Theta_R^{(\alpha)} [\phi_{m+1}] R(\phi_{m+1}) \left[ \frac{w^{(\alpha)}(\phi_{m+1})}{\sum_{\beta} w^{(\beta)}(\phi_{m+1})} \right] \Theta_{\mu_s}^{(\alpha)} \right\} \Theta_{\text{cut}} [\Phi_m^{(\alpha)}(\phi_{m+1})] \\
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 \end{aligned}$$

fix: make them multiplicative

# KrkNLO

## KrkNLO matching for colour-singlet processes

---

Pratixan Sarmah,<sup>a</sup> Andrzej Siódmok,<sup>a</sup> James Whitehead<sup>a,b</sup>

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**ABSTRACT:** Matched calculations combining perturbative QCD with parton showers are an indispensable tool for LHC physics. Two methods for NLO matching are in widespread use: Mc@NLO and POWHEG. We describe an alternative, KrkNLO, reformulated to be easily applicable to any colour-singlet process. The primary distinguishing characteristic of KrkNLO is its use of an alternative factorisation scheme, the ‘Krk’ scheme, to achieve NLO accuracy. We describe the general implementation of KrkNLO in Herwig 7, using diphoton production as a test process. We systematically compare its predictions to those produced by Mc@NLO with several different choices of shower scale, both truncated to one-emission and with the shower running to completion, and to ATLAS data from LHC Run 2.

**KEYWORDS:** QCD, LHC, NLO matching, parton showers, factorisation schemes, hadron colliders

## Main idea:

- change PDF factorisation scheme  
(‘Krk’ scheme: not MSbar!)
- matching becomes multiplicative
- no subtraction: weights become positive

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## Progress:

- Drell–Yan *Jadach et al* [arXiv: [1503.06849](#)]
- Higgs *Jadach et al* [arXiv: [1607.06799](#)]
- general (q-qb) colour singlet processes now implemented  
*Sarmah, Siódlok, JW* [arXiv: [2409.16417](#)]
- ongoing complementary theory, pheno and computational studies

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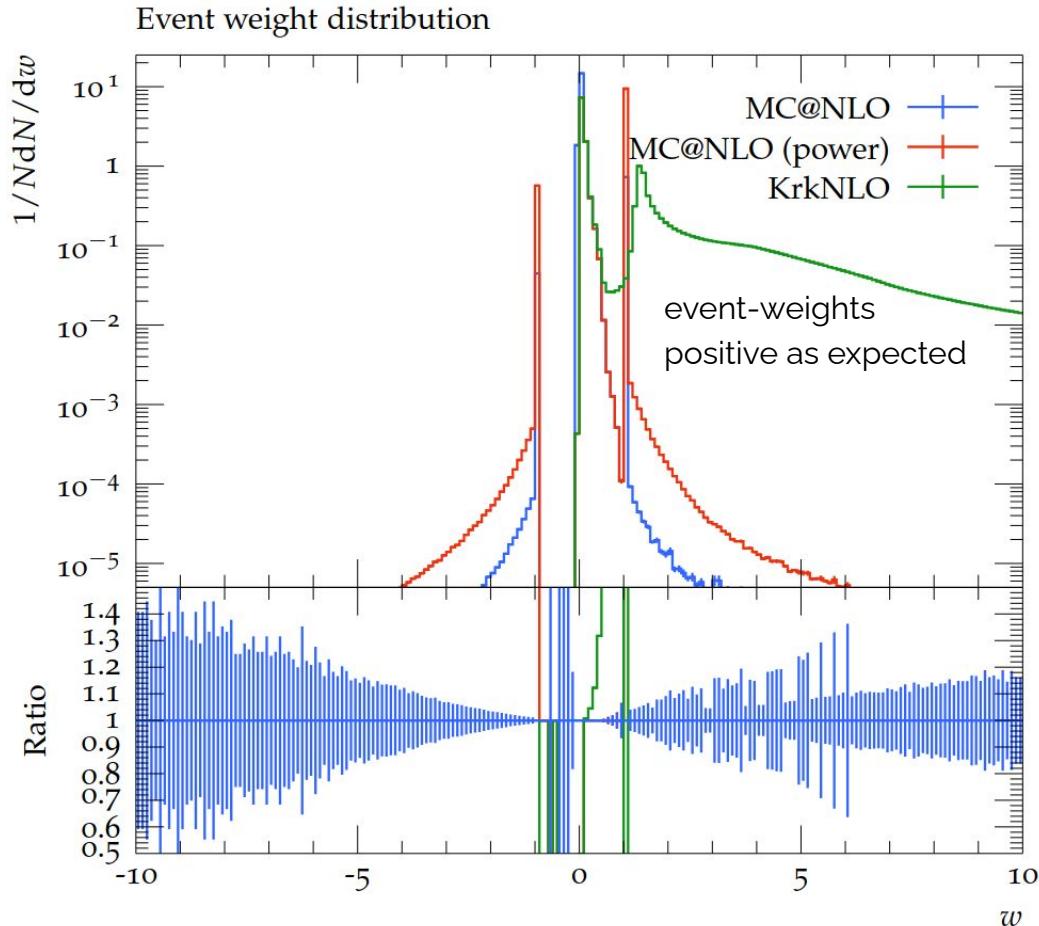
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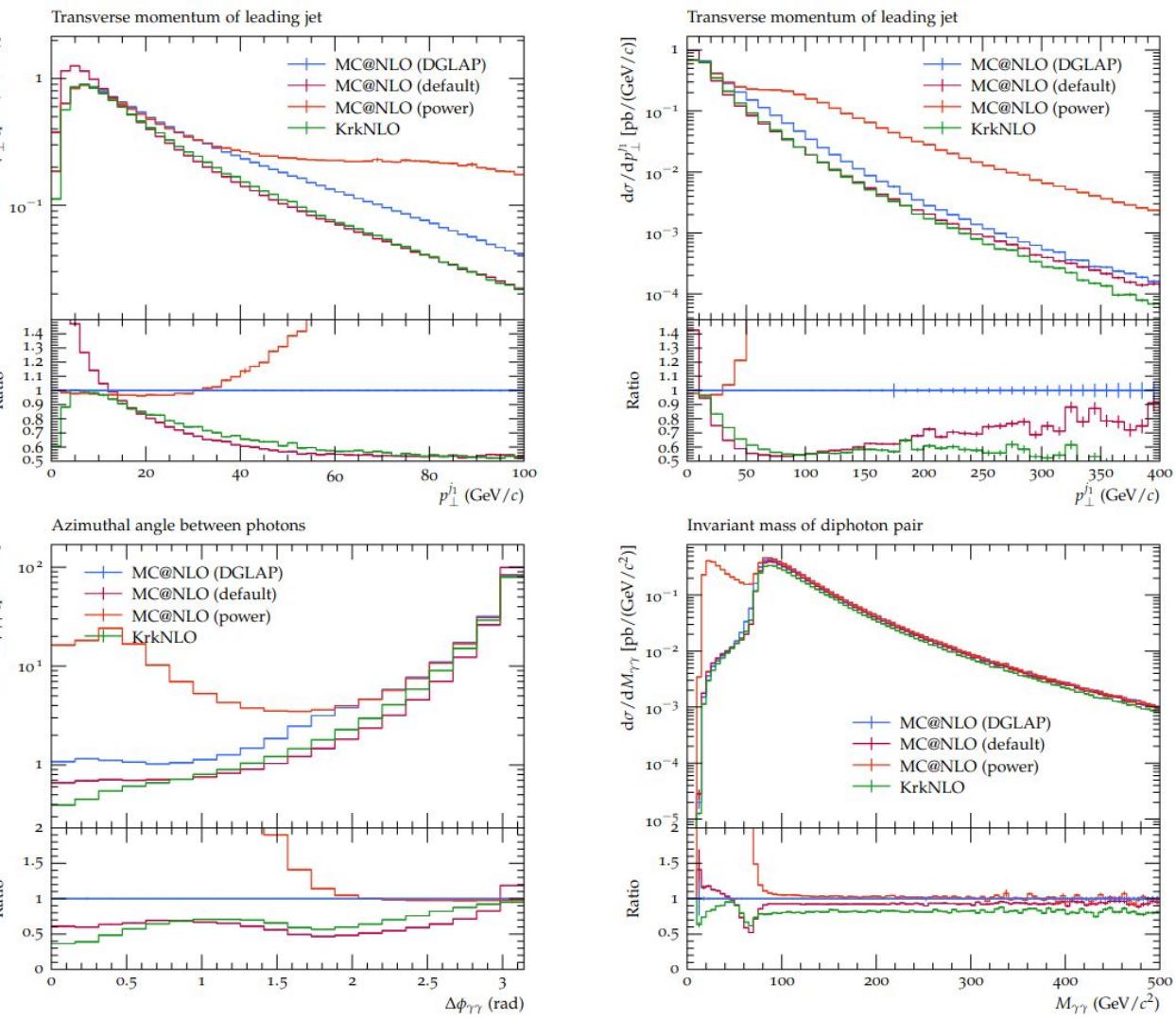
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## Outlook:

- due to be included in Herwig 7.4.0
- pheno studies in progress
- possible extensions to NLO merging, non-singlets, (NNLO?)

# MC@NLO with Matchbox

'Make them multiplicative' for MC@NLO:

- restructure MC@NLO code in Matchbox to generate reweights in place of subtractions

$$\begin{aligned}
 & d\phi_m u(\phi_m) \Theta_{\text{cut}}[\phi_m] \left[ \left\{ B(\phi_m) + V(\phi_m) + \sum_{\alpha} \left[ I^{(\alpha)}(\phi_m) + dx(P+K)^{(\alpha)}(x; \phi_m) \right] \right\} \right. \\
 & + \sum_{\alpha} dq^{(\alpha)} \left\{ \Theta_R^{(\alpha)} [\Phi_{m+1}^{(\alpha)}(\phi_m; q)] R(\Phi_{m+1}^{(\alpha)}(\phi_m; q)) \left[ \frac{w^{(\alpha)}(\Phi_{m+1}^{(\alpha)}(\phi_m; q))}{\sum_{\beta} w^{(\beta)}(\Phi_{m+1}^{(\beta)}(\phi_m; q))} \right] \Theta_{\mu_s}^{(\alpha)} - D^{(\alpha)} (\Phi_{m+1}^{(\alpha)}(\phi_m; q)) \right\} \\
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 & + d\phi_{m+1} u(\phi_{m+1}) \left[ R(\phi_{m+1}) \Theta_{\text{cut}}[\phi_{m+1}] \right. \\
 & - \sum_{\alpha} \left\{ \Theta_R^{(\alpha)} [\phi_{m+1}] R(\phi_{m+1}) \left[ \frac{w^{(\alpha)}(\phi_{m+1})}{\sum_{\beta} w^{(\beta)}(\phi_{m+1})} \right] \Theta_{\mu_s}^{(\alpha)} \right\} \Theta_{\text{cut}} [\Phi_m^{(\alpha)}(\phi_{m+1})] \\
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 \end{aligned}$$

fix: make them multiplicative

# Matchbox restructuring

reducing the fraction of negative weights

(including new flexibility to study matching uncertainty)

## old components:

- real shower subtraction
- ‘virtual shower subtraction’
  - generate real-type
  - subtractive projections
- born-type

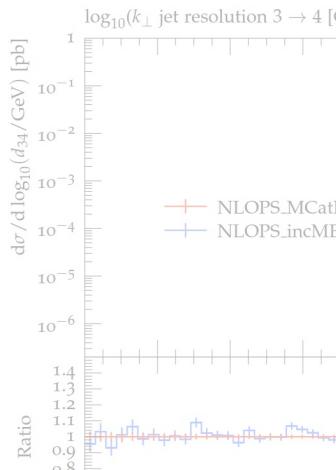
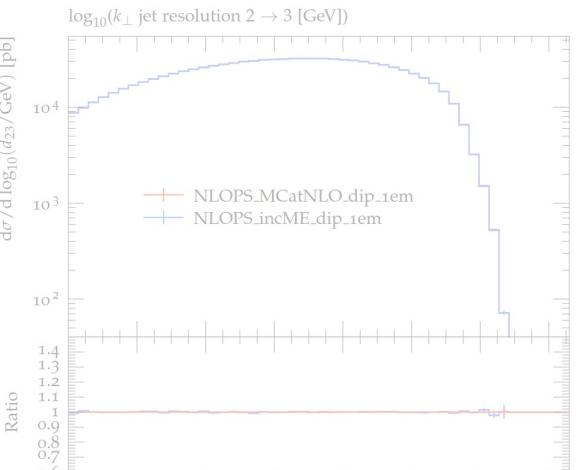
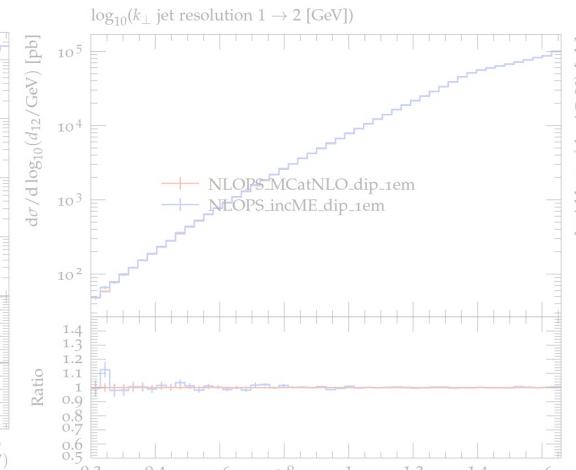
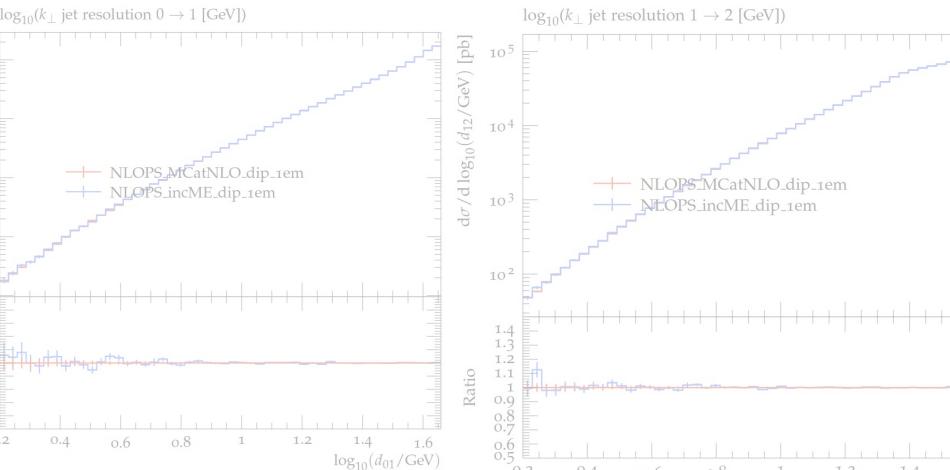
## additional new component:

- ‘inclusive ME’
  - generate born-type
  - radiative splittings

# Matchbox restructuring

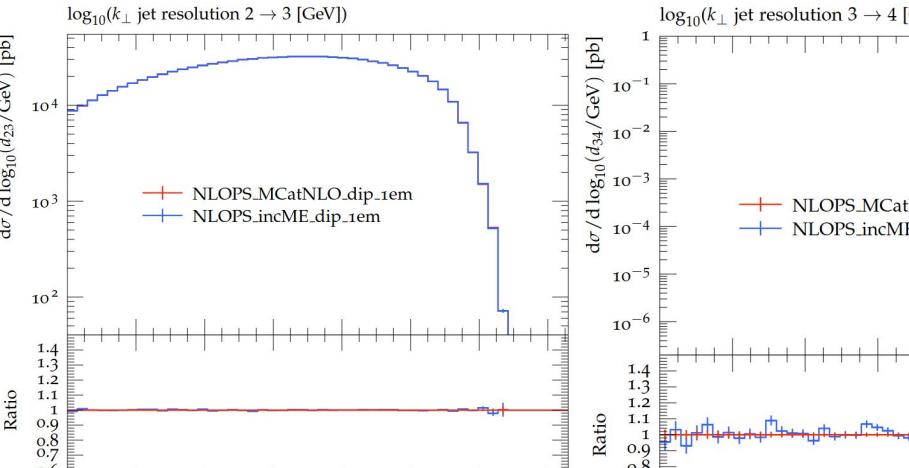
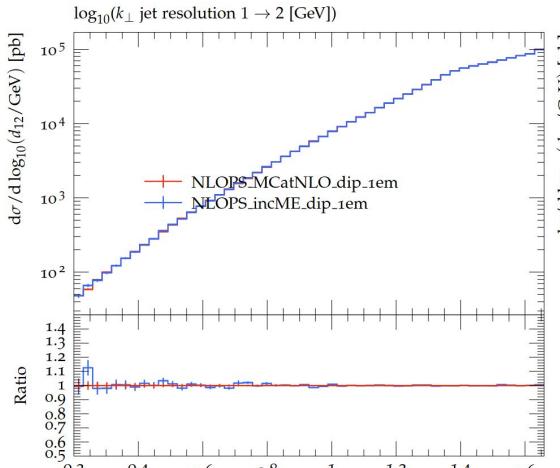
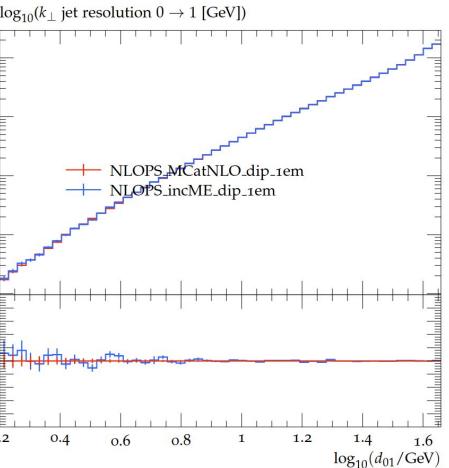
reducing the fraction of negative weights

(including new flexibility to study matching uncertainty)



# Matchbox restructuring

validation ongoing (preview)



—

# Thank you!

# Parton showers in **Herwig 7**

**angular-ordered vs Herwig dipole shower**

different choices of

1. emission kernels  $P_m^{(\alpha)}(\Phi_{+1}^{(\alpha)})$
2. phase-space mappings  $\Phi_m(p_1, p_2) \xrightarrow{\Phi_{+1}} \Phi_{m+1}^{(\alpha)}$
3. evolution variable  $t(\Phi_{m+1}^{(\alpha)})$

**customisable:**

4. starting scale  $t_1(\Phi_m)$ , cut-off scale  $t_0$
5. renormalisation scales  $\mu^{(\alpha)}(\Phi_{m+1}^{(\alpha)})$

**different (reasonable) choices encapsulate different physics**  
several others are also available (Pythia, Sherpa CSS, Vincia, Dire, Alaric etc)

# Angular-ordered ('q-tilde')

## New formalism for QCD parton showers

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**ABSTRACT:** We present a new formalism for parton shower simulation of QCD jets, which incorporates the following features: invariance under boosts along jet axes, improved treatment of heavy quark fragmentation, angular-ordered evolution with soft gluon coherence, more accurate soft gluon angular distributions, and better coverage of phase space. It is implemented in the new HERWIG++ event generator.

**KEYWORDS:** QCD, Jets, Heavy Quark Physics.

A crucial ingredient of modern parton showering algorithms<sup>1</sup> is *angular ordering*, which ensures that important aspects of soft gluon coherence are included in an azimuthally-averaged form. The angular shower evolution variable [2] used in the event generator program HERWIG [3] is good for ensuring that angular ordering is built in from the outset, but the phase space is complicated and not invariant under any kind of boosts. Evolution in virtuality looks natural but then angular ordering must be imposed afterwards, as is done in PYTHIA [4].

## 2. New variables for parton branching

### 2.1 Final-state quark branching

virtuality  $Q_g^2$  for gluons and light quarks. Therefore from eq. (2.5) the evolution variable is

$$\tilde{q}^2 = \frac{\mathbf{p}_\perp^2}{z^2(1-z)^2} + \frac{\mu^2}{z^2} + \frac{Q_g^2}{z(1-z)^2} \quad (2.7)$$

where  $\mu = \max(m, Q_g)$ .

Angular ordering of the branching  $q_i \rightarrow q_{i+1}$  is defined by

$$\tilde{q}_{i+1} < z_i \tilde{q}_i .$$

$$dP(q \rightarrow qg) = \frac{\alpha_s}{2\pi} \frac{d\tilde{q}^2}{\tilde{q}^2} P_{qq} dz = \frac{C_F}{2\pi} \alpha_s [z^2(1-z)^2 \tilde{q}^2] \frac{d\tilde{q}^2}{\tilde{q}^2} \frac{dz}{1-z} \left[ 1 + z^2 - \frac{2m^2}{z\tilde{q}^2} \right]$$

### 2.2 Gluon splitting

$$\tilde{q}^2 = \frac{q^2}{z(1-z)} = \frac{\mathbf{p}_\perp^2 + m^2}{z^2(1-z)^2}$$

$$dP(g \rightarrow q\bar{q}) = \frac{T_R}{2\pi} \alpha_s [z^2(1-z)^2 \tilde{q}^2] \frac{d\tilde{q}^2}{\tilde{q}^2} \left[ 1 - 2z(1-z) + \frac{2m^2}{z(1-z)\tilde{q}^2} \right] dz$$

$$dP(g \rightarrow gg) = \frac{C_A}{2\pi} \alpha_s [z^2(1-z)^2 \tilde{q}^2] \frac{d\tilde{q}^2}{\tilde{q}^2} \left[ \frac{z}{1-z} + \frac{1-z}{z} + z(1-z) \right] dz$$

# Dipole shower

## Coherent Parton Showers with Local Recoils

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**ABSTRACT:** We outline a new formalism for dipole-type parton showers which maintain exact energy-momentum conservation at each step of the evolution. Particular emphasis is put on the coherence properties, the level at which recoil effects do enter and the role of transverse momentum generation from initial state radiation. The formulated algorithm is shown to correctly incorporate coherence for soft gluon radiation. Furthermore, it is well suited for easing matching to next-to-leading order calculations.

**KEYWORDS:** QCD, Jets, NLO Calculations.

Having however observed that we can reproduce the correct Sudakov anomalous dimension, while avoiding soft double counting we additionally note that within the variables chosen

$$p_\perp^2 = 2 \frac{p_i \cdot q}{p_i \cdot p_k} q \cdot p_k \quad (2.30)$$

for emission of a gluon of momentum  $q$  off a dipole  $(i, k)$ . Ordering emissions in this variable therefore corresponds to an ordering reproducing the most probable history of multiple gluon emission according to the eikonal approximation in the limit of soft gluons strongly ordered in energy.

### 3.1 Final State Radiation

#### 3.1.1 Final State Spectator

Final state radiation with a final state spectator does represent the generic version of the splitting kinematics chosen here. For a splitting  $(p_i, p_j) \rightarrow (q_i, q, q_j)$  we choose the standard Sudakov decomposition

$$q_i = z p_i + \frac{p_\perp^2}{z s_{ij}} p_j + k_\perp \quad (3.1)$$

$$q = (1 - z) p_i + \frac{p_\perp^2}{(1 - z) s_{ij}} p_j - k_\perp \quad (3.2)$$

$$q_j = \left(1 - \frac{p_\perp^2}{z(1 - z)s_{ij}}\right) p_j , \quad (3.3)$$

$$dP = \frac{\alpha_s}{2\pi} \langle V(p_\perp^2, z) \rangle \left(1 - \frac{p_\perp^2}{z(1 - z)s_{ij}}\right) \frac{dp_\perp^2}{p_\perp^2} dz$$

$$\langle \mathbf{V}^{q_a g_i, b}(x_{i,ab}) \rangle = C_F \left\{ \frac{2}{1 - x_{i,ab}} - (1 + x_{i,ab}) \right\} ,$$

$$\langle \mathbf{V}^{q_a q_i, b}(x_{i,ab}) \rangle = C_F \left\{ x_{i,ab} + 2 \frac{1 - x_{i,ab}}{x_{i,ab}} \right\} ,$$

$$\langle \mathbf{V}^{g_a g_i, b}(x_{i,ab}) \rangle = 2C_A \left\{ \frac{1}{1 - x_{i,ab}} + \frac{1 - x_{i,ab}}{x_{i,ab}} - 1 + x_{i,ab}(1 - x_{i,ab}) \right\}$$

$$\langle \mathbf{V}^{q_a q_i, b}(x_{i,ab}) \rangle = T_R \{1 - 2x_{i,ab}(1 - x_{i,ab})\} .$$

# MC@NLO

$$\begin{aligned} d\sigma_{\text{mod}} &= \left( B(\Phi_B) + \hat{V}(\Phi_B) + \int R^{(\text{MC})}(\Phi_B, \Phi_{\text{rad}}) d\Phi_{\text{rad}} \right) d\Phi_B \\ &+ \left( R(\Phi_B, \Phi_{\text{rad}}) - R^{(\text{MC})}(\Phi_B, \Phi_{\text{rad}}) \right) d\Phi_B d\Phi_{\text{rad}}, \end{aligned}$$

## NEXT-TO-LEADING-ORDER EVENT GENERATORS

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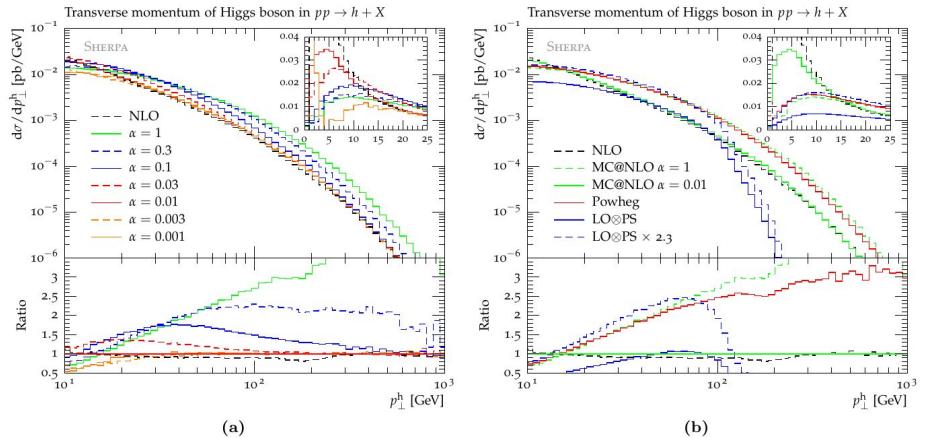
### Abstract

We review the methods developed for combining the parton shower approximation to QCD with fixed-order perturbation theory, in such a way as to achieve next-to-leading-order (NLO) accuracy for inclusive observables. This has made it possible to

# Powheg

$$d\sigma = d\Phi_B \bar{B}^S \left[ \Delta_S(Q_0) + \Delta_S(p_T) \frac{R^S}{B} d\Phi_{\text{rad}} \right] + R^F d\Phi_R,$$

$$\bar{B}^S = B + \hat{V} + \int R^S d\Phi_{\text{rad}}, \quad \Delta_S(p_T) = \exp \left[ - \int \frac{R^S}{B} d\Phi_{\text{rad}} \theta(p_T(\Phi_{\text{rad}}) - p_T) \right]$$



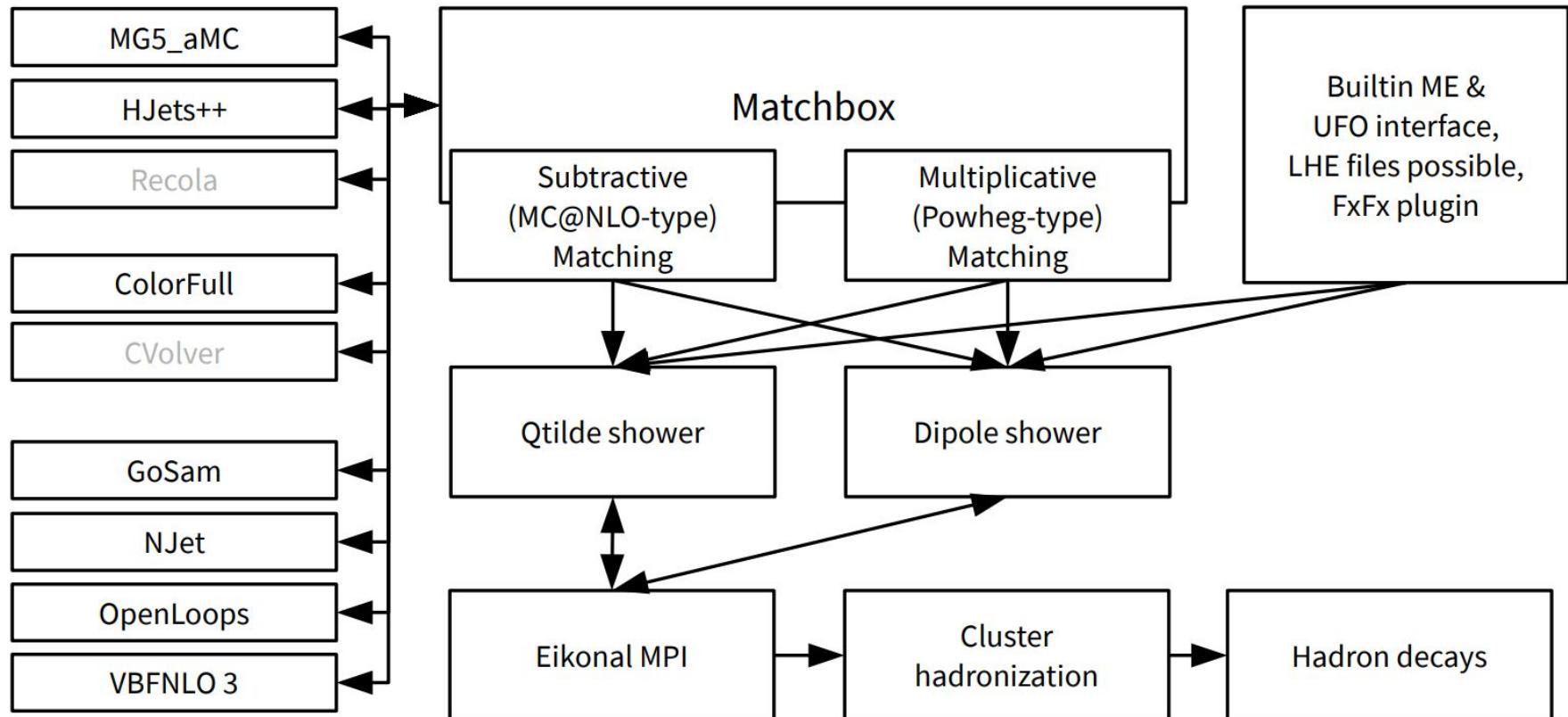
**Figure 1:** Transverse momentum of the Higgs boson in inclusive Higgs boson production ( $m_h = 120$  GeV) at  $E_{\text{cm}} = 7$  TeV. The variation of MC@NLO predictions with varying  $\alpha_{\text{cut}}$  (denoted  $\alpha$  in the legend) is shown in Fig. (a) while Fig. (b) compares the MC@NLO, POWHEG and LO\*PS methods.

# Overview of H7

Full-featured Monte Carlo event generator:

- NLO+PS matching with *Matchbox* (using dipole subtraction)
  - loops: MadGraph/OpenLoops/GoSam/NJet/(any BLHA2)
  - pdfs: LHAPDF
- interchangeable parton showers (dipole, angular-ordered)
- interchangeable hadronisation models (cluster, or string via Pythia)
- analysis: Rivet/HepMC





Output: HepMC, Rivet, built-in analyses.