# Jet fragmentation and substructure at the LHC

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# Jet fragmentation

In leading-order QCD, well-separated jets and partons are exactly equivalent

Broken by evolution from fixed-order to "real" jets, including both perturbative QCD radiation and non-perturbative hadronisation

Collectively this process can be considered as the *fragmentation* of a parton into the multi-hadron spray of a particle-level jet

Measuring jet fragmentation ⇒ understanding the emergence of jet structure from a mixture of parton flavours and configurations



Light-jet fragmentation

# Earlier jet fragmentation measurements

**Previous LHC measurements of jet fragmentation:** 

**Eur. Phys. J. C 76 (2016) 322** — Measurement of the charged-particle multiplicity inside jets from  $\sqrt{s}$  = 8 TeV pp collisions with the ATLAS detector arXiv:1602.00988

**Phys. Rev. D 93 (2016) 052003** — Measurement of jet charge in dijet events from  $\sqrt{s=8}$  TeV pp collisions with the ATLAS detector, arXiv:1509.05190

**Eur. Phys. J. C 71 (2011) 1795** — Measurement of the jet fragmentation function and transverse profile in proton-proton collisions at a center-of-mass energy of 7 TeV with the ATLAS detector, arXiv:1109.5816

**Phys.Rev.D 83 (2011) 052003** — Study of jet shapes in inclusive jet production at 7 TeV with the ATLAS detector, arXiv:1101.0070

# ATLAS jet fragmentation at 13 TeV — arXiv:1906.09254

Uses 33 fb<sup>-1</sup> dataset of 13 TeV pp collisions from 2016

- Increased phase space & jet  $p_{\tau}$  reach wrt 7, 8 TeV
- Makes use of Run 2 tracker upgrades, e.g. IBL
- Dense-environment tracking, for  $\langle \mu \rangle \approx 25$

At least two reco jets with  $|\eta| < 2.1$ , and  $p_T > 60$  GeV

- $|\eta|$  requirement for full containment in tracker
- $p_{T1}/p_{T2} < 1.5$  balance to simplify interpretation
- $p_{T} > 100 \text{ GeV}$  at fiducial level
- Charged tracks ghost-associated to calo jets



## Unfolded average observables

Average observables vs  $p_T$ generally well-described by main shower MC codes (Pythia8.1xx, Herwig++ and Sherpa 2.1)

Hints of deviation from Sherpa, particularly in radial profiles standard component of MC via 7 TeV jet shapes ... for jet  $p_T < 500$  GeV!

*Need to check vs Sherpa 2.2.x* 



### Unfolded observable moments & weighted sums

Also observables computed as moments and weighted sums with the  $p_T$  fraction  $\zeta$  raised to powers  $\kappa = 0.5$  and  $\kappa = 2$ :

$$\begin{split} \langle \zeta^{\kappa} \rangle &= \int \zeta^{\kappa} F(\zeta) d\zeta / \int F(\zeta) d\zeta \\ \langle \sum_{i \in \text{jet}} \zeta_{i}^{\kappa} \rangle &= \int \zeta^{\kappa} F(\zeta) d\zeta \end{split}$$

Pythia 8 and Herwig++ mostly well-behaved; major discrepancies seen for Sherpa 2.1, esp. for  $\kappa = 2$ [effectively a var( $\zeta$ ) measurement]





#### Differential distributions of every core variable in bins of jet $p_{\tau}$

#### A treasure-trove of data for jet modelling & resummation studies! Rivet soon



# CMS quark & gluon jet substructure

**36 fb<sup>-1</sup>, 13 TeV** *pp* dataset, using akT4 & 8 jets with  $p_{T} > 30$  GeV, |y| < 1.7 (cf. tracker acceptance)

**Dual event selection: dijets and Z+jets** (two OS muons,  $p_T > 26$  GeV,  $|m_{\mu\mu} - m_Z| < 20$  GeV)

#### JJ and ZJ asymmetry and separation required

Compare to LO event simulations with MG5+Py8 (+  $\leq$  4 partons) and H++. Higher multiplicity MG5+Py8 unsurprisingly describes  $p_T$  spectra better  $\Rightarrow$  used as nominal MC

5 x generalised angularity observables cf. diagram:



# CMS quark & gluon jet substructure

CMS-PAS-SMP-20-010

Observables distinguished by:

- event-selection
- central/forward dijet-event jet
- $p_{\mathrm{T}}$ -bin, and
- reco method: particle-flow, charged-only, and groomed



# CMS quark & gluon jet substructure



# Selections identified with *q*/*g* enhancement:

- "gluon" = central jet in dijet events
- "quark" = Z+jet at low- $p_T$ (regions 1,3-5), and forward jet of dijet system at high  $p_T$

**Mean rates:** MCs follow data trends, some large spreads. q worse?  $\Rightarrow$  tuning

**b-jet fragmentation** 

# **b-jet fragmentation**

# Heavy quark/jet production crucial both for QCD and EW/BSM physics

**EW/BSM:** *b*-jet signatures ubiquitous in many BSM models, top-quarks, and SM & BSM  $H \rightarrow bb$  channels

#### QCD: sensitivities to, for example...

- hard-scatter formalism between PDF / ME
- PS scale choices and mass effect on radiation pattern
- *b*-hadron production fractions



# Earlier *b*-tagged jet fragmentation measurements

Previous measurements of *b*-jet fragmentation:



JHEP 12 (2013) 039 — CMS angular correlations in *Z*-boson with *b*-hadrons, arXiv:1310.1349

JHEP 03 (2011) 136 — CMS *BB* angular correlations from SV reconstruction, arXiv:1102.3194



14

# ATLAS *b*-fragmentation in *tt*

*b*-jet fragmentation moments, via secondary vertices and track-jets 13 TeV analysis, partial Run 2 dataset of 36/fb

- R = 0.4 calo jets with standard ATLAS *b*-tagging (70% eff)
- Event selection: = 2 OS  $e+\mu$ , = 2 jets,  $\Delta R_{ii}$  > 0.5; tag & probe, both ways
- Variable-radius track jets ghost-associated to calo jets
- Track-jet PV and SV tracks: SV/(PV+SV) ~ *b*-hadron/*b*-quark



#### ATLAS-CONF-2020-050

# ATLAS *b*-fragmentation in *tt*

n<sub>ch</sub> moment

- #SV tracks ≈ *b*-hadron
- Fit shifts away from the input-MC prior
- Reweightings of
   Pow+Py8 to probe-jet
   n<sub>sv</sub> as systematic
- Check of hadron fractions & decays: Sherpa > 2.2.8 improvements



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*n<sub>b</sub><sup>ch</sup> bin* 

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#### ATLAS-CONF-2020-050

# ATLAS *b*-fragmentation in *tt*

- *z*<sub>ch,L</sub> (longitudinal) moment
  - Experimental proxy for the theoretical fragmentation function: tunings from LEP and SLD valid?
  - Descriptions generally good, with Herwig a slight outsider (much improved from v7.0.4)



6

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z<sup>ch</sup> bin

# ATLAS *b*-fragmentation in *tt*

0.8

0.7

0.5

1.5

Sensitivities to Sherpa tunes, Pw+Hw versions, Pw+Py8  $r_{\rm B}$  tunes,  $\alpha_{\rm S}$  variations:

z variables: little sensitivity to  $r_{\rm p}$  param Data ATLAS Preliminary 2.2 Sherpa 2.2.1 2.2 /s = 13 TeV, 36 fb<sup>-</sup> Sherpa 2.2.8 (Z + bb tune — Data — Data Data  $\begin{array}{c} & \mbox{Pow}+\mbox{Py8} \ r_B = 0.855 \ \alpha_{S}^{FSR} = 0.127 \\ - & \mbox{Pow}+\mbox{Py8} \ r_B = 0.855 \ \alpha_{S}^{FSR} = 0.111 \\ - & \mbox{Pow}+\mbox{Py8} \ r_B = 0.855 \ \alpha_{S}^{FSR} = 0.139 \\ - & \mbox{Pow}+\mbox{Py8} \ r_B = 1.050 \ \alpha_{S}^{FSR} = 0.127 \end{array}$ Sherpa 2.2.8 defaults  $\begin{array}{c} \hline & \mathsf{Pow} + \mathsf{Py8} \; r_B = 0.855 \; \alpha_F^{\mathsf{SR}} = 0.127 \\ \hline & --- \; \mathsf{Pow} + \mathsf{Py8} \; r_B = 0.855 \; \alpha_F^{\mathsf{SR}} = 0.111 \\ \hline & \mathsf{Pow} + \mathsf{Py8} \; r_B = 0.855 \; \alpha_F^{\mathsf{SR}} = 0.139 \\ \hline & --- \; \mathsf{Pow} + \mathsf{Py8} \; r_B = 1.050 \; \alpha_S^{\mathsf{FSR}} = 0.127 \end{array}$  $\begin{array}{c} \hline & \mathsf{Pow+Py8} \ r_{\mathsf{B}} = 0.855 \ \alpha_{\mathsf{SR}}^{\mathsf{FSR}} = 0.127 \\ \hline & \mathsf{Pow+Py8} \ r_{\mathsf{B}} = 0.855 \ \alpha_{\mathsf{SR}}^{\mathsf{FSR}} = 0.111 \\ \hline & \mathsf{Pow+Py8} \ r_{\mathsf{B}} = 0.855 \ \alpha_{\mathsf{SR}}^{\mathsf{FSR}} = 0.139 \end{array}$ --- Sherpa 2.2.10 1.6 ----- Pow+Pv8  $r_B = 1.050 \, \alpha_{PSR}^{FSR}$ 1.8 1.8 Ratio to data 1.2 ATLAS Preliminary 1.4 ATLAS Preliminary ATLAS Preliminary  $\sqrt{s} = 13 \text{ TeV}.36 \text{ fb}^{-1}$ 1.6 1.6  $\sqrt{s} = 13 \text{ TeV} \cdot 36 \text{ fb}^{-1}$  $\sqrt{s} = 13 \,\text{TeV}, 36 \,\text{fb}^{-1}$ 1.2 Ratio to data Ratio to data 1.1 1.4 1.4 1 1.2 1.2 0.8 0.6 0.9 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0 0.8 0.8 0.8 Data 0.6 0.6 Pow+Her 7.0.4 13 ----- Pow+Her 7.1.3 0.7 0.4 0.5 1.5 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.2 0.3 0.5 0.6 0.7 0.8 1.2 ATLAS Preliminary  $\sqrt{s} = 13 \text{ TeV}, 36 \text{ fb}^$ to data Latest Sherpa models b-frag better Ratio Smooth effects of FSR  $\alpha_s$  and frag function parameters 0.9

on Py8 data/MC agreement: perfect tuning inputs

19

# ATLAS *b*-fragmentation with mesons

Explicit reconstruction of  $B^{\pm} \rightarrow J/\psi K$  decay channel

- Two muons:  $p_T > 6$  GeV, 2 < m<sub>µµ</sub> < 9 GeV
- Third track, cuts on vtx  $\chi^2$  & pair/triplet masses

Unfold to particle-level with kin cuts on  $\mu$  and  $K p_{T}$ 

Measure fragmentation functions:

$$z = \frac{\vec{p}_B \cdot \vec{p}_j}{|\vec{p}_j|^2}; \quad p_{\mathrm{T}}^{\mathrm{rel}} = \frac{|\vec{p}_B \times \vec{p}_j|}{|\vec{p}_j|}$$





# ATLAS *b*-fragmentation with mesons

Unfolding more limited by transfer resolution for  $p_{T,rel}$  than z





Limiting systematics a balance btw *B* reco, jet reco, and unfolding uncertainties

# ATLAS *b*-fragmentation with mesons

### Longitudinal and transverse frag functions in jet- $p_{T}$ bins

⇒ Herwig7 showers and Sherpa cluster hadronisation show deviations wrt data



# ATLAS *b*-fragmentation with mesons

Average values of frag functions vs jet  $p_{\tau} \Rightarrow$  flags O(10%) mismodelling



#### CMS *b*-jet fragmentation from *tt* decays CMS-PAS-TOP-18-012

CMS' version is more directly tied to the Lund-Bowler fragmentation function ansatz and fitting of its  $r_b$  parameter

Explicit reconstruction of  $J/\psi$  and  $D^0$ mesons (the latter with and without a muon-tagged decay)

Use mesons as final-state proxies for the decayed *b*-hadron. Distributions of momentum fractions used to fit  $r_b$ 



#### CMS *b*-jet fragmentation from *tt* decays CMS-PAS-TOP-18-012



Set of three proxy fragmentation fractions extracted, used to constrain  $x_{B}$ 

# Significant precision improvements wrt LEP/SLD *Z*-pole tunes:



# ATLAS $g \rightarrow bb$ at small opening angles

Focus on final-state  $g \rightarrow bb$  splitting kinematics in boosted region  $p_T > 450$  GeV R=1 akT jets, 33/fb of 13 TeV *pp* data

g manna g

Require two *b*-tagged, ghost-assoc VR track-jets as *b* proxies, 60% working point

Flavour fit, via signed-impact-parameter distributions for subleading track, per observable bin, e.g.  $\Delta R_{bb}$  right: Mostly slight *BB*-fraction overestimates



Phys. Rev. D 99 (2019) 052004,

arXiv:1812.09283,

Plot page

# ATLAS $g \rightarrow bb$ at small opening angles

#### Flavour-fraction fits, per bin of each observable

(BB ~good, large differences in B and L+C)



Jet fragmentation in tt

arXiv:1808.07340 / Phys. Rev. D 98 (2018) 092014

# 36 fb<sup>-1</sup> of 13 TeV *pp* dataset, with semileptonic top-pair selection

Exactly 1 tight, isolated lepton; 63% *b*-tag working point  $\Rightarrow$  94%-pure *tt* 

#### akT4 jets, $p_{\rm T}$ > 30 GeV, flavour groups:

- inclusive
- *b*-jet: via tag, incl  $g \rightarrow bb$
- q-enh: via W-mass window, 50% pure
- g-enh: neither of the above, 58% pure

Particle-level flavour  $\Rightarrow$  ghost matching &  $m_{ii}$ 







arXiv:1808.07340 / Phys. Rev. D 98 (2018) 092014

#### Lots of substructure observables:

- constituent-multiplicity &  $p_{T}$ -dispersion
- angularities: width, LHA, jet thrust
- eccentricity
- soft-drop fraction and groomed  $N_{\rm ch}$
- groomed-subjet angles
- N-subjettiness ratios
- ECFs C<sub>1,2,3</sub>, M<sub>2</sub>, N<sub>2,3</sub>

Several observables measured for both charged and charged+neutral constituents!





arXiv:1808.07340 / Phys. Rev. D 98 (2018) 092014





Breakdowns of observables by flavour category, plus correlations: will be ideal for MC dev & tuning via Rivet

# Other jet structure measurements

#### **Top-decay**

**Eur. Phys. J. C 78 (2018) 847** — ATLAS 13 TeV measurement of colour flow between  $W \rightarrow qq'$  jets in *tt* with jet-pull observables arXiv:1805.02935

#### **Boosted large-***R***jets**



JHEP 08 (2019) 033 — ATLAS 13 TeV measurements of jet substructure in top-quark, *W*-boson, and light jets arXiv:1903.02942

JHEP 11 (2018) 113 — CMS 13 TeV jet mass distributions in dijet events, arXiv:1807.05974

Phys. Rev. D 86 (2012) 072006 — ATLAS 7 TeV properties of boosted jets arXiv:1206.5369

JHEP 1205 (2012) 128 — ATLAS 7 TeV jet mass and substructure arXiv:1203.4606

# Conclusions

- Measurements sensitive to jet fragmentation have grown far beyond direct measurements cf. LEP
  - A multitude of angularities, correlation functions, substructure observables from both ATLAS and CMS
  - Use of track-based & all-particle reconstructions, and dig into jet-flavour dependence
  - Ghost-association of track-jets or reconstructed hadrons, esp. for *b*-quark studies
  - Grooming algorithms reduce pile-up dependence, provide another facet
  - Also large-*R* jets and boosted phase-space
- Ways to improve syst precision? Most analyses only 36/fb so far!!
- Dawn of Run 3 a good time to revisit 7 TeV MC tunes & studies



# ATLAS g→bb fragmentation — arXiv:1812.09283

# Super-quick summary: b-tagged track subjets in boosted jets

Fiducial differential cross-sections in b-subjet separation, mass,  $p_T$  balance, and polarisation angle

Key: flavour fit via signed impact param





### **Observables**

Fragmentation function *D* defined vs  $\zeta = p_T$  fraction of hadron *h* wrt its containing jet  $p_T$ , from parton *p*  $\Rightarrow$  DGLAP pQCD evolution; mirror image of PDFs

This paper uses charged hadrons, but full (calo) jet  

$$\Rightarrow \langle n_{ch} \rangle$$
 and differential  $1/N_{iet} dN_{iet}/d\langle n_{ch} \rangle$ 

- + summed fragmentation function: differential in  $p_T$  fraction  $\zeta$  and jet  $p_T \Rightarrow$  extract partial fractions, moments & weighted sums
- Relative transverse momentum
   Radial profile (non-p<sub>T</sub>-weighted)

$$\mu \frac{\partial}{\partial \mu} D_p^h(\zeta,\mu) = \sum_{p'} \int_{\zeta}^1 \frac{d\zeta'}{\zeta'} \frac{\alpha_{\rm S}(\mu) P_{p' \leftarrow p}(\zeta',\mu)}{\pi} D_{p'}^h\left(\frac{\zeta}{\zeta'},\mu\right)$$

 $\langle n_{\rm ch} \rangle (p_{\rm T}^{\rm jet}) = \sum_{p} f_{p}(p_{\rm T}^{\rm jet}) \sum_{h \text{ charged}} \int_{\rm threshold/p_{\rm T}^{\rm jet}}^{1} d\zeta D_{p}^{h}(\zeta, p_{\rm T}^{\rm jet})$ 

$$F(\zeta, p_{\rm T}^{\rm jet}) = \sum_{p} f_p(p_{\rm T}^{\rm jet}) \sum_{h \text{ charged}} D_p^h(\zeta, p_{\rm T}^{\rm jet})$$

$$p_{\rm T}^{\rm rel} \equiv p_{\rm T}^{\rm charged \ particle} \sin \Delta \phi$$
$$\rho_{\rm ch}(r, p_{\rm T}^{\rm jet}) = (1/N_{\rm jet}) dn_{\rm ch}/2\pi r dr$$

# **Detector correction & uncertainties**

Unfolding from detector obs to fiducial phase space: particle-level tracks & jets from particles with  $cT_0 > 10$  mm; muons and neutrinos excluded from jets



Unfolding by 2D iterative Bayes method (1 iter) sandwiched by explicit in/out migration corrs.

Main uncertainties: tracking, jet scale, binning & unfolding, depending on observable



### **Detector-level variables**

Raw distributions of  $n_{trk}$ , track momentum fraction, track  $p_{T,rel}$ , and track radial profile

For a 1 TeV jet, most probable  $n_{trk}$  is ~15, and most probable momentum fraction ~1%

Track  $p_{T,rel}$  and r (radial profile) distributions peak at zero since radiation dominantly collinear



# Unfolded partial sums: $n_{\rm ch}$ fraction in bins of $\zeta$

 $\int_0^X F(\zeta) d\zeta / \int F(\zeta) d\zeta = n_{ch}(\zeta < X) / n_{ch}$ Fractions of charged particles with  $\zeta \le 10\%$ , 1%, and 0.1% vs jet  $p_{\tau}$ 

Fraction of small-fraction particles increases with jet  $p_T$ , cf. hadronisation scale Small mismodelling of 10% by Herwig; with Sherpa & Py8 in less inclusive bins



# Quark/gluon jet discrimination

An important application of jet structure data is development of methods to extract information about quark/gluon jet origins

Ideally in a well-defined, QCD-aware way!

- Central/forward jet: roughly, central and low-p<sub>T</sub> jets are more likely to be gluon-initiated
- → Extract q/g components with an MC-template procedure
- New: model-independent q/g extraction by data-driven "topic" modelling



# Mean observables with central/forward-jet split

Aim of central/forward jet distinction is to bias quark or gluon jet origin

Biases allow extraction of separate q/g-like fragmentation functions by comparison of forward and central jet ones

Note Pythia mismodelling of split  $n_{ch}$  distributions, unlike inclusive. Most c/f-split mean observables are well-described



42

## Model-dependent quark/gluon jet characterisation

q/g extraction by use of MC flavour fractions *f*, nominally from Pythia:

$$h_{i}^{f} = f_{q}^{f} h_{i}^{q} + (1 - f_{q}^{f}) h_{i}^{g}$$
  
$$h_{i}^{c} = f_{q}^{c} h_{i}^{q} + (1 - f_{q}^{c}) h_{i}^{g}$$

Jet flavour defined by hardest parton geometrically associated to the jet: many theory issues, and potential sources of uncertainty

Extracted q/g-like fragmentation observables fit expectations:



# Model-independent quark/gluon jet characterisation

# Novel approach is to use "topic modeling" extraction.

The categories are defined by data rather than MC internals:

$$h_{i}^{T_{1}} = \frac{h_{i}^{f} - \left(\min_{j}\{h_{j}^{f}/h_{j}^{c}\}\right) \times h_{i}^{c}}{1 - \min_{j}h_{j}^{f}/h_{j}^{c}}$$
$$h_{i}^{T_{2}} = \frac{h_{i}^{c} - \left(\min_{j}\{h_{j}^{c}/h_{j}^{f}\}\right) \times h_{i}^{f}}{1 - \min_{j}h_{j}^{c}/h_{j}^{f}}$$



Interesting new approach. Limitation: alignment of topics to q and g template ideas relies on the existence of bins dominated by q or g: applies to  $n_{ch}$  distribution only

# Comparing quark/gluon jet characterisations

**Pythia-based vs topic modeling:** good description by Pythia for quarks in both; less good for gluons. "Quark" topic also aligns well with quarks, worse for gluons.

pQCD normalization-anchored, since can't handle non-perturbative physics: compares well to q/g extractions





45

#### ATLAS-CONF-2020-050

Data

with uncertainty

with uncertaint

# ATLAS *b*-fragmentation

#### p moment

- Ratio of *b*-hadron  $p_{\tau}$ to average of charged lepton  $p_{\tau}$ 's comparison of the b momentum to the *tt* parent event scale
- Lepton  $p_{T}$  more precisely measurable than *b*-jets or *tt*
- Sensitive to QCD radiation not contained in the *b*-jets



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> 1.5 probe-jet / Total Signal modeling \_.\_.\_ Tracking Pileup ······ Other 0.005 0.000 0 ρ bin

#### ATLAS-CONF-2020-050

# ATLAS *b*-fragmentation

- z<sub>ch,T</sub> (transverse) moment
  - *p*<sub>T,rel</sub> (projected *p*<sub>T</sub> wrt the parent jet axis)
     proved difficult to measure
  - Correlated with longitudinal projection, plus some residual information about directional kicks from radiation



# CMS Z+BB cross sections at 7 TeV

 Measure the production of a Z boson in association with B hadrons as a function of angular correlation especially the B-hadron pair production at small angular separation where there are significant theoretical uncertainties in the description of collinear production







### CMS Z+BB cross sections at 7 TeV



• ALPGEN well describes data in collinear regions ( $\Delta R_{BB} < 0.7$ ) while MADGRAPH and amc@NLO are lower than data

• At large  $\Delta R_{BB}$ , all predictions agree with data

### CMS Z+BB cross sections at 7 TeV



# CMS angular correlations between BB at 7 TeV

JHEP03 (2011) 136

- *BB* production at 7 TeV
- B hadrons are identified using reconstructed secondary vertex → probe small separation angle
- Simulation is normalized to regions > 2.4



- None of the predictions describe the data very well
- amc@NLO mismodels at small angle where gluon splitting is significant

### CMS jet mass in dijet events at 13 TeV arXiv:1807.05974

Uses 33 fb<sup>-1</sup> dataset of 13 TeV pp collisi



52

# CMS jet mass in dijet events at 13 TeV arXiv:1807.05974



53