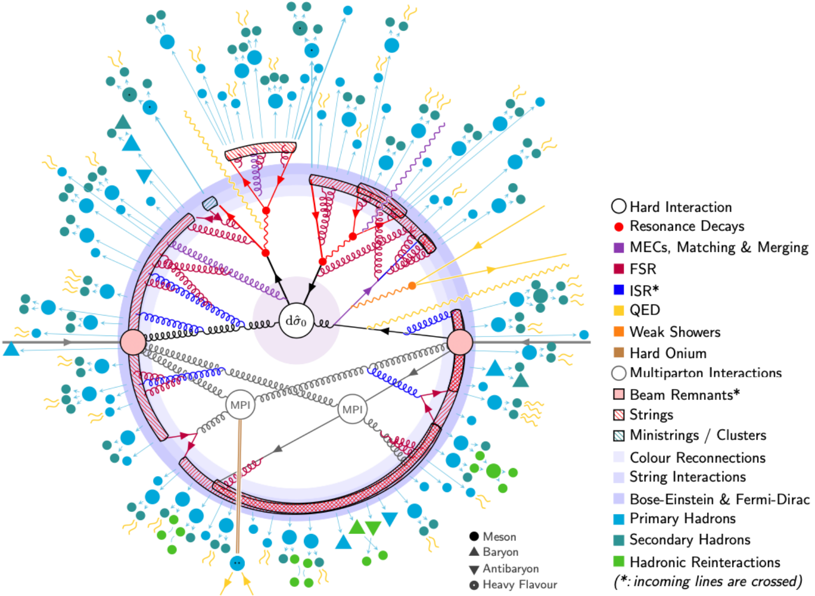
Top-quark physics with PYTHIA

Christian T Preuss (University of Wuppertal)

LHC TOP WG Meeting
30/11/2023

BERGISCHE
UNIVERSITÄT
WUPPERTAL

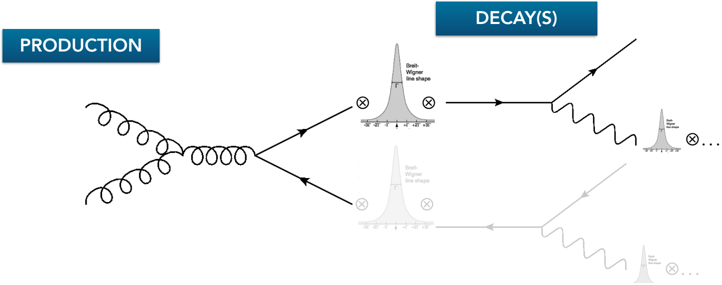
Top production in PYTHIA



Resonance-final showers

The MC "truth" top-quark mass distribution in PYTHIA

First step: $\frac{\Gamma_t}{m_t} \ll 1 \Rightarrow$ factorise production and decay(s) ("pole approximation")
$+$ Breit-Wigner-improved pole approximation $\Rightarrow$ tops with BW mass distribution
(skewed by PDF effects: more incoming partons at lower invariant masses)



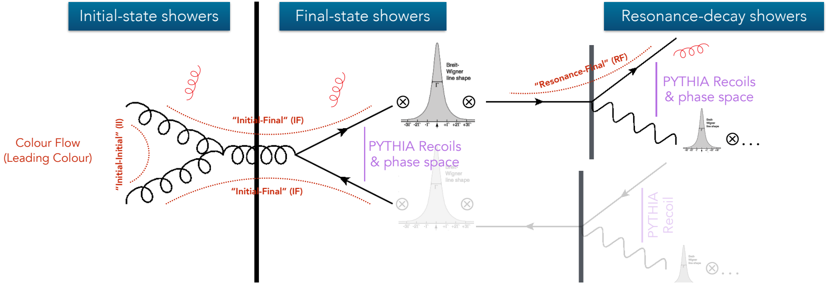
Note: for external events (POWHEG, MC@NLO, ...) this might be done differently.

Slide adapted from P. Skands.

Radiative corrections – PYTHIA

PYTHIA's default shower model ("simple shower") is anchored in collinear (DGLAP) limits
⇒ **Separate** initial-state, final-state, and resonance-decay showers

Coherence for soft radiation across these boundaries is not automatic
No notion of **resonance-final** recoils, must use **final-final** ones instead.

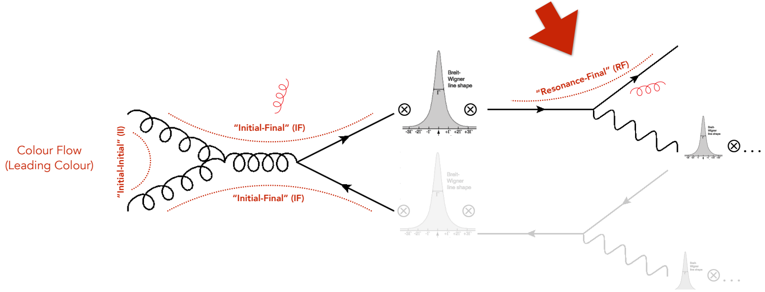


Slide adapted from P. Skands.

Radiative corrections – VINCIA

Bremsstrahlung
Colour flow determines (leading-colour) coherent radiation pattern

In VINCIA (`PartonShowers:model = 2`)
Unique coherent **“resonance-final”** antenna pattern *and* recoils [Brooks, Skands 1907.08980]

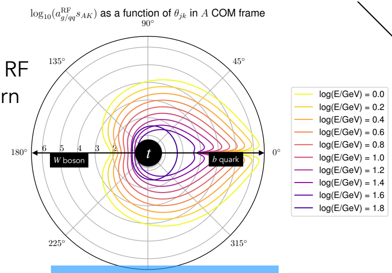


Slide adapted from P. Skands.

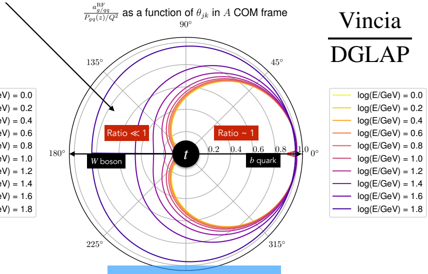
Coherence in top decays [Brooks, Skands 1907.08980]

First emission: not much difference
Phase space: limit set by $m_t - m_W$ in both cases
Recoils: VINCIA RF recoils to $t - b = W \leftrightarrow$ PYTHIA FF recoils to W
RF pattern suppressed at wide angles compared to DGLAP (but PYTHIA has **MEC**)

Vincia RF pattern



Log of antenna function



Ratio to AP kernel

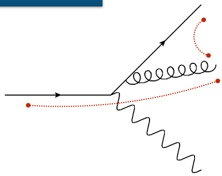
Brooks, Skands, 2019

Slide adapted from P. Skands.

Coherence in top decays [Brooks, Skands 1907.08980]

Second emission: big differences
Neither controlled by POWHEG nor by MECs.
Not as important as first emission, but still highly significant if goal is per-mille precision on m_t.

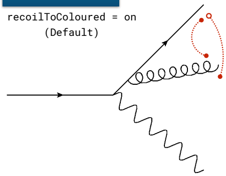
VINCIA RF



tg RF antenna:
Phase space & recoils set by:
$t - g = b + W$
Collective recoil

PYTHIA

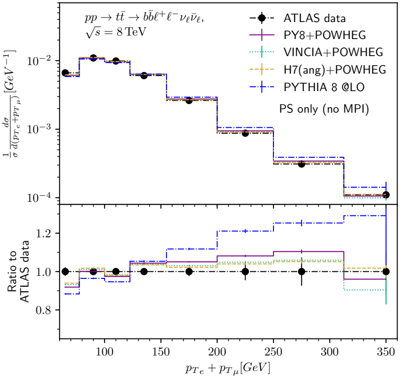
`recoilToColoured = on`
`(Default)`

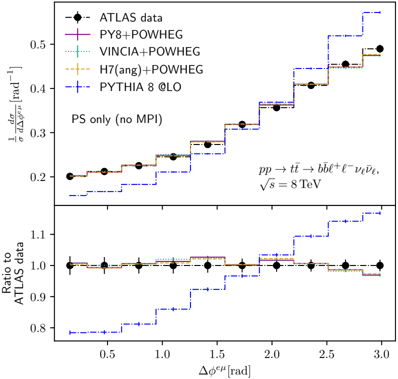


$g - t$ dipole treated as $g - b$:
Phase space & recoils set by b
Affects b fragmentation

Slide adapted from P. Skands.

Radiative corrections – consequences [Brooks, Skands 1907.08980]





Interleaved EW showers

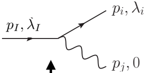
EW showers [Kleiss, Verheyen 2002.09248]

Real corrections: EW gauge bosons, tops, Higgs part of jets

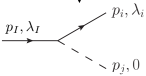
Virtual corrections: universal Sudakov logs of type $\frac{\alpha}{\pi}\log^2\left(\frac{s}{Q^2_{\mathrm{EW}}}\right)$

Features of the EW sector

- Chiral ⟶ Helicity showers   Larkoski, Lopez-Villarejo, Skands 1301.0933; Fischer, Lifson, Stands, 1708.01736
- EW-scale mass corrections
- Longitudinal polarisations / Goldstone bosons
- Neutral boson interference
- Double-counting between QCD and EW
- Resonance-like branchings



$$\epsilon_0^\mu(p) = \frac{1}{m}\left(p^\mu - \frac{m^2}{p\cdot k}k^\mu\right)$$



Slide adapted from R. Verheyen.

EW antenna functions

Every SM $1 \to 2$ splitting included $(V \to f\bar{f}, V \to VH, H \to HH, \ldots)$
$\Rightarrow \mathcal{O}(1000)$ **different branching types** (helicity dependent!)

$$a^{FF}_{f_\lambda \mapsto f_\lambda V_\lambda} = 2(v - \lambda a)^2 \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} \frac{1}{x_j}$$

$$a^{FF}_{f_\lambda \mapsto f_\lambda V_{-\lambda}} = 2(v - \lambda a)^2 \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} \frac{x_i^2}{x_j}$$

$$a^{FF}_{f_\lambda \mapsto f_{-\lambda} V_\lambda} = 2 \frac{1}{(m_{ij}^2 - m_I^2)^2} \left((v - \lambda a) m_i \frac{1}{\sqrt{x_i}} - (v + \lambda a) m_I \sqrt{x_i} \right)^2$$

$$a^{FF}_{f_\lambda \mapsto f_\lambda V_0} = \frac{1}{(m_{ij}^2 - m_I^2)^2} \left[(v - \lambda a) \left(\frac{m_I^2}{m_j} \sqrt{x_i} - \frac{m_i^2}{m_j} \frac{1}{\sqrt{x_i}} - 2 m_j \frac{\sqrt{x_i}}{x_j} \right) + (v + \lambda a) \frac{m_I m_i}{m_j} \frac{x_j}{\sqrt{x_i}} \right]^2$$

$$a^{FF}_{f_\lambda \mapsto f_{-\lambda} V_0} = \frac{(m_I (v + \lambda a) - m_i (v - \lambda a))^2}{m_j^2} \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} x_j.$$

$$a^{FF}_{V_\lambda \mapsto f_\lambda \bar{f}_{-\lambda}} = 2(v - \lambda a)^2 \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} x_j^2$$

$$a^{FF}_{V_\lambda \mapsto f_{-\lambda} \bar{f}_\lambda} = 2(v + \lambda a)^2 \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} x_i^2$$

$$a^{FF}_{V_\lambda \mapsto f_{-\lambda} \bar{f}_{-\lambda}} = 2 \frac{1}{(m_{ij}^2 - m_I^2)^2} \left((v + \lambda a) m_i \sqrt{\frac{x_j}{x_i}} + (v - \lambda a) m_j \sqrt{\frac{x_i}{x_j}} \right)^2$$

$$a^{FF}_{V_0 \mapsto f_\lambda \bar{f}_\lambda} = \frac{((v + \lambda a) m_i - (v - \lambda a) m_j)^2}{m_I^2} \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2}$$

$$a^{FF}_{V_0 \mapsto f_\lambda \bar{f}_{-\lambda}} = \frac{1}{(m_{ij}^2 - m_I^2)^2} \times \left[(v - \lambda a) \left(2 m_I \sqrt{x_i x_j} - \frac{m_i^2}{m_I} \sqrt{\frac{x_j}{x_i}} - \frac{m_j^2}{m_I} \sqrt{\frac{x_i}{x_j}} \right) + (v + \lambda a) \frac{m_i m_j}{m} \frac{1}{\sqrt{x_i x_j}} \right]^2.$$

$$a^{FF}_{f_\lambda f_\lambda H} = \frac{e^2}{4 s_w^2} \frac{m_i^4}{s_w^2} \frac{1}{(m_{ij}^2 - m_I^2)^2} \left(\sqrt{x_i} + \frac{1}{\sqrt{x_i}} \right)^2$$

$$a^{FF}_{f_\lambda f_{-\lambda} H} = \frac{e^2}{4 s_w^2} \frac{m_i^2}{s_w^2} \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} x_j.$$

$$a^{FF}_{V_\lambda \mapsto V_\lambda V_\lambda} = 2 g_v^2 \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} \frac{1}{x_i x_j}$$

$$a^{FF}_{V_\lambda \mapsto V_\lambda V_{-\lambda}} = 2 g_v^2 \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} \frac{x_i^3}{x_j}$$

$$a^{FF}_{V_\lambda \mapsto V_{-\lambda} V_\lambda} = 2 g_v^2 \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} \frac{x_j^3}{x_i}$$

$$a^{FF}_{V_\lambda \mapsto V_\lambda V_0} = g_v^2 \frac{1}{(m_{ij}^2 - m_I^2)^2} \frac{(m_I^2 - m_i^2 - \frac{1+x_i}{x_j} m_j^2)^2}{m_j^2}$$

$$a^{FF}_{V_\lambda \mapsto V_0 V_\lambda} = g_v^2 \frac{1}{(m_{ij}^2 - m_I^2)^2} \frac{(m_I^2 - m_j^2 - \frac{1+x_j}{x_i} m_i^2)^2}{m_i^2}$$

$$a^{FF}_{V_\lambda \mapsto V_0 V_0} = \frac{g_v^2}{2} \frac{(m_I^2 - m_i^2 - m_j^2)^2}{m_i^2 m_j^2} \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} x_i x_j.$$

$$a^{FF}_{V_\lambda \mapsto V_\lambda H} = \frac{e^2}{s_w^2} \frac{m_v^4}{m_w^2} \frac{1}{(m_{ij}^2 - m_I^2)^2}$$

$$a^{FF}_{V_\lambda \mapsto V_0 H} = \frac{e^2}{2 s_w^2} \frac{m_v^2}{m_w^2} \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} x_i x_j$$

$$a^{FF}_{V_0 \mapsto V_\lambda H} = \frac{e^2}{2 s_w^2} \frac{m_v^2}{m_w^2} \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2} \frac{x_j}{x_i}$$

$$a^{FF}_{V_0 \mapsto V_0 H} = \frac{e^2}{4 s_w^2} \frac{1}{m_w^2} \frac{1}{(m_{ij}^2 - m_I^2)^2} \left(m_I^2 - 2 m_i^2 \left(x_i + \frac{1}{x_i} \right) \right)^2.$$

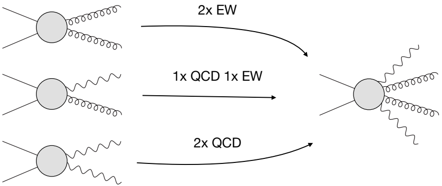
$$a^{FF}_{H \mapsto f_\lambda \bar{f}_\lambda} = \frac{e^2}{4 s_w^2} \frac{m_i^2}{s_w^2} \frac{\tilde{m}_{ij}^2}{(m_{ij}^2 - m_I^2)^2}$$

$$a^{FF}_{H \mapsto f_\lambda \bar{f}_{-\lambda}} = \frac{e^2}{4 s_w^2} \frac{m_i^4}{s_w^2} \frac{1}{(m_{ij}^2 - m_I^2)^2} \left(\sqrt{\frac{x_i}{x_j}} - \sqrt{\frac{x_j}{x_i}} \right)^2.$$

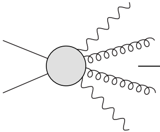
Slide adapted from R. Verheyen.

Overlap veto

Double-counting problem



Veto procedure



Last emission QCD? $\longrightarrow d_{ij}^{\text{Last}} < \min\left(d_{ij}^{\text{EW}}\right)$ → Accept Branching

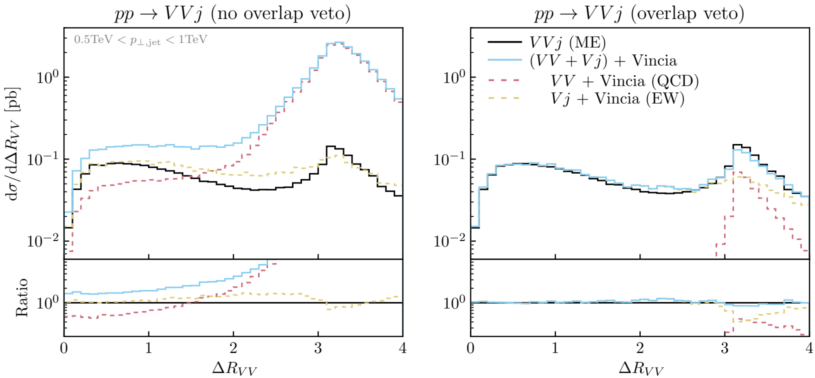
Last emission EW? $\longrightarrow d_{ij}^{\text{Last}} < \min\left(d_{ij}^{\text{QCD}}\right)$ → Accept Branching

$$d_{ij} = \min\left(k_{T,i}^2, k_{T,j}^2\right)\frac{\Delta_{ij}}{R} + m_i^2 + m_j^2 - m^2$$

Slide adapted from R. Verheyen.

Overlap veto – in action

[Brooks, Skands, Verheyen 2108.10786]



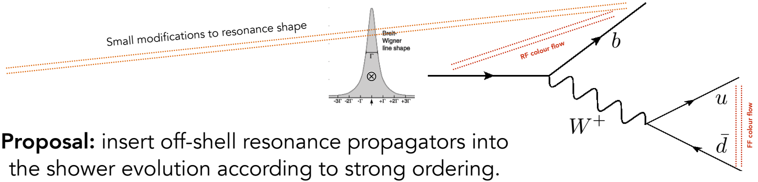
Finite-width effects

Physically, **short-lived fluctuations** do not have time to form **long-wavelength emissions**.

In **parton showers**, this is reflected by **strong ordering**.

However, **resonance decays** are usually treated **sequentially**; **no strong ordering**!

Expect initial-final interference effects at scales below Γ_t

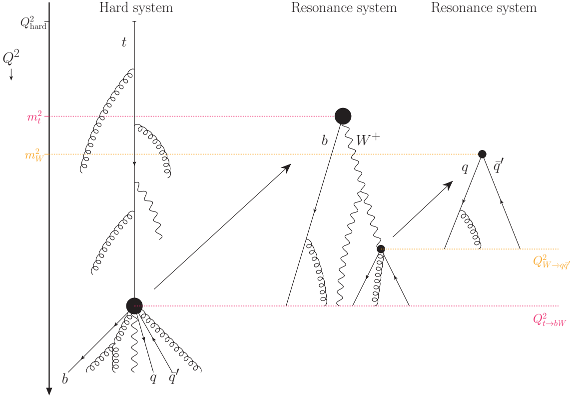


Proposal: insert off-shell resonance propagators into the shower evolution according to strong ordering.

Uniquely treated in VINCIA via "interleaved resonance decays"

Slide adapted from P. Skands.

Interleaved resonance decays



Sequential

- Complete evolution of the hard system
- Perform resonance shower

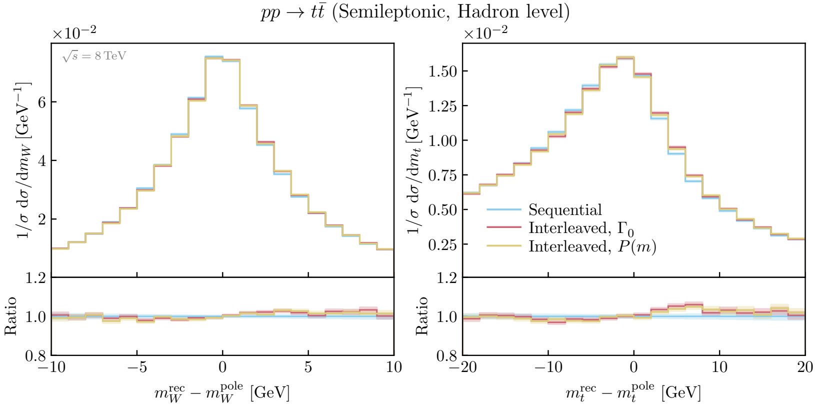
Interleaved

- Evolution up to offshellness scale of the resonance
- Perform resonance shower
- Insert showered decay products and continue evolution

Slide adapted from R. Verheyen.

Interleaved resonance decays – consequences

[Brooks, Skands, Verheyen 2108.10786]



Matching (and) Uncertainties

MC@NLO and MC@NLO-Δ with PYTHIA

Reduction of negative weights in MC@NLO-type matching:
MC@NLO-Δ [Frederix, Frixione, Prestel, Torrielli 2002.12716]

$$\mathrm{d}\sigma^{\Delta,\mathbb{H}} = \left(\mathrm{d}\sigma^{\mathrm{NLO,E}} - \mathrm{d}\sigma^{\mathrm{MC}}\right)\Delta$$

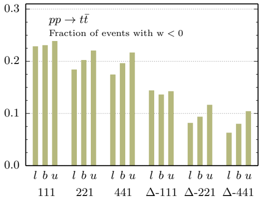
$$\mathrm{d}\sigma^{\Delta,\mathbb{S}} = \mathrm{d}\sigma^{\mathrm{MC}}\Delta + \sum_{\alpha} \mathrm{d}\sigma^{\mathrm{NLO},\alpha} + \mathrm{d}\sigma^{\mathrm{NLO,E}}(1-\Delta)$$

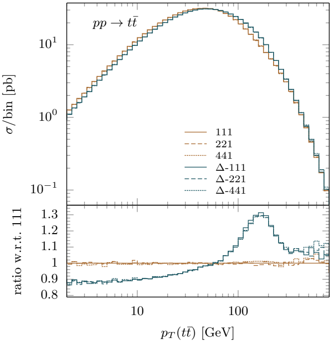
with (Sudakov-like) factor

$$0 \leq \Delta \leq 1\,, \quad \Delta \to \begin{cases} 0 & \text{soft and collinear} \\ 1 & \text{hard regions} \end{cases}$$

Supported since PYTHIA 8.309.

Two **different** matching methods!
⇒ **systematic differences** beyond **formal NLO accuracy**.





Note: still only default "simple shower" with global recoil supported by MADGRAPH _AMC@NLO!

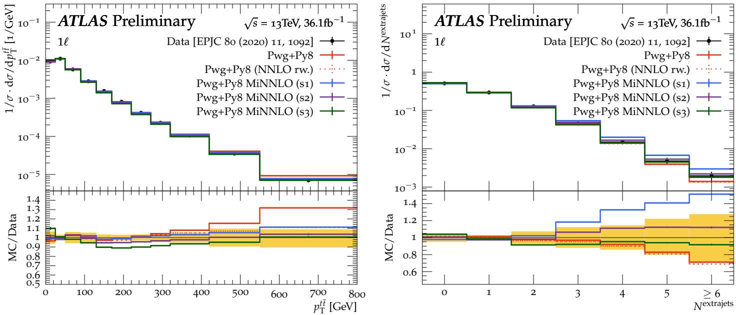
Matching uncertainties in MiNNLO$_{\text{PS}}$+PYTHIA → Katharina Voß' talk

MiNNLO$_{\text{PS}}$ achieves formal NNLO accuracy in showered $t\bar{t}$ events [Mazzitelli et al. 2012.14267].

$$\tilde{B}_{0j} = \mathrm{e}^{-\tilde{S}_{0j}} \left[B_{1j}\left(1+\frac{\alpha_s}{2\pi}\tilde{S}^{(1)}_{0j}\right) + V_{1j} + R_{1j} + D^{\geq 3}_{0j} F^{\text{corr}}_{1j} \right]$$

$$\sim \text{Sudakov}_{0j} \times [\text{POWHEG}_{1j} + \text{corrections}]$$

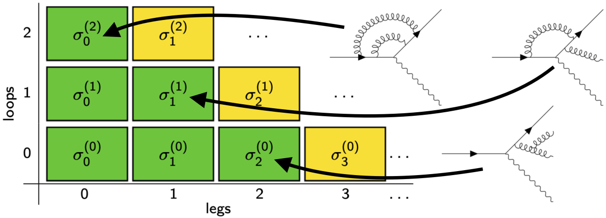
Problem: mismatch between "POWHEG p_{T}" and "PYTHIA p_{T}" leaves "matching scale" ambiguous **despite vetoed showers** [Hamilton et al. 2301.09645]



[ATLAS Collaboration ATL-PHYS-PUB-2023-029]

⇒ Need to consider *matching uncertainties* **separately** from renormalisation scale variations!

Towards fully-differential NNLO+PS [Campbell, Höche, Li, CTP, Skands 2108.07133]



Idea: "POWHEG at NNLO" without auxiliary scales and approximations

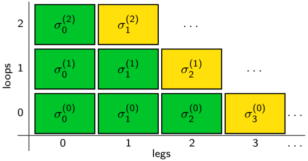
$$\langle O \rangle^{\mathrm{VINCIA}}_{\mathrm{NNLO+PS}} = \int \mathrm{d}\Phi_2 \, \mathrm{B}(\Phi_2) \underbrace{k_{\mathrm{NNLO}}(\Phi_2)}_{\text{local } K\text{-factor}} \underbrace{\mathcal{S}_2(t_0, O)}_{\text{shower operator}}$$

Need:

1. (1) Born-local NNLO K-factors
2. (2) shower filling ordered and unordered regions of 1- and 2-emission phase space
3. (3) tree-level MECs in ordered and unordered shower paths
4. (4) NLO MECs in the first emission

Valid for **all shower components** (FF, IF, II, **RF**), can be **iterated** ($t \to bW$, $W \to q\bar{q}'$, ...).

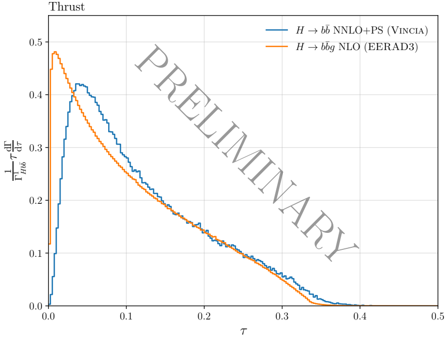
NNLO+PS matching in resonance decays

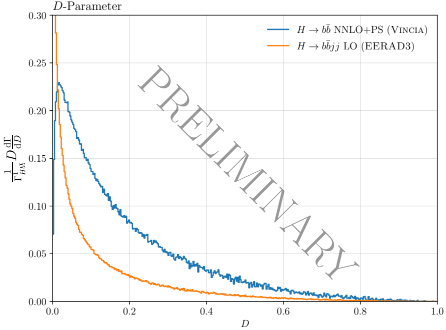


By construction, partial width is accurate to **NNLO**.

NNLO accuracy at Born level also implies
NLO correction in first emission and
LO correction in second emission.

E.g. $H \to b\bar{b}$ (VINCIA, parton level):





Conclusions

	Coherence: $pp \to t\bar{t}$ shower	Coherence: $t \to bW$ shower	Mass effects for b (and t)	Finite-Width effects (Γ_t, Γ_W)	Matrix-Element Corrections: $pp \to t\bar{t}$ shower	Matrix-Element Corrections: $t \to bW(\to q\bar{q})$ showers
	~ Approximate dipole treatment	🚫 Best is recoilToTop?	✓ Via iterated MECs	~ **BW** + Sequential Decays	🚫 → use PowHeg	1 — 1st order MECs for $t \to bWg$ & $W \to q\bar{q}g$
VINCIA	(✓) **Coherent** Initial-Final and Resonance-Final antennae + global (coherent) **resonance-final recoils.** (IF and FF recoils still local → ongoing work.)	(✓)	✓ **Massive** eikonals & **exact** massive antenna phase spaces	(✓) **BW** + **Interleaved** Decays. (Still missing a formal proof)	🚫 → 1 Under development. Can also use PowHeg	🚫 → 2 Under development. MECs up to $t \to bWgg$ & $W \to q\bar{q}gg$

Adapted from P. Skands.

VINCIA as of PYTHIA 8.310:

RF shower, interleaved EW shower, multipole QED shower, CKKW-L merging, POWHEG hooks

Soon:

NNLO MECs in resonance decays

PYTHIA helpdesk authors@pythia.org

Stay tuned: pythia-news@cern.ch

VINCIA tutorial: http://skands.physics.monash.edu/slides/files/Pythia83-VinciaTute.pdf

Backup

Resonance matching

Branchings like $t \to bW$, $Z \to q\bar{q}$ etc.

- Large scales:
  EW shower offers best description
- Small scales:
  Breit-Wigner distribution

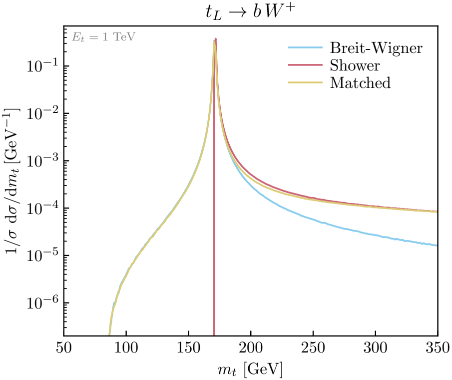
$$\mathrm{BW}(Q^2) \propto \frac{m_0 \Gamma(m)}{Q^4 + m_0^2 \Gamma(m)^2}$$

Matching:

- Sample mass from Breit-Wigner upon production
- Suppress shower by factor

$$\frac{Q^4}{(Q^2 + Q_{\mathrm{EW}}^2)^2}$$

- Decay when shower hits off-shellness scale



Slide adapted from R. Verheyen.

NNLO+PS with sector showers

Key aspect

up to matched order, include **process-specific** **NLO corrections** into shower evolution:

(1) correct first branching to exclusive ($< t'$) NLO rate:

$$\Delta^{\mathrm{NLO}}_{2\mapsto 3}(t_0, t') = \exp\left\{ -\int_{t'}^{t_0} \mathrm{d}\Phi_{+1}\, \mathrm{A}_{2\mapsto 3}(\Phi_{+1}) w^{\mathrm{NLO}}_{2\mapsto 3}(\Phi_2, \Phi_{+1}) \right\}$$

(2) correct second branching to LO ME:

$$\Delta^{\mathrm{LO}}_{3\mapsto 4}(t', t) = \exp\left\{ -\int_{t}^{t'} \mathrm{d}\Phi'_{+1}\, \mathrm{A}_{3\mapsto 4}(\Phi'_{+1}) w^{\mathrm{LO}}_{3\mapsto 4}(\Phi_3, \Phi'_{+1}) \right\}$$

(3) add direct $2 \mapsto 4$ branching and correct it to LO ME:

$$\Delta^{\mathrm{LO}}_{2\mapsto 4}(t_0, t) = \exp\left\{ -\int_{t}^{t_0} \mathrm{d}\Phi^{>}_{+2}\, \mathrm{A}_{2\mapsto 4}(\Phi_{+2}) w^{\mathrm{LO}}_{2\mapsto 4}(\Phi_2, \Phi_{+2}) \right\}$$

$\Rightarrow$ entirely based on **MECs** and **sectorisation**

$\Rightarrow$ **by construction**, expansion of extended shower **matches** NNLO singularity structure

But shower kernels **do not** define **NNLO subtraction terms**[1] (!)

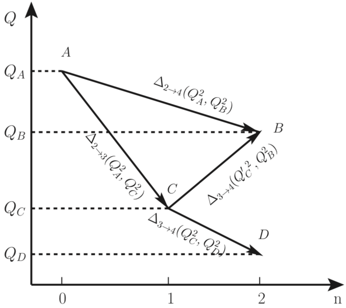
---

[1] This would be required in an "Mc@Nnlo" scheme, but difficult to realise in antenna showers.

Interleaved single and double branchings

A priori, direct $2 \mapsto 4$ and iterated $2 \mapsto 3$ branchings **overlap in ordered** region.

In **sector showers**, iterated $2 \mapsto 3$ branchings are **always strictly ordered**.



Divide double-emission phase space into **strongly-ordered** and **unordered** region: [Li, Skands 1611.00013]

$$\mathrm{d}\Phi_{+2} = \underbrace{\mathrm{d}\Phi_{+2}^{>}}_{\text{u.o.}} + \underbrace{\mathrm{d}\Phi_{+2}^{<}}_{\text{s.o.}}$$

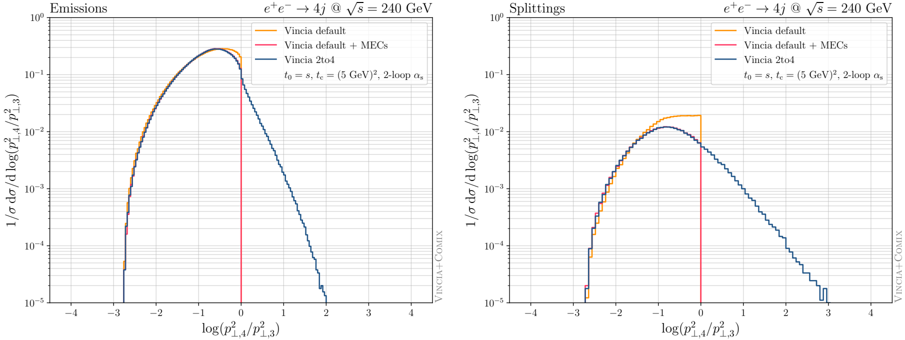
$\mathrm{d}\Phi_{+2}^{<}$: **single-unresolved** limits $\Rightarrow$ iterated $2 \mapsto 3$
$\mathrm{d}\Phi_{+2}^{>}$: **double-unresolved** limits $\Rightarrow$ direct $2 \mapsto 4$

Restriction on double-branching phase space enforced by additional veto:

$$\mathrm{d}\Phi_{+2}^{>} = \sum_{j} \theta\left(p_{\perp,+2}^2 - \hat{p}_{\perp,+1}^2\right) \Theta_{ijk}^{\mathrm{sct}}\, \mathrm{d}\Phi_{+2}$$

Real and double-real corrections

Direct $2 \mapsto 4$ shower component fills **unordered region** of phase space $p^2_{\perp,4} > p^2_{\perp,3}$.



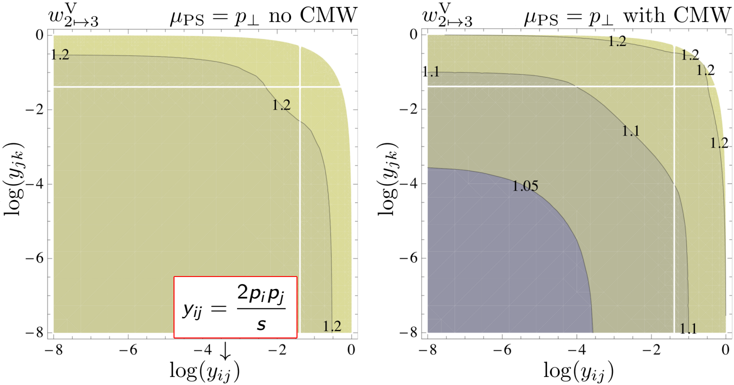
Sectorisation enforces **strict** cutoff at $p^2_{\perp,4} = p^2_{\perp,3}$ in iterated $2 \mapsto 3$ shower. **No recoil effects**!

Real-virtual corrections

Real-virtual correction factor ("local K-factor")

$$w^{\mathrm{NLO}}_{2\mapsto 3} = w^{\mathrm{LO}}_{2\mapsto 3}\left(1 + w^{\mathrm{V}}_{2\mapsto 3}\right)$$

studied **analytically** in detail for $Z \to q\bar{q}$ in [Hartgring, Laenen, Skands 1303.4974]:



Now: **generalisation** & **(semi-)automation** in VINCIA in form of NLO MECs