LHC EWWG — 10th July 2024

MC Tuning Prospects in ATLAS

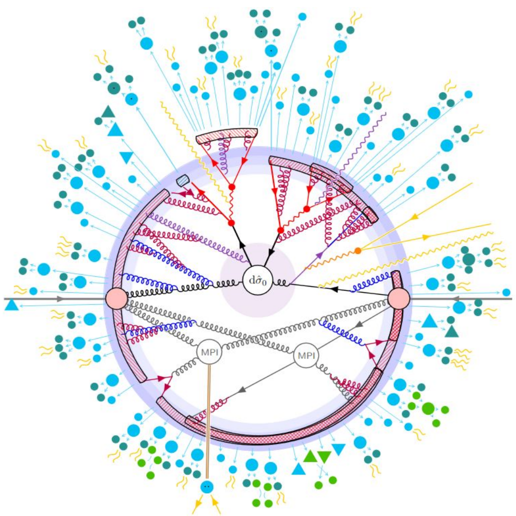
Ynyr Harris (University of Bonn) with input from Tim Martin (University of Warwick)

Tuning is the fitting of the free parameters of the **phenomenological models** used in MC event generators to describe [LHC] data

Stages of a MC event generator

- Hard Scatter (e.g. DY qq → ee)
- Parton Shower (PS)
- Hadronisation (Had)
- Colour Reconstruction (CR)
- Multiple Parton Interactions (MPI)

Underlying Event (UE) / 'everything else'



Pythia 8.3 schematic event

Pheno.-driven models, all implemented differently in the main generators (Pythia, Sherpa, Herwig, Epos, …), all with many free parameters that aren't known in advance

Today

What do recent measurements bring to a potential MC tuning campaign?

- Overview of tuning methodology
- Snapshot of new models available in MC event generators
  - Non-exhaustive list just to indicate development
- Overview of recent measurements sensitive to model choices and tunes
  - With contributions from ATLAS Jet/Photon, Soft QCD, W/Z, and Top groups

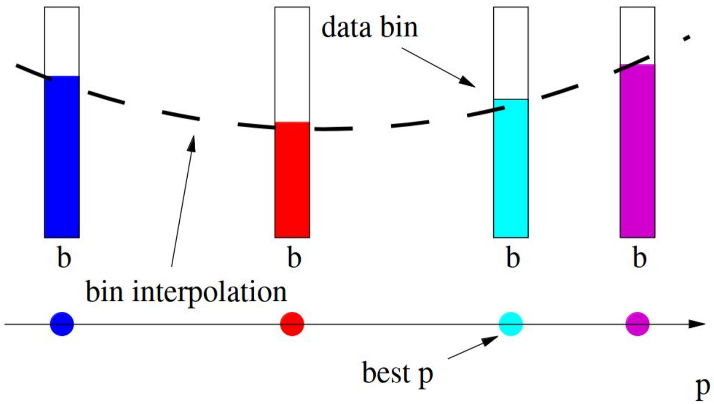
***Throughout: ‘new’ ~ new for use in tuning**

Overview of Current Tuning Methodology

Use the tried-and-tested Professor toolkit

[0907.2973, hepforge]

$$\mathrm{MC}_b(\boldsymbol{p}) \approx f^{(b)}(\boldsymbol{p}) = \alpha_0^{(b)} + \sum_i \beta_i^{(b)} p'_i + \sum_{i\leq j} \gamma_{ij}^{(b)} p'_i p'_j$$



- Polynomial interpolation of bin response to changes of the parameter vector ***p***
- Bin-weighted χ^2 -minimisation wrt data

$$\chi^2(\boldsymbol{p}) = \sum_{\mathcal{O}} w_{\mathcal{O}} \sum_{b\in\mathcal{O}} \frac{(f^{(b)}(\boldsymbol{p}) - \mathcal{R}_b)^2}{\Delta_b^2}$$

  - Weights are user-defined and depend on tune priorities
- Current ATLAS tunesets: A3 for MB, A14 for UE + Had, AZ for Z pT (+ more)

See this talk by Stefan Kiebacher (Herwig) for recent methodological ideas

Making tuning more convenient / less expert-dependent

New Features in Pythia

SU(3)-based CR [1505.01681]

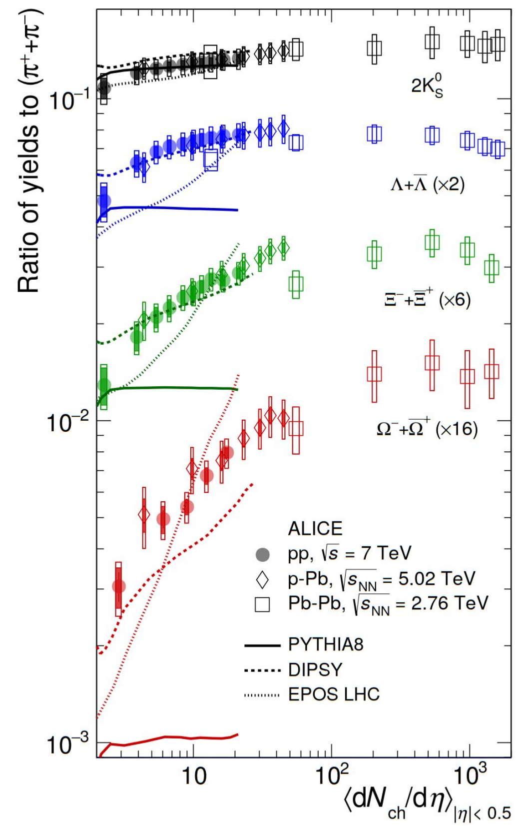
- MPI counteracts $1/N_C^2$ suppression
- Full multiplet structure enables string junction formation (baryons) [2404.12040] ✔

Colour ropes [1412.6259]

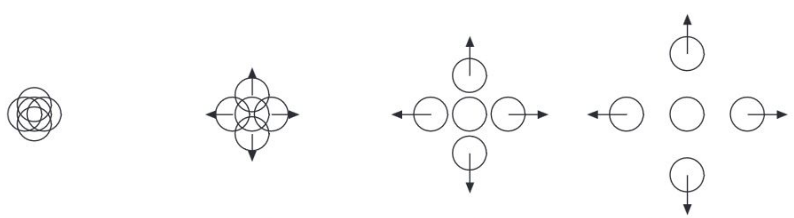
- Colour strings can overlap, forming ‘ropes’
- Ropes have higher string tension κ
  - Enhances strange production (probability ~ $\exp(-\pi m_S^2 / \kappa)$) ✔

String shoving [1612.05132]

- Pressure gradient between inside and out ropes generates k_T
  - Induces flow/collective effects ✔



Strange enhancement seen by ALICE [1606.07424] and everywhere



New Features in Pythia

Interesting new features that have never been tuned together in Pythia 8.3 (?)

Conclusion of [2404.12040] and conversations with Harsh (Pythia) [NPTA Workshop]

SU(3)-based CR [1505.01681]

- MPI counteracts $1/N_C^2$ suppression
- Enables string junction formation (baryons) [2404.12040]

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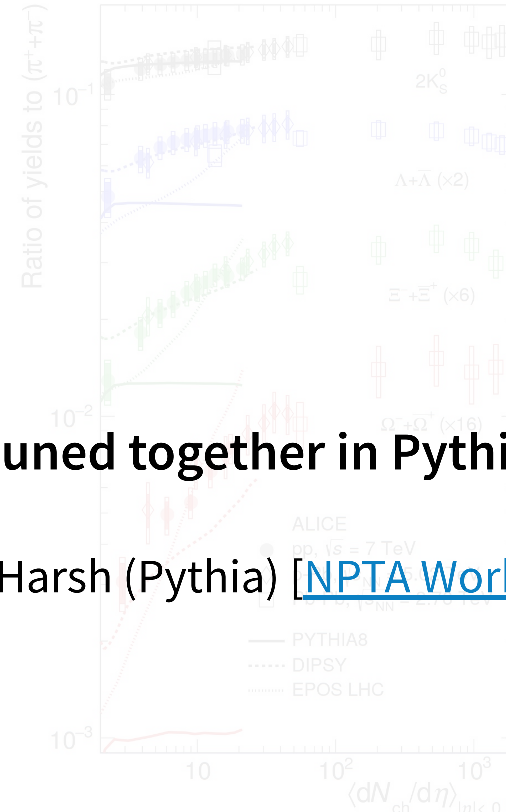


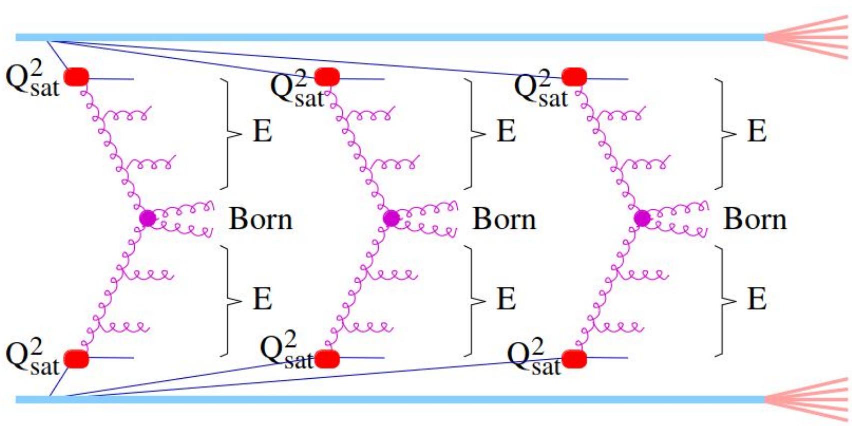
Strange enhancement seen by ALICE [1606.07424] and everywhere

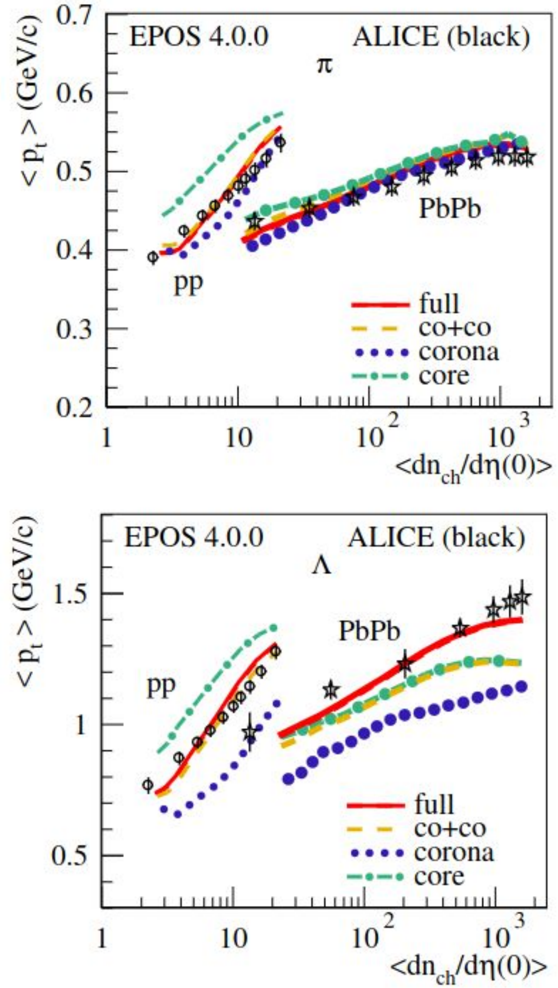
New Features in EPOS

EPOS 4 presented in [2301.12517](2301.12517) and by Tanguy Pierog at the NPTA Workshop

EPOS 4 solves conceptual problems (to do with maintaining factorisation during parallel scatters) w.r.t. EPOS-LHC. Now good for:

- “Normal” high-pT *pp* physics
- High-multiplicity *pp* physics
- *AA* scattering at LHC and RHIC



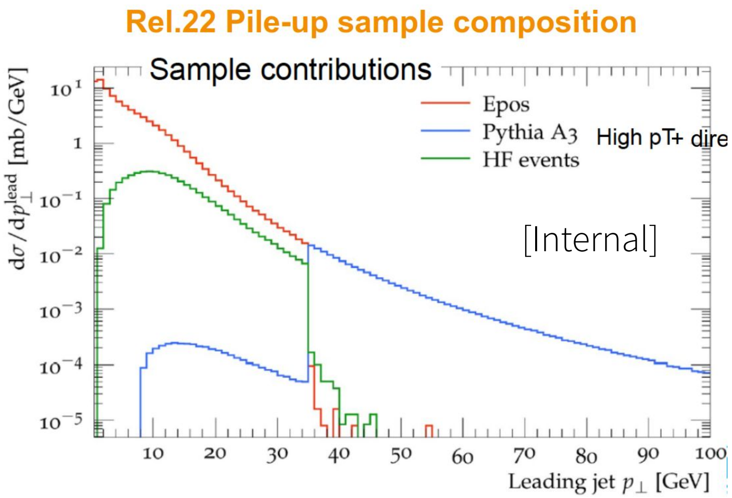


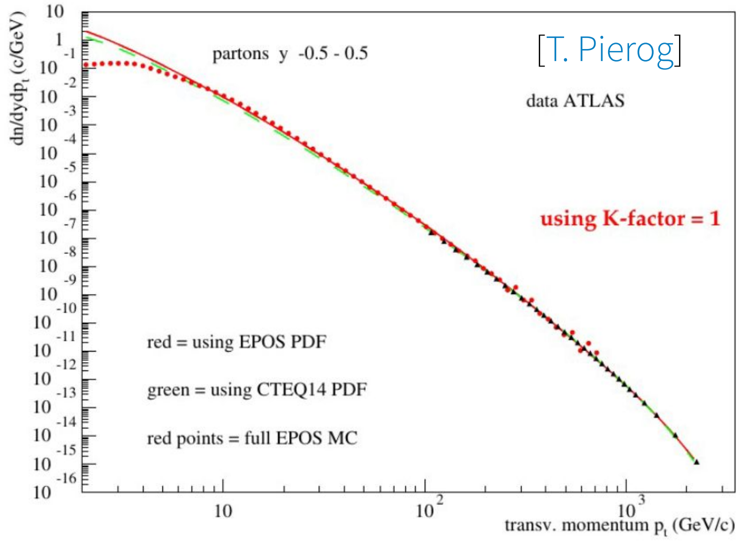
Consistent description of *pp* and *AA* [2301.12517]

EPOS 4 For Pile-Up Modelling?

ATLAS Run 3 pileup-modelling strategy involves mixing Pythia 8 A3 + EPOS-LHC based on leading jet-pT

With EPOS 4 good for high-pT physics, consider EPOS only?





Jet Measurements

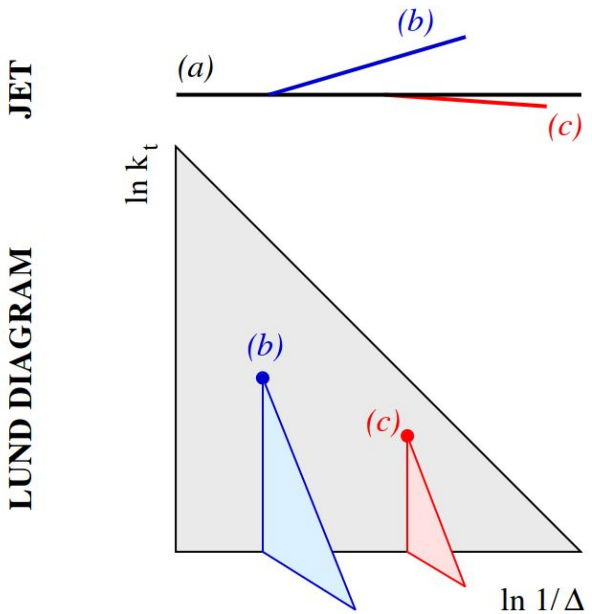
Thanks to Josu Contero for input.

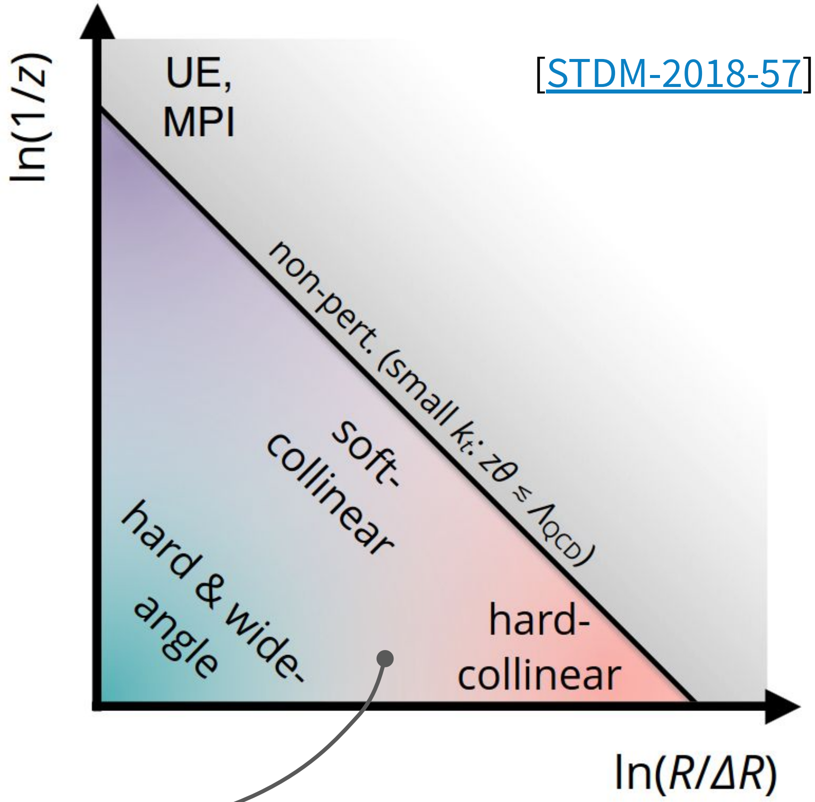
Analysis	**Models Probed**				**Rivet?** [Rivet coverage]
	UE/MB	**PS**	**CR**	**Had**	
Lund Jet Plane (ATLAS)		✔	✔	✔	ATLAS_2020_I1790256
Lund Multiplicities (ATLAS)		✔	✔	✔	No
Multijet Event Shapes (ATLAS)		✔			ATLAS_2020_I1808726
Multijet Event Isotropies (ATLAS)		✔			No
TEECs (ATLAS)		✔			ATLAS_2023_I2625697
TEECs (CMS)		✔			No
Intra-Jet Properties (ALICE)		✔	✔	✔	No

✔ in model column ~ model **particularly** sensitive to measurement

Lund Jet Plane @ 13 TeV

LJP construction from 1807.04758:





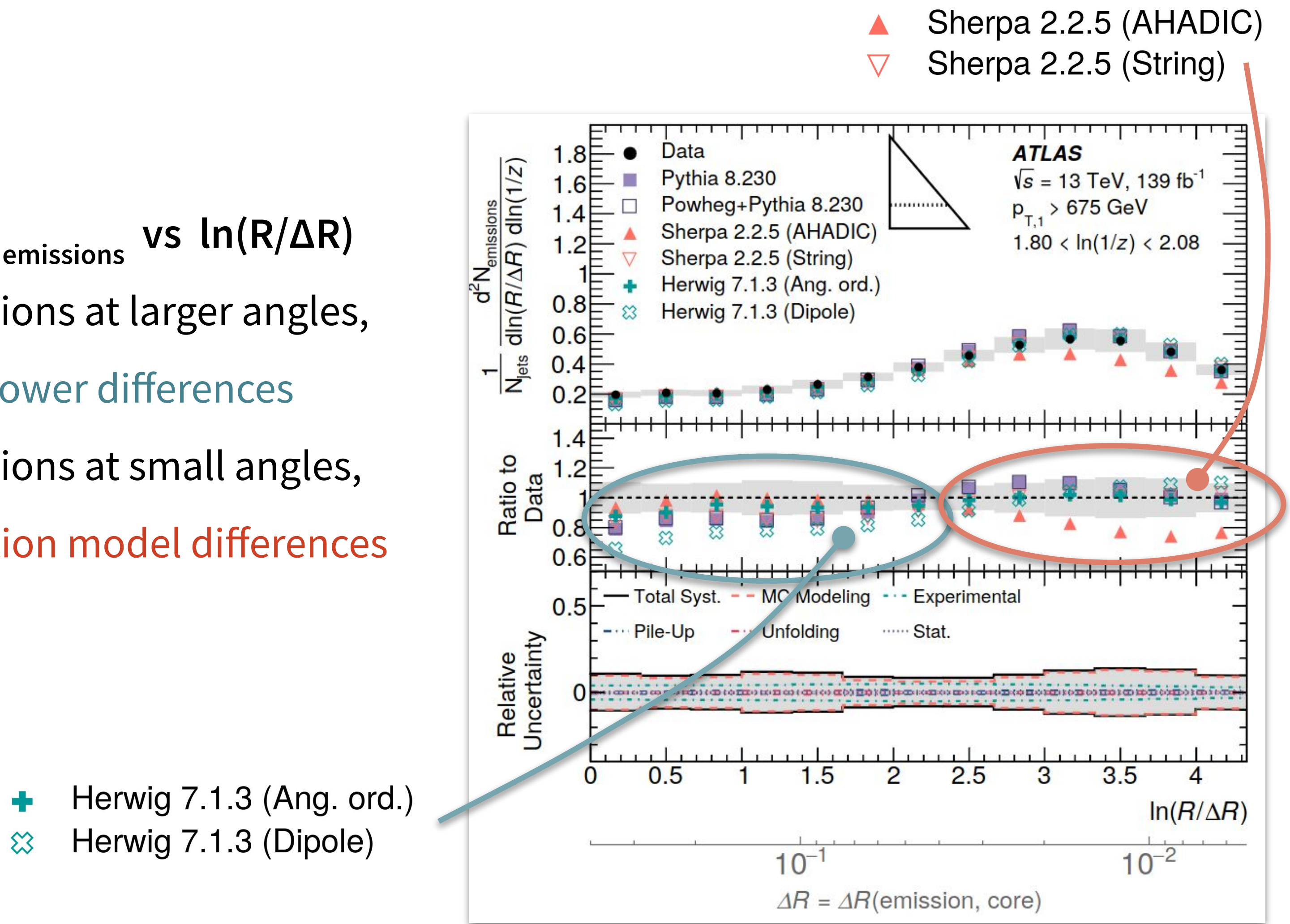
LJP separates physical effects

This is a great phase space for tuning, and has never been used before (?)!

Lund Jet Plane @ 13 TeV

E.g. this plot of $d^2N_{emissions}$ vs ln(R/ΔR)

- For hard emissions at larger angles, note parton shower differences
- For hard emissions at small angles, see hadronisation model differences



Fixed kT slice

[STDM-2018-57]

Transverse Energy-Energy Correlators (TEECs) @ 13 TeV

STDM-2018-51 published last year

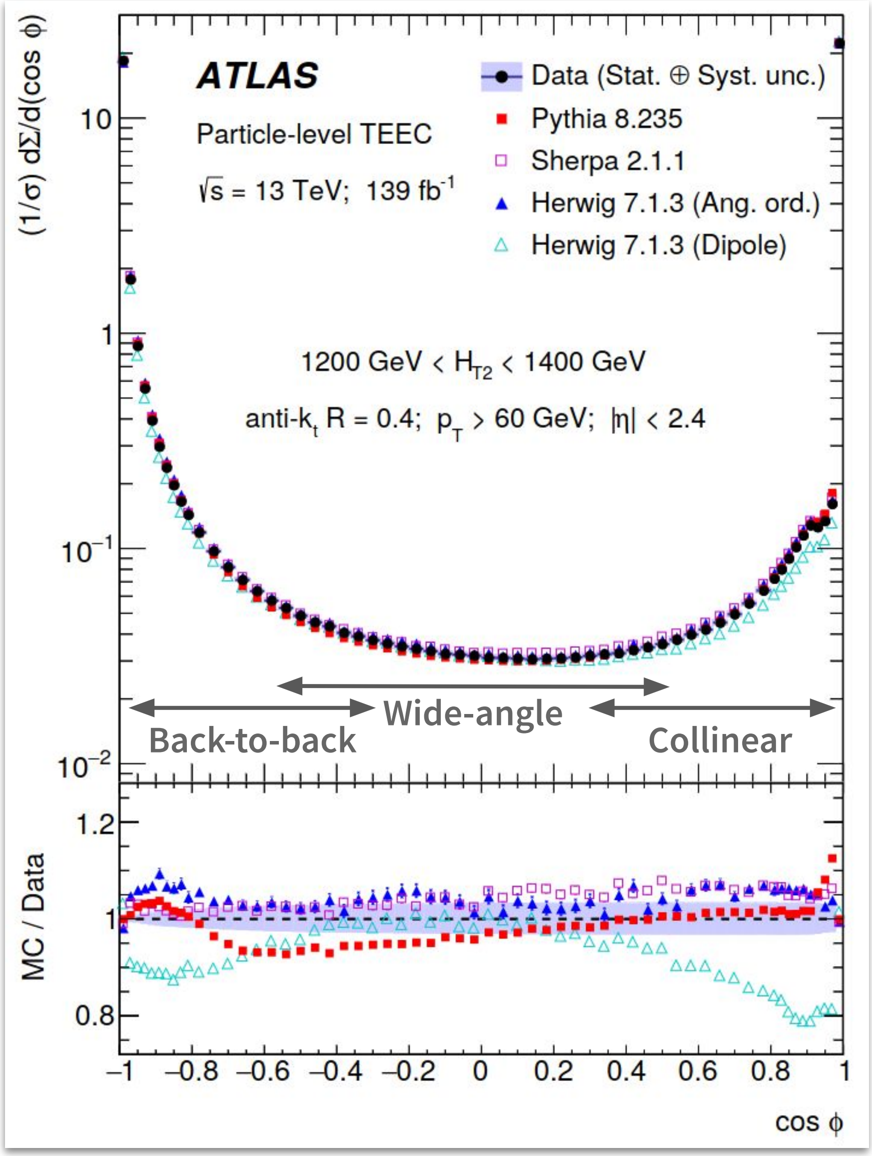
E_T-weighted azimuthal differences

$$\frac{1}{\sigma}\frac{d\Sigma}{d\cos\phi} = \frac{1}{N}\sum_{A=1}^{N}\sum_{ij}\frac{E_{Ti}^{A}E_{Tj}^{A}}{\left(\sum_k E_{Tk}^{A}\right)^2}\delta(\cos\phi - \cos\varphi_{ij})$$

between pairs of jets

Another Event Shape that's infrared and collinear-safe, sensitive to α_S, and isolates parton shower effects

Also measured by CMS [SMP-22-015]



Soft QCD Measurements

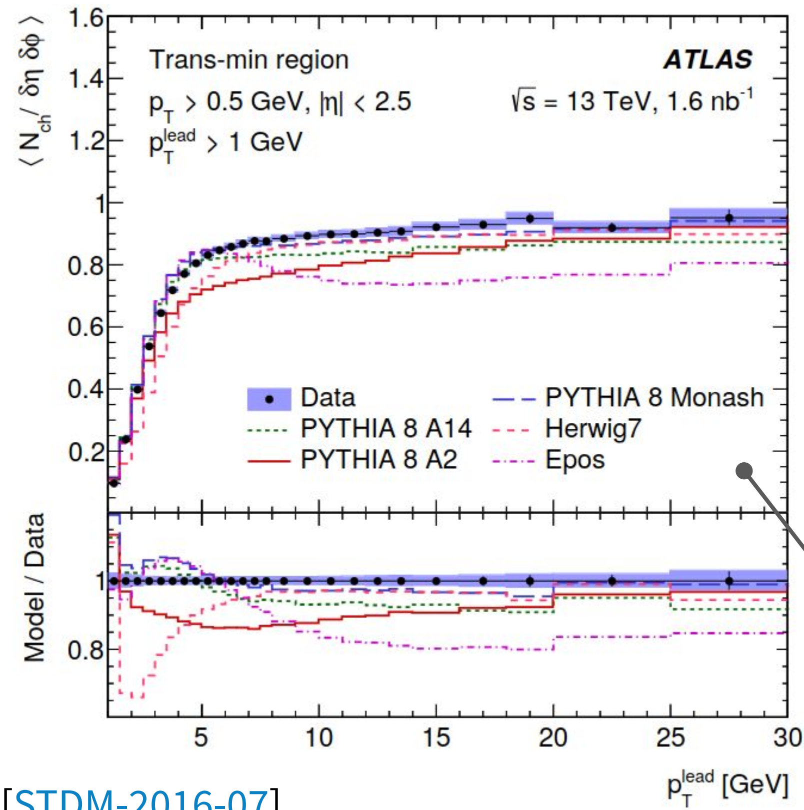
Thanks to Karel Cerny for input.

Analysis	Models Probed				Rivet? [Rivet coverage]
	UE/MB	PS	CR	Had	
Leading-track UE (ATLAS) 🔗	✔		✔		ATLAS_2017_I1509919
Z boson UE (ATLAS) 🔗	✔		✔		ATLAS_2019_I1736531
Strange UE (ATLAS) 🔗	✔		✔	✔	Coming soon
Azimuthal ordering (ATLAS) 🔗	✔		✔	✔	ATLAS_2012_I1091481
Tracks-based Event Shapes (CMS) 🔗	✔		✔	✔	Coming soon
Transverse spherocity (ALICE) 🔗	✔		✔	✔	No

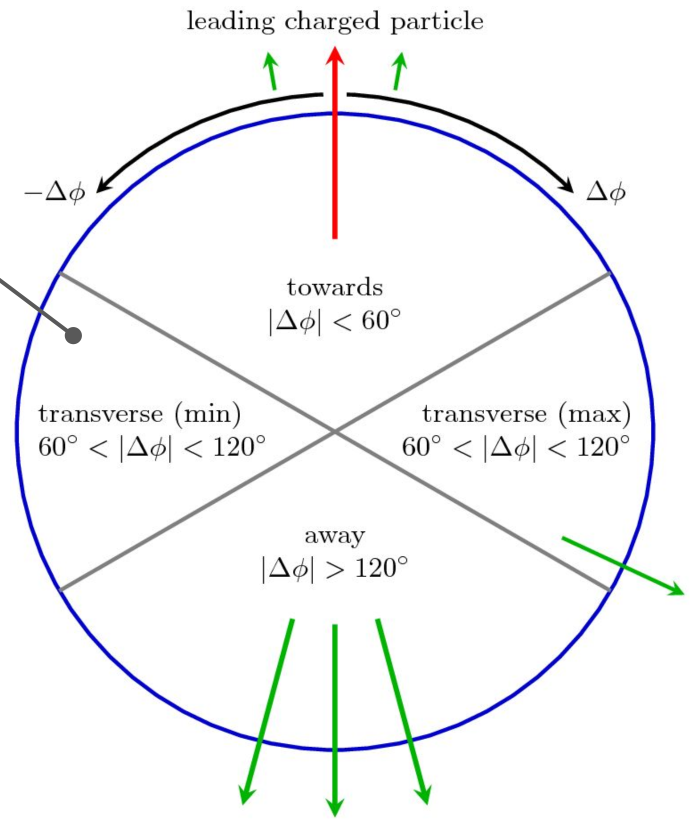
✔ in model column ~ model **particularly** sensitive to measurement

Leading-track UE @ 13 TeV

Study kinematic variables like p_T^{lead}, N_{ch}, Σp_T in the region transverse to dijet activity



[STDM-2016-07]



Take profiles in p_T^{lead} to study dependence on ~scale of the hard scatter. Usually see significant disagreements!

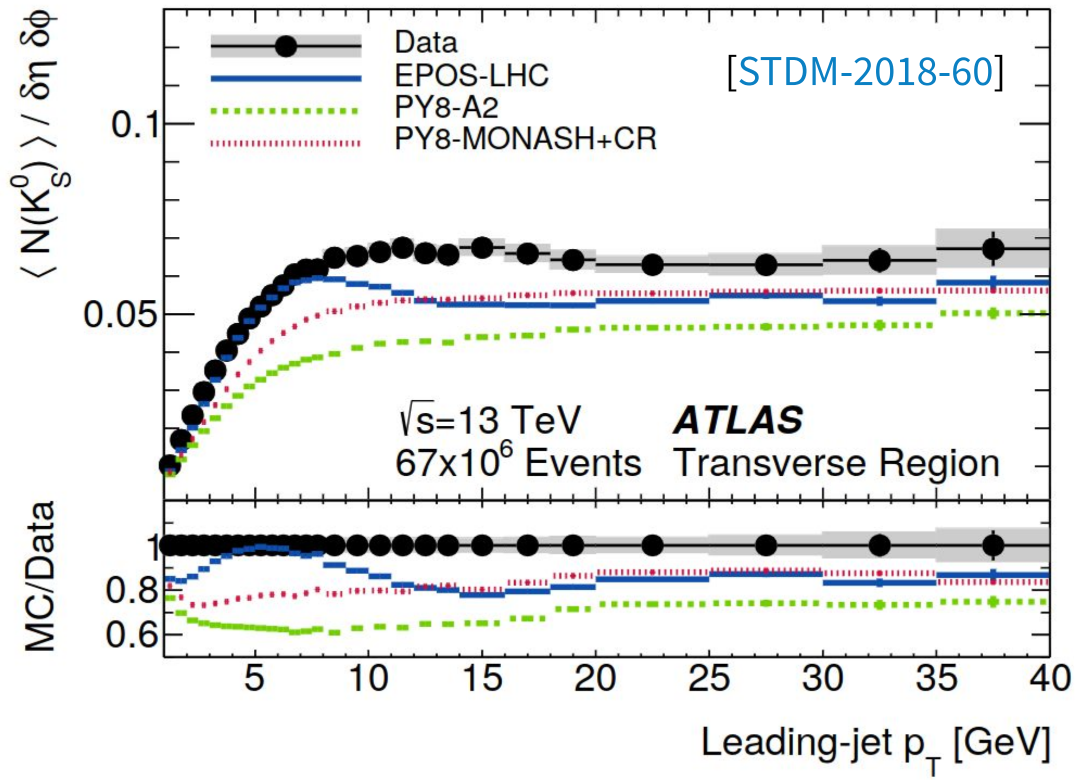
Strange UE @ 13 TeV

Like the leading-track UE but this time counting strange hadrons K_S^0 and Λ

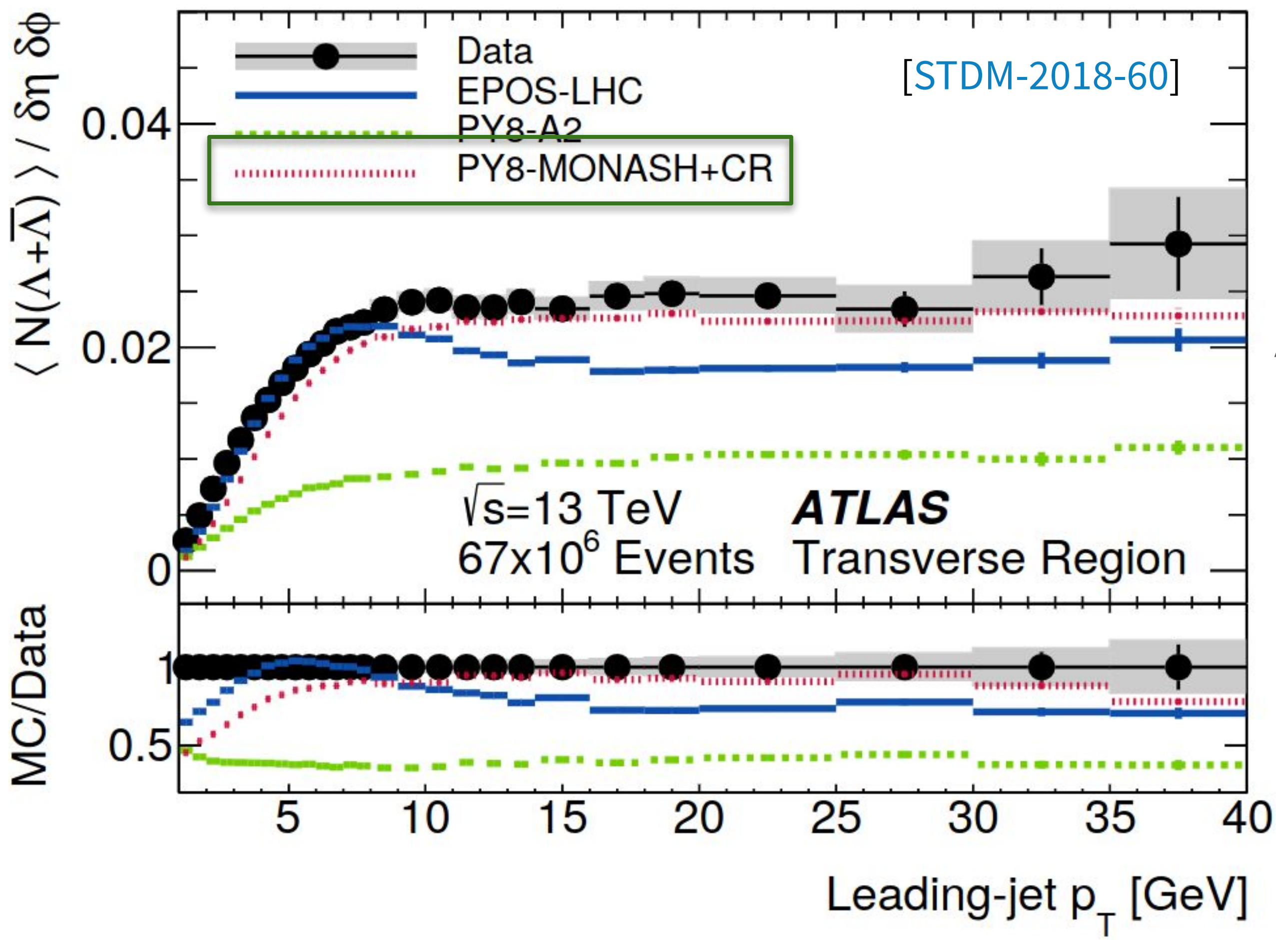
Strange hadron masses ~ Λ_{QCD} makes this measurement very sensitive to hadronisation

Counting Λ baryons makes it sensitive to three-way colour reconnection

See Tim Martin's talk for more information



Strange UE @ 13 TeV

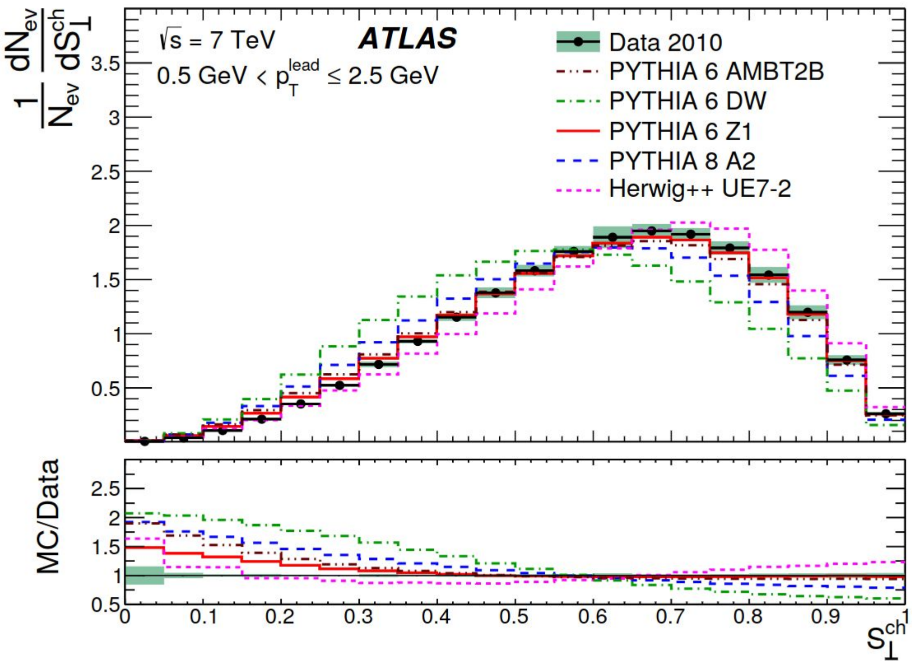


Strangeness + baryon enhancement compared to Py8 A2

See effects of Pythia's SU(3)-based CR model on baryon multiplicities

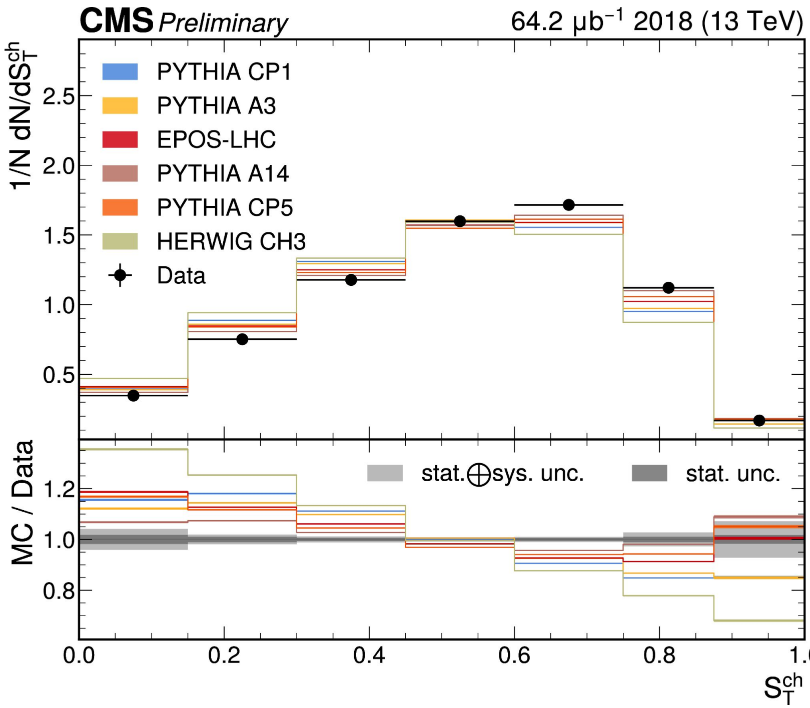
What's Going On With "Event Shapes"?

Simple observation: tracks-based Event Shapes appear to have always been quite mis-modelled, with data tending to be more isotropic



ATLAS 7 TeV version

[1207.6915]



CMS @ 13 TeV

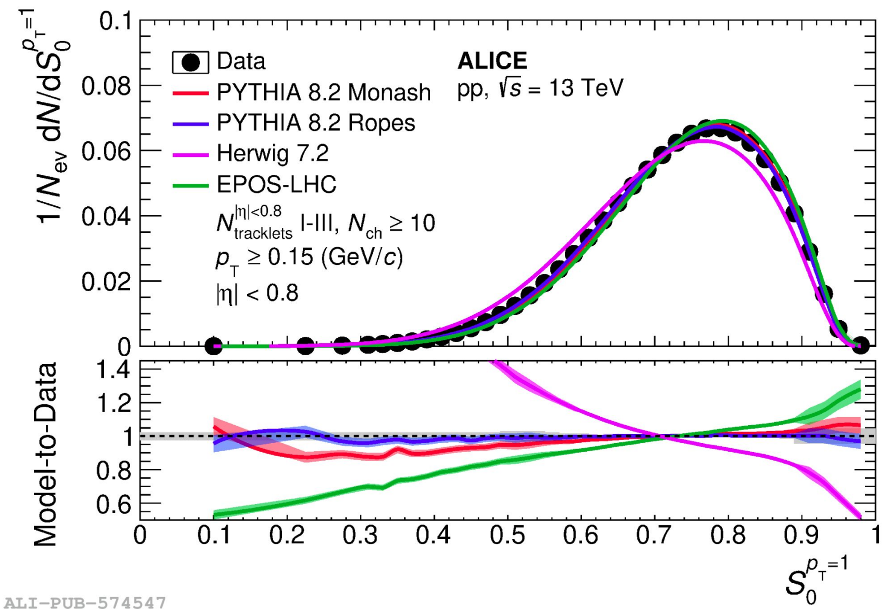
[SMP-23-008]

What's Going On With "Event Shapes"?

[JHEP 05 (2024) 184]

Curious that **Pythia 8 + Ropes** appears to describe transverse spherocity well (although the string shoving wasn't included)

(Measure Event Shapes with tracks again, like CMS just did [SMP-23-008], and compare latest models?)



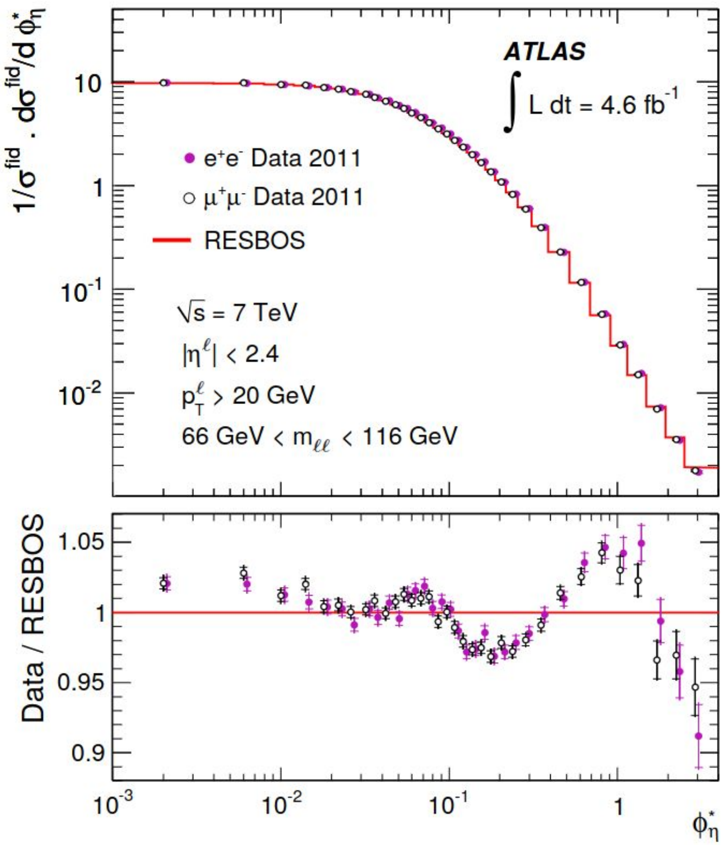
$$S_{\mathrm{O}}^{p_{\mathrm{T}}=1} = \frac{\pi^2}{4} \min_{\hat{n}} \left(\frac{\Sigma_i |\hat{p_{\mathrm{T},i}} \times \hat{n}|}{N_{\mathrm{trks}}} \right)^2$$

pT-unweighted 'spherocity'

The Z p_T spectrum isolates initial state effects (ISR and primordial k_T) important for low p_T^V -modelling — this motivated a dedicated tuning in the past

Pythia 8 tuned to Z ϕ_η^* distribution (correlated to pT but less sensitive to systematics [1009.1580]) → AZ tunes [ATL-PHYS-PUB-2013-017]

⇒ In principle improves W pT modelling, and reduces W mass error



Z pT @ 7 TeV used for AZ tunes [1211.6899]

Measurements of W/Z Bosons

Thanks to Stefano Camarda for input.

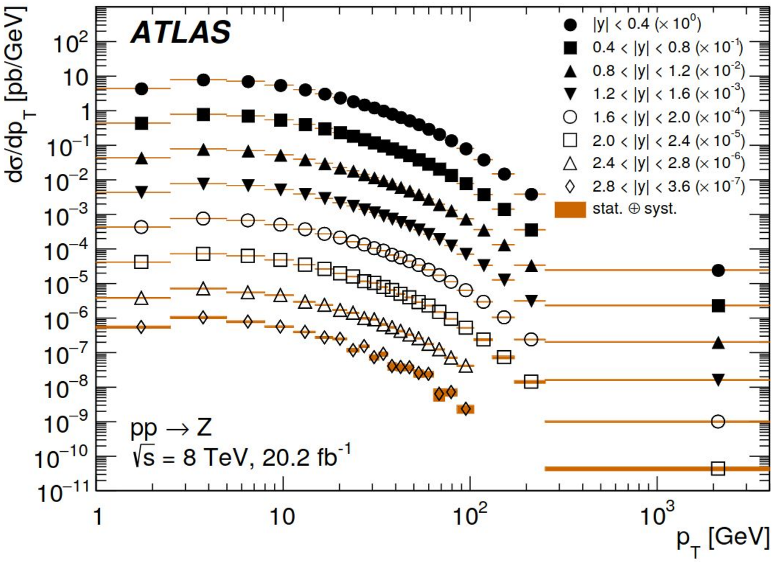
Special mention: double-differential Z pT and

rapidity distributions @ 13 TeV

[STDM-2018-05]

Factorise-away the analytic dependence on polaristion!

$$\frac{d\sigma}{dp_T\, dy\, dm\, d\cos\theta\, d\phi} = \frac{3}{16\pi} \boxed{\frac{d\sigma^{U+L}}{dp_T\, dy\, dm}} \Big\{(1+\cos^2\theta) + \frac{1}{2} A_0(1-3\cos^2\theta) + A_1 \sin 2\theta \cos\phi + \frac{1}{2} A_2 \sin^2\theta \cos 2\phi + A_3 \sin\theta \cos\phi + A_4 \cos\theta + A_5 \sin^2\theta \sin 2\phi + A_6 \sin 2\theta \sin\phi + A_7 \sin\theta \sin\phi \Big\}.$$



- ~ 5% agreement with state-of-the-art pQCD predictions in pT
- 0.2 – 0.5% accuracy in rapidity

Tune Z pT again?

Measurements of Tops

Top-antitop events used in the past for their PS and Had information [A14]

Analysis	Models Probed				Rivet? [Rivet coverage]
	UE/MB	PS	CR	Had	
Strange production (ATLAS)		✔	✔	✔	ATLAS_2019_I1746286
Top mass $m_{l\mu}$ (ATLAS)		✔	✔	✔	No
b-fragmentation with tracks (ATLAS)		✔		✔	No
CR observables (ATLAS)		✔	✔		ATLAS_2022_I2152933
Jet substructure (ATLAS)		✔	✔		No

Now a pertinent question: **does the top quark colour reconnect?**

Colour reconnection scale ~ 1 fm > top-quark decay length ~ 0.2 fm

Measurements of Tops

Top-antitop events used in the past for their PS and Had information [A14]

Analysis	Models Probed				Rivet? [Rivet coverage]
	UE/MB	PS	CR	Had	
Strange production (ATLAS)		✔	✔	✔	ATLAS_2019_I1746286
Top mass $m_{l\mu}$ (ATLAS)		✔	✔	✔	No
b-fragmentation with tracks (ATLAS)		✔		✔	No
CR observables (ATLAS)		✔	✔		ATLAS_2022_I2152933
Jet substructure (ATLAS)		✔	✔		No

Focussed measurements of *b* fragmentation-sensitive variables

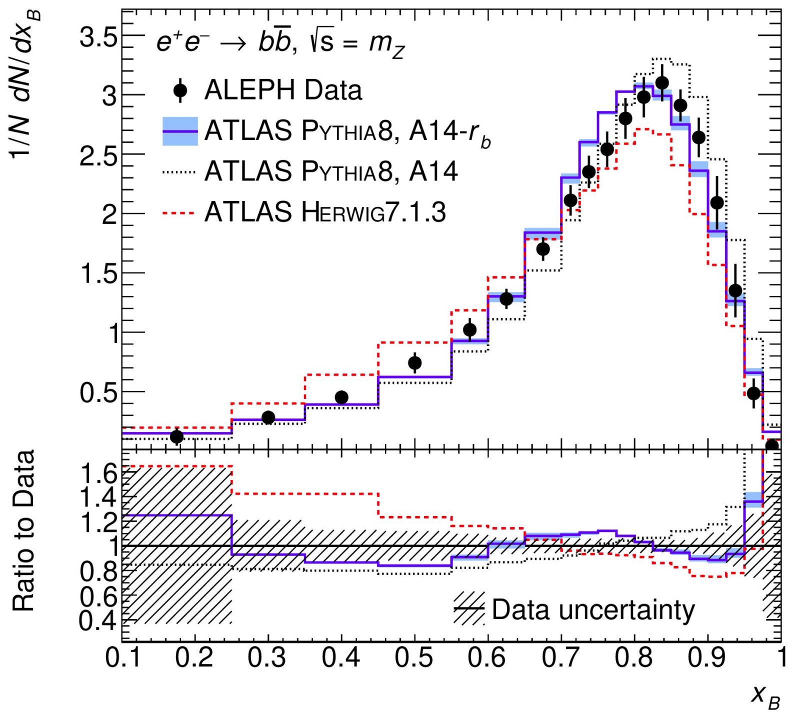
b-Fragmentation With Soft Muon Tags

The r_b parameter of the Lund-Bowler b-fragmentation function affects top mass extraction [TOPQ-2017-17] — A14-r_b tune produced to control this

$$f(z) = \frac{1}{z^{1+br_b m_b^2}}(1-z)^a \exp(-bm_T^2/z)$$

New ATLAS analysis (kicked off **last Monday!**) plans to measure fragmentation-sensitive variables using soft muons from B-hadron decays

Higher r_b — softer x_B



Fraction of b-quark energy ending up in the B-hadron

Conclusion

- Presented an arbitrary assortment of new models and recent measurements
- **Currently a good environment for tuning, with lots of new ideas and data!**
  - As has recently been discussed in ATLAS (though there's no central effort **yet**)
- Theorists provide default tunes, experimentalists make precision tunes!
  - Complete with systematic uncertainties
- More accurate models + tunes → physics understanding, smaller systematics, …

ChatGPT advice (courtesy of Stefan Kiebacher):

4. Continual Improvement: The tuning process is ongoing as new experimental data becomes available or as theoretical understanding advances. Regularly revisit the tuning procedure to incorporate new information and improve the accuracy of the event generator.

EXTRAS

Recent Methodological Ideas

For an active expert's overview, see this recent talk by Stefan Kiebacher (Herwig)

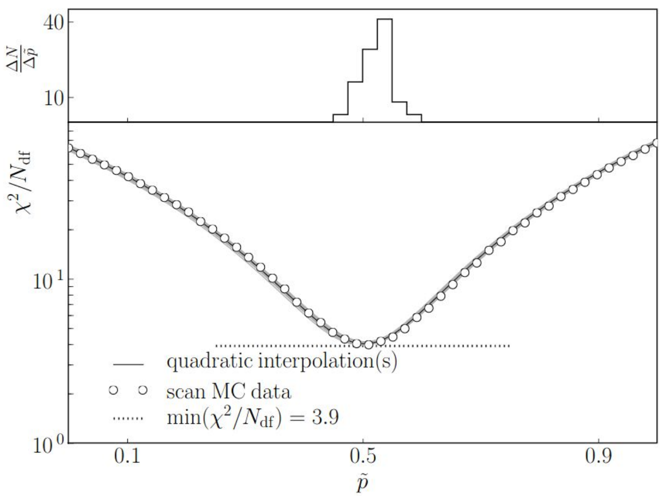
- Include a percentage "theory" uncertainty of ~ 5% `Professor`
  - Avoid over-fitting to high-statistics bins at the expense of others
- Regularised goodness-of-fit functions `Professor`
  - Exclude bins that cannot be described
- Reject bins if data not in the envelope of of sampled parameters `Apprentice`
- Find decorrelated subspaces to tune in `AutoTunes`

Systematic Uncertainties on Tunesets

What's the best way to produce uncertainties on tunesets ?

The "eigentunes" method of Professor — usually underestimates uncertainties.

Define a 'tolerance' as is done in PDF fitting [2112.11266]? $\Delta\chi^2 = N_{df} / 2$ was used in A14



Take the spread of an ensemble of fits [1812.07424]? Laborious but meaningful

Some effort to automate tune variations on-the-fly [P. Skands, 2308.13459] !

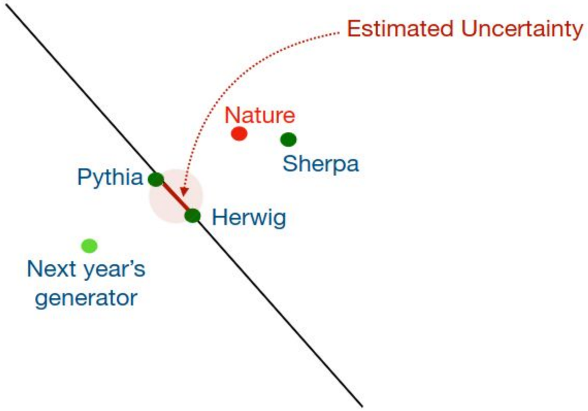
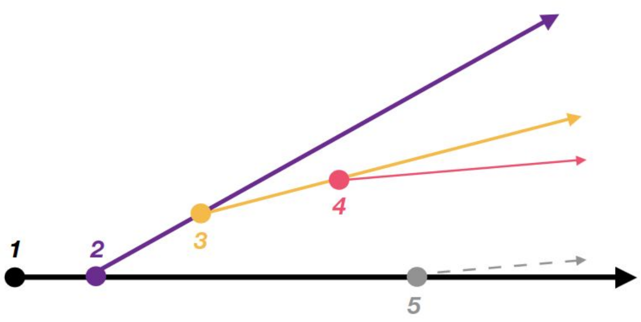


Illustration of 2-point uncertainty meaning
Ghosh & Nachman [2109.08159]

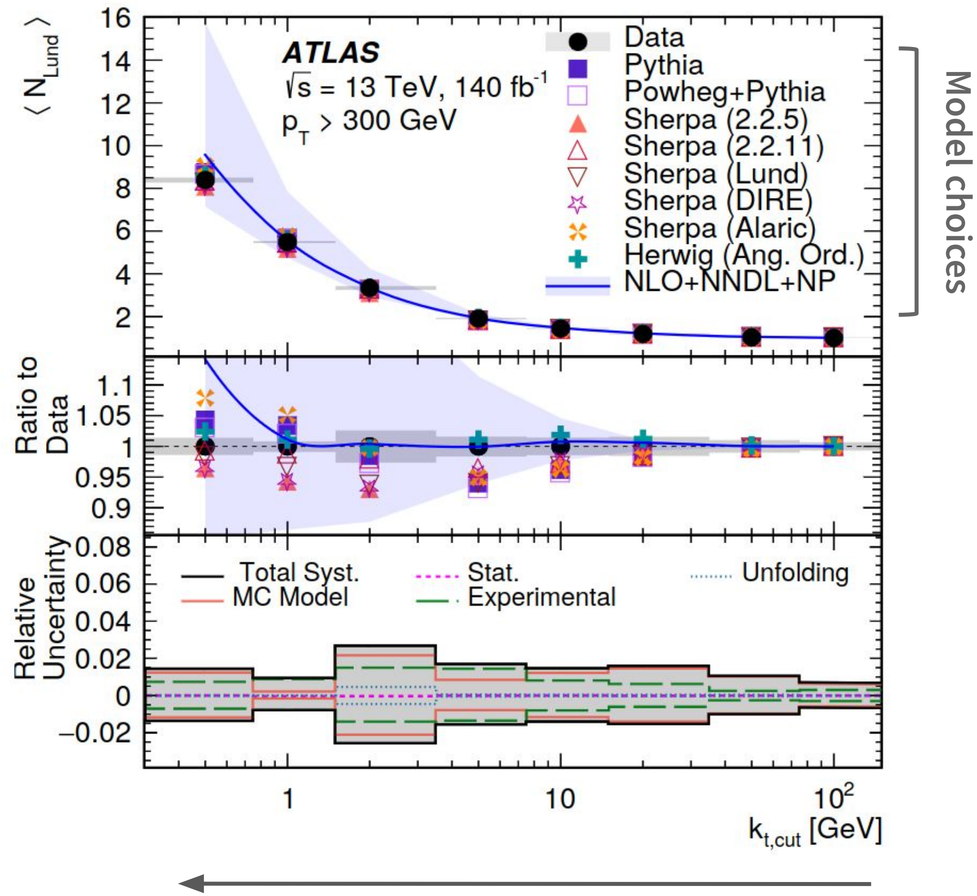
Lund Subjet Multiplicities @ 13 TeV

Similar to the LJP measurement, but this time counting emissions [STDM-2023-07]:



$N_{Lund} = 5$

N_{Lund} measured in bins of jet p_T for increasing emission-k_t requirements



More non-perturbative

Multijet Event Shapes @ 13 TeV

[STDM-2020-20]

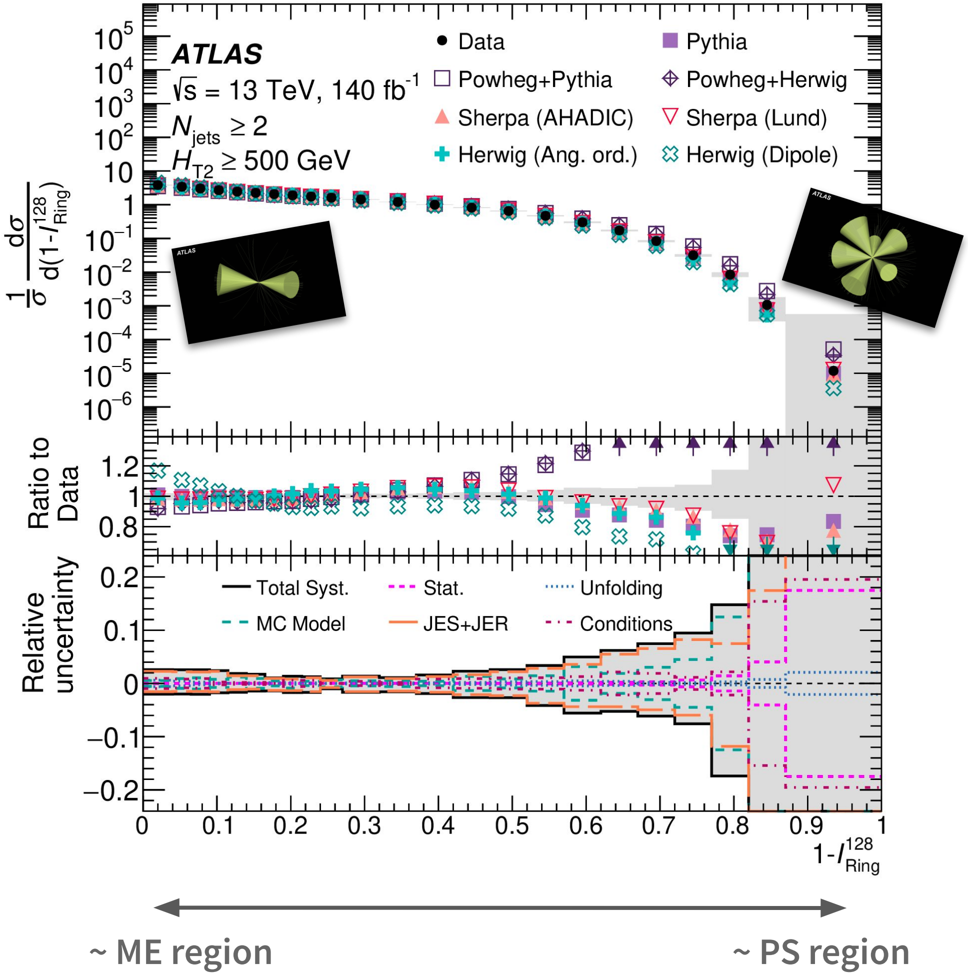
Measurements of multijet

Event Isotropies [STDM-2020-20]

and Event Shapes [STDM-2019-02]

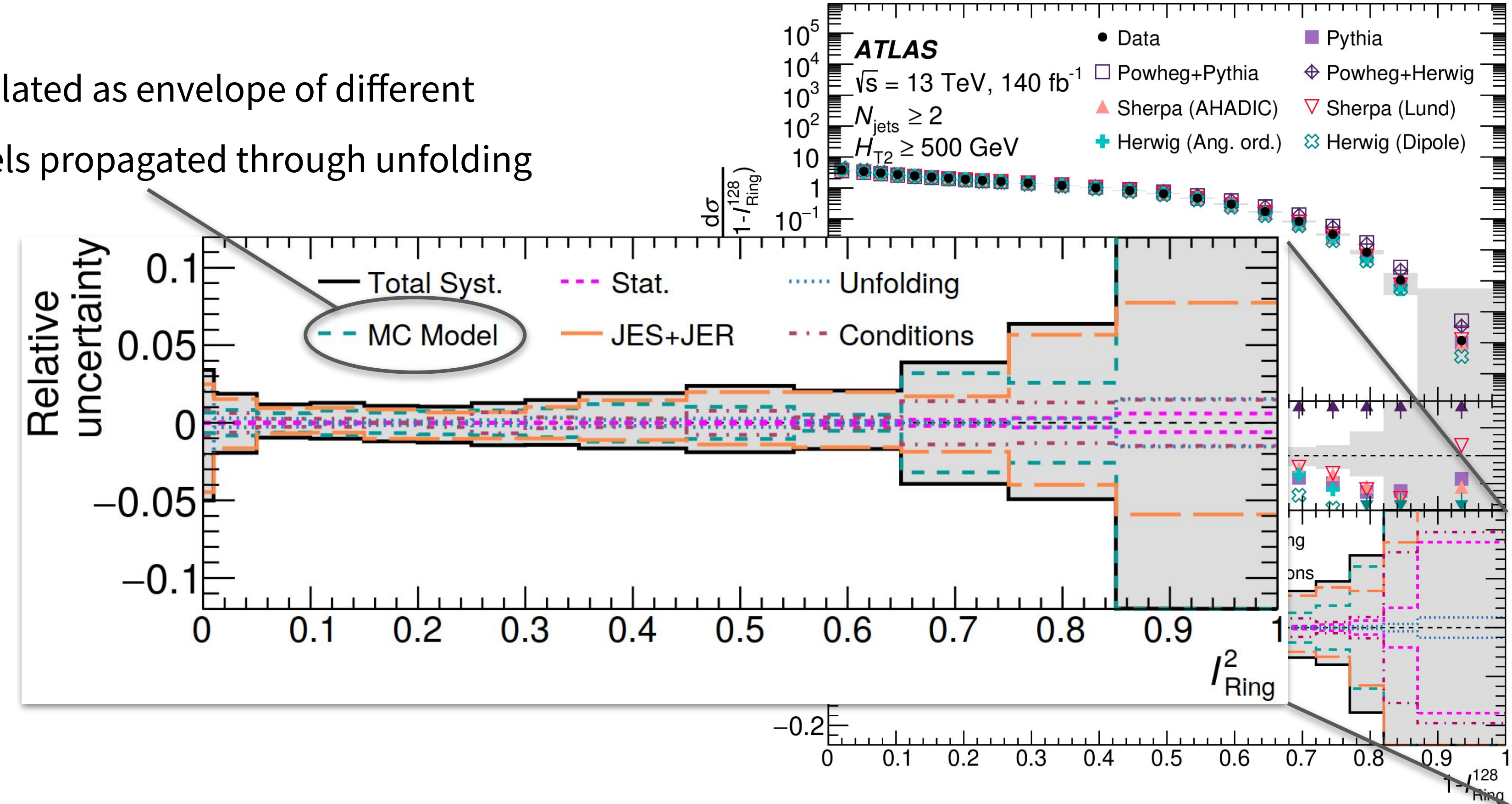
are sensitive to choice of

parton shower model



Common Theme From These Jet/Photon Analyses

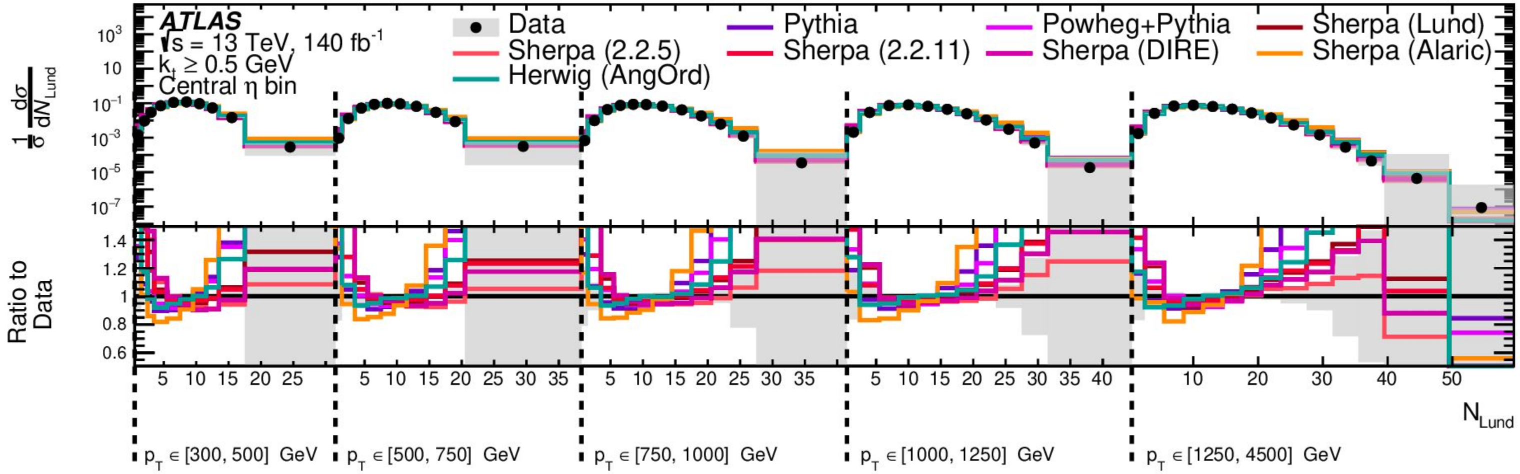
Calculated as envelope of different models propagated through unfolding

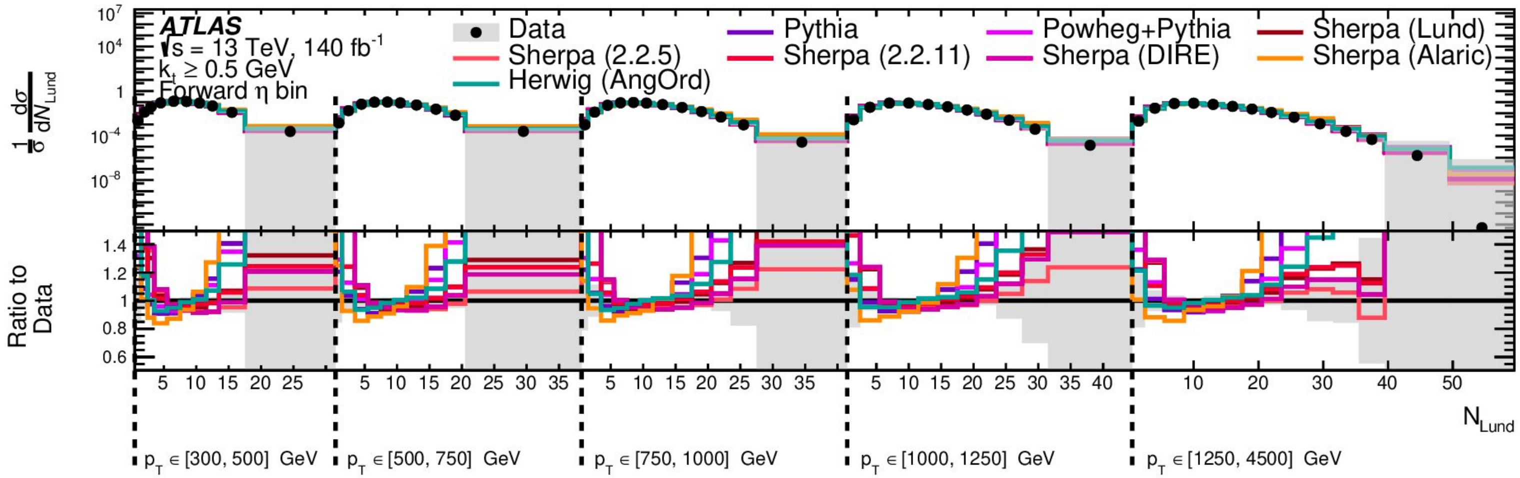


‘MC modelling’ uncertainty is a dominant systematic. Modelling also affects JES.

Bad for physics analysis, but great for tuning!

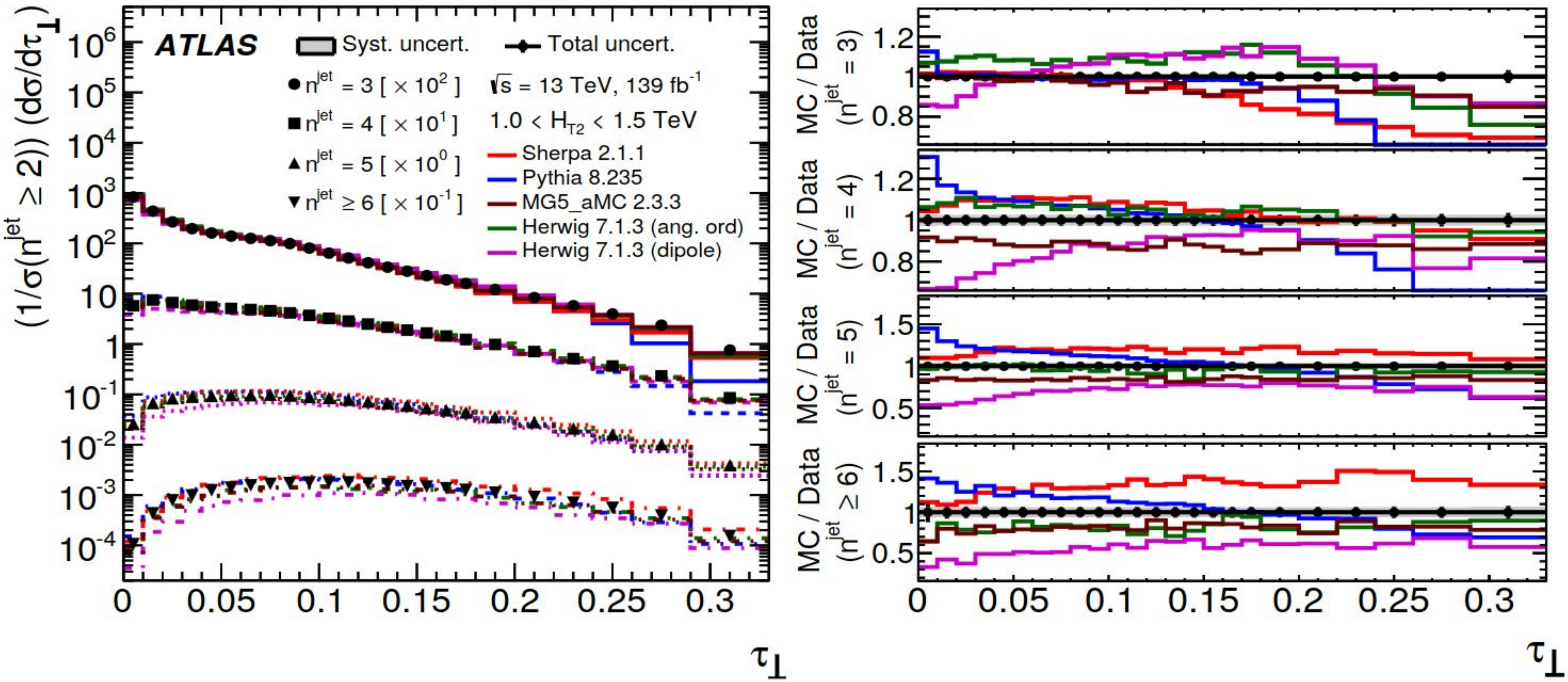
Lund Subjet Multiplicities @ 13 TeV





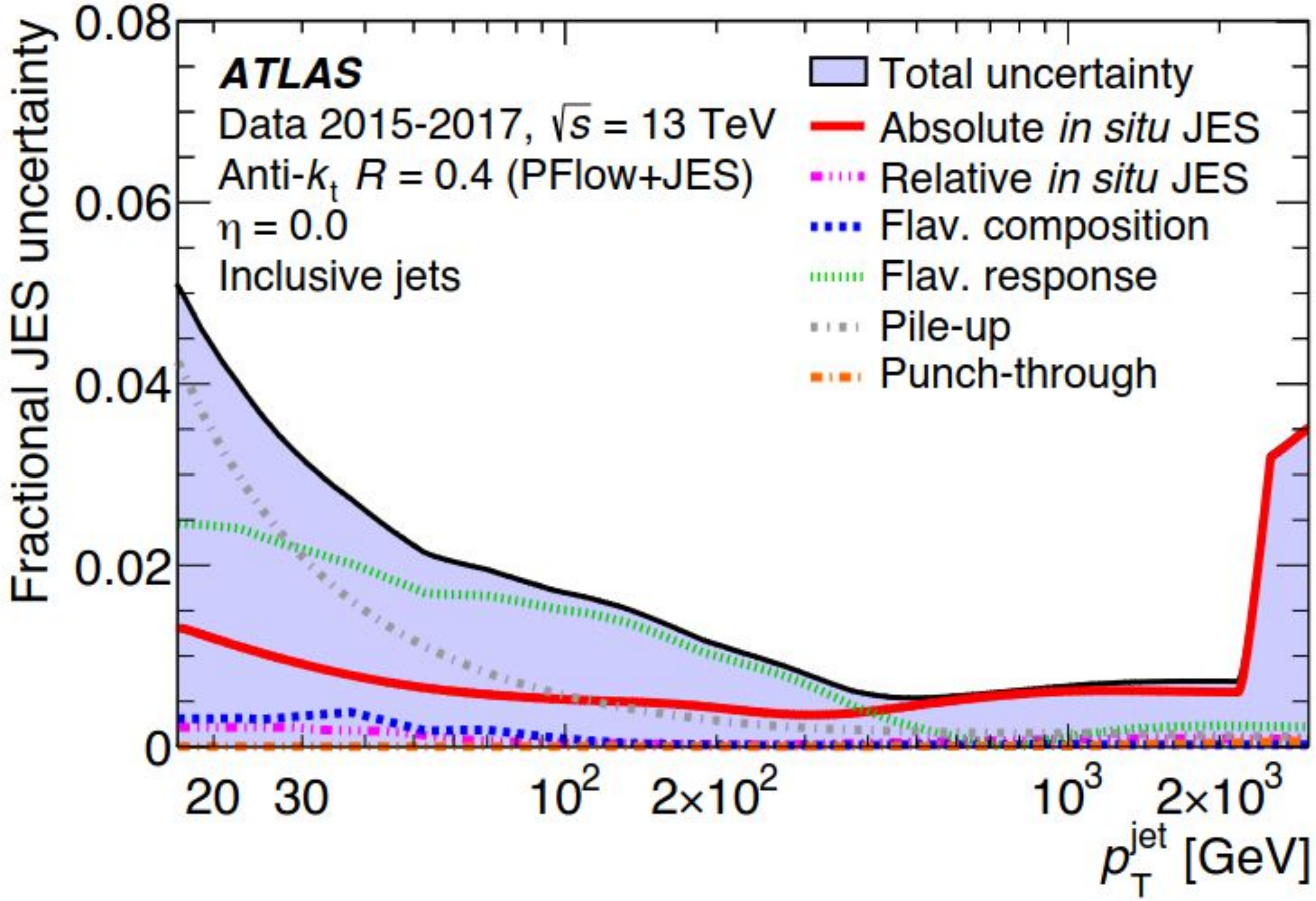
[STDM-2023-07]

Hadronic Event Shapes @ 13 TeV



[STDM-2019-02]

Effects of MC Modelling on JES Uncertainty, e.g.



[JETM-2018-05]