Pythia and Colour Reconnections

Peter Skands *(Monash University)*

Colour **Reconnections** ➤ increasingly seen as part of broader spectrum of (non-perturbative) 'collective effects'. New models.

Shower Uncertainties in PYTHIA.

Colour **Connections**: colour flows in tt and coherence in PYTHIA and VINCIA.

(t→)b→B fragmentation and tuning.

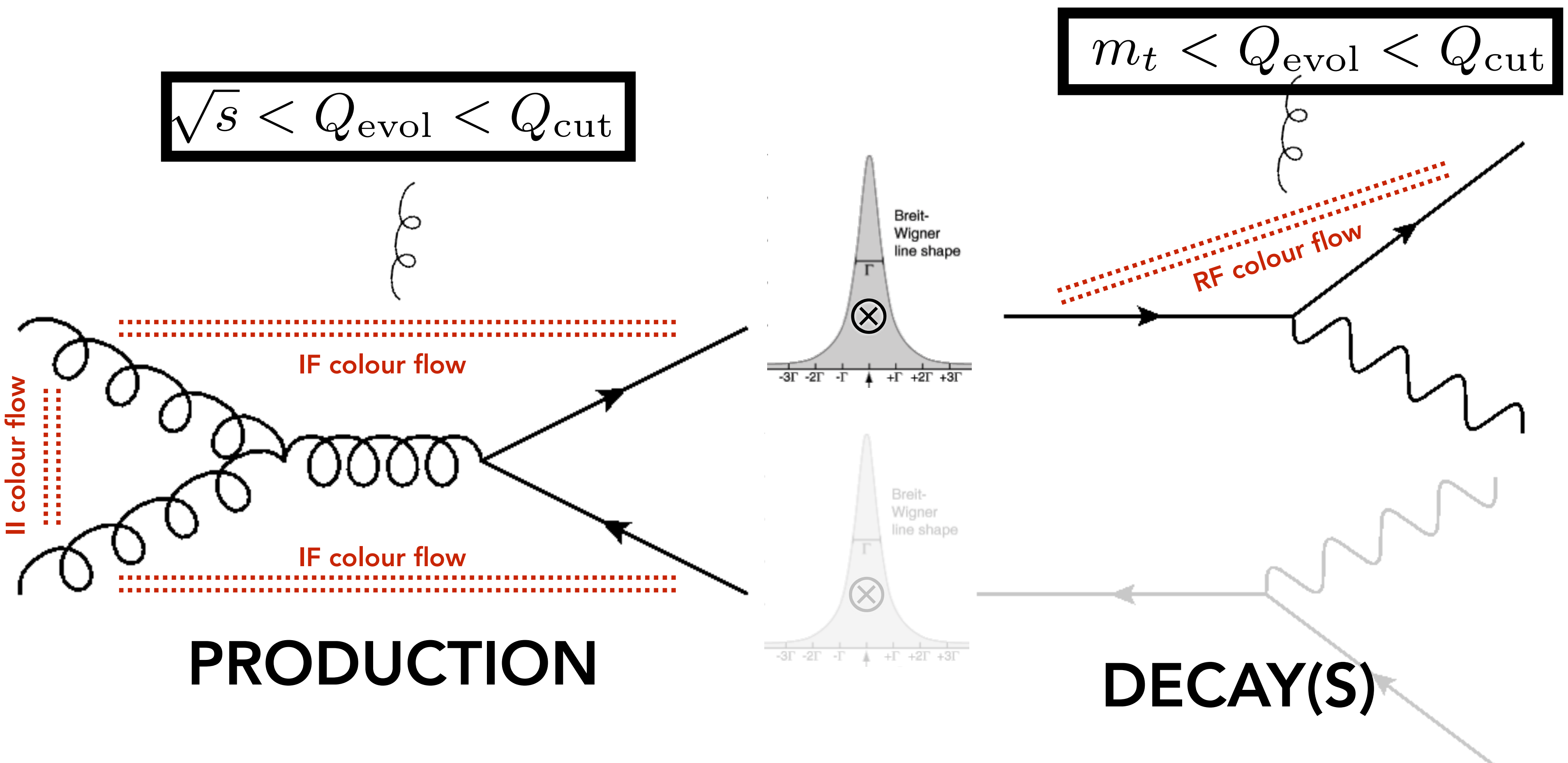
LHC Top WG Meeting
CERN, November 2019

Modelling Top Pair Production and Decay

In limit $\Gamma_t \sim 0$, factorise **production** and **decay**

These stages are showered independently.

I: initial
F: final
R: resonance



Production ISR + FSR shower preserves Breit-Wigner shape

Resonance-Decay FSR shower preserves Breit-Wigner shape

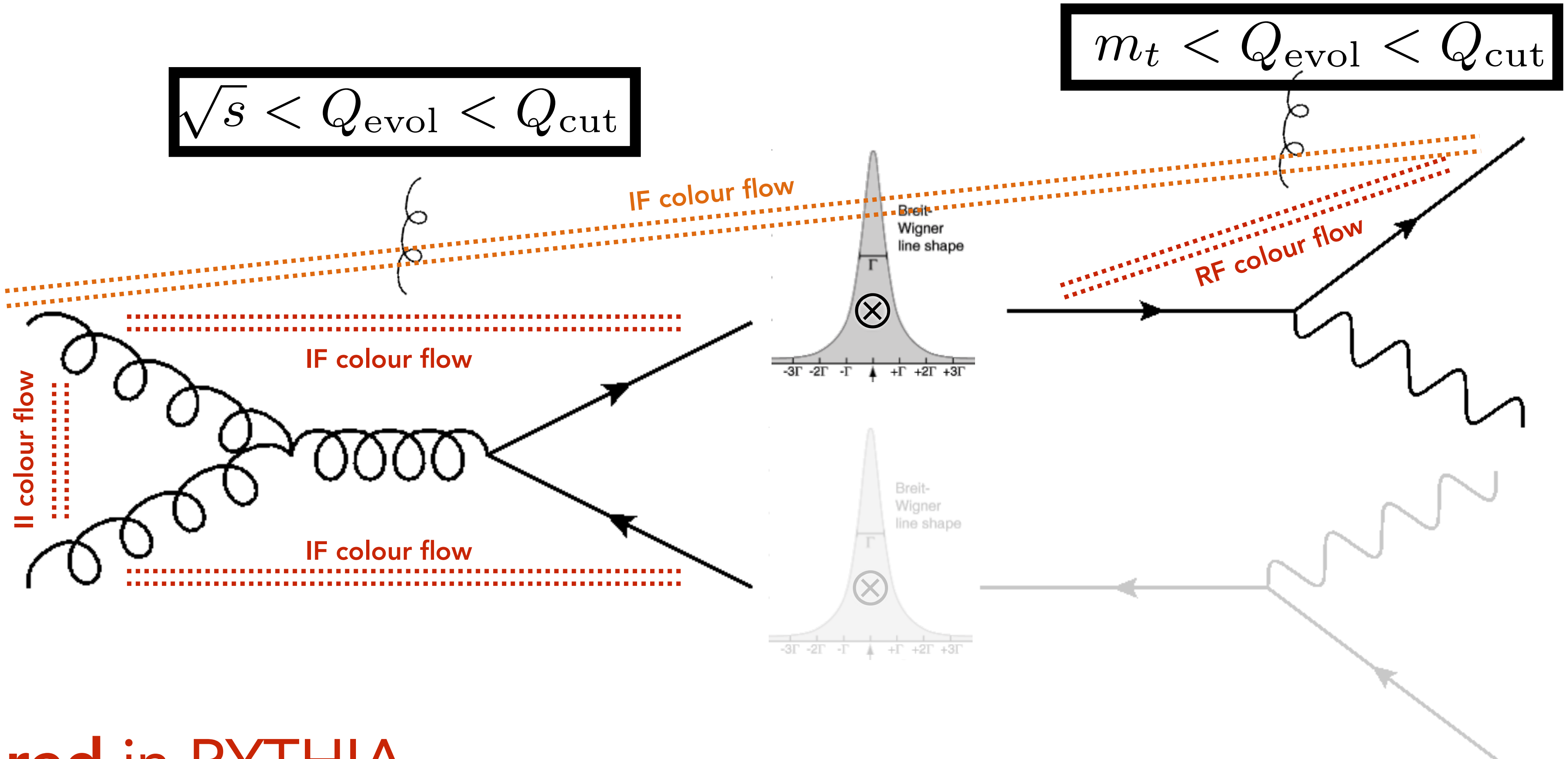
Would modify BW shape.

But expect small effects. Cutoff of perturbative shower $Q_{cut} \sim 1$ GeV ; $\Gamma_t \sim 1.5$ GeV (in SM); Interference only from scales $1 \text{ GeV} < Q < 1.5 \text{ GeV}$

I: initial

F: final

R: resonance



- **Ignored** in PYTHIA.

Production showered to Q_{cut}, decay as well.

An e^+e^- study found $\Delta m_t < 50$ MeV but not repeated for LHC (to my knowledge)

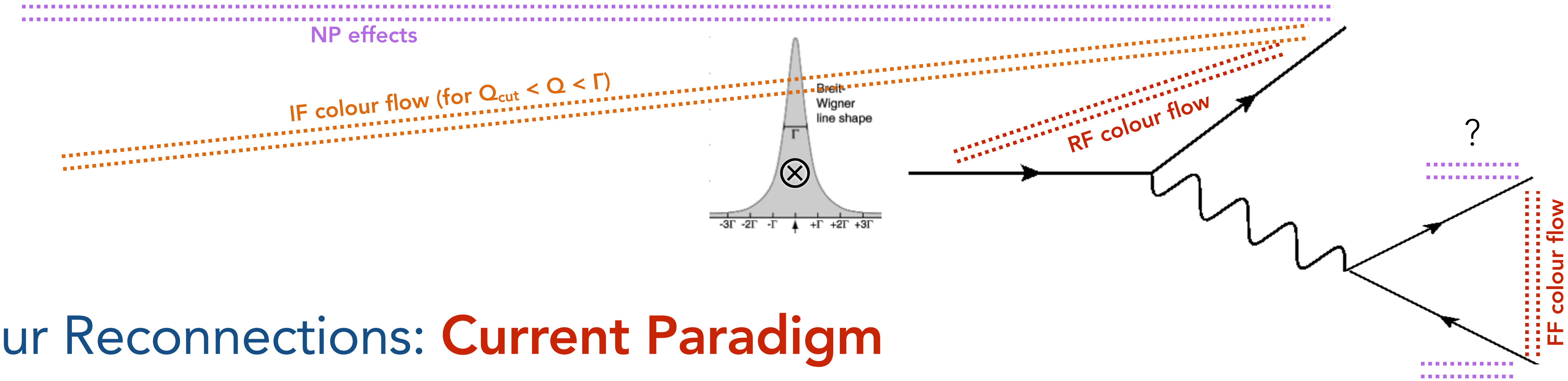
Khoze, Sjöstrand, Phys.Lett. B328 (1994) 466

Non-perturbative effects: MPI, CR, etc

Will modify BW shape.

Affects hadronisation in b-jet and may (?) affect b→B transition.

May (?) affect hadronic W hadronisation.



Colour Reconnections: Current Paradigm

Partons from different MPI (or ee→WW) can be "close" in phase space.

Nature can make use of **non-LC possibilities** to minimise the confinement potentials. This motivated the **"QCD-inspired"** model in PYTHIA, and in various more or less explicit ways informs most other CR models.

NB: momentum transfer happens due to **ambiguities** in colour space; indirect

New / Emerging Paradigm

LHC has discovered **new non-perturbative QCD phenomena in pp**, like CMS "ridge" and ALICE strangeness enhancement vs multiplicity

These effects do not seem to be explicable solely in terms of CR.

➤ New paradigm: new non-perturbative **dynamics** (interactions)

New Models:

Lund/NBI: **Collective Strings 1**: (Swing) + Colour Ropes + String Shoving

Monash: **Collective Strings 2**: (QCD CR) + Dynamic String Tensions + Repulsion

Lund: Strings with Spacetime Information + **Hadron Rescattering**

Herwig: Cluster Model with **spacetime CR** + Dynamic strangeness enhancement

Epos: Core/Corona picture with **QGP-like thermal effects** in core component

Expect additional hadron-level effects of order Λ_{QCD}, beyond "conventional" CR.

Good, Bad, or Irrelevant for Top Physics?

Good?

CR is difficult to pin down and constrain directly, with any confidence. That is part of the reason why we still have a plethora of models.

But strangeness and baryon enhancements leave **clear smoking-gun traces**.

Bad?

Expect additional **hadron-level effects of order Λ_{QCD}**, beyond "conventional" CR.

E.g., if strings push on each other, that could exchange momenta of order Λ_{QCD} (per unit rapidity!) between top system and MPI.

And/or if **B_s/B** and **Λ_b/B** rates are affected ➤ modifications to B spectra (+decays)

Irrelevant?

Like CR, effects may primarily affect the "soft bulk" of particle production (~ the UE),

(Tips of) **high-pT jets may not be significantly affected**. But would need explicit constraints to be sure.

Most models not tested for top physics yet. Get in touch with MC authors.

Shower Uncertainties: Scale Variations

What do parton showers do?

In principle, LO shower kernels proportional to α_s

Naively: do factor-2 variations of μ_{PS}.

There are at least 3 reasons this could be **too** conservative

1. For soft gluon emissions, we know what the NLO term is

   → even if you do not use explicit NLO kernels, you are effectively NLO (in the soft gluon limit) **if** you are coherent and use $\mu_{PS} = (k_{CMW}\ p_T)$, with 2-loop running and $k_{CMW} \sim 0.65$ (somewhat n_f-dependent). *[Though there are many ways to skin that cat; see next slides.]*

   Ignoring this, a **brute-force** scale variation **destroys** the NLO-level agreement.

2. Although hard to quantify, showers typically achieve better-than-LL accuracy by accounting for **further physical effects** like (E,p) conservation

3. We see empirically that (well-tuned) showers tend to stay far inside the envelope spanned by factor-2 variations in **comparison to data**

See e.g., Perugia radHi and radLo variations on mcplots.cern.ch

Scale Variations: How Big?

Poor man's recipe: Use $\sqrt{2}$?

Sure … but still rather arbitrary

Instead: add compensation term to preserve soft-gluon limit at $O(\alpha_s^2)$

Allowing full factor-2 outside that limit.

Several MCs now implement such compensation terms, at least in context of automated uncertainty bands.

Warning: aggressive definitions can lead to overcompensation / **extremely** optimistic predictions → very small uncertainty bands.

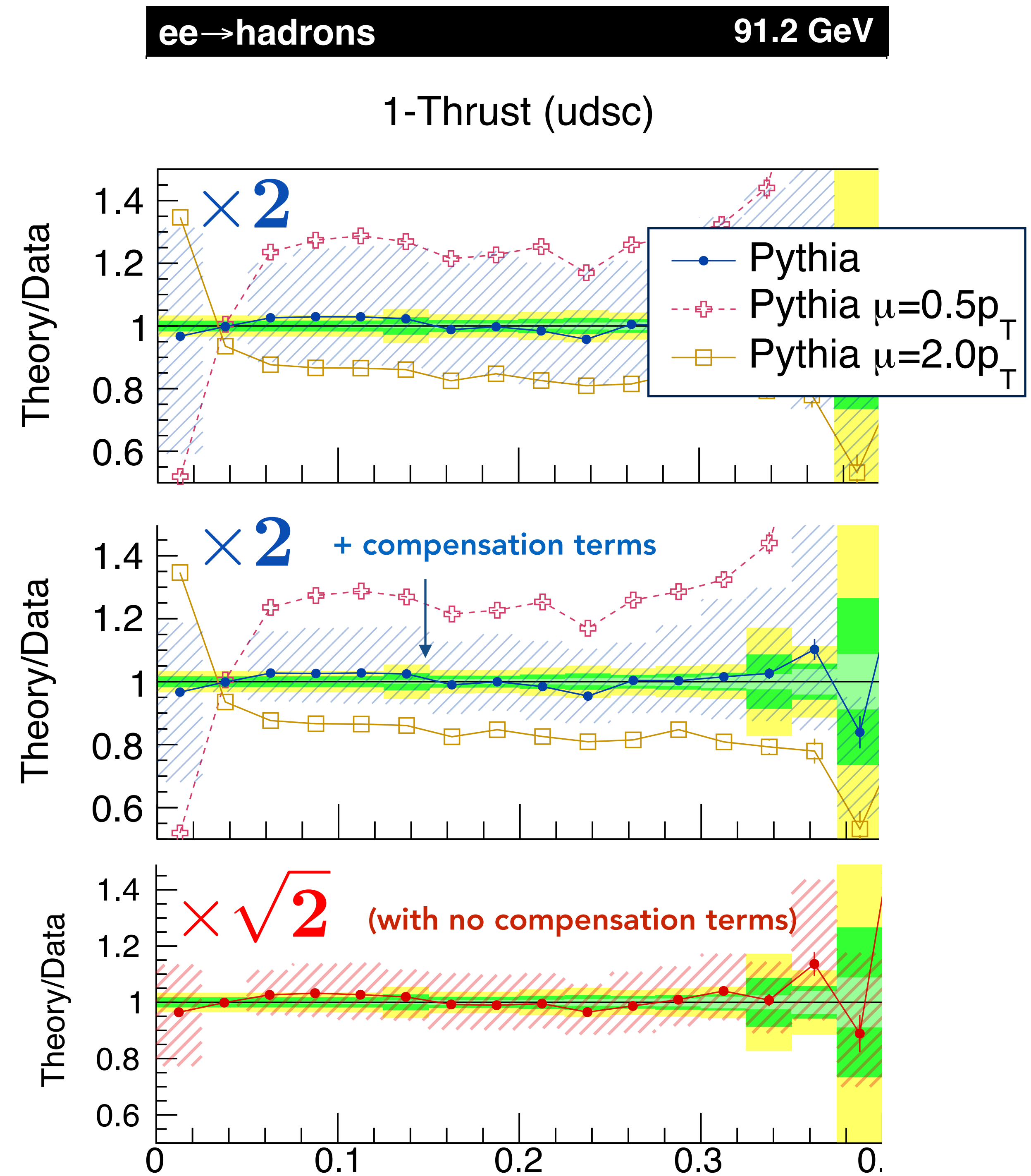
For PYTHIA, we chose a rather conservative definition ➤ larger bands.

$$P'(t,z) = \frac{\alpha_s(kp_\perp)}{2\pi}\left(1 + (1-\zeta)\frac{\alpha_s(\mu_{\max})}{2\pi}\beta_0 \ln k\right)\frac{P(z)}{t}$$

Kills the compensation outside the soft limit

Small absolute size of compensation

$$\zeta = \begin{cases} z & \text{for splittings with a } 1/z \text{ singularity} \\ 1-z & \text{for splittings with a } 1/(1-z) \text{ singularity} \\ \min(z,1-z) & \text{for splittings with a } 1/(z(1-z)) \text{ singularity} \end{cases}$$

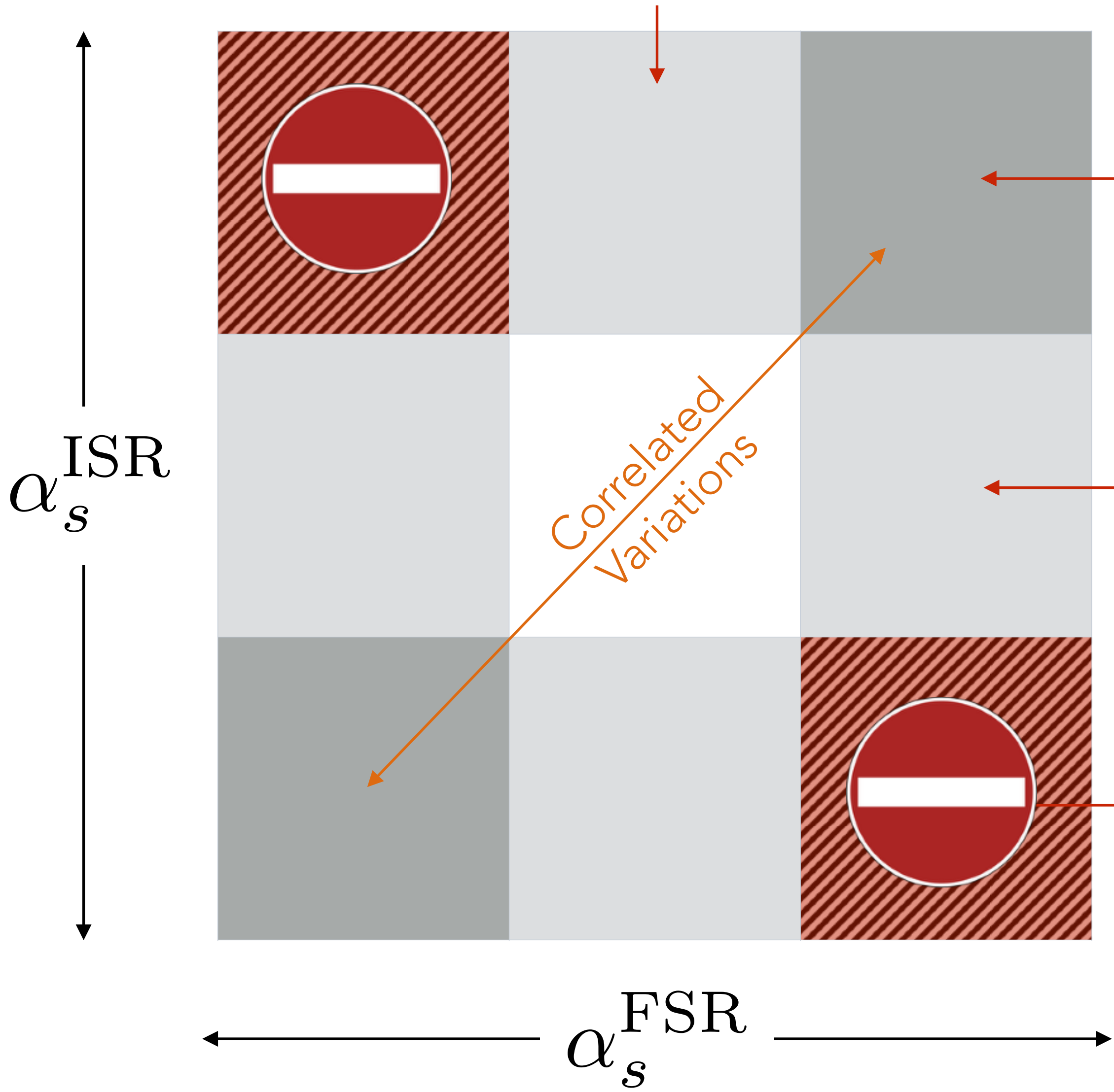


S. Mrenna & PS: PRD94(2016)074005; arXiv:1605.08352

Correlated or Uncorrelated?

What I would do: **7-point variation** (resources permitting → use the automated bands?)

Increasing only ISR
➠ More H_T and N_{jets}; similar core jet shapes



Increasing both ISR and FSR
➠ More H_T in the events.
➠ More OOC loss (from FSR) but also more H_T and more hard ISR jet seeds → partial cancellation in N_{jets}?

Increasing only FSR
➠ More OOC loss (FSR jet broadening), acting on similar number of seed partons (no increase in ISR).
➠ Similar H_T

Increasing FSR, Decreasing ISR
➠ Double counting? Fewer ISR partons, **and** more smearing of those that remain. *(Easy to rule out?)*
➠ Also from theoretical/mathematical point of view, the artificially induced discrepancy is now proportional to ln(16) = 2.8 instead of ln(4) = 1.4.

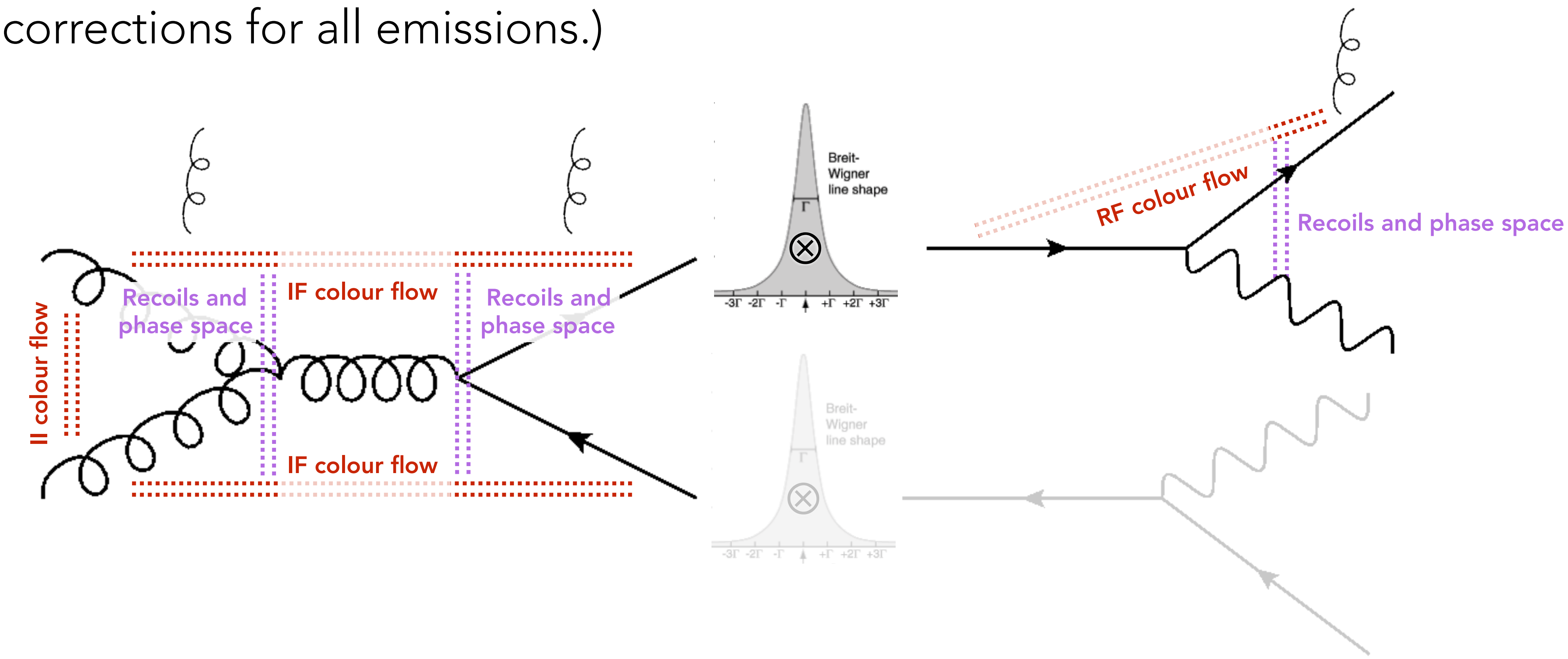
Note: I would also do splitting-kernel variations (see extra slides)

Default PYTHIA showers not fully coherent for “IF” or “RF” flows

All initial-state partons treated as II. (Some coherence by rapidity ~angular vetos)

All final-state partons treated as FF. (MECs ➤ 1st emission in top decay correct; + b mass corrections for all emissions.)

I: initial
F: final
R: resonance



RF not coherent from **2nd emission** onwards. (So eg Powheg does not help.)

Issues for soft wide-angle, recoil effects, and some phase-space effects.

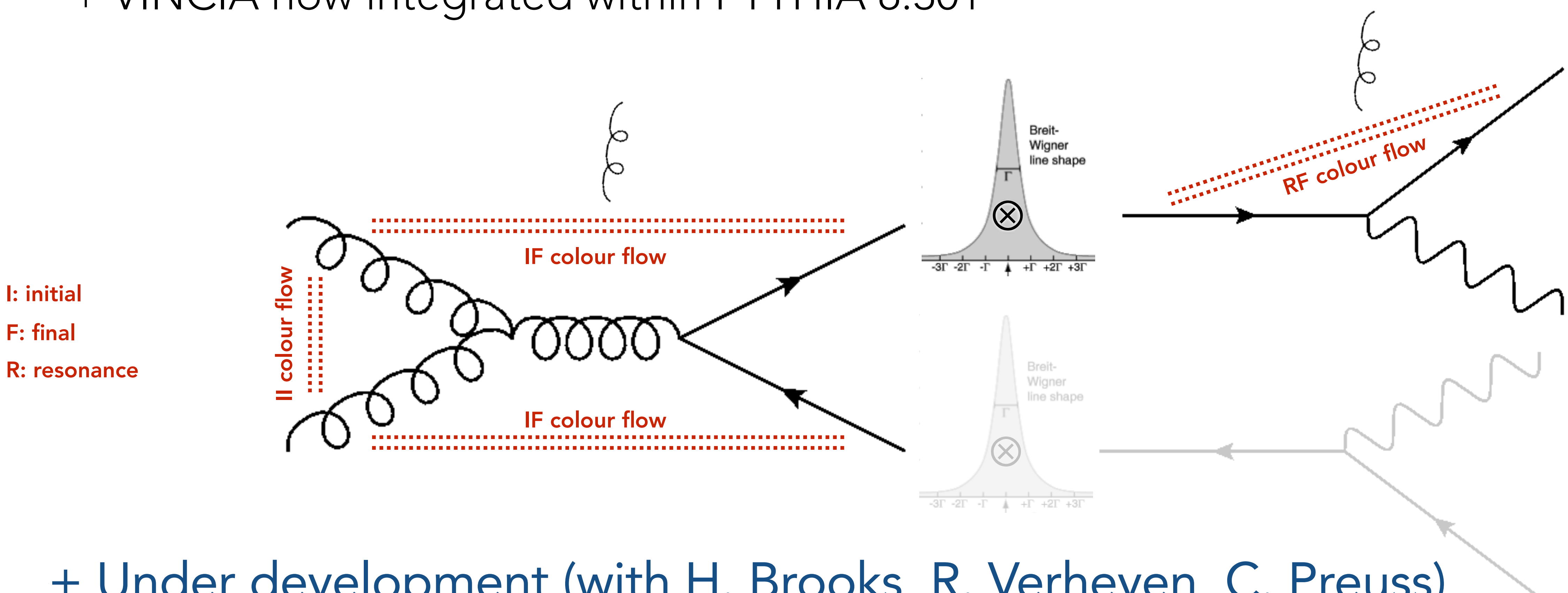
Brooks, Skands, Phys.Rev. D100 (2019) no.7, 076006 ARXIV:1907.08980

Explicit **IF** and (recently) **RF** antennae

Based on **coherent dipole-antenna** patterns, with **full t and b mass** effects.

Collective recoils for RF emissions: coherent radiation recoils against "crossed" top

+ VINCIA now integrated within PYTHIA 8.301



+ Under development (with H. Brooks, R. Verheyen, C. Preuss)

Interleaved resonance decays ➤ interference between production and decays.

Iterated Matrix-element Corrections. (So far it is a pure shower.)

Automated uncertainty variations (in the same style as internal Pythia 8 ones).

Slide from H. Brooks

arXiv:1801.03944

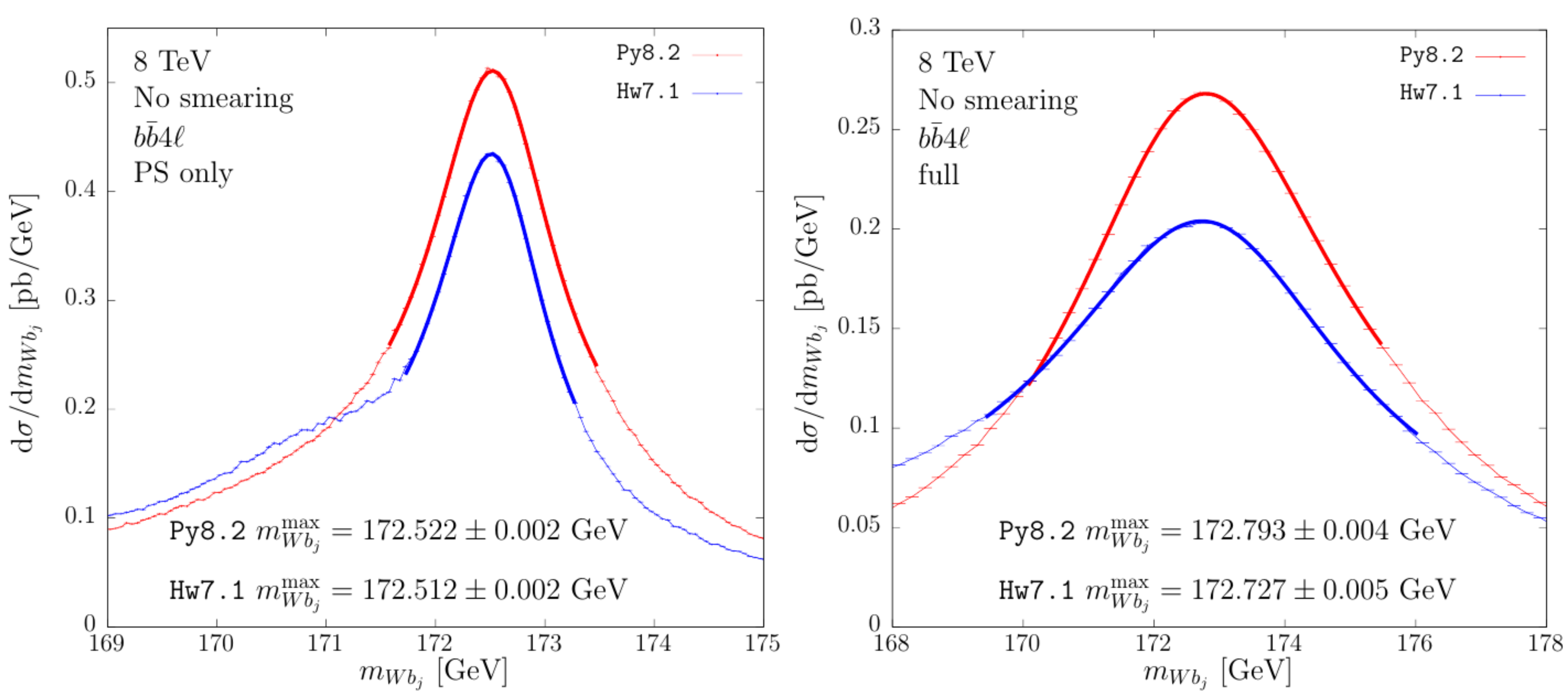
A theoretical study of top-mass measurements at the LHC using NLO+PS generators of increasing accuracy

Silvia Ferrario Ravasio,[a] Tomáš Ježo,[b] Paolo Nason,[c] Carlo Oleari[a]

[a] *Università di Milano-Bicocca and INFN, Sezione di Milano-Bicocca, Piazza della Scienza 3, 20126 Milano, Italy*

[b] *Physics Institute, Universität Zürich, Zürich, Switzerland*

[c] *CERN, CH-1211 Geneve 23, Switzerland, and INFN, Sezione di Milano-Bicocca, Piazza della Scienza 3, 20126 Milano, Italy*



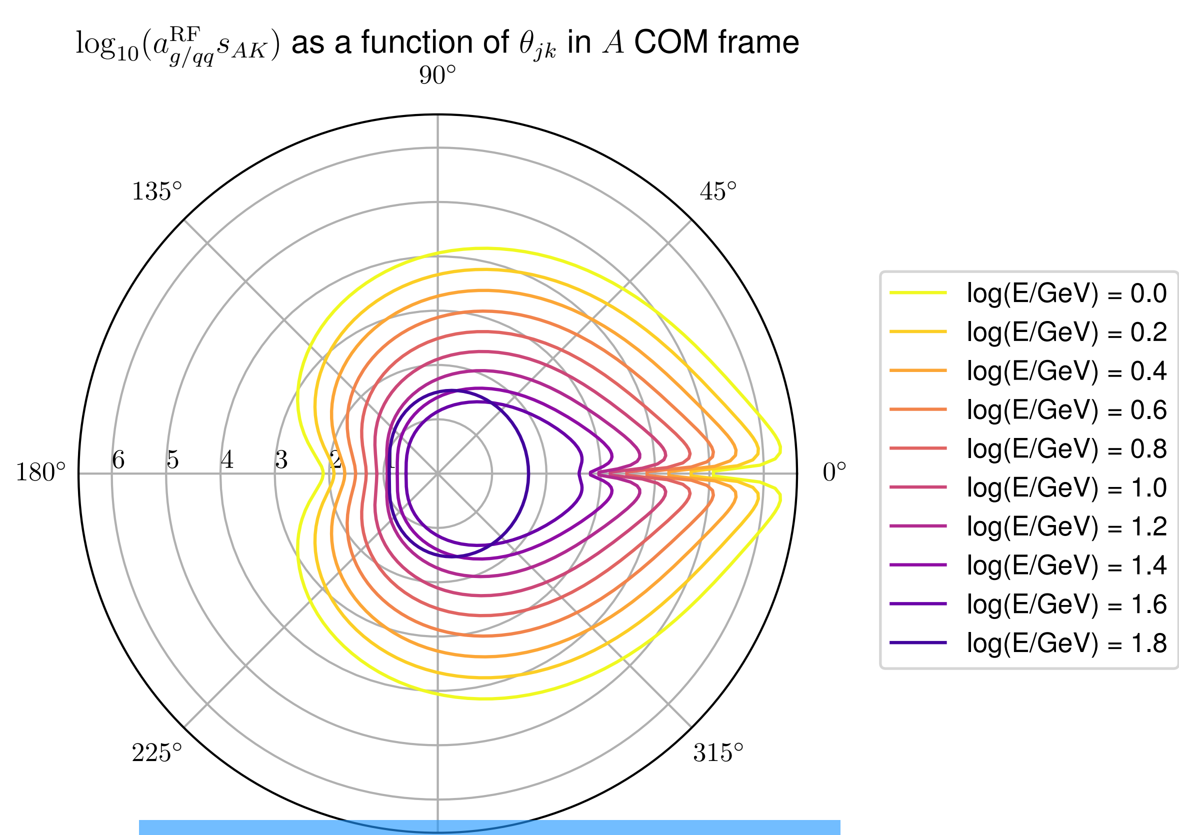
"… the very minimal message that can be drawn from our work is that, in order to assess a meaningful theoretical error in top-mass measurements, the use of different shower models, associated with different NLO+PS generators, is mandatory."

Coherence in Top Decay

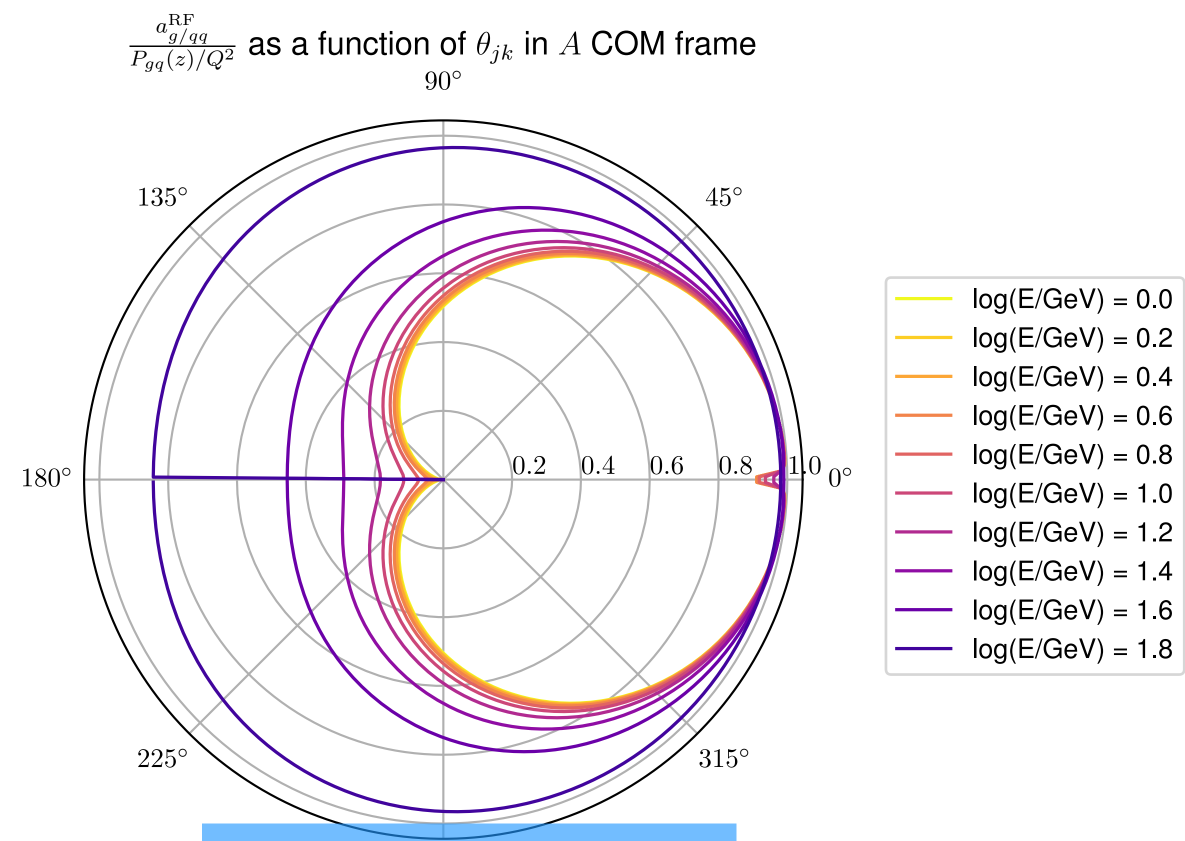
Slide from H. Brooks

Brooks, Skands, Phys.Rev. D100 (2019) no.7, 076006 [ARXIV:1907.08980]

Plot antenna function in top centre of mass frame (b along z):



Log of antenna function



Ratio to AP kernel

Antenna function ➔ b-quark DGLAP splitting function in forwards (collienar) direction; coherence results in a suppression in the backwards (wide-angle) direction ➤ narrower b-jets

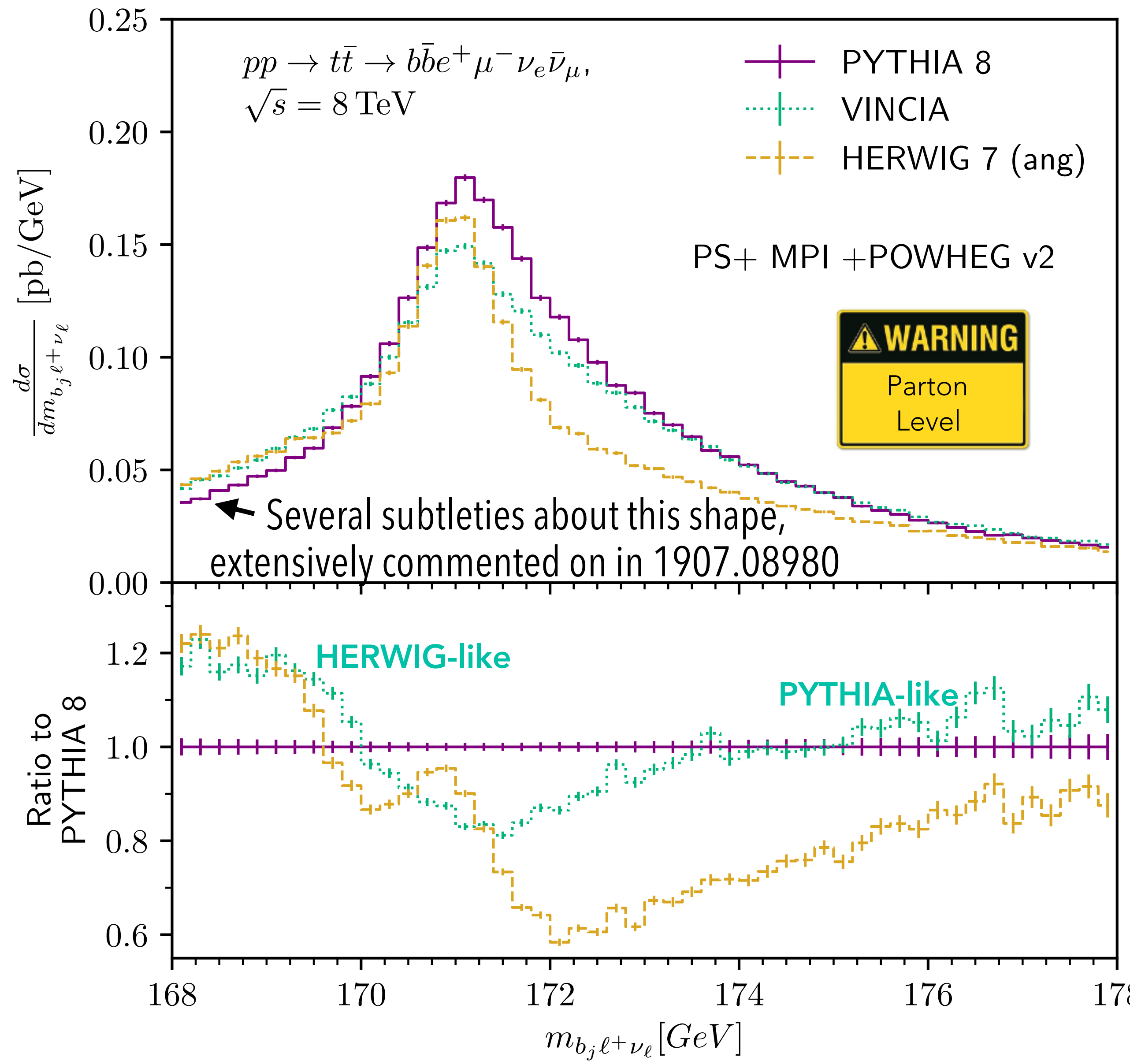
Matching with POWHEG

Brooks, Skands, Phys.Rev. D100 (2019) no.7, 076006 ARXIV:1907.08980

- Use POWHEG v2 $(t\bar{t}dec)$[1] (no need for exact finite width effects)
- **Very** similar setup to matching with PYTHIA in [2].
- Veto hardest emission in production with

  `Vincia:QmaxMatch = 1`

- Veto hardest emission in decay with `UserHooks` interface



[1] [1412.1828] [1509.0907]

PYTHIA 8.301 released. Includes VINCIA with new resonance-final showers

Not yet recommended for main production runs, but need your feedback.

Still to come in VINCIA: multi-leg MECs, automated uncertainty bands, production-decay interference, electroweak showers, NLO antenna functions,…

Comments on b fragmentation

Skands, Carazza, Rojo, Eur.Phys.J. C74 (2014) no.8, 3024

The Monash tune for heavy flavour:

Constrained by **LEP event shapes** (including b-tagged ones) + jet rates

➤ Relatively large value of TimeShower:alphaSvalue = 0.1365

Regarded at least in part as making up for NLO K-factor for ee→3 jets (Pythia only accurate to LO for 3 jets).

Consistent with 3-flavour Λ_{QCD} ~ 0.35 GeV (since we use 1-loop running)

Not guaranteed to be universal. LHC studies tend to prefer lower values

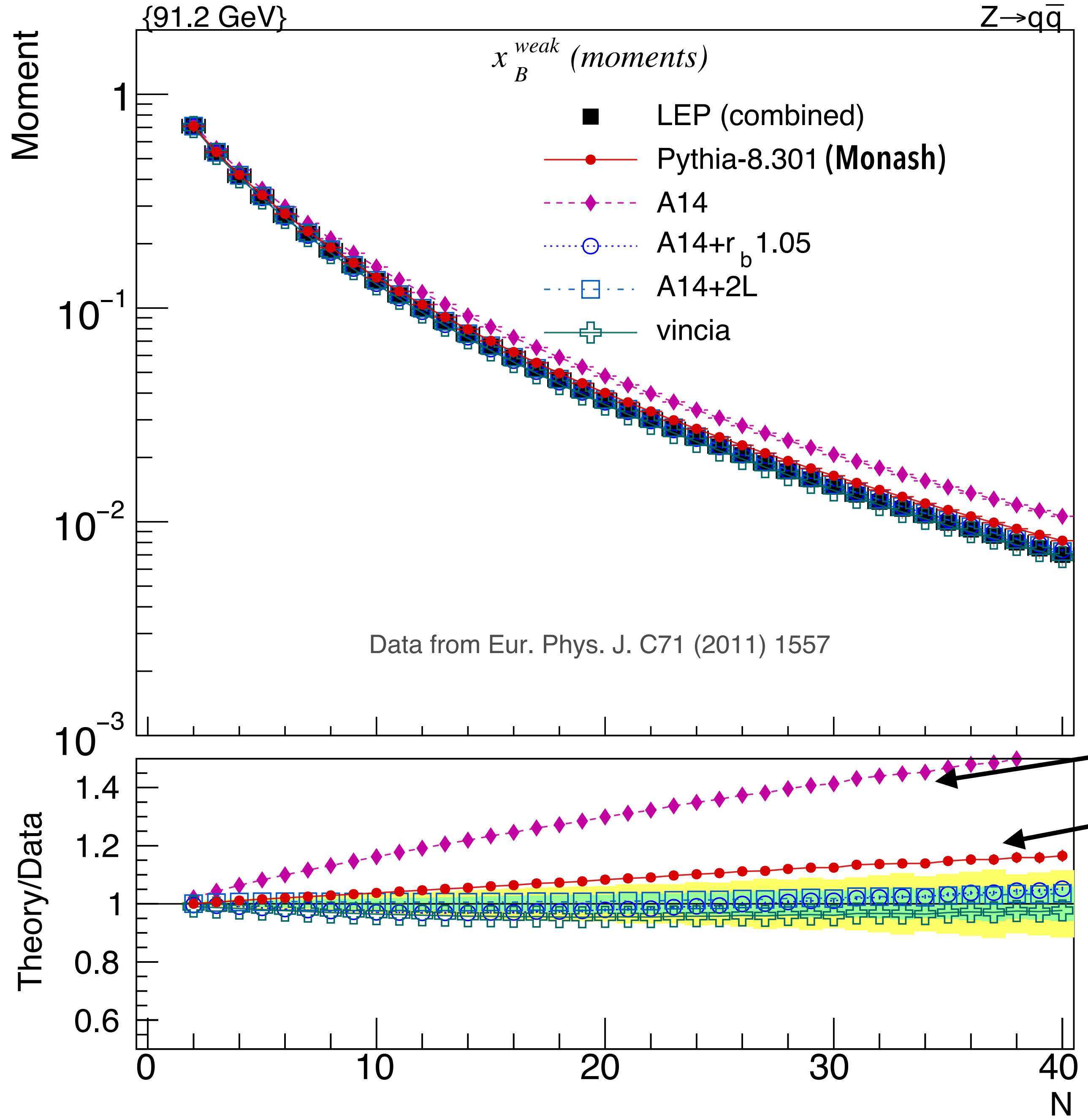
E.g., **A14** uses TimeShower:alphaSvalue = 0.129 (could be reinterpreted via CMW to MSbar alphaS(mZ) ~ 0.12 so consistent with world average.)

(but I would then also change to 2-loop running; would preserve Λ_{QCD} value)

Non-Perturbative b-fragmentation parameter r_b constrained by measured x_B spectra of weakly decaying B hadrons.

➤ StringZ:rFactB = 0.88.

LEP B Fragmentation



Moments of x_B distribution

(easier / clearer to look at than spectrum itself)

Question: possible to do in-situ constraints or at least cross checks in top / inclusive b / … at LHC?

Lower α_S ➤ B spectrum too hard

(Monash; deliberately slightly hard for global reasons)

Increasing r_b (0.88→1.05) **or** changing to 2-loop running. Both reestablish agreement **but will scale differently**

Also note: lower value of $\alpha_s(M_Z)$ ➤ **lower 3-jet rate**

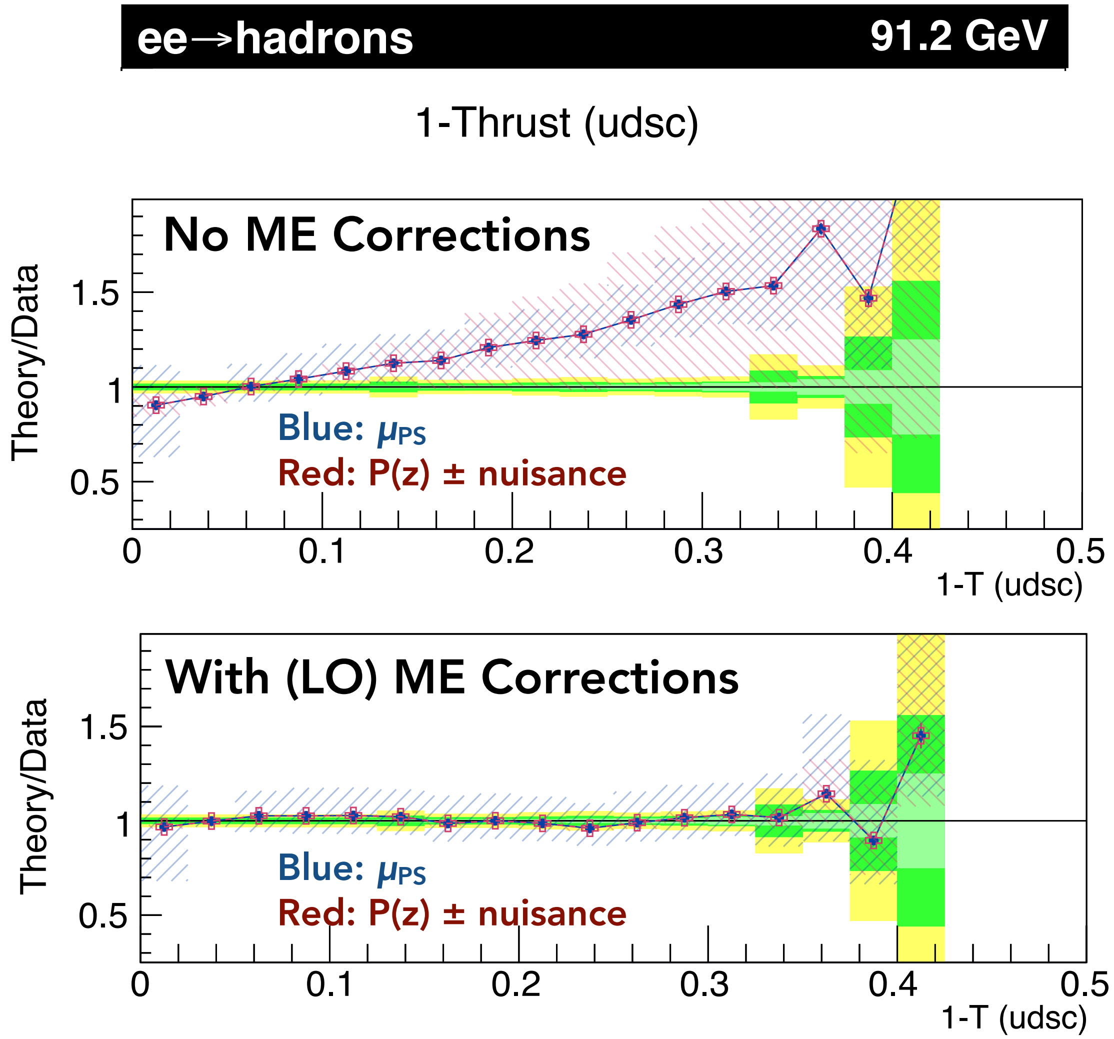
➤ wrong 2- vs 3-jet mixture (relative to data sample)? **Do reweighting?**

Questions / Discussion ?

How to test if "More" ME Corrections needed?

The soft and collinear enhanced (singular) terms in the shower kernels are universal, process-independent

- Matrix Elements contain the same information, plus process-specific **non-singular** terms.
- The shower singularities dominate for soft and collinear radiation
- The process-specific non-singular terms dominate for hard radiation



VINCIA: Giele, Kosower & PS: PRD84(2011)054003; arXiv:1102.2126

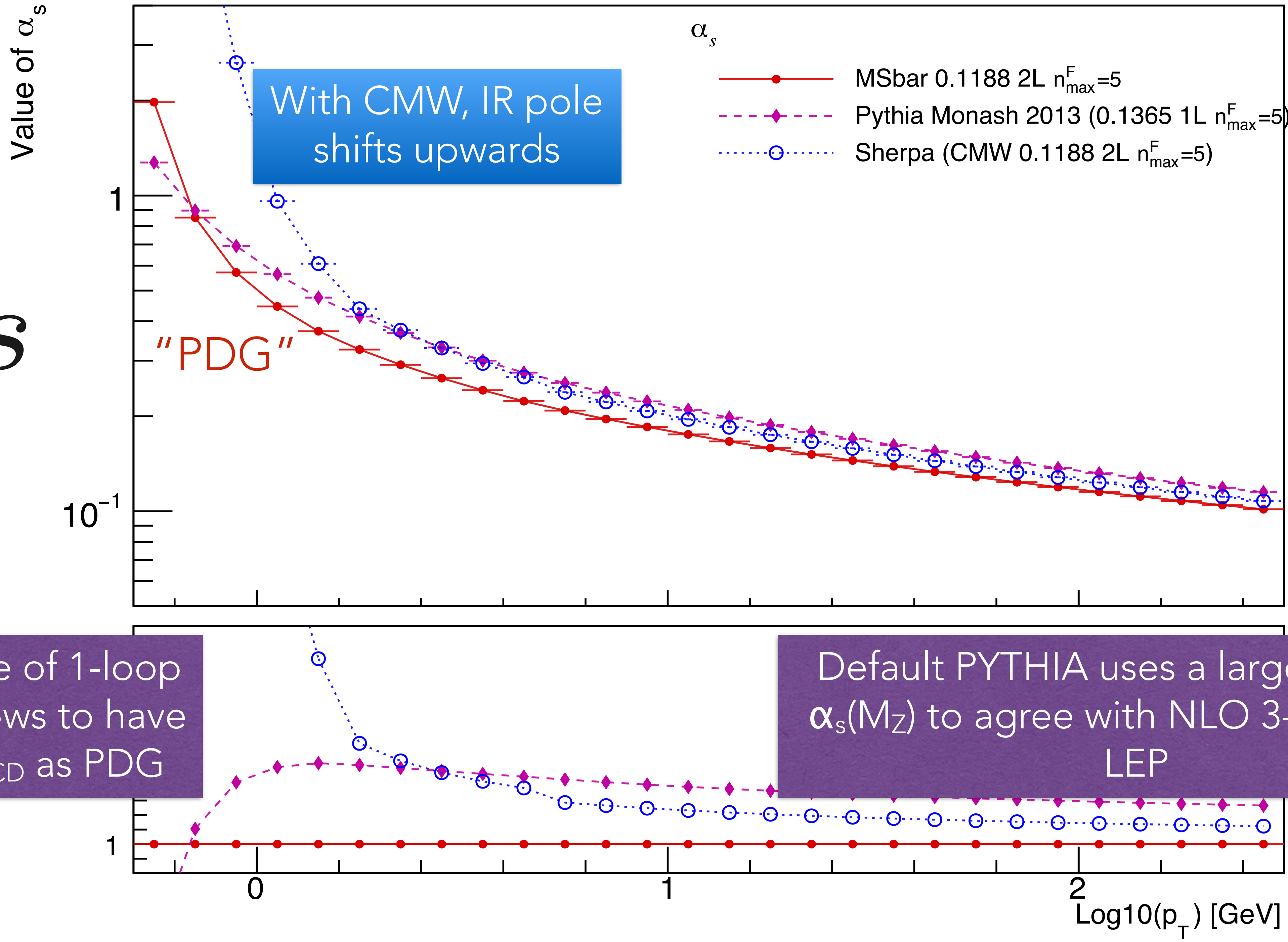
PYTHIA 8: S. Mrenna & PS: PRD94(2016)074005; arXiv:1605.08352

Suggestion: add nuisance parameter = arbitrary nonsingular term to shower kernels, and **vary** to estimate sensitivity to missing ME terms

Note: by definition, any fit of such a nuisance parameter would be process-specific

NOTE ON DIFFERENT ALPHA(S) CHOICES

α_s



With CMW, IR pole shifts upwards

Slower pace of 1-loop running allows to have similar Λ_{QCD} as PDG

Default PYTHIA uses a large value of $\alpha_s(M_Z)$ to agree with NLO 3-jet rate at LEP

SCALE VARIATIONS: HOW BIG?

Scale variations induce 'artificial' terms beyond truncated order in QFT ~ Allow the calculation to float by $(1+O(\alpha_s))$.

$$\frac{\alpha_s(k_1^2\mu^2)}{\alpha_s(k_2^2\mu^2)} \sim 1 - b_0 \ln(k_1^2/k_2^2)\alpha_s(\mu^2)$$

Flavour-dependent slope of order 1
$b_0 \sim 0.65 \pm 0.07$

Expansion around μ only sensible if this stays ≲ 1

Proportionality to $\alpha_s(\mu)$ ⟹ can get a (misleadingly?) small band if you choose central μ scale very large.

E.g., some calculations use μ ~ H_T ~ largest scale in event ?!

Worth keeping in mind when considering (uncertainty on) central μ choice

Mainstream view:

Regard scale dependence as unphysical / leftover artefact of our mathematical procedure to perform the calculations.

Dependence on it has to vanish in the 'ultimate solution' to QFT

→ Terms beyond calculated orders must sum up to at least kill μ dependence

Such variations are thus regarded as a useful indication of the size of uncalculated terms. (Strictly speaking, only a lower bound!)

Typical choice (in fixed-order calculations): k ~ [0.5,1,2]

Note: In PYTHIA you specify k^2
TimeShower:renormMultFac
SpaceShower:renormMultFac

AUTOMATED SHOWER UNCERTAINTY BANDS/WEIGHTS

Mrenna, Skands Phys.Rev. D94 (2016) 074005

Idea: perform a shower with nominal settings

Ask: what would the probability of obtaining this event have been with **different choices** of μ_R, radiation kernels, … ?

Easy to calculate **reweighting factors**

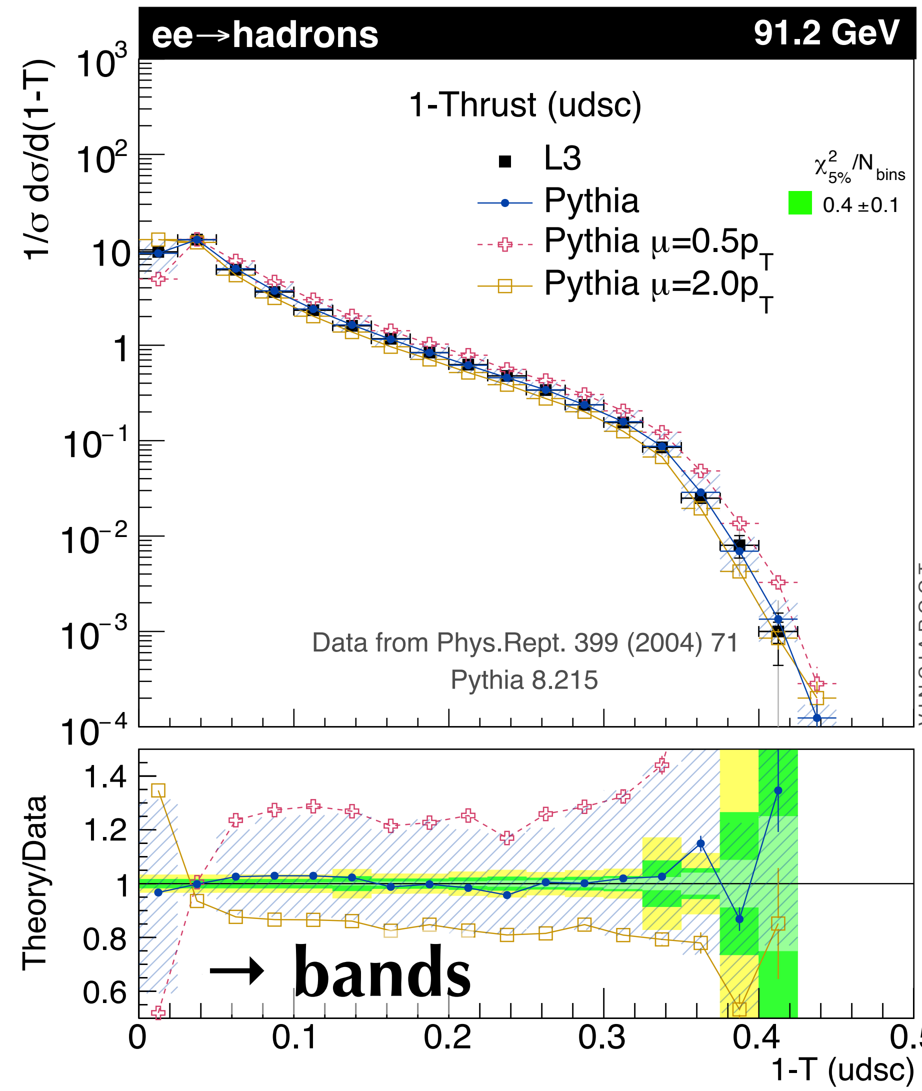
In MC accept/reject algorithm:

for **all** branchings

∀ *Accepted Branchings:* $$R'_{\rm acc}(t) = \frac{P'_{\rm acc}(t)}{P_{\rm acc}(t)}$$

∀ *Rejected Branchings:* $$R'_{\rm rej}(t) = \frac{1 - P'_{\rm acc}(t)}{1 - P_{\rm acc}(t)}$$

Giele, Kosower, Skands PRD84 (2011) 054003



Output: **vector of weights** for each event

One for the nominal settings (unity)

+ Alternative weight for each variation

(Note: similar functionality also in Herwig++ and Sherpa; see 1605.08256 1606.08753)

AUTOMATED SHOWER UNCERTAINTY BANDS/WEIGHTS

Mrenna, Skands Phys.Rev. D94 (2016) 074005

The benefits: only a single sample needs to be generated, hadronised, passed through detector simulation, etc.

Can add arbitrarily many (combinations of) variations (if supported by code)

The drawback: effective statistical precision of uncertainty bands computed this way (from varying weights) is always less than that of the central sample (which typically has all weights =

(Note: similar functionality also in Herwig++ and Sherpa; see 1605.08256 1606.08753)

HOW MANY PARAMETERS TO VARY?

There is of course only a single α_s in nature

But remember we are here just using scale variations as a stand-in for unknown higher-order terms.

ISR and FSR kernels receive different NLO corrections

Physically, ISR also has additional ambiguity tied to the PDF

ISR and FSR have different phase spaces and affect physical observables differently

- FSR: jet shapes, OOC, heavy-flavour parton energy loss, …
- ISR: Recoils to hard system; Soft ISR increases overall H_T. Hard ISR → N_{Jets}.

I therefore conceive of ISR and FSR variations as separate things

(Yes, there are overlapping cases, most obviously when colour flows from initial to final state, as in ttbar: initial-final antennae, and also for subleading colour effects.)

Not to forget (but not main topics of this talk):

PDFs, functional form of central choices of factorisation and renormalisation scales, nonsingular parameters, subleading colour, local vs global recoils …

SETTINGS FOR AUTOMATED 7-POINT VARIATION

7-Point scale variations

Based on factor-2 variations with NLO soft compensation term ON

+ some nonsingular-term variations to estimate sensitivity to process-dependent finite terms (signaling need for further ME correcti

```
UncertaintyBands:doVariations = on
UncertaintyBands:muSoftCorr = on
UncertaintyBands:List = {
  radHi fsr:muRfac=0.5 isr:muRfac=0.5,
  fsrHi fsr:muRfac=0.5,
  isrHi isr:muRfac=0.5,
  radLo fsr:muRfac=2.0 isr:muRfac=2.0,
  fsrLo fsr:muRfac=2.0,
  isrLo isr:muRfac=2.0,
  fsrHardHi fsr:cNS=2.0,
  fsrHardLo fsr:cNS=-2.0,
  isrHardHi isr:cNS=2.0,
  isrHardLo isr:cNS=-2.0
}
```

Note: the soft compensation term may be too conservative especially for ISR
We'd welcome feedback on

Colour Reconnections: Old Paradigm

LC colour flows are good approx for single system of QCD charges…

For a single shower system, coherence / angular ordering ➤ neighbours in colour space tend to also be neighbours in phase space.

LC connections from perturbative stage will tend to produce the **minimal potentials** (cluster/string sizes) for non-perturbative stage. Nature will choose those.

… but must be extended (by CR) when multiple systems are present.

In the presence of MPI (or in ee→WW), partons from different systems (unrelated in LC colour space) can be "close" in phase space. Nature will attempt to make use of non-LC possibilities to minimise the potential energy.

Motivated the **"QCD-inspired"** model in PYTHIA, and in various more or less explicit ways informs most other CR models on the market.

Note that we are here talking about **ambiguities** in colour space, with no explicit **interactions**; transfer of momentum only happens indirectly.

Using a lower value of $\alpha_s(M_Z)$: what happens?

Option 1. Keep 1-loop running ➤ lower value of Λ_{QCD}

Different IR limit of shower ➤ retune (all) non-perturbative parameters.

Problem: lower value of $\alpha_s(M_Z)$ ➤ **lower 3-jet rate**. Cannot tune to data that includes 3-jet events (like inclusive x_B) without separate 3-jet correction; do reweighting for 3-jet rate (or NLO merging).

Or: could use x_B from sample of excl 2-jet events (3-jet veto), but I am not aware that such conditional x_B spectra were measured? Could they be?

Or: if your new $\alpha_s(M_Z)$ value describes LHC jet shapes well, could you constrain r_b *in-situ* from b→B measurements at LHC?

Option 2. Change to 2-loop running ➤ keep Λ_{QCD} ~ unchanged

➤ Reduced need to retune (though **precision** would still require retuning)

(E.g. VINCIA uses CMW with alphaSvalue = 0.118, 2-loop running, and $\mu_R = 0.8 p_T$)

Perturbative stage is important in the context of (re)tuning.

Hard process + showers + merging: **$b(Q_F) \to b(Q_{cut})$**

Non-perturbative parameters (HAD+MPI+CR): **$b(Q_{cut}) \to B$**

These two components **scale differently**. Non-universal to force the latter to make up for shortcomings in the former.

At LEP, amount of perturbative radiation emitted from *b* can be validated / controlled by 3-jet rate *(in b-tagged events)*

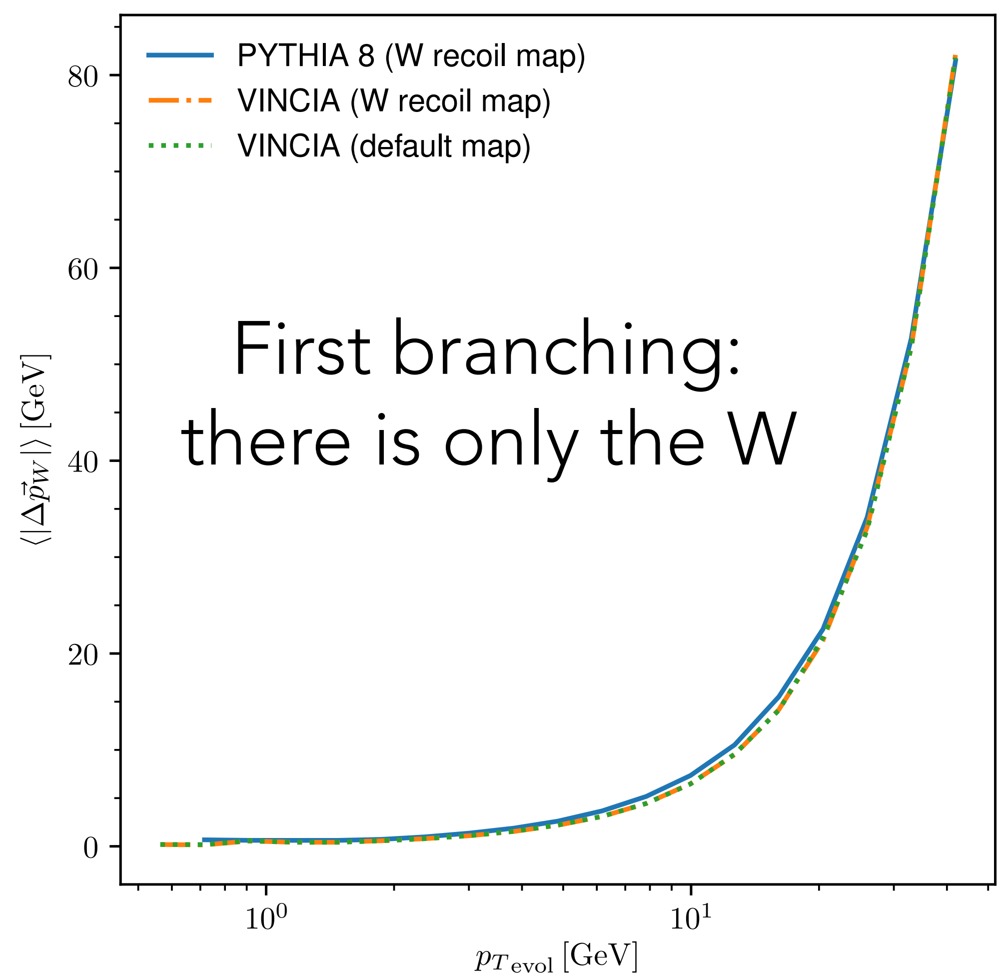
In top events, presumably *b*-jet substructure and/or rate of additional jets "near" the *b*-jet can be used to check if the b is losing the "right" amount of energy from perturbative radiation?

Constrain r_b in-situ? x_B spectra in inclusive *b* jets?

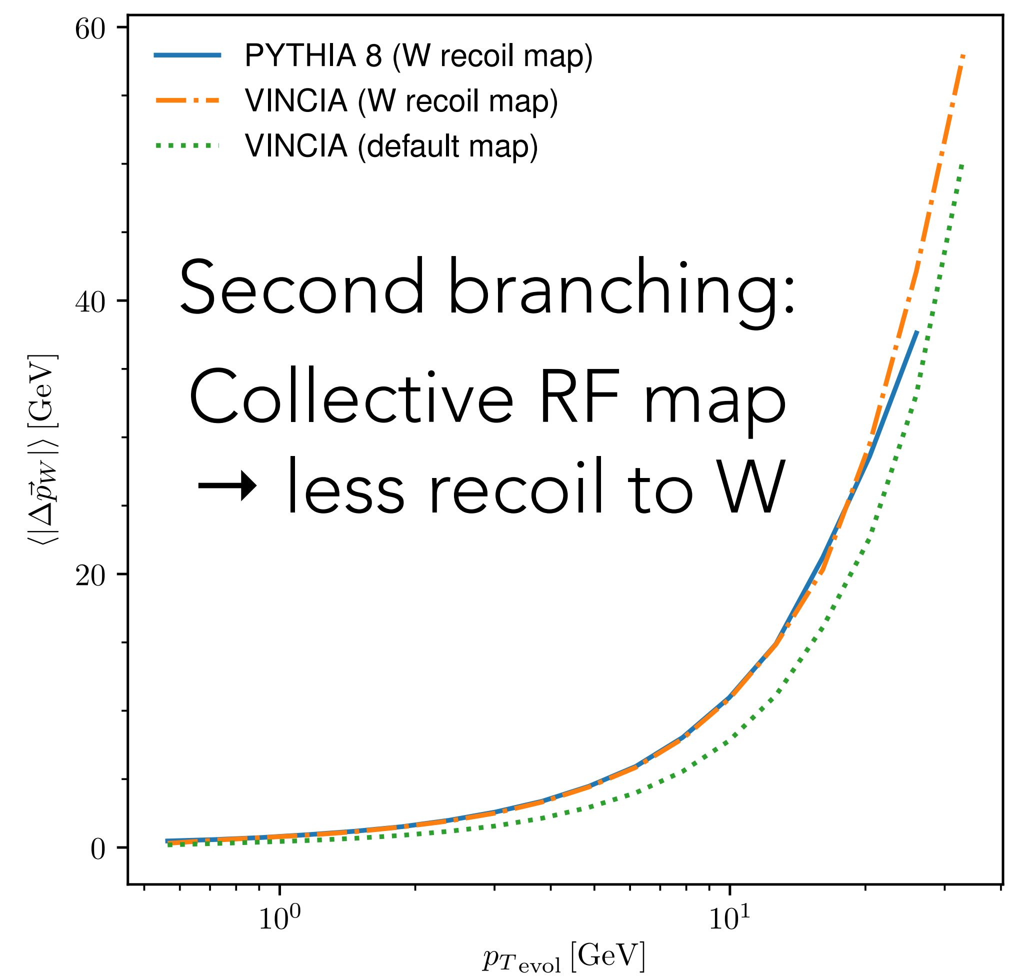
Lesson from LEP: process-dependent factors (eg NLO 3-jet rate) can affect precision tuning ➤ larger uncertainties if not carefully controlled.

Consider average recoil $|\Delta\vec{p}_W|$, after first and second emission(s).

Recoil after first:

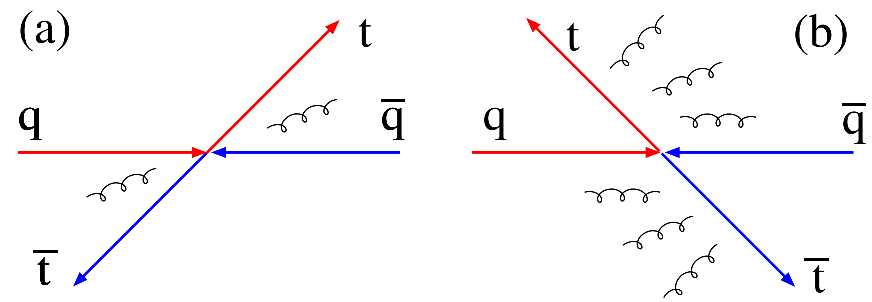


Recoil after second:



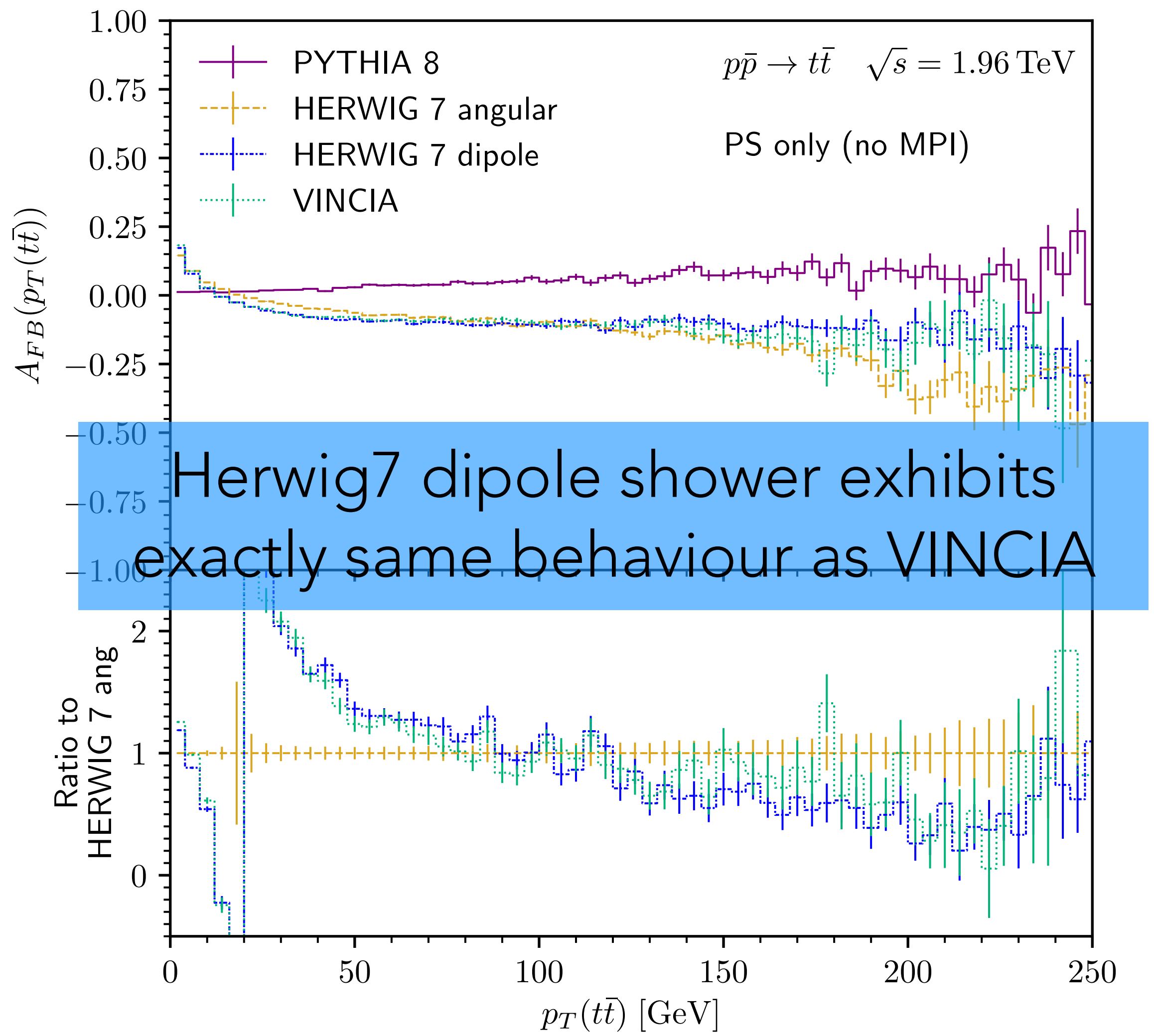
(Coherence In Production)

Well-studied effect in p-pbar collisions
Top quark FB asymmetry



PS, Webber, Winter JHEP 1207 (2012) 151

Coherent showers produce a p_T-dependent asymmetry



Herwig7 dipole shower exhibits exactly same behaviour as VINCIA

Forward-backwards asymmetry:

$$A_{FB}(\mathcal{O}) = \frac{\left.\frac{d\sigma}{d\mathcal{O}}\right|_{\Delta y>0} - \left.\frac{d\sigma}{d\mathcal{O}}\right|_{\Delta y<0}}{\left.\frac{d\sigma}{d\mathcal{O}}\right|_{\Delta y>0} + \left.\frac{d\sigma}{d\mathcal{O}}\right|_{\Delta y<0}}$$

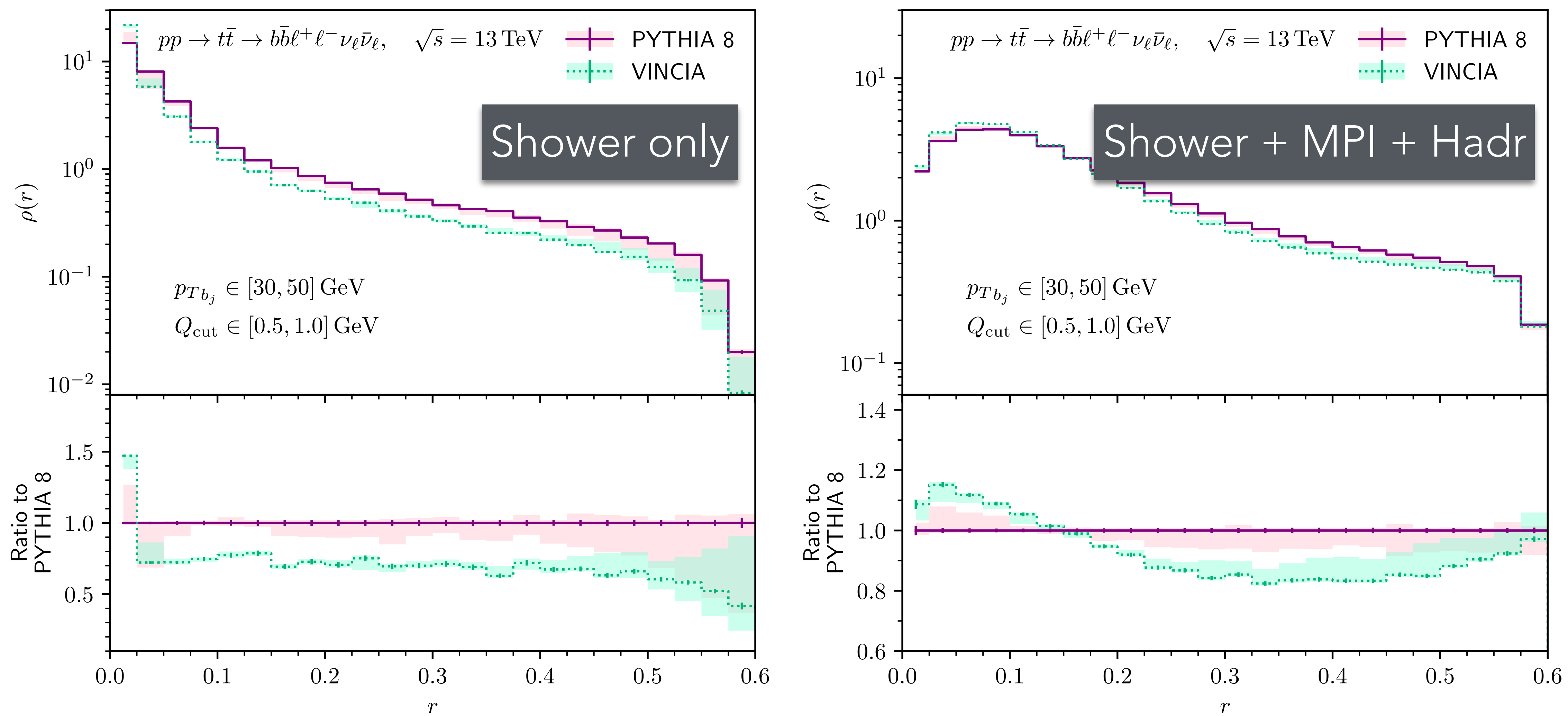
Coherent showers include part of the real emission correction that generates a FB asymmetry that becomes negative for large $p_T(t\bar{t})$. [1205.1466]

B-Jet Profiles

VINCIA gives narrower b-jets than Pythia 8

Effect survives MPI + hadronisation

Differential jet shape ρ(r)



Tentative conclusion: more coherence ~ more wide-angle suppression?

*Also agrees with intuition from dipole language where "top dipole" can be negative

Top Mass Profile @ 8 TeV : Parton Level

Slide from H. Brooks

Brooks, Skands, Phys.Rev. D100 (2019) no.7, 076006 ARXIV:1907.08980

$p\bar{p} \to t\bar{t}$ @ 8 TeV: $m_{b_j \ell \nu}$

Monte-Carlo "truth" (parton-level) analysis:

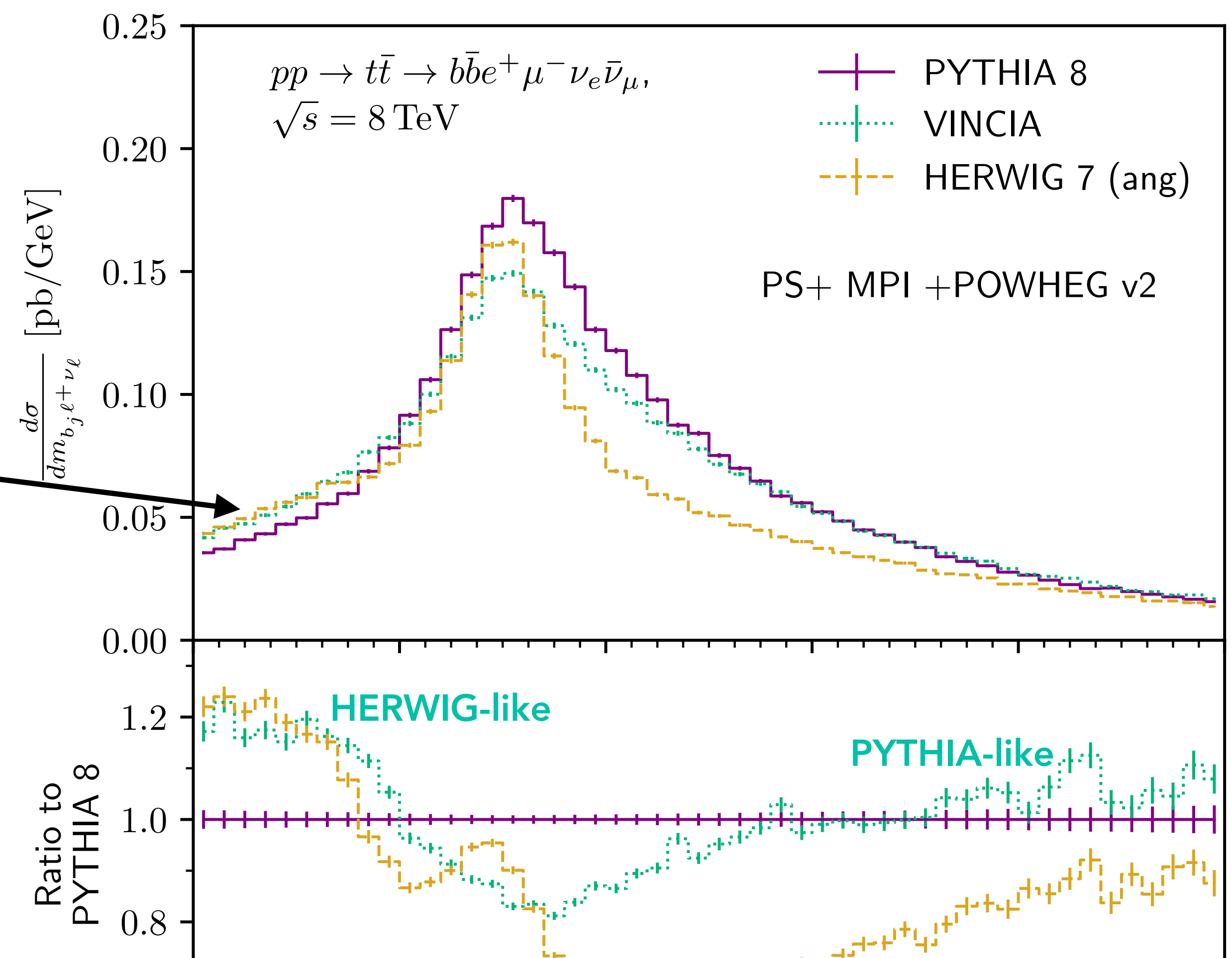
- Assumes we can reconstruct p_ν and match correct ℓ, b_j pair.

Pythia has little population in the low tail. Ascribed to an artificially small phase space (due to a non-coloured dipole) from the 2nd emission onwards.

Many subtleties related to this, especially when combined with POWHEG.

Commented on and illustrated extensively in arXiv:1907.08980

"Cured" in VINCIA.



WARNING

Parton Level

VINCIA

~ HERWIG-like below m_t

~ PYTHIA-like above m_t

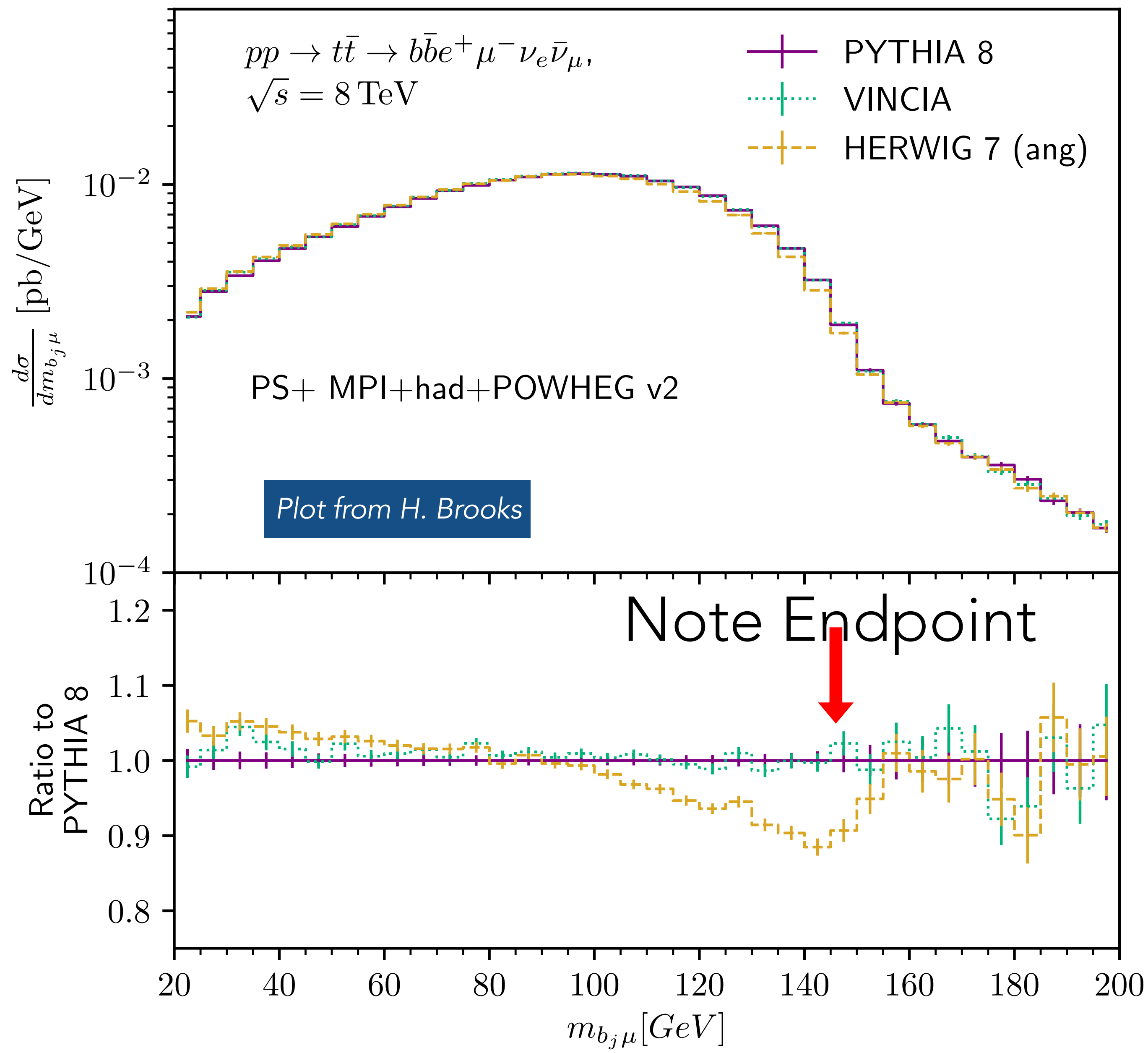
PYTHIA 8.301 released. Includes VINCIA with new resonance-final showers

Not yet recommended for main production runs, but need your feedback.

Still to come in VINCIA: multi-leg MECs, automated uncertainty bands, production-decay interference, electroweak showers, NLO antenna functions,…

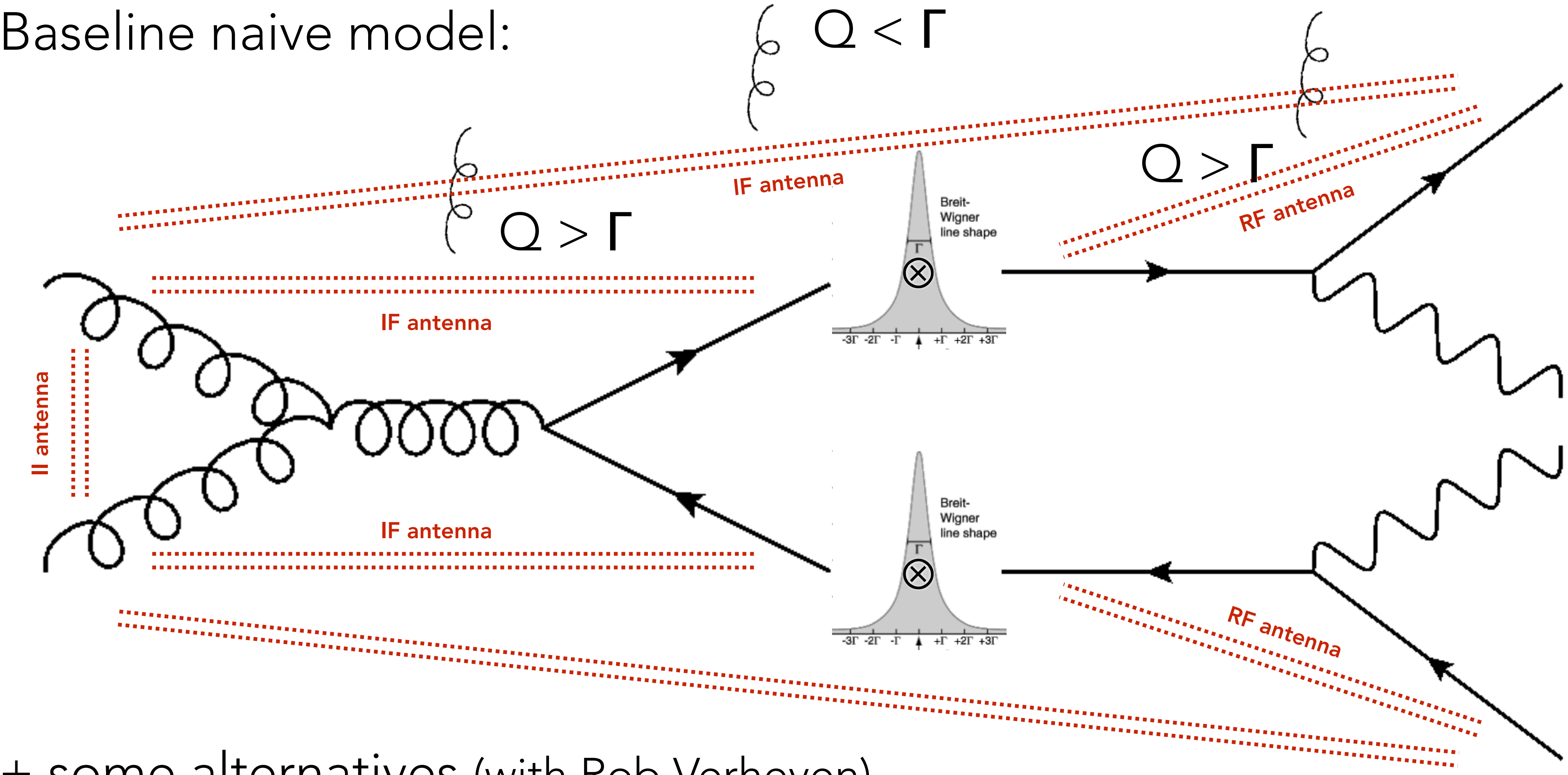
$p\bar{p} \to t\bar{t}$ @ 8 TeV: $m_{b_j\mu}$ (example of a realistic observable)

Full hadron-level analysis: choose pairing for ℓ, b_j that minimise average mass.



Finite-width effects

Baseline naive model:



+ some alternatives (with Rob Verheyen)

Note: we do not expect these effects to be large for top decays, cf e.g., Khoze & Sjöstrand Phys.Lett. B328 (1994) 466-476

Shower Architectures

Table from H. Brooks

Type	Singularities		Coherence?	No dead zones?	Examples
	soft	collinear			
DGLAP	part.	full	✗	✗	
Angular	full+veto	full+veto	✓	✗	H7 $\tilde{q}$
Dipole	part.	part.	✗	✓	Pythia 8
C-S	part.	part.	✓	✓	Sherpa, H7 dip
Antenna (global)	full	part.	✓	✓	Vincia
Antenna (sector)	full	full+veto	✓	✓	Vincia

Sum over all dipoles / antennae should reproduce the leading log