Event-Generator Tuning — Overview

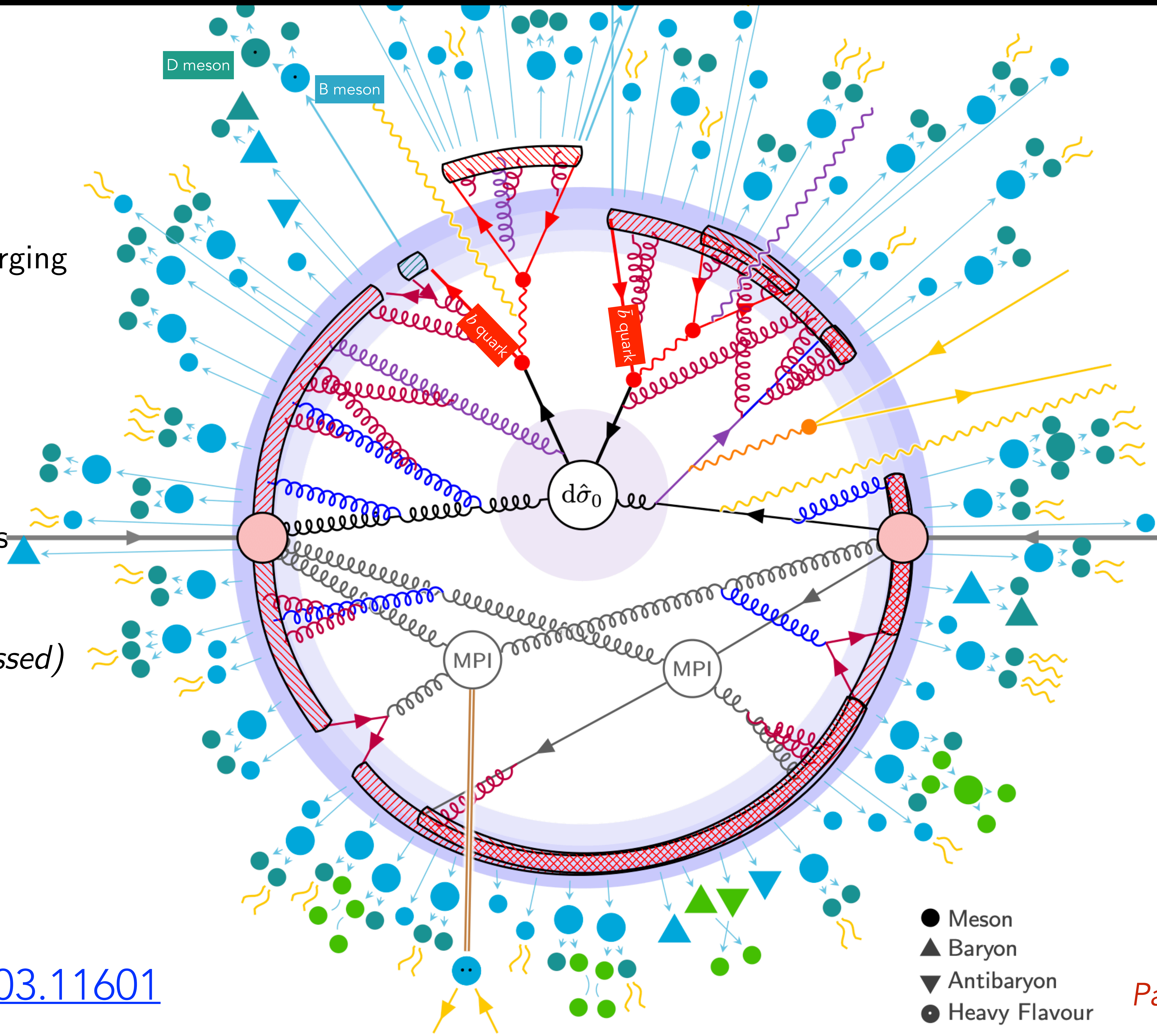
P. Skands

What are we tuning? Components of Modern Monte Carlo Event Generators:

Parton Level

- Hard Interaction
- Resonance Decays
- MECs, Matching & Merging
- FSR
- ISR*
- QED
- Weak Showers
- Hard Onium
- Multiparton Interactions
- Beam Remnants*

(: incoming lines are crossed)*



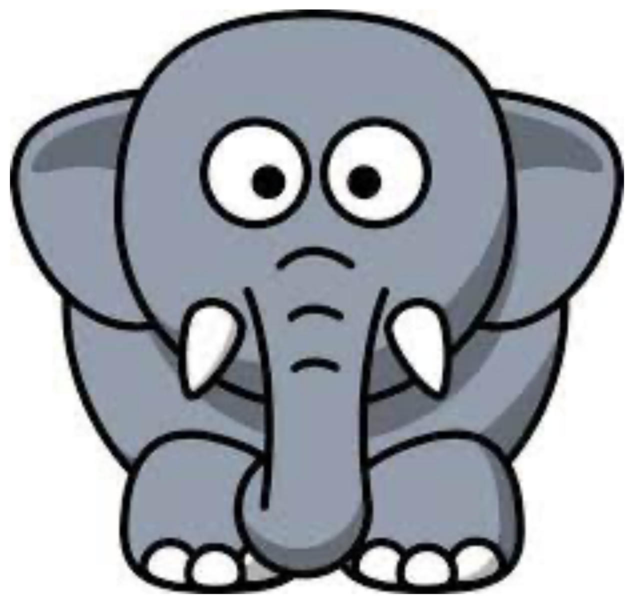
Hadron Level

- Beam Remnants*
- Strings
- Clusters
- Colour Reconnections
- String Interactions
- Bose-Einstein & Fermi-Dirac
- Primary Hadrons
- Secondary Hadrons
- Hadronic Reinteractions
- QED in Hadron Decays

(: incoming lines are crossed)*

Figure from arXiv:2203.11601

Tuning at Parton Level (?)



Purist: you should not tune perturbation theory!

Uncalculated orders / coefficients should be set to zero.

And no explicit power corrections (unless by intent)

Goal: a theory calculation that delivers a clean simple-to-understand prediction, at a stated accuracy.

It may agree or disagree with data. That's ok, consistent with the stated accuracy.

It may disagree a **lot** with data. Not your problem.

(ATLAS and CMS may end up with a problem.)

Problem: Parton showers *always* generate subleading structures …

Hard to control and generally not possible to set cleanly to zero.

Pythia Philosophy

Vice to Virtue: nothing special about zero as guess for higher orders.

Goal: deliver a description that faithfully represents as much data as possible.

Replace purist view by Sanity Limit: avoid undue violence to the underlying physics model.

1) Allow explicit/controlled coefficients to deviate from exact values

Theoretically consistent if deviation $\lesssim$ uncalculated corrections.

PYTHIA example: use effective values for $\alpha_s(M_Z)$, consistent with other LO determinations of it.

Slightly extreme: our one-loop α_s "magic trick" for NLO-level agreement at LEP.

Caveat: no guarantee of universality!

Pythia Philosophy

2) Control for non-universalities

Consider several complementary processes and contexts

Possibly weighted by how much you care about each

(and/or by how much the experiments care!)

E.g., for the effective FSR α_s value in Pythia

We have 3-jet LO MECs and use **3- and 4-jet event shapes** + ditto **jet rates** at LEP as main constraints (universality across jet multiplicities)

And then we cross check with **jet shape profiles at the LHC**.

Always a risk that this can fail. E.g., tensions between different processes at LHC (eg top); experiments retune α_s and associated worries.

One example that has not been clean to disentangle: b-quark fragmentation in the top decay jet.

+ Hard to be consistent in context of matching and merging $\Longrightarrow$ unsolved problem.

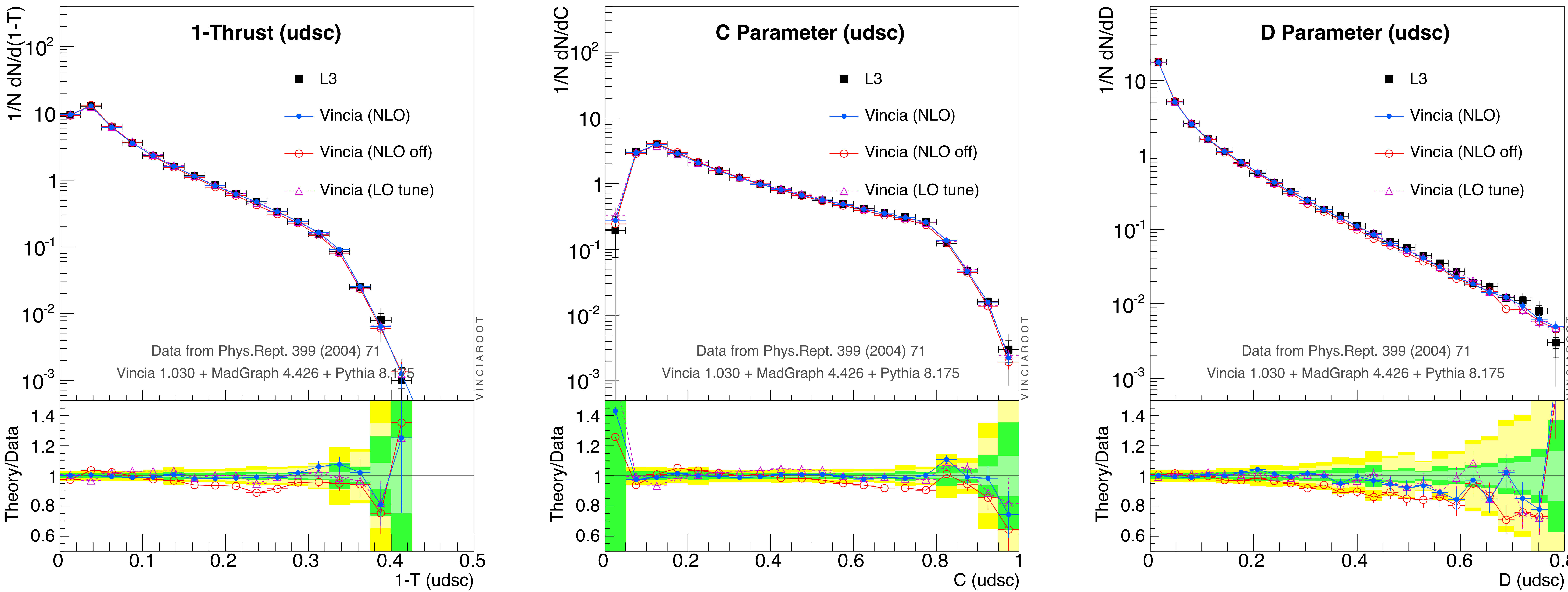
Hartgring, Laenen, Skands, arXiv:1303.4974

First LEP tune with NLO 3-jet corrections (NNLO Z Decay)

NLO tune (3-jet LO): $\alpha_s(M_Z) = 0.139$ (1-loop running, MSbar)

NNLO tune (3-jet NLO): $\alpha_s(M_Z) = 0.122$ (2-loop running, CMW)

Comparable values for Λ_{QCD}



Parameters (in PYTHIA): **FSR pQCD Parameters**

Matching

Additional Matrix Elements included?

At tree level / one-loop level? Using what matching scheme?

$\alpha_s(m_Z)$

The value of the strong coupling

In PYTHIA, you set an effective value for $\alpha_s(m_Z^2)$ ⇔ choice of k in $\alpha_s(kp_\perp^2)$

α_s Running

Renormalization Scheme and Scale for α_s

1- vs 2-loop running, MSbar / CMW scheme, choice of k in $\alpha_s(kp_\perp^2)$, cf

Subleading Logs

Ordering variable, coherence treatment, effective 1→3 (or 2→4), recoil strategy, …

Branching Kinematics (z definitions, local vs global momentum conservation), hard parton starting scales / phase-space cutoffs, masses, non-singular terms, …

Hadron energy fractions

Fragmentation Function

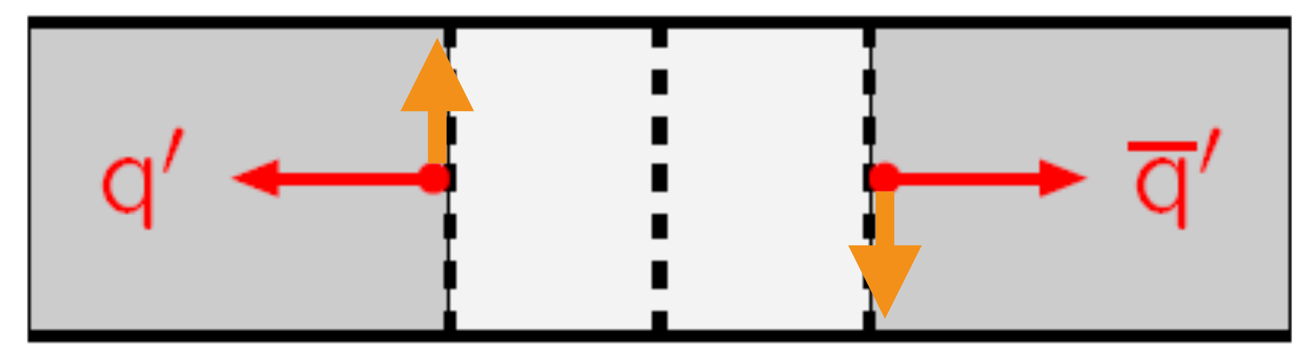
The "Lund a and b parameters" (and $\Delta a_{\mathrm{diquark}}$ for baryons)

Or use a and $\langle z \rangle$ instead (less correlated) A. Jueid et al., *JCAP* 05 (2019) 007

p_T in string breaks

Scale of string-breaking process

Shower cutoff and $\langle p_\perp \rangle$ in string breaks



Meson Multiplets

Mesons

Strangeness suppression, **Vector/Pseudoscalar**, η, η′, …

Baryon Multiplets

Baryons

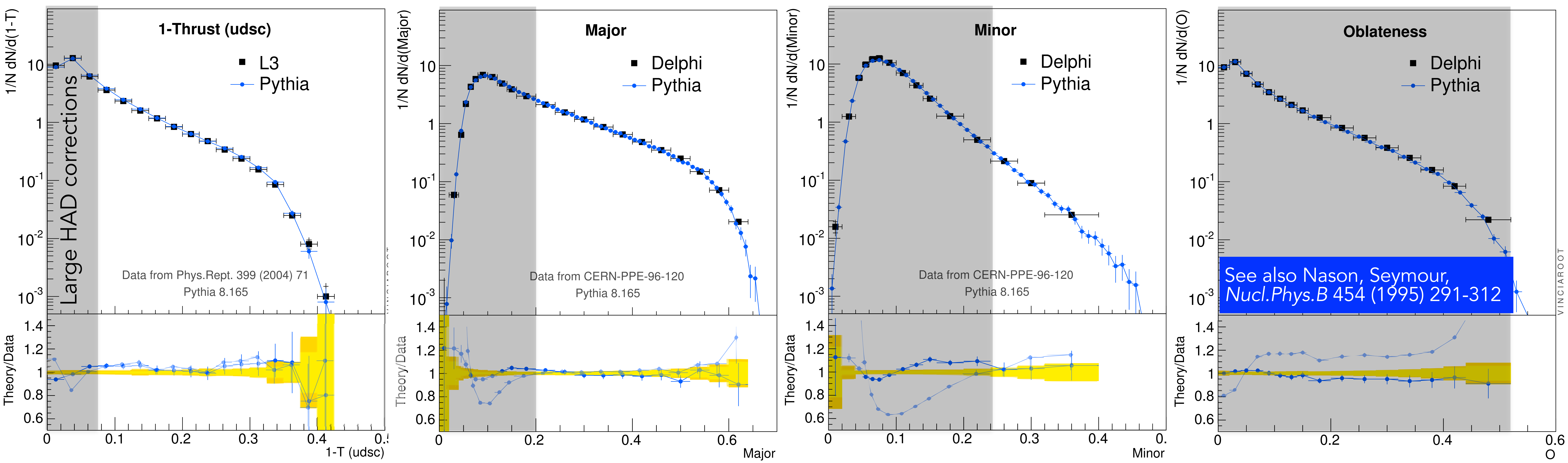
Baryon-to-meson ratios, **Spin-3/2 vs Spin-1/2**, "popcorn", colour reconnections (junctions), … ?

Sensitivity to Hadronization Parameters

PYTHIA 8 (hadronization on) Vs (hadronization off)

Important point: These observables are **IR safe ➜ minimal hadronisation corrections**

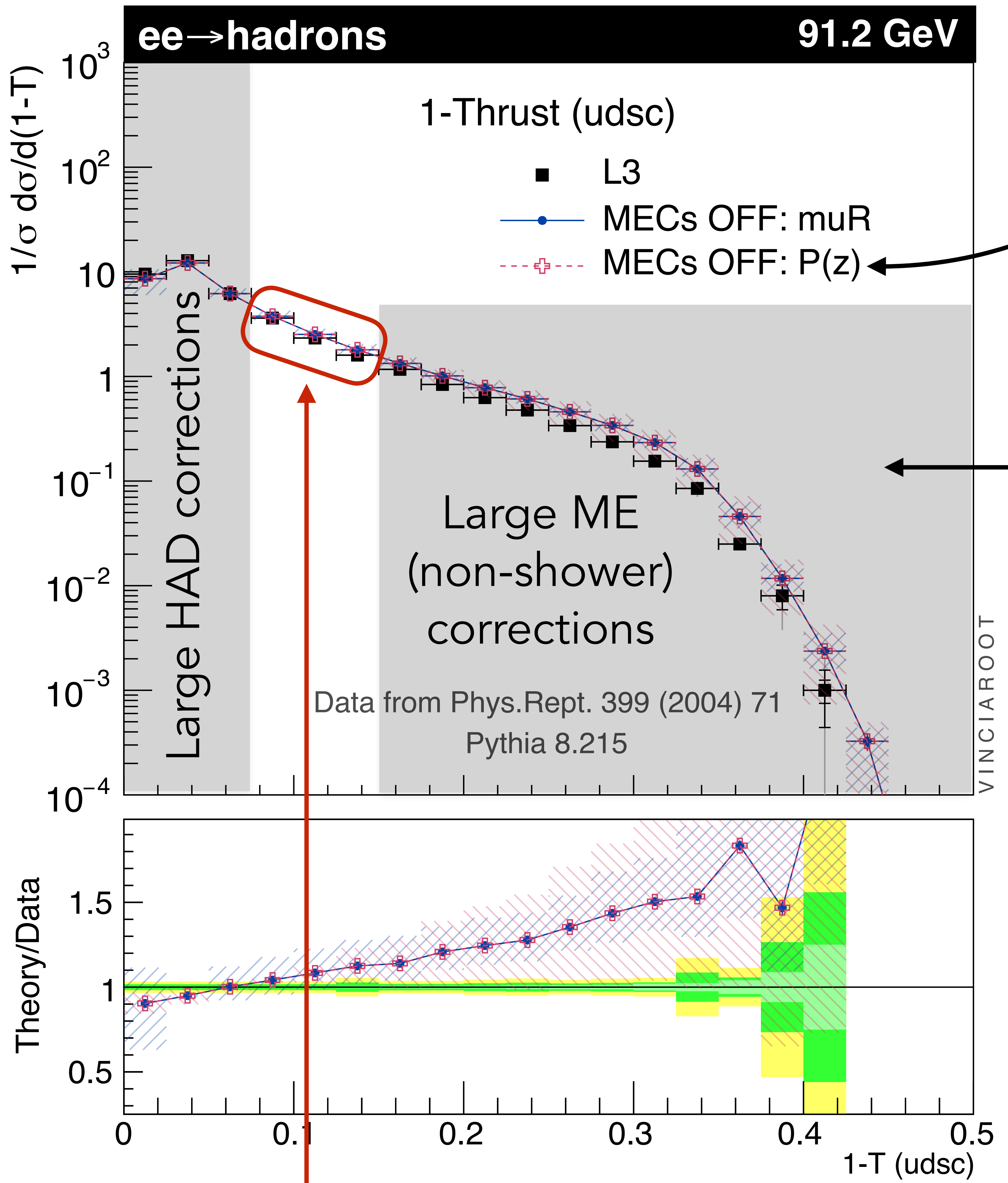
Big differences in **how** sensitive each of these are to hadronisation & over what **range**



The shaded bins provide constraints for the non-perturbative tuning stage.
You want your hadronization power corrections to do the "right thing" at low Thrust.

… and **sensitivity** to **fixed-order** corrections

(Adding nuisance terms $\Delta P(z) \propto Q^2$ to the splitting kernels beyond shower accuracy)



These points are quite sensitive to MECs / Matching / Merging.

➜ we should ensure we do MECs / matching / merging if we want to use them (or something equivalent to that.)

These points are relatively insensitive to **both** hadronization **and** matching/merging

Hadronization Corrections: Fragmentation Tuning

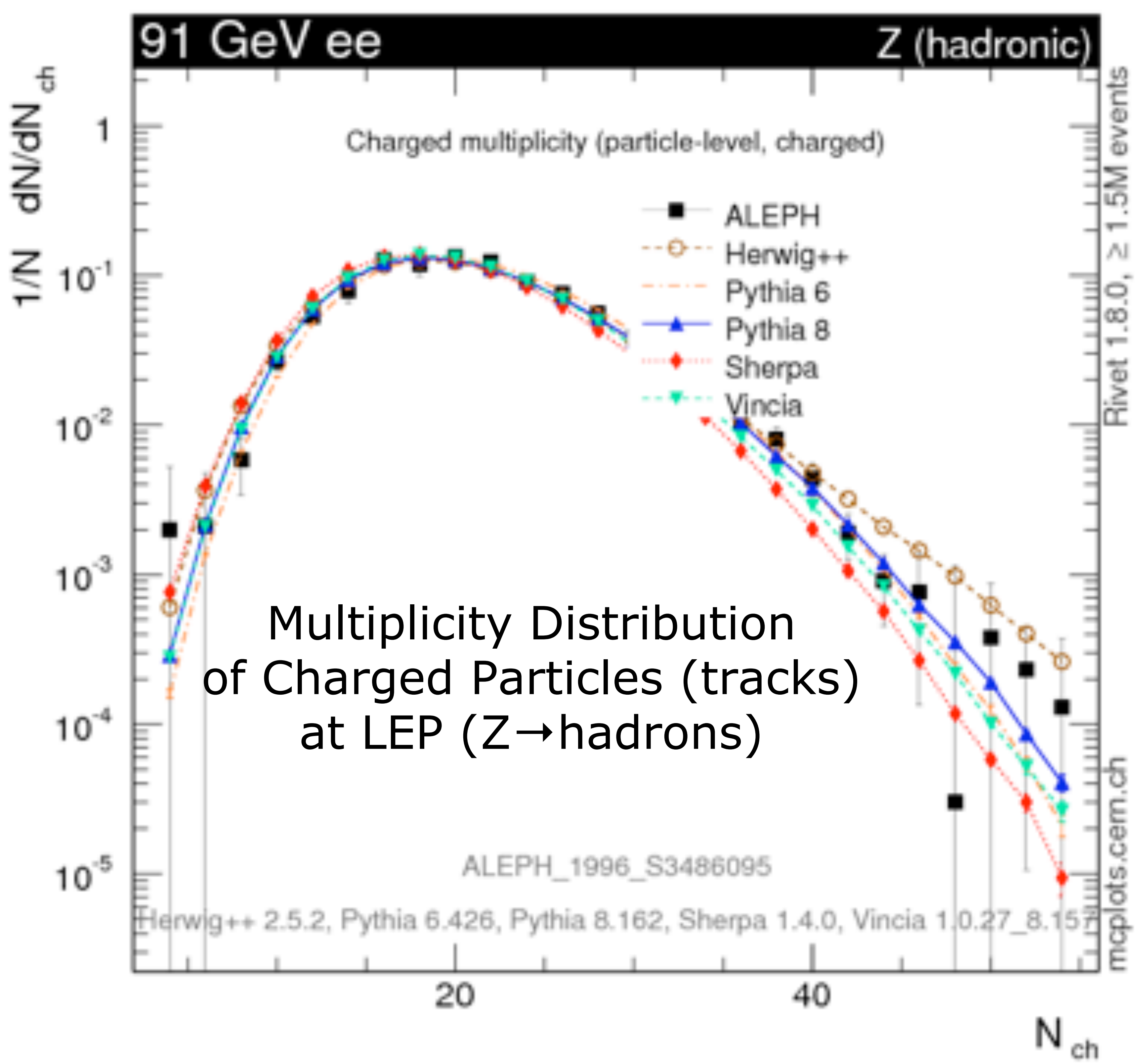
Now use infrared **sensitive** observables - sensitive to hadronization
+ first few bins of previous (IR safe) ones

Longitudinal FF parameters *a* and *b*.

Transverse p_T broadening in string breaks (curtails high-N tail, and significantly affects event shapes)

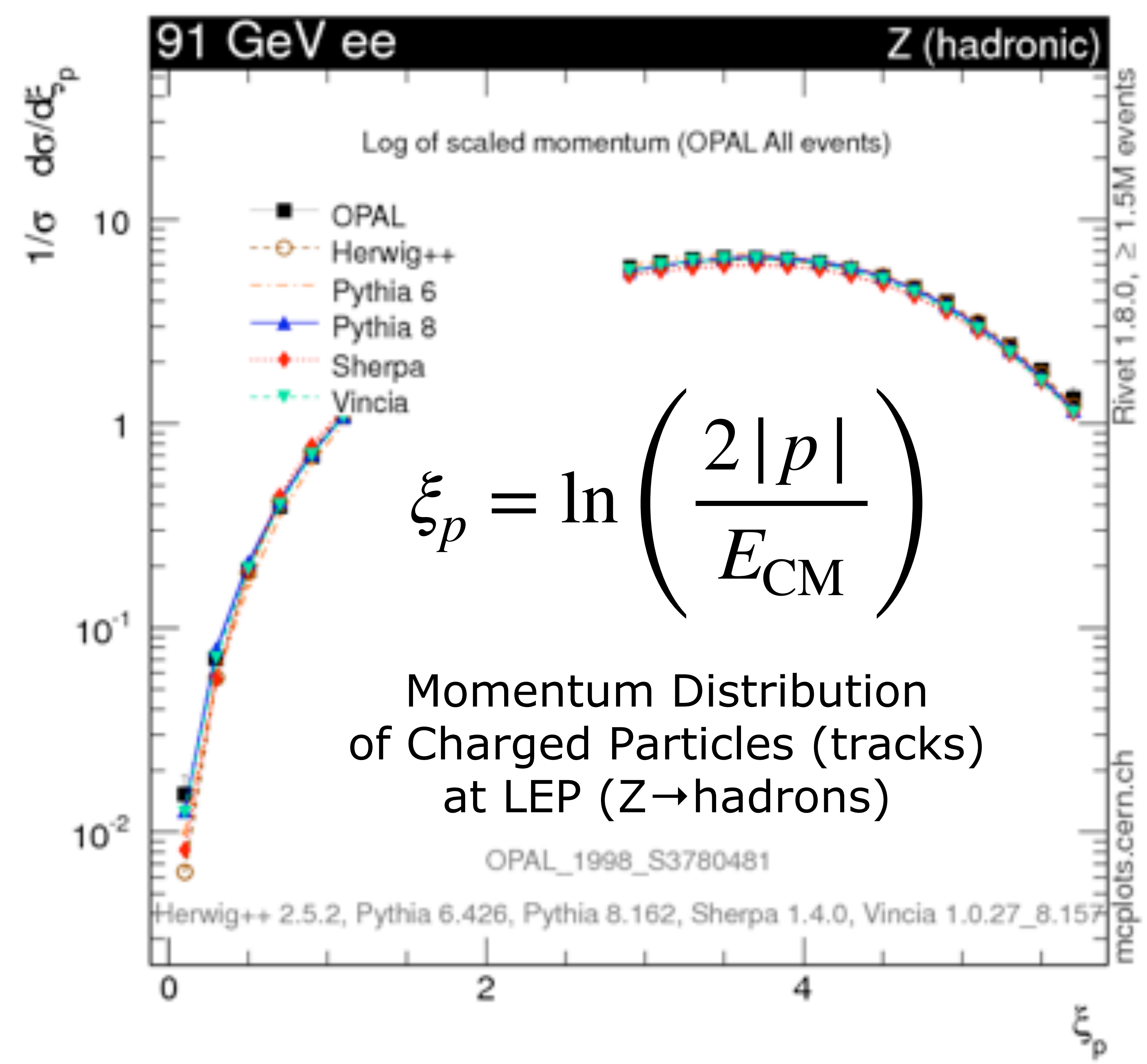
Further parameter $a_{diquark}$ requires looking at a baryon spectrum

How many hadrons do you get?



$\langle N_{ch}(M_Z)\rangle \sim 21$

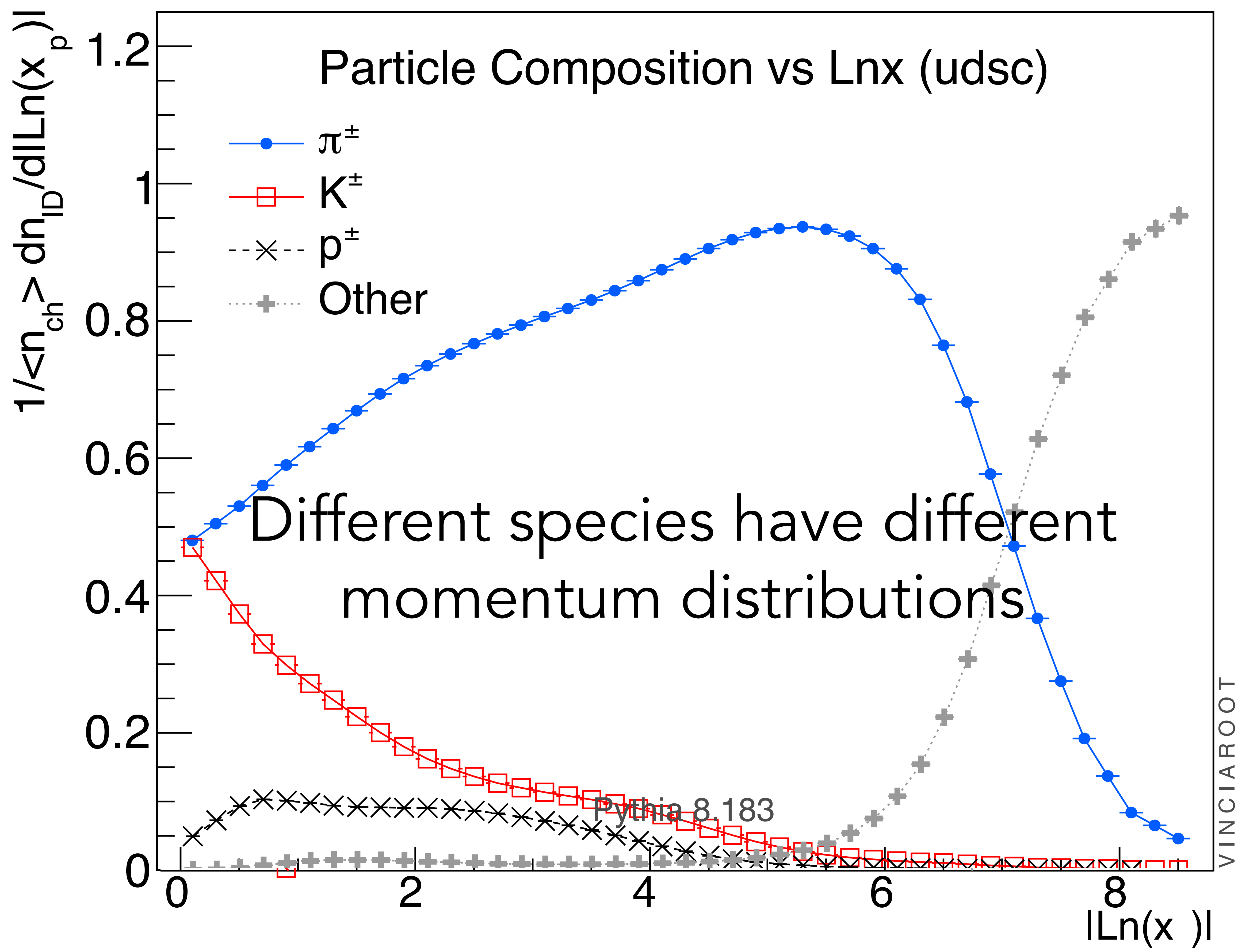
And how much momentum do they carry?



Fragmentation Tuning

Somewhat sensitive to particle composition: **heavier hadrons are harder!**

Know what **physics** goes in



Different species have different momentum distributions

+ effects of feed-down!

(e.g., $\rho \to \pi\pi,\ K^* \to K\pi,\ \eta \to \pi\pi\pi,\ \ldots$)

If you get the longitudinal and transverse FF aspects right, I would hope the particle composition would not need much work.

But of course good to check. There is a PDG Rivet routine but it may have some issues. I have a Monash-tune Pythia main program I could share too.

Final Note on Fragmentation Tuning

Tuning: the higher up the chain you change something, the more it will affect the large-scale event structure ➜ Start at the top, and work your way down.

Divide and Conquer: Use Infrared Safety, **Exclusivity**, and **Ratios** to exploit factorisations!

3-jet events have a larger $\langle N_{\mathrm{ch}} \rangle$ than 2-jet events

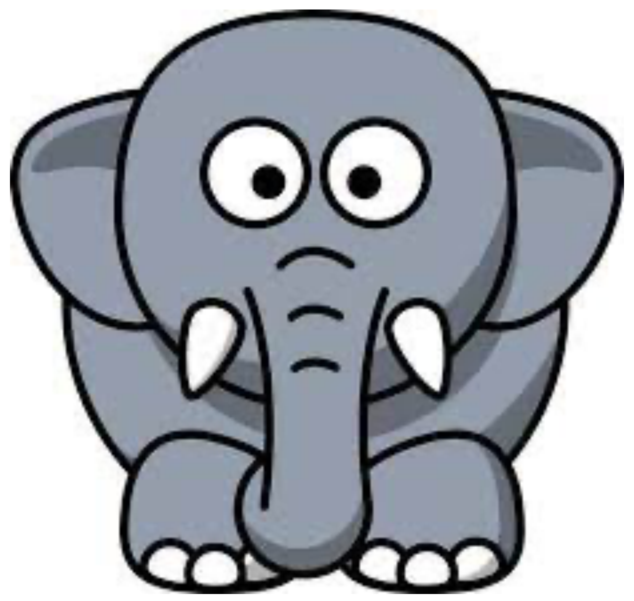
So if you don't get the relative mixture of 2- to 3-jet events right, then you would be in unsafe territory trying to fit your **lower-scale** non-perturbative parameters to an inclusive measurement of $\langle N_{\mathrm{ch}} \rangle$.

What can you do? Adjust shower α_s, or use NNLO merging, or use reweighting, or use $\langle N_{\mathrm{ch}} \rangle$ in an **exclusive 2-jet sample** that does not depend on the relative 2-to-3-jet ratio. **But don't do nothing.**

Similarly, the total number of particles is different

But **relative ratios** like $\langle N_{\mathrm{K}} \rangle / \langle N_{\pi} \rangle$ should be more universal

Another elephant in the room: Automated vs Manual tuning



Professor is a powerful tool. I would (by now) recommend using it. Wisely.

Some Dangers

Overfitting: extremely precisely measured data points can generate large χ^2 values even if the generator gets within what one would naively consider a "reasonable" agreement.

- Fit reacts by sacrificing agreement elsewhere (typically in tails) to improve χ^2 in peaks.
- Professor now has facility to include a "sanity limit" (e.g., 5%) "theory uncertainty"
- ➤ Fit no longer gets rewarded (much) for improving agreement beyond that point. More freedom in tails.
- This also tends to produce $\chi^2_{5\%}$ values in the neighbourhood of unity → meaningful uncertainty bands?

Incompatibilities: a model may be ***unable*** to agree at all with (some part of) a given measurement.

- Example: trying to force a "wimpy shower" to agree with p_{TZ} in bins above m_Z.
- Fit reacts by desperately trying to reduce order-of-magnitude differences in bins it shouldn't have been asked to fit in the first place, at cost of everything else ➤ total garbage.
- Choose carefully. + Professor now has facility to not penalise χ^2 beyond some maximum deviation.

Wouldn't it be nice if there was a tool:

That could automatically detect correlations between parameters and observables.

And tell you which "groups" they fall into naturally : which parameter sets you should ideally tune together, and which are more nicely factorised.

This is (at least partly) what the tool AutoTunes does

Bellm, Gellersen, Eur.Phys.J.C 80 (2020)

I won't have time to discuss that today, but I think it looks promising

I encourage you to study it and use it:

You may also be interested in Apprentice

Krishnamoorthy et al., EPJ Web Conf. 251 (2021) 03060

Variance reduction to semi-automate how to weight observables & bins

Parameters (in PYTHIA): Initial-State Radiaton

Matching & Merging

Additional Matrix Elements included?

At tree level / one-loop level? What matching scheme?

+ PDF Choice

Size of Phase Space

Starting scale

Relation between Q_{PS} and Q_F (Vetoed showers? Suppressed? cf matching)

Coherence

Initial-Final interference

I-F colour-flow interference effects (eg VBF & Tevatron $t\bar{t}$ asym) & interleaving

α_s

Value and running of the strong coupling

Governs overall amount of radiation (cf FSR)

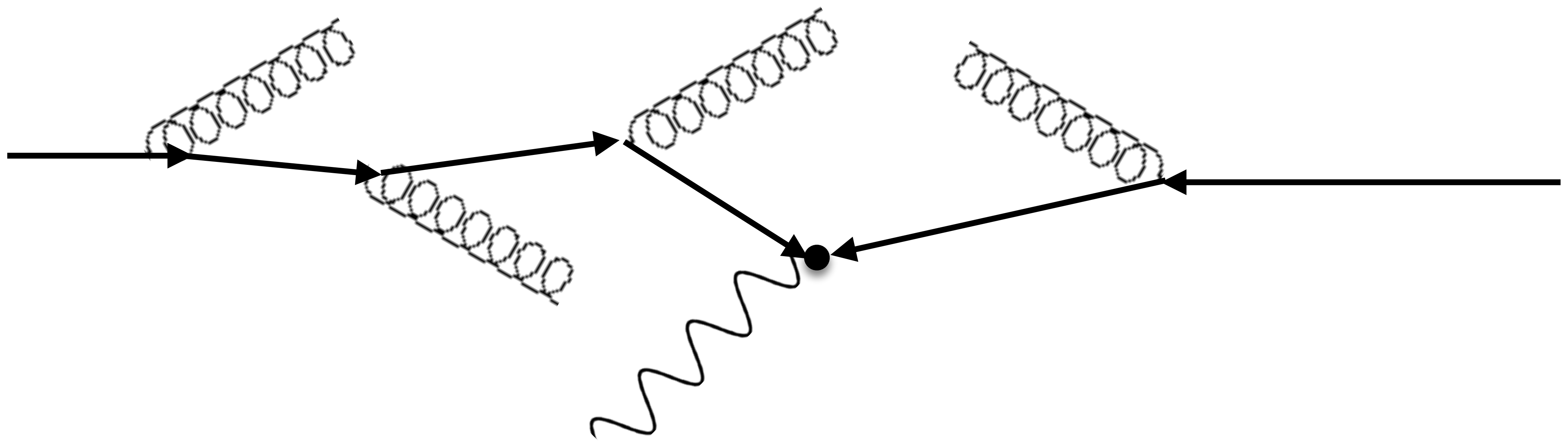
"Primordial kT"

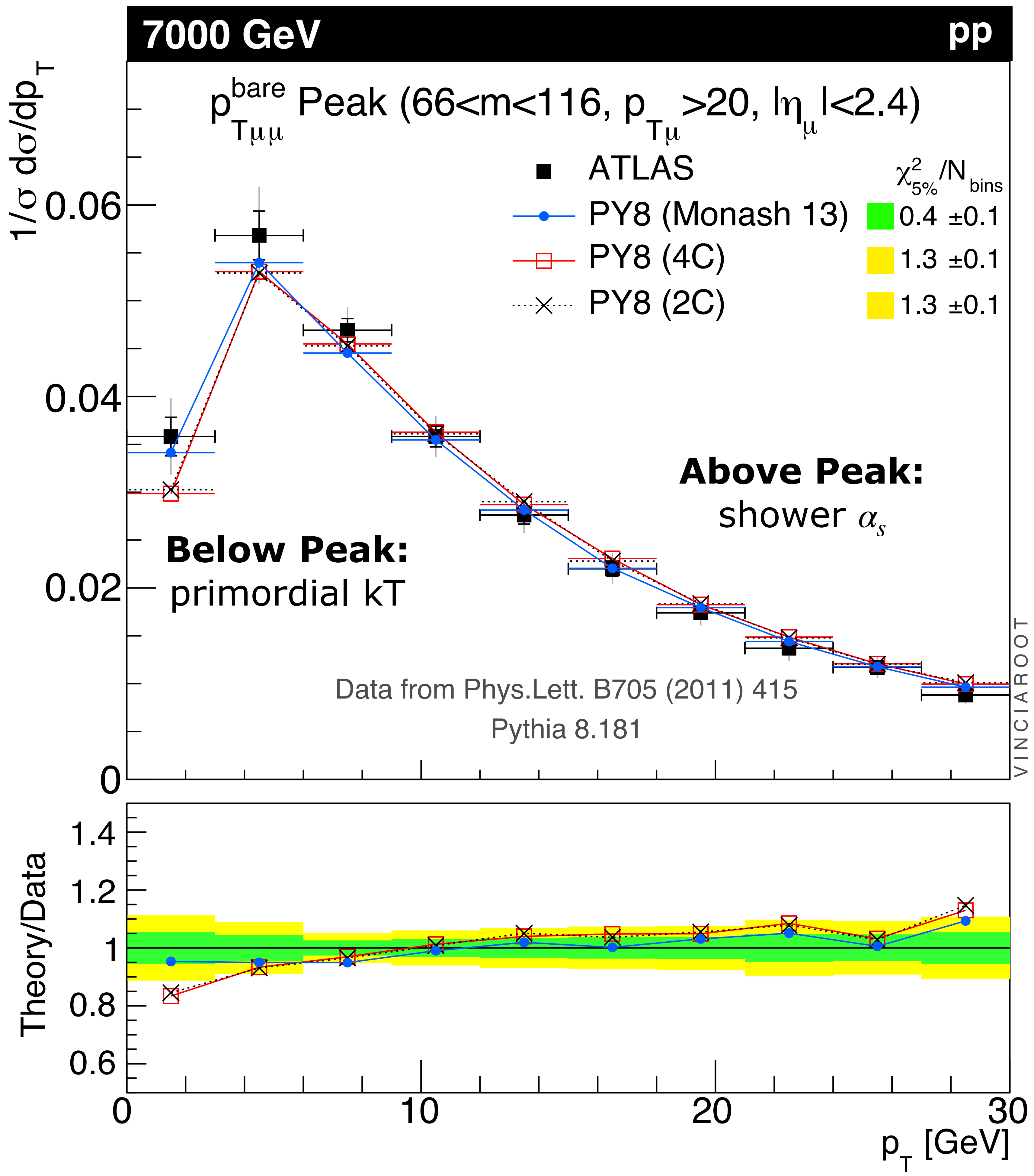
A small additional amount of "unresolved" kT

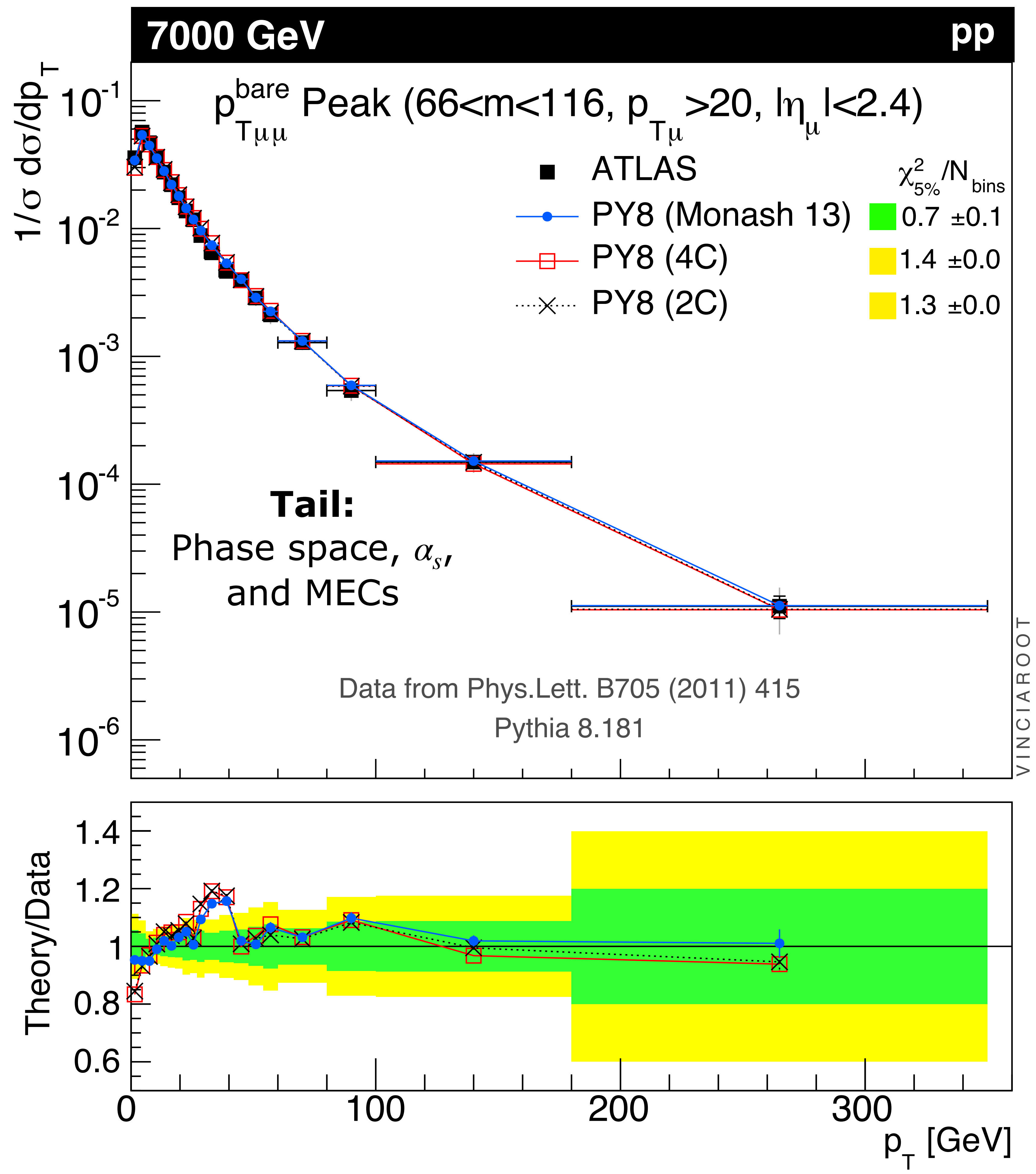
Fermi motion + unresolved ISR emissions + low-x effects?

ISR + Primordial kT

Drell-Yan pT distribution

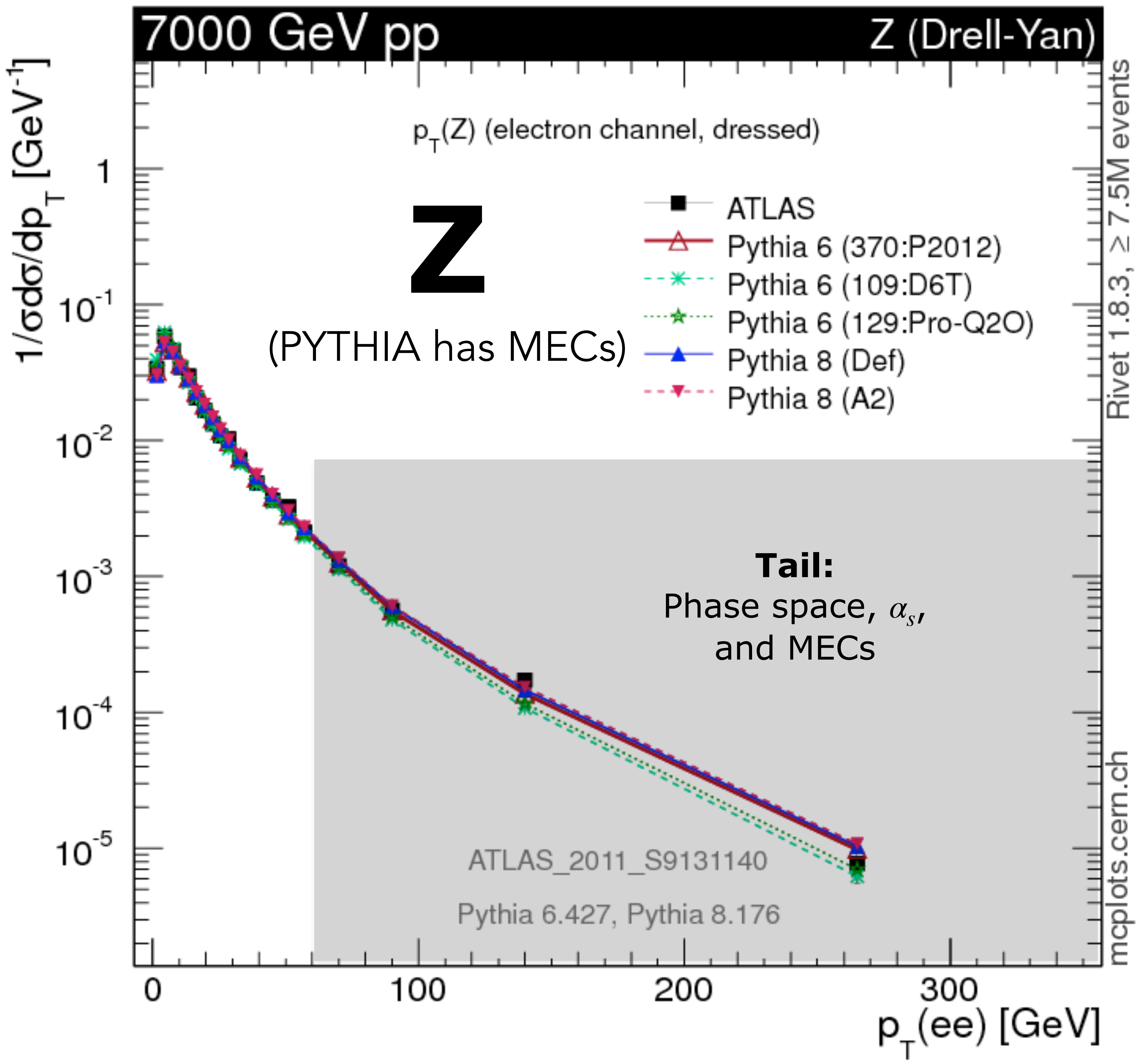






Controlling for Process Dependence!

Note: these distributions rely on Pythia's "Power Showers"



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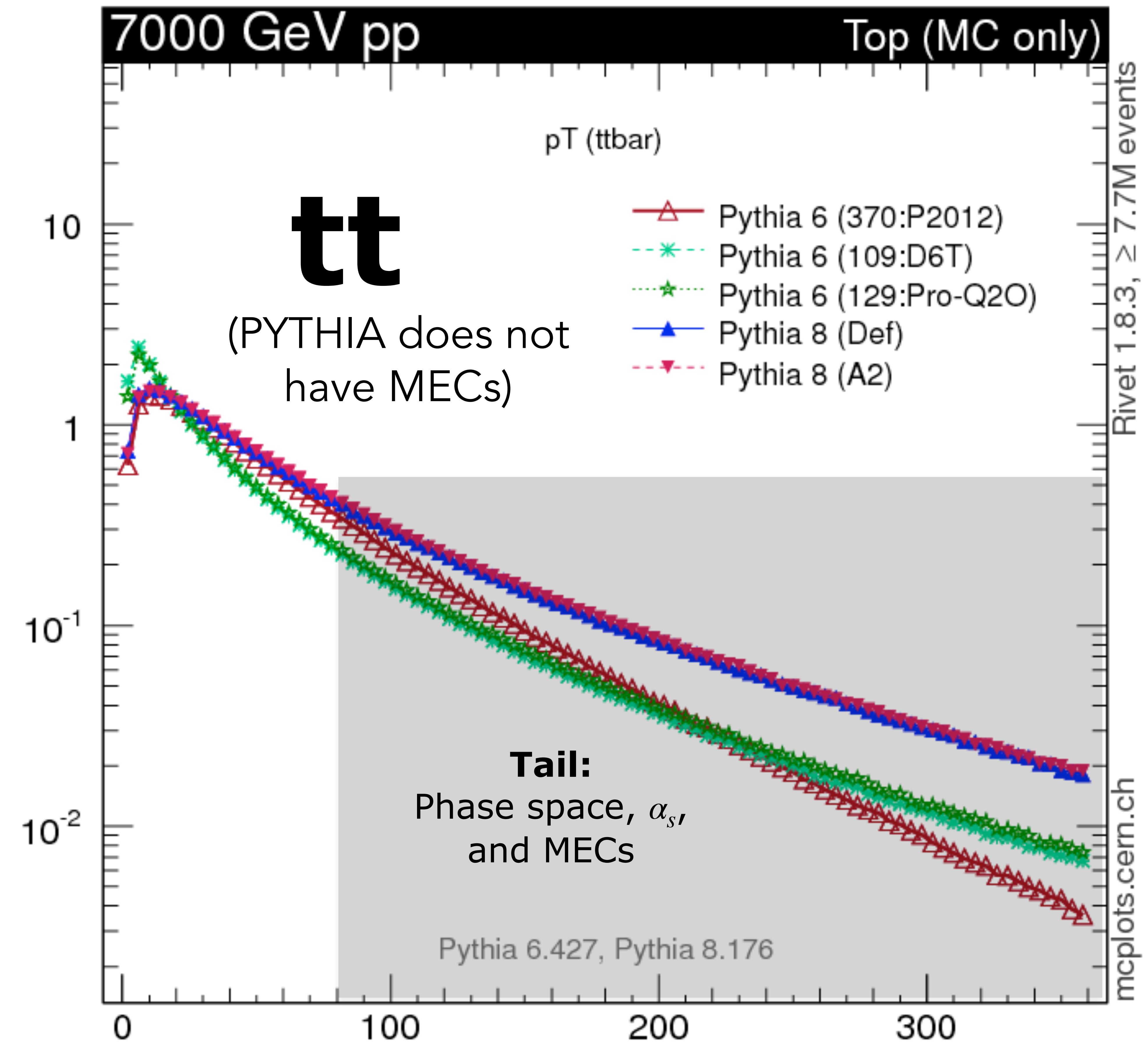
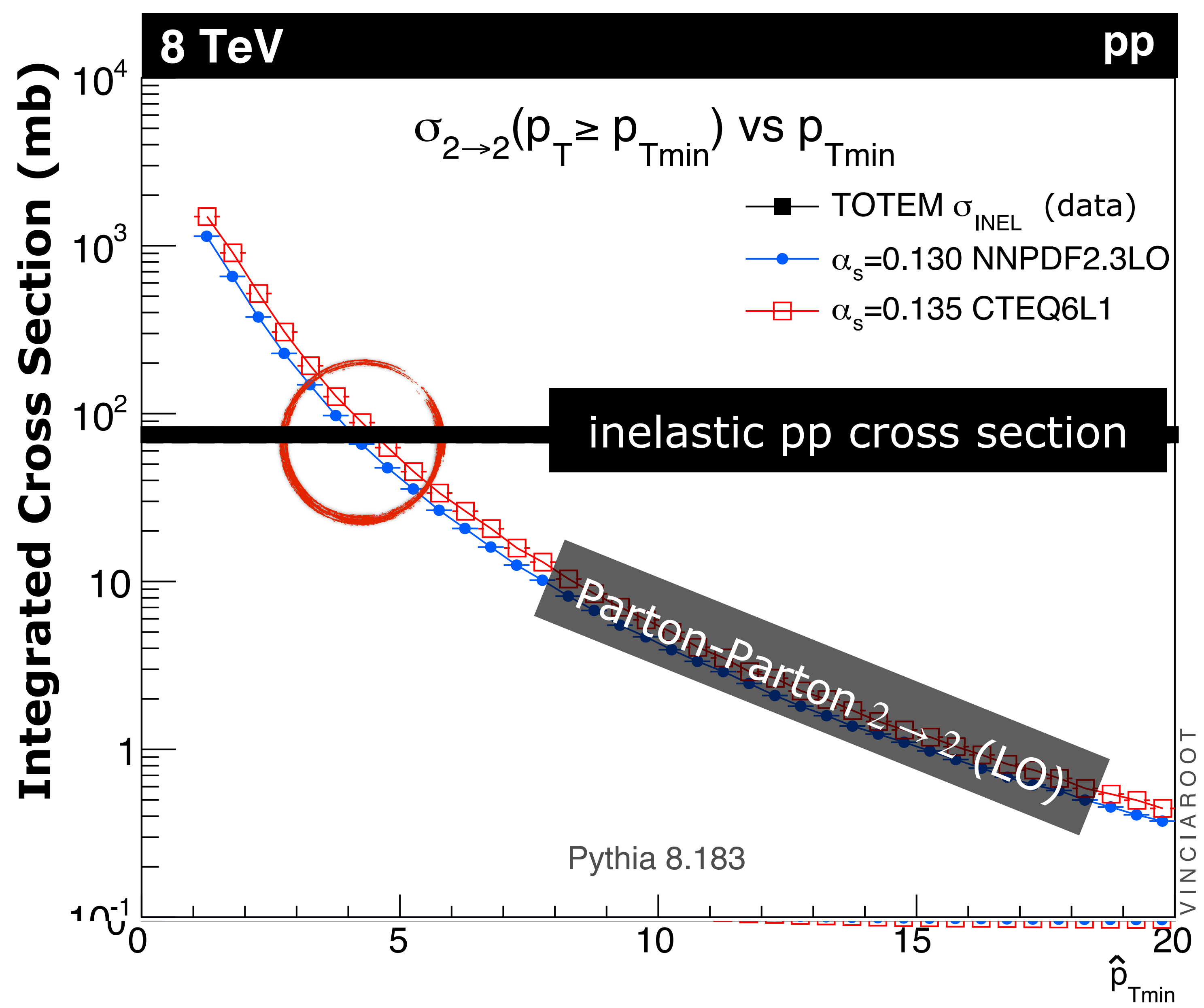


➜ we should ensure we do MECs / matching / merging if we want to use them (or something equivalent to that.)

A Brief History of MPI in PYTHIA

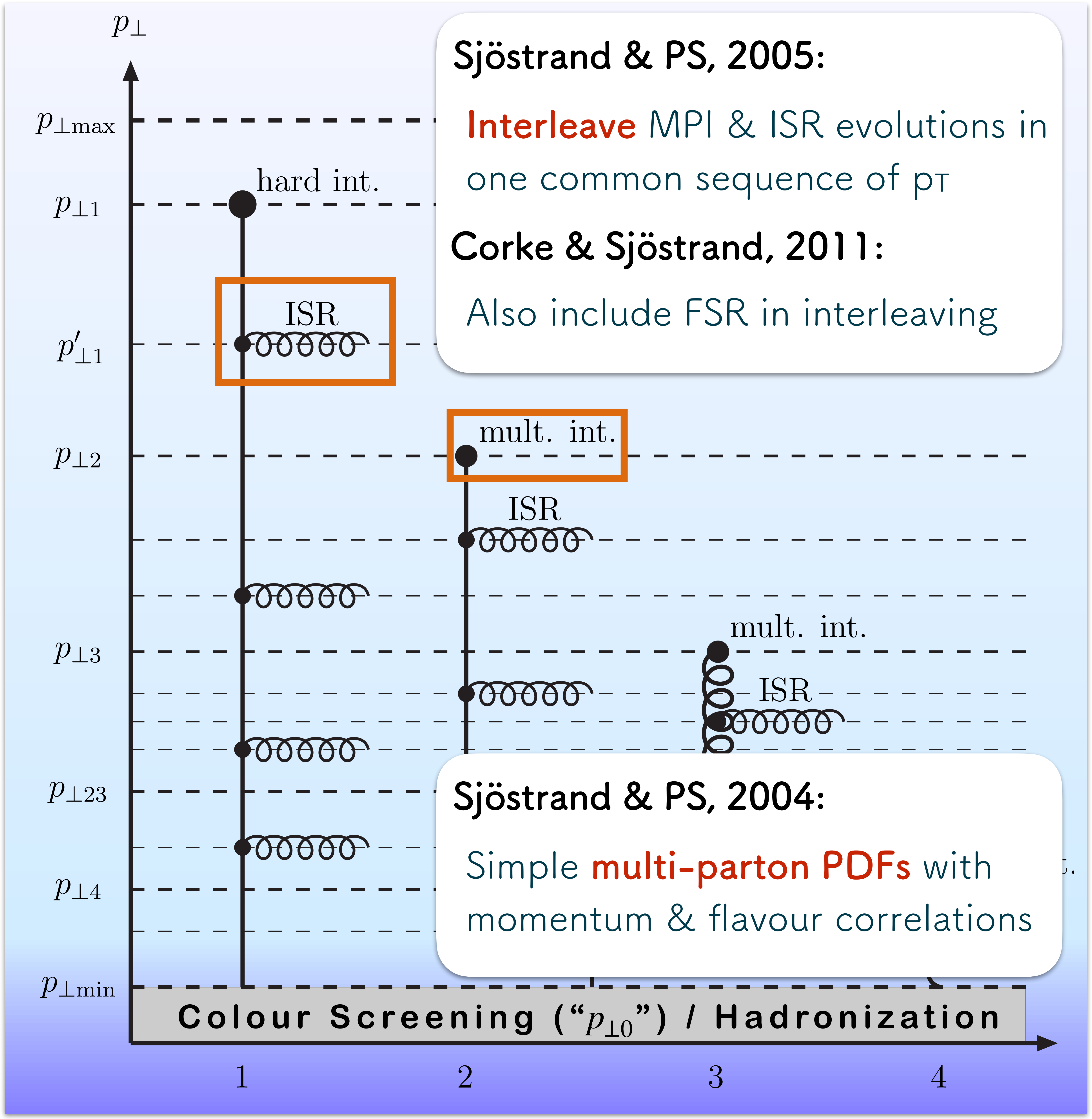
$$\frac{\sigma_{\text{parton-parton}}(\hat{p}_\perp)}{\sigma_{\text{hadron-hadron}}} > 1$$

$\Longrightarrow$ several parton-parton interactions *per* hadron-hadron interaction: **MPI**



Sjöstrand & van Zijl, 1985:

Cast as **Sudakov-style evolution equation**, analogous to the $\sigma_{X+\text{jet}}(p_\perp)/\sigma_X$ one of showers



Sjöstrand & PS, 2005:

Interleave MPI & ISR evolutions in one common sequence of pT

Corke & Sjöstrand, 2011:

Also include FSR in interleaving

Sjöstrand & PS, 2004:

Simple **multi-parton PDFs** with momentum & flavour correlations

Figure from Sjöstrand & PS, 2005

Minimum-Bias & Underlying Event

Number of MPI

Infrared Regularization scale $p_{\perp 0}$ for the QCD 2→2 (Rutherford) scatterings used for multiple parton interactions

→ average number of MPI, sets size of overall UE activity

Note: **strongly correlated with choice of PDF set!** (low-x gluon)

Pedestal Rise

Proton transverse mass distribution → difference between central (more active) **vs peripheral** (less active) **collisions**

Strings per Interaction

Color correlations between multiple-parton-interaction systems (aka colour *reconnections* — relative to LC)

→ shorter or longer strings → less or more hadrons per MPI

Affect <p_T> vs N_{ch} balance: High CR ➜ fewer particles, each carrying more p_T

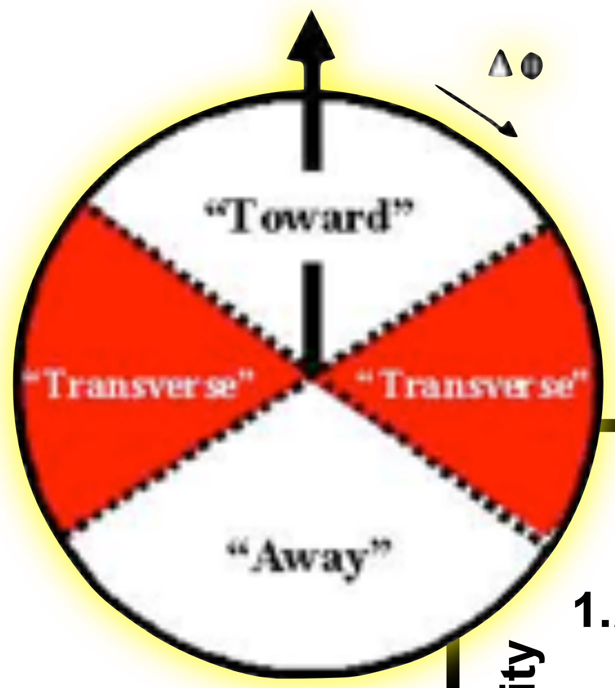
$\sqrt{s}$ scaling

Evolution of UE, $\langle dN/d\eta \rangle$, … with collider CM energy

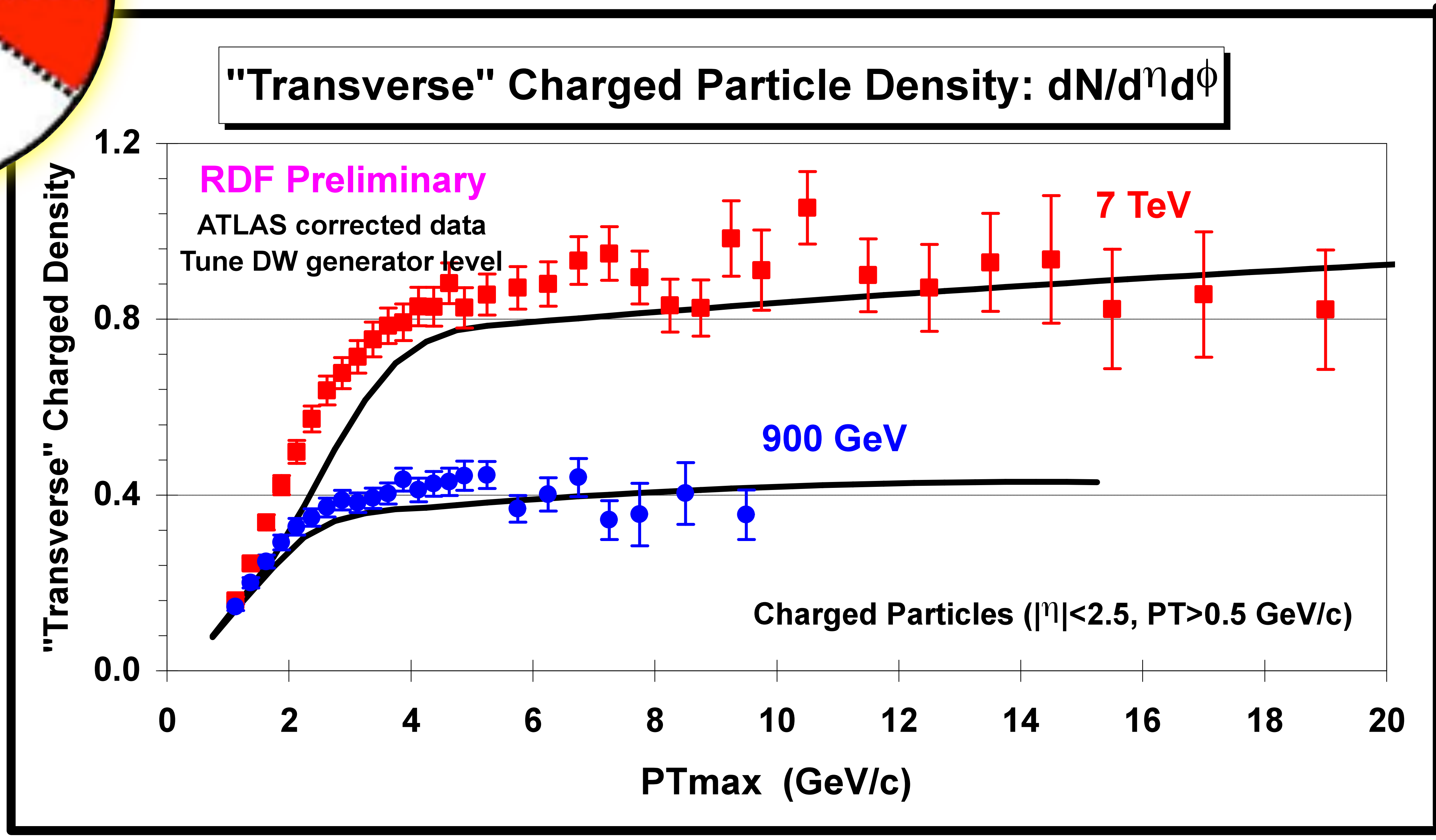
Cast as energy evolution of p_{T0} parameter.

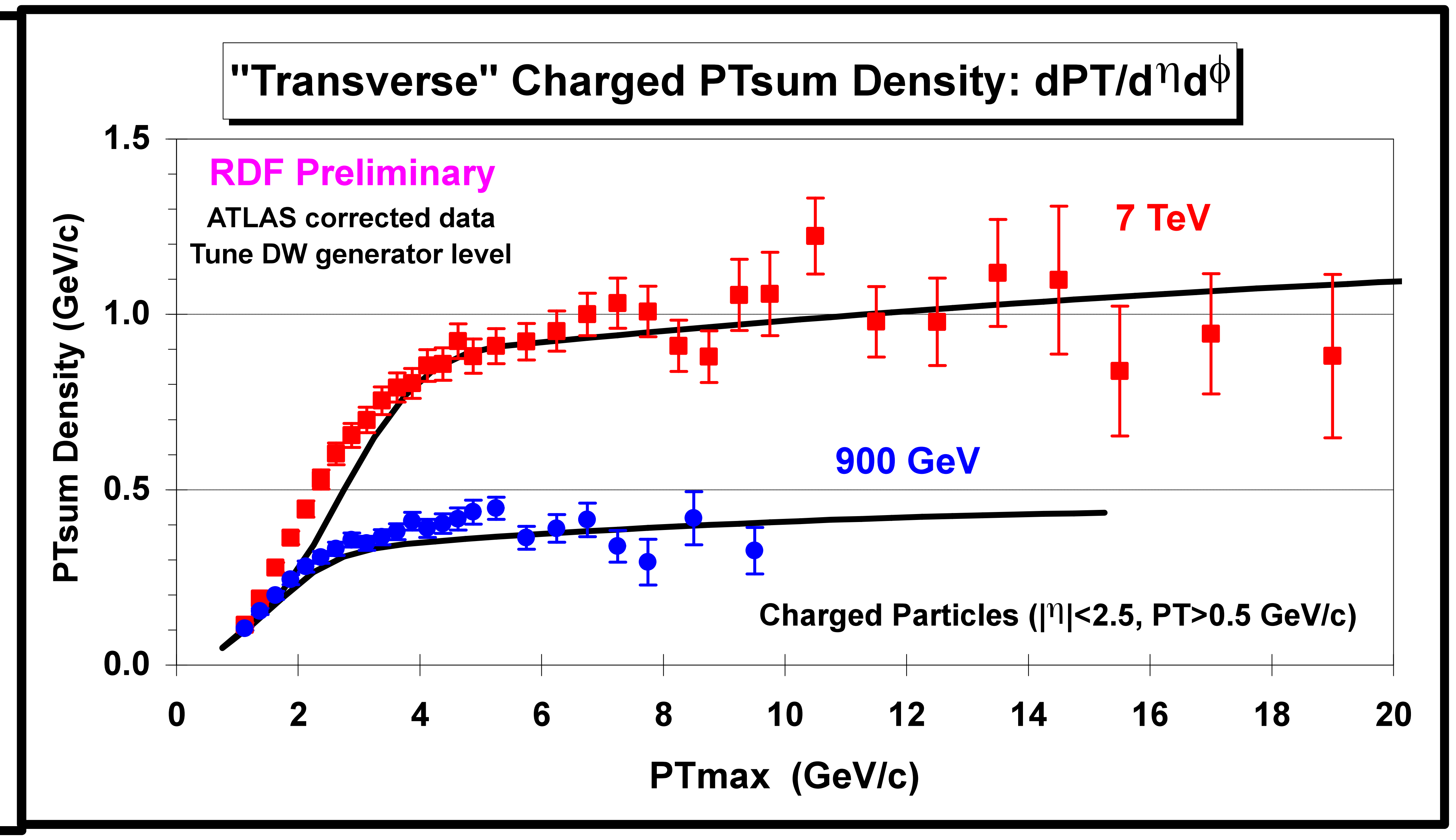
Underlying Event

Same thing as before: how many particles do you get? And how much p_T do they carry?



UE - LHC from 900 to 7000 GeV - ATLAS





As you trigger on progressively higher p_T, the entire event increases …

… until you reach a plateau ("max-bias") also called the "jet pedestal" effect

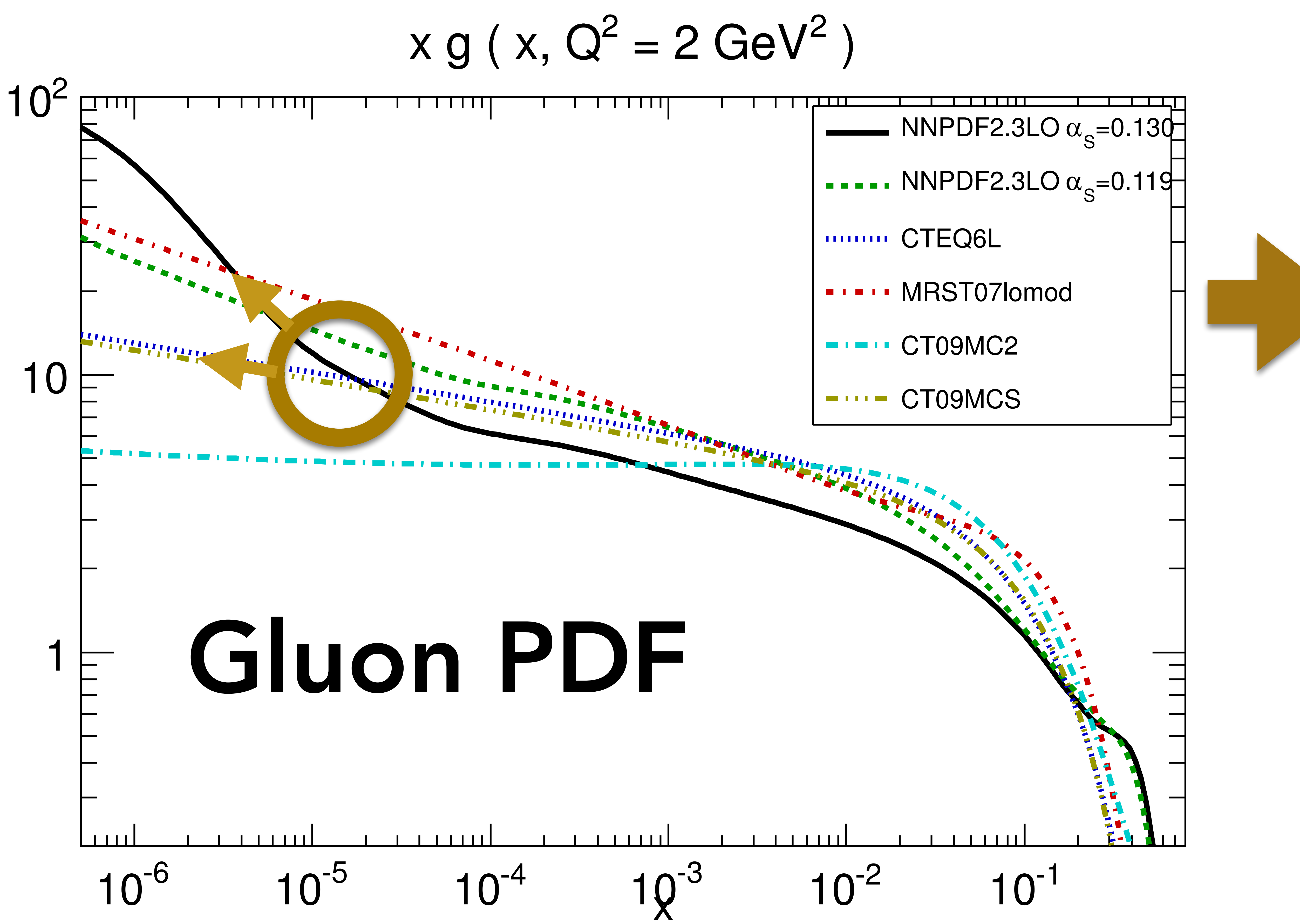
Interpreted as impact-parameter effect

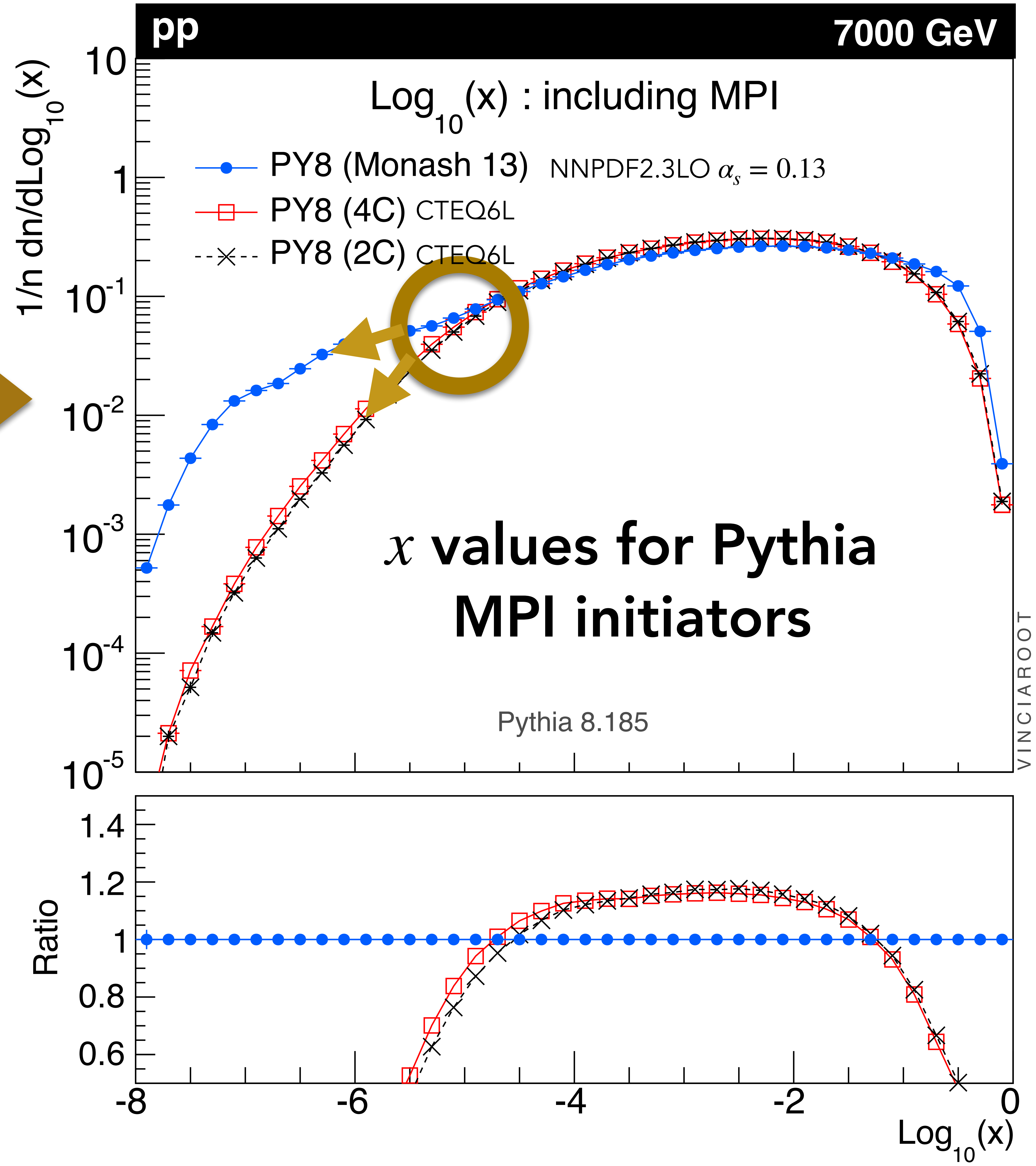
Qualitatively reproduced by MPI models

Relative size of this plateau / min-bias depends on pT0, PDF, *and* b-profile

Interplay between MPI and PDF set

Some PDFs that were available at the time of the Monash tune

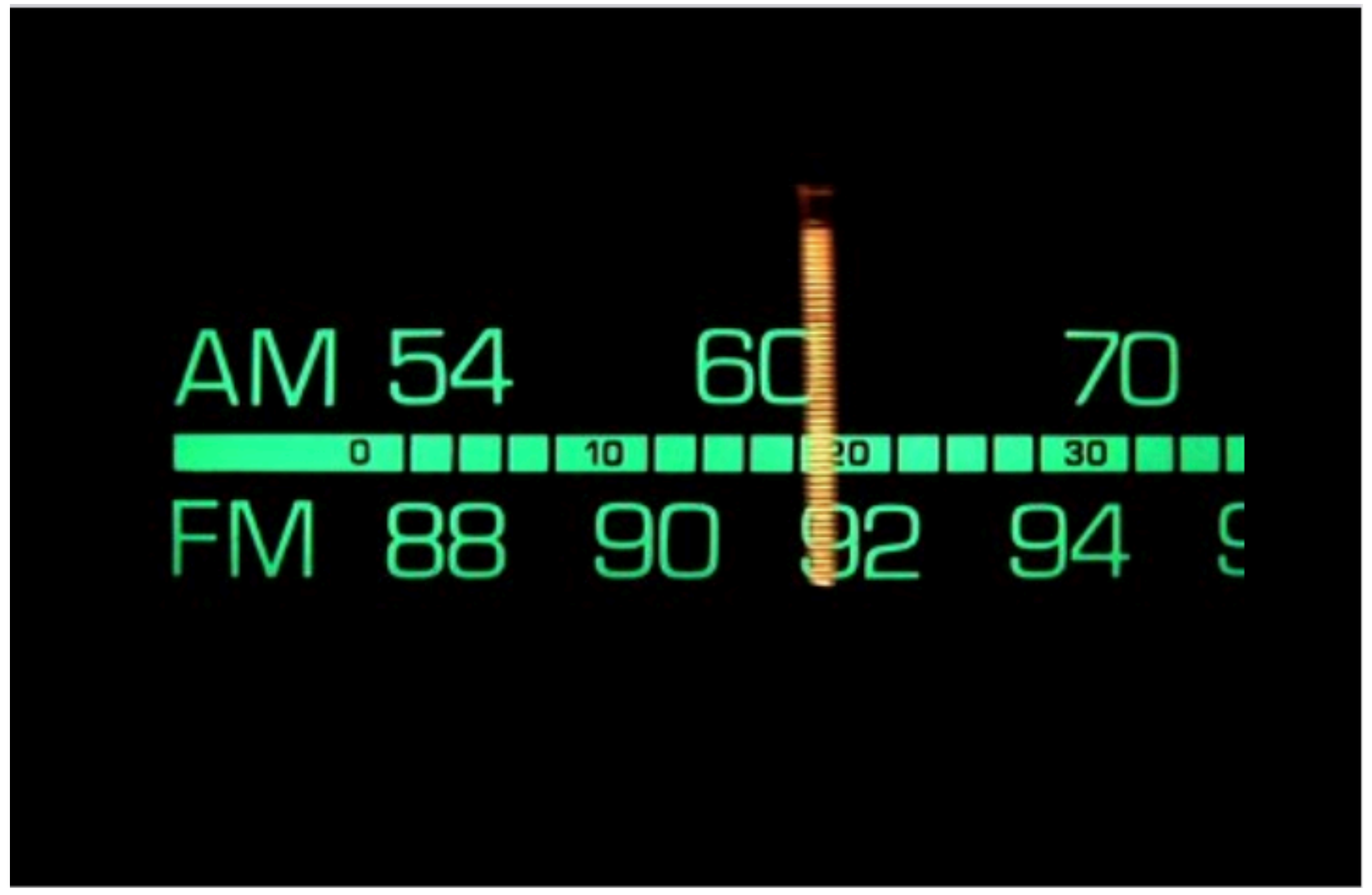




Need sensible behaviour down to very low x, and very low Q ~ ISR/MPI cutoff ~ 1 GeV

Negative PDFs not an option. Shower and MPI kernels are LO.

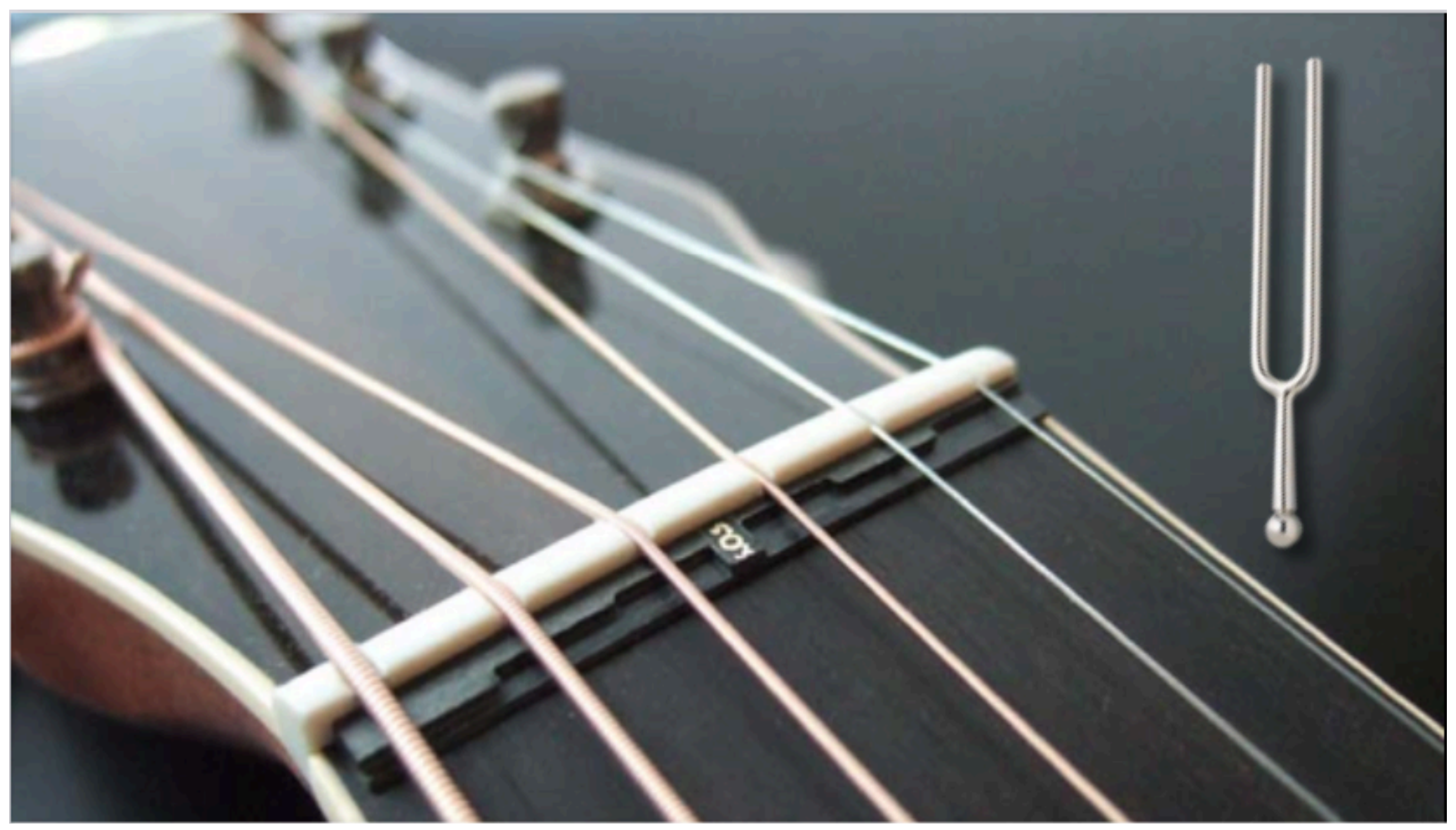
Tuning: What do you want it to be?



Sensible

A set of physically sensible central parameter values, with good universality.

What does "physically sensible" and "good universality" really mean?



Sophisticated

High-precision & specialised parameter sets, with reliable uncertainties

Tuning in the context of N^{n}LO matching & precision/theory applications. Theory uncertainties. Rigorous scientific analyses of parameter spaces.

Best Fit?

A pure optimisation problem. The **best fit** you can get. Ask questions later.

Risky. Overfitting, oversimplification, GIGO, black-box syndrome, tunnel vision, how to define "best", loss of insight & scientific rigour,…

Notes on PDFs for MPI Models

The issue with NLO gluons at low x

(Summary of note originally written by T. Sjöstrand, from discussions with R. Thorne though any oversimplifications or misrepresentations are our own)

Low-x gluon

Key constraint: DIS F_2

Low x: $\mathrm{d}F_2/\mathrm{d}\ln(Q^2)$ driven by $g \to q\bar{q}$

LO $P_{q/g}(z)$ ~ flat $\Longrightarrow$ x of measured quark closely correlated with x of mother gluon.

NLO Integral over $P_{q/g}(z) \propto 1/z$ for small z $\Longrightarrow$ approximate $\ln(1/x)$ factor.

➤ Effectively, the NLO gluon is probed more "non-locally" in x.

$\mathrm{d}\ln F_2/\mathrm{d}Q^2$ at small x becomes too big unless positive contribution from medium-to-high-x gluons (derived from $\mathrm{d}\ln F_2/\mathrm{d}Q^2$ in that region, and from other measurements) is combined with a negative contribution from low-x gluons.

Mathematically (toy NLO Calculation with just one x):

$$\frac{\mathrm{ME}_{\mathrm{NLO}}}{\mathrm{ME}_{\mathrm{LO}}} = 1 + \alpha_{\mathrm{s}}(A_1 \ln(1/x) + A_0)$$

$\ln(1/x)$ largely compensated in def of NLO PDF:

$$\frac{\mathrm{PDF}_{\mathrm{NLO}}}{\mathrm{PDF}_{\mathrm{LO}}} = 1 + \alpha_{\mathrm{s}}(B_1 \ln(1/x) + B_0)$$

➤ Product well-behaved at NLO if we choose $B_1 \approx A_1$
Cross term at $\mathcal{O}(\alpha_s^2)$ is beyond NLO accuracy … →

For large x and small $\alpha_s(Q^2)$, e.g. $\alpha_s A_1 \ln(1/x) \sim 0.2$:

$$\frac{\mathrm{ME}_{\mathrm{NLO}}\,\mathrm{PDF}_{\mathrm{NLO}}}{\mathrm{ME}_{\mathrm{LO}}\,\mathrm{PDF}_{\mathrm{LO}}} = (1+0.2)(1-0.2) = 0.96$$

👍 log terms cancel

But if x and Q^2 are small, say $\alpha_s A_1 \ln(1/x) \sim 2$:

$$\frac{\mathrm{ME}_{\mathrm{NLO}}\,\mathrm{PDF}_{\mathrm{NLO}}}{\mathrm{ME}_{\mathrm{LO}}\,\mathrm{PDF}_{\mathrm{LO}}} = (1+2)(1-2) = -3$$

👎 Cross term dominates;
The PDF becomes negative

Not so important for high-p_T processes because 1) DGLAP evolution fills up low-x region, 2) kinematics restricted to higher x, 3) smaller α_s

Some Desirable Properties for PDFs for Event Generators

General-Purpose MC Generators are used to address very diverse physics phenomena and connect (very) high and (very) low scales ➤ **Big dynamical range!**

1. Stable (& positive) evolution to **rather low Q^2 scales**, e.g. $Q_0 \lesssim 1\,\mathrm{GeV}$

   ISR shower evolution and MPI go all the way down to the MC IR cutoffs ~ 1 GeV

2. **Extrapolates sensibly to very low** $x \sim 10^{-8}$ (at LHC), especially at low $Q \sim Q_0$.

   "Sensible" ~ positive and smooth, without (spurious) structure

   Constraint for perturbative MPI: $\hat{s} \geq (1\,\mathrm{GeV})^2 \implies x_{\mathrm{LHC}} \gtrsim 10^{-8}$ $(x_{\mathrm{FCC}} \geq 10^{-10})$

   Main point: MPI can probe a **large range of** x, beyond the usual $\sim 10^{-4}$

   (Extreme limits are mainly relevant for ultra-forward / beam-remnant fragmentation)

3. **Photons** included as partons

   Bread and butter for part of the user community

4. **LO** or equivalent in some form (possibly with α_s^{eff}, relaxed momentum sum rule, …)

   Since MPI Matrix Elements are LO; ISR shower kernels also LO (so far)

5. Happy to have **N^{n}LO** ones in a similar family.

   E.g., for use with higher-order MEs for the hard process.

   Useful (but possible?) for these to satisfy the other properties too?