

**Physics Institute** 



# Parton showers and event generators studies and modeling

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QCD@LHC 2024

# Underlying event, proton structure and particle production

#### Underlying-event studies with strange hadrons in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

axiv:2405.05048

Study of Z boson plus jets events using variables sensitive to doubleparton scattering in pp collisions at √s = 13 TeV (CMS) arxiv:2105.14511

Energy scaling behavior of intrinsic transverse momentum parameters in Drell-Yan simulation (CMS) arxiv:2409.17770

affects the MC





$$K_S^0 \to \pi^+ \pi^-, \Lambda \to \pi^- p, \bar{\Lambda} \to \pi^+ \bar{p}$$

 $\rightarrow$  use displaced two-particle vertices to reconstruct them

#### Measure:

- Strange hadron density or fraction
- In Towards, Transverse or Away regions
- In bins of leading jet  $p_{T} % \left( p_{T} \right) = p_{T} \left( p_{T} \right) \left( p_{T} \right)$

Hadronization & multiple-parton interaction (MPI) models

The data can be used to tune

Strange hadron production in UE

Measure them

https://arxiv.org/abs/2405.05048



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\ N(K<sup>0</sup>) / ۵۱ ک Data EPOS-LHC Low leading jet  $p_T$ **PY8-A2** 0.1 PY8-MONASH+CR ~ soft scattering region • Increase of  $K^0_S$  density versus jet  $p_T$ 0.05 EPOS-LHC describes the data √s=13 TeV ATLAS  $\rightarrow$  different pp collision model 67x10<sup>6</sup> Events **Transverse Region** (hydrodynamic) from Pythia MC/Data • Pythia A2 & color-reconnection 0.8 tune under-estimates 30 35 10 15 20 25 5 40 Leading-jet  $p_{\perp}$  [GeV] Color-reconnection tune performs better the A2 tune N(K<sup>0</sup>) / N(ch) Data 0.04 EPOS-LHC PY8-A2 PY8-MONASH+CR 0.03 0.02 None of the generators describe well the  $K_{\rm S}^0$  / Nch(prompt) √s=13 TeV ATLAS 0.01 67x10<sup>6</sup> Events Transverse Region MC/Data 1.2 0.8 0.6 5 10 15 20 25 30 35 40 Leading-jet  $p_{T}$  [GeV] University of Zürich Weijie Jin



Low leading jet  $p_T$ ~ soft scattering region

- Increase of  $K^0_S$  density versus jet  $p_T$
- EPOS-LHC describes the data

   → different pp collision model
   (hydrodynamic) from Pythia
- Pythia A2 & color-reconnection tune under-estimates
- Color-reconnection tune performs better the A2 tune

• None of the generators describe well the  $K_S^0$  / Nch(prompt)



## High leading jet $p_T$ ~ hard scattering region



- Weak dependence on jet  $p_T$ 
  - Dominated by non-diffractive hard collisions
  - $\rightarrow$  the measured  $K_S^0$  dominated by MPI
  - $\rightarrow$  especially in region transverse to leading jet

#### • EPOS-LHC mismodeling

- not monotonic & underestimates the data
- $\rightarrow$  probably because of lack of hard scattering model
- Pythia tunes predicts the shape well but under estimates the yield overall





**Enhancement** of  $K_S^0$  and  $\Lambda + \overline{\Lambda}$  / Nch (prompt) in towards region of leading jet  $\rightarrow$  the feature is captured by **EPOS-LHC** 

#### Summary

- These strangeness observables are sensitive to hadronization models (e.g. color reconnection)
   → inputs for generator tuning
- They reflect non-perturbative effects in pp collisions (difference between EPOS & Pythia)
  - $\rightarrow$  useful for investigating non-perturbative phenomena e.g. quark-gluon plasma

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#### Double parton scattering (DPS) in Z+jets events arxiv:2105.14511

 $Z \rightarrow \mu\mu$  production is experimentally clean and theoretically well understood

 $\rightarrow$  use it to explore the simultaneously occurred scatterings — presence of MPI, typically DPS

The kinematics of jets tend to be **correlated** with Z & **balance** the Z momentum

The jets are less likely to balance each other

Design variables about Z&jet, Z&dijet, and two jets relations

- sensitive to momentum correlation
- sensitive to momentum balance University of Zürich

Z+jets from double parton scattering (DPS)

The jets more likely to balance each other

 $\rightarrow$  the kinematics of jets are **less correlated** with Z

→ the jets are less likely to balance the Z momentum

Two separate scatters

The measurements reflect DPS modeling

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#### Azimuthal angle between Z and leading jet University of Zürich





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The variables show high sensitivity to DPS

• The tunes were **fit** to data from **soft QCD process** → **generally describes well** these variables from hard scattering process (Z production)

Input for DPS-specific tunes & global tunes with other soft QCD measurements

$$\Delta_{\rm rel} p_{\rm T}(j_1, j_2) = \frac{|\vec{p}_{\rm T}(j_1) + \vec{p}_{\rm T}(j_2)|}{|\vec{p}_{\rm T}(j_1)| + |\vec{p}_{\rm T}(j_2)|}.$$

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#### Intrinsic $k_T$ in generators probed by Drell-Yan $p_T$

**Parton Shower** 

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#### Intrinsic kT:

The transverse momenta of the partons in the incoming

colliding hadrons

 $\rightarrow$  Not calculable in perturbative QCD

 $\rightarrow$  Described by phenomenological models



Use Drell-Yan  $p_T$  to probe the intrinsic  $k_T$ 

- DY  $p_T(l^+l^-)$  measured from precisely reconstructed  $l^+l^-$
- DY  $p_T(l^+l^-)$  reflects the intrinsic  $k_T$  from incoming partons  $\rightarrow$  especially the low  $p_T(l^+l^-)$  region

arxiv:2409.17770

**Generator models** of intrinsic  $k_T$ :

- Fermi motion of partons (non-perturbative)
- Soft parton emissions not included by the parton shower in initial state radiation (ISR) (perturbative + non-perturbative)



### Intrinsic $k_T$ in generators probed by Drell-Yan $p_T$

Intrinsic  $k_T$  parameter is tuned to DY differential XS at low  $p_T(l^+l^-)$ 

 $\rightarrow$  Tune results gives hints on parton Fermi motions and soft ISR, non-perturbative and perturbative

Tune both **Pythia** and **Herwig** with a few underlying-event (UE) tunes + NLO DY matrix elemens  $\rightarrow$  Study the impact of **parton shower** and **UE** model

Tune to data from experiments of various  $\sqrt{s}$  and hadron types

- NuSea, R209, PHENIX, D0, CDF, CMS, ATLAS, LHCb
- +  $\sqrt{s}$ : 38.8 GeV— 13 TeV,  $m(l^+l^-)$  5 GeV—1 TeV



For each  $\sqrt{s}$ , tune intrinsic  $k_T$  separately for various  $m(l^+l^-) \sim$  hard scattering scale

 $\rightarrow$  Stable tune results versus  $m(l^+l^-) \sim x_1 x_2 \sqrt{s}$  under fixed  $\sqrt{s}$ 

 $\rightarrow$  Weak/no dependence on parton momentum fraction  $x_1, x_2$ 



### Intrinsic $k_T$ in generators probed by Drell-Yan $p_T$



Tune intrinsic  $k_T$  under various  $\sqrt{s}$ 

- Tune results increase with  $\sqrt{s}$
- Power-law scaling behaviour log(intrinsic  $k_T$ )  $\propto$  log( $\sqrt{s}$ )



Parton Fermi motion cannot depend on  $\sqrt{s}$ 

 $\rightarrow$  the behaviour comes from missing ISR in parton shower



The trend is similar for Pythia & Herwig  $\rightarrow$  The scaling behaviour is **robust versus parton shower model** ( $p_T$ -ordered or angular-ordered)

Tuning result with CASCADE (arxiv:2312.08655) shows a weaker dependence on  $\sqrt{s}$ 

CASCADE simulation uses **parton-branching** method to **describe transverse momentum dependent PDF** 

 $\rightarrow$  Different from the Pythia and Herwig parton shower and collinear PDF

 $\rightarrow$  Includes more non-perturbative soft gluon emissions

The **intrinsic**  $k_T - \sqrt{s}$  scaling behaviour in Pythia & Herwig probably related non-perturbative gluon emissions

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## Jets and jet substructure

#### Dependence of the Jet Energy Scale on the Particle Content of Hadronic Jets in the ATLAS Detector ATL-PHY-PUB-2022-021

Measurement of energy correlators inside jets and determination of the strong coupling  $\alpha_S(m_Z)$  (backup)

covered by Oleg Kuprash arxiv:2402.13864

#### Calibration of jets depending on simulation models ATL-PHY-PUB-2022-021



#### Reconstructed jet energy does not exactly equal to the truth

- $\rightarrow$  calibration (jet energy scale) needed based on MC models of jets and detector simulation
- Electromagnetic shower can be correctly reconstructed  $\langle E_{reco}/E_{true}\rangle = 1$
- Energy deposit of hadronic shower is not fully reconstructed (non-compensation hadronic calorimeter)

 $E_{reco}$  depends on **MC models of jet** 

– hadron contents & kinematics

→ Jet models affects the calibration

- Averagely under-calibrated  $\langle E_{reco}/E_{true} \rangle < 1$
- $\langle E_{reco}/E_{true} \rangle$  depends on energy/type of hadrons

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#### **Calibration of jets depending on simulation models**

Ratio of Simulated jet response  $(p_T^{reco}/p_T^{true})$  to Pythia response



#### Calibration of jets depending on simulation models





Quark jets and gluon jets have different jet response

- $\rightarrow$  different **fragmentation pattern**  $\rightarrow$  hadron momentum spectrum
- $\rightarrow$  different hadron contents e.g. fraction of baryons & kaons

Important to model the jet fragmentation pattern and hadron contents

#### **Calibration of jets depending on simulation models**



The modeling differences of hadron contents are investigated by Baryon Energy Fraction  $f_{baryon}$  & Kaon Energy Fraction  $f_{kaon}$ 



Reweighting Herwig to Pythia by  $f_{baryon}$  and  $f_{kaon}$  versus  $p_T^{jet} \rightarrow$  closer jet response !



First quantitive estimate of the effects of hadron contents on jet reconstruction  $\rightarrow$  encourages improvement on hadronization models for jet calibration & precision measurements

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# Modeling of Top processes

#### Simulation of on- and off-shell *ti* production with the Monte Carlo generator b\_bbar\_4I at CMS <u>CMS-NOTE-2023-015</u>

Study of matrix element correction in *tī* events using MG5\_aMC@NLO+Pythia8

ATL-PHYS-PUB-2024-002

Studies on the improvement of the matching uncertainty definition in topquark processes simulated with Powheg+Pythia 8 <u>ATL-PHYS-PUB-2023-029</u>

#### **State-of-the-art MC simulation of** $t\bar{t}$ **at NLO**

CMS-NOTE-2023-015



Sketch of  $t\overline{t}$  processes



One of the top quarks goes off-shell  $\rightarrow$  Large interference with tW processes



For precise modeling of  $t\bar{t}$  kinematics  $\rightarrow$  **Full NLO calculation** of  $pp \rightarrow b\bar{b}l^+l^-\nu\bar{\nu}$  needed (assume leptonic final states)

 $\rightarrow$  CMS simulation on board

**b\_bbar\_41 (bb41)** generator in POWEG BOX RES package + matched PYTHIA shower (CP5 tune)

### **State-of-the-art MC simulation of** $t\overline{t}$ **at NLO**

CCMS



MC tests on a variable sensitive to  $t\bar{t}$ , tW interference

Lower accuracy MC samples assuming stable top: NLO  $t\bar{t}$  production in narrow width approximation (NWA) NLO tW production in NWA + interference treatment to prevent double counting • diagram removal (DR) scheme  $\rightarrow t\bar{t} + tW$ , DR • diagram subtraction (DS) scheme  $\rightarrow t\bar{t} + tW$ , DS

 $m_{b\ell}^{\min} = \min \left[ \max \left( m_{b_1 \ell_1}, m_{b_2 \ell_2} \right), \max \left( m_{b_1 \ell_2}, m_{b_2 \ell_1} \right) \right]$ 

+ LO top quark decay

**bb41** describes data better than  $t\bar{t} + tW$ , DR,  $t\bar{t} + tW$ , DS in regions sensitive to off-shell  $t\bar{t}$  and interference

NLO  $t\overline{t}$  production and NLO top quark decay + LO treatment of  $t\overline{t}$ , tW interference  $\rightarrow$  **ttb\_NLO\_dec** 

**ttb\_NLO\_dec** and **bb41** matches data similarly

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#### **State-of-the-art MC simulation of** $t\bar{t}$ **at NLO**



Prediction of top quark mass spectrum is significantly different for **bb41** and  $t\bar{t} + tW$ , **DR**,  $t\bar{t} + tW$ , **DS**  $\rightarrow$  indicates the effects of off-shell top production and NLO top decay  $\rightarrow$  expect to give **bb41** to give a more accurate

prediction



#### Studies of matrix element correction (MEC) in $t\bar{t}$ events using MG5\_aMC@NLO+Pythia8

#### ATL-PHYS-PUB-2024-002



 $t\bar{t}$  production at NLO by MG5\_aMC@NLO (narrow width approximation) + Pythia shower of  $t\bar{t}$ 

Already including NLO corrections in top production





MEC added in Pythia shower for hard recoils (new recommendation for Pythia\*)

- Higher order corrections to top decays
- More precise than NL parton shower

\* Frixione, S., Amoroso, S., & Mrenna, S. (2023). Matrix element corrections in the Pythia8 parton shower in the context of matched simulations at next-to-leading order. *The European Physical Journal C*, *83*(10), 970.

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#### Studies of matrix element correction (MEC) in $t\bar{t}$ events using MG5\_aMC@NLO+Pythia8

ATLAS EXPERIMENT

MC test for MG5\_aMC@NLO

• Inclusive  $t\overline{t}$  production (MG5aMC)

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Pythia shower with/without MEC

•  $t\overline{t}$  production + FxFx merging up to two partons at the Born level (**FxFx**)



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#### ATL-PHYS-PUB-2023-029

Matrix element (ME) calculation of the hard scatter ------ Parton shower

Match

Double counting or holes in the phase space  $\rightarrow$  Matching uncertainty

**Previous** uncertainty estimation

- Difference between PowhegBox+Pythia and MG5\_aMC@NLO+Pythia
- $\rightarrow$  includes **multiple effects**: shower adjustments to ME generator, top-decay settings
- → Over-coverage for matching uncertainty

New prescription for the matching uncertainty:

- Both Powheg and Pythia have emissions based a  $p_T$  based variable "hardness"
- Pythia vetos the emission above the "hardness" to avoid double counting
- $\rightarrow$  Use various choices of "hardness" ( $p_T^{hard}$ ) definition to estimate the uncertainty





**Powheg+Pythia**  $p_T^{hard}$  = 2 "hardness" as the minimal  $p_T$  of all the Powheg final-state partons

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Some effects previously covered by **PowhegBox** and **MG5\_aMC@NLO** differences are not included

Modeling of top decay lineshape

 $\rightarrow$  corresponding new prescriptions for them

- Modeling of  $\operatorname{top} p_T\operatorname{spectrum}$ 

Similar approach in **PowhegBox** and **MG5\_aMC@NLO** for top production and decay

- narrow width approximation for top production
  - + smear mass by Breit-Wigner distribution
  - + reshuffle momenta of other particles for energy-momentum conservation



model difference for the two generators

- top decay lineshape difference

→ isolate this effect: replace the reshuffling method of PowhegBox with the MG5\_aMC@NLO one (MadSpin)

top decay lineshape difference is approximated by the PowhegBox and PowhegMadSpin difference

Some effects previously covered by PowhegBox and MG5\_aMC@NLO differences are not included

- Modeling of top decay lineshape
- Modeling of top  $p_T$  spectrum

Several NLO+PS generator shows a similar trend of mismodeling  $\rightarrow$  Mismodeling comes from NNLO contribution



Solution: reweight **PowhegBox+Pythia** to NNLO calculation by  $m^{t\bar{t}}$  and  $p_T^{t\bar{t}}$ 

•••••• reweighted sample

Description to data is improved by reweighting



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#### **Summary**

#### Non-perturbative QCD effects & modeling in pp collisions

- Underlying event study: strange hadron measurement in UE
- **Double parton scattering**: use Drell-Yan process as a standard candle to measure the extra scatter
- Intrinsic  $k_T$  in generators: how the parameter scales with  $\sqrt{s}$  and hard-scattering scale

#### Jets as a probe for generator models

- How the hadron content modeling of jets affect the jet calibration
- Use jet substructure to extract the strong coupling constant  $\alpha_S(m_Z)$

#### **Development of top process models**

- Full **NLO simulation** of on-shell and off-shell  $t\bar{t}$  at the CMS
- Adding matrix element corrections to improve  $t\bar{t}$  simulation with MG5\_aMC@NLO at the ATLAS
- Improved matching uncertainty estimation subscription in top processes from Powheg at the ATLAS

#### **Studies not discussed in the talk**

- Measurement of the mass dependence of the transverse momentum of lepton pairs in Drell--Yan production in proton-proton collisions at  $\sqrt{s} = 13$  TeV (<u>CMS-SMP-20-003</u>)
- Measurement of double-parton scattering in inclusive production of four jets with low tranverse momentum in proton-proton collisions at  $\sqrt{s} = 13 \text{ TeV} (\underline{\text{CMS-SMP-20-007}})$
- Study of quark and glon jet substructure in Z+jet and dijet events from pp collisions (CMS-SMP-20-010)
- Measurement of jet multiplicity and jet transverse momentum in multijet events in proton-protn collisions at  $\sqrt{s} = 13 \text{ TeV} (CMS-SMP-21-006})$
- Measurement of inclusive and differential cross sections for single top quark production in association with a W boson (<u>CMS-TOP-21-010</u>)
- Measurement of differential cross sections for the production of top quark pairs and of additional jets (<u>CMS-TOP-20-006</u>)
- Measurement of the top quark pole mass using pair produced top quarks (CMS-TOP-21-008)
- Measurement of the inclusive and differential tty cross section (<u>CMS-TOP-21-004</u>)
- Measurement of the shape of the b quark fragmentation function using charmed mesons produced inside b jets from (<u>CMS-TOP-18-012</u>)
- Studies of Monte Carlo predictions for the  $t\bar{t}bb$  process (<u>ATL-PHYS-PUB-2022-006</u>)
- Measurements of observables sensitive to colour reconnection in  $t\bar{t}$  events with the ATLAS detector at  $\sqrt{s} = 13 \text{ TeV} (\underline{\text{TOPQ-2019-01}})$
- Modelling and computational improvements to the simulation of single vector-boson plus jet processes for the ATLAS experiment (<u>PMGR-2021-01</u>)



#### **Double parton scattering in 4-jet events with low** $p_T$ <u>CMS-SMP-20-007</u>

Multijet is the background for many measurements  $\rightarrow$  important to improve the theoretical models of multijet



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![](_page_35_Picture_6.jpeg)

#### Double parton scattering in 4-jet events with low $p_T$

![](_page_36_Figure_1.jpeg)

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#### Double parton scattering in 4-jet events with low $p_T$

![](_page_37_Figure_1.jpeg)

CMS

Azimuthal angular difference between the hard and soft jet pairs

$$\Delta S = \arccos\left(\frac{(\vec{p}_{\text{T},1} + \vec{p}_{\text{T},2}) \cdot (\vec{p}_{\text{T},3} + \vec{p}_{\text{T},4})}{|\vec{p}_{\text{T},1} + \vec{p}_{\text{T},2}| |\vec{p}_{\text{T},3} + \vec{p}_{\text{T},4}|}\right)$$

← More robust MC behaviours under various shower models

Suitable for extracting the DPS contribution and DPS-specific tunes

#### **Energy correlators in jets & extraction of** $\alpha_S(m_Z)$

![](_page_38_Picture_1.jpeg)

arxiv:2402.13864

Cross section of jet production

![](_page_38_Figure_3.jpeg)

#### Energy correlators in jets & extraction of $\alpha_S(m_Z)$

![](_page_39_Figure_1.jpeg)

#### **Energy correlators in jets & extraction of** $\alpha_S(m_Z)$

![](_page_40_Picture_1.jpeg)

![](_page_40_Figure_2.jpeg)

Measure the E3C/E2C versus  $x_L$  slope at various  $p_T^{jet}$ 

Generate MC predictions from various  $\alpha_S(m_Z)$   $\rightarrow$  Interpolate

Fit MC templates to data  $\rightarrow$  measured  $\alpha_S(m_Z)$  $0.1229^{+0.0014}_{-0.0012} \text{ (stat)}^{+0.0030}_{-0.0033} \text{ (theo)}^{+0.0023}_{-0.0036} \text{(exp)}$ 

Most precise  $\alpha_{S}(m_{Z})$  from jet substructures