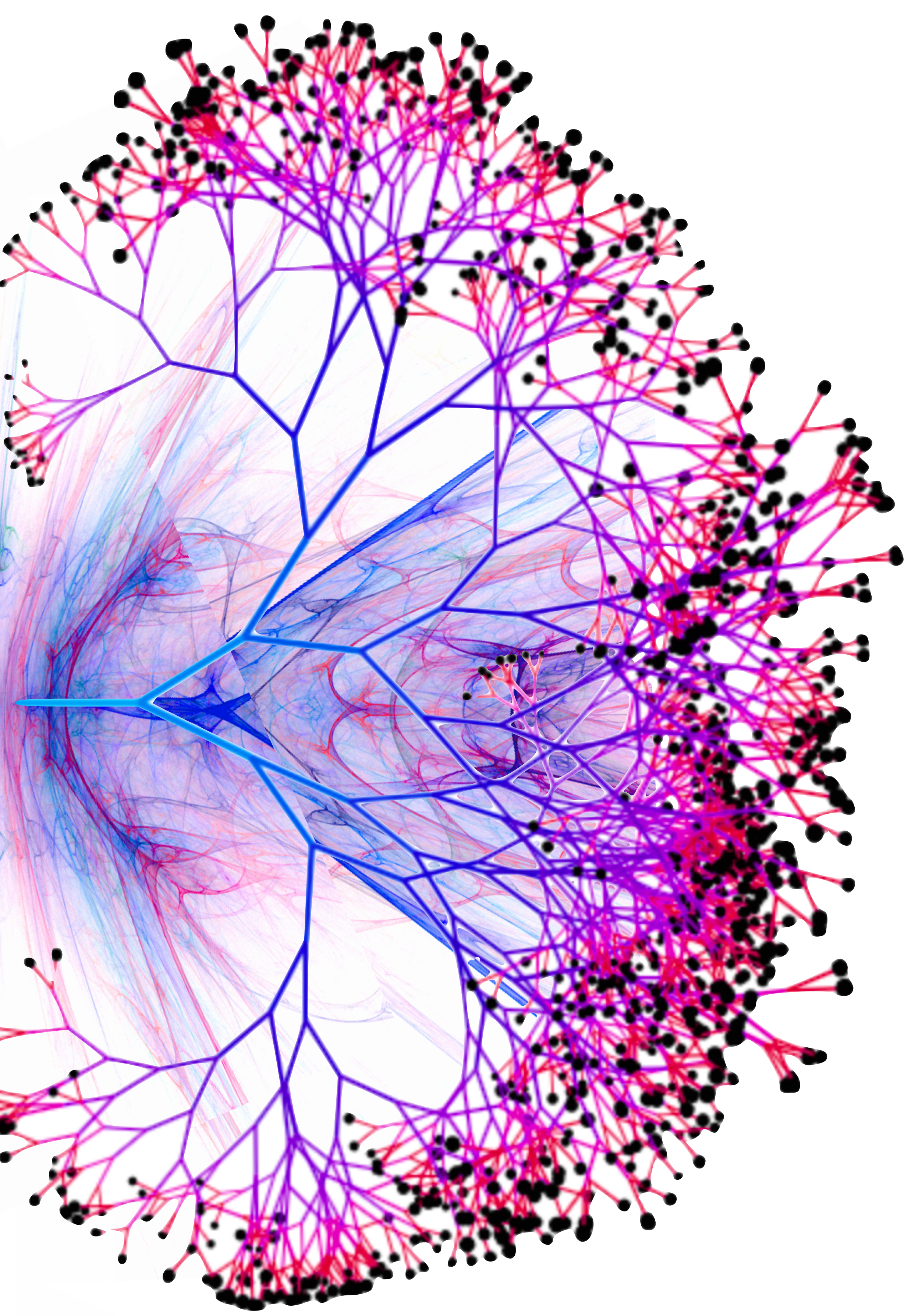
Soft QCD in MC Event Generators

(A selection of topics focusing on pp, with emphasis on Pythia)



1. **Hadronization Uncertainties** for **Precision Studies**
2. **Multiple Parton Interactions** & **PDFs**
3. **Colour Reconnections** & **Heavy-Flavour** Baryons
4. **Strangeness**, Ropes, and (Advanced) Close-Packing

Peter Skands
University of Oxford & Monash University

QCD@LHC
Durham — September 2023

1. **Hadronization Uncertainties** for **Precision Studies**

Hadronization

Map: Partons (defined at a low factorisation scale, after showering) → **Hadrons**

Inclusive sums ↑

- Fully Inclusive: **Power Corrections** (to IRC Safe Observables)
- Semi-Inclusive: **Fragmentation Functions**: One hadron species at a time
- Fully Exclusive: **Dynamical Models** in MC Event Generators

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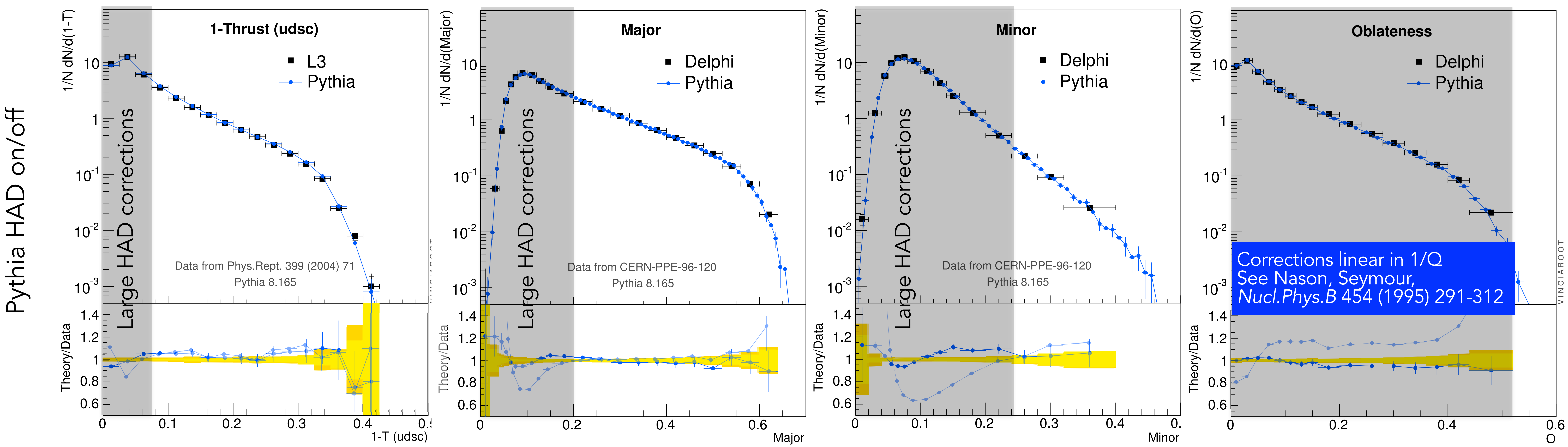

Important point: even for nominally IRC safe observables, **peaks** of distributions often involve low scales where **HAD sensitivity is highest** ⟹ NP peak shifts.

Uncertainties

High-Precision Measurements ↔ Rigorous & Exhaustive Uncertainties

- **Expensive** to construct & perform all salient parm variations individually ➞ GEANT …

  Not just question of CPU; also **environmental impact**, cost, inefficient duplication of man-hours & higher risk of mistakes/inconsistencies (by non-authors) + risk that lessons learned aren't perpetuated

- **Sophisticated:** reweighting methods developed for Parton Showers

  Based on reinterpreting the veto algorithm's accept and reject probabilities

  [VINCIA 1102.2126; SHERPA 1605.04692; HERWIG 1605.08256; PYTHIA 1605.08352]

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Hadronization Uncertainties: More parameters and lots of subtleties

Interplay between **perturbative** (eg N_{jets}) and **nonperturbative** (eg $N_{hadrons}$) observables

Parameter correlations; for a helping hand, see AutoTunes [Bellm & Gellersen, 1908.10811]

Risk of purely data-driven methods (eg eigentunes) to **overfit** precise data points at expense of tails / asymptotics / less statistically dominant (but perhaps theoretically important) data

Tensions between different measurements

- Recent elaborate studies with PYTHIA 8, see eg: [Jueid et al., 1812.07424; 2202.11546; 2303.11363]

Another aspect of the problem

Pythia, Herwig, Sherpa all tuned to ~ same data ➤ risk central tunes being "too" similar?

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Borrowed slide from A Ghosh ↔ Machine Learning of/for Theory Models

EPJC:s10052.022.10012.w: **Aishik Ghosh**, Benjamin Nachman

*Personal Comment: I would kind of hope next year's generator would be **closer** to Nature, not further from it…*

Instruction to ML: "Please shrink Pythia vs Herwig difference" **Model will learn to fool you !**

ML methods don't often generalise the way you would hope

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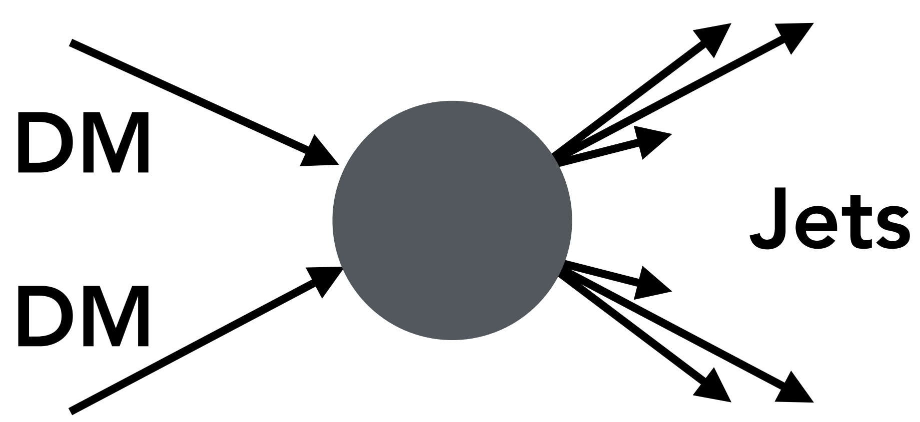
Example: The Strong Force Meets the Dark Sector

Based on A. Jueid et al., 1812.07424 (gamma rays, *eg for GCE*) and 2202.11546 (antiprotons, *eg for AMS*) + **2303.11363 (all)**

QCD uncertainties on Dark-Matter Annihilation Spectra



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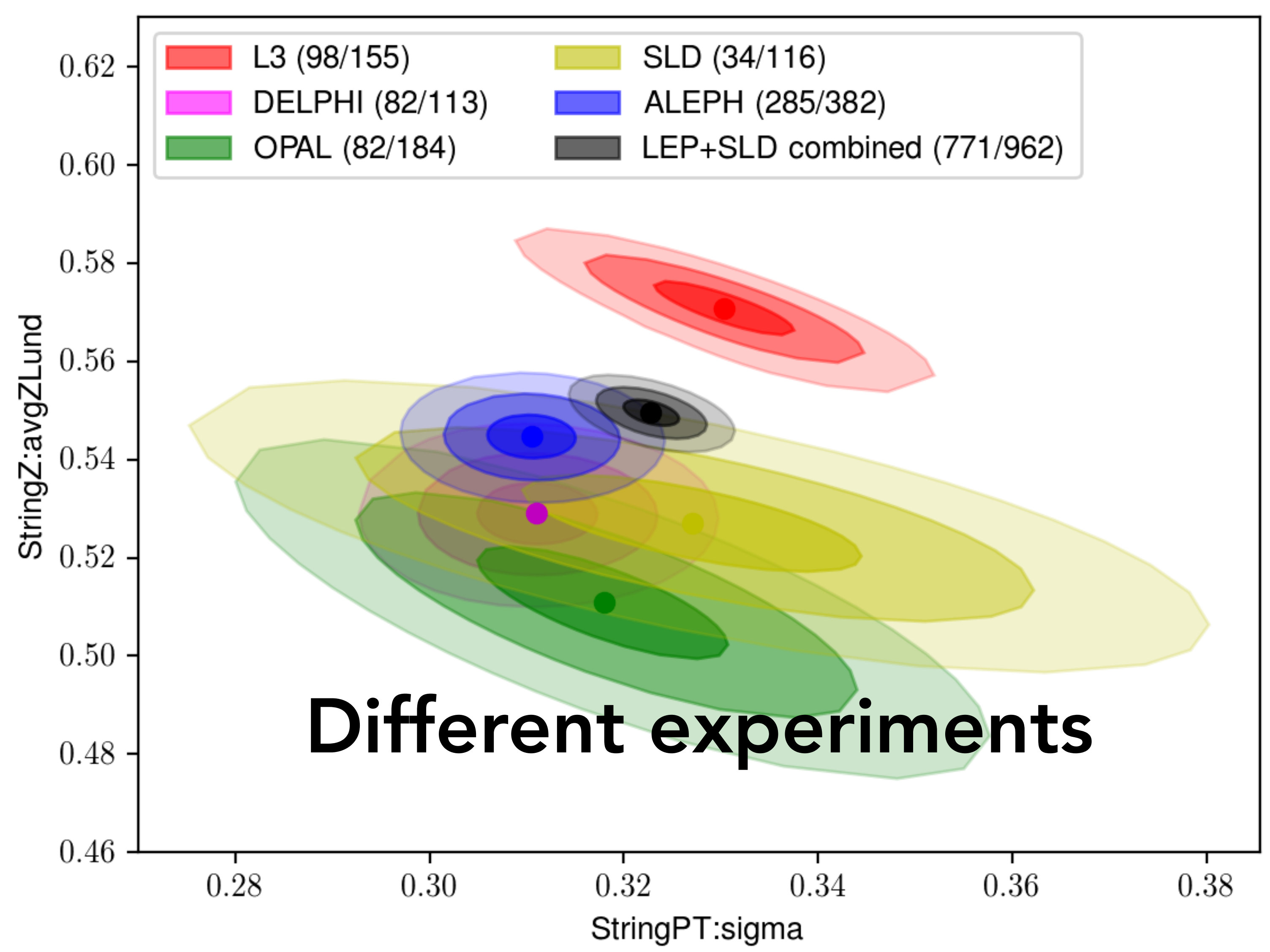
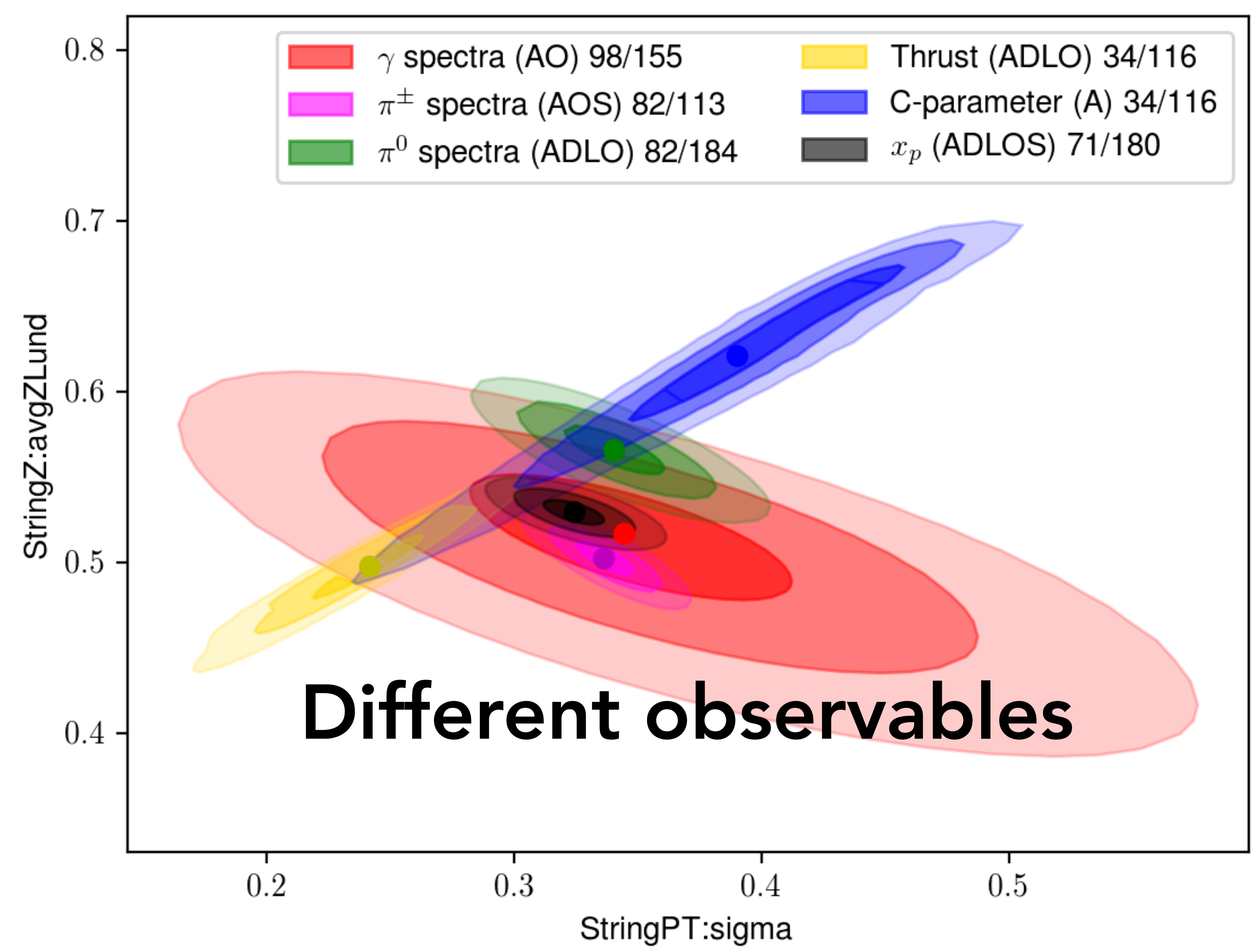
- Instead, did **parametric refittings** of LEP data within PYTHIA's modelling
  - $\langle z \rangle$, bLund, σ_{p_T} : **also useful for collider studies of hadronization uncertainties**

+ universality tests: identifying and addressing tensions, overfitting & universality/consistency





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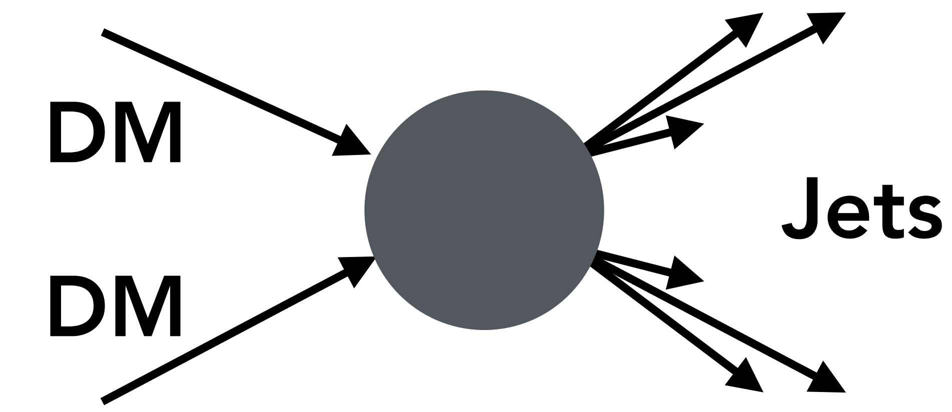

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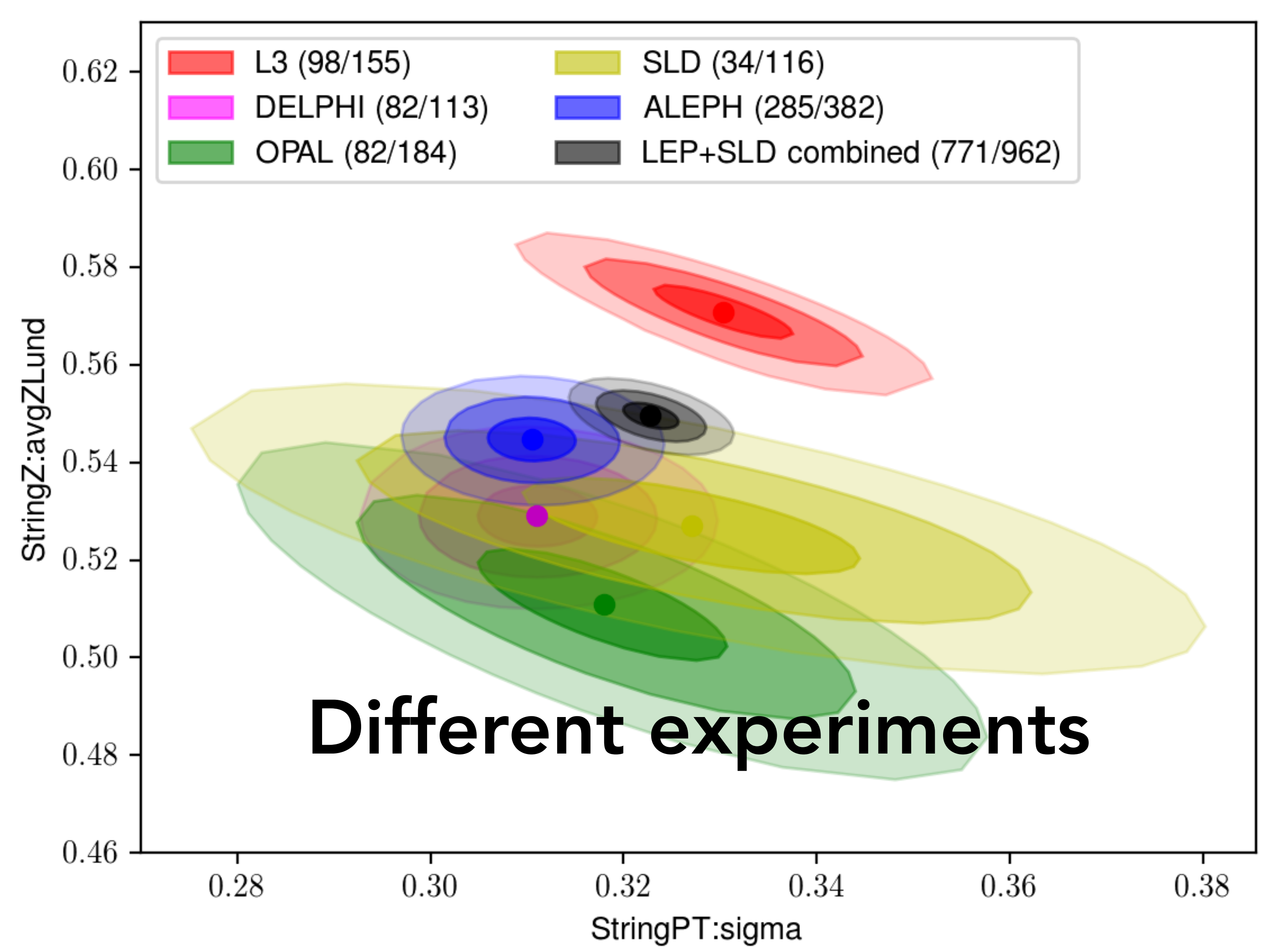

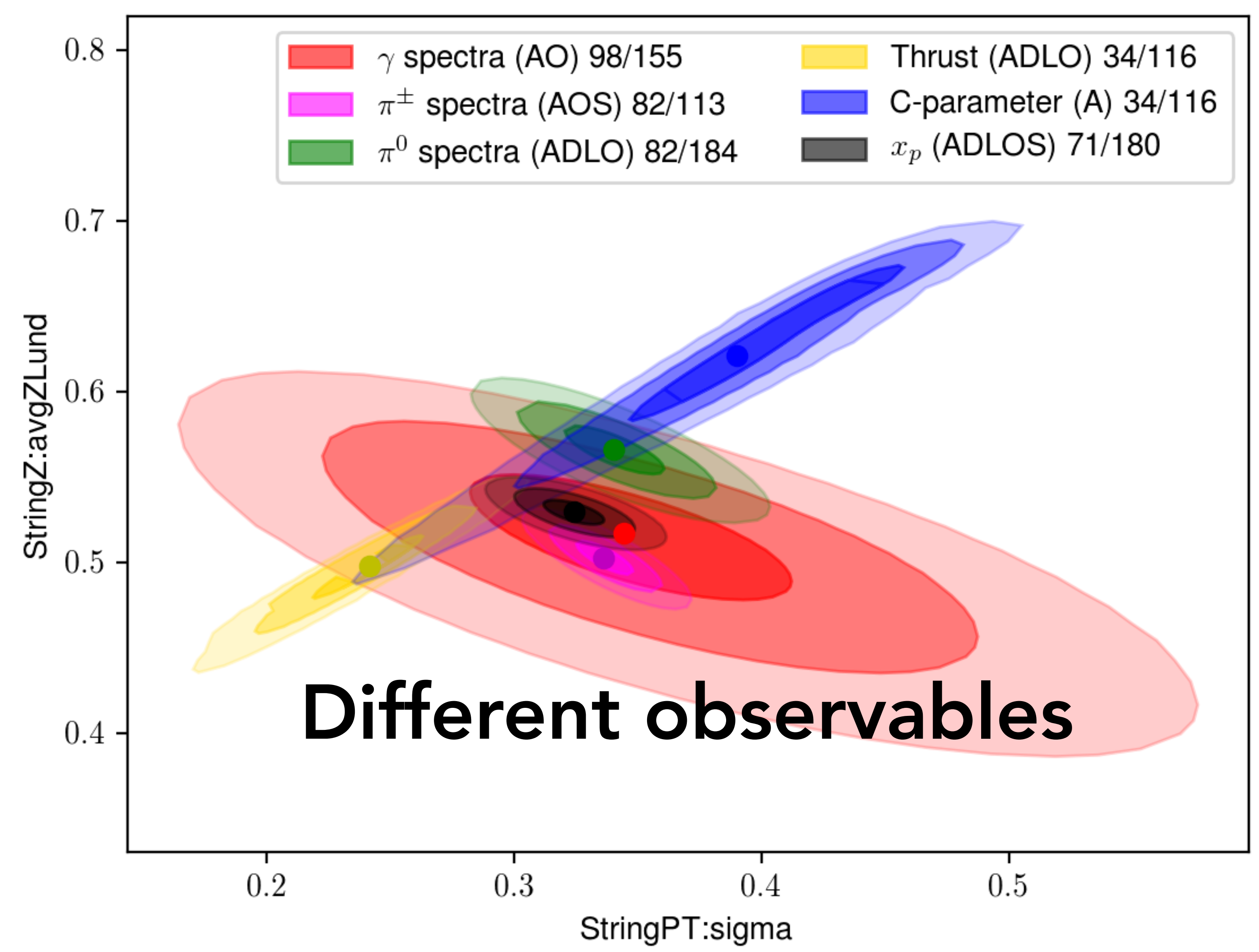

Simple sanity limit / overfit protection / tension resolution:
add blanket 5% baseline TH uncertainty
(+ exclude superseded measurements)

Parameter	without 5%	with 5%
StringPT:Sigma	$0.3151^{+0.0010}_{-0.00010}$	$0.3227^{+0.0028}_{-0.0028}$
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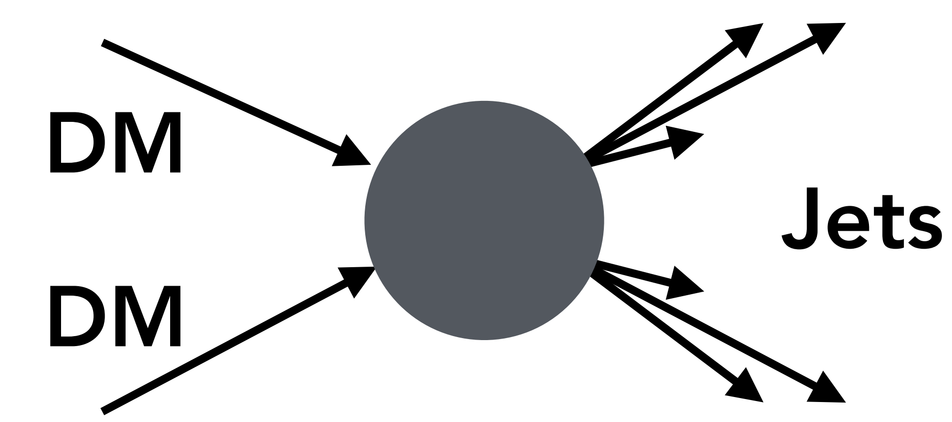

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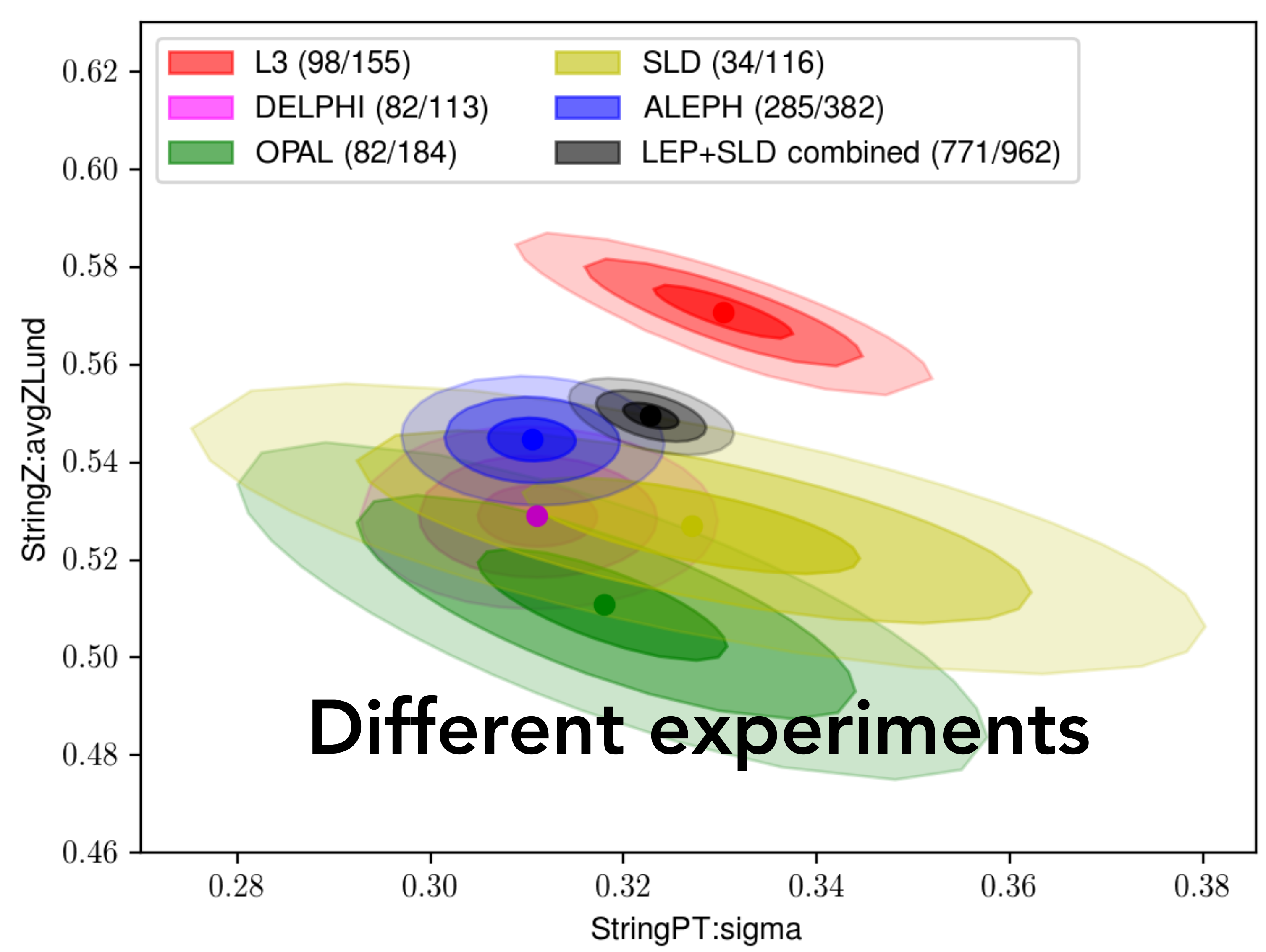

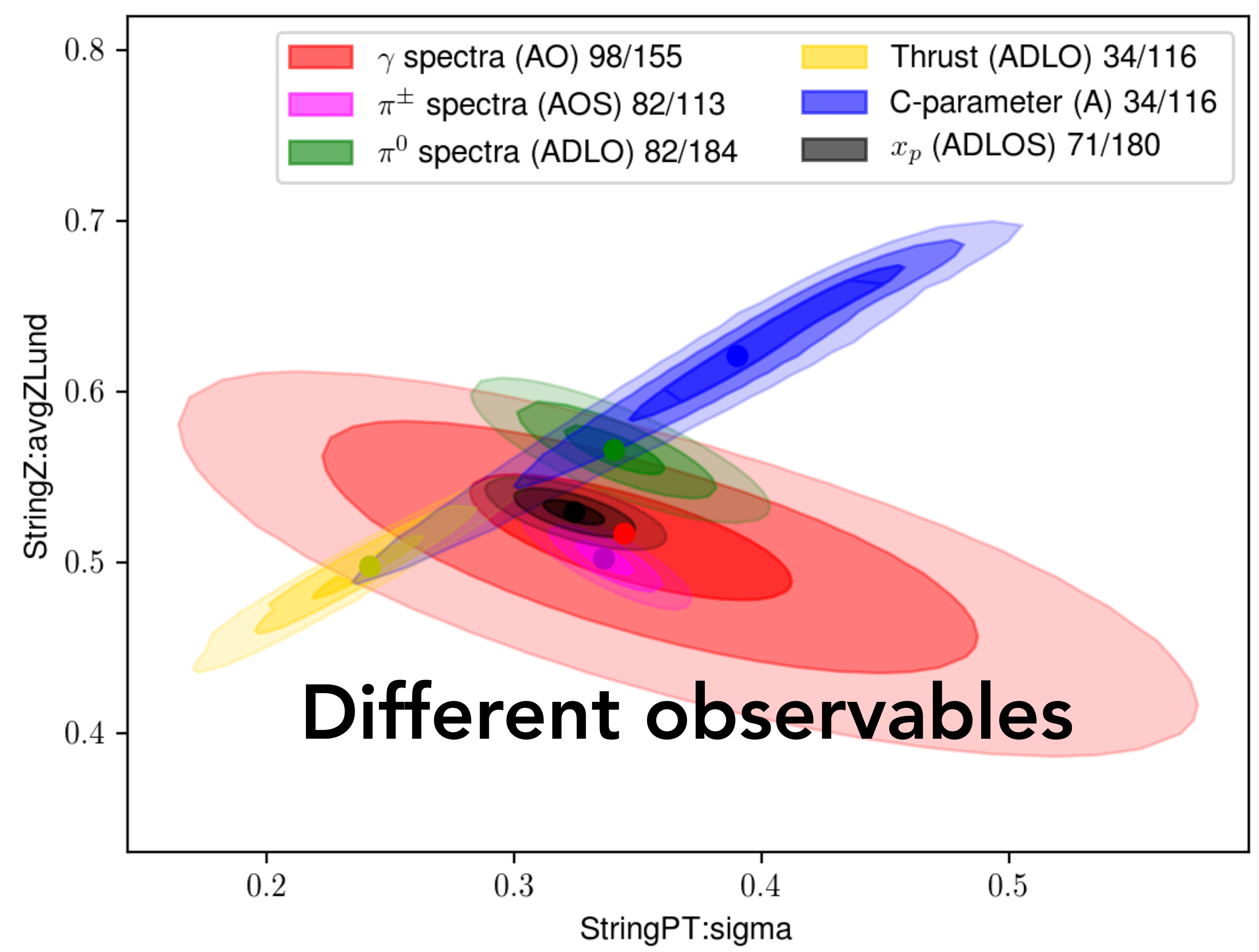

Other possible universality tests (eg in pp):

Different CM energies …
Different fiducial windows …
Different hard processes …
Quarks vs Gluons …

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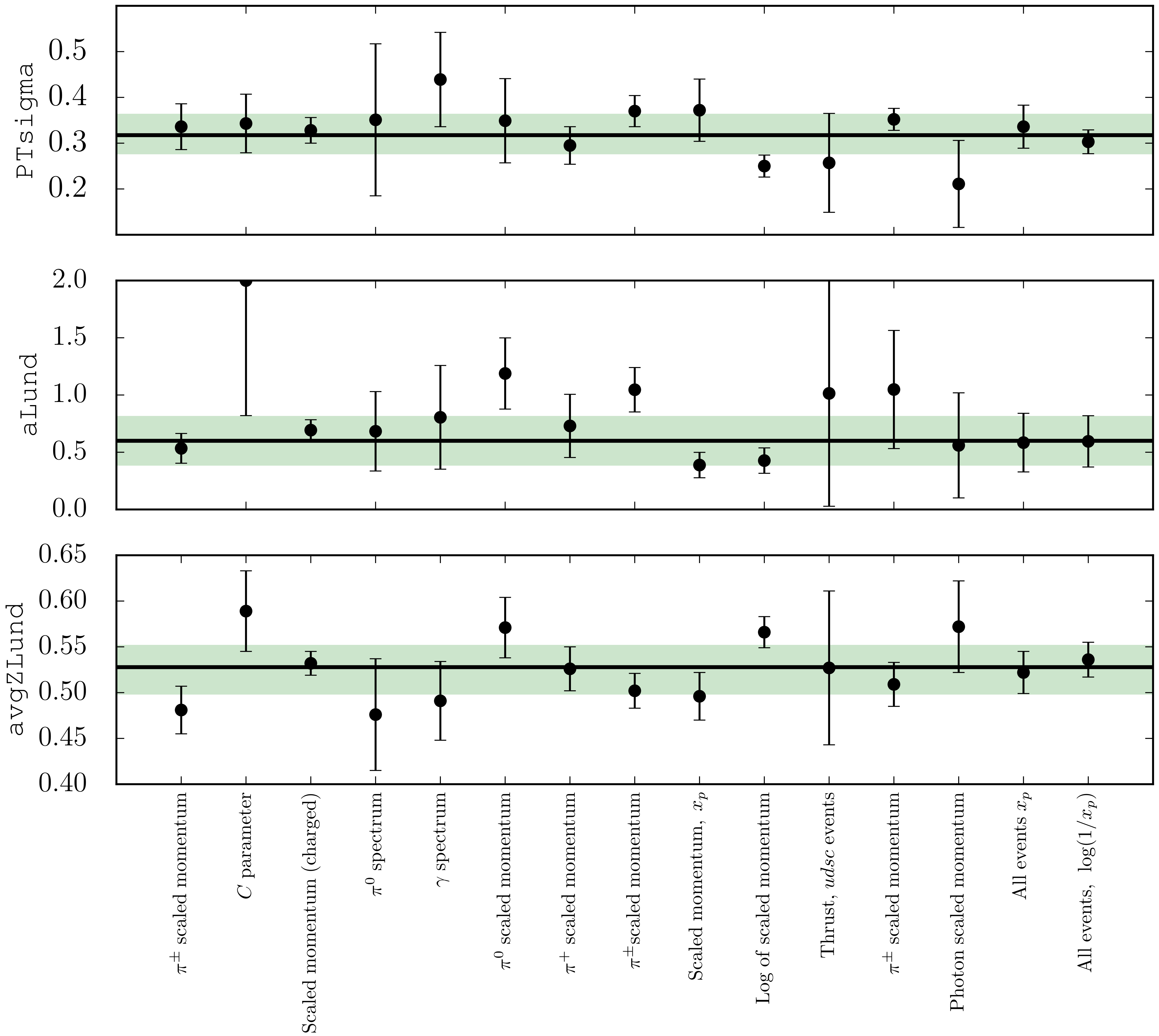
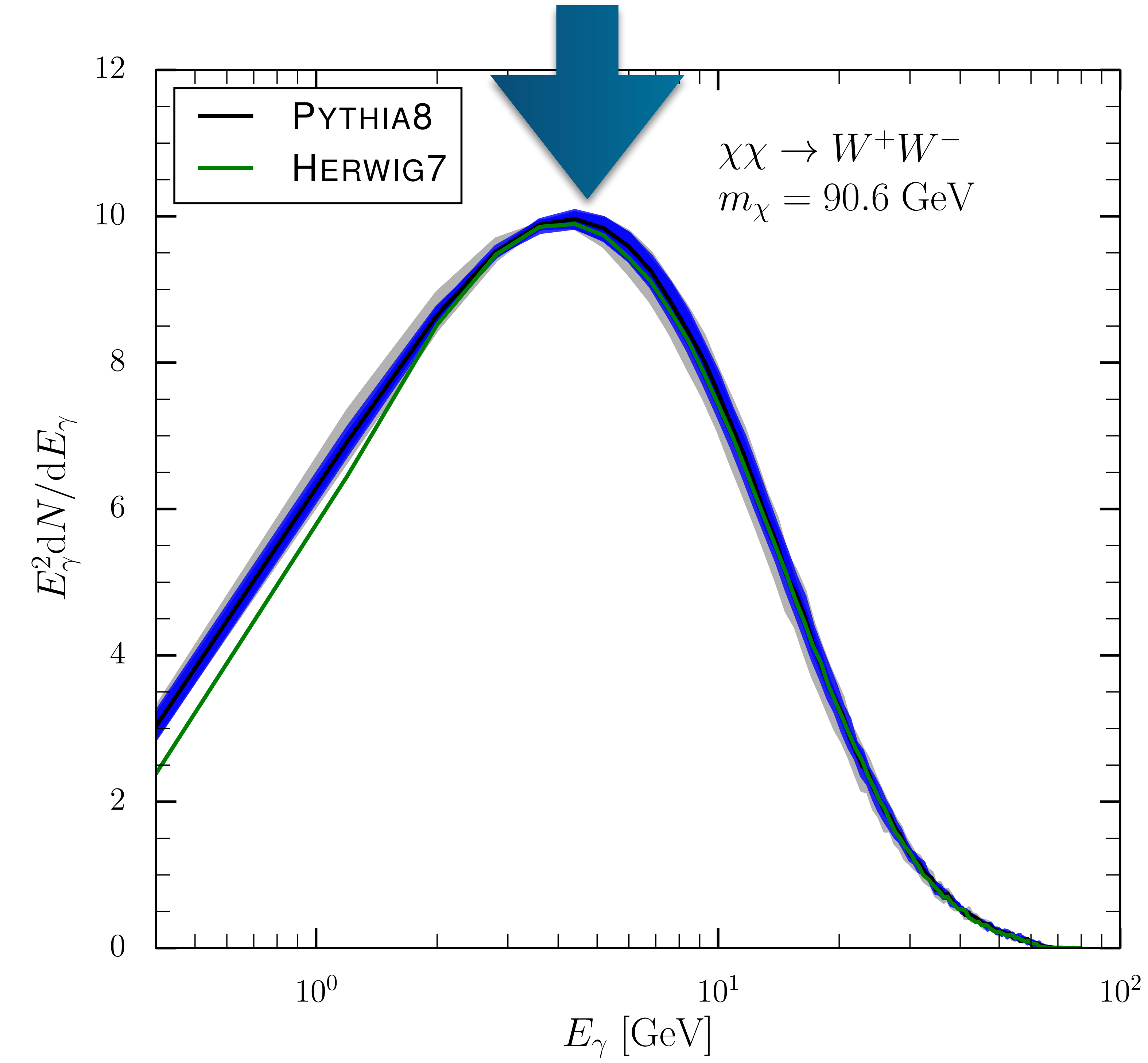


Weighted Average: good consistency across observables

10-point variations ➤ **Fairly convincing** uncertainty bands?



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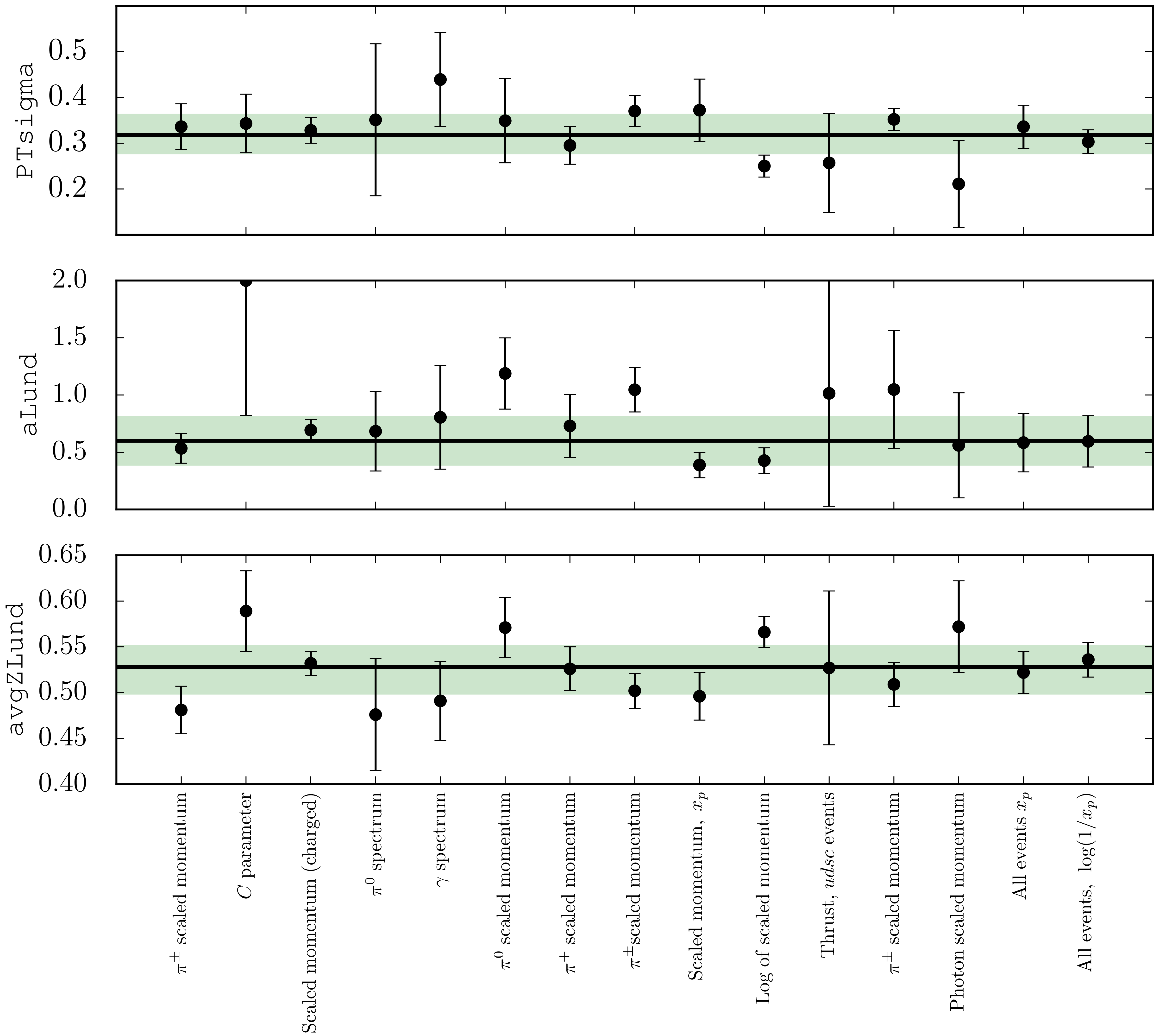

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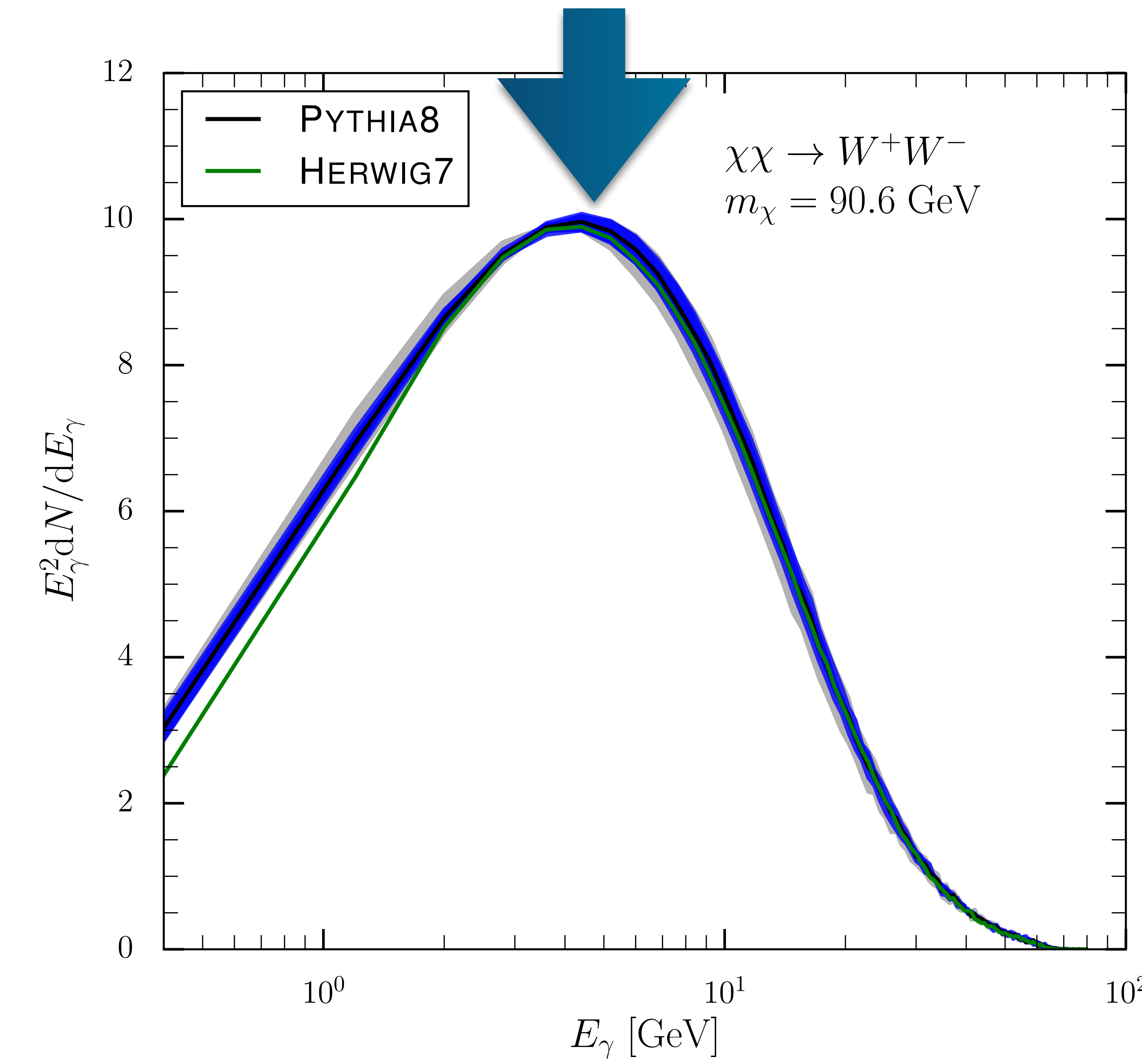

Same done for antiprotons, positrons, antineutrinos

Main Contact: adil.jueid@gmail.com

- Tables with uncertainties available on request. Also the spanning tune parameters of course.

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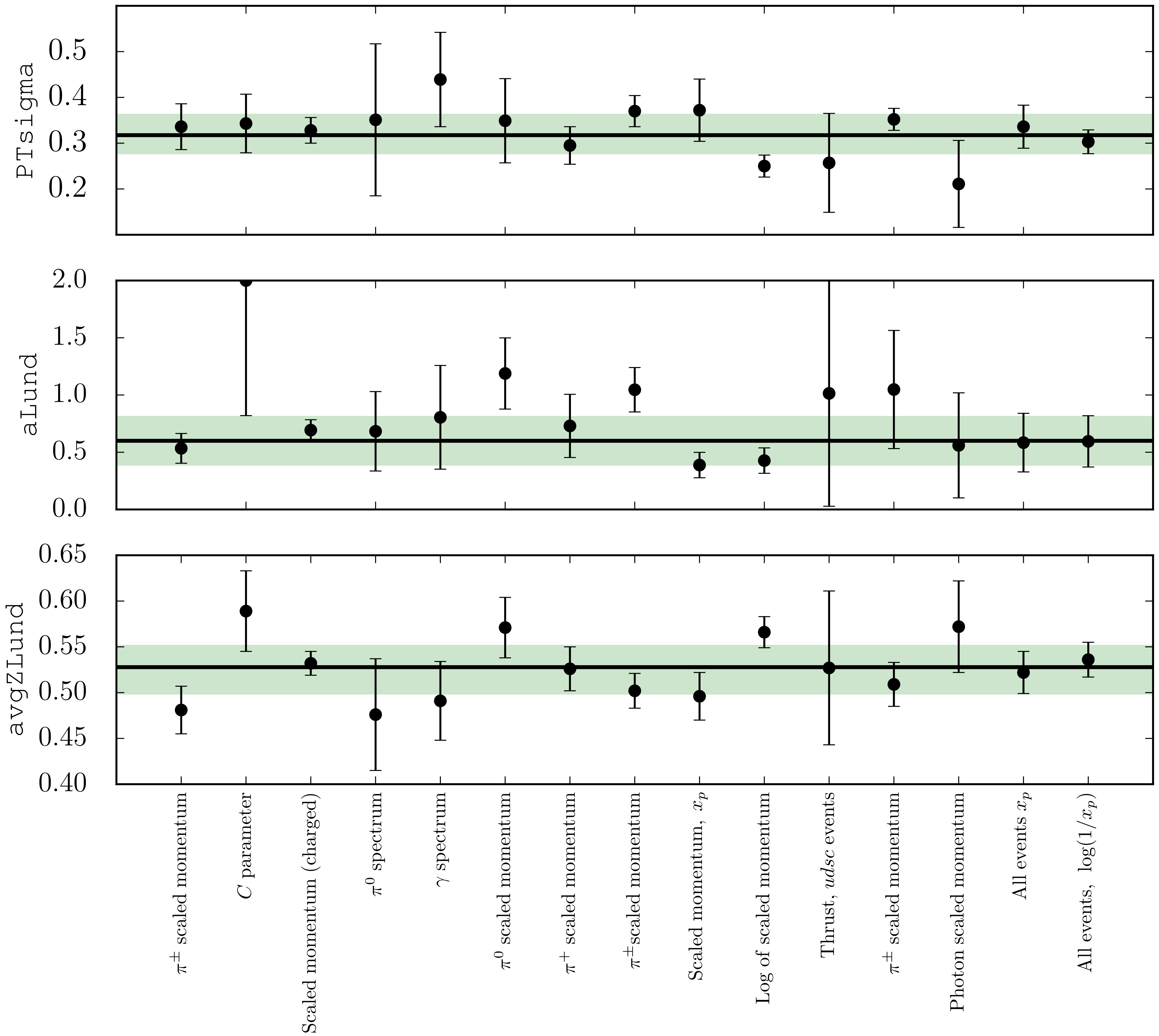

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Expensive?

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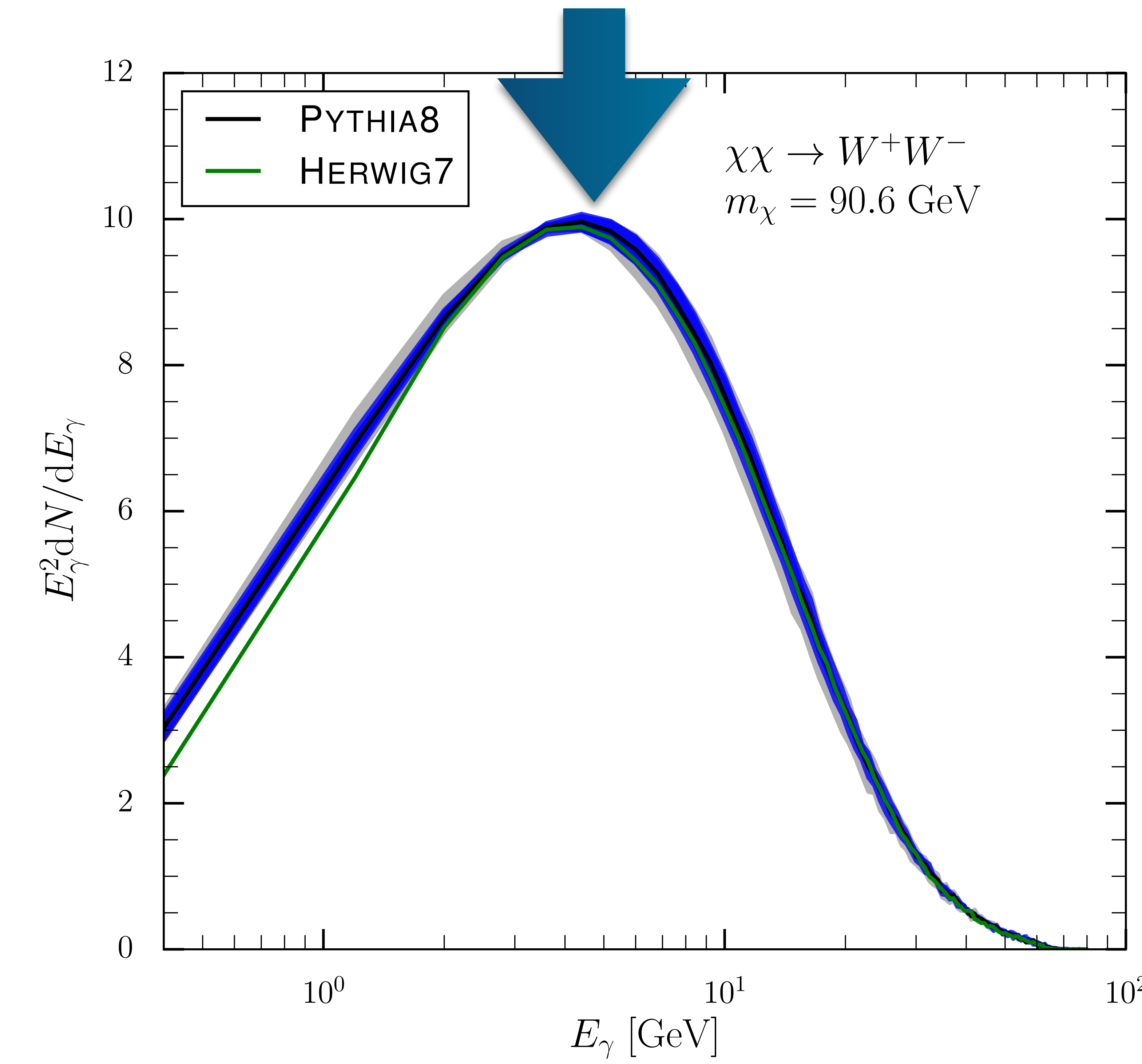

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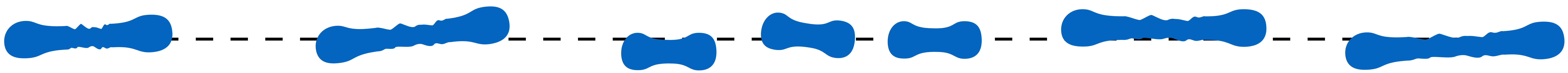
Problem:

- Given a colour-singlet system that (randomly) broke up into a specific set of hadrons:



- What is the relative probability that same system would have resulted, if the fragmentation parameters had been somewhat different?
- Would this particular final state become more likely ($w' > 1$)?
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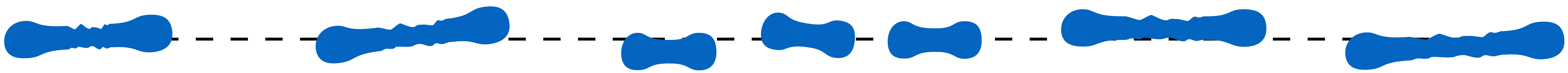

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Aug 25: Bierlich, Ilten, Menzo, Mrenna, Szewc, Wilkinson, Youssef, Zupan

[*Reweighting MC Predictions & Automated Fragmentation Variations in Pythia 8*, 2308.13459]

Method is general; demonstrated on variations of the 7 main parameters governing longitudinal and transverse fragmentation functions in PYTHIA 8

https://gitlab.com/uchep/mlhad-weights-validation

Examples

Transverse FF (Gaussian)

$$\frac{1}{2\pi\sigma_{p_T}^2}\exp\left(-\frac{(\Delta p_x)^2+(\Delta p_y)^2}{2\sigma_{p_T}^2}\right)$$

For each p_T (Box-Muller transform):

$$w' = \frac{\sigma^2}{\sigma'^2}\exp\left(-\kappa\left(\frac{\sigma^2}{\sigma'^2}-1\right)\right)$$

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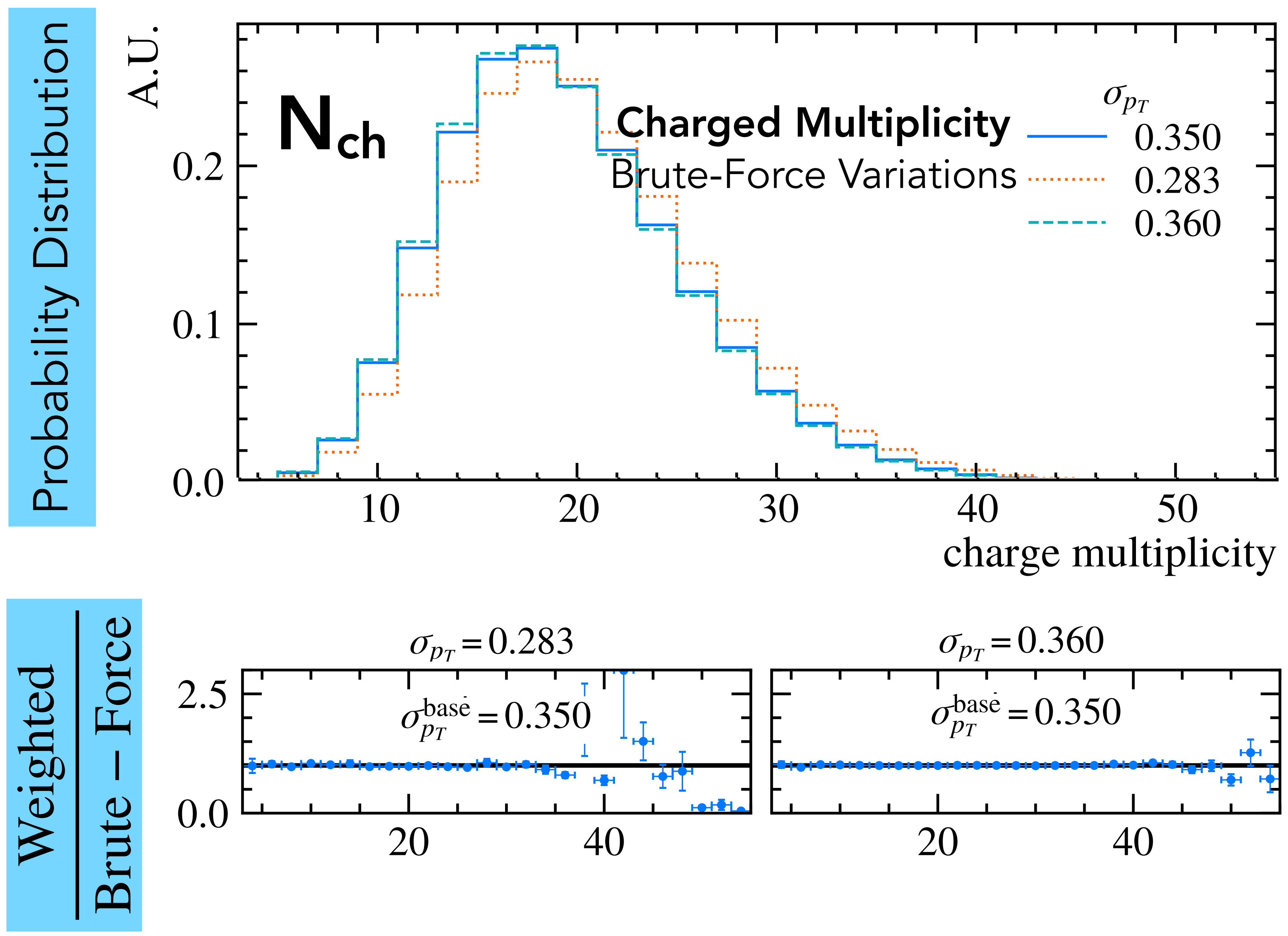

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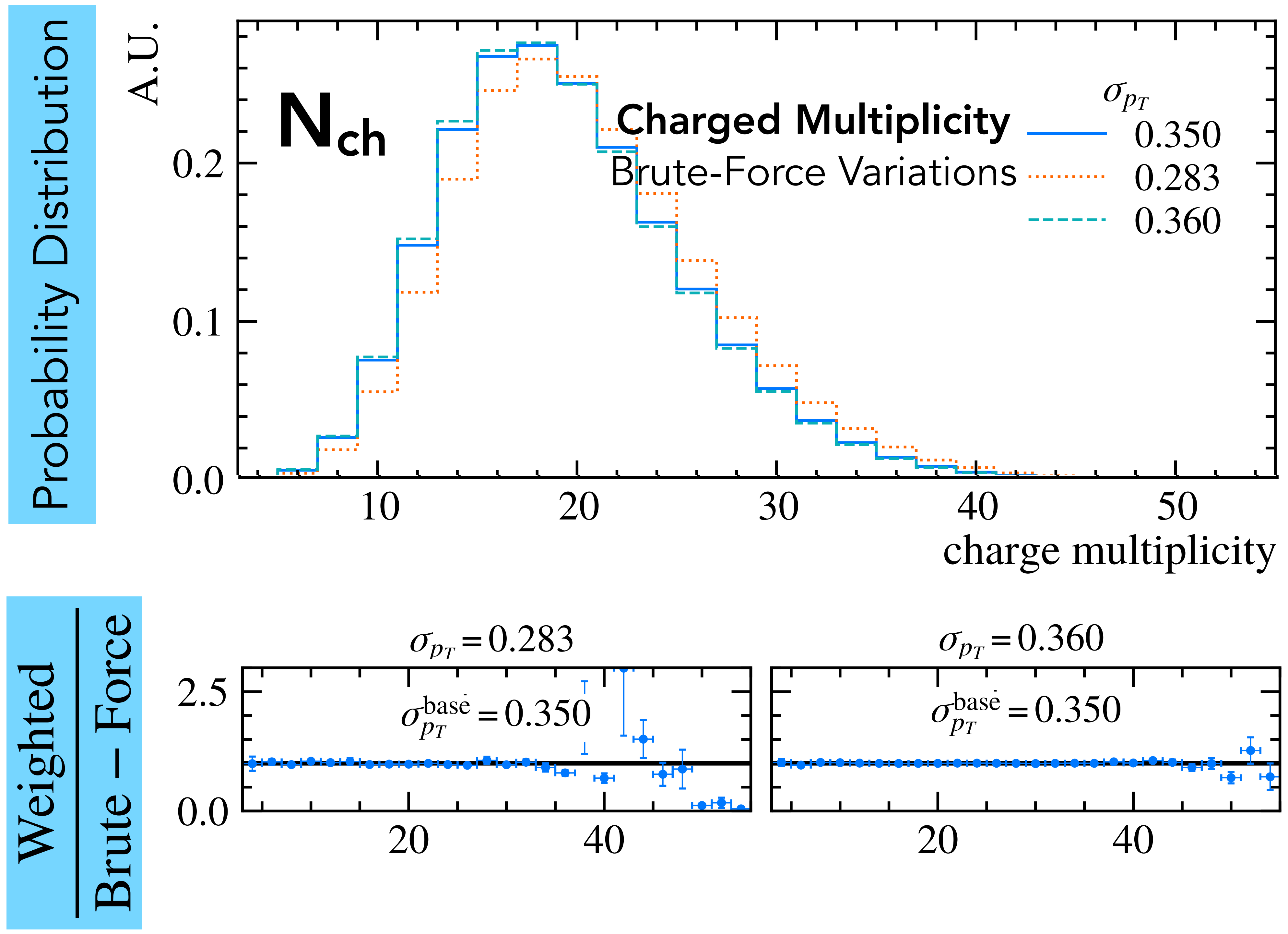

Longitudinal FF (Lund Symmetric FF)

f(z) ~ *scaled* light-cone hadron momentum fraction $\propto \frac{1}{z^{1+r_Q b m_Q^2}}(1-z)^a \exp\left(-\frac{bm_\perp^2}{z}\right)$

Accept-Reject Algorithm

$$w' = w \prod_{i\in\text{accepted}} R'_{i,\text{accept}}(z) \prod_{j\in\text{rejected}} R'_{j,\text{reject}}(z),$$

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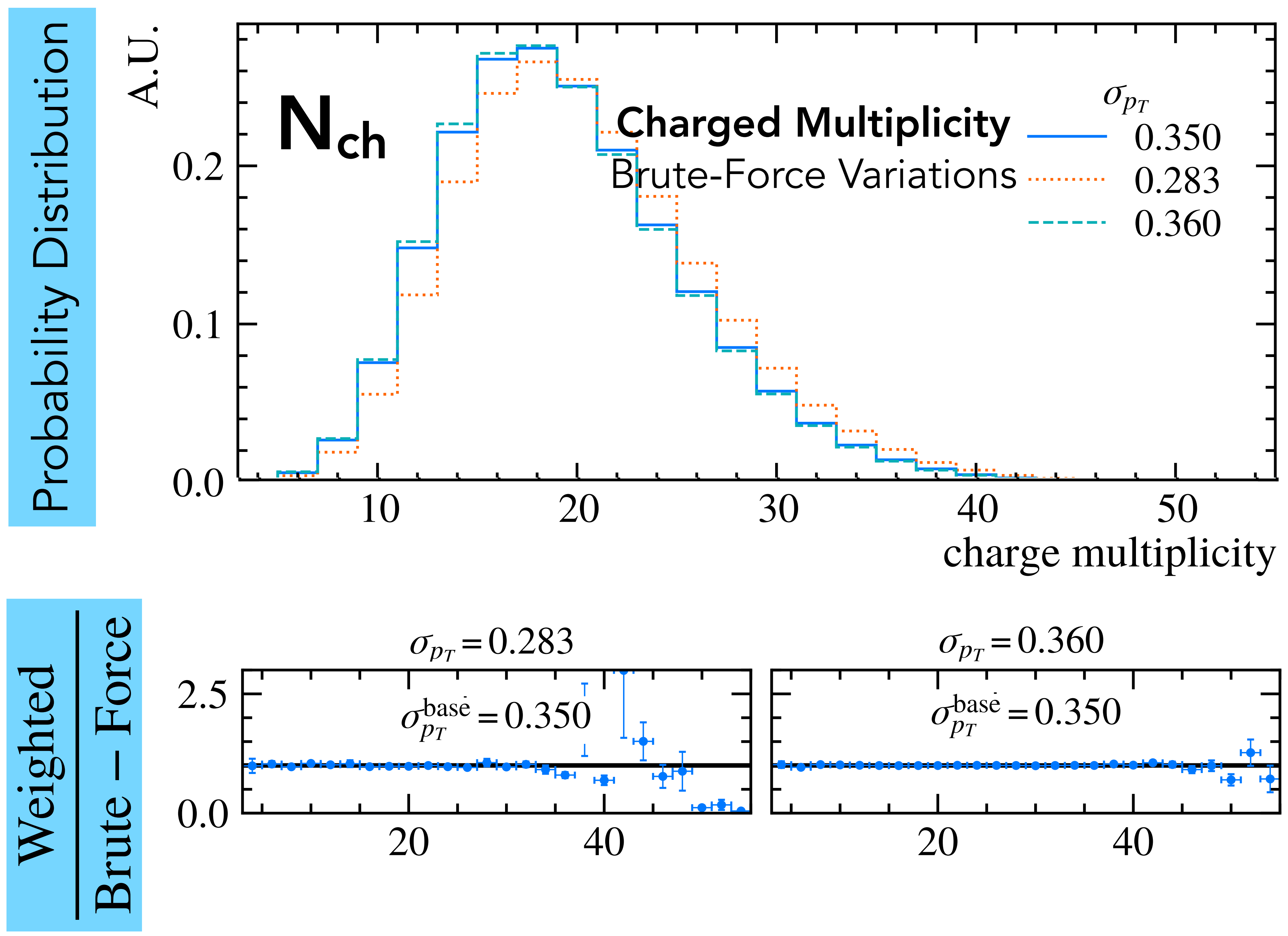

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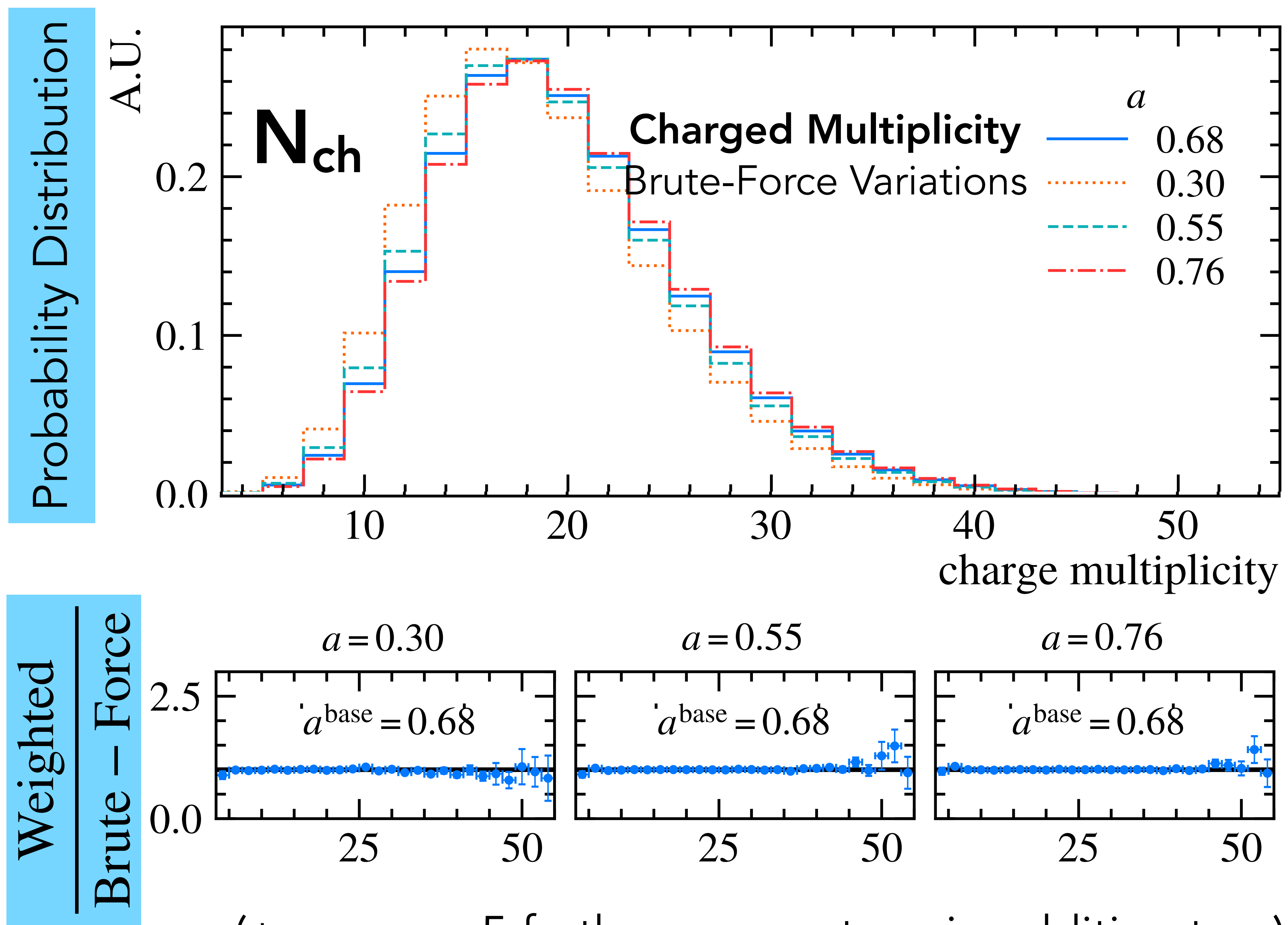

(+ can vary 5 further parameters, in addition to *a*)

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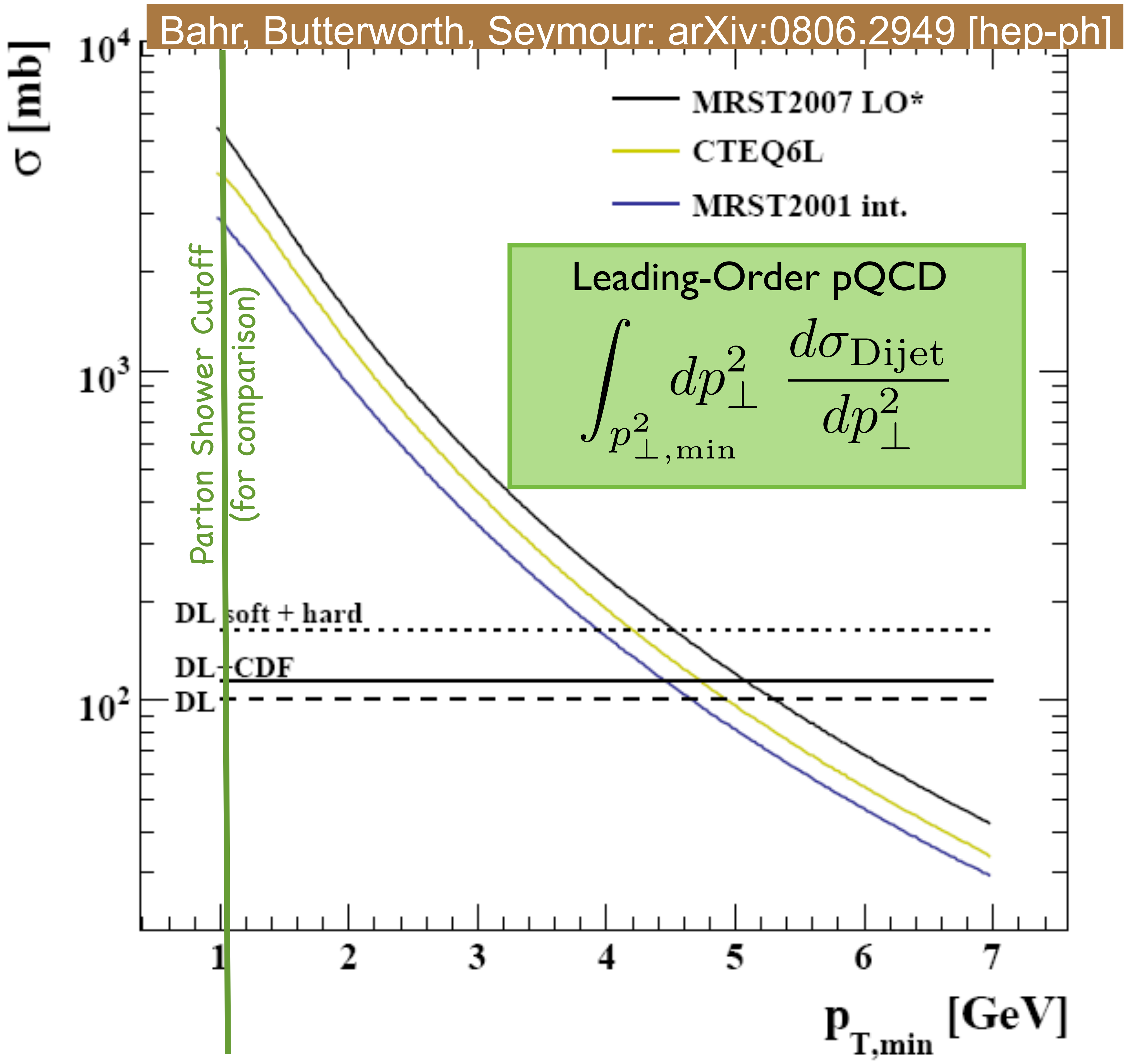
QCD dijet cross section (cumulative)



Lesson from bremsstrahlung in pQCD:

Divergences → fixed-order breaks down

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Unitarity: Divergent cross section for one emission reinterpreted as finite cross section for a **divergent number of emissions**

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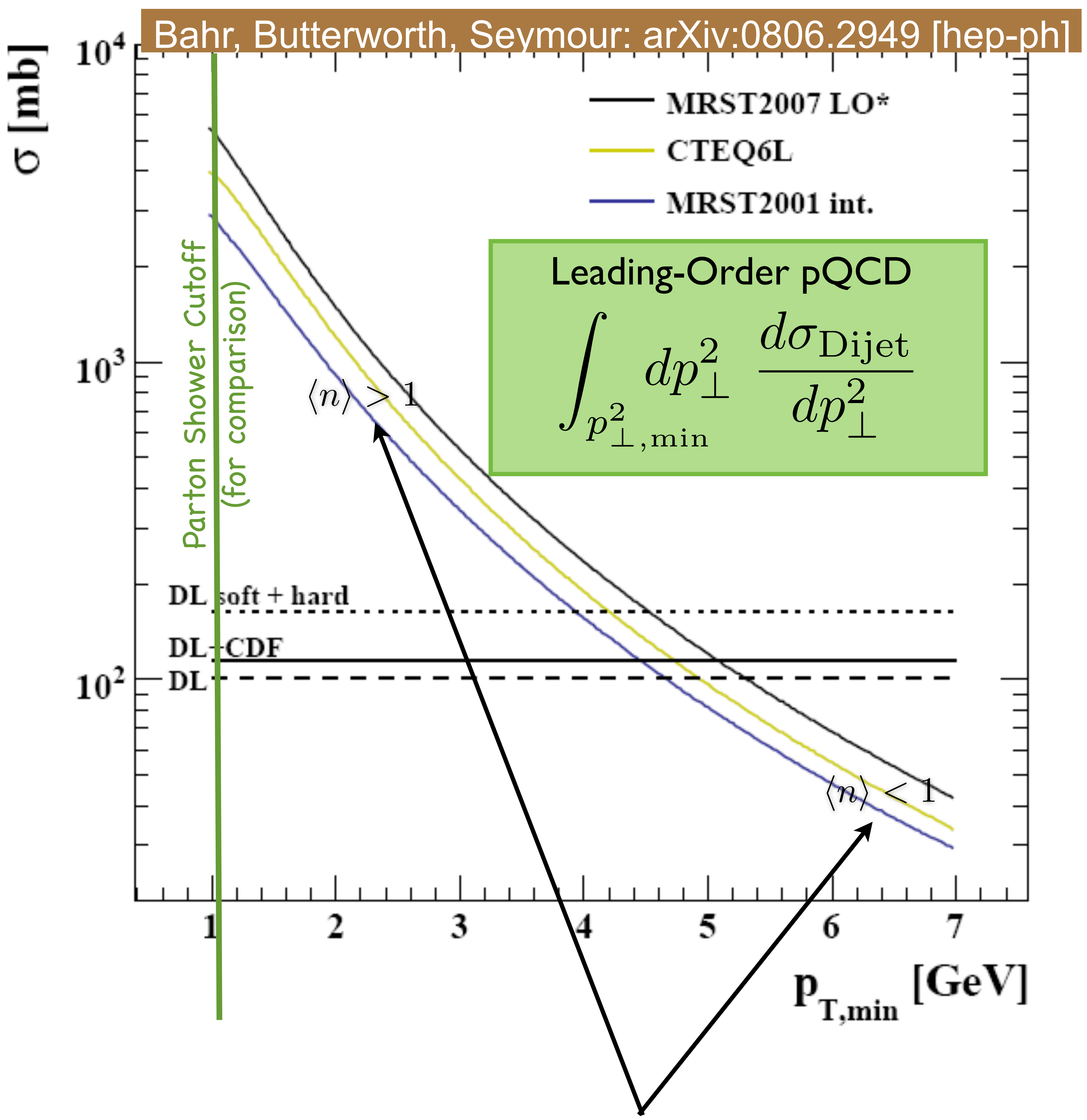

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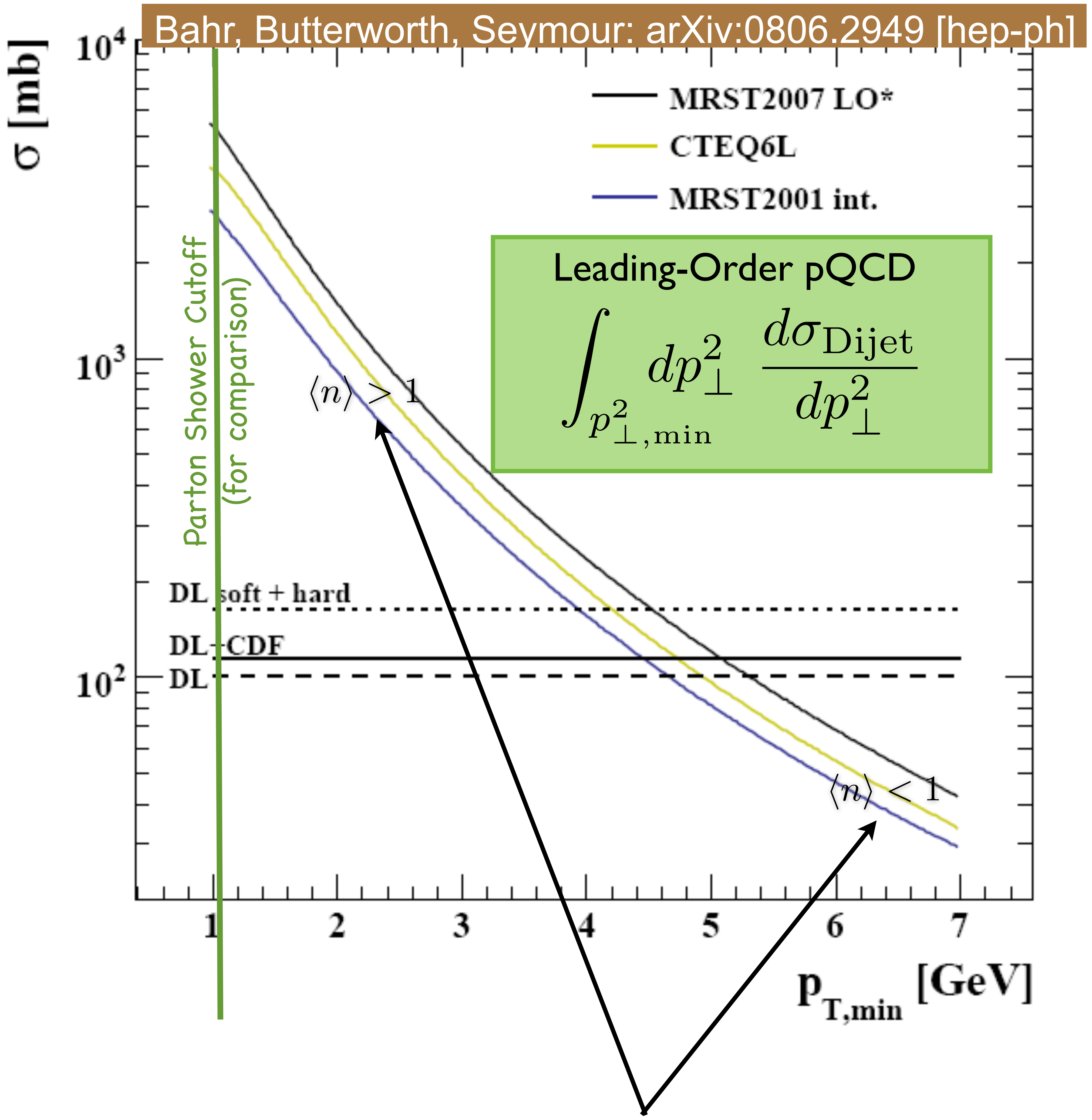

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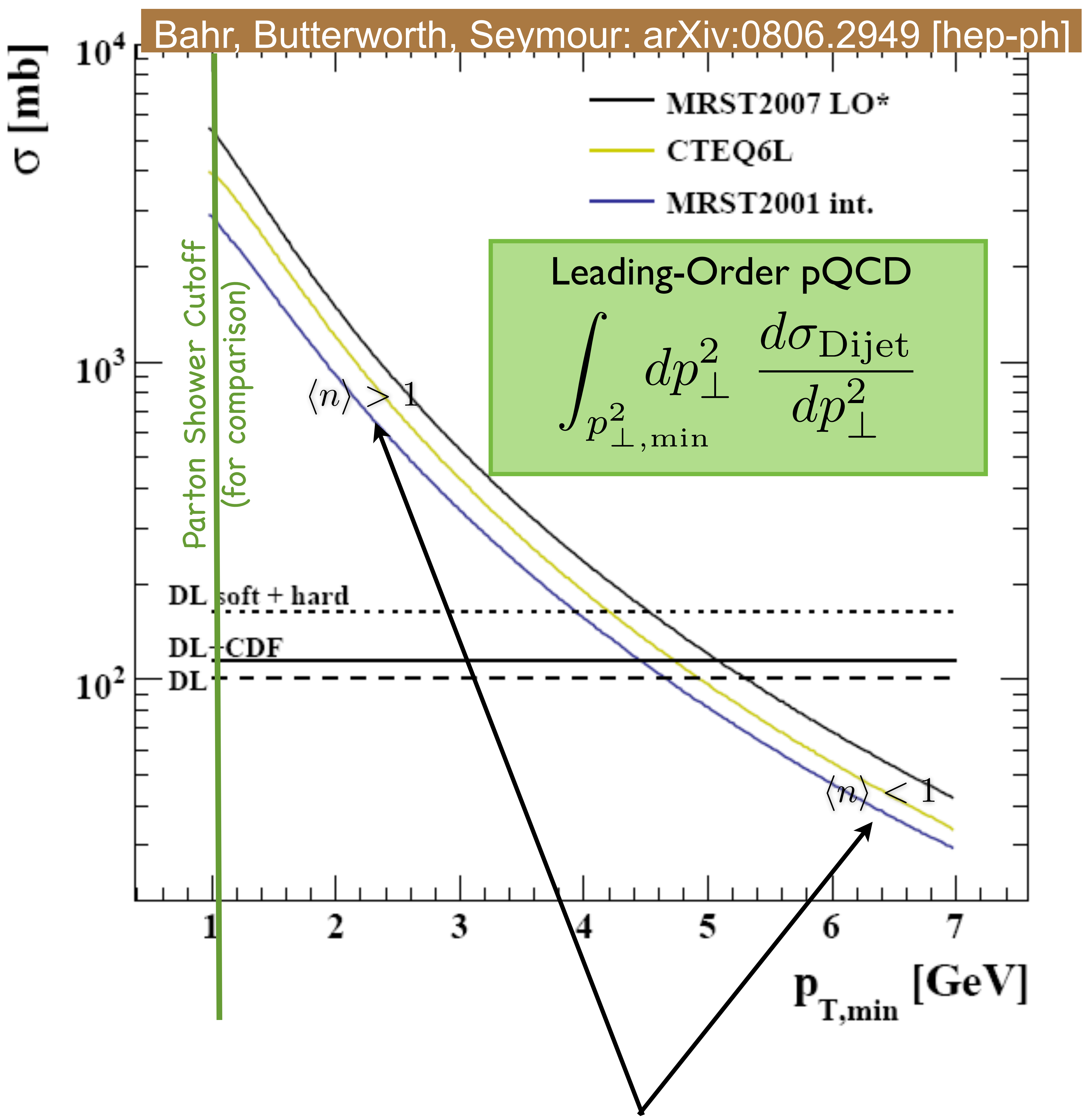

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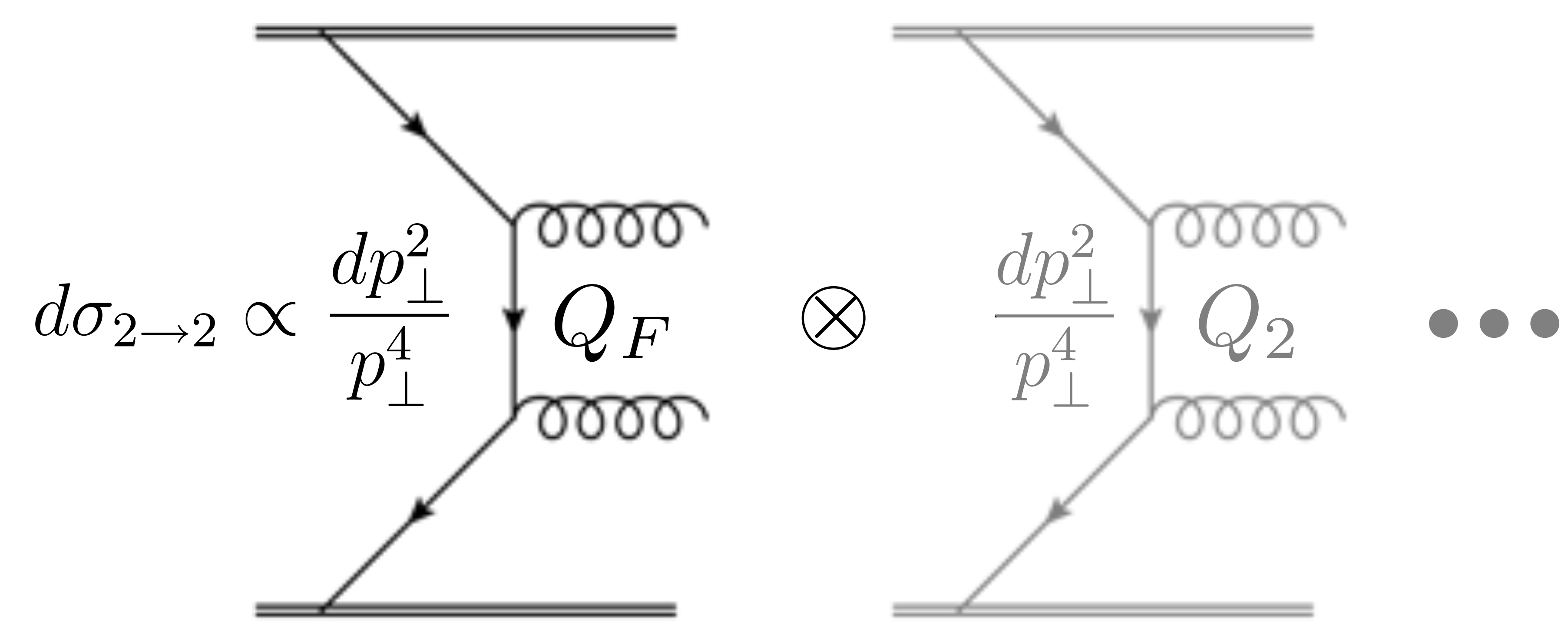

MPI probe low p_T scales down to $Q \sim 1\,\mathrm{GeV}$

And very low x scales, down to $x \sim 1/s_{\mathrm{hh}}$

Earliest MC model ("old" PYTHIA 6 model) Sjöstrand, van Zijl PRD36 (1987) 2019

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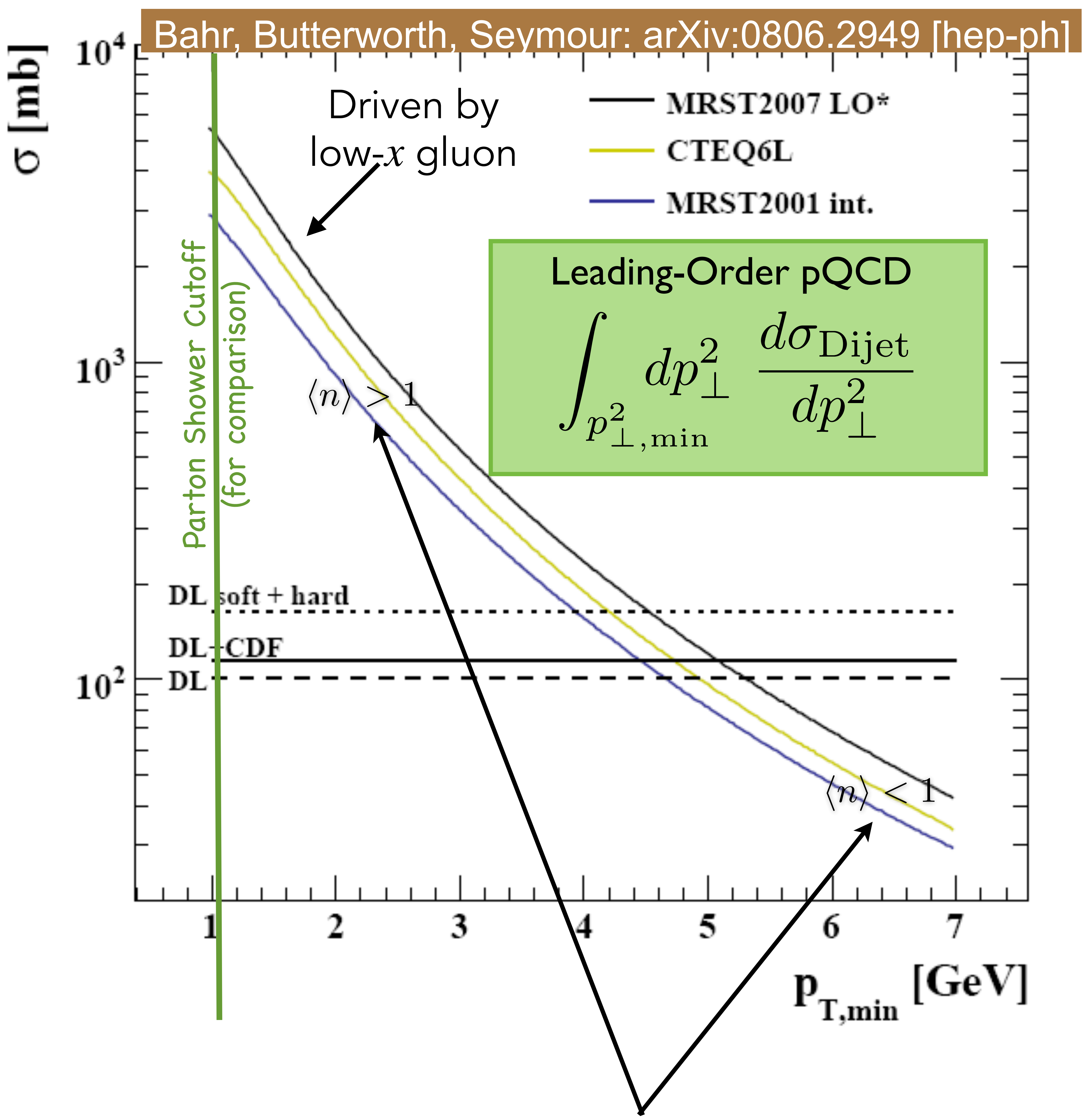

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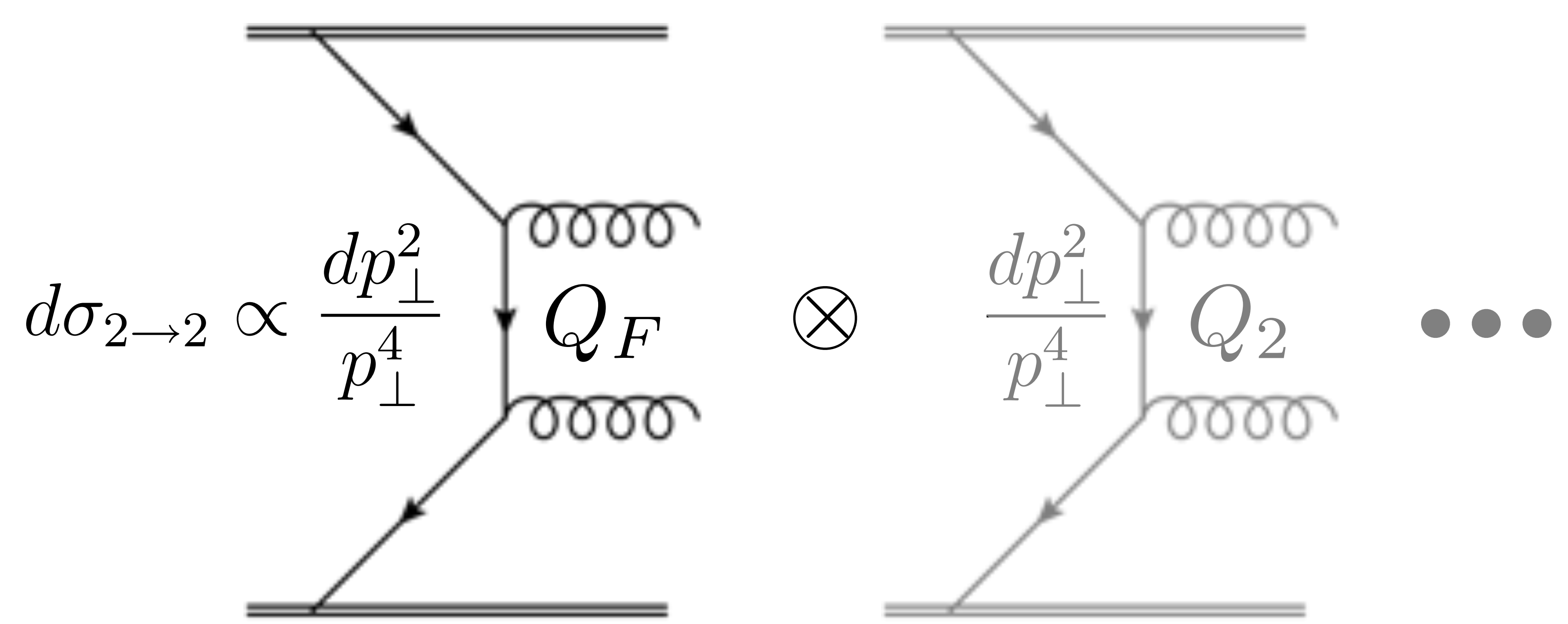

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The issue with NLO gluons at low x

(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 $P_{q/g}(z) \propto 1/z$ for small z $\Longrightarrow$ Integral over z produces an 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**.

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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.

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

$$\frac{\mathrm{ME_{NLO}\,PDF_{NLO}}}{\mathrm{ME_{LO}\,PDF_{LO}}} = (1+0.2)(1-0.2) = 0.96$$

👍 log terms cancel

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

$$\frac{\mathrm{ME_{NLO}\,PDF_{NLO}}}{\mathrm{ME_{LO}\,PDF_{LO}}} = (1+2)(1-2) = -3$$

👎 Cross term dominates; The PDF becomes negative

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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!**

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   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?

3. **Colour Reconnections** & **Heavy-Flavour** Baryons

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Hadronization

- Map: Partons (defined at a low factorisation scale, after showering) → Hadrons
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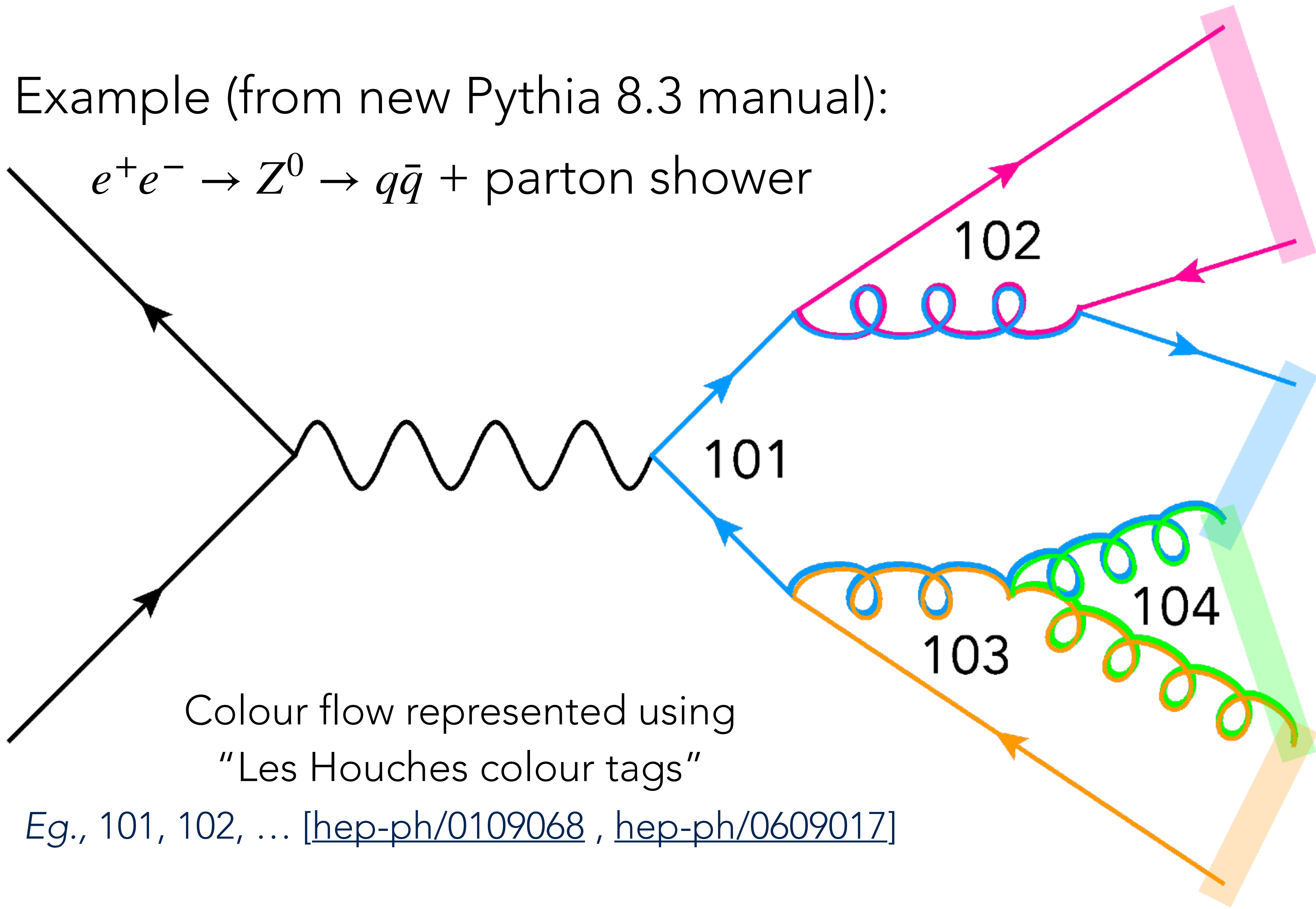
$\Longrightarrow$ Probability for any given colour charge to accidentally be same as any other $\to 0$.

$\Longrightarrow$ Each colour appears only once & is matched by a unique anticolour.

Example (from new Pythia 8.3 manual):

$e^+e^- \to Z^0 \to q\bar{q}$ + parton shower



Colour flow represented using "Les Houches colour tags"

Eg., 101, 102, … [hep-ph/0109068 , hep-ph/0609017]

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In e^+e^- collisions (LEP):

- Corrections to the Leading-Colour picture suppressed by $1/N_C^2 \sim 10\,\%$
- Also: coherence $\Longrightarrow$ not much overlap in phase space (except in WW → 4q)

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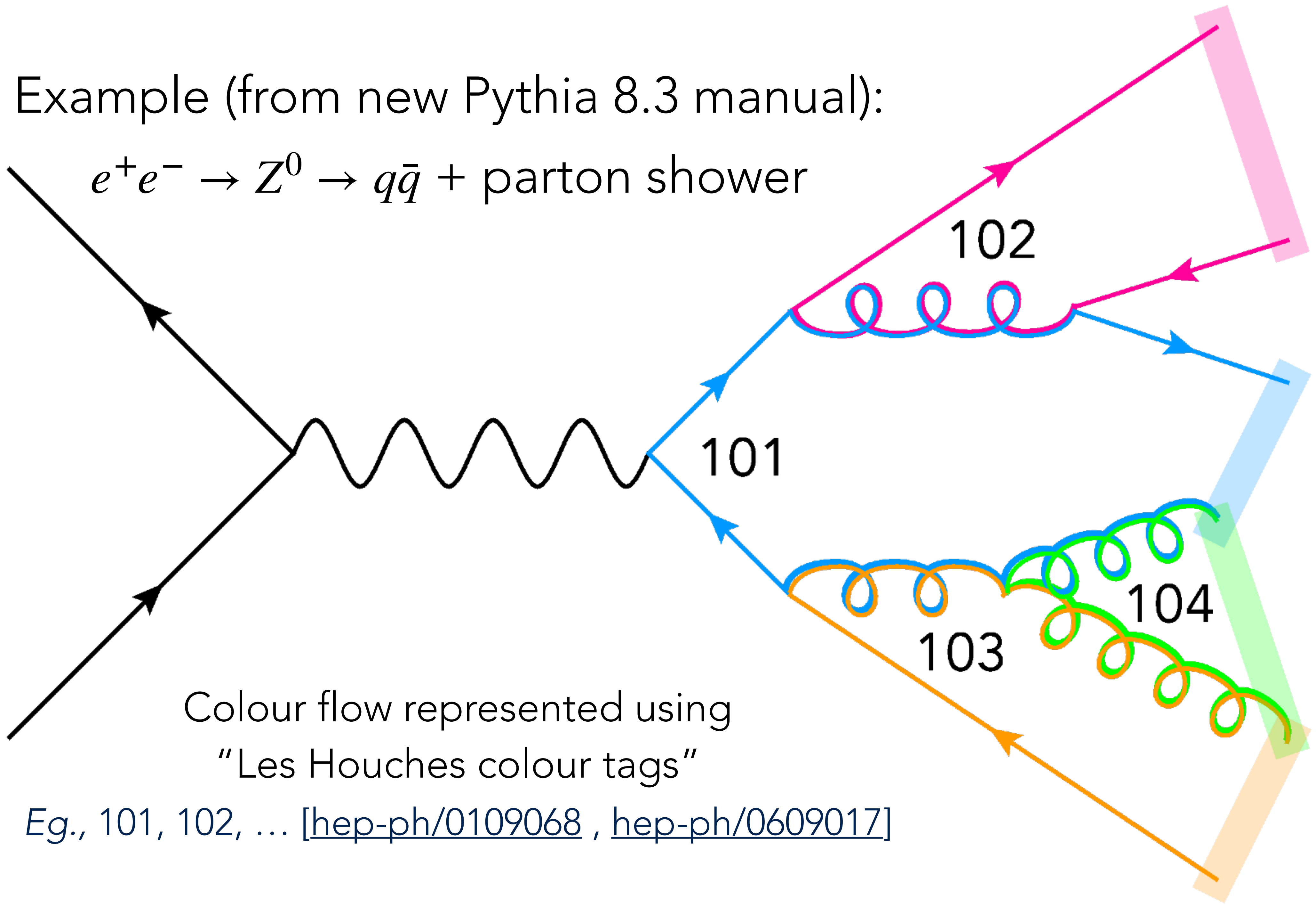

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High-energy pp collisions with QCD bremsstrahlung + multi-parton interactions

- Final states with very many coloured partons
- With significant overlaps in phase space
- Who gets confined with whom?
- If each has a colour ambiguity ~ 10%, CR becomes more likely than not

$$\text{Prob(no CR)} \propto \left(1 - \frac{1}{N_C^2}\right)^{n_{\mathrm{MPI}}}$$

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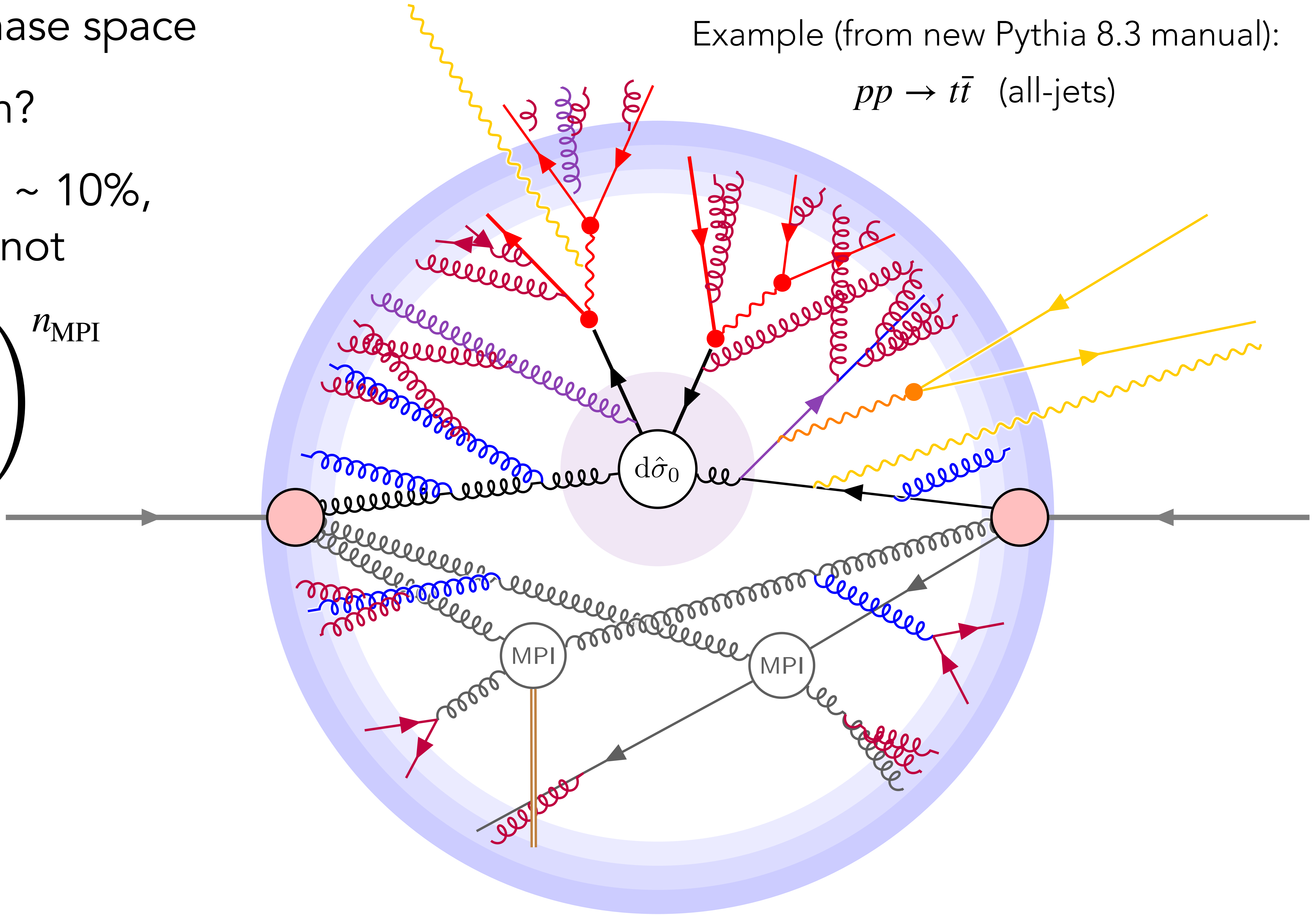
$pp \to t\bar{t}$ (all-jets)



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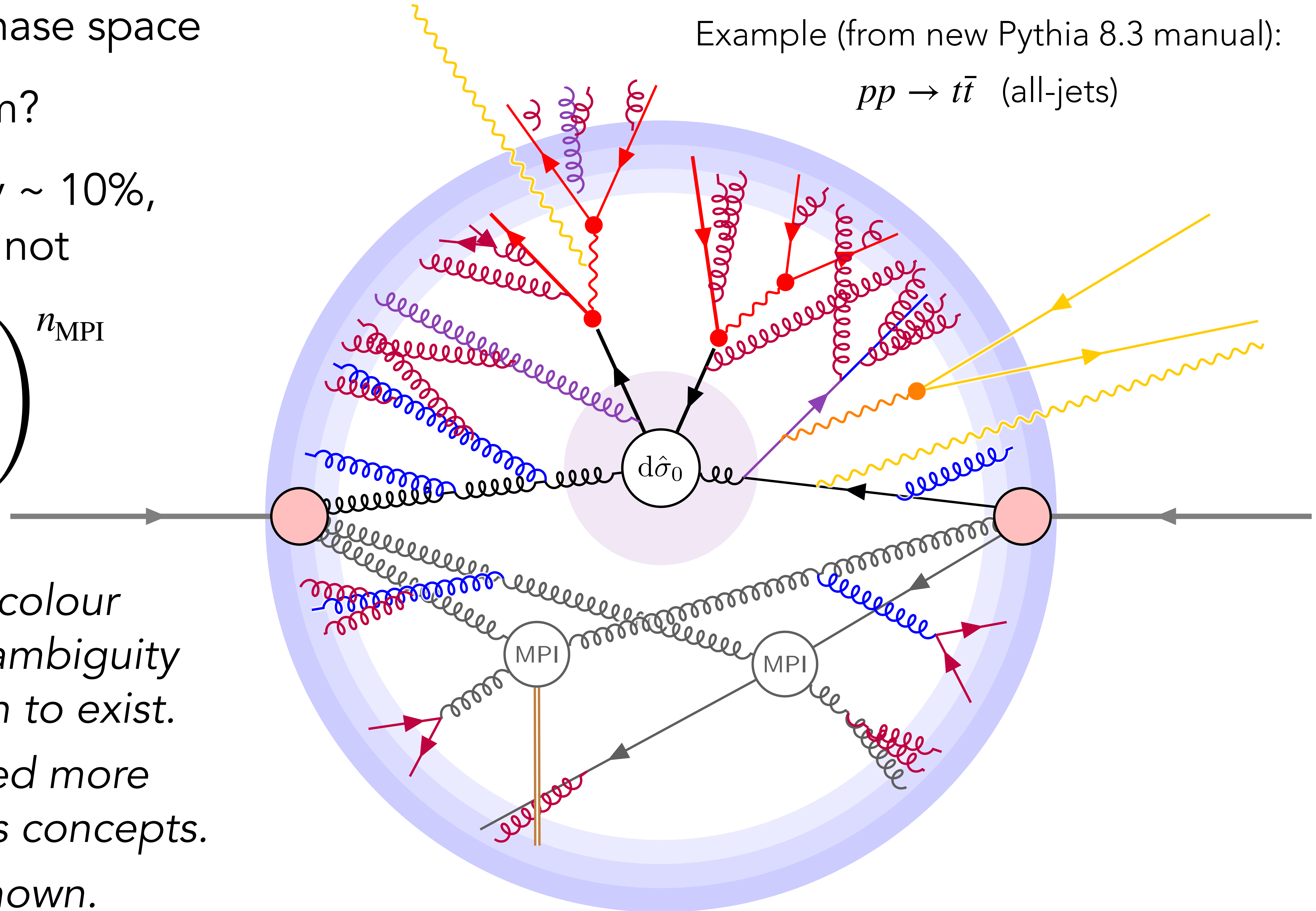

Note: in this context, the word "colour reconnections" simply refers to an ambiguity beyond Leading N_C, which is known to exist.

But the term "CR" can also be used more broadly to incorporate further physics concepts.

Detailed physics not yet fully known.

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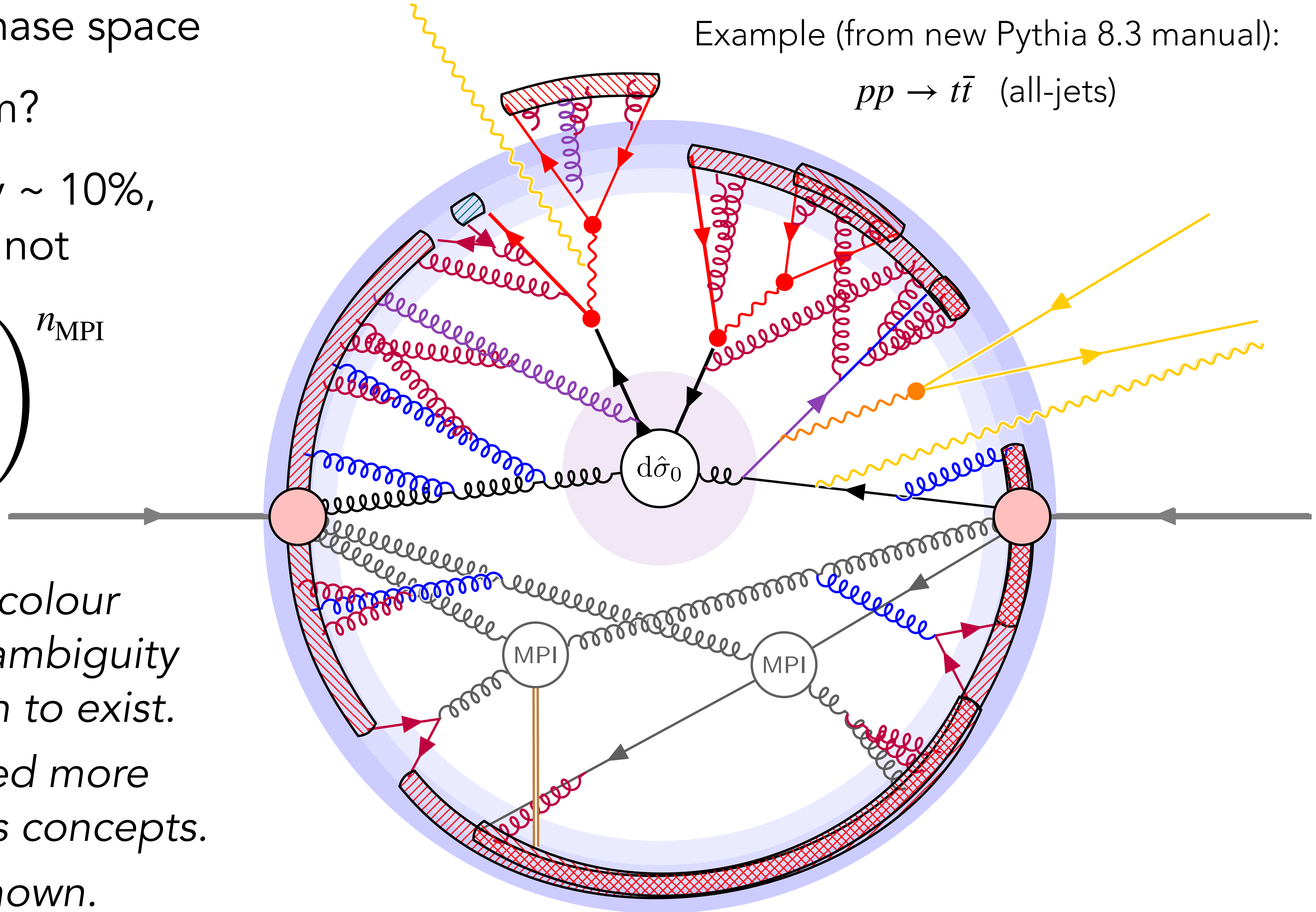

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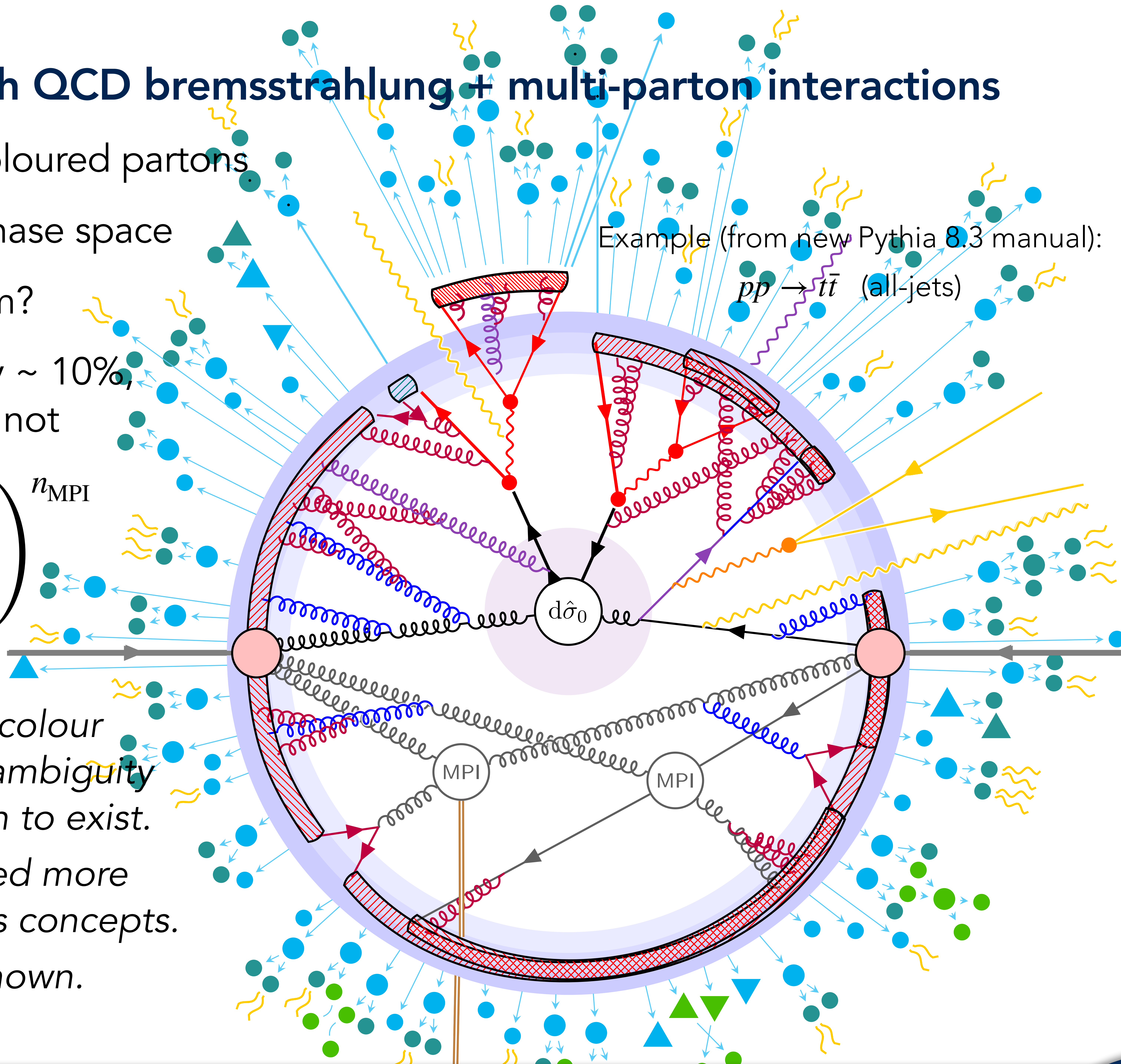
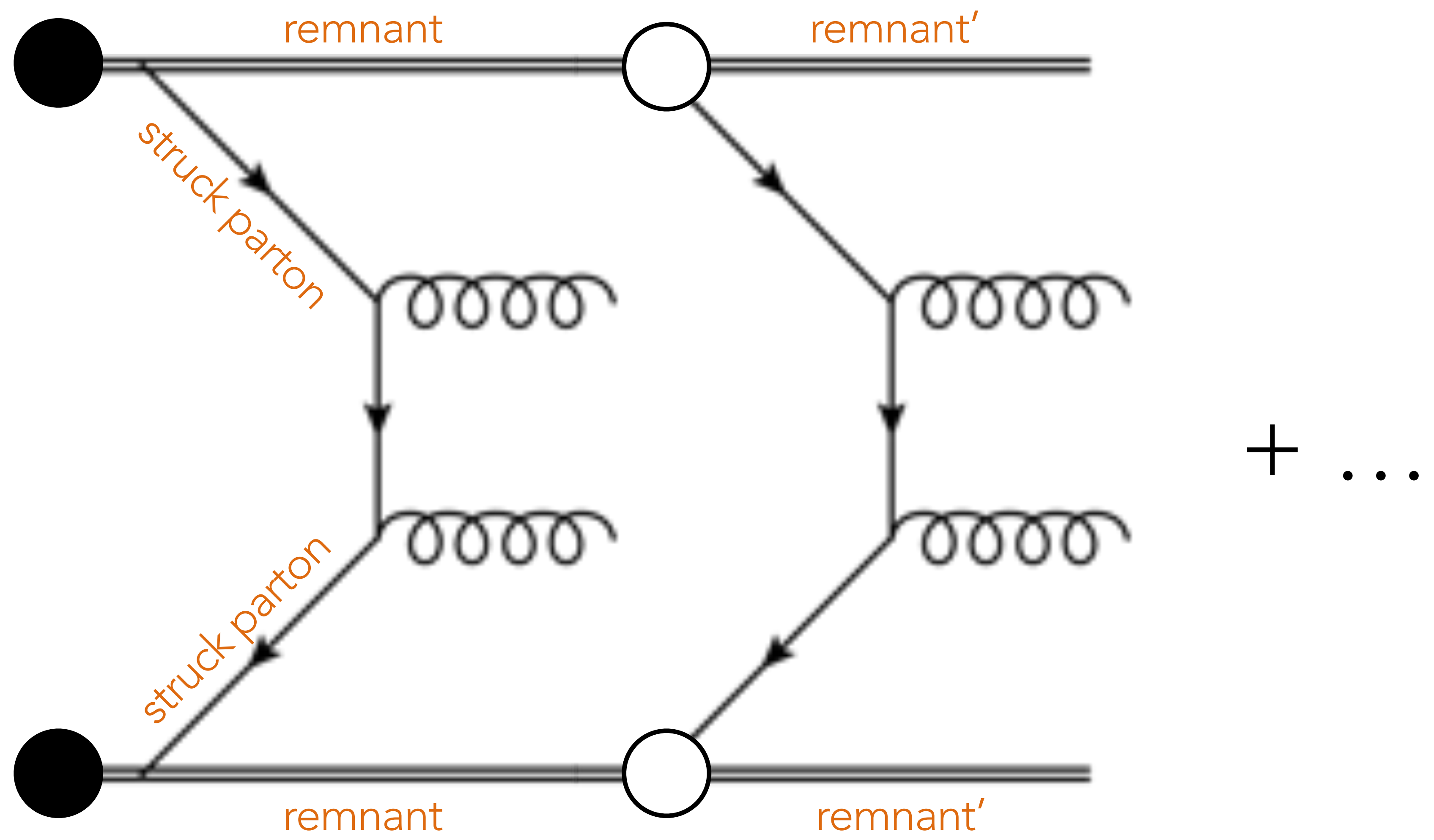
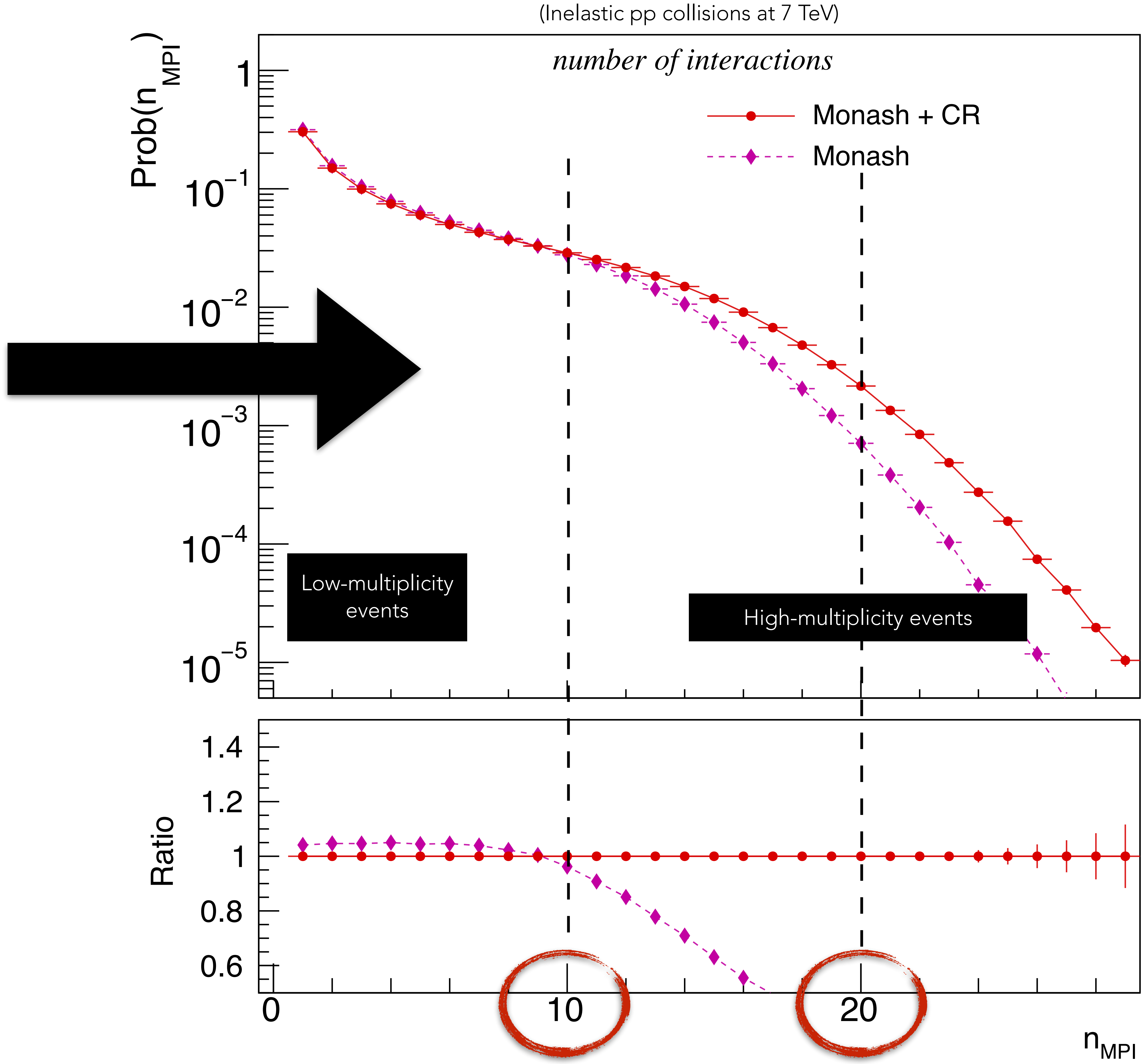


How many MPI are we talking about?

How many parton-parton systems are there in pp collisions? DPS? 3PS? ...?

Multi-Parton Interactions (MPI)





$\Longrightarrow$ can have **very** many parton systems within a single pp collision (esp. in high-multiplicity events)

All within ~ transverse size of a proton (= right on top of each other)

[Baryon Number Violation & String Topologies: Sjöstrand & PS hep-ph/0212264]

“Colour reconnection” modelling based on stochastic sampling of SU(3) group probabilities: allows for random (re)connections [String Formation Beyond Leading Colour: Christiansen & PS 1505.01681]

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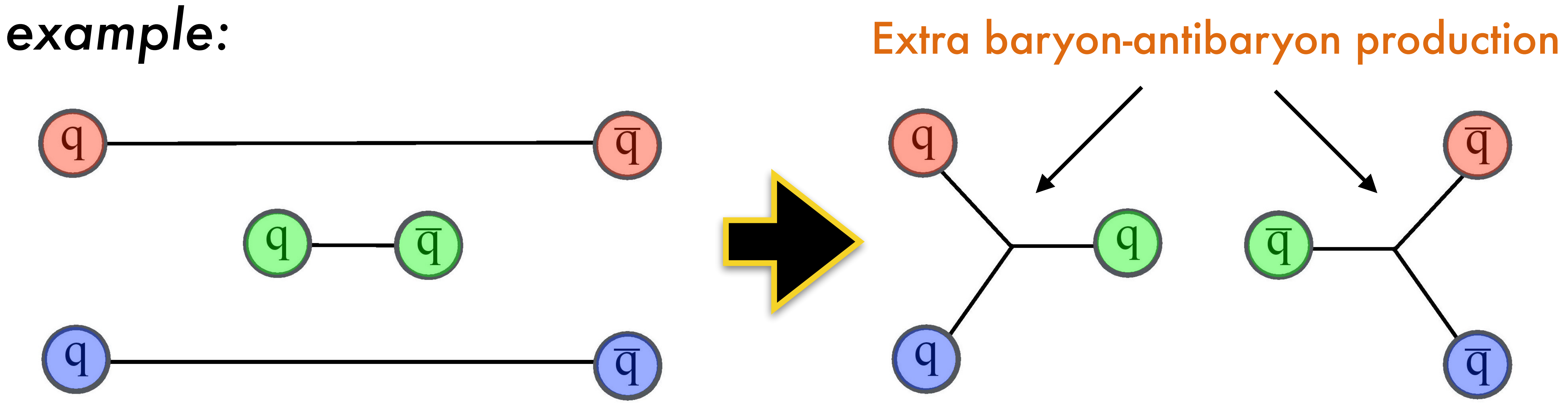

Unique feature of SU(3): Y-Shaped 3-String "Junctions" ➤ Baryons

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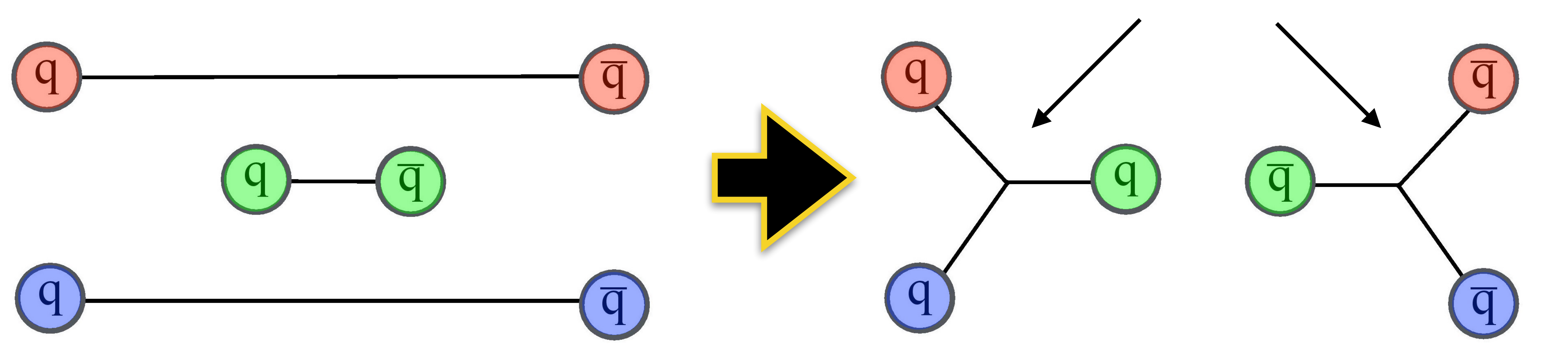

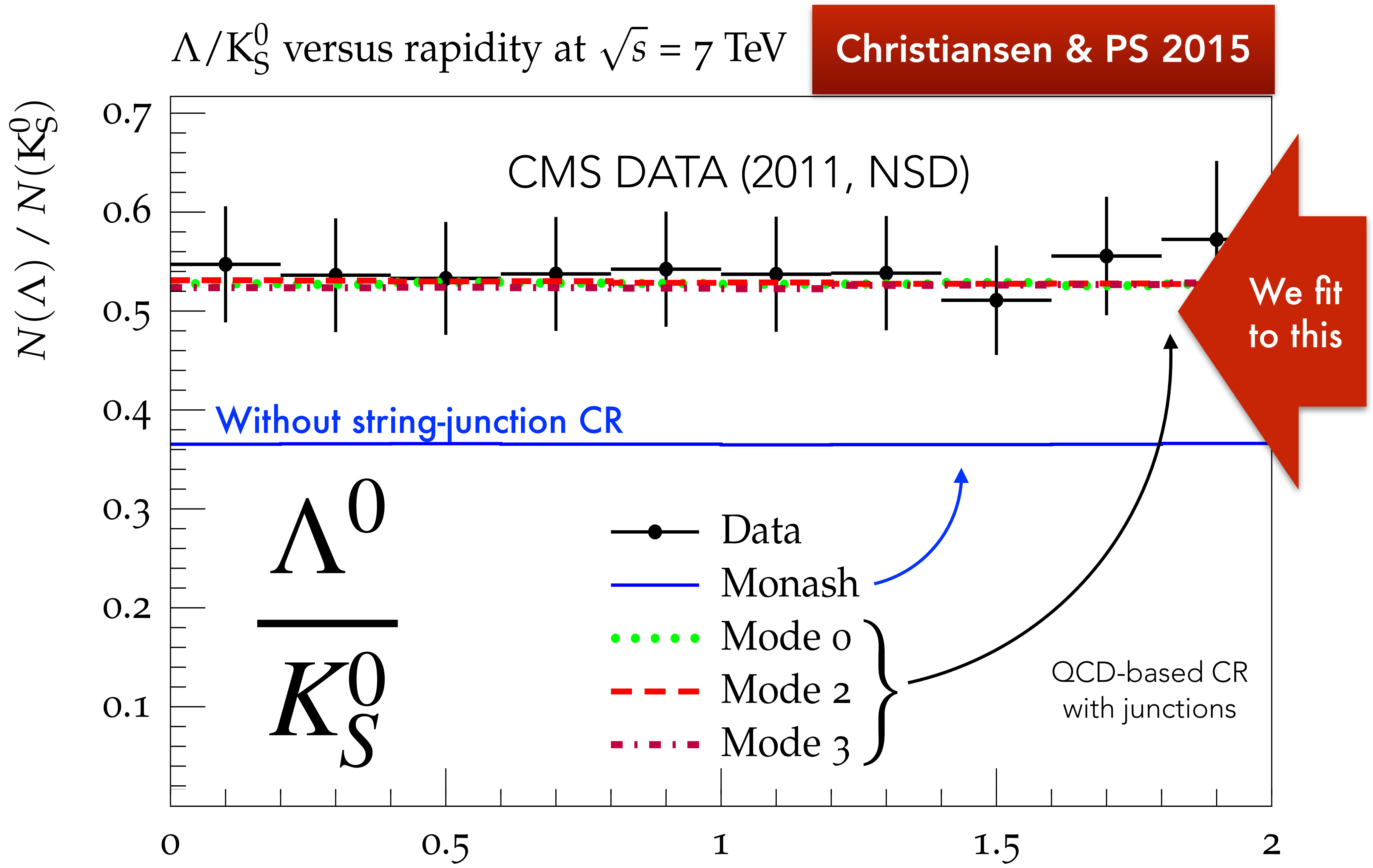

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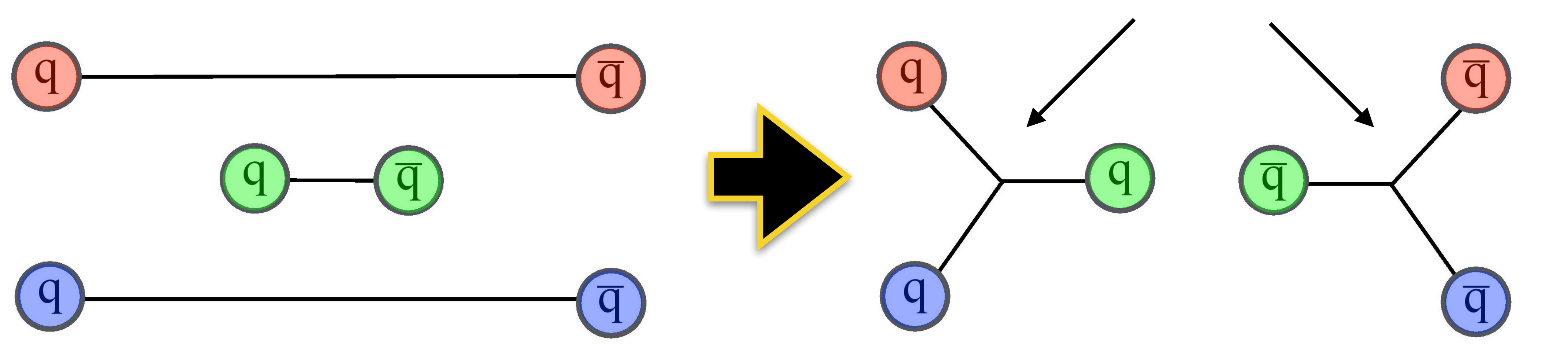

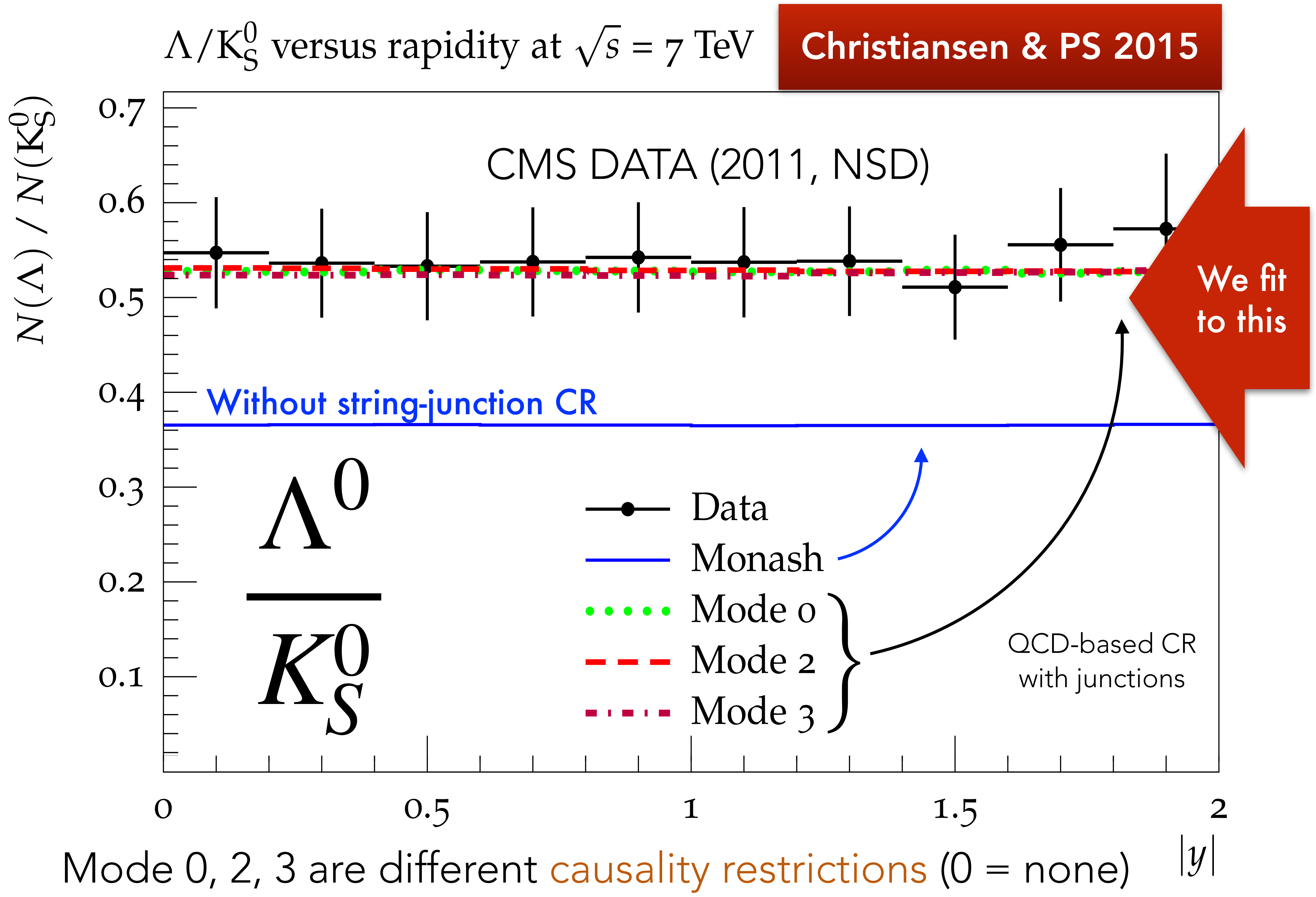

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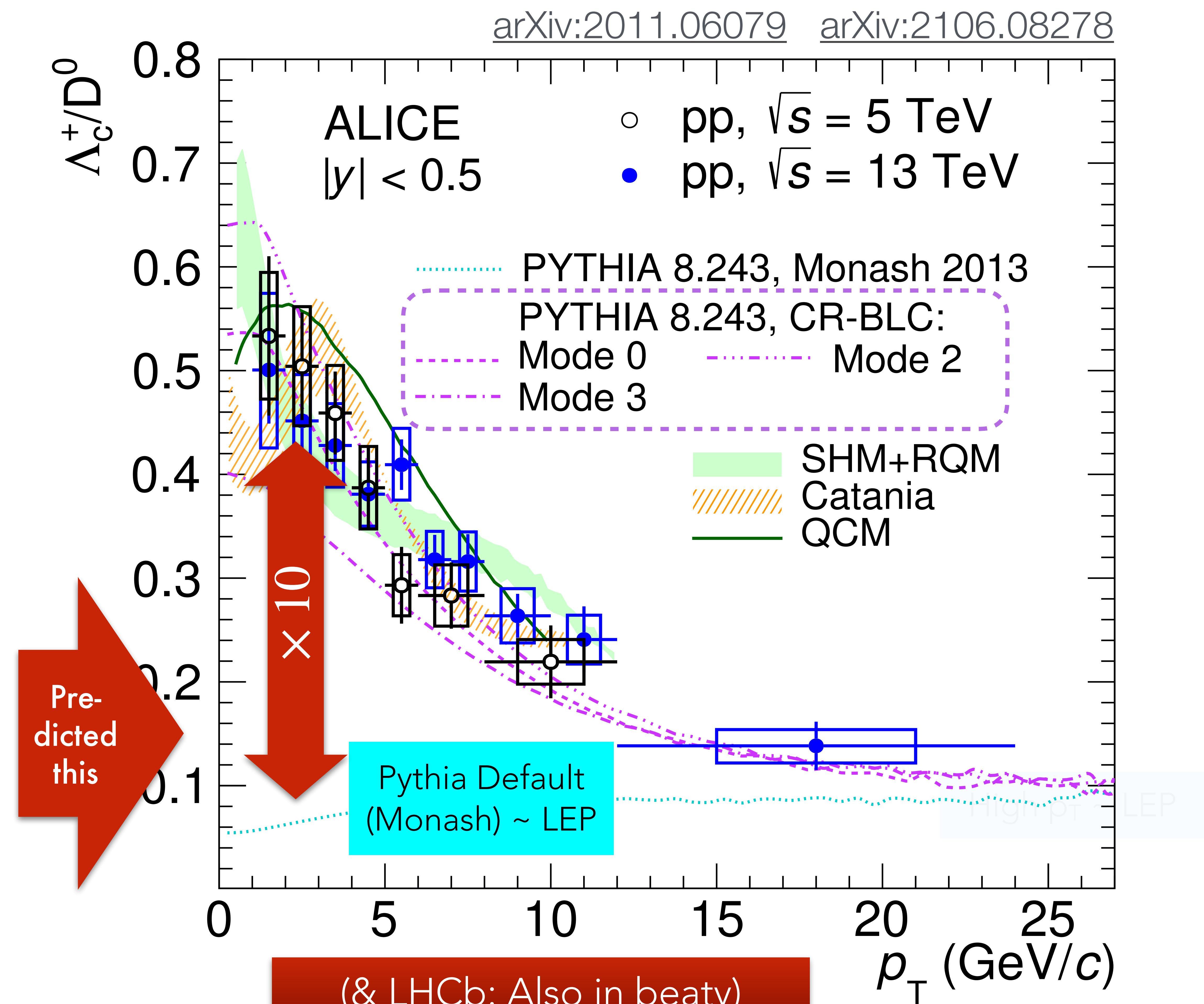
ALICE 2021: also in charm



(& LHCb: Also in beaty)

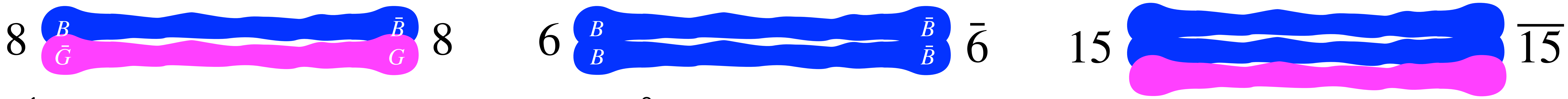
4. **Strangeness**, Ropes, and (Advanced) Close-Packing

Clear observations of strangeness enhancements in high-multiplicity pp collisions (relative to LEP and low-multiplicity pp) [e.g., ALICE Nature Phys. 13, 535 (2017)]

- Much activity to understand *dynamics* of effective breakdown of strangeness universality

In string context, MPI + Colour Ropes [e.g., Bierlich et al. 1412.6259] have been proposed:

- Casimir scaling of effective string tension $\Longrightarrow$ less strangeness suppression in string breaks



p=1 q=1 $C_8 = C_A = 2.25\, C_F$

p=2 q=0 $C_6 = 2.5\, C_F$

p=2 q=1 $C_{15} = 4\, C_F$

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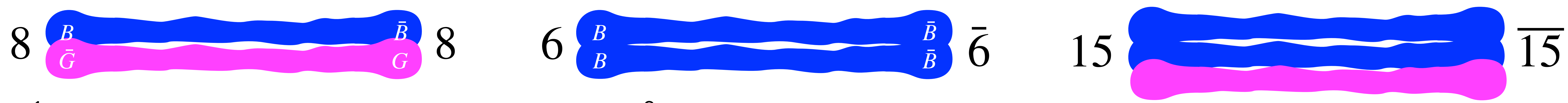
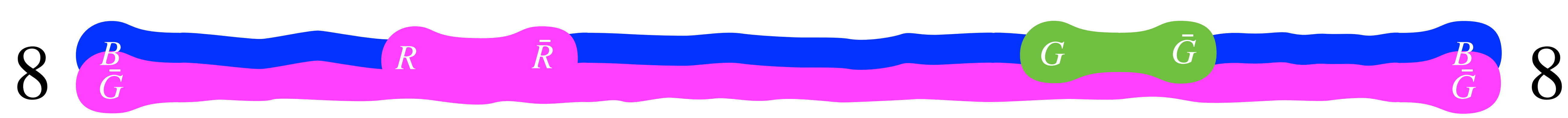


p=1, q=1: $C_8 = C_A = 2.25\,C_F$ p=2, q=0: $C_6 = 2.5\,C_F$ p=2, q=1: $C_{15} = 4\,C_F$

Simplified alternative: Close-Packing [Fischer, Sjöstrand 1610.09818] string tension scales with effective background ∝ n_{MPI} (global) or $n_{strings}$ (local)

- Local version updated with Monash student J. Altmann to account for **directional colour flows** (p and q), **junction topologies**, and effective **diquark suppression** in octet-type fields ("*Altmann mechanism*"):



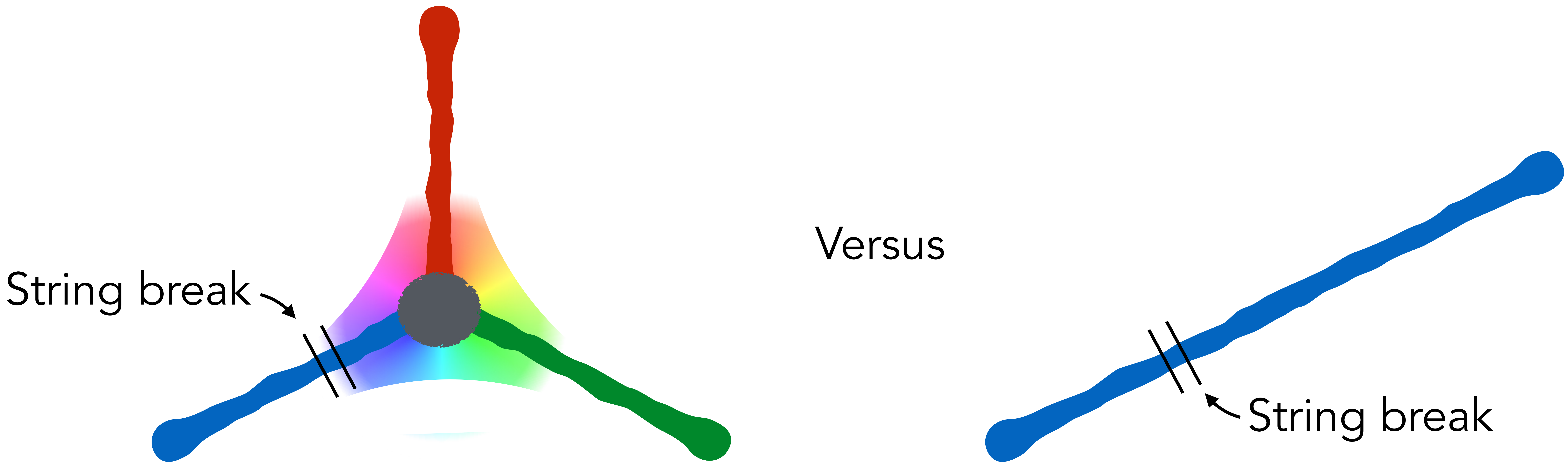
"Popcorn picture" in which diquark formation is viewed as a fluctuation of first one colour followed by another of a different colour

$R\bar{R}$ (or $\bar{R}R$) fluctuation increases tension from C_8 to C_6

$G\bar{G}$ (or $\bar{G}G$) fluctuation Can just break the other string

What do we really know about the field strength near a QCD junction?

- Probably related to baryon spectroscopy / lattice, but unaware of any specific answers



Effective energy density per unit length could be different from vacuum case near a junction?

New: Strange Junctions

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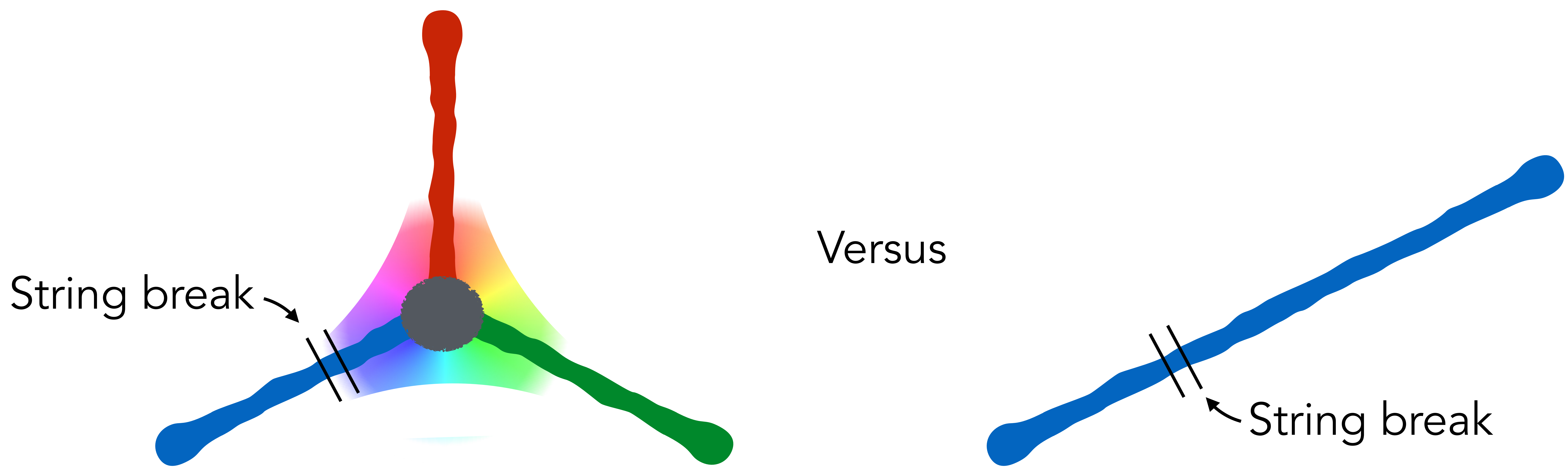

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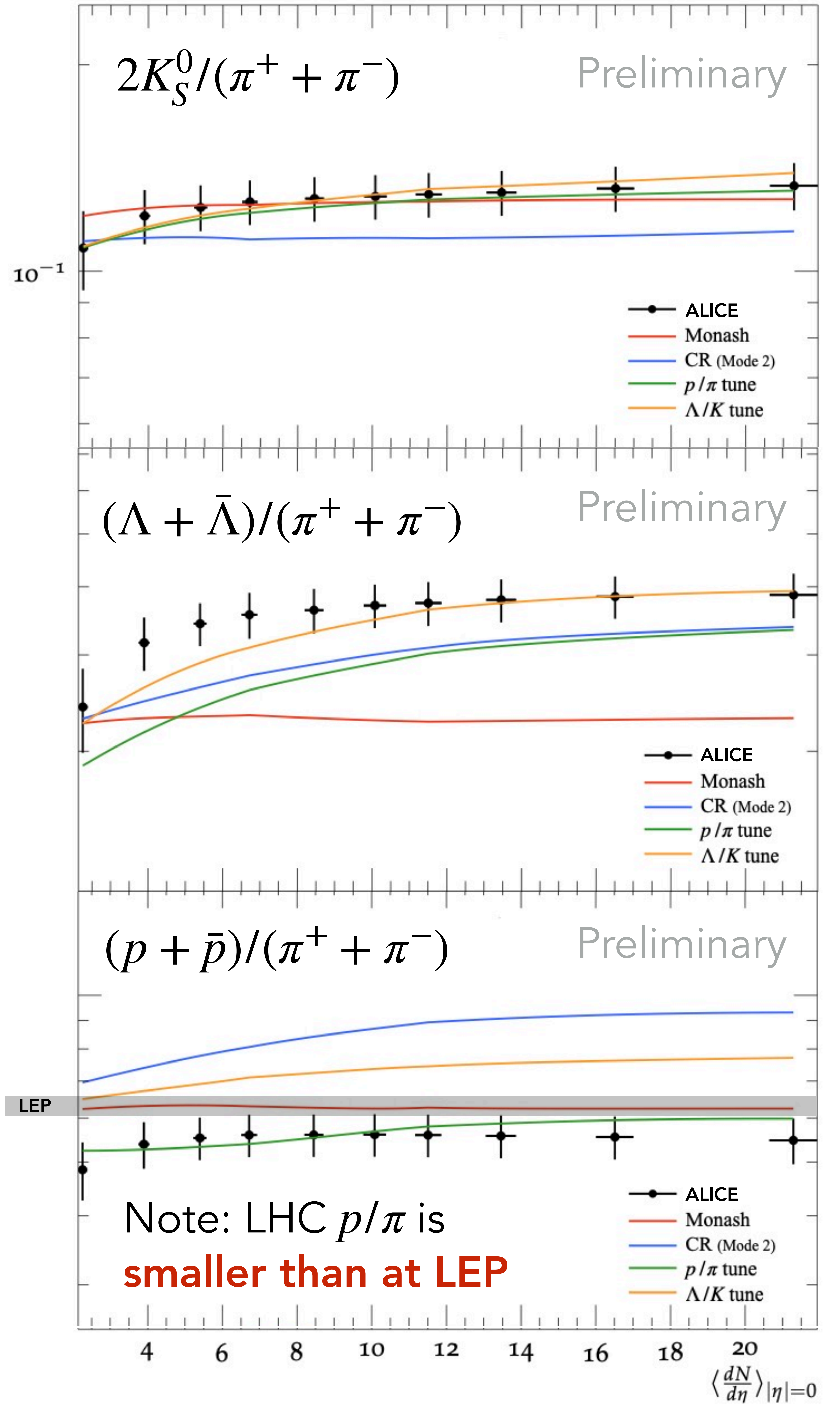
Enhanced string tension on the string breaks closest to junction?

→ Model of **"strange junctions"** (with Monash PhD student Javira Altmann)

Mechanism for strangeness enhancement specifically for junction baryons

QCD CR + Advanced Close-Packing: First Results



Note: LHC p/π is **smaller than at LEP**

- **Monash** (no QCD CR, no close-packing) ~ LEP
- **QCD CR** (mode 2); no close-packing
- **QCD CR + ACP**: p/π tune
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		p/π	Λ/K	
`StringPT:tension`	=	0.05	0.11	← Close-packing
`StringPT:qqFac`	=	0.7	0.23	← Altmann Mechanism
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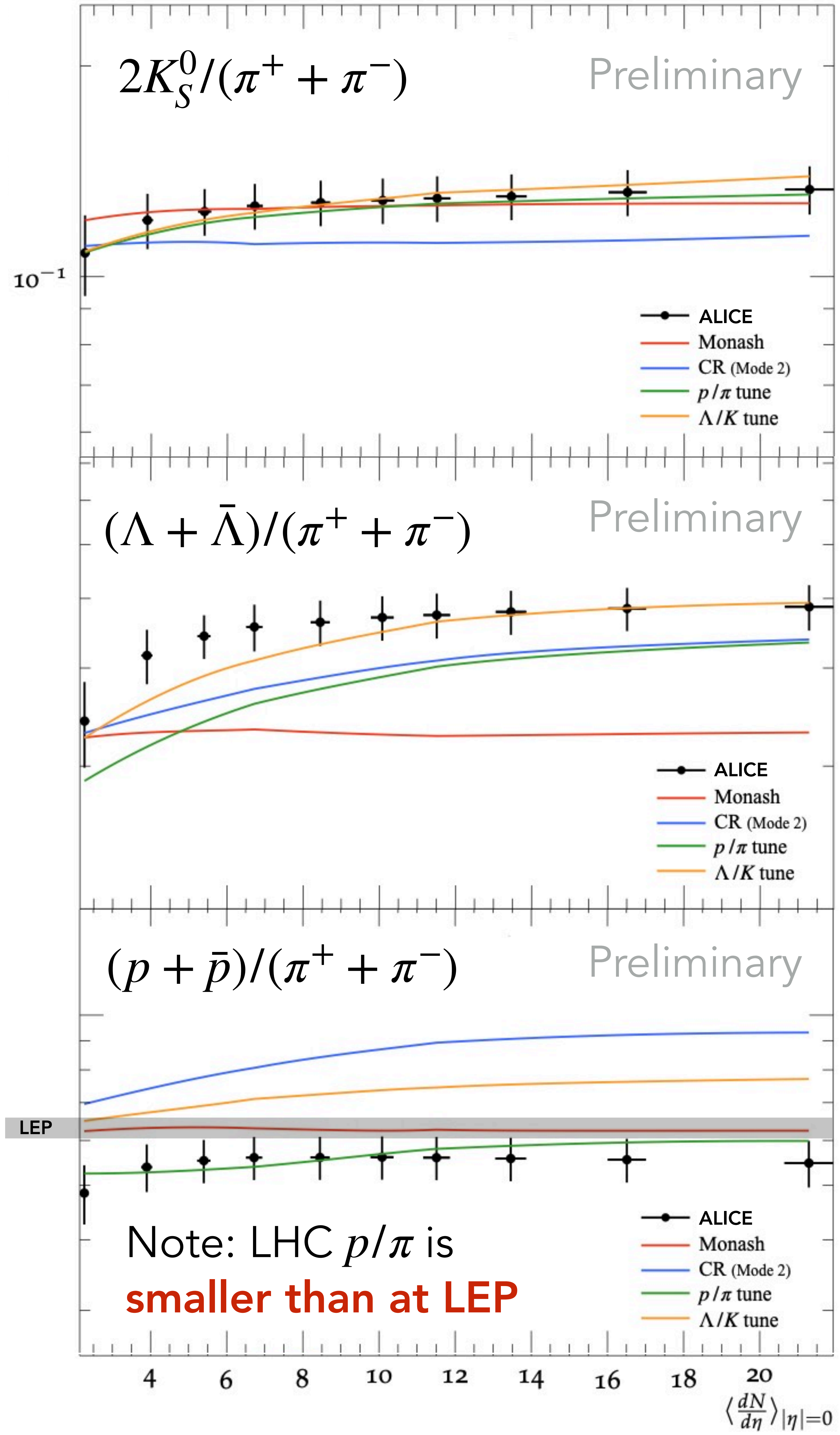

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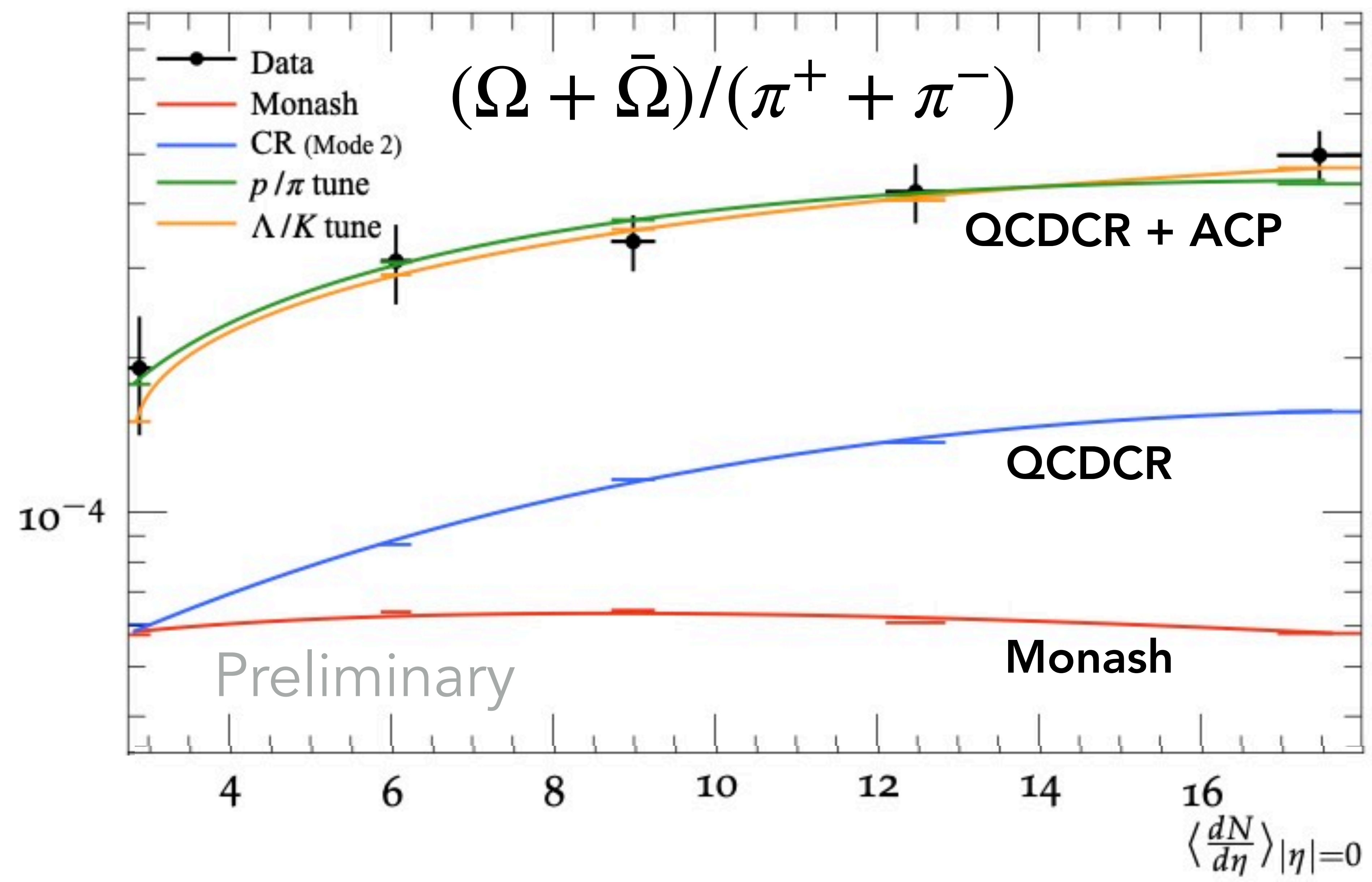

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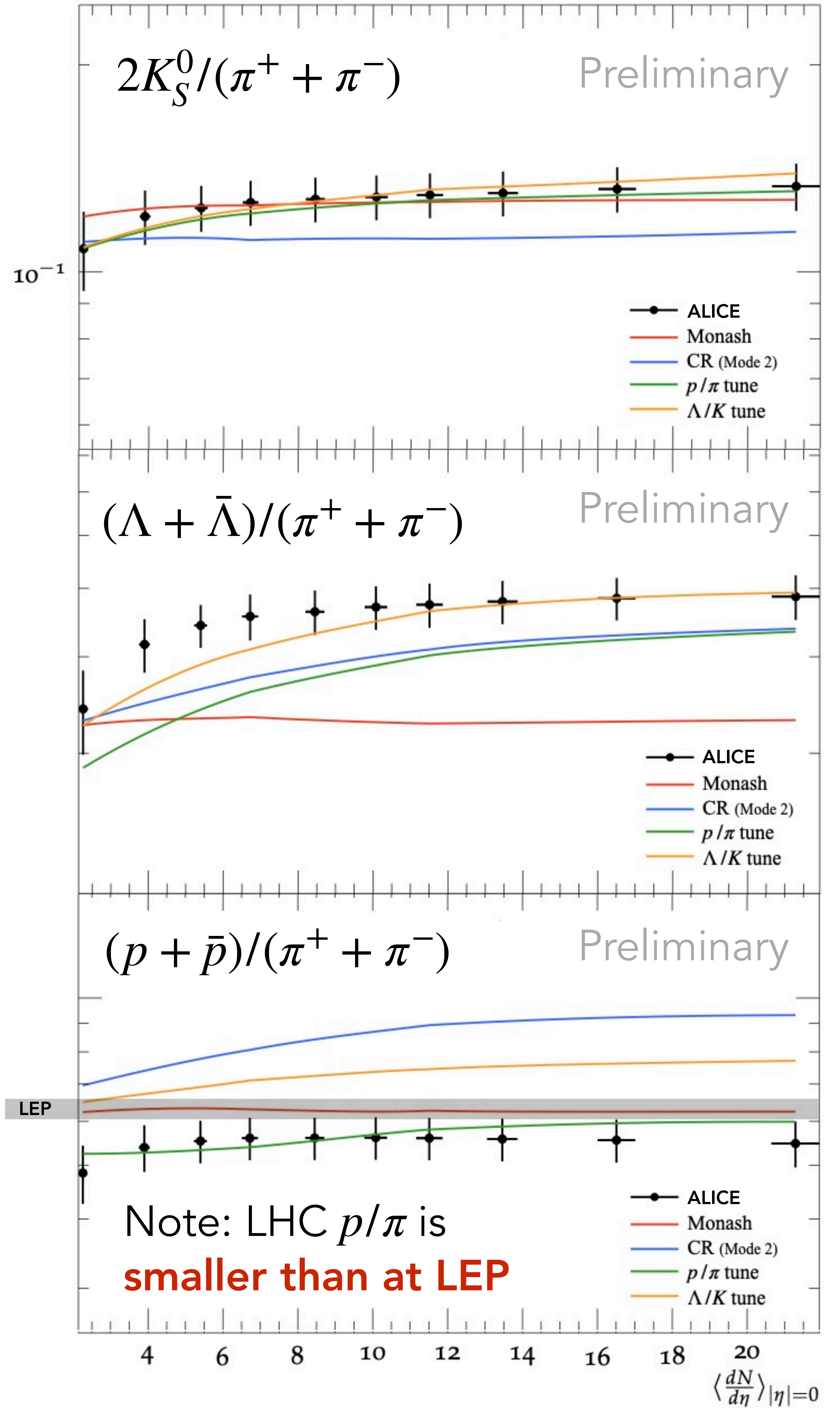

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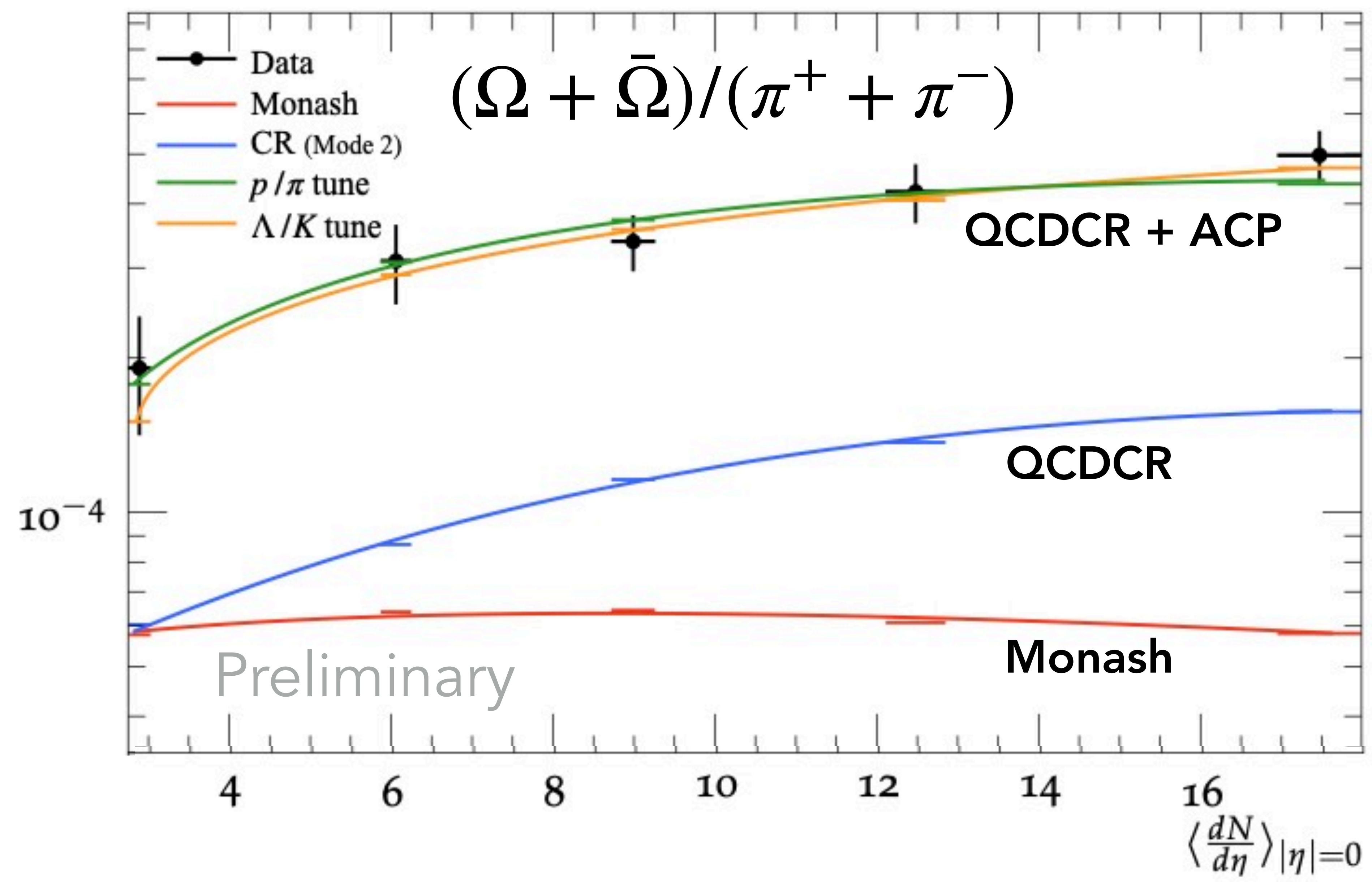

Being finalised now, with publication on the way.

J. Altmann, PS

5. If there is time …

Cosmic-Ray Air Showers

Single incident particle ➡ billions of final-state particles (forget about GEANT).

Recently started a collaboration with CORSIKA 8 fast/optimised air-shower tracker

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- Provide **hadron-air cross sections** ⊕ **perform collisions** ⊕ simulate **hadron decays**

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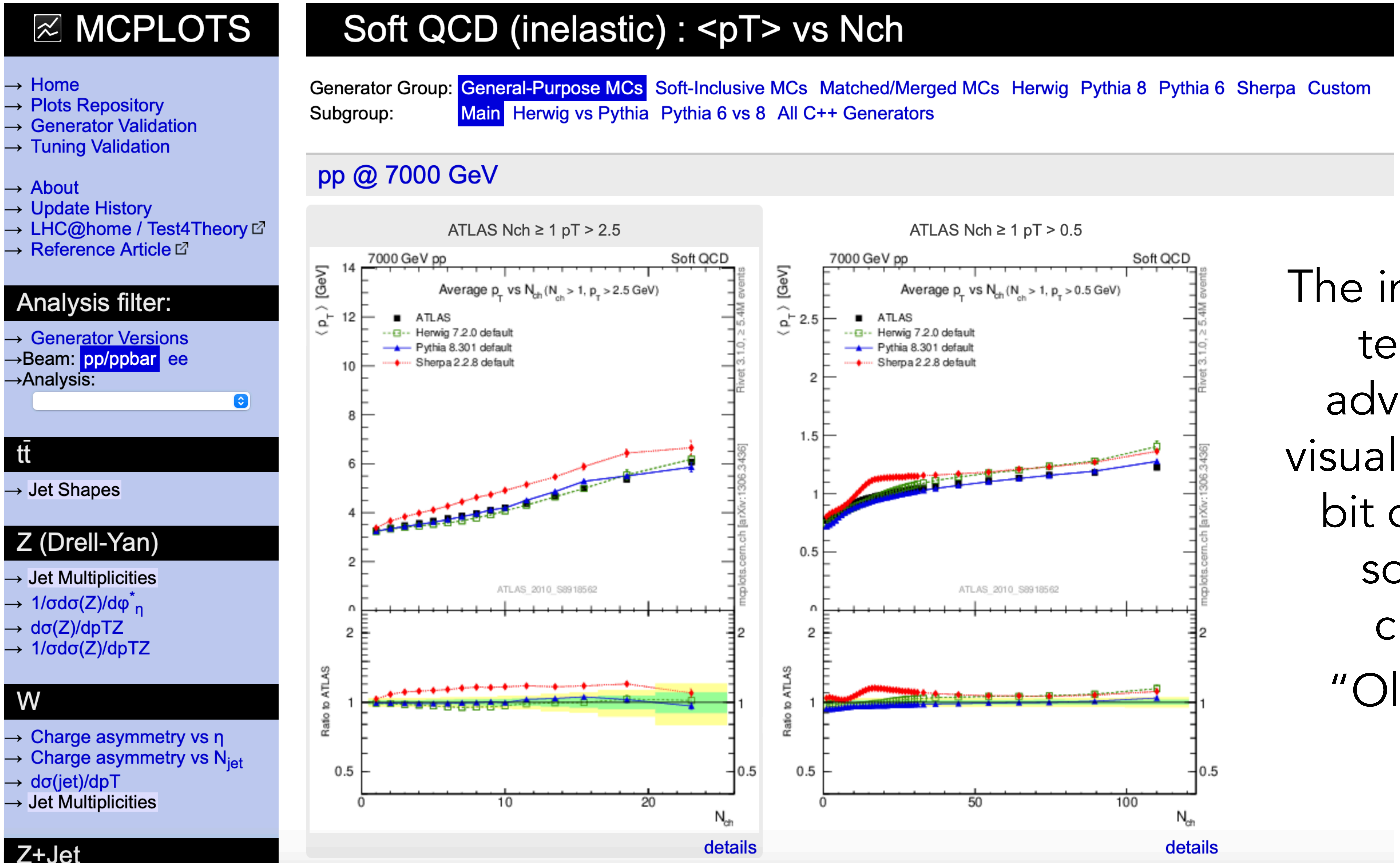
- A positive technical note: native C++ simplifies CORSIKA 8 - PYTHIA 8 interfacing

See also M. Reininghaus et al. *Pythia 8 as hadronic interaction model in air shower simulations*, **2303.02792**

Last: mcplots.cern.ch — New and Updated coming soon!

mcplots.cern.ch started in 2010, as browsable repository of MC validations (via Rivet)

- Running continuously on ~ 1000 cores donated by BOINC LHC@home volunteers (+ Grid backfill)



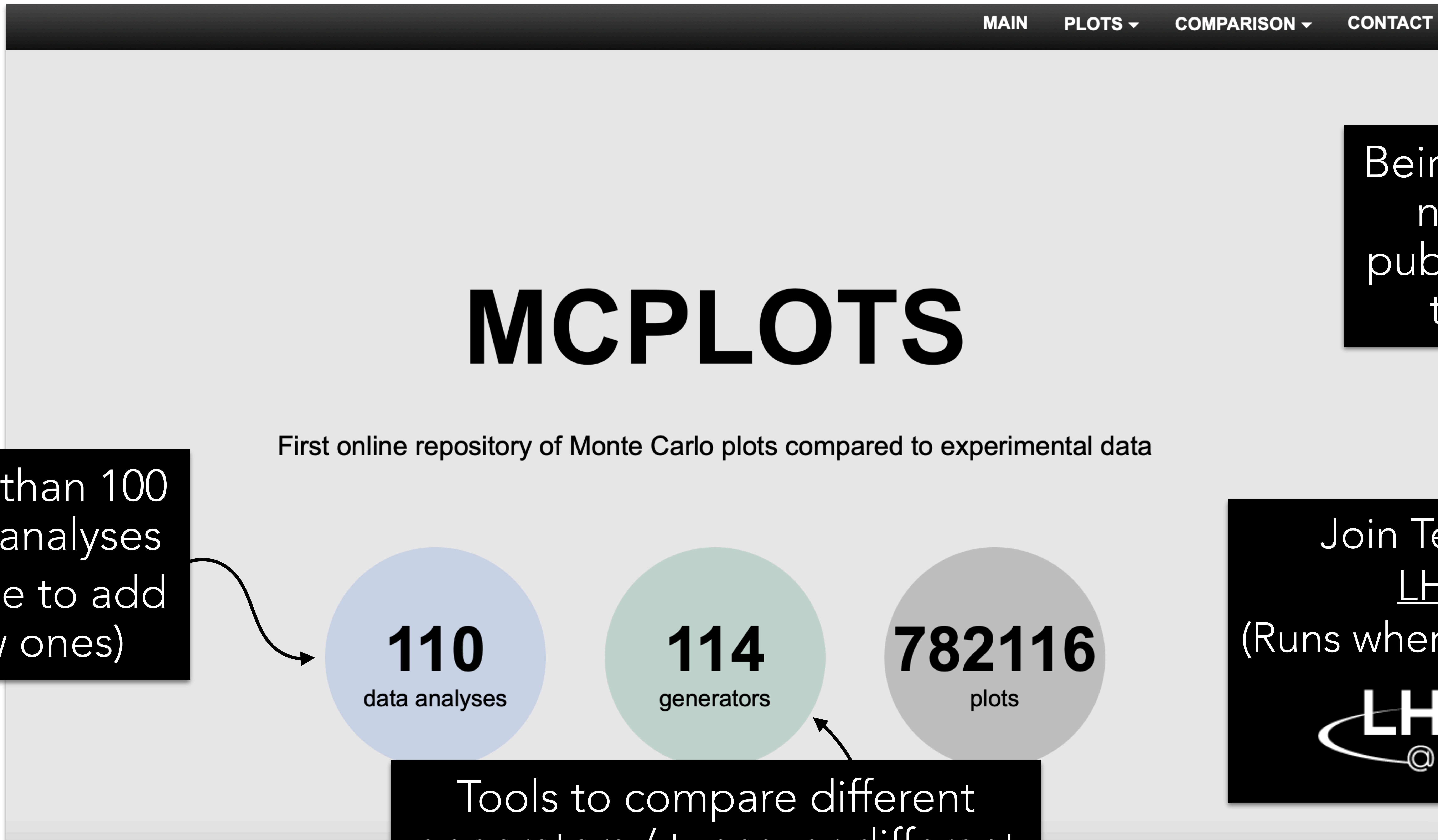
The interface was technically advanced but visually perhaps a bit dated, and somewhat cluttered

"Old School"

mcplots.cern.ch — New and Updated coming soon!

Modern clean interface developed through 2023 (+ many improvements under the hood)

- Mainly driven by Natalia Korneeva, now an adjoint at Monash U (with support from LPCC)



Being finalised now, with publication on the way.

More than 100 Rivet analyses (simple to add new ones)

Join Test4Theory on LHC@home (Runs when computer is idle)

Volunteer computing for the LHC

Tools to compare different generators / tunes, or different versions of same generator

Extra Slides

An Achilles' Heel? **Protons!**

So far, physics models have focused heavily on strangeness

- The original ALICE paper from 2017 also included the proton/pion ratio
- In many model setups, enhancement of strangeness is accompanied by more heavier states in general $\Longrightarrow$ **non-strange baryons also enhanced**
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Baryon-to-Meson Ratios

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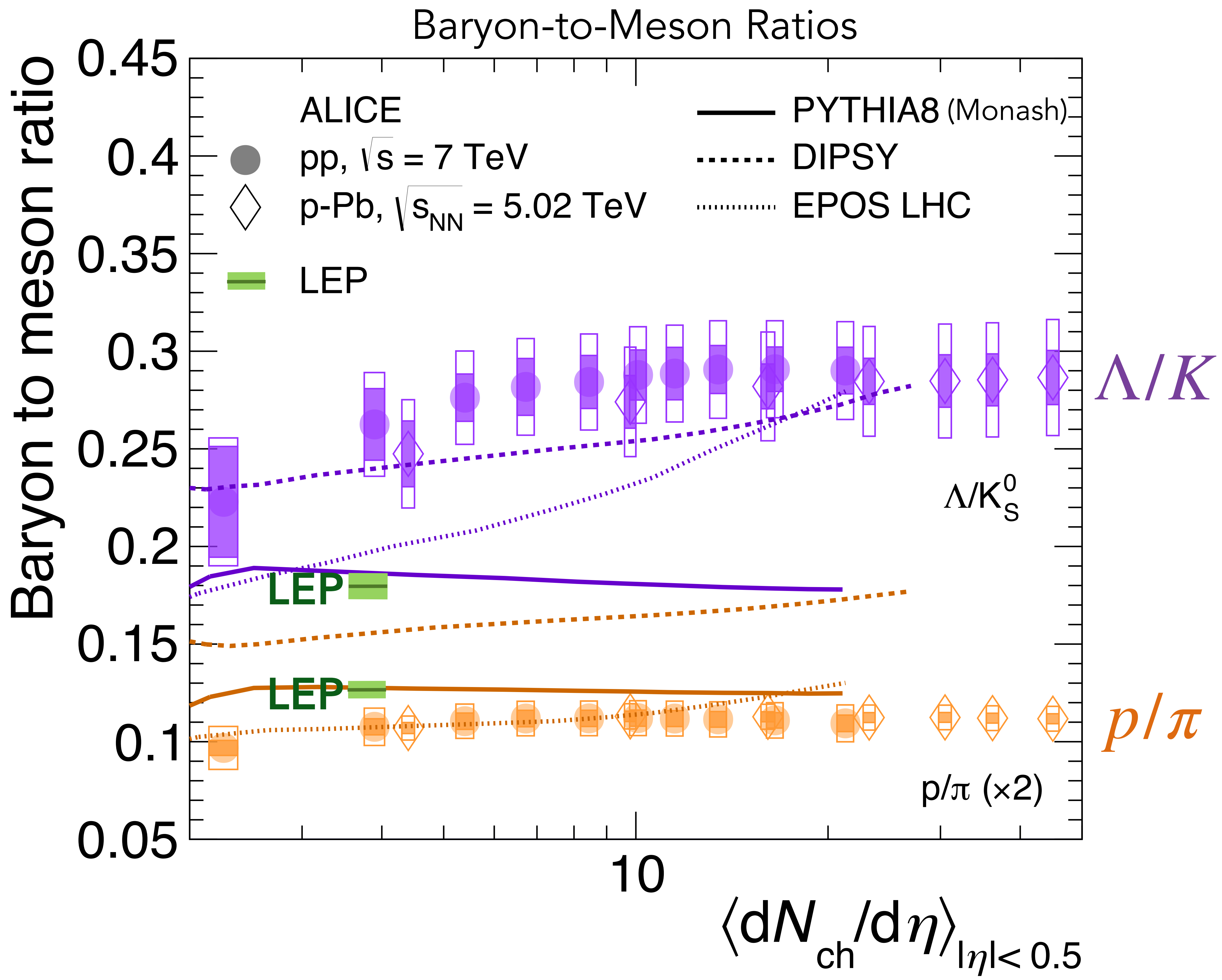

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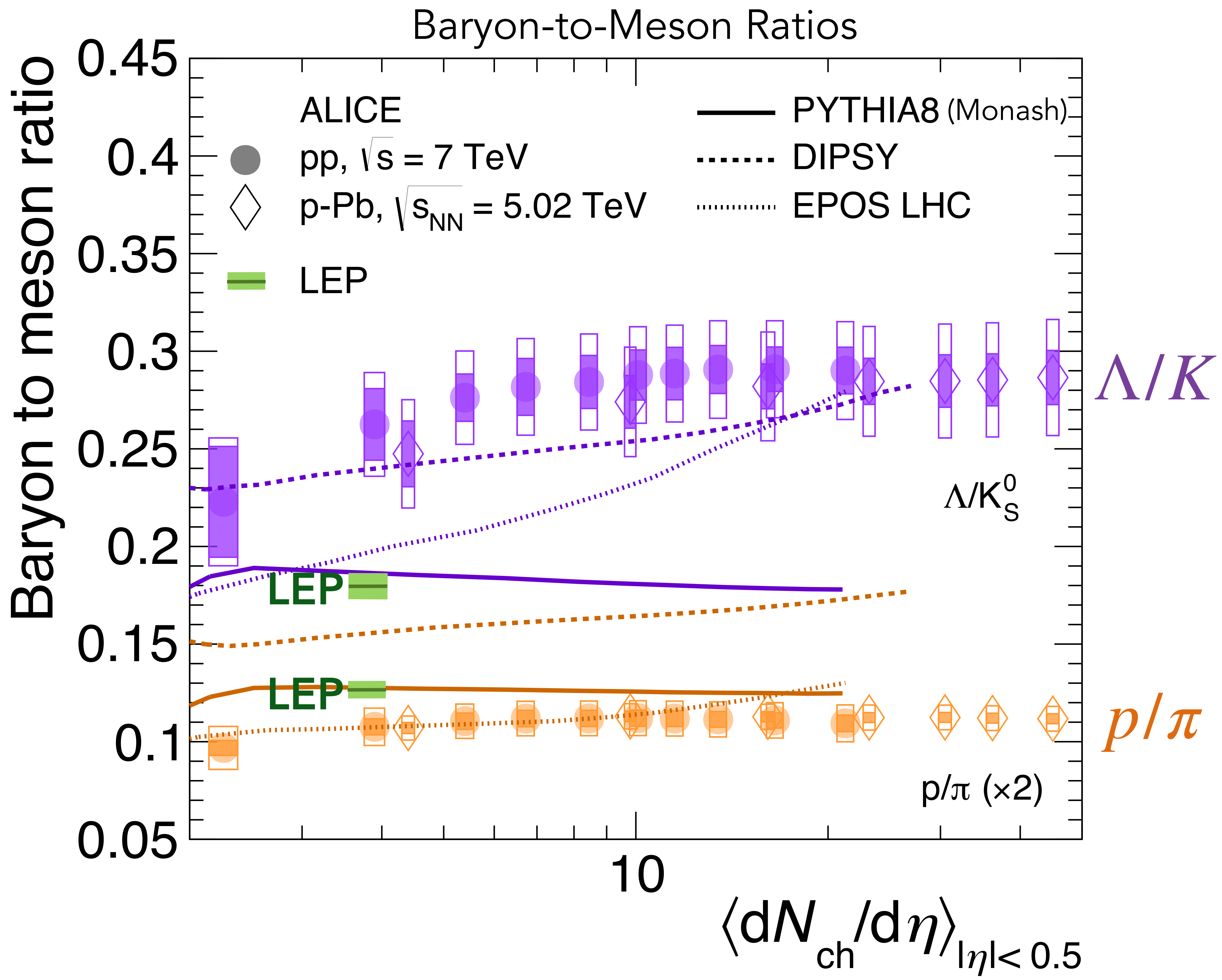

Data shows that the p/π ratio at LHC is a bit *smaller* than at LEP!

With ~ no evolution with N_{ch}

Protons are the most abundant baryons!

EPOS captures this behaviour

(what about @ LEP?)

From a CR perspective, baryon enhancement appears *very* correlated with strangeness …