# Parton-shower and matching uncertainties in top-pair production with Herwig 7



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# SETTING THE SCENE

#### HEP EVENT GENERATORS



- Parton picture of the proton (QCD asymptotic freedom); PDFs; resolve quarks and gluons at high energies.
- Single hard interaction between partons (hard matrix elements); determined from first principles.
- QCD radiation in initial and final state (PDFs and parton showers); evolution from first principles.
- Hadronization and hadron decays (QCD confinement); no first principles, needs modelling.
- Multiple parton interactions (MPI) / Underlying event; modelling of soft QCD.

#### HEP EVENT GENERATORS

- Event generators aim at exclusive final states with O(100 1000) particles.
- Fixed order calculations can only do a limited number of legs.
   LO and NLO automatization: Up to 5 10 particles in the final state.
   NNLO: Selected processes with 2 or 3 particles in the final state.
- Logarithmic enhancements in the soft/collinear regions of phase space. Need to be resummed to all orders in α<sub>s</sub>.
  - Fixed-order matrix elements (ME)
- For large-angle and/or hard radiation: Exact results at a certain fixed order.
- Soft/collinear regions: Missing effects of the all-order summation of large logarithms.

- Parton showers (PS)
- Generate a large amount of partons, due to multiple emissions in the soft/collinear approximation. Evolving an inclusive cross section at a hard scale into an exclusive final state at a lower cut-off scale.
- Approximate the matrix element to "all" orders in the soft/collinear regions, i.e. resummation at leading log (next-to-leading log) accuracy.
- X The hard regions of phase space are naturally described badly.

- Matching/Merging
  - Combine PS and ME by correcting (or replacing) the hardest emission(s) of the PS.
  - The more MEs get involved, the better → Hard regions by the MEs, soft/collinear regions by the PS.
  - There is double counting between PS and MEs → Matching and merging: Derive formulae for auxilliary cross sections, or algorithms to combine multiple inclusive calculations, upon which a parton shower can be applied without leading to double counting.
  - Stick to matching in this talk.

• Condensed master formula to compute a physics observable:

omitting flux factors and initial-state averaging



• For an observable with LO prediction through an *n*-parton tree-level amplitude:

$$\begin{aligned} \alpha_s^{n-2} |\mathcal{A}_n|^2 &= \alpha_s^{n-2} \left( |\mathcal{A}_n^{(0)}|^2 + \alpha_s 2\mathcal{R}e(\mathcal{A}_n^{(0)*}\mathcal{A}_n^{(1)}) + \alpha_s^2 2\mathcal{R}e(\mathcal{A}_n^{(0)*}\mathcal{A}_n^{(2)}) + \alpha_s^2 |\mathcal{A}_n^{(1)}|^2 + \dots \right) \\ \alpha_s^{n-2} |\mathcal{A}_{n+1}|^2 &= \alpha_s^{n-2} \left( \alpha_s |\mathcal{A}_{n+1}^{(0)}|^2 + \alpha_s^2 2\mathcal{R}e(\mathcal{A}_{n+1}^{(0)*}\mathcal{A}_{n+1}^{(1)}) + \dots \right) \\ \alpha_s^{n-2} |\mathcal{A}_{n+2}|^2 &= \alpha_s^{n-2} \left( \alpha_s^2 |\mathcal{A}_{n+2}^{(0)}|^2 + \dots \right) \quad \text{etc.} \end{aligned}$$

- LO: *n*-parton contribution; NLO: *n* and (*n*+1)-parton contribution
- O IR safe means  $O_{n+1} \rightarrow O_n$  if +1 is soft or any two partons of n+1 are collinear

• NLO real 
$$\left(R = \left|\mathcal{A}_{n+1}^{(0)}\right|^2\right)$$
 plus virtual  $\left(V = 2\mathcal{R}e\left(\mathcal{A}_n^{(0)*}\mathcal{A}_n^{(1)}\right)\right)$  in the soft/collinear limit:  
$$\int_{n+1} O_{n+1}R + \int_n O_n V \longrightarrow \int_n O_n\left(\int_{+1}^R + V\right)$$

#### LO and NLO contributions in a condensed notation:

the "inclusiveness" and thus IR safety breaks down for identified partons (here through initial state PDFs), thus if initial state partons are present, a counterterm  $\int O_n C$  is needed to subtract additional collinear divergences;

$$\langle O \rangle^{LO} = \int_{n} O_{n}B \qquad \langle O \rangle^{NLO} = \int_{n+1} O_{n+1}R + \int_{n} O_{n}V + \int_{n} O_{n}C$$

$$V \propto \int dV$$
, w/  $dV \propto d^4 k f(p_i, m_i, k)$ 



Loop integration may lead to soft  $(|k_i| \rightarrow 0)$ , collinear  $(k_i||k_j)$  and ultraviolet  $(|k| \rightarrow \infty)$  divergences.

 $R \propto$  squared real-emission amplitude



Integration over +1 real-emission phase space may lead to soft  $(|p_i| \rightarrow 0)$  and collinear  $(p_i||p_i)$  divergences.

- UV divergences removed by renormalization: V denotes the renormalized virtual piece
- Squared amplitude level: IR divergences cancel between virtual and real emission
- Observable level: Only IR safe observables guarantee the cancellation of IR divergences cf previous slide

- Dimensional regularization in  $D = 4 2\varepsilon$  dimensions ( $|\varepsilon| \ll 1$ ): Divergences yield  $\varepsilon$ -poles.
- Analytical many-body phase-space integration impossible → Numerical integration. keep in mind that numerical integration is in finite four dimensions
- Different phase-space dimensions of both NLO contributions → Combined Monte Carlo integration in finite four dimensions impossible.
- Need to cancel IR divergencies for the *n* and *n*+1 parts separately. keep in mind that UV poles are already removed
- A popular method is the subtraction method:

$$\langle O \rangle^{NLO} = \int_{n+1} \left[ O_{n+1}R \Big|_{\varepsilon=0} - O_nA \Big|_{\varepsilon=0} \right] + \int_n \left[ O_nV + O_n \int_{+1}A \right]_{\varepsilon=0}$$

Using QCD factorization properties, one may devise a subtraction term A, such that

- A has the same pointwise singular behaviour as R.  $O_{n+1} \rightarrow O_n$  in the soft/collinear limit:  $O_nA$  acts as local counterterm to  $O_{n+1}R$ .
- A is analytically integrable over the +1-parton sub-space in D dimensions. The resulting soft/collinear ε-poles cancel the explicit soft/collinear ε-poles of V. together with the poles from the initial-state collinear counterterm, if present
- The first bracket is finite by definition. The second bracket is free of ε-poles. Separate numerical integration of both brackets in four dimensions possible.

- Most NLO QCD calculations nowadays use the subtraction method to regularize the soft/collinear divergencies between the two different phase spaces of the virtual and real corrections.
- The bottleneck used to be the virtual contributions  $\rightarrow$  NLO revolution:

Past 10 - 15 years. Automation of NLO QCD corrections. Breakthroughs in understanding underlying principles & implementation of efficient algorithms, particularly for one-loop calculations. NLO QCD corrections for virtually any SM process "at the push of a button".

Paradigm shift:

Dedicated ME providers (OLPs; one-loop providers) & MC event generators interface on the code level. Let the MC event generator steer the computation (process setup, real subtraction, phase-space integration, ...), possibly also showering and hadronization, ... Use the OLPs for ME input, as e.g. suggested in the BLHA(2) accord.

#### Automated QCD NLO OLPs:

OpenLoops, Recola, MadLoop w/ MG5\_aMC@NLO, GoSam, NLOX, NJet, Helac-NLO, Black-Hat, ....

Automated QCD MC frameworks:

BBMC, MoCaNLO, Munich, Sherpa, MG5\_aMC@NLO, Herwig 7, Powheg-Box, Powhel, VBFNLO, MCFM, ....

Some of the MC event generators are fixed-order event generators, to be interfaced to shower programs like Herwig 7, Sherpa, or Pythia (mostly via Les Houches event files).

Some of the MC event generators go one step further and collect all under one hood: e.g. Herwig 7 and Sherpa have their own showers and hadronization but rely largely on external OLPs (interface on the code level), on the other hand e.g MG5\_aMC@NLO has its own OLP but interfaces to external shower providers (internally also through LH event files).

### PARTON SHOWERS

- Cutting perturbative calculations at a certain fixed order: accompanied by spurious logarithms L of ratios of process dependent scales √s<sub>i</sub> by a non-physical cut-off scale μ.
  - Enhanced in regions where the ratios are small (or large)  $\rightarrow$  large logs.
  - Problematic for perturbative convergence if  $L\alpha_s \approx 1$ .
- 2) Current fixed-order calculation are not sufficient to describe the momenta of outgoing jets well in an exclusive picture of the process (including jet structures, i.e. distributions of associated particles).
- A way to deal with all that is through parton showers, by dressing the hard process with additional soft/collinear QCD radiation.
  - Approximate the matrix element in the soft and collinear regions, where contributions are enhanced.
  - Built on the factorization of an n+1 particle state into an n particle state times a one-particle phase space and universal splitting function (enhanced for z = 0, 1)

$$d\sigma_{n+1} = \sigma_n \frac{dt}{t} dz P(z)$$

- Iterative algorithm to generate multiple emissions, successively off the *n* particle state, the *n*+1 particle state, etc.
- Fast production of many-particle final states in enhanced regions.
- Summing up high orders in α<sub>s</sub>; in the soft/collinear approximation takes all the leading large logarithms into account.
- Evolving, in a cascade like fashion, from an inclusive hard process at some large scale, to an exclusive manyparticle state at some low scale at which QCD confinement (hadronization) takes over.



For small angles:  $p_a^2 = t = (p_b + p_c)^2$  $= z(1-z)E_a^2(\Theta_b + \Theta_c)^2$ 

• Given a LO process with total cross section  $\sigma_n$ , the associated (differential) NLO cross section factorizes in the collinear limit ( $\theta_{ji} \ll \pi/2$ ):

$$\mathrm{d}\sigma_{n+1}^{j} \approx \sigma_{n} \sum_{\mathrm{emitters}\,i} \frac{\alpha_{s}}{2\pi} \frac{\mathrm{d}\theta_{ji}}{\theta_{ji}} \mathrm{d}z_{\mathrm{ji}} P_{ji}(z_{ji}, \phi_{ji}) \frac{\mathrm{d}\phi_{\mathrm{ji}}}{2\pi} = \sigma_{n} \sum_{\mathrm{emitters}\,i} \mathrm{d}\mathcal{P}_{ji}(\theta_{ji}, z_{ji}, \phi_{ji})$$

- Hard configuration of emitters i, accompanied by a collinear parton j with energy fraction z<sub>ji</sub>, wrt i.
- θ<sub>ji</sub>: Emission angle between i and j.
- φ<sub>ji</sub>: Azimuth of j around the i-axis.
- $P_{ji}(z_{ji}, \phi_{ji})$ : Spin-dependent splitting functions

Enhanced for  $z_{ji} = 0$  or also  $z_{ji} = 1$ , depending on the type of splitting.

Independent of the precise def. of z in the collinear limit: energy fraction, light-cone momentum fraction - or similar. Neglecting spin correlations  $\rightarrow$  spin-averaged splitting functions  $P_{ji}(z_{ji})$ .

- ▶ Instead of  $\frac{dt}{t} = \frac{d\theta^2}{\theta^2}$  one may also choose e.g.  $\frac{dq^2}{q^2}$ ,  $\frac{dk_{\perp}^2}{k_{\perp}^2}$  or  $\frac{d\tilde{q}^2}{\tilde{q}^2} \rightarrow \text{diff. choices for the evol. variable:}$ 
  - $q^2 = z(1-z)E^2\theta^2$  the virtuality of the off-shell emitter propagator, with energy *E*.
  - ►  $k_{\perp}^2 = z^2 (1-z)^2 E^2 \theta^2$  the emitted parton's transverse momentum wrt the emitter.
  - $\tilde{q}^2 = E^2 \theta^2$  (used e.g. by Herwig 7 in its angular-ordered shower, aka  $\tilde{q}$  shower; generalized for masses).
  - All of these choices are identical in the collinear limit, but extrapolate differently away from it.

- So far: Inclusive emission distribution of all emissions j off i.
  - Consider e.g. only j = gluon. Consider further the virtuality  $q^2$  of the internal emitter line.
  - The total probability for all gluon branchings off a parton *i* between  $q^2$  and  $q^2 + dq^2$  is

$$\mathrm{d}\mathcal{P}_i(q^2) = \frac{\alpha_s}{2\pi} \frac{\mathrm{d}q^2}{q^2} \int_{\mathcal{Q}_0^2/q^2}^{1-\mathcal{Q}_0^2/q^2} \mathrm{d}z P_{ji}(z)$$

- How to single out the distributions of individual gluons? How to know that a certain branching is the "first" or the "hardest"?
  - Introduce order: the virtuality  $q^2$  serves as "ordering" variable.
  - Introduce  $\Delta_i(Q^2, q^2)$ : the probability that there is no branching between  $q^2$  and a certain max. virtuality  $Q^2 > q^2$ .
  - The probability to emit nothing at all, while evolving all the way down to a shower cut-off Q<sup>2</sup><sub>0</sub>, is Δ<sub>i</sub>(Q<sup>2</sup>, Q<sup>2</sup><sub>0</sub>).
  - The probability to have the first emission at a scale  $q^2$  is

$$\frac{\mathrm{d}\Delta_i(Q^2,q^2)}{\mathrm{d}q^2} = \Delta_i(Q^2,q^2) \frac{\mathrm{d}\mathcal{P}_i(q^2)}{\mathrm{d}q^2}$$

Thus the solution for the Sudakov form factor is

$$\Delta_i(Q^2, q^2) = \exp\left\{-\int_{q^2}^{Q^2} \mathrm{d}\mathcal{P}_i(k^2)\right\} = \exp\left\{-\int_{q^2}^{Q^2} \frac{\alpha_s}{2\pi} \frac{\mathrm{d}k^2}{k^2} \int_{Q_0^2/k^2}^{1-Q_0^2/k^2} \mathrm{d}z P_{ji}(z)\right\}$$

- ▶ We've sneaked in a resolution scale / a lower cut-off Q<sub>0</sub>. Why?
  - Soft/collinear configurations → divergences arise universaly Physical measurements have a finite resolution → Cannot differ an exact soft/collinear config. from just one parton
- Above Q<sub>0</sub>: (finite) resolvable emission For the relative k<sub>⊥</sub> between emitter and emission (cut-off Q<sub>0</sub> = k<sub>⊥,0</sub>), we cut on soft and collinear simultaneously.
- Integrate the distribution below  $Q_0$ Probability for non-resolvable emission: divergent  $\rightarrow$  add it to the loop correction of the hard process
- Unitarity: The total probability of either emitting s.th. or not emitting at all is one, or

 $\mathcal{P}(\text{no emission}) = 1 - \mathcal{P}(\text{all emissions})$ 

- Parton showers built on this principle include loop corrections implicitly.
   Exact for soft/collinear contributions. Hard non-collinear loops yield in general a finite correction.
- Formally, this defines a parton shower operation on an observable *O*, over an *n*-parton seed configuration: dropped sums over parton species shower cut-off Q<sup>2</sup><sub>0</sub> = μ<sup>2</sup><sub>IR</sub>

$$PS[Q^{2}, \mu_{IR}^{2}, \{\Phi_{n}, O\}] = \Delta(Q^{2}, \mu_{IR}^{2})O_{n} + \int_{\mu_{IR}^{2}}^{Q^{2}} d\mathcal{P}(q^{2})\Delta(Q^{2}, q^{2})PS[q^{2}, \mu_{IR}^{2}, \{\Phi_{n+1}, O\}]$$

- Back substitution gives the series solution for the modified DGLAP evolution equations.
- Each splitting generates one order more in α<sub>s</sub>. Summing the leading contributions of repeated parton branchings to "all" orders in α<sub>s</sub>.

- By choosing the angle as ordering variable one can show that coherence effects of soft gluons are properly included → angular-ordered showers
  - One can show that color coherence leads to emissions of successively smaller opening angles.
  - In a p<sub>T</sub> or virtuality ordered shower, one would have to manually veto any emission that is larger in angle than the previous one.
- ► However, for certain applications one would like to include color coherence and still be able to have the transverse momentum as ordering variable → dipole showers
  - ► Uses color dipoles and 2 → 3 splittings: emission off a color dipole; conserve on-shell conditions by using additional color-connected parton as momentum-balancing third party.
  - Since color coherence effects enter naturally, one does not have to enforce them through explitic angular ordering.
- ► Using a running  $\alpha_s$  in the splittings, with  $p_{\perp}$  as argument, i.e.  $\alpha_s(q^2 = p_{\perp}^2)$ , a tower of certain higher order loop insertions can be resummed.
  - The value of  $\alpha_s$  increases with decreasing  $p_{\perp} \rightarrow$  increasing multiplicity; phase space fills with soft gluons.
  - ▶ To avoid regions of  $\alpha_s \approx 1$  need to place the cut-off  $Q_0 = \mu_{IR}$  higher  $\rightarrow$  not a technical cut anymore.

Above is in the form of a final-state evolution. An initial-state evolution can be formulated too, as backwards evolution, taking into account PDF evolution.

- HERWIG 7 e.g. implements an angular-ordered parton shower (using q̃ as ordering variable) as well as a dipole shower, based on Catani-Seymour dipoles (which are also used in the NLO real subtraction in HERWIG 7).
- In terms of scales so far:

Hard process scale ( $\mu_H = \mu_R = \mu_F$ ), hard veto scale, aka shower start scale ( $Q = Q_{\perp}$ ), shower scale ( $\mu_S$  in shower  $\alpha_s(\mu_S)$ ), lower cut-off scale ( $\mu_{IR}$ ). For matching uncertainties we are interested in the first three.

# MATCHING

### PARTON SHOWERS AND FIXED ORDERS

#### Plots: [arXiv:1101.2599]

- ▶ Look at terms that enter in the  $\alpha_s$  expansion of a jet cross section, e.g. in  $e^+e^- \rightarrow jets$ .
  - For each order  $\alpha_s^n$  there is a set of large logs  $L^m$ , with  $m \leq 2n$ .



► Terms in a jet cross section in e.g. e<sup>+</sup>e<sup>-</sup> → jets that are correctly included (filled blobs) e.g. by a NLL parton shower.



- Terms correctly included in a tree-level matrix element of order α<sup>n</sup><sub>s</sub>. Here, a 4-jet observable in e.g. e<sup>+</sup>e<sup>-</sup> → jets with LO prediction at order α<sup>2</sup><sub>s</sub>.
- To get as many blobs as possible: combine fixed-order calculations and parton showers.
- However, notice that there is double counting if one does that naively.
- Avoid double counting in NLO+PS: NLO matching; essentially two methods, MC@NLO and Powheg.
- Variants thereof are built into various programs nowadays.
   HERWIG 7 e.g. implements variants of both.

Remember

$$\begin{aligned} & \text{member} \\ & \text{PS}[Q^2, \mu_{\text{IR}}^2, \{\Phi_n, O\}] = \Delta(Q^2, \mu_{\text{IR}}^2) O_n + \int_{\mu_{\text{IR}}^2}^{Q^2} d\mathcal{P}(q^2) \Delta(Q^2, q^2) \text{PS}[q^2, \mu_{\text{IR}}^2, \{\Phi_{n+1}, O\}] \\ & \Delta(Q^2, \mu_{\text{IR}}^2) = \exp\left[-\int_{\mu_{\text{IR}}^2}^{Q^2} d\mathcal{P}(q^2)\right] = 1 - \int_{\mu_{\text{IR}}^2}^{Q^2} d\mathcal{P}(q^2) + \mathcal{O}(\alpha_s^2) \end{aligned}$$

and further

w/

$$O_{\rm NLO} = \int \mathrm{d}\Phi_n \Big(\mathcal{B} + \bar{\mathcal{V}}\Big) O_n + \int \mathrm{d}\Phi_{n+1} \Big(\mathcal{R}O_{n+1} - \mathcal{A}O_n\Big), \text{ with } \bar{\mathcal{V}} = \mathcal{V} + \int d\Phi_1 \mathcal{A}$$

• Up to NLO in  $\alpha_s$ : PS[ $Q^2, \mu_{IR}^2, \{\Phi_n, O_{NLO}\}$ ]

$$=\int \mathrm{d}\Phi_n \left(\mathcal{B} + \bar{\mathcal{V}}\right) O_n + \int \mathrm{d}\Phi_{n+1} \left(\mathcal{R}O_{n+1} - \mathcal{A}O_n\right) + \int \mathrm{d}\Phi_n \mathcal{B} \int_{\mu_{\mathrm{IR}}^2}^{Q^2} \mathrm{d}\mathcal{P}(q^2) \left(O_{n+1} - O_n\right)$$

Double-counting between PS & real emission and PS & real subtraction Total inclusive cross section unaffected (replace  $O_n$  and  $O_{n+1}$  by 1)

 NLO Matching: Restore the correct NLO expression at the observable level Subtract PS contribution, so that PS[O<sup>matchd</sup><sub>NLO</sub> = O<sub>NLO</sub> + O(NNLO α<sub>s</sub>)

$$O_{\text{NLO}}^{\text{matched}} = \int \mathrm{d}\Phi_n \left( \mathcal{B} + \bar{\mathcal{V}} \right) O_n + \int \mathrm{d}\Phi_{n+1} \left( \mathcal{R}O_{n+1} - \mathcal{A}O_n \right) - \int \mathrm{d}\Phi_n \, \mathcal{B} \int_{\mu_{\text{IR}}^2}^{Q^2} \mathrm{d}\mathcal{P}(q^2) \left( O_{n+1} - O_n \right)$$

Plot by D. Rauch (first steps with HERWIG++ and MATCHBOX beta for top-pair production; Master's thesis in 2014)



- Red: NLO calculation; the low energy region is dominated by large logarithms
- Blue: LO + parton shower
  - the low energy region is properly Sudakov suppressed
  - the high energy region is only described with LO accuracy
- Yellow: MC@NLO-like matching (pretty much the matching subtraction formula) with angular-ordered parton shower the low energy region shows the correct sudakov suppression the high energy tail is described with NLO accuracy



- Exclusive event generation in particle collisions at had-had, had-lep and lep-lep colliders (up to the particle level)
- HERWIG 7 is written in C++ and based on THEPEG [https://herwig.hepforge.org/, https://thepeg.hepforge.org/]

Supports LHAPDF, as well and HepMC output and/or Rivet

- Perturbative physics
  - Hard process at NLO QCD
    - LHE file input
    - Built-in LO and NLO matrix elements (MEs)
    - Automated assembly of NLO QCD calculations
    - Interfacing various external ME providers
  - Parton shower Monte Carlo
    - Angular-ordered parton shower
    - Dipole shower
    - Decays of heavy resonances (incl. spin correlations)
    - Dedicated Powheg matched / matrix element corrected
    - Automated matching machinery, algorithms based on MC@NLO and Powheg
- Non-perturbative and soft physics
  - Hadronization
  - Cluster hadronization model
  - Color reconnection
  - Decays

- Underlying event
  - MPI (eikonal multiple interaction model)
- Diffractive processes
- BSM machinery: Built-in processes as well as UFO model file input



▶ HERWIG 7 ∈ MCnet

[http://www.montecarlonet.org/]

[http://www.montecarlonet.org/index.php?p=Projects/herwig]



- HERWIG++ has been developed over the course of ~10 years [hep-ph/0311208, ..., 0803.0883, ..., 1310.6877] Intention: Fully replace and supersede the capabilities of FORTRAN HERWIG [hep-ph/0011363, hep-ph/0210213]
- Paradigm shift towards NLO → Release of HERWIG 7 [arXiv:1512.01178] The current version is Herwig 7.1.5 (top-pair study in [arXiv:1810.06493] done with 7.1.4). Herwig 7.2 in the making.
- As the successor of the HERWIG++2 and HERWIG 6 series HERWIG 7 supersedes the physics capabilities of both its predecessors Focusing greatly on precission and NLO automatization Greatly improved installation, steering and documentation
- The MATCHBOX module forms the basis for the automated NLO capabilities of HERWIG 7 Fully integrated framework for automated NLO matching, with full control over the fixed order input
  - Automated setup for a full NLO QCD calculation in the subtraction formalism
  - Implementation of the CS dipole subtraction method (massless [Catani, Seymour, '96] and massive [Catani, Dittmaier, Seymour, Trocsanyi, '02])
  - Fixed-order input: In-house calculations and Interfaces to various external matrix-element providers

- Automated diagram based multi-channel phase-space sampling and adaptive phase-space integration
- Fully automated matching algorithms: Subtractive (based on MC@NLO [Frixione, Webber, '02, '06]) and multiplicative (based on Powheg [Nason '04; Aliolo, Nason, Oleari, Re '08])
- Plug-ins to the two shower variants in HERWIG 7

All in one framework: External matrix-element codes fully interfaced, no event files to move around anymore MATCHBOX already introduced previously [Plätzer, Gieseke '12]. Beta tested in Herwig++.

# NLO MATCHING IN HERWIG 7

Remember

$$O_{\text{NLO}}^{\text{matched}} = \int \mathrm{d}\Phi_n \left(\mathcal{B} + \bar{\mathcal{V}}\right) O_n + \int \mathrm{d}\Phi_{n+1} \left(\mathcal{R}O_{n+1} - \mathcal{A}O_n\right) - \int \mathrm{d}\Phi_n \mathcal{B} \int_{\mu_{\text{IR}}^2}^{Q^2} \mathrm{d}\mathcal{P}(q^2) \left(O_{n+1} - O_n\right)$$

• Rearranging wrt  $O_n$  and  $O_{n+1}$  (so-called *S*- and *H*-events)

$$\begin{split} O_{\mathsf{NLO}}^{\mathsf{matched}} &= \left[ \int \mathrm{d} \Phi_n \left( \mathcal{B} + \bar{\mathcal{V}} \right) \ - \ \int \mathrm{d} \Phi_{n+1} \mathcal{A} \ + \ \int \mathrm{d} \Phi_n \mathcal{B} \int_{\mu_{\mathrm{IR}}^2}^{Q^2} \mathrm{d} \mathcal{P}(q^2) \ \right] O_n \\ &+ \left[ \int \mathrm{d} \Phi_{n+1} \mathcal{R} \ - \ \int \mathrm{d} \Phi_n \mathcal{B} \int_{\mu_{\mathrm{IR}}^2}^{Q^2} \mathrm{d} \mathcal{P}(q^2) \ \right] O_{n+1} \end{split}$$

•  $O_n$  and  $O_{n+1}$  contributions are separately not finite: Add extra term  $A_{\text{bridge}}$  below shower cut-off  $\mu_{\text{IR}}$ 

$$\int \mathrm{d}\Phi_{n+1}\mathcal{A}_{\mathrm{bridge}}(\Phi_{n+1})\Theta(q^2 < \mu_{\mathrm{IR}}^2) \Big(O_n - O_{n+1}\Big)$$

Subtract real-emission divergencies in the n+1-parton bin and those of  $\mathcal{A}$  in the n-parton bin For IR safe observables only adds power corrections below  $\mu_{IR}$  (conserves the log behaviour) Choose  $\mathcal{A}_{bridge} = \mathcal{A}$ 

#### MATCHING SUBTRACTION IN HERWIG 7



- Interfaces at amplitude level
- Built-in (one-loop) helicity sub-amplitudes, spinor helicity library and caching facilities
- MG5\_AMC@NLO [https://launchpad.net/mg5amcnlo] (color-ordered sub-amplitudes)
   Color bases: COLORFULL [M. Sjödahl, S. Plätzer], CVOLVER [S. Plätzer]
- In-house calculations, e.g. parts of HJETS++ [F. Campanario, T. Figy, S. Plätzer, M. Sjödahl]

### Matchbox

- Interfaces at squared amplitude level
  - Dedicated interfaces [ HEJ [https://hej.hepforge.org/]; NLOJET++ [www.desy.de/ znagy/Site/NLOJet++.html] ]
  - BLHA(2) [ GOSAM [https://gosam.hepforge.org/]; NJET [https://bitbucket.org/njet/njet/]; OPENLOOPS [https://openloops.hepforge.org/]; VBFNLO [https://www.itp.kit.edu/vbfnlo/] ]
- Shower plugins:
  - Angular ordered P(q̃) or Dipole shower D(p⊥)
  - MEC R<sub>MEC</sub>(p<sub>⊥</sub>)

$$O_{\rm NLO}^{\rm matched} = \left[ \int \mathrm{d}\Phi_n \left( \mathcal{B} + \bar{\mathcal{V}} \right) + \int \mathrm{d}\Phi_n \mathcal{B} \int_{\mu_{IR}^2}^{Q^2} \mathrm{d}\mathcal{P}(q^2) - \int \mathrm{d}\Phi_{n+1} \mathcal{A} \Theta(q^2 > \mu_{IR}^2) \right] O_n \qquad \mathsf{S}$$

$$+ \left[ \int \mathrm{d}\Phi_{n+1} \ \mathcal{R} \ - \int \mathrm{d}\Phi_n \ \mathcal{B} \ \int_{\mu_{I\!R}^2}^{Q^2} \mathrm{d}\mathcal{P}\!\left(q^2\right) \ - \int \mathrm{d}\Phi_{n+1} \ \mathcal{A} \ \Theta\!\left(q^2 < \mu_{I\!R}^2\right) \right] O_{n+1} \qquad \mathbf{H}^{-1}$$

 MC@NLO-type (subtractive matching; NLO⊕): The matching subtraction formula from before. For the dipole shower things get particularly easy, as BP ≈ A.
 For the *q̃* shower the emission of a single-emission kinematic also reduces to dipole kinematic. S ~ (B+V)dφ<sub>n</sub> & H ~ (R − A)dφ<sub>n+1</sub> ~ Rdφ<sub>n+1</sub> − Bdφ<sub>n</sub>dP

Powheg-type (multiplicative matching; NLO⊗): Replace BP ≈ R. S ~ (B + V̄)dφ<sub>n</sub> + (R − A)dφ<sub>n+1</sub>Θ(q<sup>2</sup> > μ<sub>IR</sub><sup>2</sup>) The amount of negative events, i.e. the ones in the O<sub>n+1</sub> bracket, reduces. But not completely! Powheg matching goes along with having to have the first emission also the hardest. For the q̃ shower this is not the case → truncated, vetoed shower. For practical reasons, as evaluating real-emission MEs is expensive, only the first emission is replaced by BP ≈ R.

### HARD VETO SCALE

### SHOWER START SCALE

**PROFILE SCALES** 

- The parton shower hard scale is limited from above, by an upper limit Q = Q⊥ on the transverse momentum available to the shower, to avoid summation of an unphysical tower of logarithms in the Sudakov exponent.
- Not all of the emission phase-space should be available to the shower. Instead of a fixed scale, use a functional profile, i.e. smear the hard veto scale Q<sub>⊥</sub> with κ(Q<sub>⊥</sub>, p<sub>⊥</sub>), with p<sub>⊥</sub> the transverse momentum of the splitting.
- ► Known from the hfact profile used as damping factor in PowhegBox, where  $\kappa(Q_{\perp}, p_{\perp}) = 1/(1+x^2)$ , with  $x = p_{\perp}/Q_{\perp}$ .
- Profile scales can be applied generically, though. We will look at it in MC@NLO matching, comparing with another profile scale choice, i.e. the resummation profile

$$\kappa(\mathcal{Q}_{\perp}, p_{\perp}) = \begin{cases} 1 & , x \leq 1 - 2\rho , \\ 1 - \frac{(1 - 2\rho - x)^2}{2\rho^2} & , x \in (1 - 2\rho, 1 - \rho] , \\ \frac{(1 - x)^2}{2\rho^2} & , x \in (1 - \rho, 1] , \\ 0 & , x > 1 , \end{cases}$$

In Herwig 7.1.4  $\rho = 0.3$ .

- The resummation profile  $\rightarrow 1$  for  $p_{\perp} < (1 2\rho)Q_{\perp}$ ,  $\rightarrow 0$  for  $p_{\perp} > Q_{\perp}$ , and quadratically interpolates between these regions. Expected to reproduce the desired towers of logarithms, and switches off the resummation smoothly towards the hard region.
- ▶ hfact → 1 in the resummation region, for  $p_{\perp} < Q_{\perp}$ , → 0 in the fixed-order region, for  $p_{\perp} > Q_{\perp}$ . Does not produce the desired towers of logarithms. Not close enough to one in the Sudakov region,  $p_{\perp} \ll Q_{\perp}$ ; does not enforce a sufficient cutoff on the shower emissions in the hard region,  $p_{\perp} \gg Q_{\perp}$ .



- ► The resummation profile  $\rightarrow 1$  for  $p_{\perp} < (1 2\rho)Q_{\perp}$ ,  $\rightarrow 0$  for  $p_{\perp} > Q_{\perp}$ , and quadratically interpolates between these regions. Expected to reproduce the desired towers of logarithms, and switches off the resummation smoothly towards the hard region.
- hfact → 1 in the resummation region, for p<sub>⊥</sub> < Q<sub>⊥</sub>, → 0 in the fixed-order region, for p<sub>⊥</sub> > Q<sub>⊥</sub>. Does not produce the desired towers of logarithms. Not close enough to one in the Sudakov region, p<sub>⊥</sub> ≪ Q<sub>⊥</sub>; does not enforce a sufficient cutoff on the shower emissions in the hard region, p<sub>⊥</sub> ≫ Q<sub>⊥</sub>.

### Hard Veto Scale / Starting Scale $(Q_{\perp})$ Choices

Starting scale for the  $p_{\perp}$ -ordered DS. Veto scale for the angular-ordered PS.

S- and H-events are showered separately for NLO matched predictions. In MC@NLO-type matching we expect a fraction of low- $p_{\perp}$  H-events. In those cases choosing  $Q_{\perp}$  at the order of the corresponding real-emission  $p_{\perp}$  is unnatural.

Per default  $Q_{\perp} = \mu_H = \mu_F = \mu_R$ .

Low- $p_{\perp}$  real emission:

transverse masses largely unaffected.  $Q_{\perp} \sim$  scale similar to that had there been no emission. High- $p_{\perp}$  real emission:

sum of transverse masses increases.  $Q_{\perp}$  increases accordingly.

Common choices for  $\mu_H$  involve the top and antitop transverse masses, often in a linear or quadratic sum:  $\mu_H = \mu_1 = (m_{\perp,t} + m_{\perp,\bar{t}})/2$ , or  $\mu_H = \mu_2 = (m_{\perp,t} + m_{\perp,\bar{t}})/4$ , or  $\mu_H = \mu_3 = m_{\bar{t}\bar{t}}$ .

 $Q_{\perp}$  and  $\mu_H$  may also be chosen independently.

Choose a  $Q_{\perp}$  that better reflects the scales of the objects outgoing from the hard proc.

Low- $p_{\perp}$  real emission:  $Q_{\perp} \sim$  larger scale.

High- $p_{\perp}$  real emission:  $Q_{\perp} \sim$  scale of real emission.

Consider  $Q_{\perp} = \mu_a$ , with  $\mu_a^2 = (\sum_{i \in n_{out}} m_{\perp,i}^2)/n_{out}$ , taking into account the extra emission in the hard event

(quadratic mean of the transverse masses of all outgoing particles).

Low- $p_{\perp}$  real emission:  $\mu_a$  is much larger than the scale of the real emission.

High- $p_{\perp}$  real emission:  $\mu_a$  is sensitive to the scale of this real emission.

### SCALE STUDIES

RESULTS

### SCALE STUDIES

- 1) Scale variations.
- ► MC@NLO- (NLO⊕) / Powheg-type (NLO⊗) matching to angular-ordered (PS) / dipole shower (DS).
- ► Variations of hard process scales ( $\mu_H = \mu_R = \mu_F$ ), hard veto scale ( $Q_{\perp}$ ), shower scales ( $\mu_S$ ; arguments in shower  $\alpha_s$  and shower PDFs)
  - PS: argument of α<sub>s</sub> ~ related to transv. momentum of emitted parton, differing for fin.- and in.-state evolution. argument of PDFs ~ the ordering var. of in.-state evolution.
  - **b** DS: transv. momentum of emitted parton used for both (in  $\alpha_s$  and in PDFs).
  - Defaults:  $Q_{\perp} = \mu_H$ , resummation profile.
- Scale variations are by factors of 2 up and down: either combined (27-fold scale variation), or broken down according to the individual scale variations.
- 2) Impact of the choice of the profile scale (only MC@NLO-type matching).
  - Vary between resummation and hfact profile.
  - Defaults:  $Q_{\perp} = \mu_H$ .
- 3) Impact of the choice of the hard veto scale (only MC@NLO-type matching).
  - Vary choices of  $\mu_H = \mu_{1,2,3}$ , while looking at different choices for  $Q_{\perp}$ , either  $(\mu_H, Q_{\perp} = \mu_H)$  or  $(\mu_H, Q_{\perp} = \mu_a)$ .
  - Defaults: resummation profile.

#### SCALE VARIATION

Parton-level (production-level) benchmarks, for stable top quarks:

13 TeV COM, only QCD radiation,  $\mu_{IR} = 1 GeV$  (min. transverse momentum cut-off in shower emissions),  $m_t = 174.2$  GeV in the hard process and subsequent showering, all other quarks massless. MMHT2014nlo68cl,  $\alpha_s$  2-loop running, with  $\alpha_s(M_Z) = 0.12$ , done in H7 rather than using the PDF one. Purpose built RIVET analysis.

$$\mu_H = \frac{m_{\perp,t} + m_{\perp,\overline{t}}}{4} \,,$$

Motivated in [arXiv:1606.03350]

Particle-level comparisons to data, for unstable top quarks:

In addition to A), top quark decays, hadronization and hadron decays. Publicly available RIVET analyses, and COMs of the corresponding experimental results. Default tunes of Herwig 7.1.1.

$$\mu_H = \frac{m_{\perp,t} + m_{\perp,\bar{t}}}{2},$$

Found to give rise to reasonable predictions of several observables sensitive to jet activity using MC@NLO-type matching.

H7.1.4, MG5 for tree amplitudes, OpenLoops for one-loop amplitudes.

For the shower improvements, further details, as well as further comparisons, please have a look at [arXiv:1810.06493], containing a comprehensive overview on the currently implemented details.

- PS: Spin correlations. Improved decay of heavy particles.
- DS: (Improved) decay of heavy particles new in H7.1.4. Spin correlations to come.

#### [arXiv:1810.06493]

▶ Plot envelope of all scale variations (overall scale variations), but also breakdown into variations of  $\mu_H$ ,  $\mu_S$ ,  $Q_{\perp}$  separately



- *p*<sub>⊥</sub>(*t*) well described by LO ME, showers have limited impact (overall scale variation equally dominated by μ<sub>H</sub>, μ<sub>S</sub>, Q<sub>⊥</sub>)
- With only LO ME,  $\Delta R(\vec{n}, j_1)$  sensitive to showers (overall scale variation equally dominated by  $\mu_S, Q_{\perp}$  below  $\pi$  and by  $Q_{\perp}$  only above  $\pi$ )
- ▶ Both showers describe similar distributions for  $p_{\perp}(t)$  and  $\Delta R(t\bar{t},j_1)$

[arXiv:1810.06493]



- With only LO ME, n<sub>jets</sub> (p<sub>⊥</sub> > 25GeV) sensitive to showers (Q<sub>⊥</sub>, µ<sub>S</sub> have increasing effect with increasing n<sub>jets</sub>; Q<sub>⊥</sub> dominates), DS predicts more many-jet events
- With only LO ME, p⊥(ti) very sensitive to showers (Q⊥ dominates), DS predicts more high-p⊥(ti) events

[arXiv:1810.06493]



- NLO matched
- $\Delta R(\bar{t}, j_1)$  probes hard process and parton shower (above  $\pi$  already described by only NLO ME; largest uncertainty below  $\pi$  from  $\mu_S$ )
- for both showers both matchings describe similar distributions

NLO  $\otimes$  DS

 $\mu_{\rm H}$ 

 $\mu_{\rm H}$ 

6

 $\Delta R(t\bar{t}, j_1)$ 

 $\mathbf{5}$ 

[arXiv:1810.06493]



- NLO matched
- $n_{\text{jets}}(p_{\perp} > 25 \text{GeV}) = 0, 1$  formally accurate to NLO
- for both showers both matchings agree up to 3 jets, above 3 jets Powheg-type matching predicts more many-jet events
- Overall  $Q_{\perp}$  significant, but  $\mu_S$  and  $\mu_H$  contribute visibly (in NLO $\otimes$ PS  $\mu_S$  seems more pronounced)

[arXiv:1810.06493]



- NLO matched
- much improved overall scale uncertainties in p<sub>⊥</sub>(*iī*), as the showers have a smaller impact (exclusively dominated by μ<sub>H</sub>)
- for both showers both matchings agree well

### $tar{t}$ PRODUCTION - PARTON LEVEL - RESUMMATION VS HFACT

#### [arXiv:1810.06493]

► Looking at different cut-off profiles of the hard veto scale Q<sub>⊥</sub> in MC@NLO-type matching, one reminiscent of hfact in PowhegBox, one inspired by resummation



- In p⊥(j<sub>1</sub>) hfact overshoots resummation for high p⊥
- In  $\Delta \phi(t\bar{t},j_1)$  hfact overshoots resummation for low  $\Delta \phi$
- Comparing hfact and resummation inspired for  $p_{\perp}(j_1)$ :  $\sim 20\%$  effects at high  $p_{\perp}(j_1)$  and low  $\Delta \phi$

#### $tar{t}$ PRODUCTION - PARTON LEVEL - RESUMMATION VS HFACT

#### [arXiv:1810.06493]



- In n<sub>jets</sub> (p<sub>⊥</sub> > 25GeV) for large n<sub>jets</sub> (shower described) hfact undershoots resummation with PS, and overshoots it with DS
- In n<sub>jets</sub> (p<sub>⊥</sub> > 80GeV) hfact always overshoots for large n<sub>jets</sub>
- Comparing hfact and resummation inspired (in shower described regions):  $\sim 20\%$  effects for  $n_{\text{jets}}(p_{\perp} > 25 \text{GeV})$ ,  $\sim 300\%$  effects for  $n_{\text{jets}}(p_{\perp} > 80 \text{GeV})$

#### $t\bar{t}$ PRODUCTION - PARTON LEVEL - HARD PROCESS AND VETO SCALE CHOICE [arXiv:1810.06493]

► Vary choices of  $\mu_H$ , while looking at different choices for  $Q_{\perp}$ ,  $(\mu_H, Q_{\perp} = \mu_H)$  or  $(\mu_H, Q_{\perp} = \mu_a)$ 

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- $\mu_H = \mu_1 = (m_{\perp,t} + m_{\perp,\bar{t}})/2$ , or  $\mu_H = \mu_2 = (m_{\perp,t} + m_{\perp,\bar{t}})/4$ , or  $\mu_H = \mu_3 = m_{\bar{t}\bar{t}}$
- $\mu_a^2 = (\sum_{i \in n_{out}} m_{\perp,i}^2)/n_{out}$ , taking into account the extra emission in the H event



- $p_{\perp}(j_1)$ : hardest jet  $j_1$  is described correctly at NLO.
- Sensitive to the hard veto scale as it sets the upper limit on the scale of the first shower emission and affects the available phase space for subsequent emissions. Increase in Q<sub>⊥</sub> should yield increase in p<sub>⊥</sub>(j<sub>1</sub>).
- However above some scale we expect all distributions to agree regardless of the choice of Q<sub>⊥</sub>, as the hardest jet is produced as a NLO real emission in H events.

#### $tar{t}$ PRODUCTION - PARTON LEVEL - HARD PROCESS AND VETO SCALE CHOICE

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[arXiv:1810.06493]



- $p_{\perp}(j_2)$ : second hardest jet  $j_2$  is produced from the shower.
- Also sensitive to the hard veto scale as it sets the upper limit on the scale of the first shower emission and affects the available phase space for subsequent emissions, especially the first subsequent emission.
- Major effects at high scales, as j<sub>2</sub> is not described at NLO.

#### $tar{t}$ PRODUCTION - PARTON LEVEL - HARD PROCESS AND VETO SCALE CHOICE

[arXiv:1810.06493]





- ▶  $n_{\text{jets}}(p_{\perp} > 25 \text{GeV})$
- Major effects, especially with DS
- ▶ Expect an increase in Q<sub>⊥</sub> to produce an increase in the rate of events with high jet multiplicity.

#### $tar{t}$ PRODUCTION - PARTON LEVEL - HARD PROCESS AND VETO SCALE CHOICE

[arXiv:1810.06493]



►  $p_{\perp}(t\bar{t})$ 

Should closely reflect the behaviour observed in the  $p_{\perp}(j_1)$  distribution.

### $tar{t}$ PRODUCTION - PARTICLE LEVEL - SCALE UNCERTAINTIES

[arXiv:1810.06493]

- ►  $H_{\perp}$  distribution (sum of all jet  $p_{\perp}$ 's) measured in semileptonic 8 TeV  $pp \rightarrow t\bar{t}$  events by CMS [arXiv:1607.00837]
- Plot envelope of all scale variations (overall scale uncertainties), but also breakdown into variations of  $\mu_H, \mu_S, Q_{\perp}$  separately



► LO + shower description: above 300 GeV sensitive to showers ( $Q_{\perp}$  variation dominates,  $\mu_S$  variation visible), PS and DS predict similar rates (except in the lower bins), DS has larger overall uncertainties towards high- $H_{\perp}$  events (driven by  $Q_{\perp}$  variation; reflecting the difference in phase space of the two showers)

### $t\bar{t}$ PRODUCTION - PARTICLE LEVEL - SCALE UNCERTAINTIES

[arXiv:1810.06493]

►  $H_{\perp}$  distribution (sum of all jet  $p_{\perp}$ 's) measured in semileptonic 8 TeV  $pp \rightarrow t\bar{t}$  events by CMS [arXiv:1607.00837]



- NLO + shower description: better uncertainties and description of data in both showers with both matching variants, DS undershoots a bit towards higher H<sub>⊥</sub>, but has slightly larger overall uncertainties
- In both showers the overall uncertainties with MC@NLO-type are larger than with Powheg-type matching, but in neither there is a clear single dominant source of uncertainty (in NLO⊕DS the Q⊥ variation seems more prominent, though)

# tt PRODUCTION - PARTICLE LEVEL - HARD PROCESS AND VETO SCALE CHOICE 46 [arXiv:1810.06493] 46

- ►  $H_{\perp}$  distribution measured in semileptonic 8 TeV  $pp \rightarrow t\bar{t}$  events by CMS [arXiv:1607.00837]
- ▶ Vary choices of  $\mu_H$ , while looking at different choices for  $Q_{\perp}$ ,  $(\mu_H, Q_{\perp} = \mu_H)$  or  $(\mu_H, Q_{\perp} = \mu_a)$
- $\mu_H = \mu_1 = (m_{\perp,t} + m_{\perp,\bar{t}})/2$ , or  $\mu_H = \mu_2 = (m_{\perp,t} + m_{\perp,\bar{t}})/4$ , or  $\mu_H = \mu_3 = m_{\bar{t}\bar{t}}$
- $\mu_a^2 = (\sum_{i \in n_{out}} m_{\perp,i}^2)/n_{out}$ , taking into account the extra emission in the H event





# tt PRODUCTION - PARTICLE LEVEL - HARD PROCESS AND VETO SCALE CHOICE 47 [arXiv:1810.06493] 47

- Gap fraction measured by ATLAS in dileptonic 7 TeV  $pp \rightarrow t\bar{t}$  events [arXiv:1203.5015]
- ▶ Veto region |y| < 2.1,</p>
- ▶ Vary choices of  $\mu_H$ , while looking at different choices for  $Q_{\perp}$ ,  $(\mu_H, Q_{\perp} = \mu_H)$  or  $(\mu_H, Q_{\perp} = \mu_a)$
- $\mu_H = \mu_1 = (m_{\perp,t} + m_{\perp,\bar{t}})/2$ , or  $\mu_H = \mu_2 = (m_{\perp,t} + m_{\perp,\bar{t}})/4$ , or  $\mu_H = \mu_3 = m_{\bar{t}\bar{t}}$

•  $\mu_a^2 = (\sum_{i \in n_{out}} m_{\perp,i}^2)/n_{out}$ , taking into account the extra emission in the H event





#### SUMMARY

- NLO plus parton shower matched predictions for  $t\bar{t}$  production at the LHC with Herwig 7.
- ► MC@NLO- (NLO⊕) / Powheg-type (NLO⊗) matching to angular-ordered (PS) / dipole shower (DS).
- Studied various sources of uncertainty: Scale variations, hard scale choices, profile scale choices. No single scale variation encompasses the entire set of independent variations. All sources need to be considered to obtain a reliable uncertainty estimate. NLO matching provides improvements over a LO plus parton shower simulation where expected. However, higher jet multiplicities do suffer from large uncertainties, even using NLO matching. (to be considered when using tuned predictions) (multi-jet merged study of similar nature should be a natural continuation)
- Hard veto scale and profile scale choices: Play an important role in the handling of real-emission corrections present in the NLO matching. "Inappropriate" choices can lead to artificially suppressed or enhanced radiation.
- Improved radiation in production and decay of heavy quark flavours new in the dipole shower (not discussed in the talk) [arXiv:1810.06493].
- Also considered boosted topologies, looking at observables that are sensitive to the decay process, focusing on N-subjettiness ratios, highlighting the internal structure of the jets (not discussed in the talk) [arXiv:1810.06493].

# Thank you!