Shower & Hadronisation Uncertainties for Precision Top Physics

Peter Skands (Monash U)

Scale Variations: How big and how correlated?

 \rightarrow 7-point variations, with (conservative) soft compensation terms Provided automatically as vector of event weights?

ME Corrections

Estimating sensitivity to process-specific non-singular terms

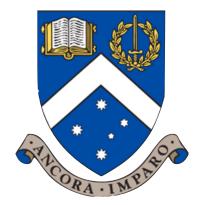
Alternative Shower Models?

Relevant variations in baseline PYTHIA + Status of DIRE and VINCIA

Colour Reconnections

Interesting physics & annoying complication: proposals for top

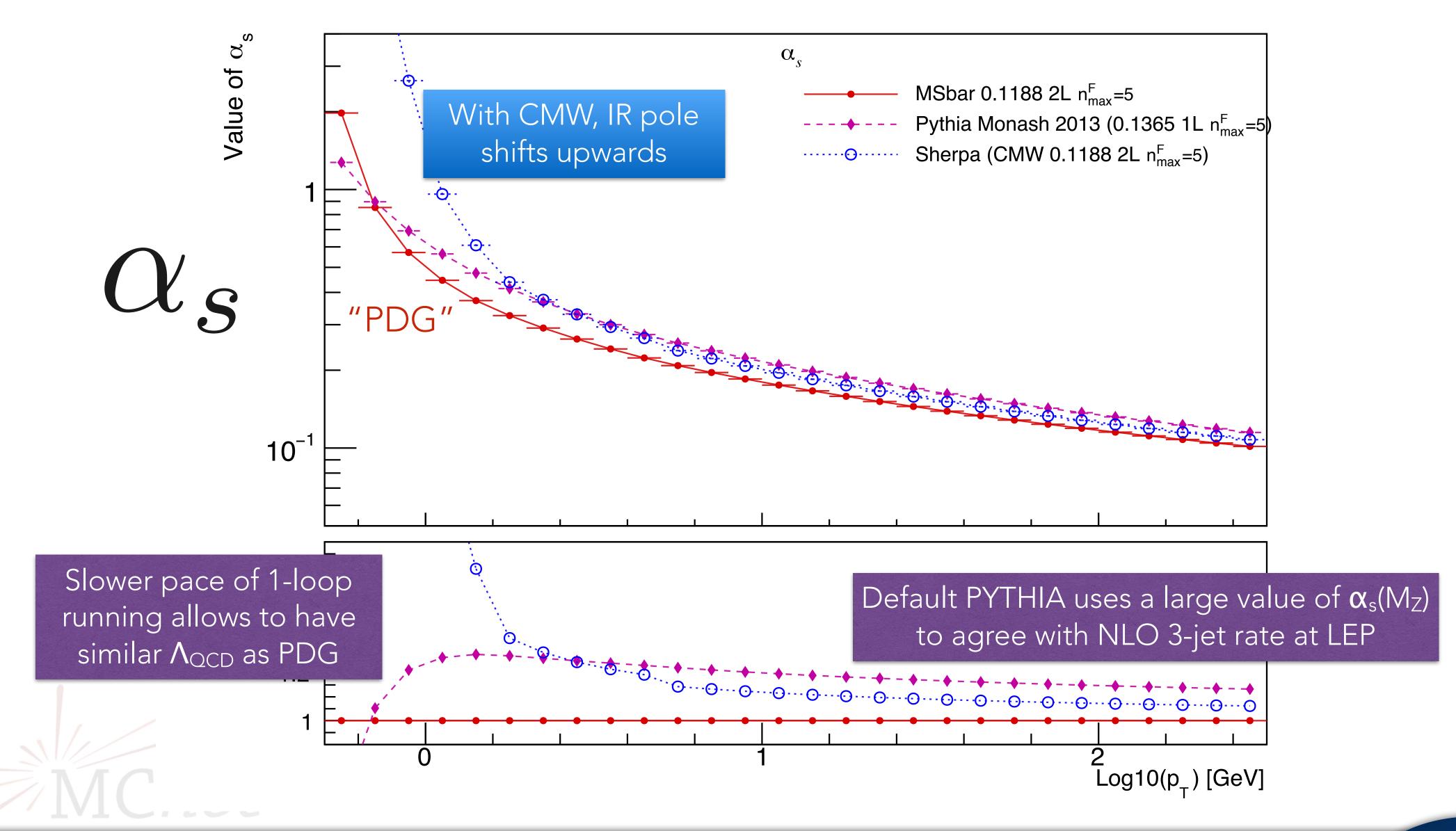
(+ Ambiguity of MC mass definition?)







NOTE ON DIFFERENT ALPHA(S) CHOICES



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SCALE VARIATIONS: HOW BIG?

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

$$\frac{\alpha_s(k_1^2\mu^2)}{\alpha_s(k_2^2\mu^2)} \sim 1 - b_0 \ln(k_1^2/k_2^2) \alpha_s(\mu^2) \leftarrow \begin{array}{l} \text{Proportionality to } \alpha_s(\mu) \Longrightarrow \text{can get a (misleadingly?) small band if you choose central } \mu \text{ scale very large.} \\ \text{E.g., some calculations use } \mu \sim \text{H}_\text{T} \sim \text{largest scale in event ?!} \\ \text{Worth keeping in mind when considering (uncertainty on) central } \mu \text{ choice} \\ \text{Worth keeping in mind when considering (uncertainty on) central } \mu \text{ choice} \\ \text{Results of the proportionality to } \alpha_s(\mu) \Longrightarrow \text{can get a (misleadingly?) small band if you choose central } \mu \text{ scale very large.} \\ \text{E.g., some calculations use } \mu \sim \text{H}_\text{T} \sim \text{largest scale in event ?!} \\ \text{Worth keeping in mind when considering (uncertainty on) central } \mu \text{ choice} \\ \text{Results of the proportionality to } \alpha_s(\mu) \Longrightarrow \text{can get a (misleadingly?) small band if you choose central } \mu \text{ scale very large.} \\ \text{E.g., some calculations use } \mu \sim \text{H}_\text{T} \sim \text{largest scale in event ?!} \\ \text{Worth keeping in mind when considering (uncertainty on) central } \mu \text{ choice} \\ \text{Results of } \mu \sim 0.65 \pm 0.07$$

Expansion around µ only sensible if this stays ≤ 1

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

 \rightarrow 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): $k \sim [0.5, 1, 2]$

Note: In PYTHIA you specify k²

TimeShower:renormMultFac SpaceShower:renormMultFac

SCALE VARIATIONS: HOW BIG?

What do parton showers do?

In principle, LO shower kernels proportional to α_{s}

Naively: do the analogous 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
 - \rightarrow 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.]
 - 0.03 (Somewhat In-dependent). [mough there are many ways to skin that cat, see hext sindes.
 - 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 <u>mcplots.cern.ch</u>

SCALE VARIATIONS: HOW BIG?

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

Sure ... but still somewhat arbitrary

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

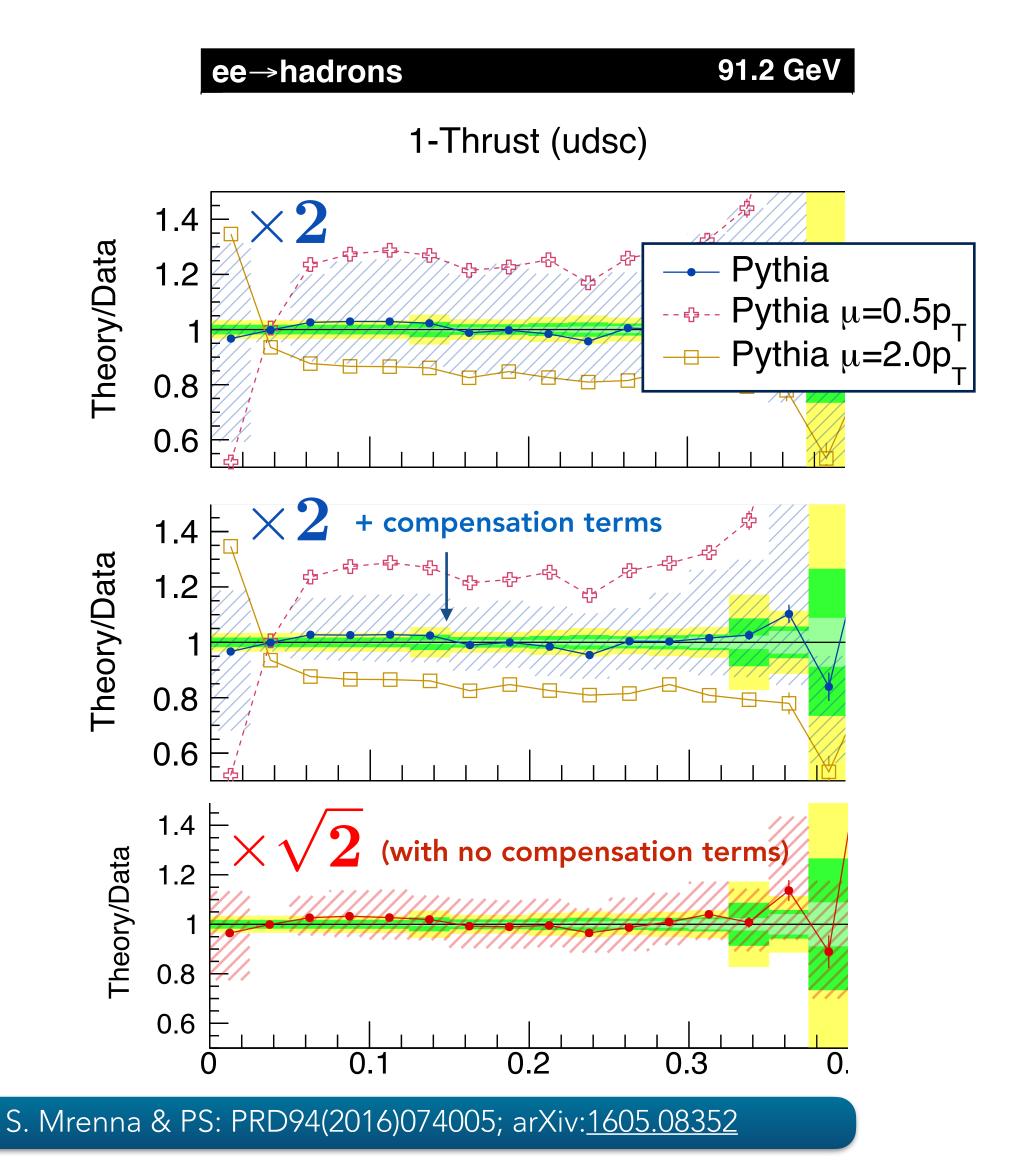
Still allowing full factor-2 outside that limit.

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

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

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

$$P'(t,z) = \frac{\alpha_s(kp_\perp)}{2\pi} \left(1 + (1-\zeta)\frac{\alpha_s(\mu_{\max})}{2\pi}\beta_0 \ln k\right) \frac{P(z)}{t}$$
 Small absolute size of compensation outside the soft limit
$$\zeta = \begin{cases} z & \text{for splittings with a } 1/z \text{ singularity} \\ 1-z & \text{for splittings with a } 1/(1-z) \text{ singularity} \\ \min(z,1-z) & \text{for splittings with a } 1/(z(1-z)) \text{ singularity} \end{cases}$$



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HOW TO TEST IF "MORE" ME CORRECTIONS NEEDED?

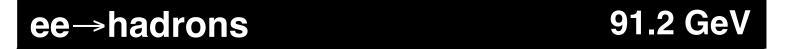
The soft and collinear enhanced (singular) terms in the shower kernels are universal, process-independent

Matrix Elements contain the same information, plus process-specific **non-singular** terms.

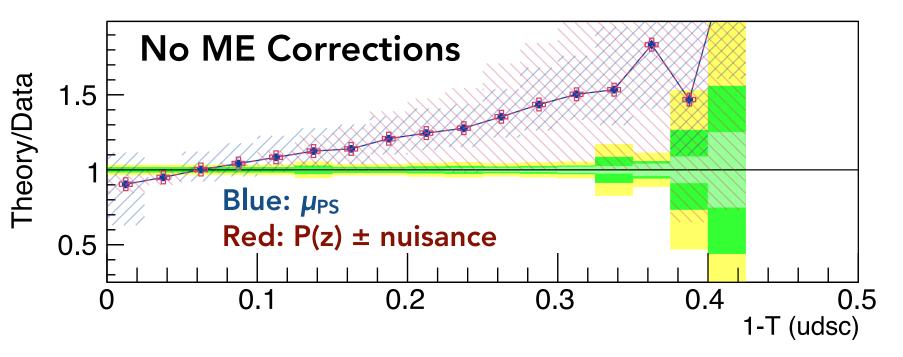
The shower singularities dominate for soft and collinear radiation

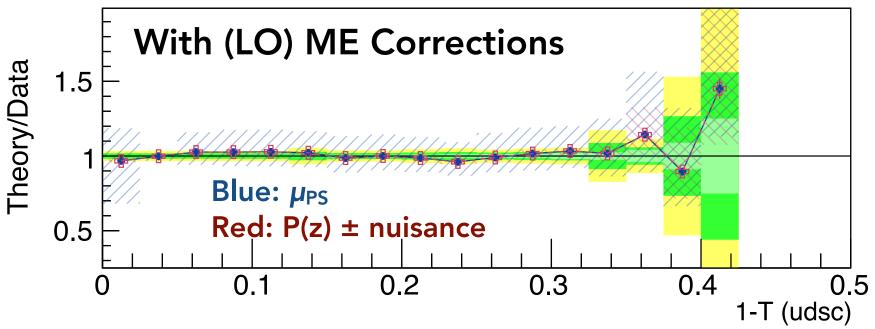
The process-specific non-singular terms dominate for hard radiation

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



1-Thrust (udsc)





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

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

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

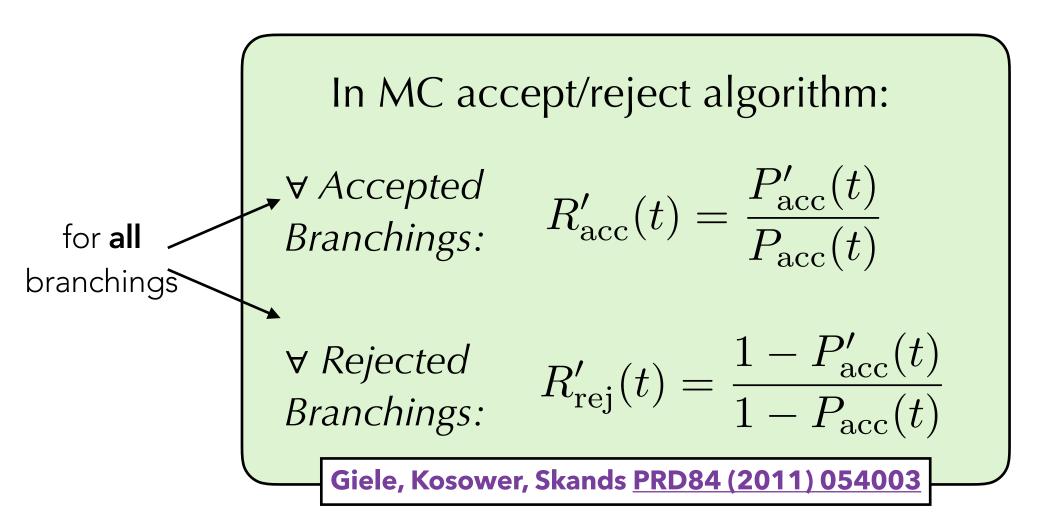
AUTOMATED SHOWER UNCERTAINTY BANDS/WEIGHTS

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, ...?

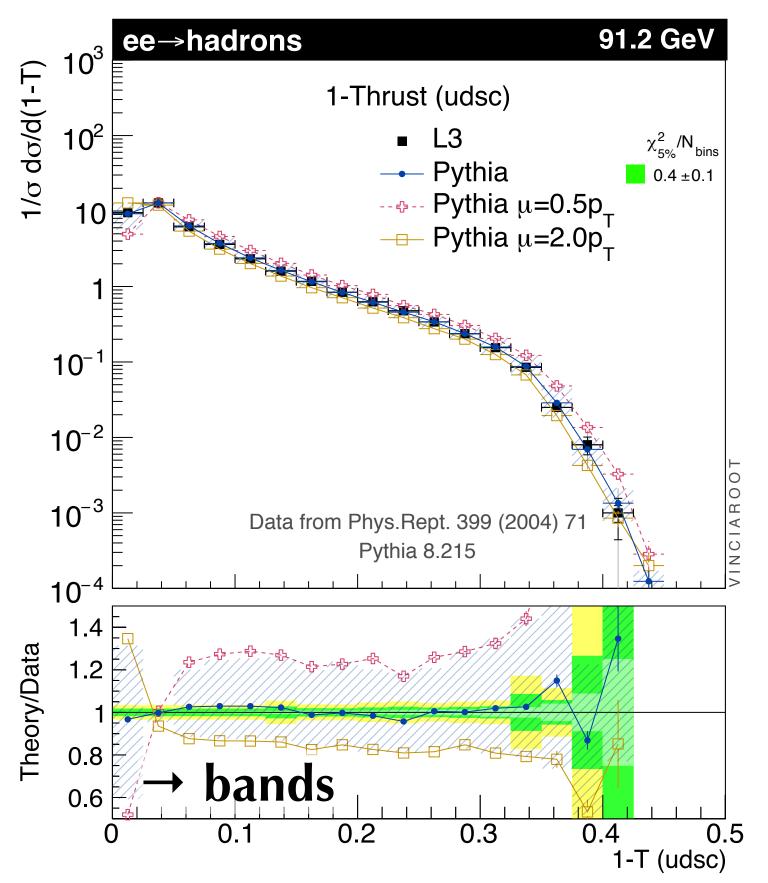
Easy to calculate reweighting factors



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)

0.0

0.6

1/o do/d(1-1

10

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 = 1).

(Improvements may be possible by combining with bias.)

(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 HT. HARD ISR -> NJETS.

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):

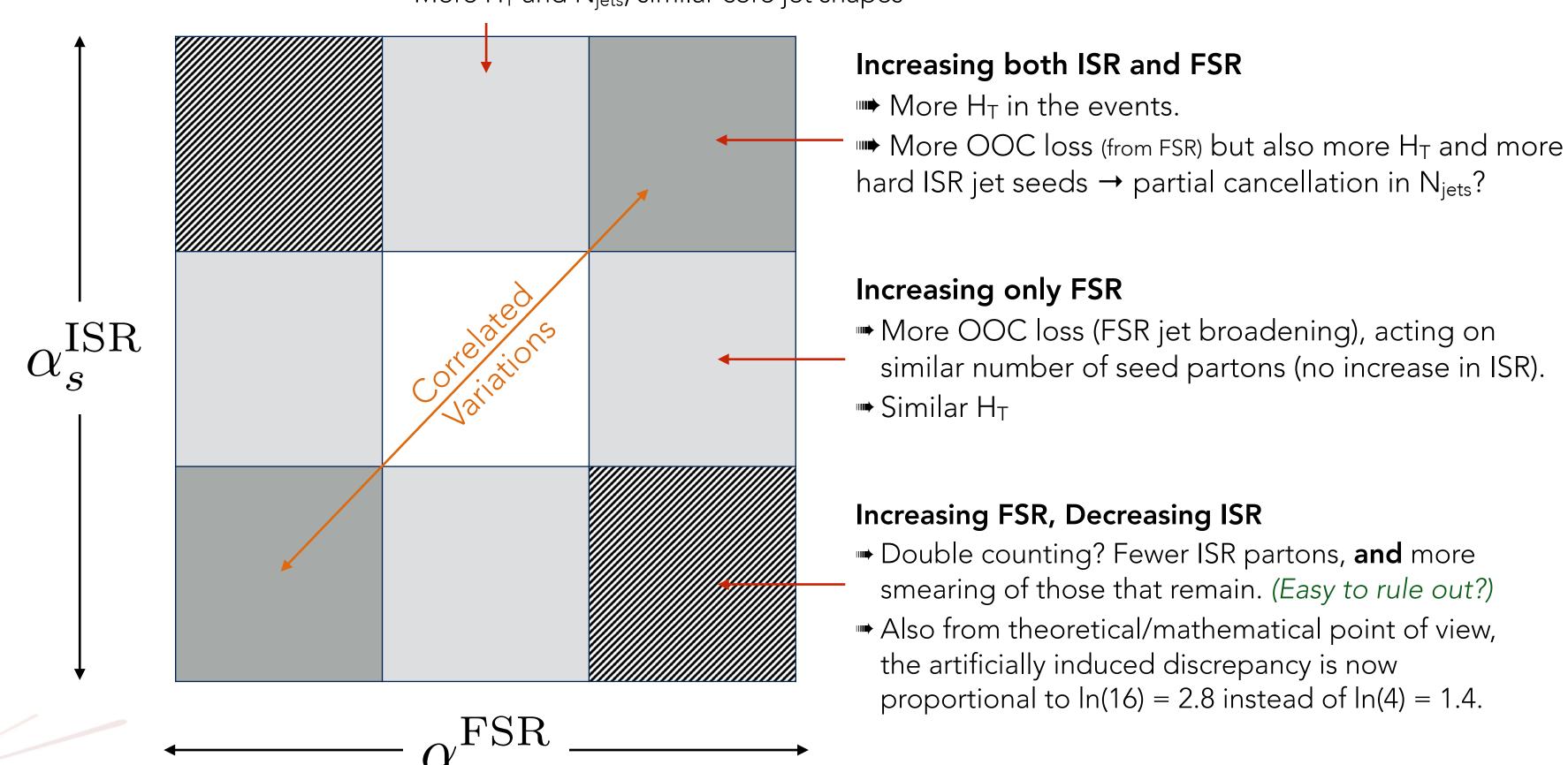
PDFs, functional form of central choices of factorisation and renormalisation scales, nonsingular parameters, subleading colour, local vs global recoils ...

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



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 corrections)

```
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,
                                                Note: the soft compensation term
  fsrHardLo fsr:cNS=-2.0,
                                                    may be too conservative
  isrHardHi isr:cNS=2.0,
                                                        especially for ISR
  isrHardLo isr:cNS=-2.0
                                                We'd welcome feedback on that.
```

WHICH PARTON SHOWER MODELS?

Baseline PYTHIA 8.2 / Monash 2013 Tune

PS: some indications that central choices for alphaS values are a bit high)

DGLAP-based parton shower, with local colour-dipole style recoils for FSR and global recoils for ISR

Not fully coherent for initial-final colour connections

SpaceShower:dipoleRecoils = on switches to more dipole/antenna-like (coherent) IF treatment, at the cost of local recoils for ISR.

There is also an option for global FSR recoils: TimeShower:globalRecoil

HERWIG

PETER SKANDS

Intrinsically coherent (angular-ordered), with global recoils (and spin correlations); quite complementary to baseline PYTHIA.

Challenging to disentangle shower effects vs cluster hadronisation effects

WHICH PARTON SHOWER MODELS?



VINCIA

Based on **QCD antennae**: combines intrinsically **coherent soft** radiation + **DGLAP limits for collinear** radiation.

Local dipole recoils.

Sophisticated treatment of quark mass effects now being reimplemented: arXiv:1108.6172

Semi-automated multi-leg ME corrections for both production and decays: arXiv:1605.06142

Helen Brooks (post doc at Monash U) currently working specifically on a new antenna-based approach to radiation in top decays

Expect news in ~ few months.

(Some elements in common with new HERWIG treatment: arXiv:1810.06493)

Main target beyond top: NLO-corrected antenna functions: arXiv:1611.00013

DIRE

Based on (Catani-Seymour style) **dipoles**: also combines coherent soft radiation + DGLAP limits for collinear radiation. Includes eikonal mass corrections.

Status: Ready for top physics (+ also here ongoing work towards NLO kernels)

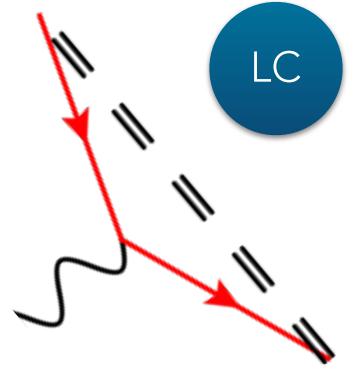
2019: Both models to be integrated into into baseline PYTHIA.

COLOUR RECONNECTIONS

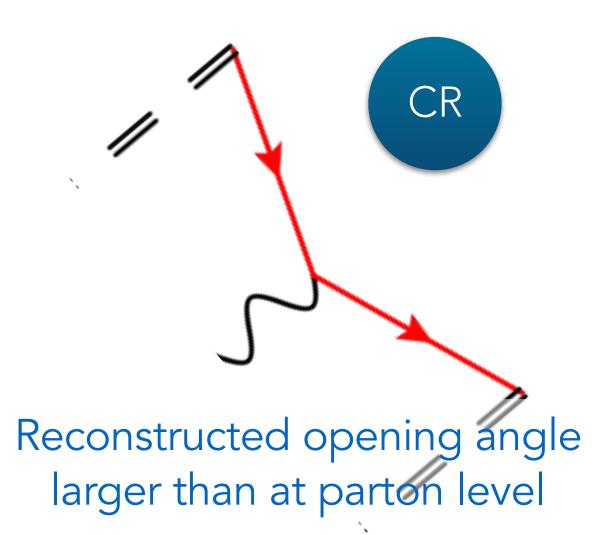
CR appears to be required to describe soft effects in pp

The basic effect on jets is 'string drag'

Simple example:
Jets from hadronic
W decay



Reconstructed opening angle smaller than at parton level



Invariant mass reconstruction highly sensitive to opening angle

We believe the effect becomes more important the more activity there is in the event (more colour kicked around; more multiparton interactions)

Could be indicated by dependence of reconstructed top mass on UE level



CR MODELS IN PYTHIA

"MPI-based scheme" (default PYTHIA / Monash 2013 model)

Has single "range" parameter. Definitely not exhausting the modelling space.

The "newer scheme"

Christiansen & PS, String Formation Beyond Leading Colour, arXiv:1505.01681

Stochastically allows random "colour-anticolour" pairings according to $\sim SU(3)_C$ weights; chooses the one with minimal string length. I consider it ~ realistic;

Predicts quite small effects at LEP, and presumably also rather small effects in top

The "Gluon move scheme" Argyropoulos & Sjöstrand, Effects of CR on tt final states at LHC, arXiv:1407.6653

Moves gluons between string pieces; can be tweaked a lot - to minimise or even maximise string length measure.

Partly devised to allow for devil's advocate uncertainty estimates to gauge 'maximal possible effect' in tt. Can produce very large effects up to $\Delta m_t \sim 1$ GeV.

+ Ongoing active research on colour ⊗ strangeness ⊗ momentum space

Lund group (Bierlich, Gustafson, Lönnblad): "Rope Model" with "shoving" Monash group (Duncan, PS): "Simplified Vortex Line Model" + repulsion

EARLY OR LATE RESONANCE DECAYS?

Top width ~ 1.5 GeV close to hadronisation scale: hadronisation already close to happening by time of top decays

Personally I don't think top decay products are much affected

+ Top boosts + high momenta of ejected topdecay debris → presumably only relatively soft hadrons from a tail of ~ slow / early top decays could be affected

→ **Default** is early resonance decays off
Secondary question: could there be CR **inside** top
decay system? LEP studies indicate not much

But we haven't **proved** it. (Nor have you?)

→ constraining CR in top?

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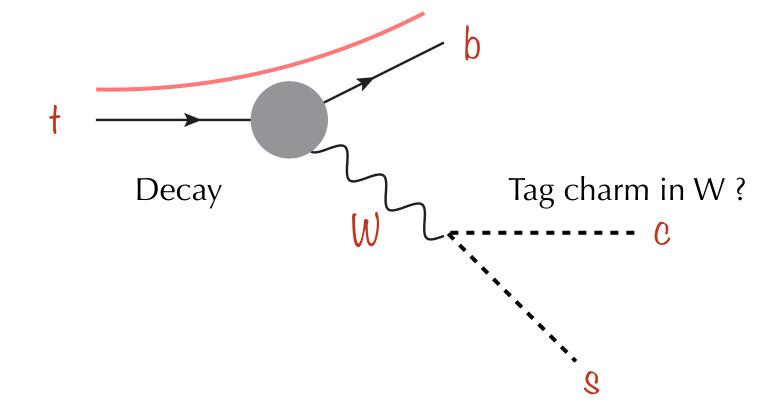
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Does B hadron spectrum depend on level of UE? On p_{TB} ? B_s/B ratio?

How about **hadrons in the b jet**? Are some of its softer hadrons affected? (Rapidity along the b-jet? p_T with respect to that axis?)

Can **D**(*) **fragmentation** spectra be measured in W → cs?

How about the other hadrons in the W jets?

Some related ideas/inspiration (not top-specific) may be found in arXiv:1603.05298

NOTE ON TOP MASS DEFINITION

Can define m_t in many ways

Pole mass, MSbar mass (at a high or low μ), 1S mass, MSR mass, ...

Which one do we (you) measure?

Measurements are calibrated to MC: effectively an "MC mass" is measured.

Jokingly called the PMAS(6,1) mass (in reference to F77 PYTHIA)

From the naive MC perspective this looks like a pole mass

Nason has formulated a series of well-considered arguments that it is indeed the pole mass, up to an ambiguity ≤ 100 MeV.

Nason: The Top Mass in Hadronic Collisions arXiv:1712.02796, + arXiv:1801.04826, 1801.03944

+ Recently (Oct 25): Ravasio, Nason, Oleari: arXiv:1810.10931, on renormalon and finite-width effects, short-distance vs pole masses.

However:

There is still a **debate** going on, and I have great respect for all of the involved people. Hoang et al argue that the ambiguity is ~ 250 MeV. [e.g, arXiv:0808.0222, arXiv:1706.08526]

Recent: arXiv:1807.06617 considered change of pole mass caused by HERWIG shower IR cutoff.

Found ~ 300 MeV and suggests ways of circumventing use of pole mass entirely.

(Still not clear to me if/how combination with well-tuned hadronisation model changes this.)

... You can disagree but at the very least I must admit I am still confused.

SUMMARY

ISR and FSR uncertainties have distinct meanings, despite some ambiguous cases: would vary them separately.

In principle, one could vary $g \rightarrow qq$ modelling separately as well ...

But I believe this is subdominant.

And/or independent variations for each shower branching

E.g., up for first emission, down for second. Little explored so far.

Recommend 7-point factor-2 variations with soft compensation terms

Nonsingular-term variations can indicate potential size of ME terms

CR & nonperturbative effects

At Tevatron, theoretical status reevaluated when $\Delta m_t \sim 1$ GeV reached.

CR toy models developed and used. Sufficient to explore uncertainties at that level.

At LHC: now reaching for $\Delta m_t \sim \Lambda_{QCD}$; Lots of dynamics at that scale. (Much still unknown.)

Devise and measure CR / fragmentation sensitive observables in situ. Publish / Rivet.

Explore broad range of CR models and rule (some of) them out. Publish / Rivet.

STILL NOT SURE WHAT TO SAY ABOUT PMAS (6,1) [SORRY, FLORENCIA]

Extra Material

OUR REFERENCE PROCESSES

Dijets

Jet Shapes

Substructure

Azimuth Decorr.

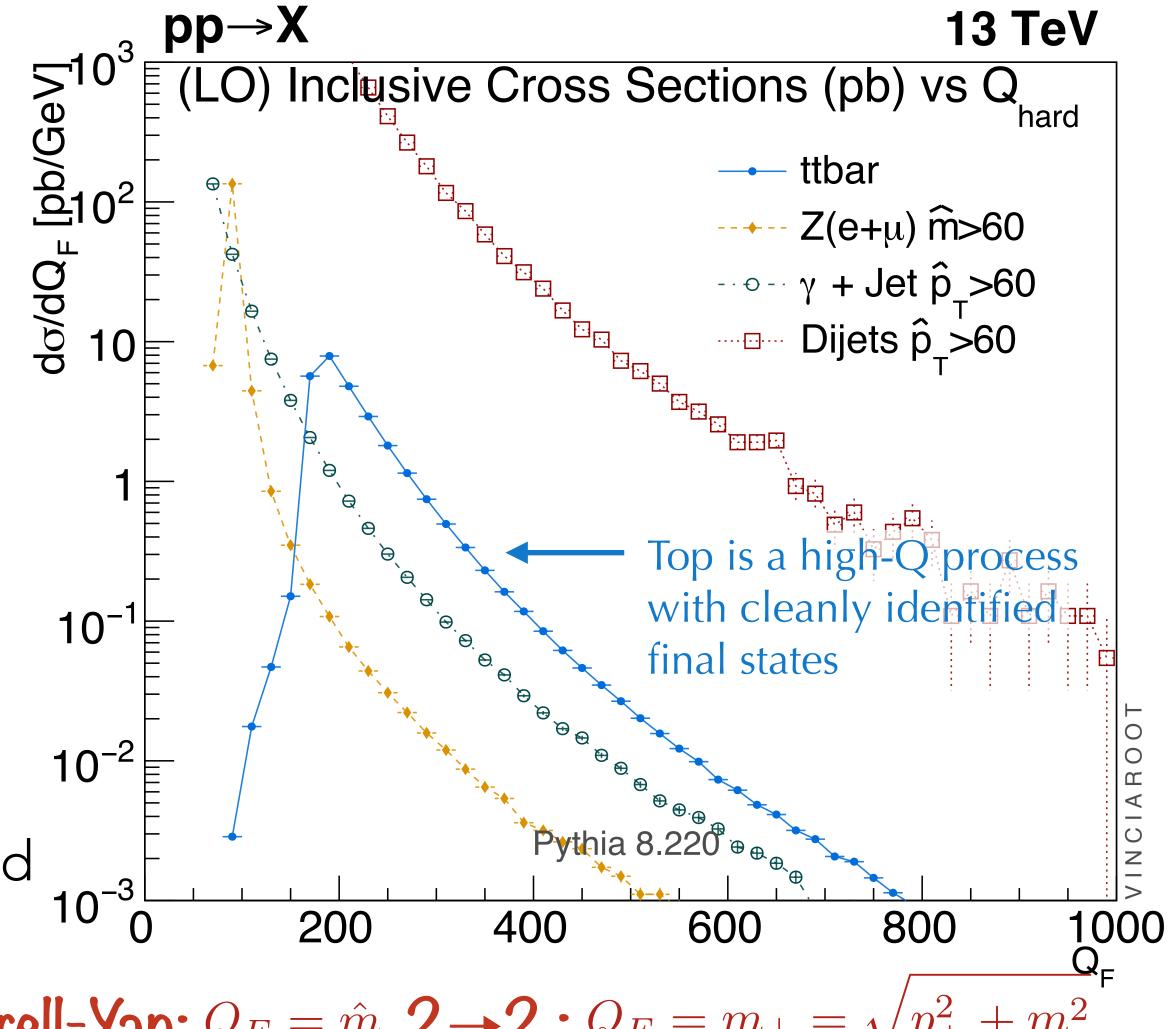
Gamma+Jet

JES Calibration

Drell-Yan

ISR with well-defined Q_F scale

Off resonance: extend to higher Q²

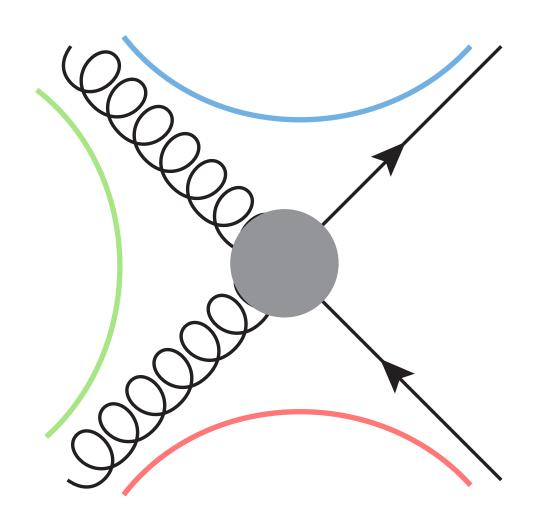


Scales in PYTHIA: Drell-Yan: $Q_F = \hat{m}$ 2-2: $Q_F = m_\perp = \sqrt{p_\perp^2 + m^2}$

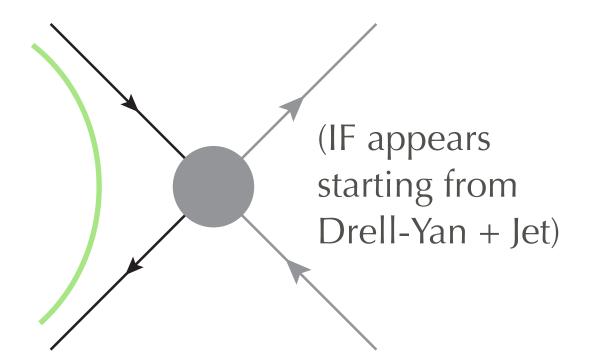
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TOP: PRODUCTION

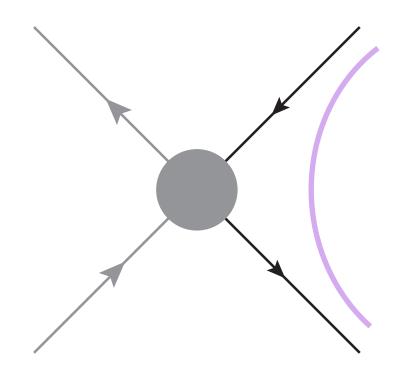
Importantly, top production involves Initial-Final colour flows



Not present in main ISR shower constraint: Drell-Yan



Not present in main FSR shower constraint: LEP



Expect strong dependence on top boosts

At threshold: no radiation from tops (only initial-state ends active)

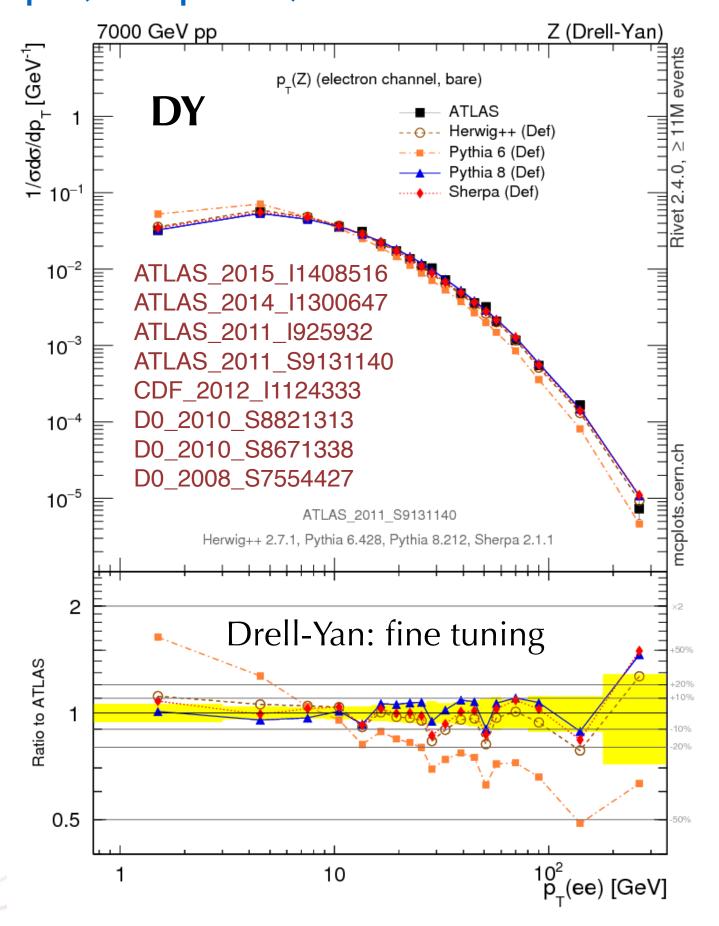
At high boosts: soft & quasi-collinear enhancements from tops

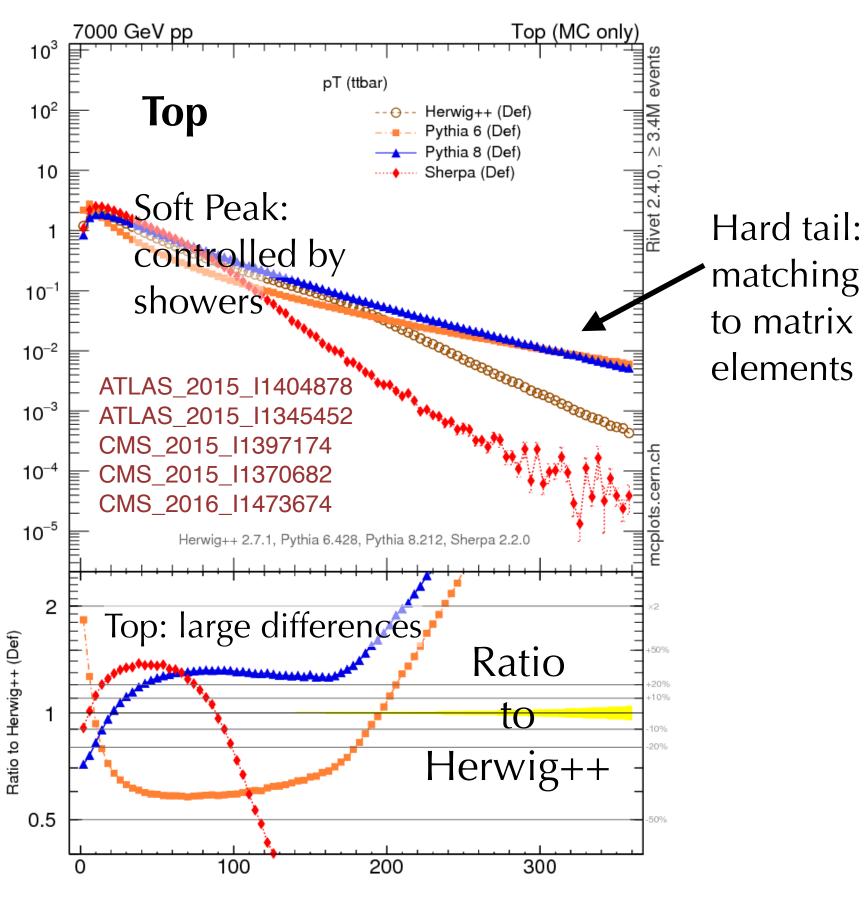
IF present in γ +Jet and Dijets as well (without mass/boost effect)

ttbar Jet Pull Angle: ATLAS_2015_I1376945

P_T(TTBAR) (& RELATED MEASUREMENTS)

Tests initial-state side of radiation in association with production, similarly to p_T (dilepton) in Drell-Yan

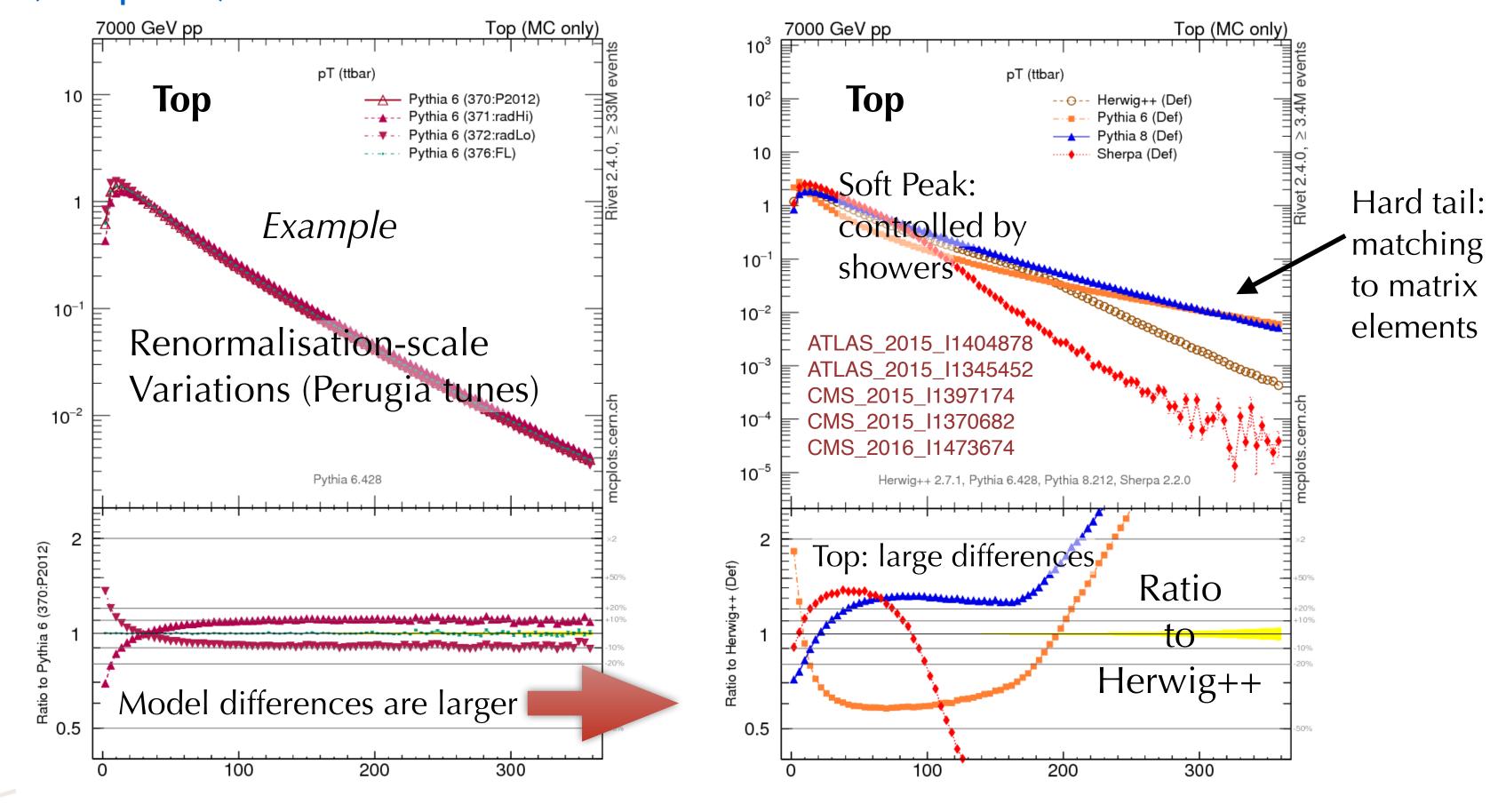




Would be nice to get these top measurements onto mcplots.cern.ch

UNCERTAINTIES

Tests initial-state side of radiation in association with production, similarly to p_T (dilepton) in Drell-Yan



Would be nice to get these top measurements onto mcplots.cern.ch

WHAT CAUSES THESE DIFFERENCES?

Suspect significant differences from alphaStrong choices (both central values and scales);

Could be (has been?) checked/validated

Treatment of Phase Space (and coherence conditions) for Initial-Final dipoles; e.g., PYTHIA 8 currently has "non-coherent" starting condition for QCD processes

See e.g., <u>arXiv:1205.1466</u>

Matching to hard region ←→ soft region via unitarity

See e.g., <u>arXiv:1003.2384</u>

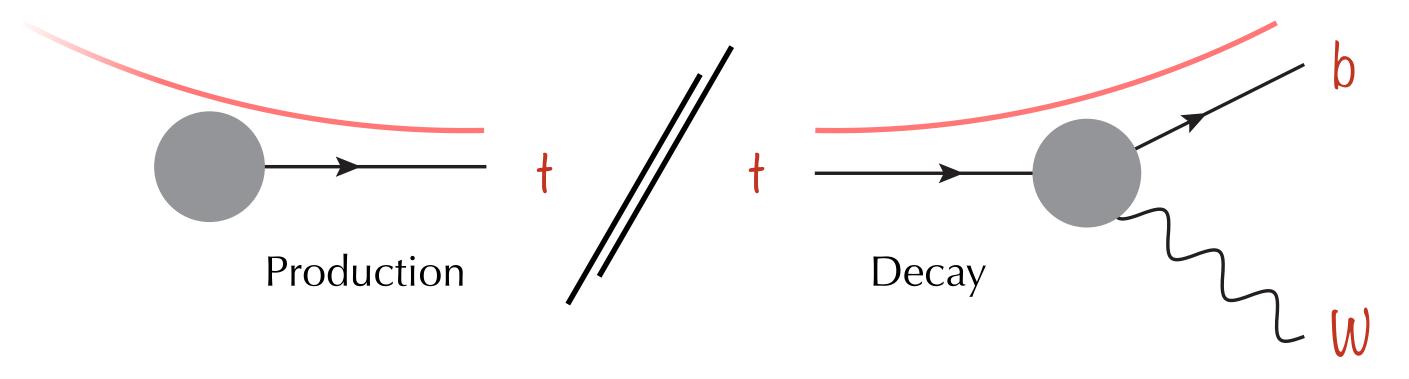
Recoil Strategies

Model differences should ideally be reduced/resolved by showers beyond LL ... work in progress. In short term: constraints + pheno + tuning

TOP DECAY

Unique: decay of a (very) massive coloured particle

Will be the go-to reference case for a lot of BSM cases



Is use of narrow-width approximation justified?

(Some ME generators allow to go beyond)

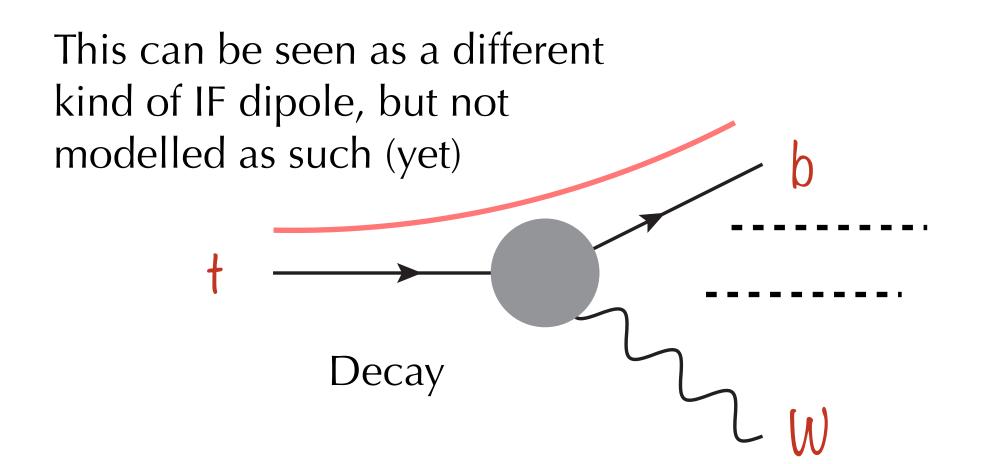
Expect cross talk for scales below $\Gamma_{top} \sim 1.5$ GeV; essentially no **perturbative** overlap

Keep in mind though, that in a generator like PYTHIA, we also average over the polarisations in the intermediate step, so any ttbar spin correlations are washed out

TOP DECAY

Unique: decay of a (very) massive coloured particle

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In PYTHIA, the b end of a fictitious bW dipole emits; equivalent to IF setup for first emission but not for subsequent ones

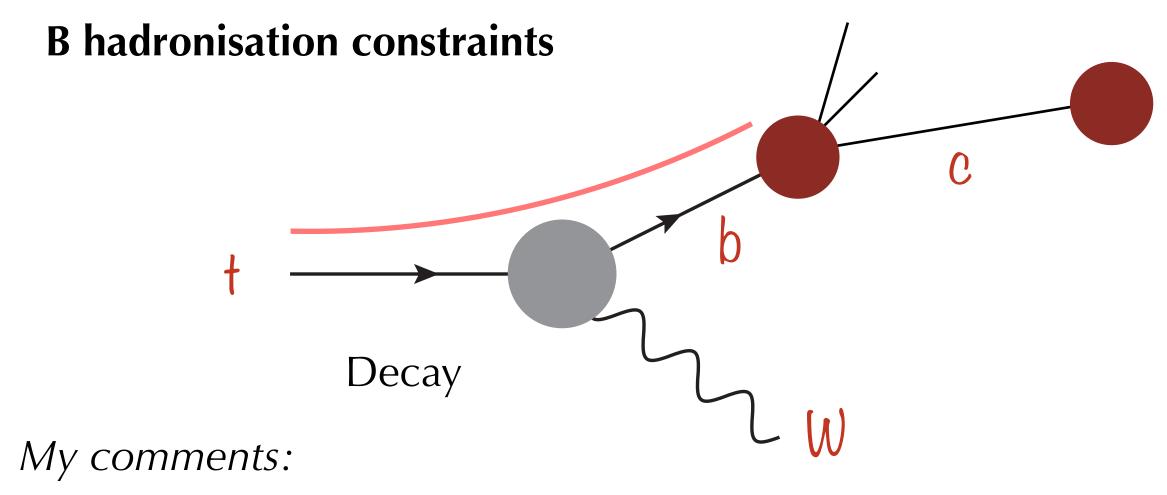
Importantly, this preserves bW invariant mass (i.e., top Breit-Wigner) But would expect recoil effects wrong/exaggerated to some extent inside the b-gluon-W system. *Develop experimental / in-situ cross checks of structure?*

Solution: now working (with S. Mrenna) on an antenna-based (IF) model for radiation in decays of massive resonances. But this will take time.

TOP DECAY

Unique: decay of a (very) massive coloured particle

Will be the go-to reference case for a lot of BSM cases



- **b fragmentation** in principle well constrained by LEP & SLD measurements; some tension between the two, may now have been resolved? Rivet 2.5.2 update includes: OPAL_2003_I599181 "Inclusive analysis of the b quark fragmentation function in Z decays" & modified DELPHI_2011_I890503, but have not yet propagated to tunes: should be checked)
- In pp, the b quark is connected to the initial state, and is embedded in the UE (is lifetime + boost from top enough to escape (most of) CR? Compare with incl b jets?)