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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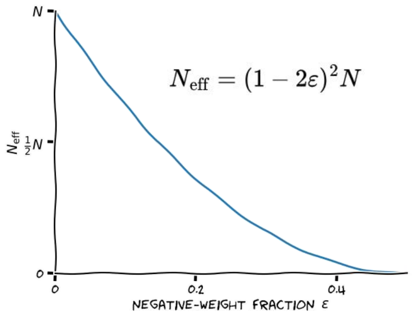


$$N_{\text{eff}} = (1 - 2\varepsilon)^2 N$$

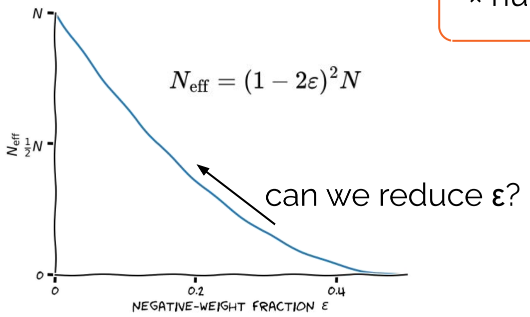
Big picture

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')

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

$$\int \mathrm{d}\hat{\sigma}^{\mathrm{NLO}} = \int \mathrm{d}\Phi_{n+1}\, \mathrm{d}\hat{\sigma}^{\mathrm{R}} + \int \mathrm{d}\Phi_n\, \mathrm{d}\hat{\sigma}^{\mathrm{V}}$$

$$\equiv \int \mathrm{d}\Phi_{n+1} \underbrace{\left[\mathrm{d}\hat{\sigma}^{\mathrm{R}} - \mathrm{d}\hat{\sigma}^{\mathrm{S}}_{\mathrm{NLO}}\right]}_{\text{finite by universality}}$$

$$+ \underbrace{\int \mathrm{d}\Phi_n \left[\mathrm{d}\hat{\sigma}^{\mathrm{V}} + \int \mathrm{d}\Phi_1\, \mathrm{d}\hat{\sigma}^{\mathrm{S}}_{\mathrm{NLO}}\right]}_{\text{finite by KLN}}$$

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

A general algorithm for calculating jet cross sections in NLO QCD ⋆

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INFN, Sezione di Firenze, and Dipartimento di Fisica, Università di Firenze, Largo E. Fermi 2, I-50125 Florence, Italy
[b] *Theory Division, CERN, CH-1211 Geneva 23, Switzerland*

Theoretical parton showers

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

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

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

Iterative operator:

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

NB: unitary!

~~Theoretical~~ **Practical** parton showers

Choose:

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

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

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(as) 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]

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}
&\mathrm{d}\phi_m\, u(\phi_m)\, \Theta_{\mathrm{cut}}\left[\phi_m\right]\Bigg[\Bigg\{\mathrm{B}(\phi_m) + \mathrm{V}(\phi_m) + \sum_\alpha \left[\mathrm{I}^{(\alpha)}(\phi_m) + \mathrm{d}x\, (\mathrm{P}+\mathrm{K})^{(\alpha)}(x;\phi_m)\right]\Bigg\} \\
&\qquad + \sum_\alpha \mathrm{d}q^{(\alpha)} \left\{\Theta^{(\alpha)}_{\mathrm{R}}\left[\Phi^{(\alpha)}_{m+1}(\phi_m,q)\right] \mathrm{R}(\Phi^{(\alpha)}_{m+1}(\phi_m,q)) \left[\frac{w^{(\alpha)}(\Phi^{(\alpha)}_{m+1}(\phi_m;q))}{\sum_\beta w^{(\beta)}(\Phi^{(\alpha)}_{m+1}(\phi_m;q))}\right] \Theta^{(\alpha)}_{\mu_s} - \mathrm{D}^{(\alpha)}\left(\Phi^{(\alpha)}_{m+1}(\phi_m;q)\right)\right\} \\
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&\qquad + \sum_\alpha \mathrm{d}q^{(\alpha)} \left\{\mathrm{M}^{(\alpha)}_{\mathrm{bridge}}(\Phi^{(\alpha)}_{m+1}(\phi_m;q))\left(1-\Theta^{(\alpha)}_{\mu_s}\right)\right\}\Bigg] \\
&+\mathrm{d}\phi_{m+1}\, u(\phi_{m+1}) \qquad \Bigg[\mathrm{R}(\phi_{m+1})\, \Theta_{\mathrm{cut}}\left[\phi_{m+1}\right] \\
&\qquad - \sum_\alpha \left\{\Theta^{(\alpha)}_{\mathrm{R}}\left[\phi_{m+1}\right] \mathrm{R}(\phi_{m+1}) \left[\frac{w^{(\alpha)}(\phi_{m+1})}{\sum_\beta w^{(\beta)}(\phi_{m+1})}\right] \Theta^{(\alpha)}_{\mu_s}\right\} \Theta_{\mathrm{cut}}\left[\Phi^{(\alpha)}_m(\phi_{m+1})\right] \\
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(based on work with Simon Plätzer and Andrzej Siódmok)

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over-subtractions cause negative weights

(based on work with Simon Plätzer and Andrzej Siódmok)

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fix: make them multiplicative

(based on work with Simon Plätzer and Andrzej Siódmok)

KrkNLO

KrkNLO matching for colour-singlet processes

Pratixan Sarmah,[a] Andrzej Siódmok,[a] James Whitehead[a,b]

[a] *Jagiellonian University, ul. prof. Stanisława Łojasiewicza 11, 30-348 Kraków, Poland*
[b] *Institute of Nuclear Physics, Polish Academy of Sciences, ul. Radzikowskiego 152, 31-342 Kraków, Poland*

E-mail: pratixan.sarmah@doctoral.uj.edu.pl, andrzej.siodmok@uj.edu.pl, james.whitehead@uj.edu.pl

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

KrkNLO

KrkNLO matching for colour-singlet processes

Pratixan Sarmah,[a] Andrzej Siódmok,[a] James Whitehead[a,b]

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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, Siódmok, **JW*** [arXiv: 2409.16417]

→ ongoing complementary theory, pheno and computational studies

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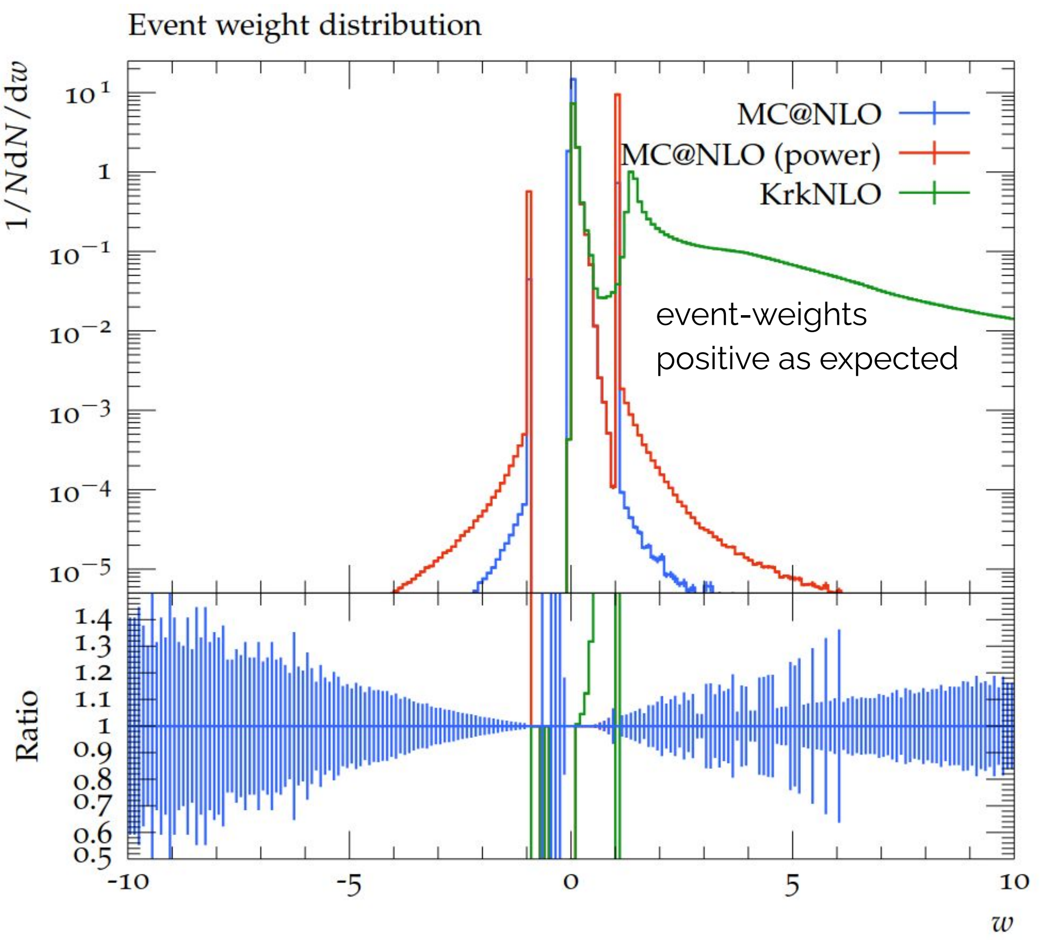

KrkNLO


arXiv:2409.16417v1 [hep-ph] 24 Sep 2024

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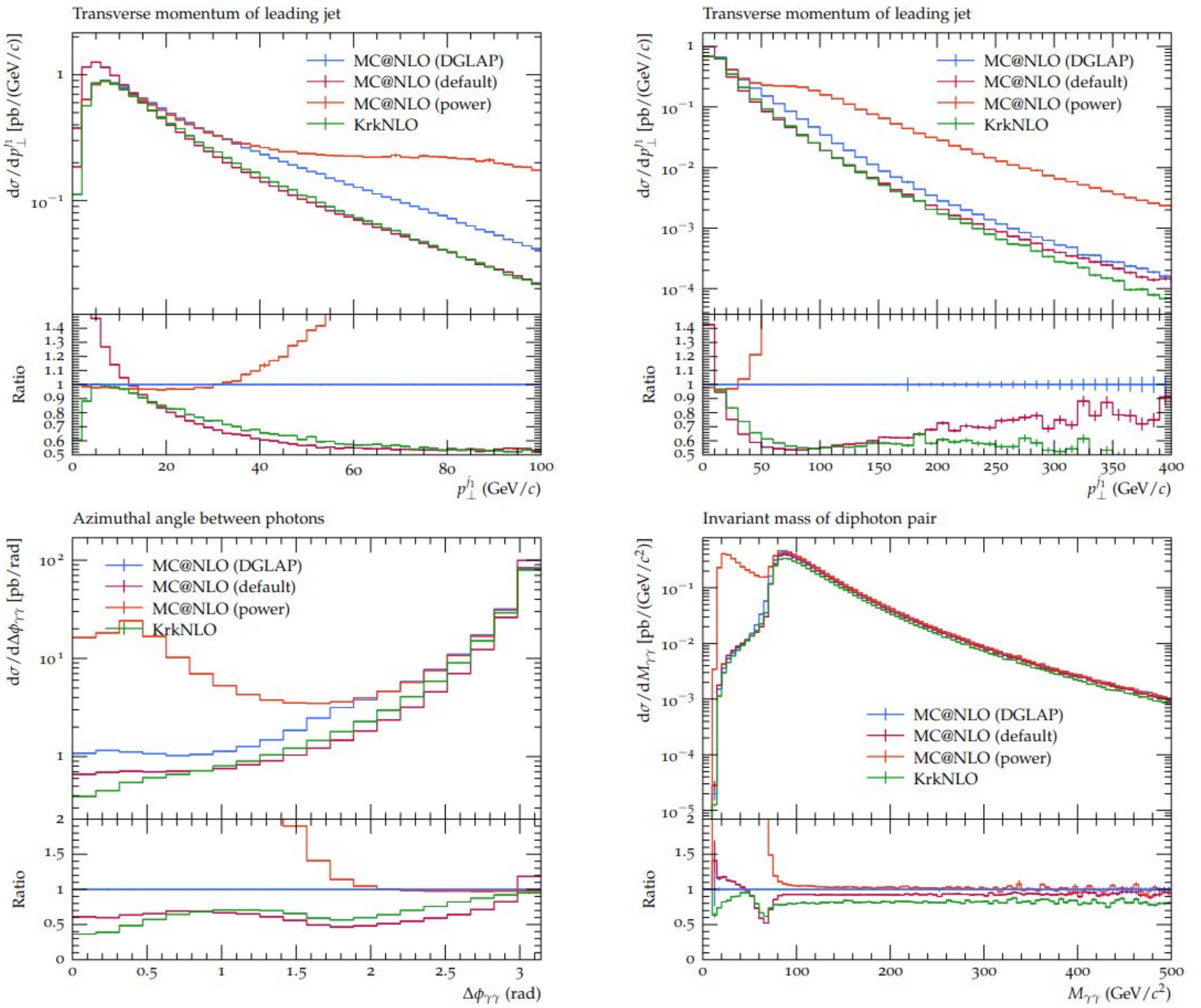

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Outlook:

→ 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 multplicative*’ for MC@NLO:

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

$$
\begin{aligned}
& \mathrm{d}\phi_m \, u(\phi_m)\, \Theta_{\mathrm{cut}}[\phi_m] \Bigg[\Bigg\{ \mathrm{B}(\phi_m) + \mathrm{V}(\phi_m) + \sum_\alpha \Big[\mathrm{I}^{(\alpha)}(\phi_m) + \mathrm{d}x\, (\mathrm{P}+\mathrm{K})^{(\alpha)}(x;\phi_m) \Big] \Bigg\} \\
& \quad + \sum_\alpha \mathrm{d}q^{(\alpha)} \Bigg\{ \Theta_{\mathrm{R}}^{(\alpha)} \Big[\Phi^{(\alpha)}_{m+1}(\phi_m, q)\Big]\, \mathrm{R}(\Phi^{(\alpha)}_{m+1}(\phi_m, q)) \left[\frac{w^{(\alpha)}(\Phi^{(\alpha)}_{m+1}(\phi_m; q))}{\sum_\beta w^{(\beta)}(\Phi^{(\alpha)}_{m+1}(\phi_m; q))} \right] \Theta^{(\alpha)}_{\mu_s} - \mathrm{D}^{(\alpha)} \left(\Phi^{(\alpha)}_{m+1}(\phi_m; q) \right) \Bigg\} \\
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\end{aligned}
$$

fix: make them multiplicative

(based on work with Simon Plätzer and Andrzej Siódmok)

*Plätzer/Siódmok/**JW*** [ongoing]

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:

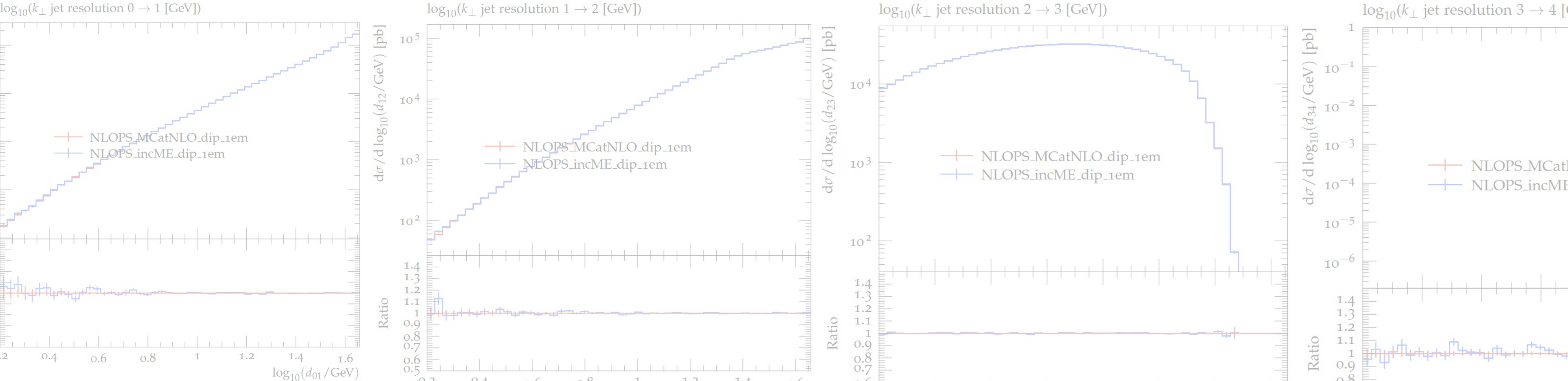
- ‘inclusive ME’
  - generate born-type
  - radiative splittings

*Plätzer/Siódmok/**JW*** [ongoing]

Matchbox restructuring

reducing the fraction of negative weights

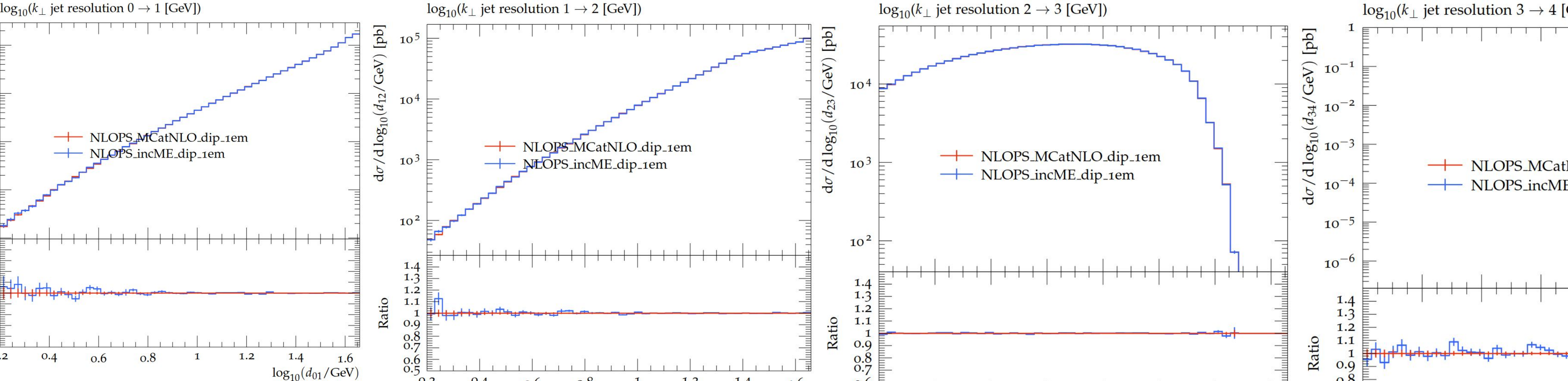
(including new flexibility to study matching uncertainty)



Plätzer/Siódmok/**JW** [ongoing]

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 $\Phi_m(p_1, p_2) \xmapsto{\Phi_{+1}} \Phi_{m+1}^{(\alpha)}$
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[1] 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

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

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

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

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

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

2.2 Gluon splitting

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

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

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

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

$$p_\perp^2 = 2\frac{p_i\cdot q\; q\cdot p_k}{p_i\cdot p_k} \tag{2.30}$$

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 $(p_i,p_j)\to(q_i,q,q_j)$ we choose the standard Sudakov decomposition

$$q_i = zp_i + \frac{p_\perp^2}{zs_{ij}}p_j + k_\perp \tag{3.1}$$

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

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

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

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

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

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

$$\langle \mathbf{V}^{q_a q_i,b}(x_{i,ab})\rangle = T_\mathrm{R}\left\{1-2x_{i,ab}(1-x_{i,ab})\right\}\,.$$

MC@NLO

Powheg

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

$$
d\sigma = d\Phi_{\mathrm{B}} \bar{B}^{\mathrm{S}} \left[\Delta_{\mathrm{S}}(Q_0) + \Delta_{\mathrm{S}}(p_{\mathrm{T}}) \frac{R^{\mathrm{S}}}{B} d\Phi_{\mathrm{rad}}\right] + R^{\mathrm{F}} d\Phi_{\mathrm{R}},
$$

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

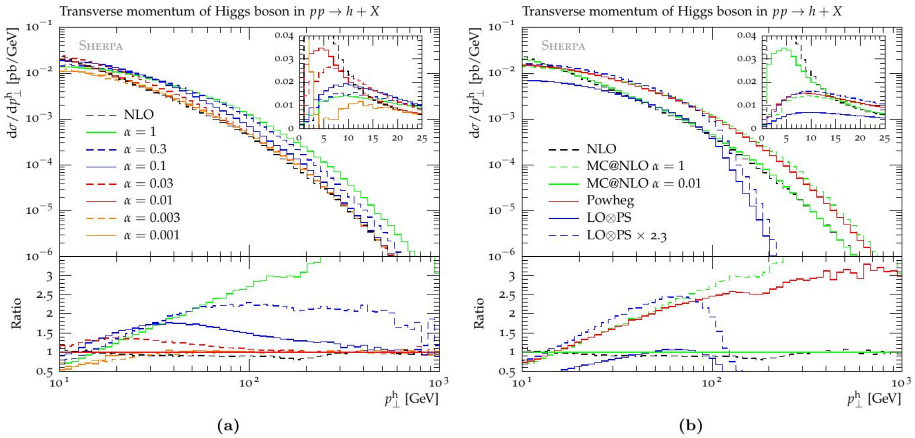

Figure 1: Transverse momentum of the Higgs boson in inclusive Higgs boson production ($m_h = 120$ GeV) at $E_{\mathrm{cms}} = 7$ TeV. The variation of MC@NLO predictions with varying α_{cut} (denoted α in the legend) is shown in Fig. (a), while Fig. (b) compares the MC@NLO, POWHEG and LO⊗PS methods.

from arxiv: 1111.1220
(Höche, Krauss, Schönherr, Siegert)

NEXT-TO-LEADING-ORDER EVENT GENERATORS

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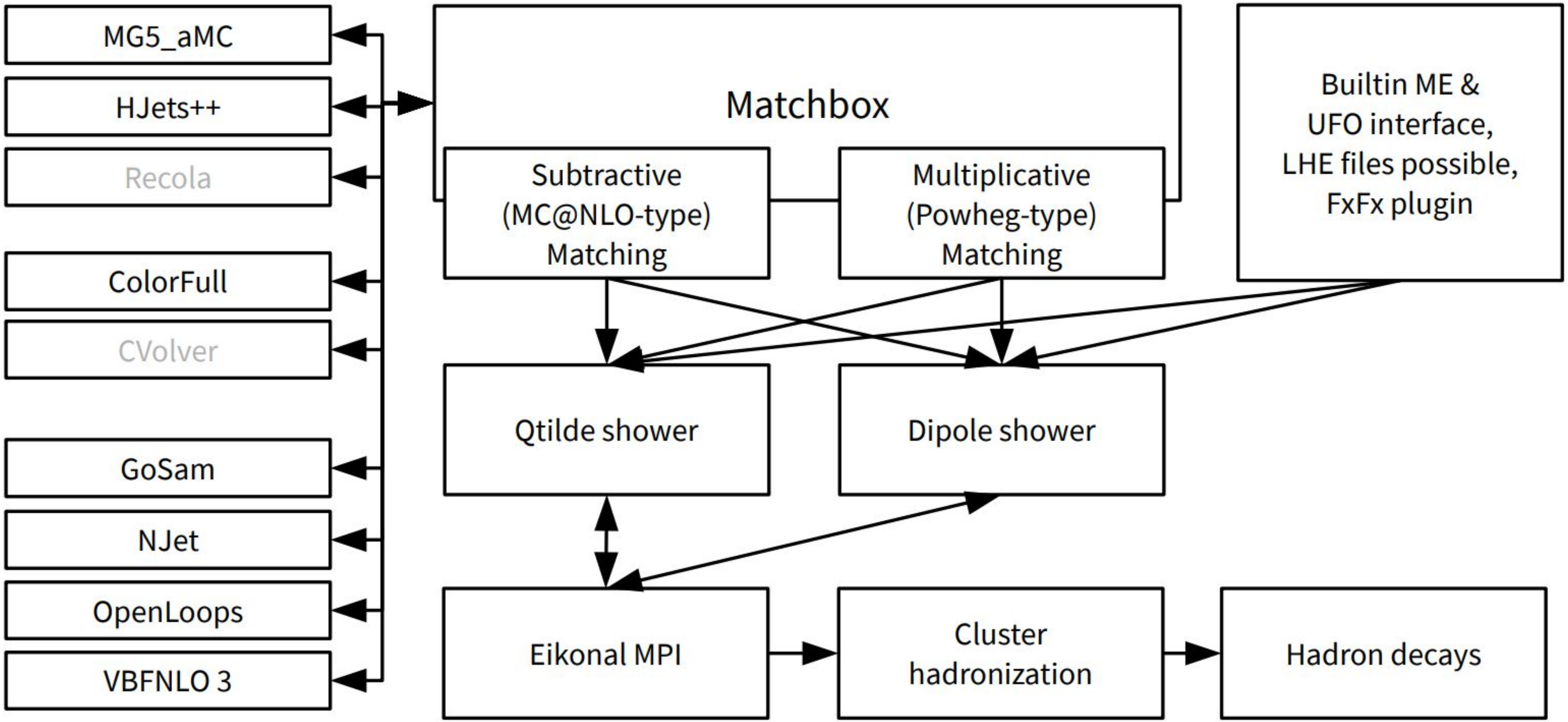
Abstract

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

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.