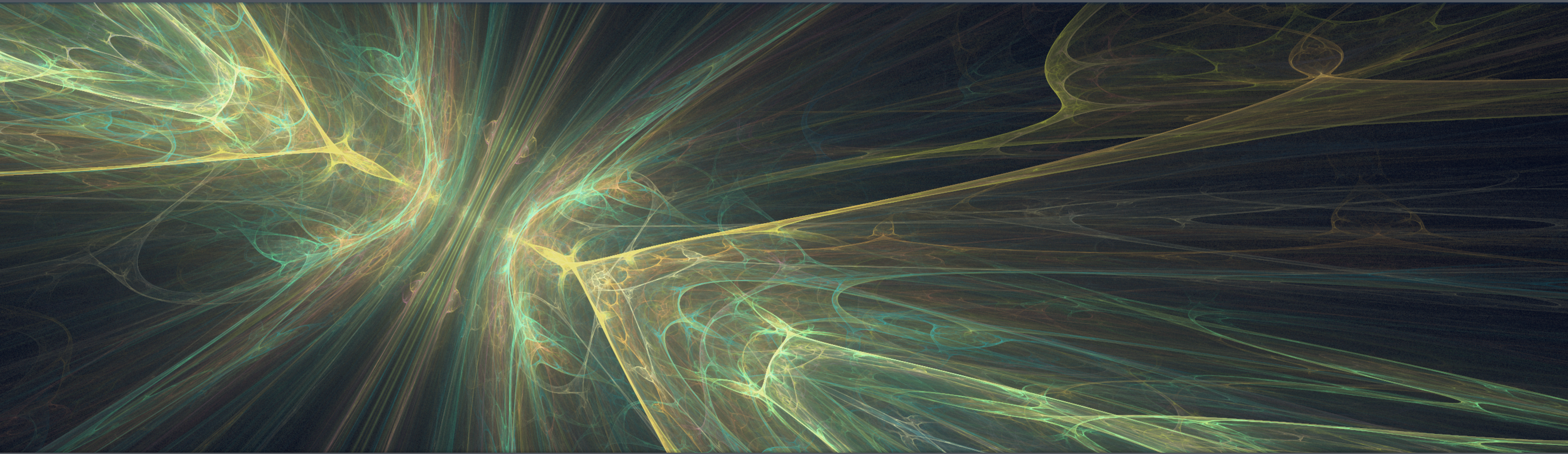
UK Theory Meeting — December 2023 — Durham

Non-perturbative Physics in Precision Event Simulations



Peter Skands

RS Wolfson Visiting Fellow, U of Oxford & Monash University

From High Energies to **Confinement**

Consider a "hard" process

"Hard" = large momentum transfers

Example: $gg \rightarrow t\bar{t}$

Here, $Q^2 \sim m_t^2 \gg \Lambda^2_{\mathrm{QCD}}$

Accelerated charges (QED & QCD)

- ➜ Bremsstrahlung (QED & QCD)
- ➜ Perturbative Methods

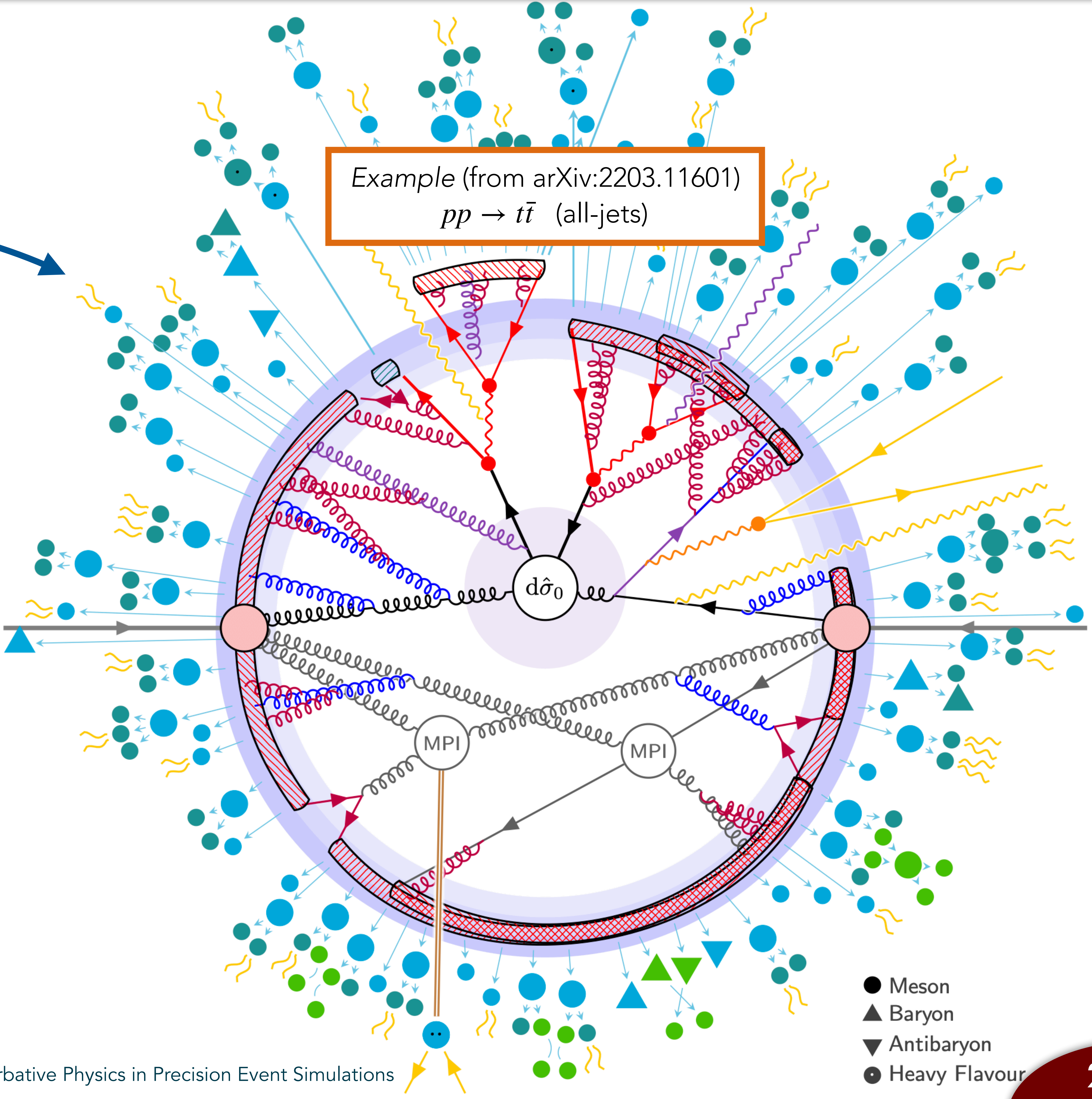
Near-Future Goal: NNLO + NNLL

➜ **Percent-level precision**

At wavelengths $\sim r_{\mathrm{proton}} \sim 1/\Lambda_{\mathrm{QCD}}$

Some dynamical process must ensure quarks and gluons become confined inside hadrons: ***Hadronization***

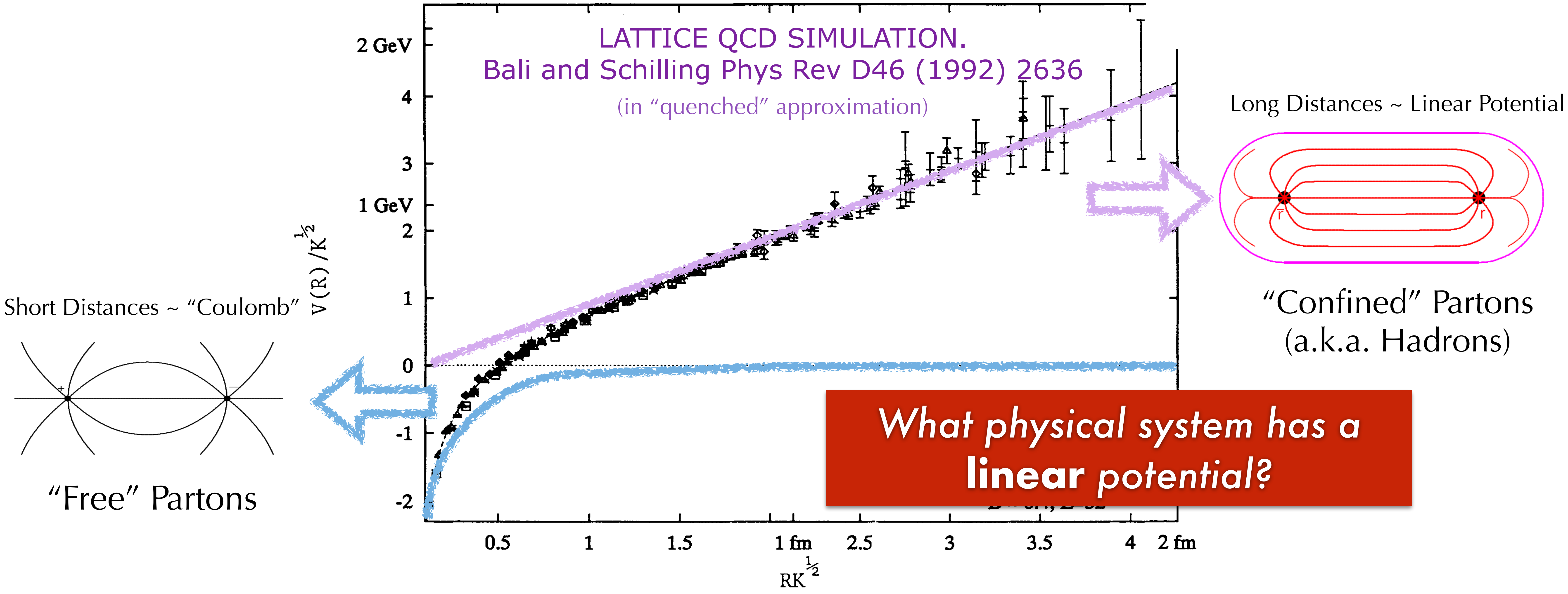
How much do we know about that?



Example (from arXiv:2203.11601)
$pp \rightarrow t\bar{t}$ (all-jets)

Linear Confinement

In lattice QCD, compute the potential energy of a colour-singlet $q\bar{q}$ state, as a function of the distance, r, between the q and $\bar{q}$



LATTICE QCD SIMULATION.
Bali and Schilling Phys Rev D46 (1992) 2636
(in "quenched" approximation)

What physical system has a* linear *potential?

"Cornell Potential" fit: $V(r) = -\frac{a}{r} + \kappa r$ with $\kappa \sim 1\ \mathrm{GeV/fm}$ (→ could lift a 16-ton truck)

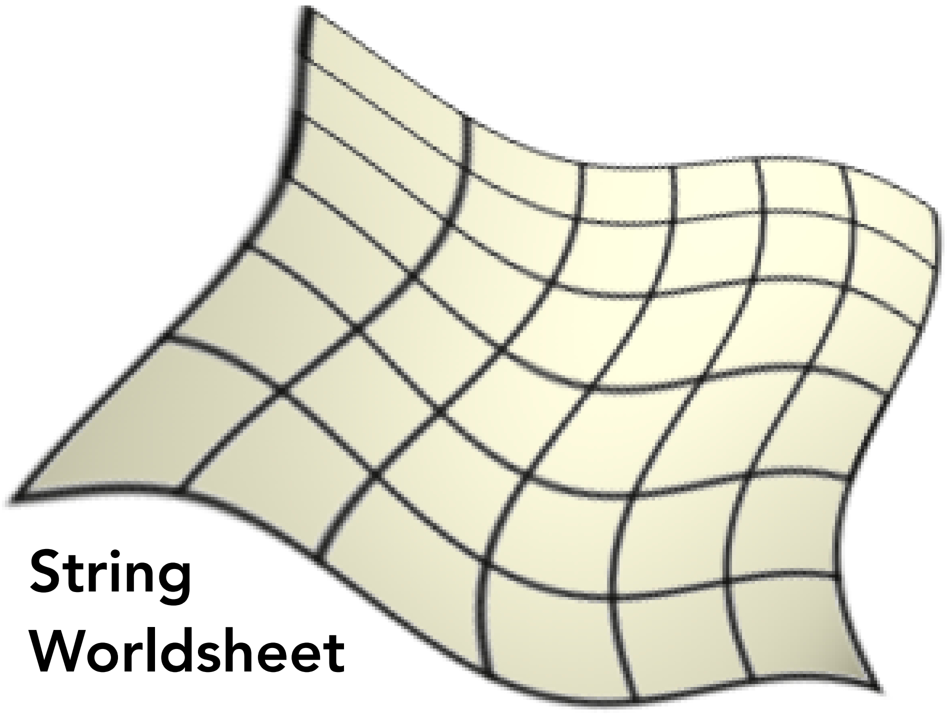
From **Partons** to **Strings**

Motivates a model:

Let colour field collapse into a narrow flux tube of uniform energy density

κ ~ 1 GeV / fm

Limit → Relativistic 1+1 dimensional worldsheet



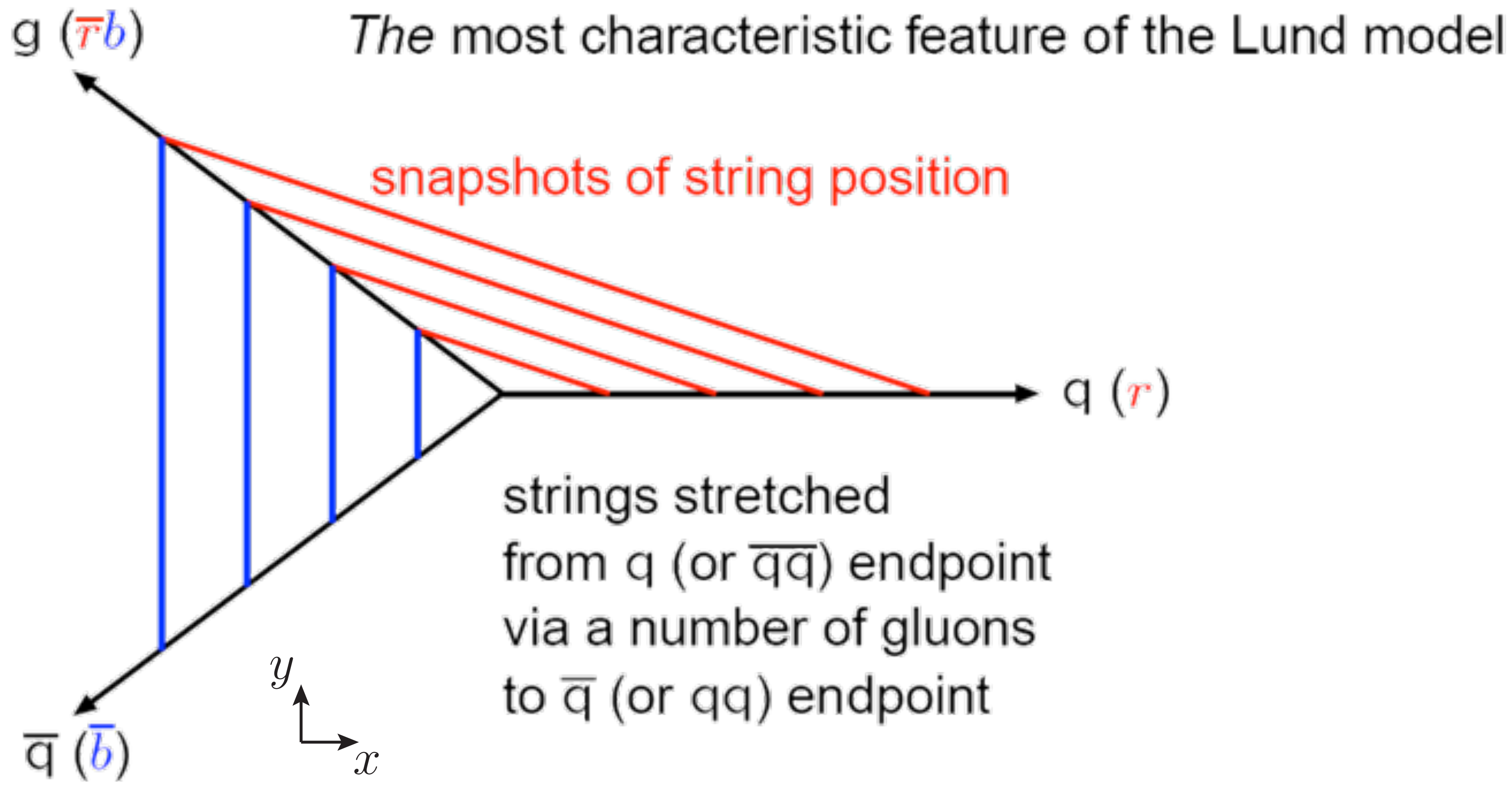
Map:

Quarks → String Endpoints

Gluons → Transverse Excitations (kinks)

Physics then in terms of string worldsheet evolving in spacetime

Nambu-Goto action $\Longrightarrow$ Area Law.



Gluon = kink on string, carrying energy and momentum

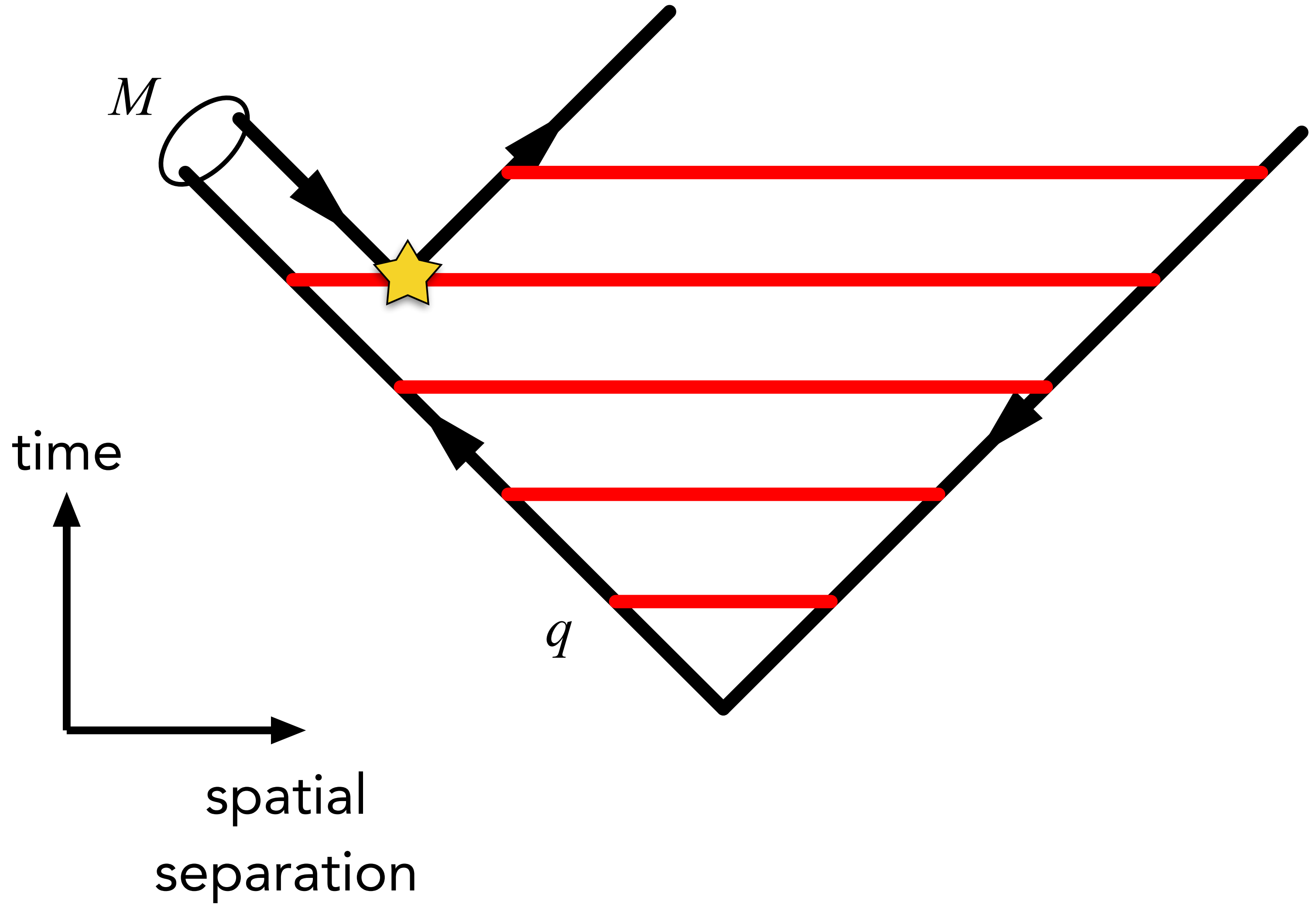
String **Breaking**

In “unquenched” QCD

$g \to q\bar{q} \implies$ The strings will “break”

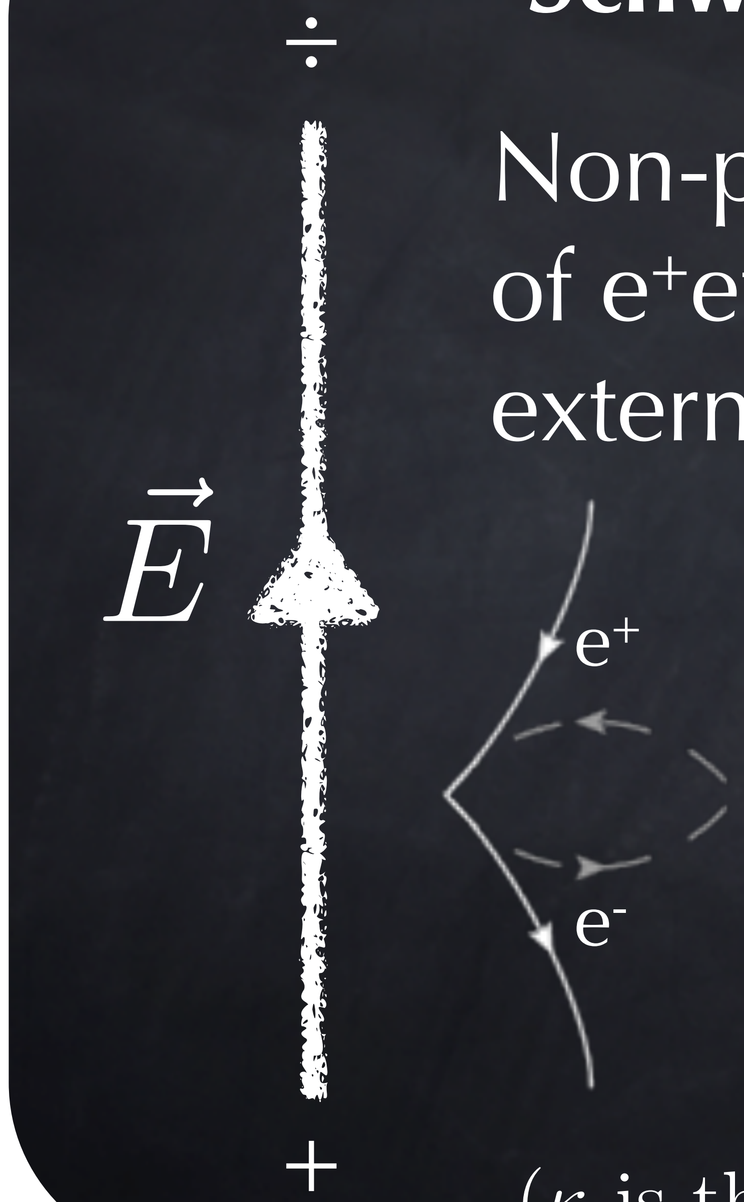
Non-perturbative so can’t use $P_{g\to q\bar{q}}(z)$

Model: Schwinger mechanism →



J. Schwinger, Phys. Rev. **82** (1951) 664

Schwinger Effect



Non-perturbative creation of e$^+$e$^-$ pairs in a strong external Electric field

Probability from Tunneling Factor

$$\mathcal{P} \propto \exp\left(\frac{-m^2 - p_\perp^2}{\kappa/\pi}\right)$$

(κ is the string tension equivalent)

$\implies$ Gaussian suppression of high $m_\perp = \sqrt{m_q^2 + p_\perp^2}$

Assume probability of string break constant per unit world-sheet area

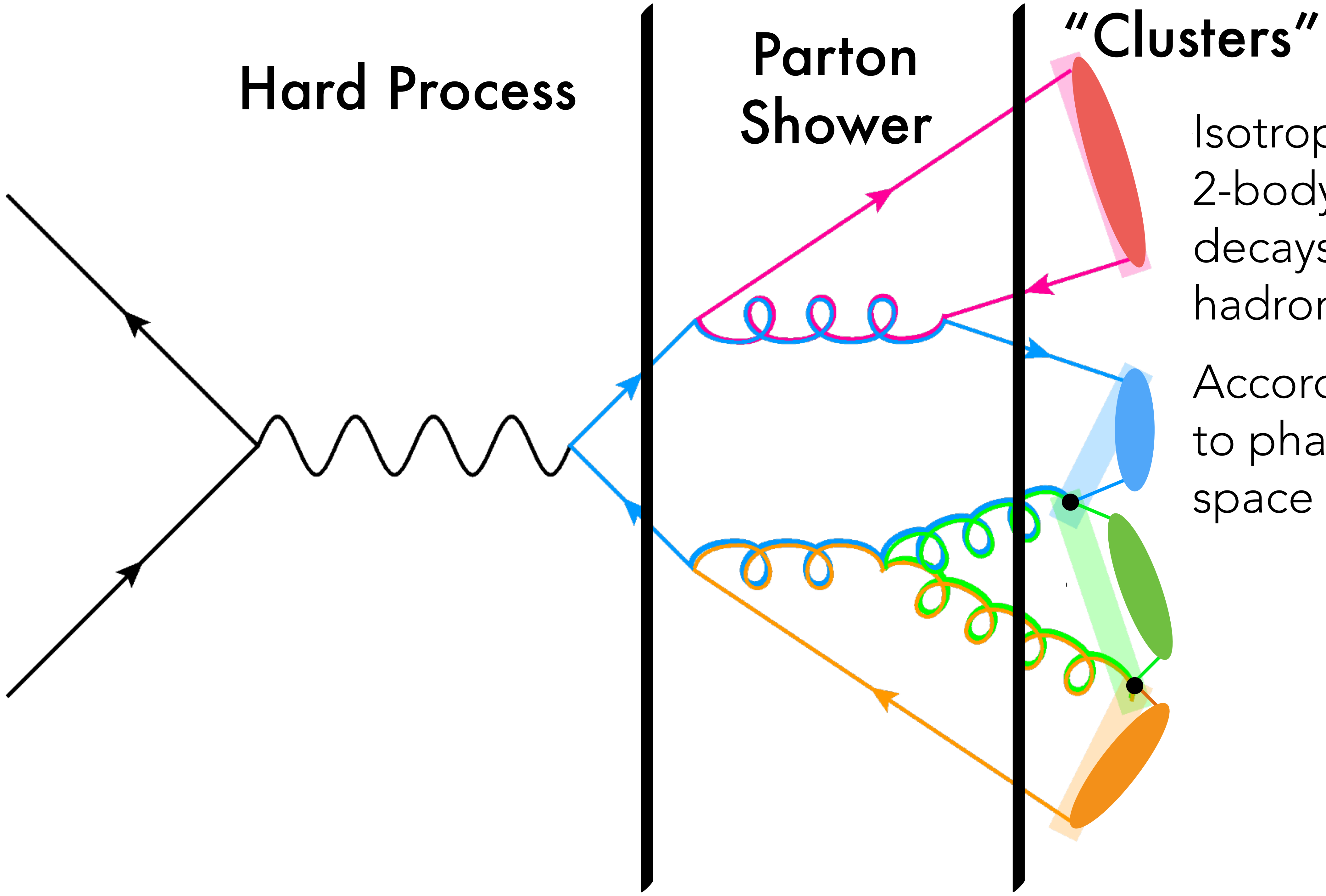
(Alternative: **The Cluster Model** — Used in Herwig and Sherpa)

In "unquenched" QCD

$g \to q\bar{q} \implies$ The strings will "break"

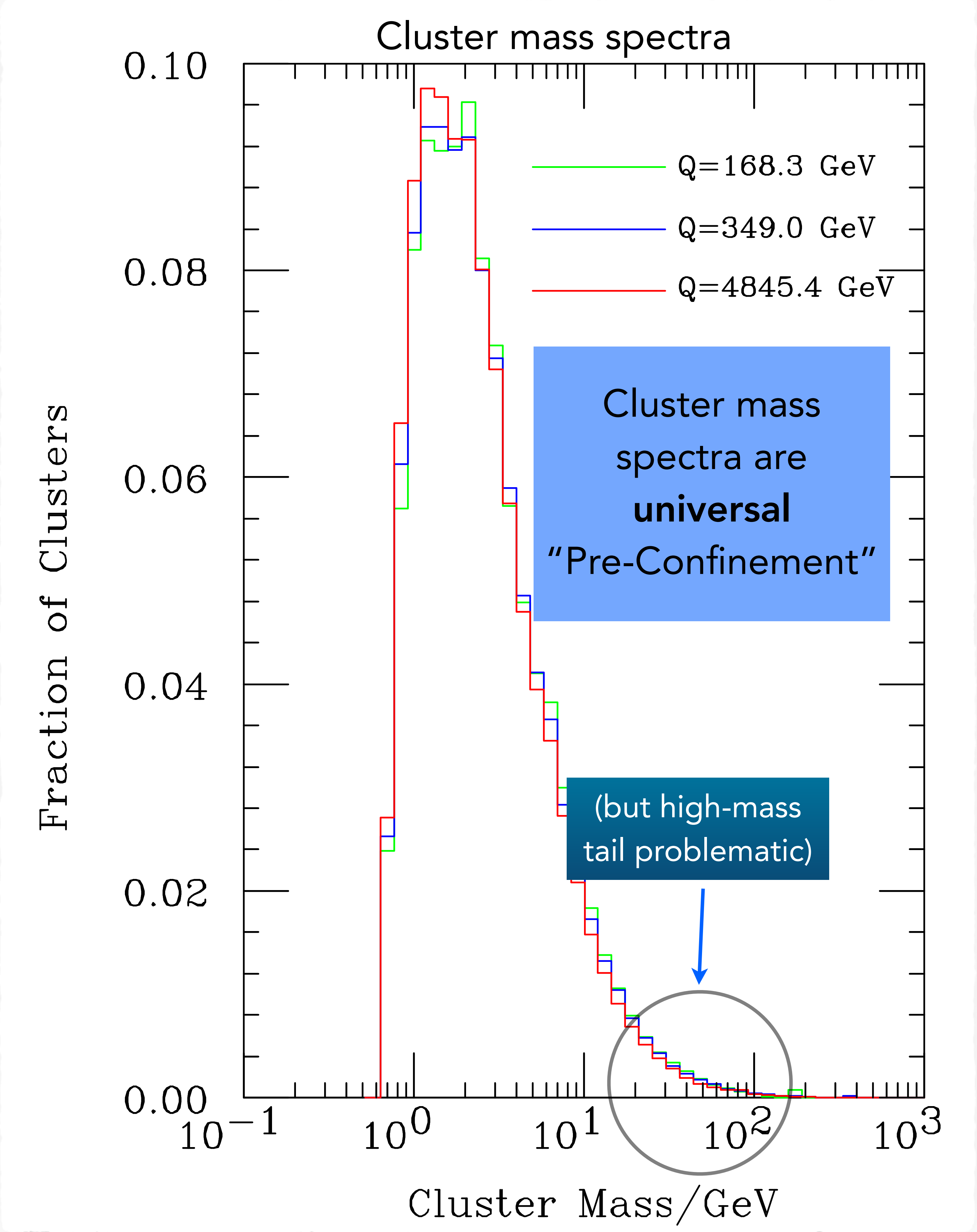
Non-perturbative so can't use $P_{g\to q\bar{q}}(z)$

Alternative: **force** $g \to q\bar{q}$ at end of shower



Isotropic 2-body decays to hadrons

According to phase space



Cluster mass spectra are **universal** "Pre-Confinement"

(but high-mass tail problematic)

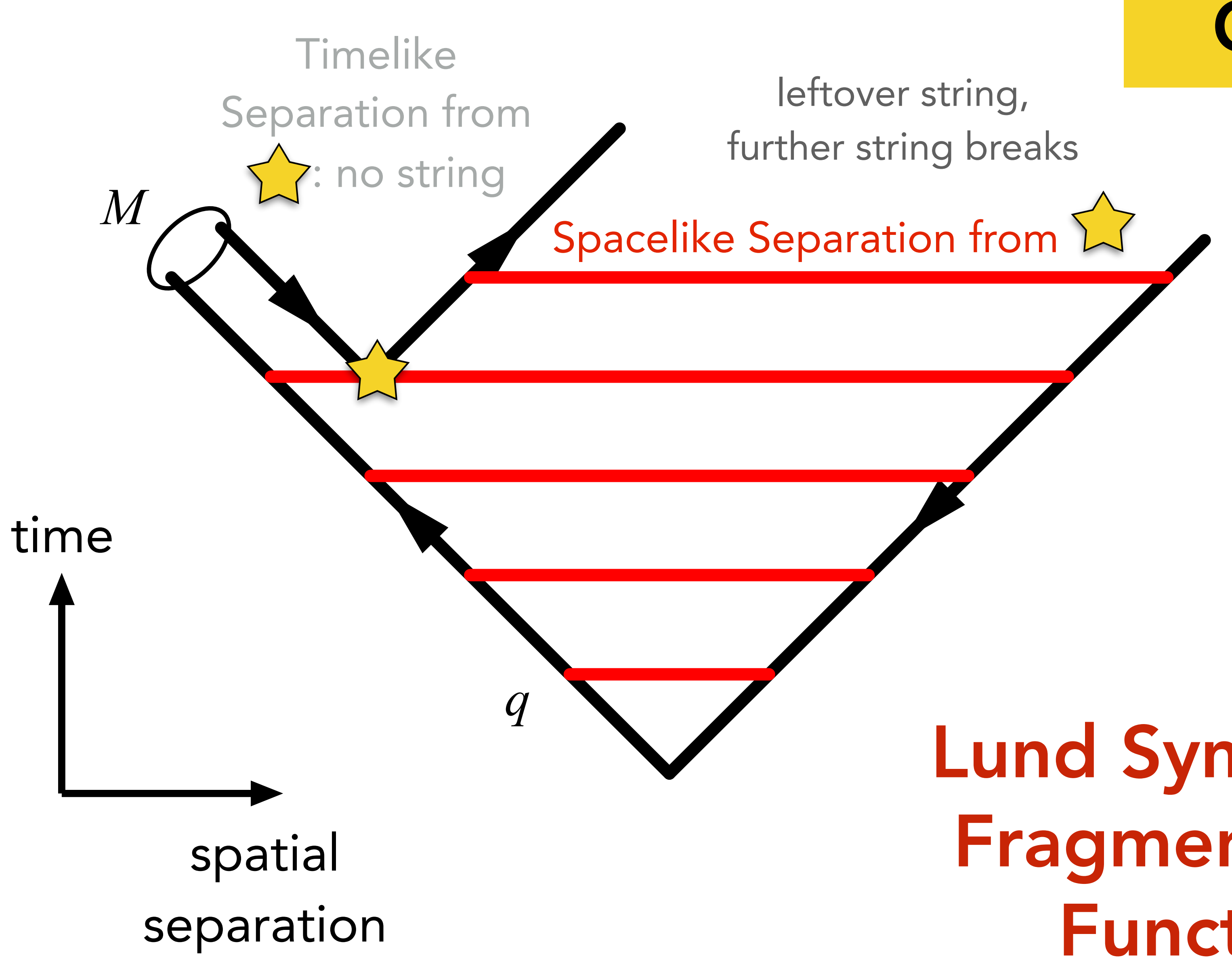
Large clusters → string-like splittings

Returning to **Strings**: the String Fragmentation Function

Schwinger $\Longrightarrow$ Gaussian $p_\perp$ spectrum (transverse to string axis) **& Prob(d:u:s) ≈ 1 : 1 : 0.2**

The meson M takes a fraction z of the quark momentum,

Probability distribution in $z \in [0,1]$ parametrised by **Fragmentation Function**, $f(z, Q^2_{\mathrm{HAD}})$



Observation: All string breaks are **causally disconnected**

Lorentz invariance $\Longrightarrow$ string breaks can be considered in *any order*. Imposes "left-right symmetry" on the **FF**

$\Longrightarrow$ **FF** constrained to a form with **two free parameters**, a & b: constrained by fits to measured hadron spectra

Lund Symmetric Fragmentation Function

$$f(z) \propto \frac{1}{z}(1-z)^{a}\exp\left(-\frac{b(m_h^2 + p_{\perp h}^2)}{z}\right)$$

↑ Supresses high-z hadrons

↑ Supresses low-z hadrons

(Note on the Length of Strings)

In Spacetime:

String tension ≈ 1 GeV/fm → a 50-GeV quark can travel 50 fm before all its kinetic energy is transformed to potential energy in the string. Then it must start moving the other way.

(→ "yo-yo" model of mesons. Note: string breaks → several mesons)

The MC implementation is formulated in momentum space

Lightcone momenta $p_\pm = E \pm p_z$ along string axis

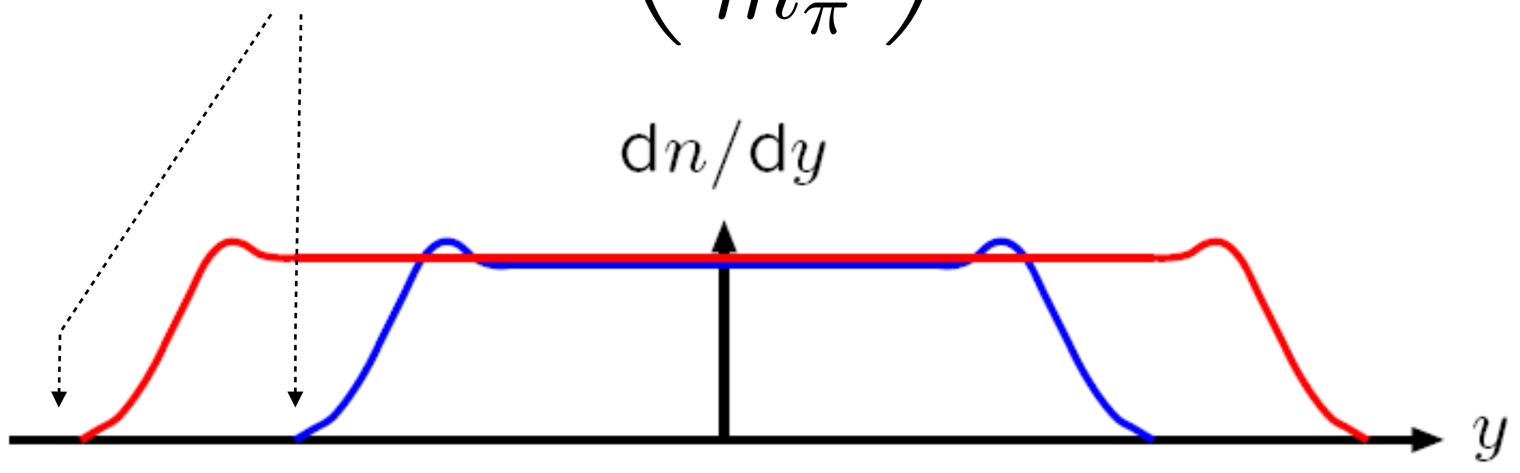
➜ Rapidity (along string axis) and $p_\perp$ transverse to it

$$y = \frac{1}{2}\ln\left(\frac{E+p_z}{E-p_z}\right) = \frac{1}{2}\ln\left(\frac{(E+p_z)^2}{E^2-p_z^2}\right)$$

If the quark gives all its energy to a single pion traveling along the z axis

$$y_{\max} \sim \ln\left(\frac{2E_q}{m_\pi}\right)$$

Increasing E_q → logarithmic growth in rapidity range



Particle Production:

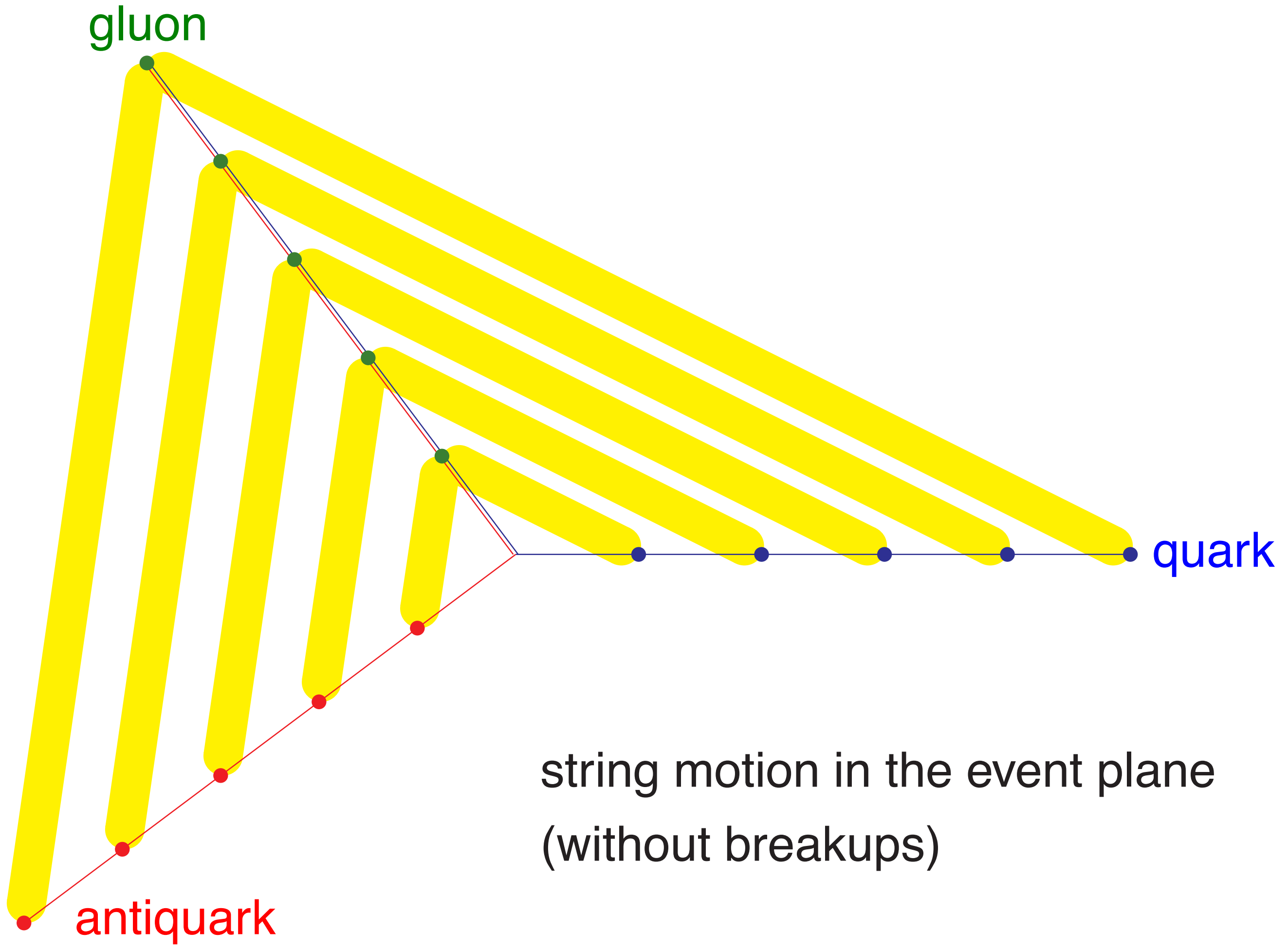
Scaling in $z \Longrightarrow$ flat in rapidity (long. boost invariance)

"Lightcone scaling"

$\langle n_{\mathrm{ch}}\rangle \approx c_0 + c_1 \ln E_{\mathrm{cm}}$, ~ Poissonian multiplicity distribution

Gluon Kinks: The Signature Feature of the Lund Model

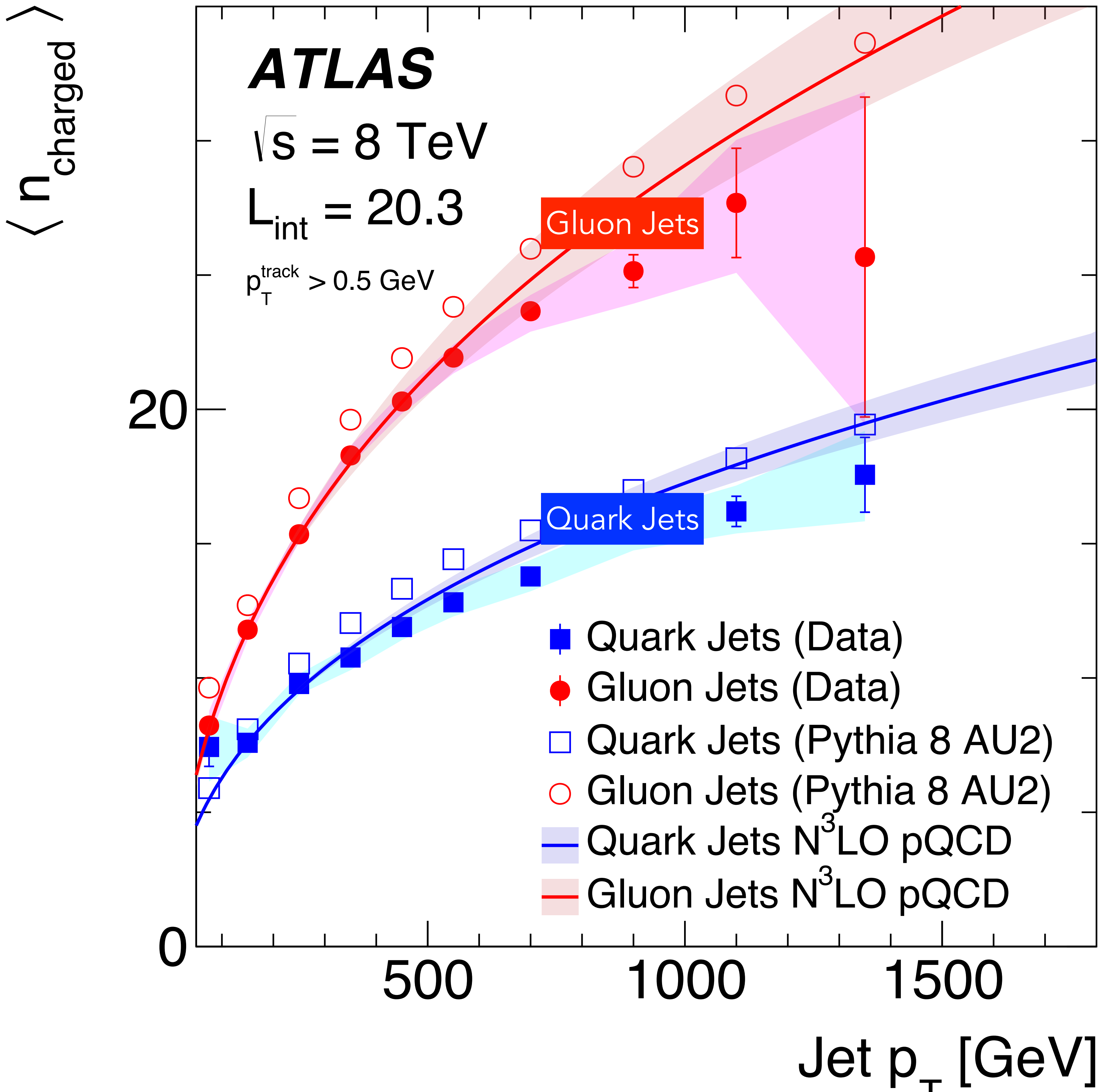
Gluons are connected to two string pieces



Each quark connected to **one** string piece

Expect factor ~ $2 \sim C_A/C_F$ more particles in gluon jets

ATLAS, Eur.Phys.J. C76 (2016) no.6, 322



Important for discriminating new-physics signals

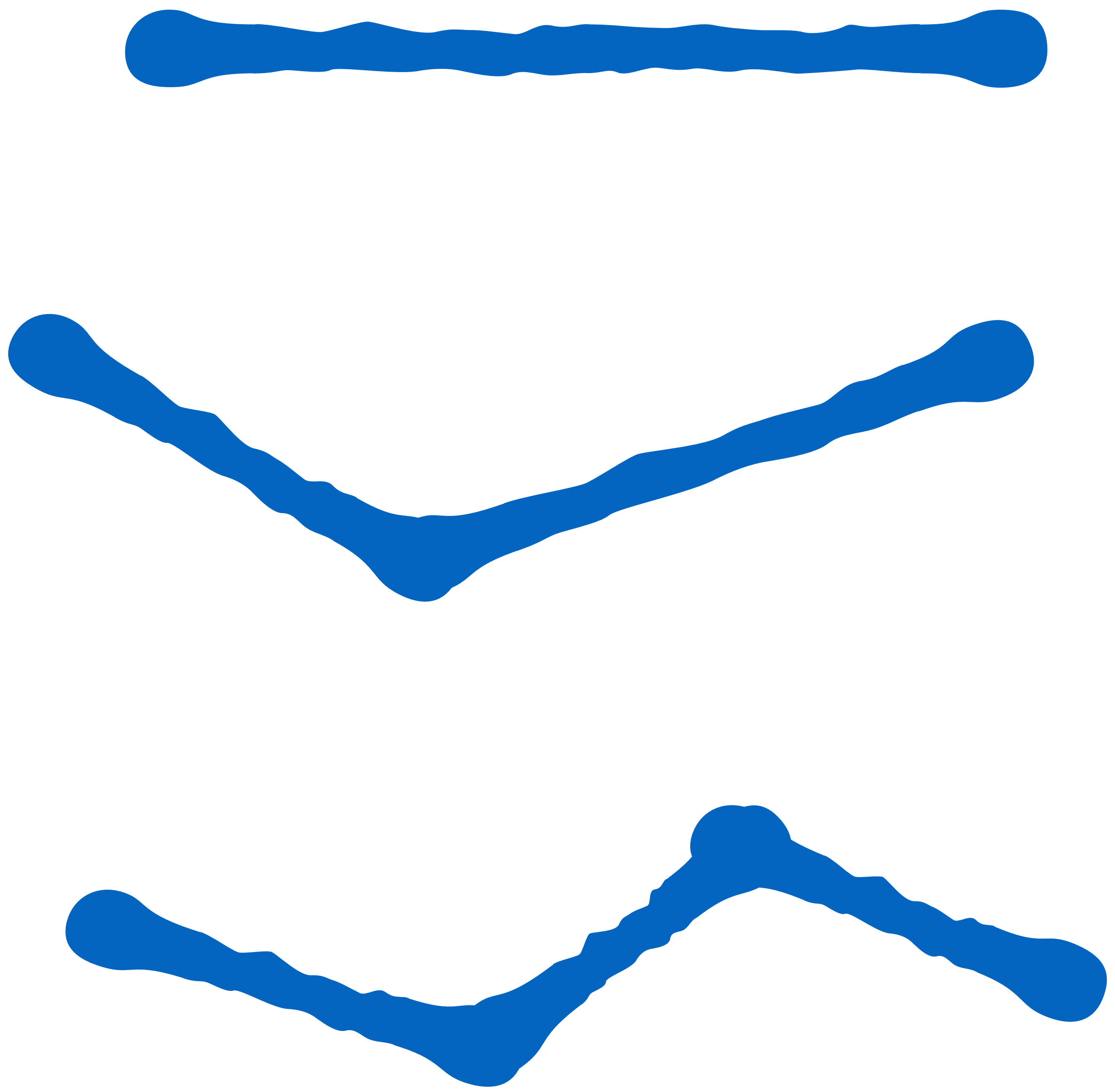
Decays to **quarks** vs decays to **gluons**,

vs composition of **background** and **bremsstrahlung** combinatorics

See also
Larkoski et al., JHEP 1411 (2014) 129
Thaler et al., Les Houches, arXiv:1605.04692

Other String Topologies

Open Strings

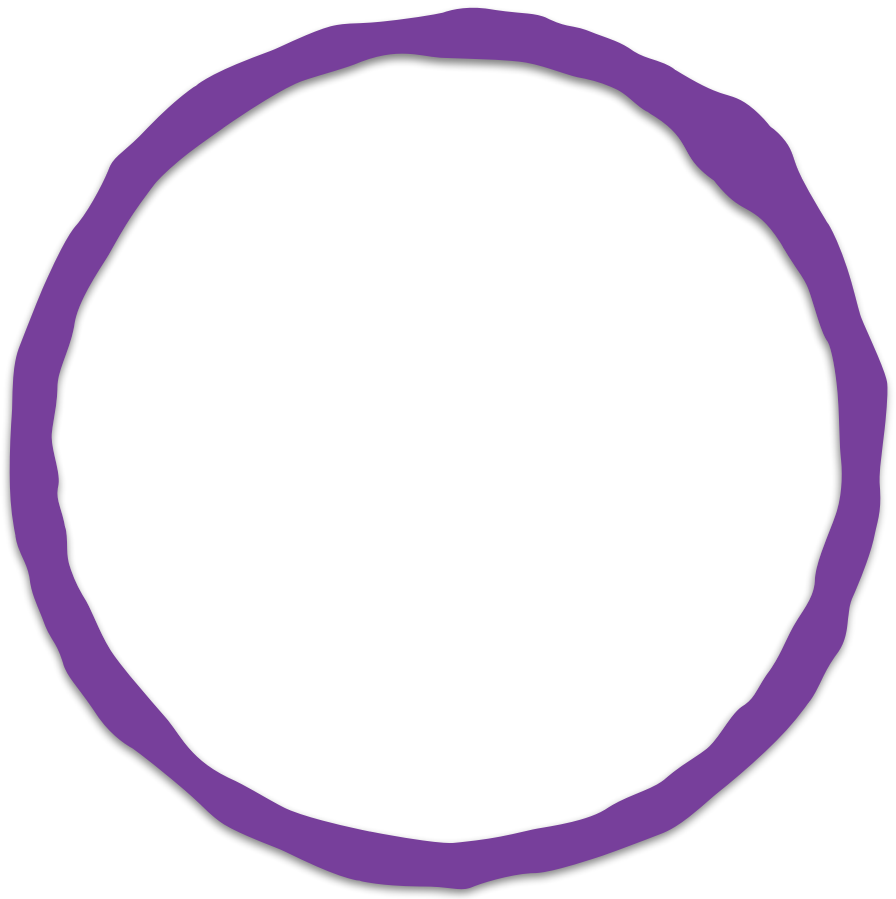


$q\bar{q}$ strings (with gluon kinks)

E.g., $Z \to q\bar{q}$ + shower

$H \to b\bar{b}$ + shower

Closed Strings



Gluon rings

E.g., $H \to gg$ + shower

$\Upsilon \to ggg$ + shower

SU(3) String Junction

Will return to these...

Open strings with $N_C = 3$ endpoints

E.g., Baryon-Number violating neutralino decay $\tilde{\chi}^0 \to qqq$ + shower

pp Collisions

In pp collisions, we are not hadronizing a simple $q - g - \ldots - g - \bar{q}$ string

Coloured initial states + gluon exchanges

$\Longrightarrow$ more complicated colour flows

Also: Protons are composite

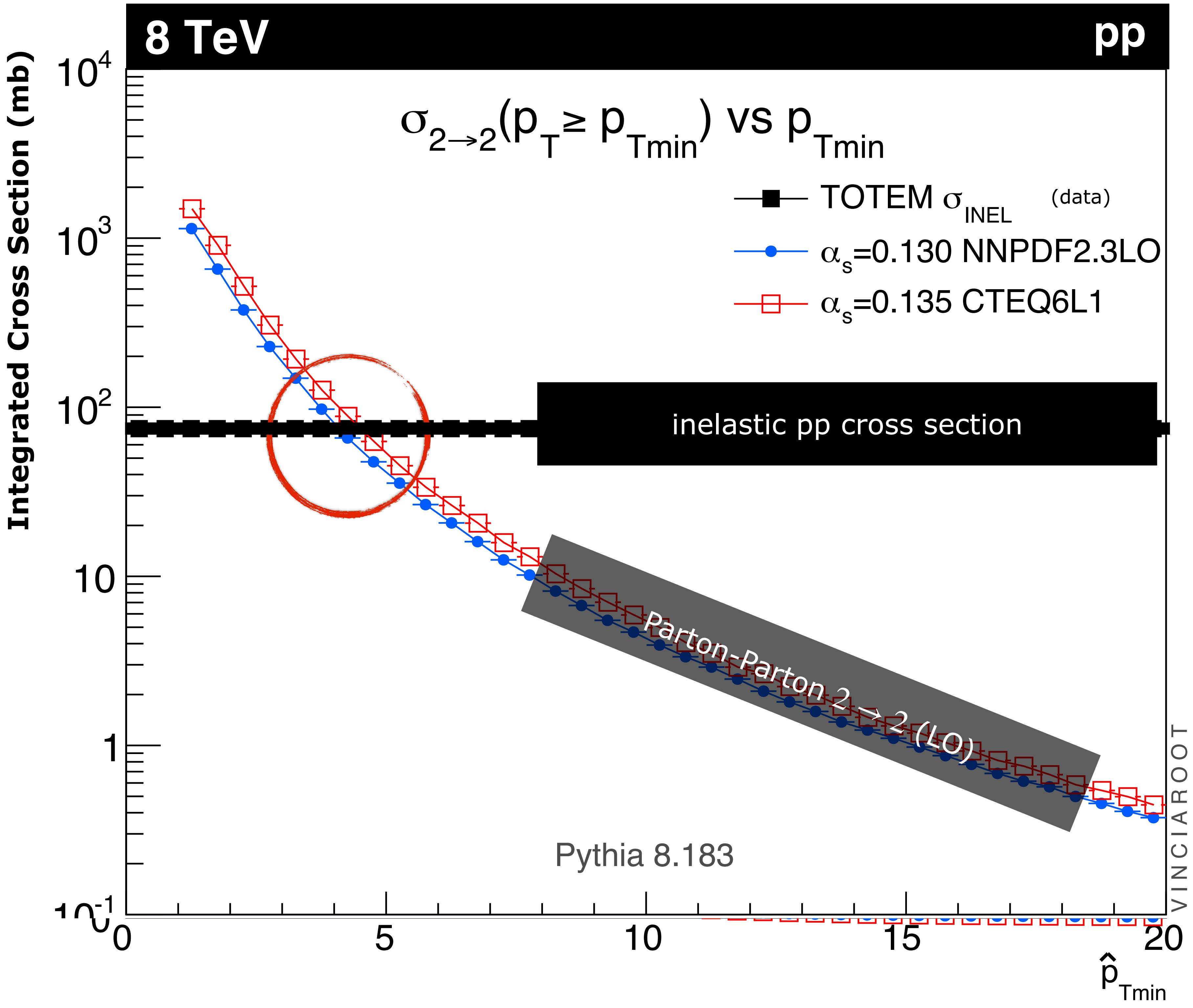
One proton = **beam** of partons

+ QCD 2 → 2 scattering diverges at low p_T

$\Longrightarrow \sigma_{\text{parton-parton}}(\hat{p}_\perp) > \sigma_{\text{proton-proton}}$ →

Interpretation: $\frac{\sigma_{\textbf{parton-parton}}(\hat{p}_\perp)}{\sigma_{\textbf{hadron-hadron}}} \sim \langle n \rangle_{\text{parton-parton}}(\hat{p}_\perp)$

(Regulated at low $\hat{p}_\perp$ by IR cutoff ~ colour screening)



Multiple Parton-Parton Interactions (MPI)

→ **Additional colour exchanges**

A Brief History of MPI (in PYTHIA)

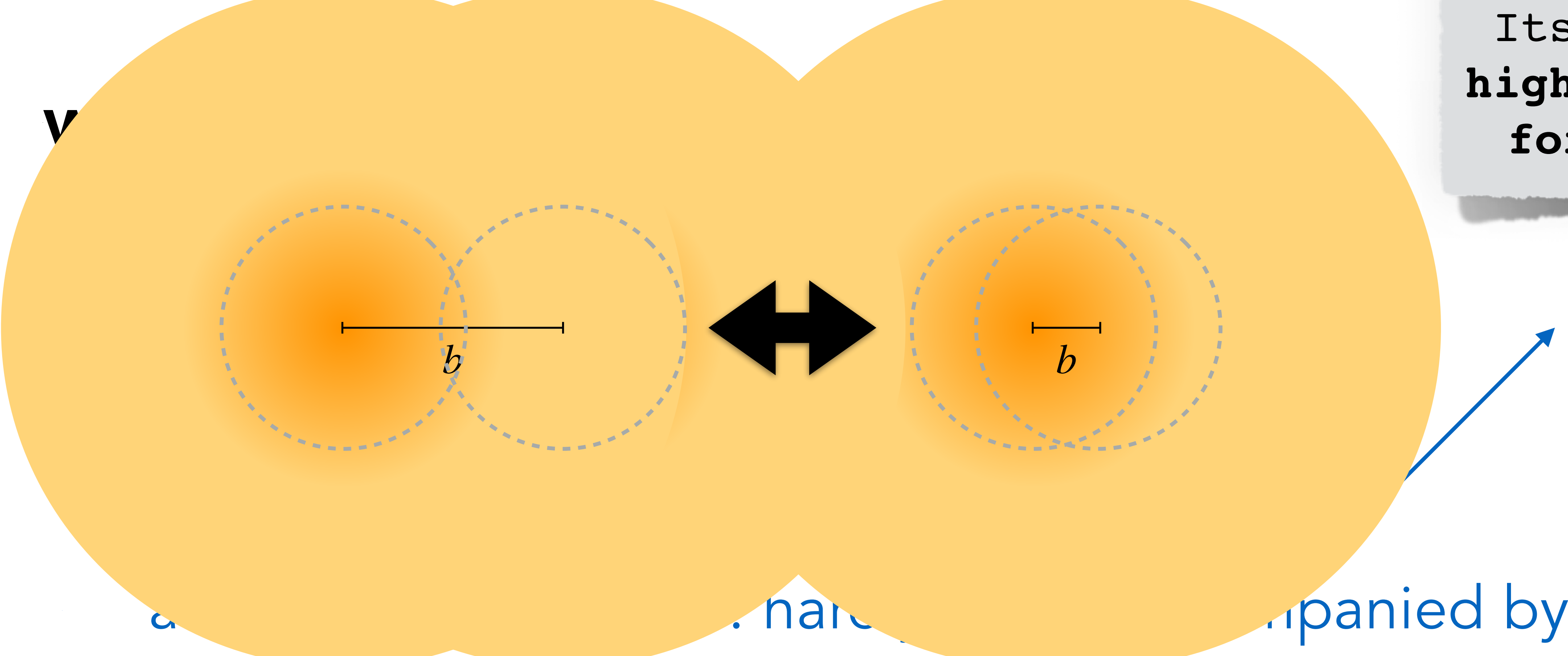
1987 [Sjöstrand & van Zijl, Phys.Rev.D 36 (1987) 2019]

Cast MPI as Sudakov-style evolution equation

Analogous to $\sigma_{\mathrm{X+jet}}(p_\perp)/\sigma_{\mathrm{X}}$ for parton showers

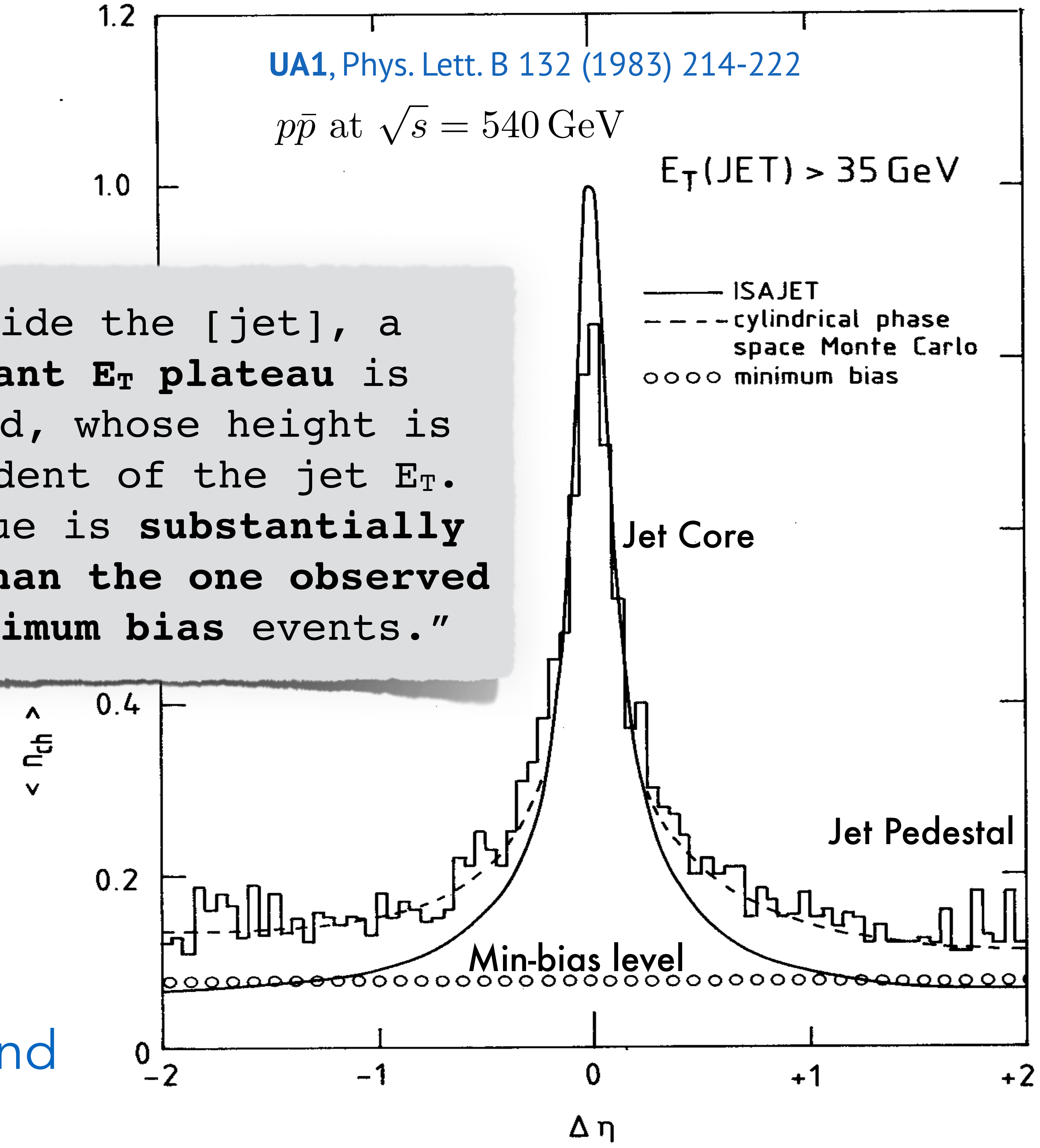
$$\frac{dP_{\mathrm{hardest}}}{d^2b\, dx_{T1}} = p(x_{T1},b)\exp\left\{-\int_{x_{T1}}^{1} p(x'_T,b)\, dx'_T\right\}$$

$p \propto \sigma_{2\to2}(x_T,b)/\sigma_{pp}$; $x_T = 2\hat{p}_\perp/\sqrt{s}$



a . hard mpanied by — and sit on top of — **higher-than average** particle densities *(compared with the average = minimum-bias pp collision)*

> "Outside the [jet], a **constant E_T plateau** is observed, whose height is independent of the jet E_T. Its value is **substantially higher than the one observed for minimum bias** events."



Interleaved Evolution in PYTHIA

2005 [Sjöstrand & **PS**, Eur.Phys.J.C 39 (2005) 129]

Interleave **MPI & ISR** evolutions in one common sequence of p_T

➜ ISR & MPI "compete" for the available x in the proton remnant.

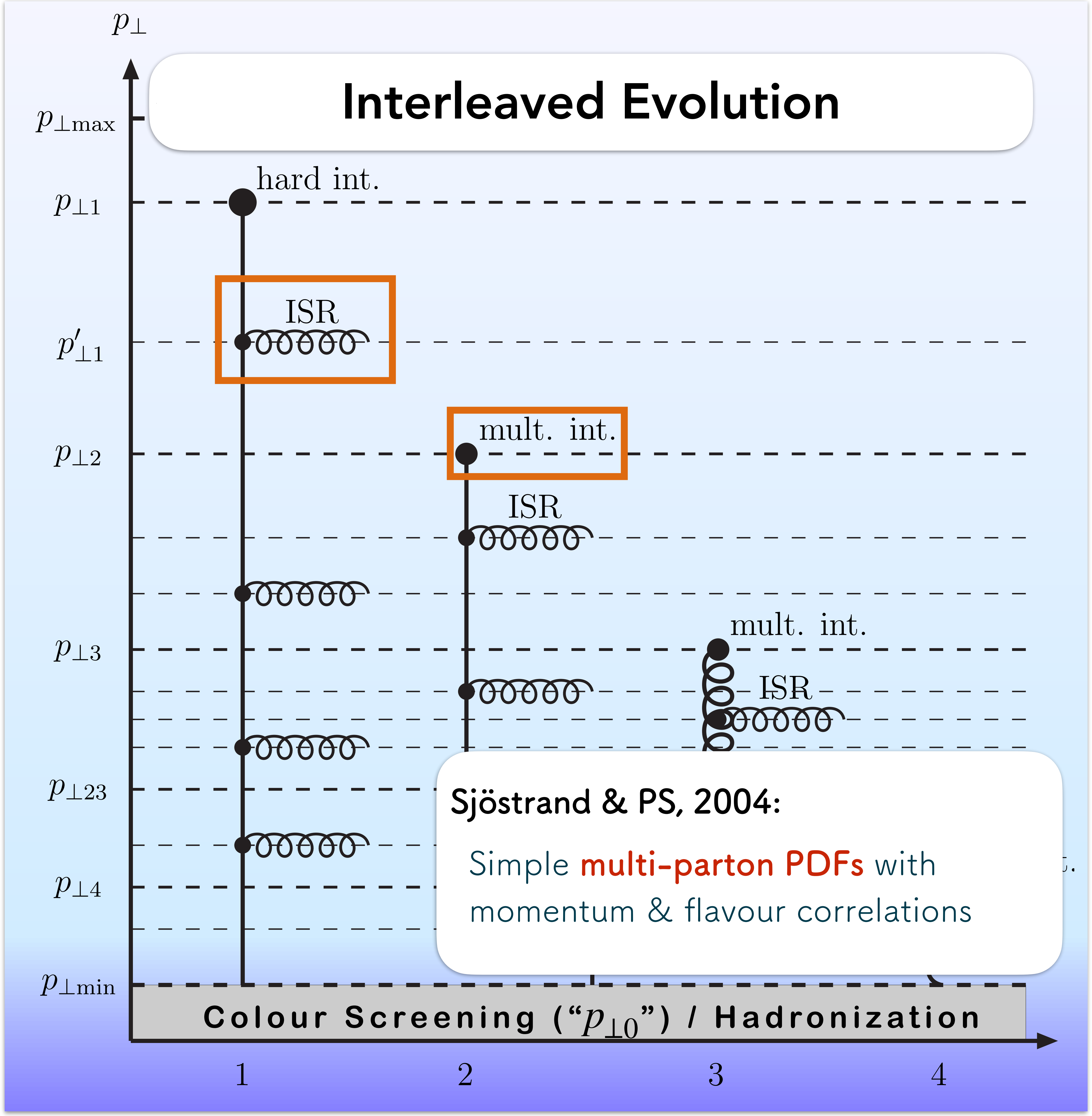
2011 [Corke & Sjöstrand, JHEP 03 (2011) 032]

Also include **FSR** in interleaving

NEW

2021 [Brooks, **PS**, Verheyen, SciPost Phys. 12 (2022) 3]

Also include **Resonance Decays** in interleaving (VINCIA)



Sjöstrand & PS, 2004:

Simple multi-parton PDFs with momentum & flavour correlations

Figure from Sjöstrand & PS, 2005

Confinement

High-energy pp collisions with MPI + QCD bremsstrahlung

Final states with **very many** coloured partons

With significant overlaps in phase space

Who gets confined with whom?

Each has a colour ambiguity $\sim 1/N_C^2 \sim 10\,\%$

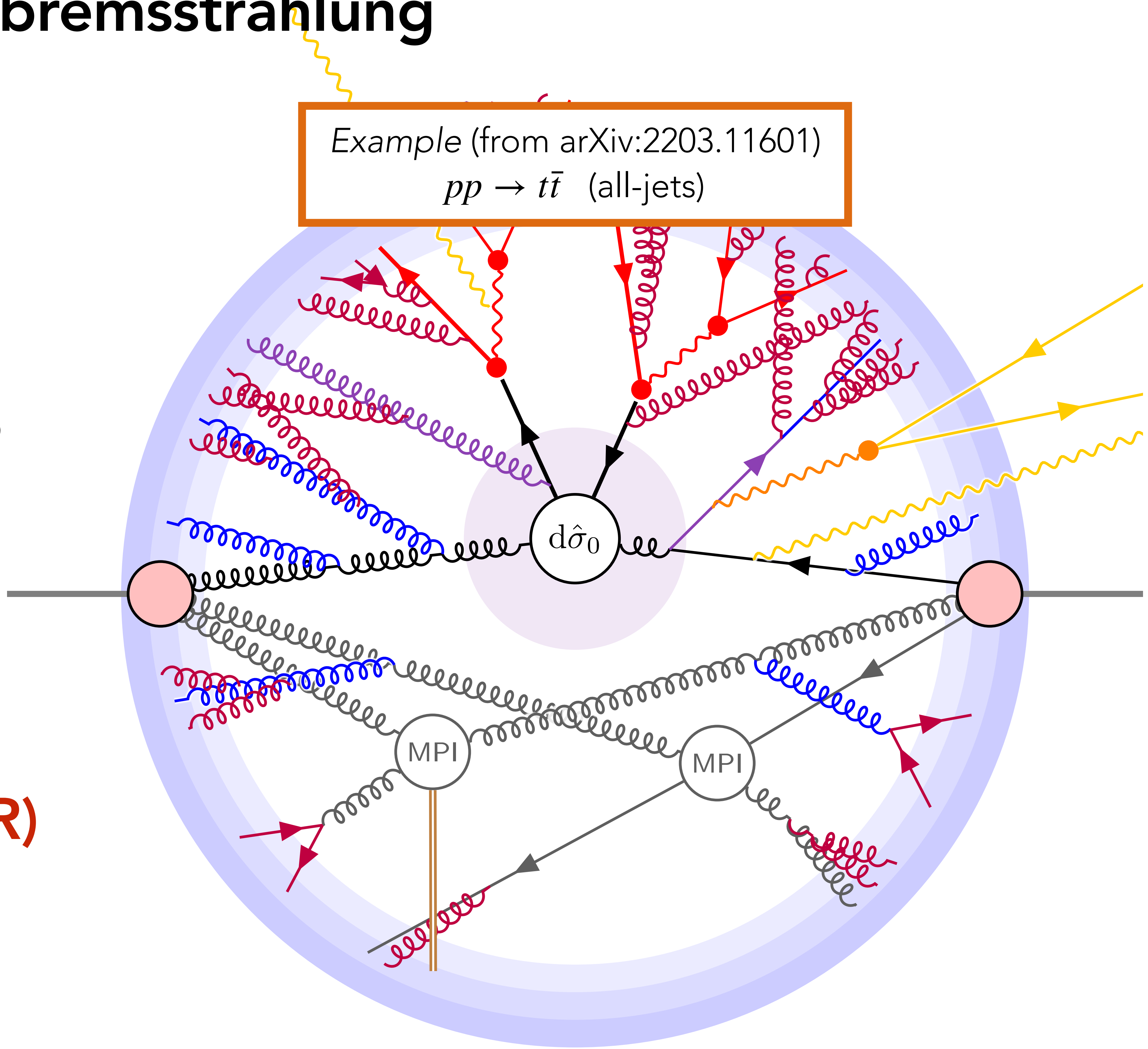
E.g.: **random triplet** charge has 1/9 chance to be in **singlet** state with **random antitriplet**:

$3 \otimes \bar{3} = 8 \oplus 1$, etc.

Many charges ➜ Colour Reconnections* (CR) more likely than not

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

Example (from arXiv:2203.11601)
$pp \to t\bar{t}$ (all-jets)



"Parton Level"

(Event structure before confinement)

*): *in this context, QCD CR simply refers to an ambiguity beyond Leading N_C, known to exist. Note the term "CR" can also be used more broadly to incorporate further physics concepts.*

Colour (Re)connections

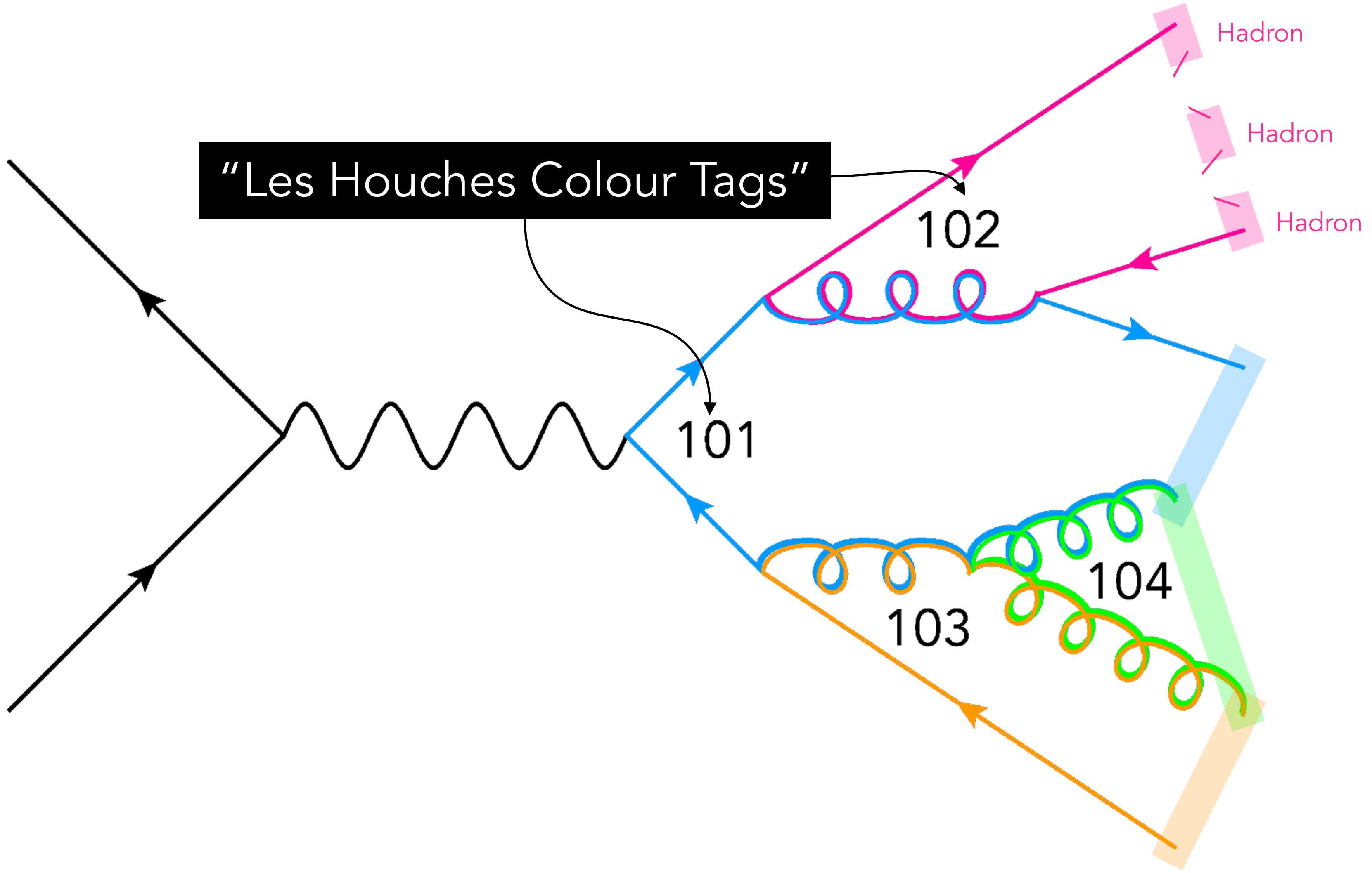
Colour Flow in MC Event Generators

Based on "Leading Colour": $8 \sim 3 \otimes \bar{3}$

Gluons ~ Direct product of 3 and $\bar{3}$

Formally corresponds to a limit $N_C \to \infty$

Unique colour flow; no interferences



2015 [Christiansen & **PS** JHEP 08 (2015) 003]

Stochastic sampling of beyond-LC **correlations in colour space** (incl MPI, etc)

Weighted by SU(3) group weights:

$3 \otimes \bar{3} = 8 \oplus 1$ $\qquad$ $3 \otimes 3 = 6 \oplus \bar{3}$

$3 \otimes 8 = 15 \oplus 6 \oplus 3$ $\qquad$ $8 \otimes 8 = 27 \oplus 10 \oplus \overline{10} \oplus 8_S \oplus 8_A \oplus 1$

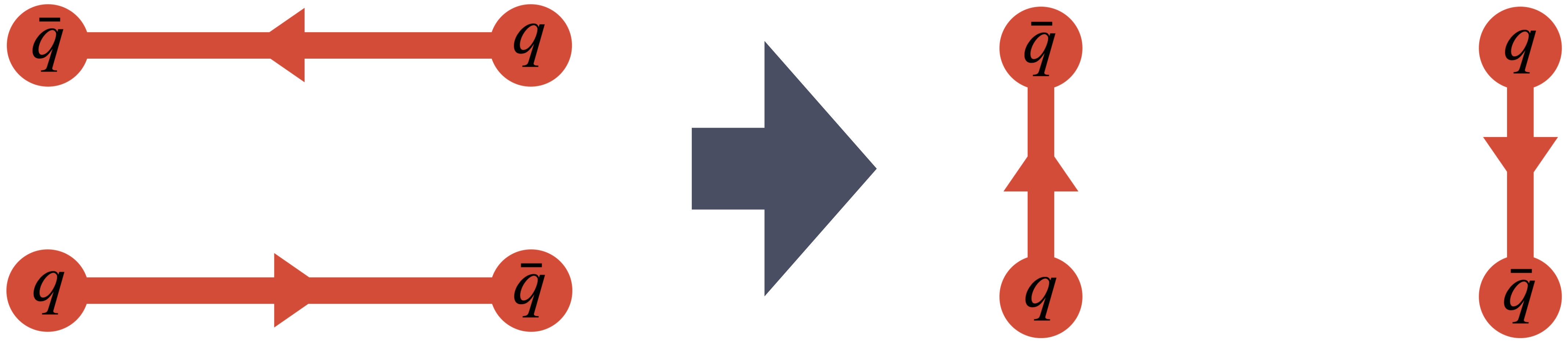
Interpret Confinement ⟷ **any** connection that can screen QCD charge

+ Use **string area law** to split degeneracies: **minimise string "length"**

QCD Reconnections ⟷ String Junctions

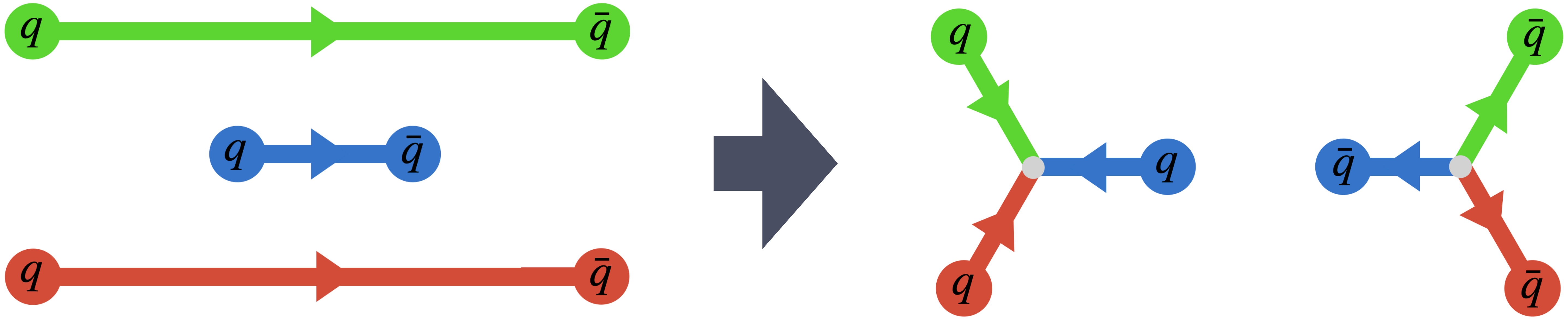
Stochastically restores colour-space ambiguities according to **SU(3) algebra**

- ➢ Allows for reconnections to minimise string lengths



Dipole-type reconnection

What about the red-green-blue colour singlet state?

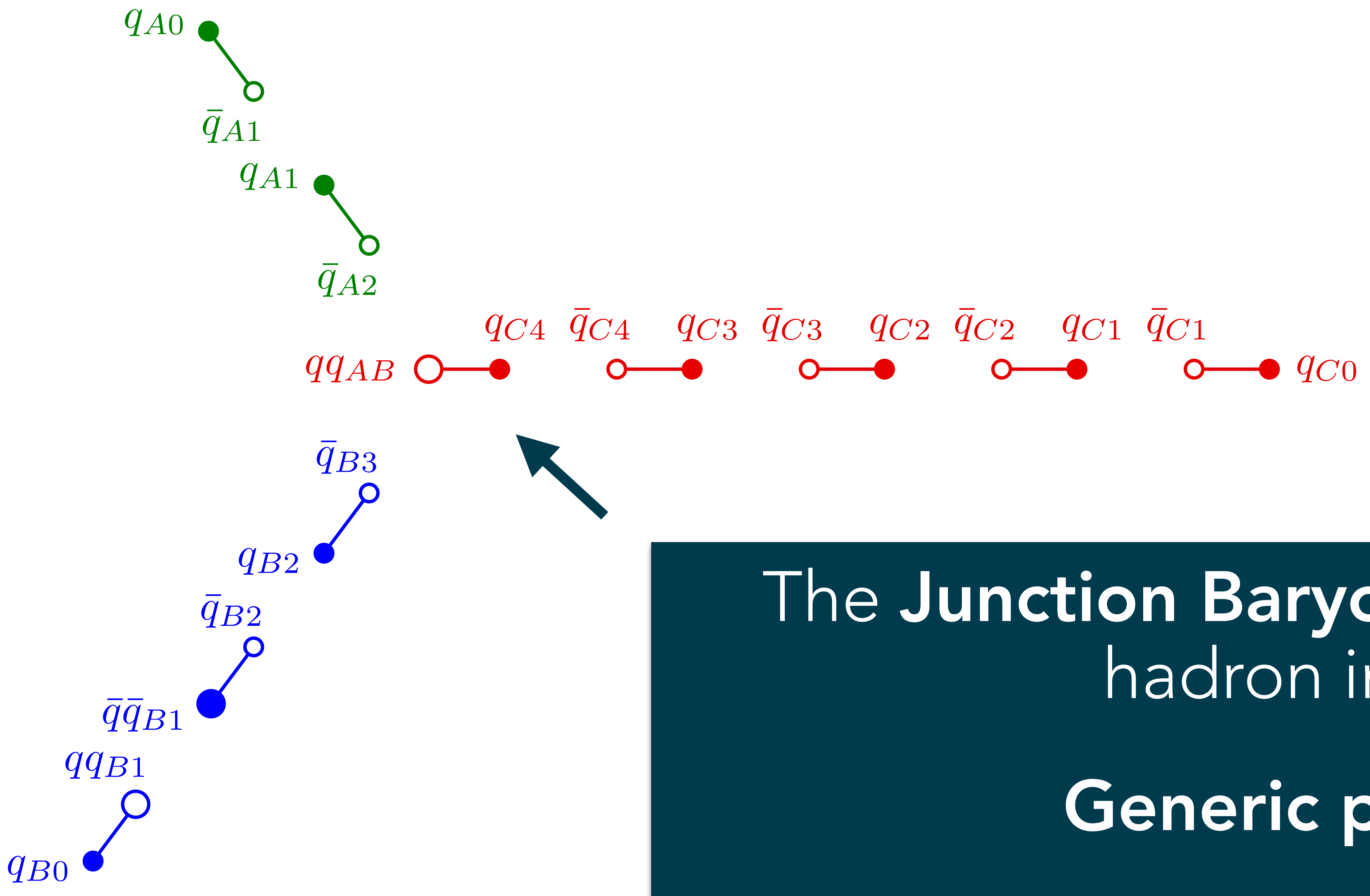


Junctions!

Fragmentation of String Junctions

Assume Junction Strings have same properties as ordinary ones (u:d:s, Schwinger p_T, etc)

➤ No new string-fragmentation parameters



The **Junction Baryon** is the most "subleading" hadron in all three "jets".

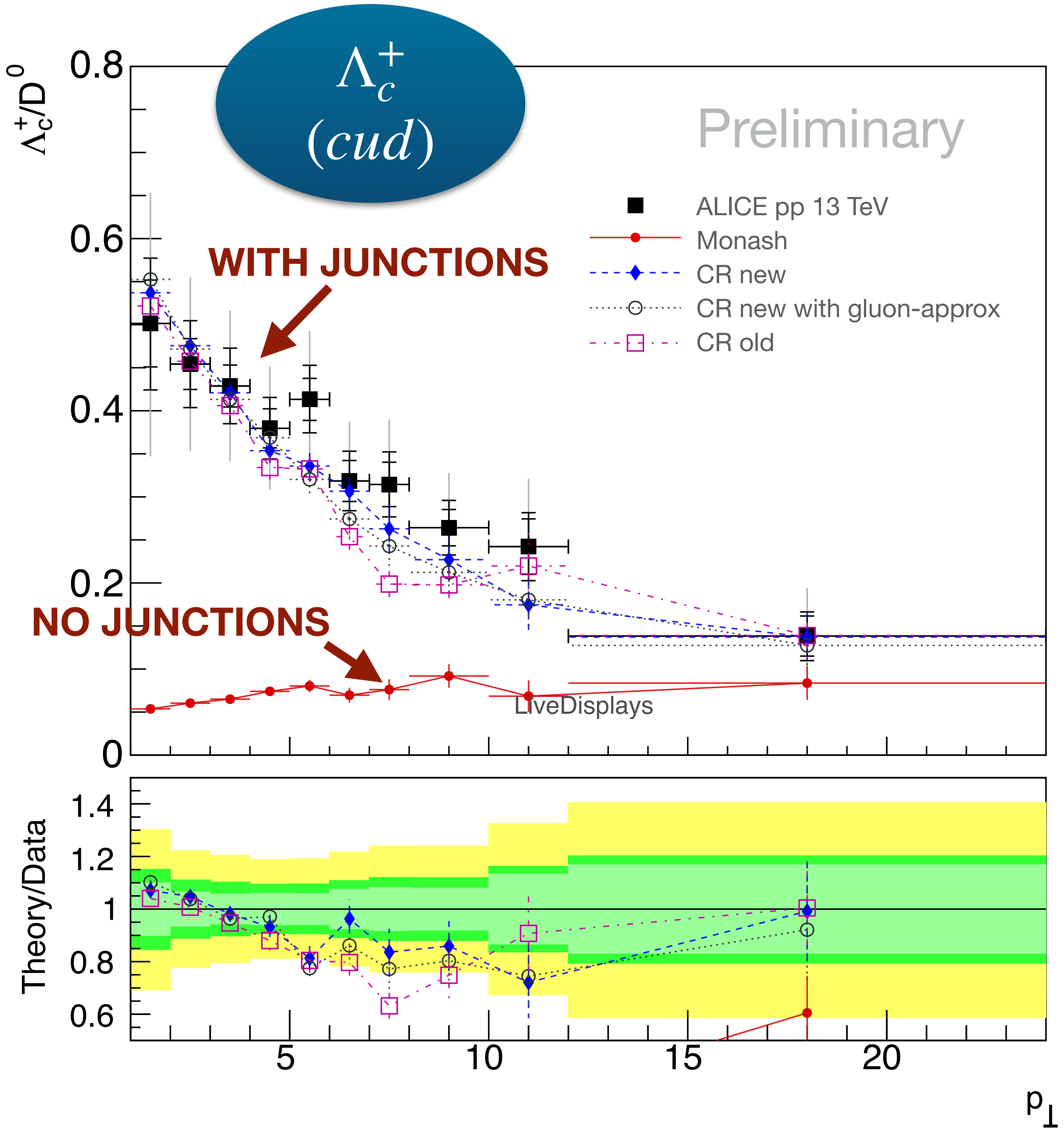
Generic prediction: low p_T

A Smoking Gun for String Junctions: Baryon enhancements at low p_T

NEW

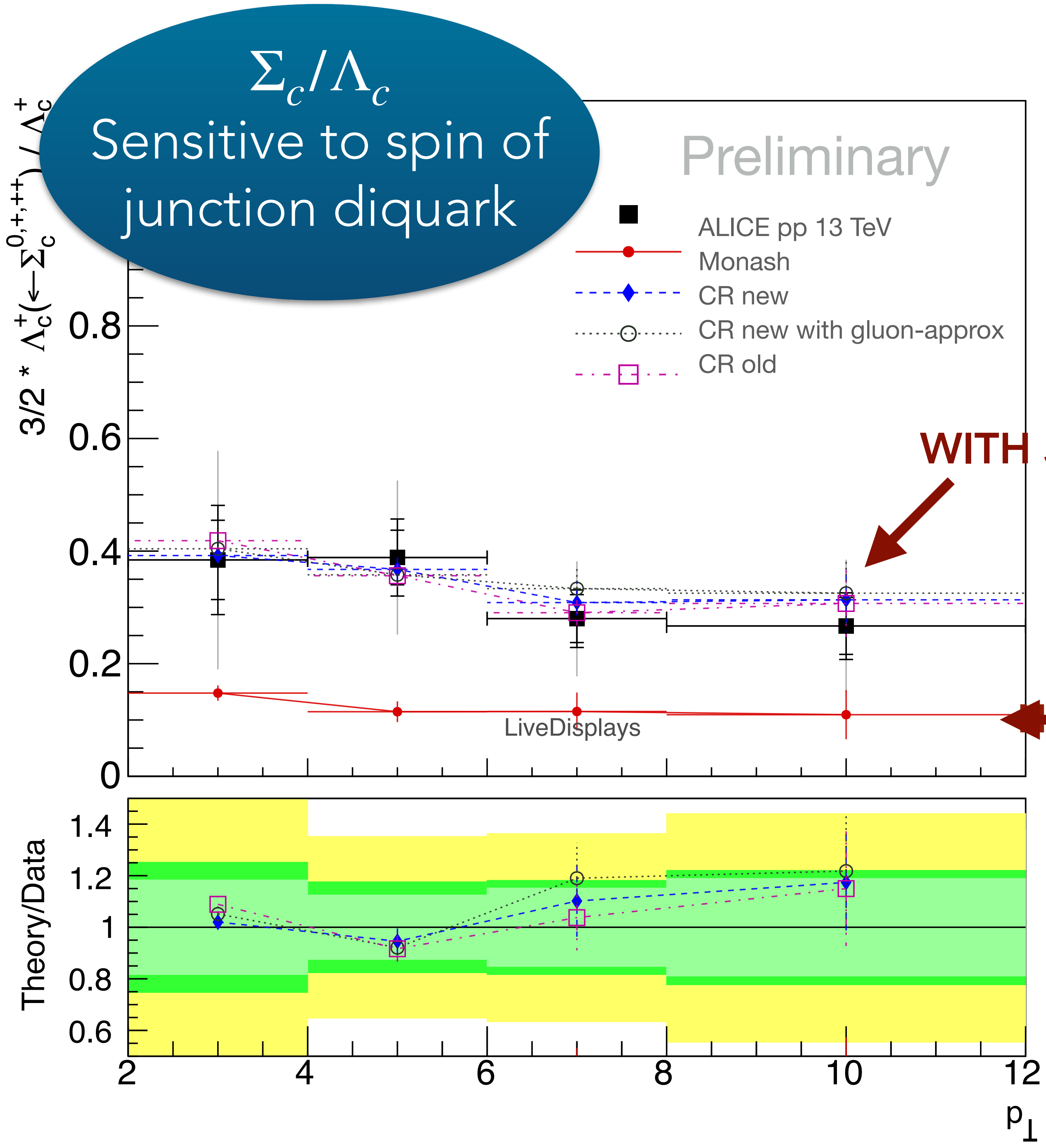
Confront with Measurements

LHC experiments report very large (factor-10) enhancements in heavy-flavour baryon-to-meson ratios at low p_T!



WITH JUNCTIONS

NO JUNCTIONS



WITH JUNCTIONS

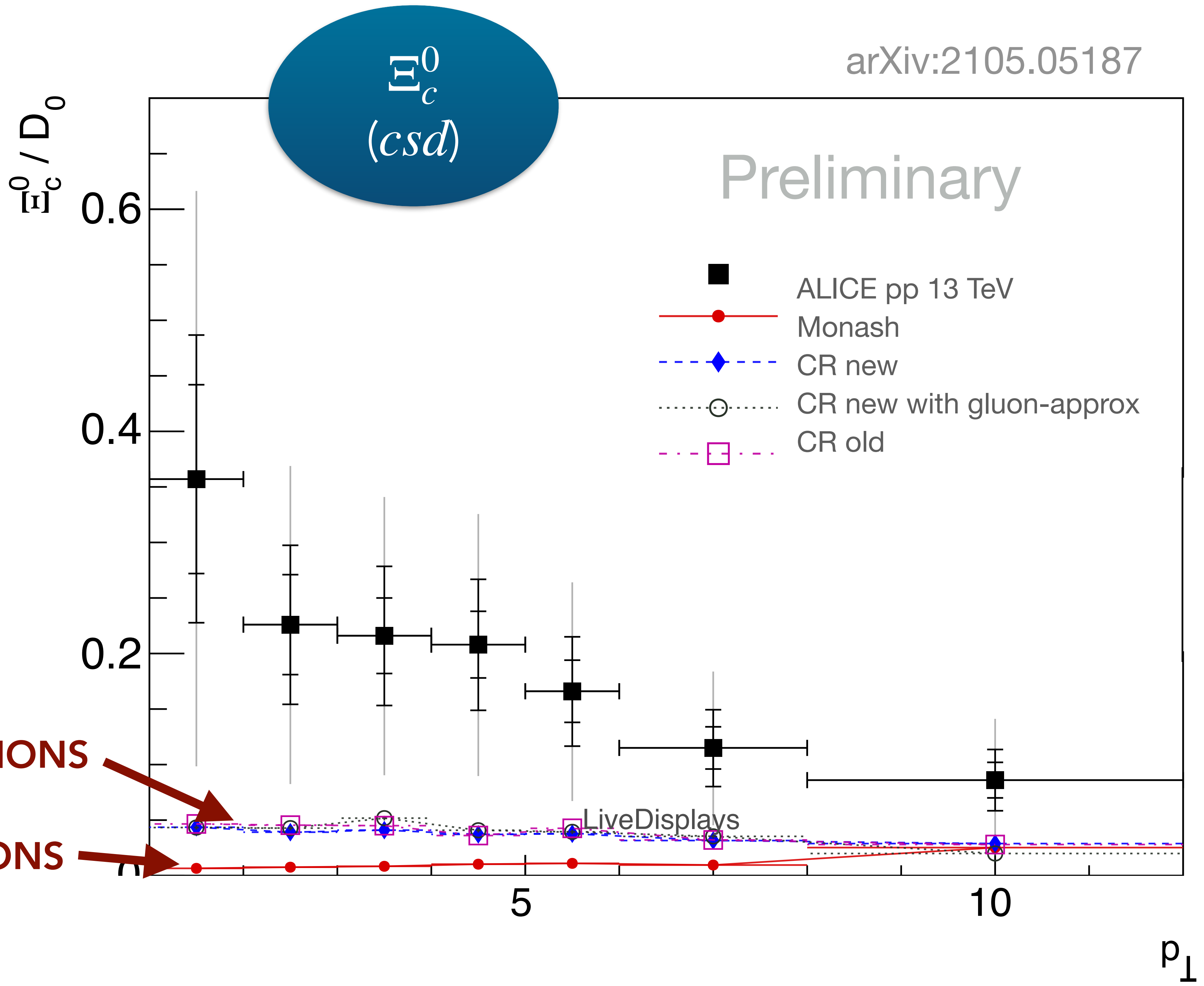
NO JUNCTIONS

Plots by
J. Altmann

Very exciting!

Confront with Measurements: **Strangeness**

What about Strange heavy-flavour baryons ?



WITH JUNCTIONS

NO JUNCTIONS

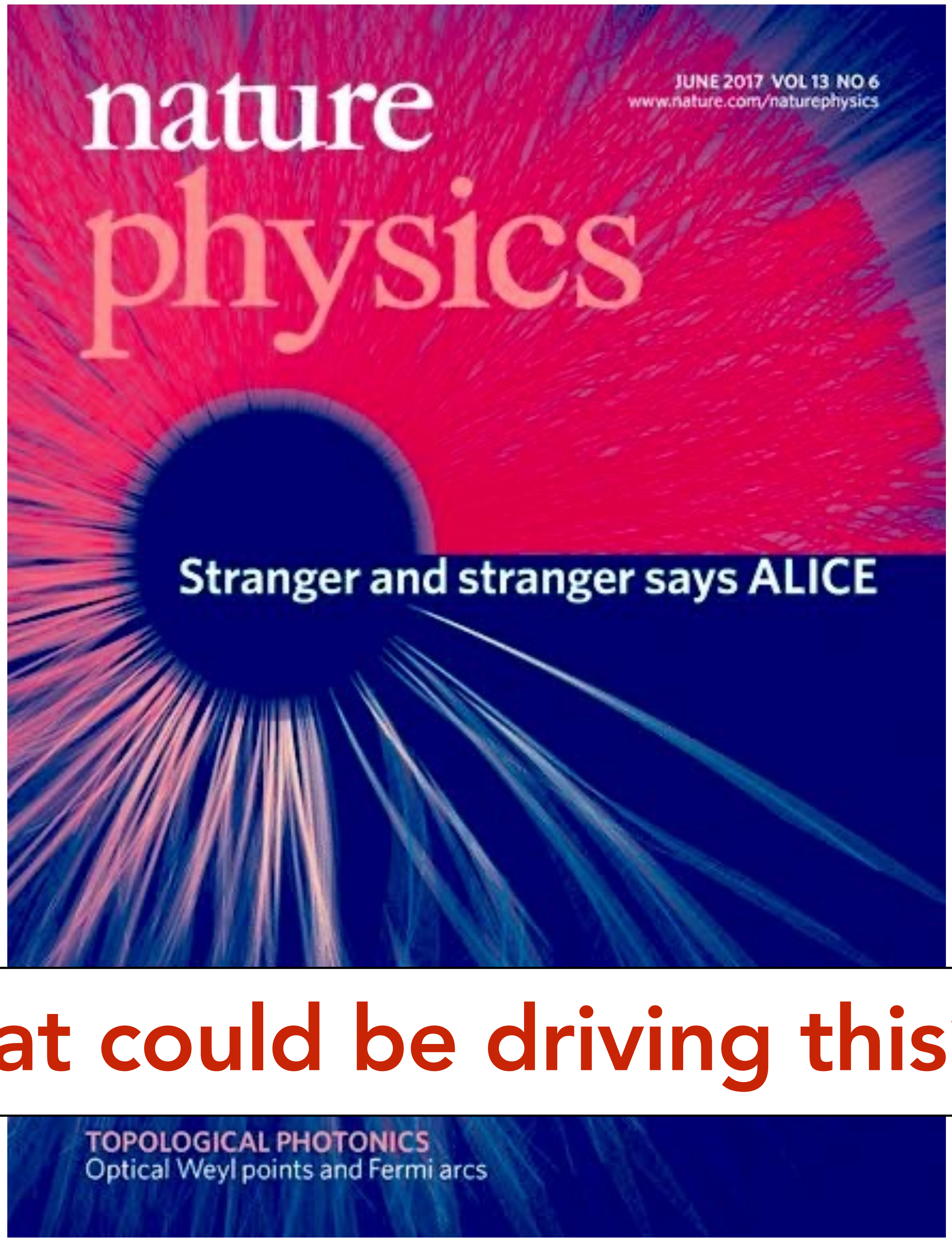
Even more exciting!

Slide adapted from J. Altmann

What a ***strange*** world we live in, said Alice

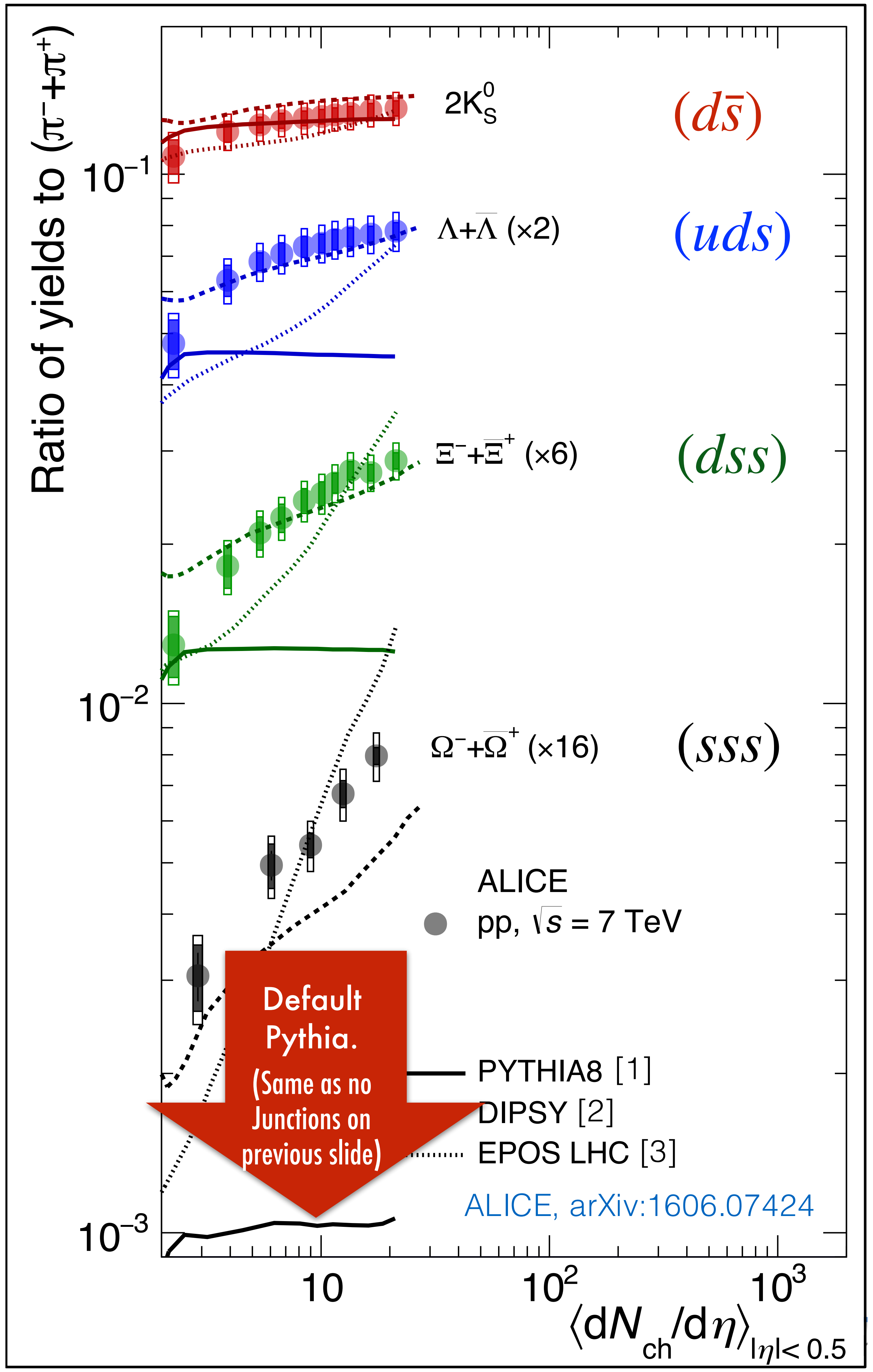
We know ratios of strange hadrons to pions strongly increase with event activity

Landmark measurement by ALICE (2017)



June 2017

What could be driving this?

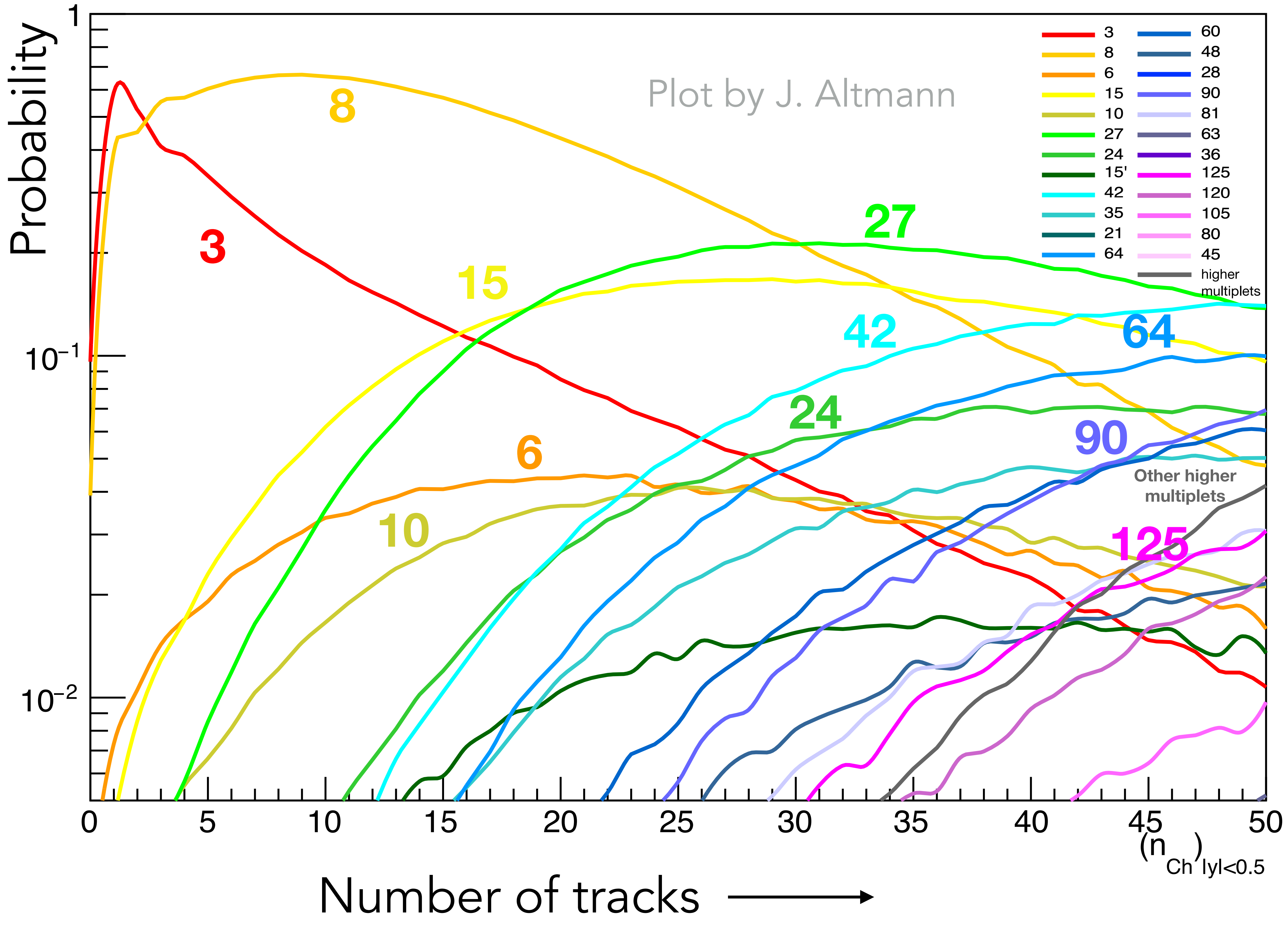


Default Pythia.
(Same as no Junctions on previous slide)

➜ Non-Linear String Dynamics?

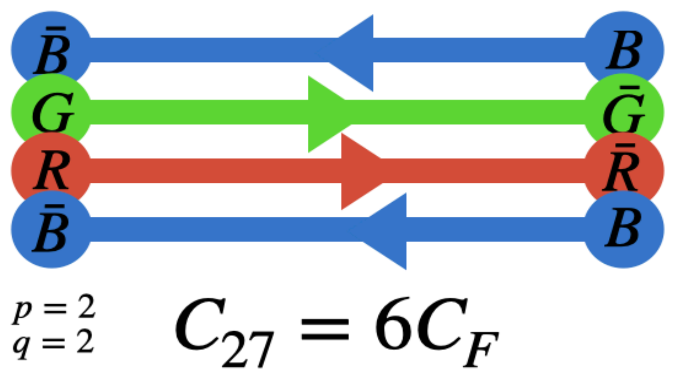
MPI $\Longrightarrow$ lots of coloured partons scattered into the final states

Count **# of flux lines** crossing $y = 0$ in pp collisions (according to PYTHIA):



Confining fields may be reaching much **higher effective representations** than simple quark-antiquark (3) ones.

E.g.: 27



27

$C_{27} = 6C_F$

Two approaches in PYTHIA:

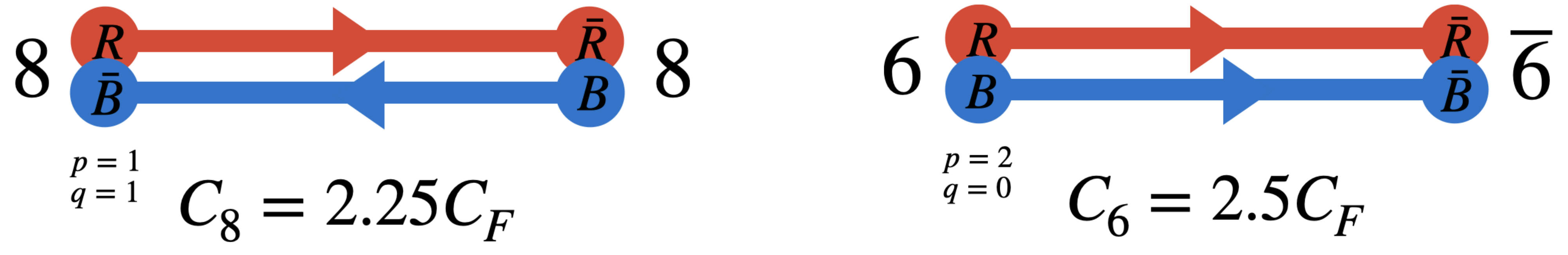
1) Colour Ropes (Lund)

2) Close-Packing (Monash)

Work in Progress: **Strangeness Enhancement from Close-Packing**

Idea: each string exists in an effective background produced by the others

Close-packing

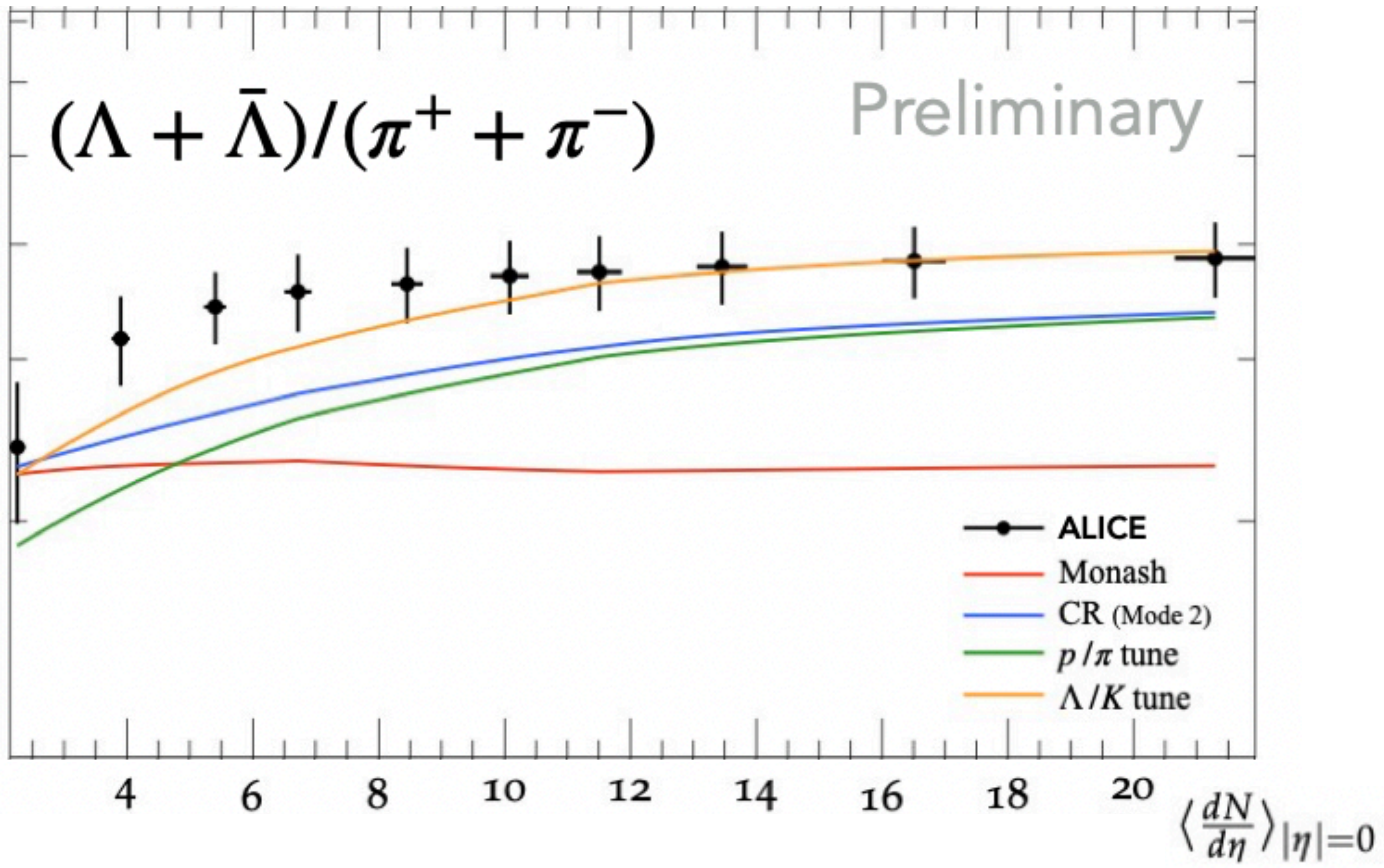


$C_8 = 2.25 C_F$ $\quad$ $C_6 = 2.5 C_F$

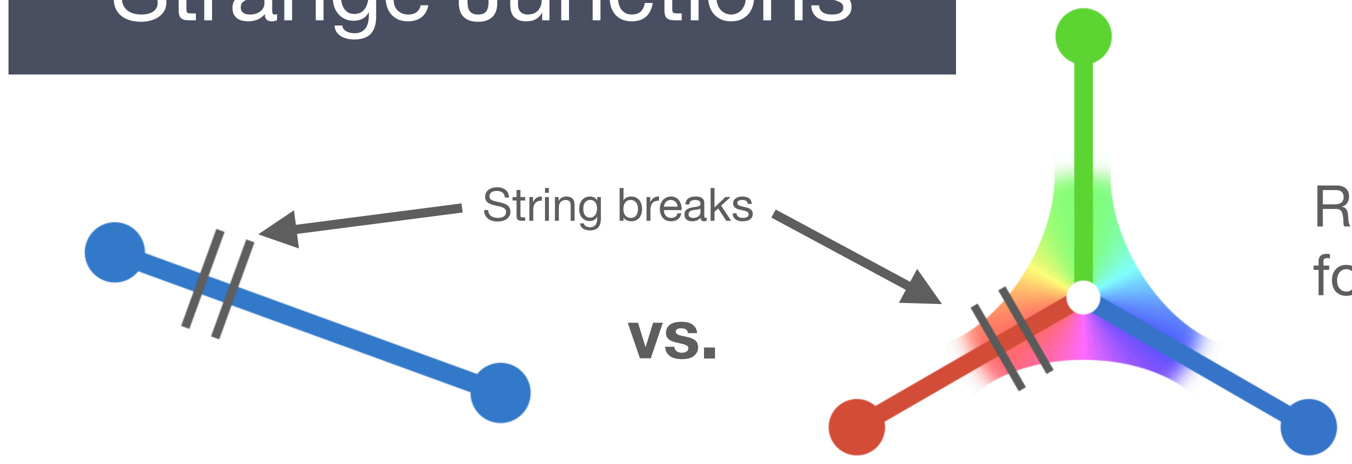
Dense string environments

→ Casimir scaling of **effective string tension**

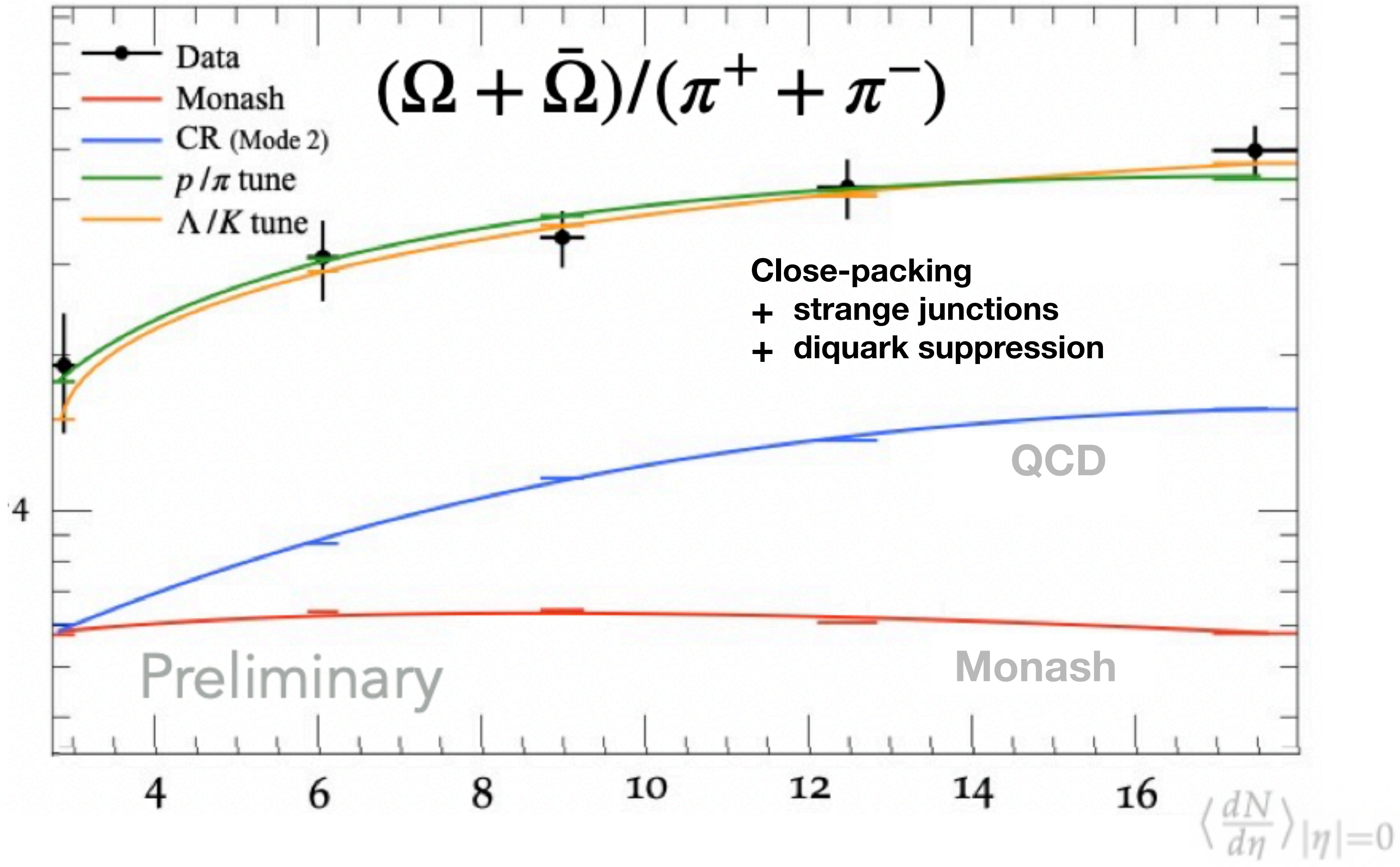
→ Higher probability of strange quarks



Strange Junctions



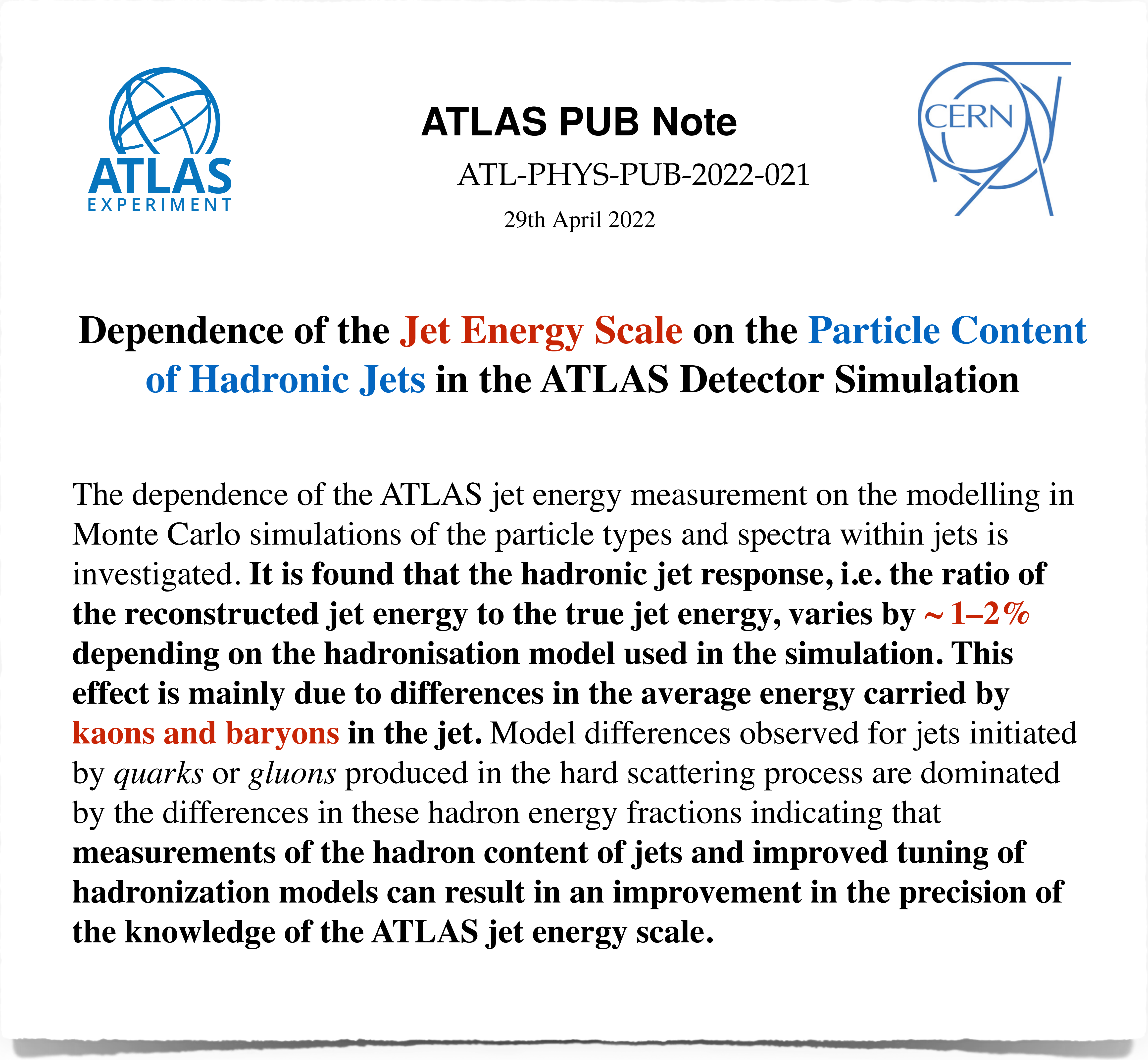
Results in strangeness enhancement focused in baryon sector



String tension could be different from the vacuum case compared to near a junction

Slide adapted from J. Altmann

Implications for Precision Event Generators



ATLAS PUB Note

ATL-PHYS-PUB-2022-021

29th April 2022

Dependence of the Jet Energy Scale on the Particle Content of Hadronic Jets in the ATLAS Detector Simulation

The dependence of the ATLAS jet energy measurement on the modelling in Monte Carlo simulations of the particle types and spectra within jets is investigated. **It is found that the hadronic jet response, i.e. the ratio of the reconstructed jet energy to the true jet energy, varies by ~ 1–2% depending on the hadronisation model used in the simulation. This effect is mainly due to differences in the average energy carried by kaons and baryons in the jet.** Model differences observed for jets initiated by *quarks* or *gluons* produced in the hard scattering process are dominated by the differences in these hadron energy fractions indicating that **measurements of the hadron content of jets and improved tuning of hadronization models can result in an improvement in the precision of the knowledge of the ATLAS jet energy scale.**

Variation largest for gluon jets

- For E_T = **[30, 100, 200] GeV**
- Max JES variation = **[3%, 2%, 1.2%]**

Fraction of jet E_T carried by baryons (and kaons) varies significantly

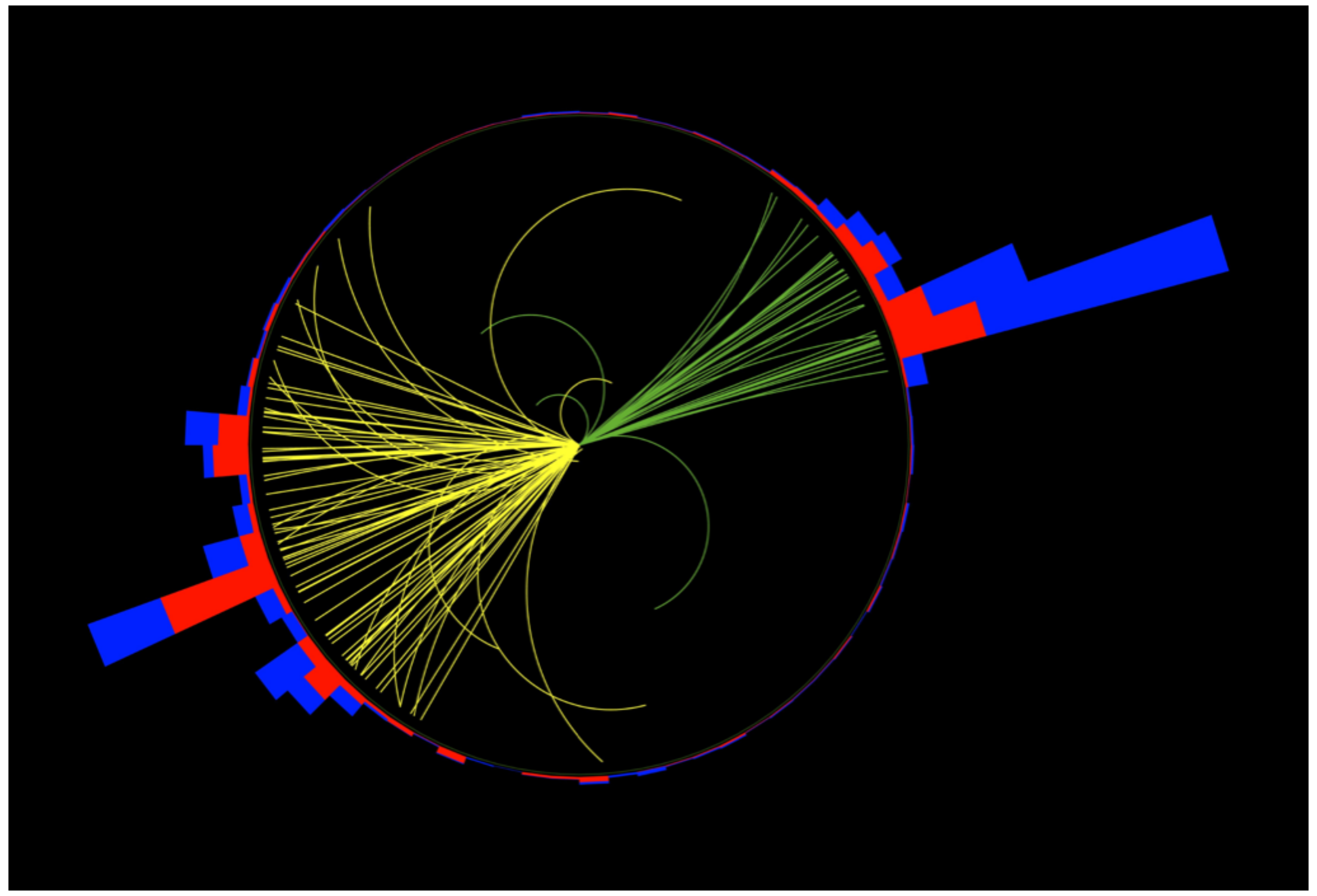
- Reweighting to force similar baryon and kaon fractions
- Max variation ➜ **[1.2%, 0.8%, 0.5%]**
- Significant potential for improved Jet Energy Scale uncertainties!

Motivates Careful Models & Careful Constraints

- Interplay with advanced UE models
- In-situ constraints from LHC data
- Revisit comparisons to LEP data

Summary

MC generators connect theory with experiment

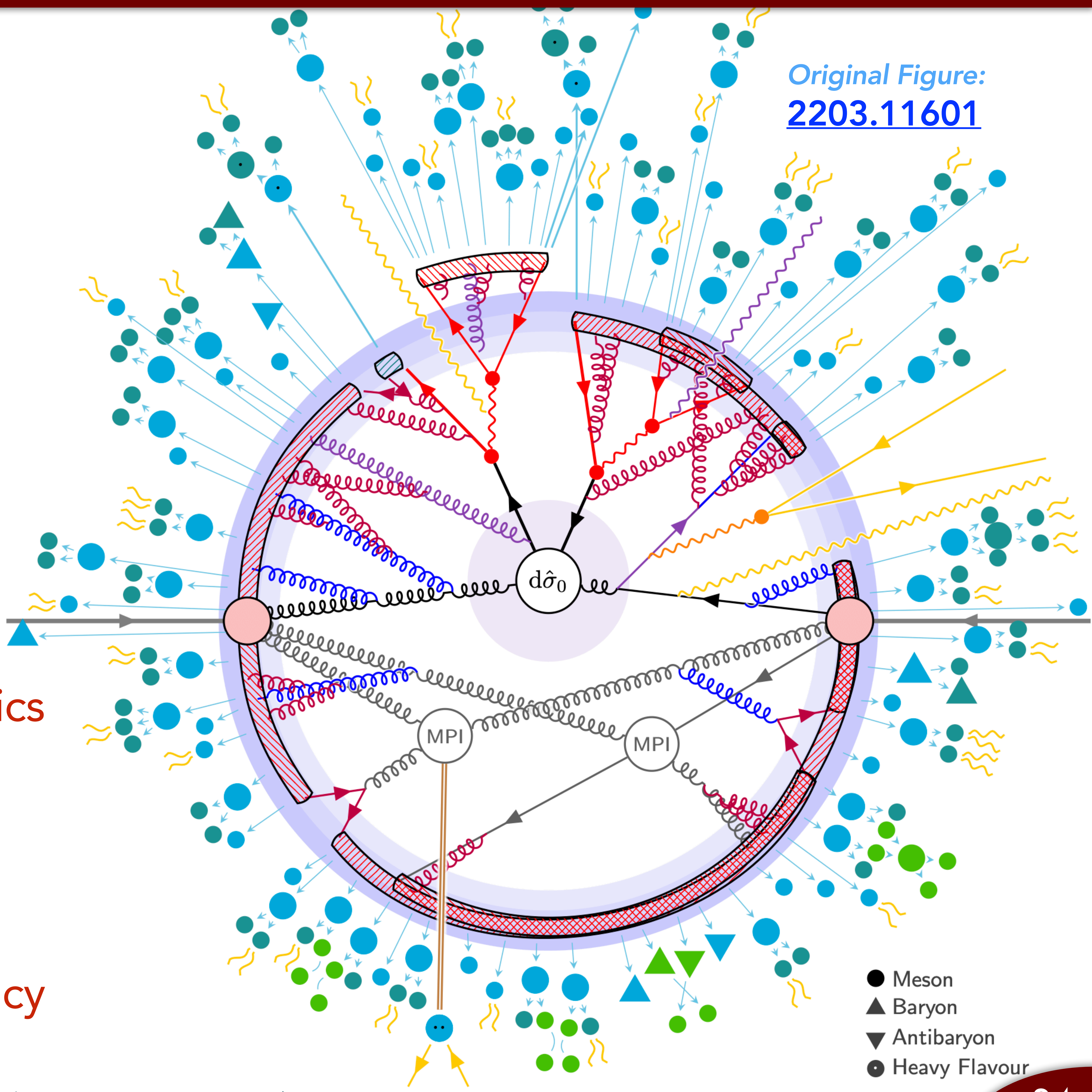


Much new work on non-perturbative physics

Driven by **new measurements** at LHC

+ expect NNLO+NNLL perturbative predictions in MCs ~ soon

➜ era of percent-level perturbative accuracy



Original Figure: 2203.11601

Extra Slides

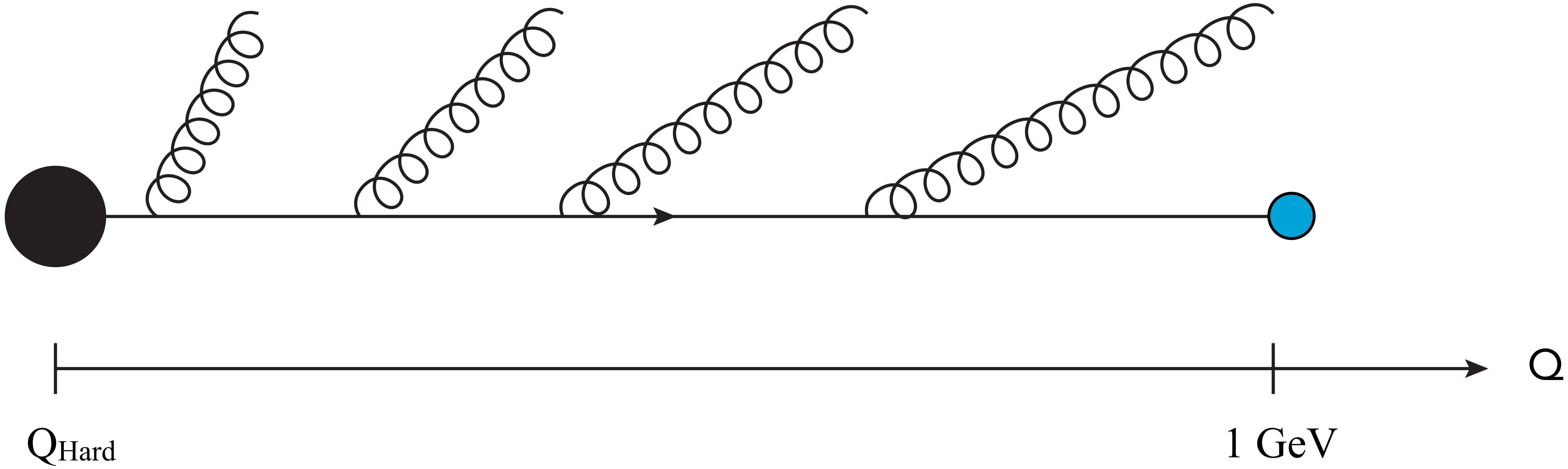
From **Partons** to **Pions**

Consider a parton emerging from a hard scattering (or decay) process

Hard:
Large momentum transfer
$Q_{\mathrm{Hard}} \gg 1\,\mathrm{GeV}$

It showers
(bremsstrahlung)

It ends up
at a low effective
factorization scale
$Q_{\mathrm{Hadronization}} \sim m_\rho \sim 1\,\mathrm{GeV}$

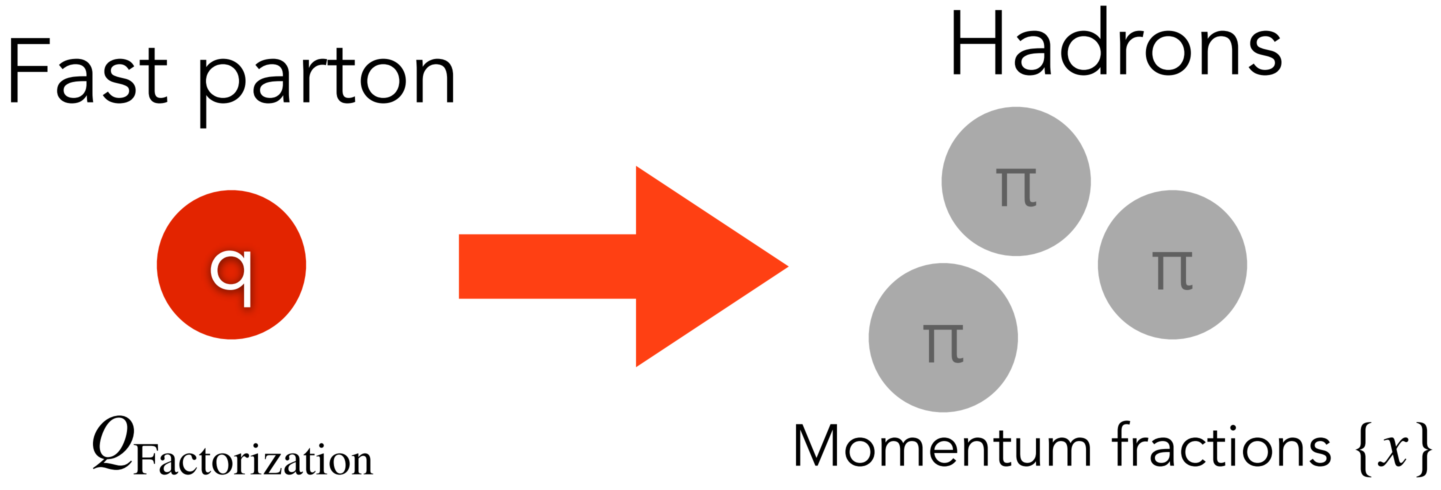


How about I just call it ~ a hadron?

→ "Local Parton-Hadron Duality"

Local Parton Hadron Duality ⟷ Independent Fragmentation

Local
Parton
Hadron
Duality

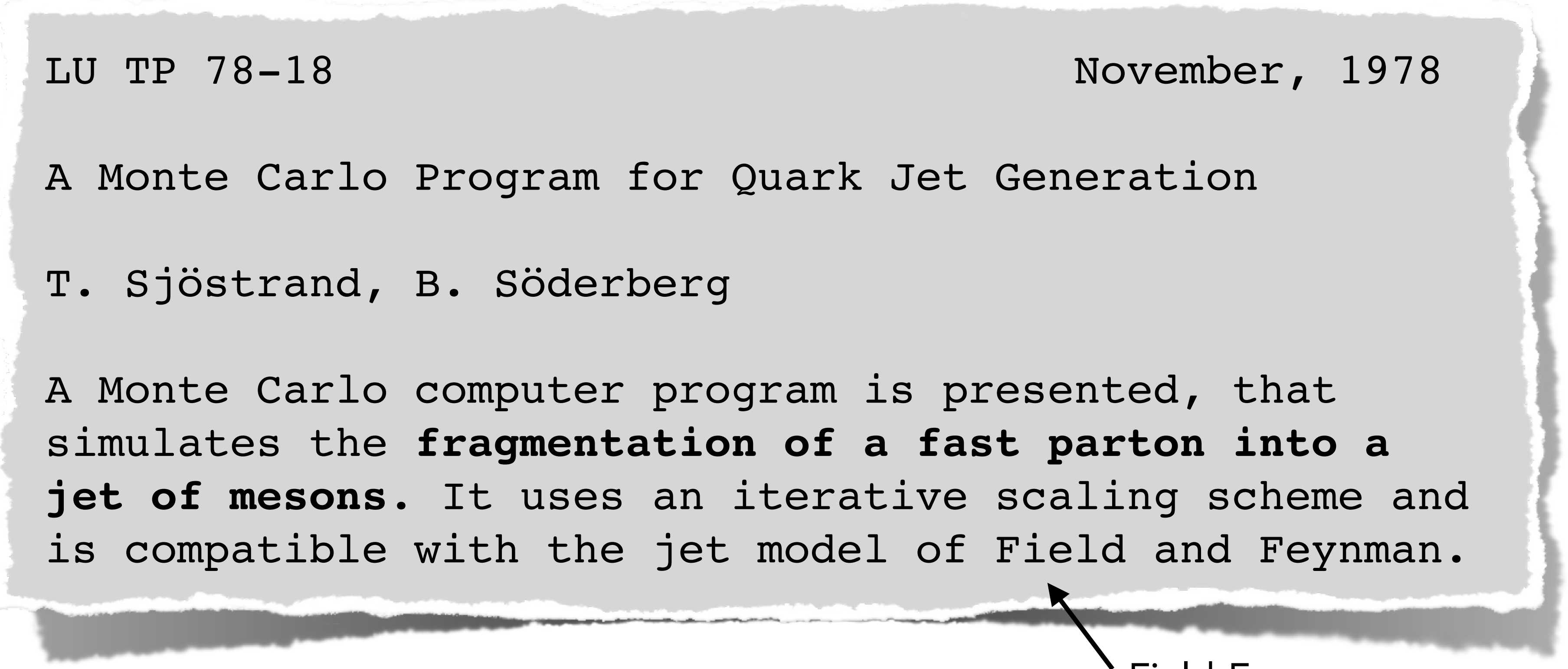


$$F_{\pi/q}(Q_F, x)$$

Fragmentation Function

Late 70s MC models: Independent Fragmentation

E.g., PYTHIA (then called JETSET) anno 1978



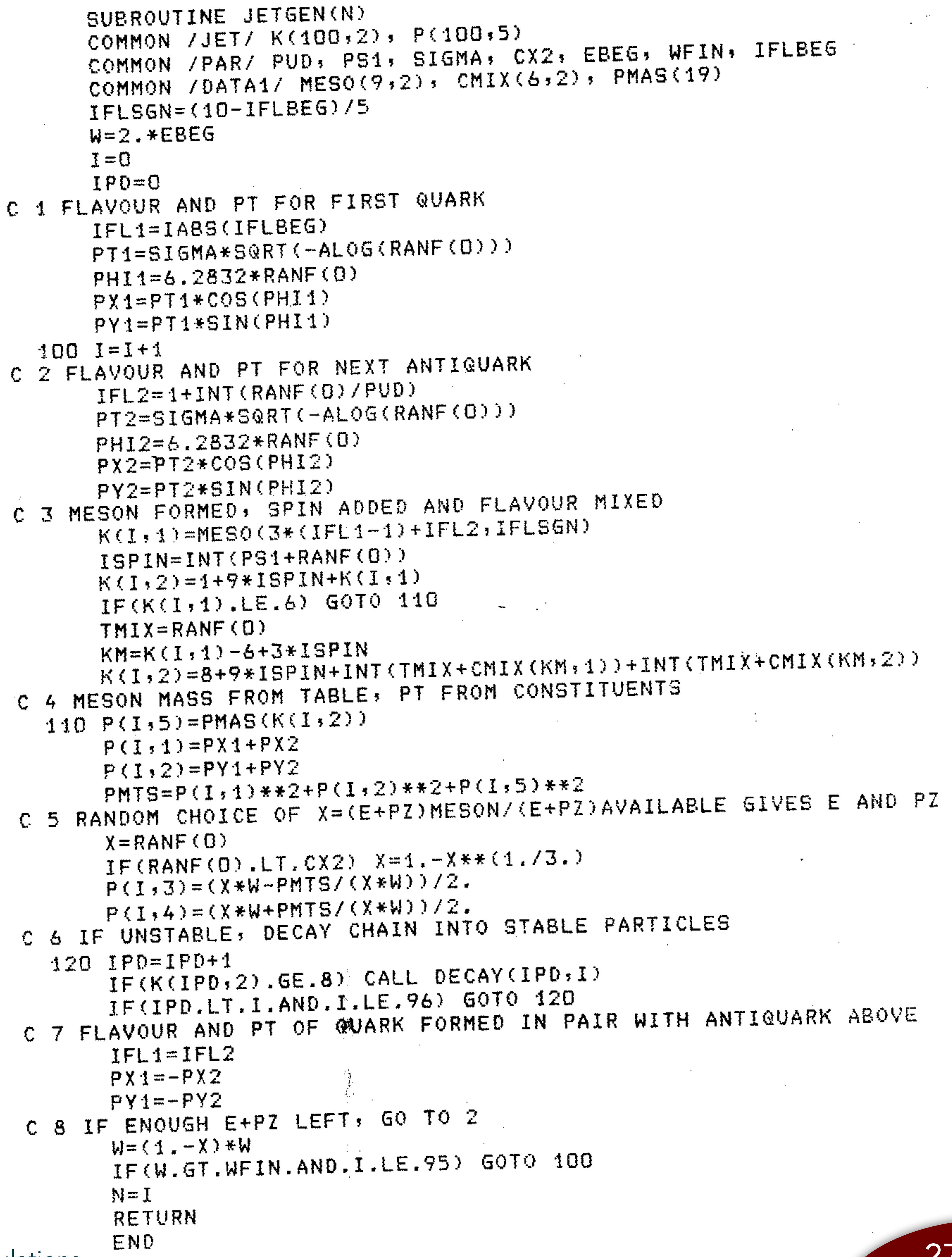
LU TP 78-18 November, 1978

A Monte Carlo Program for Quark Jet Generation

T. Sjöstrand, B. Söderberg

A Monte Carlo computer program is presented, that simulates the **fragmentation of a fast parton into a jet of mesons.** It uses an iterative scaling scheme and is compatible with the jet model of Field and Feynman.

Field-Feynman was an early fragmentation model.



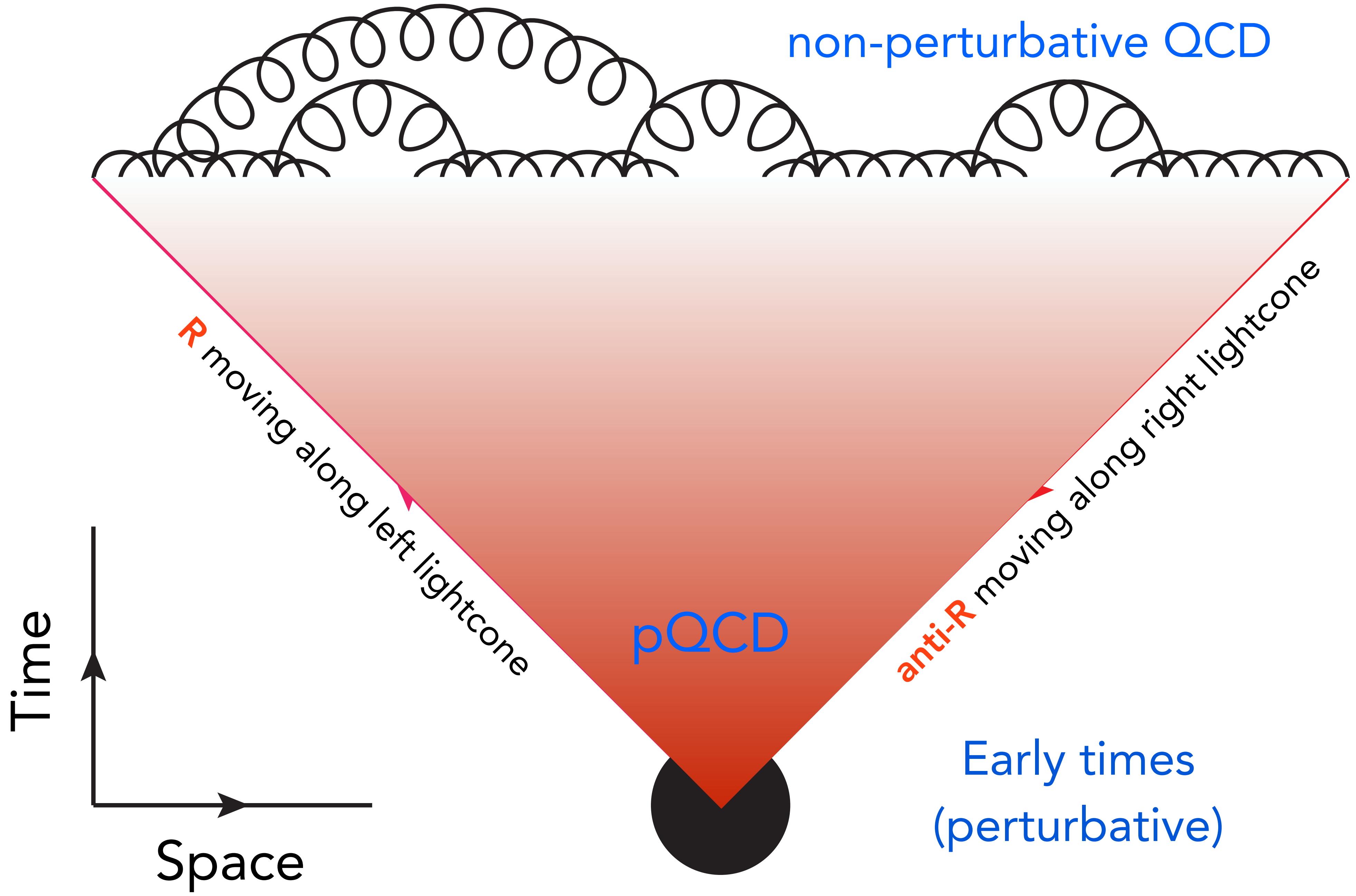
```
      SUBROUTINE JETGEN(N)
      COMMON /JET/ K(100,2), P(100,5)
      COMMON /PAR/ PUD, PS1, SIGMA, CX2, EBEG, WFIN, IFLBEG
      COMMON /DATA1/ MESO(9,2), CMIX(6,2), PMAS(19)
      IFLSGN=(10-IFLBEG)/5
      W=2.*EBEG
      I=0
      IPD=0
C 1 FLAVOUR AND PT FOR FIRST QUARK
      IFL1=IABS(IFLBEG)
      PT1=SIGMA*SQRT(-ALOG(RANF(0)))
      PHI1=6.2832*RANF(0)
      PX1=PT1*COS(PHI1)
      PY1=PT1*SIN(PHI1)
  100 I=I+1
C 2 FLAVOUR AND PT FOR NEXT ANTIQUARK
      IFL2=1+INT(RANF(0)/PUD)
      PT2=SIGMA*SQRT(-ALOG(RANF(0)))
      PHI2=6.2832*RANF(0)
      PX2=PT2*COS(PHI2)
      PY2=PT2*SIN(PHI2)
C 3 MESON FORMED, SPIN ADDED AND FLAVOUR MIXED
      K(I,1)=MESO(3*(IFL1-1)+IFL2,IFLSGN)
      ISPIN=INT(PS1+RANF(0))
      K(I,2)=1+9*ISPIN+K(I,1)
      IF(K(I,1).LE.6) GOTO 110
      TMIX=RANF(0)
      KM=K(I,1)-6+3*ISPIN
      K(I,2)=8+9*ISPIN+INT(TMIX+CMIX(KM,1))+INT(TMIX+CMIX(KM,2))
C 4 MESON MASS FROM TABLE, PT FROM CONSTITUENTS
  110 P(I,5)=PMAS(K(I,2))
      P(I,1)=PX1+PX2
      P(I,2)=PY1+PY2
      PMTS=P(I,1)**2+P(I,2)**2+P(I,5)**2
C 5 RANDOM CHOICE OF X=(E+PZ)MESON/(E+PZ)AVAILABLE GIVES E AND PZ
      X=RANF(0)
      IF(RANF(0).LT.CX2) X=1.-X**(1./3.)
      P(I,3)=(X*W-PMTS/(X*W))/2.
      P(I,4)=(X*W+PMTS/(X*W))/2.
C 6 IF UNSTABLE, DECAY CHAIN INTO STABLE PARTICLES
  120 IPD=IPD+1
      IF(K(IPD,2).GE.8) CALL DECAY(IPD,I)
      IF(IPD.LT.I.AND.I.LE.96) GOTO 120
C 7 FLAVOUR AND PT OF QUARK FORMED IN PAIR WITH ANTIQUARK ABOVE
      IFL1=IFL2
      PX1=-PX2
      PY1=-PY2
C 8 IF ENOUGH E+PZ LEFT, GO TO 2
      W=(1.-X)*W
      IF(W.GT.WFIN.AND.I.LE.95) GOTO 100
      N=I
      RETURN
      END
```

Colour Neutralisation

A **physical** hadronization model

Should involve at least **two** partons, with opposite colour charges

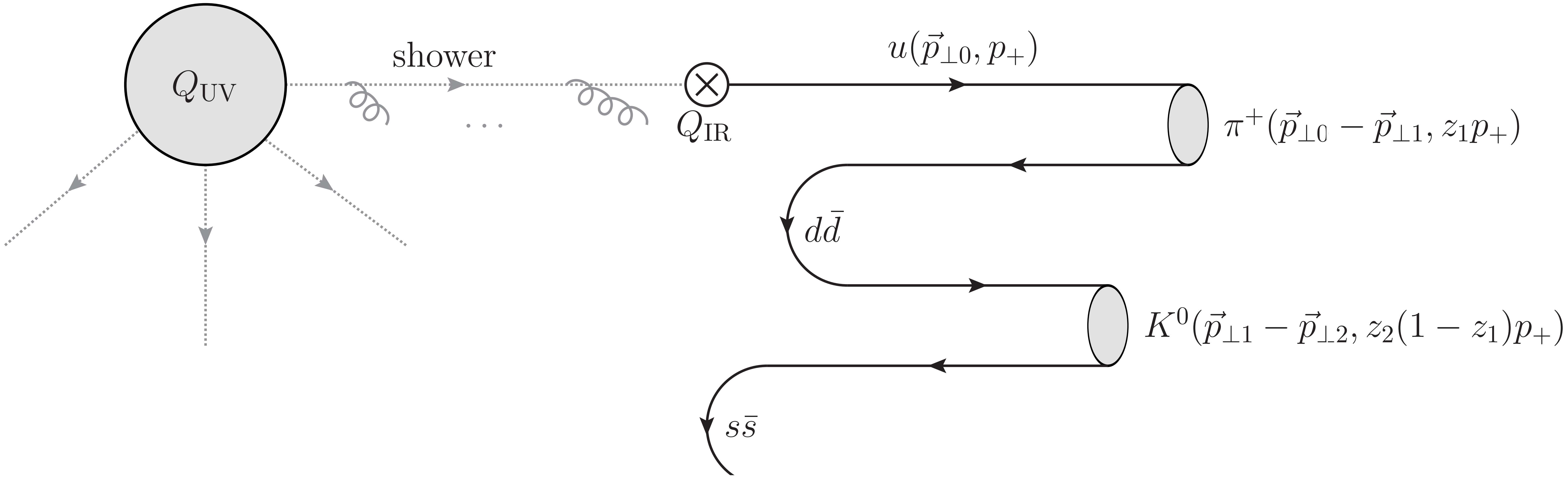
A strong **confining field** emerges between the two when their separation ≳ 1fm



Iterative String Breaks

Causality → May iterate from outside-in

Note: using light-cone coordinates: $p_+ = E + p_z$



On average, expect energy of n^{th} "rank" hadron ~ $E_n \sim \langle z\rangle^n E_0$

Fragmentation of String Junction Systems

Assume vortex-line string picture still OK

Which topology? Y, Δ, V, T, …?

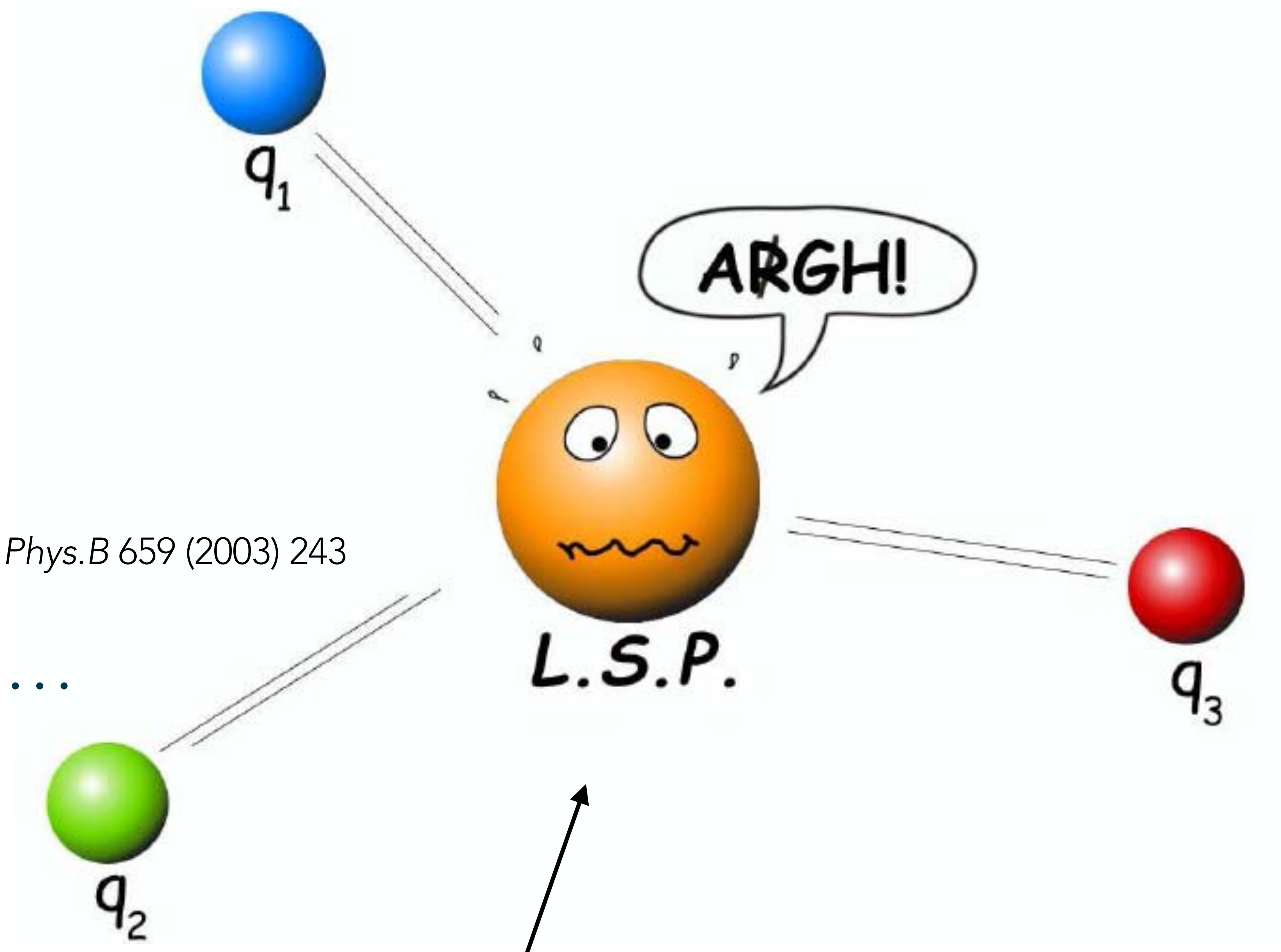
Baryon wave functions & minimal string length

⟹ Picture of Y-shaped topology with "string junction"

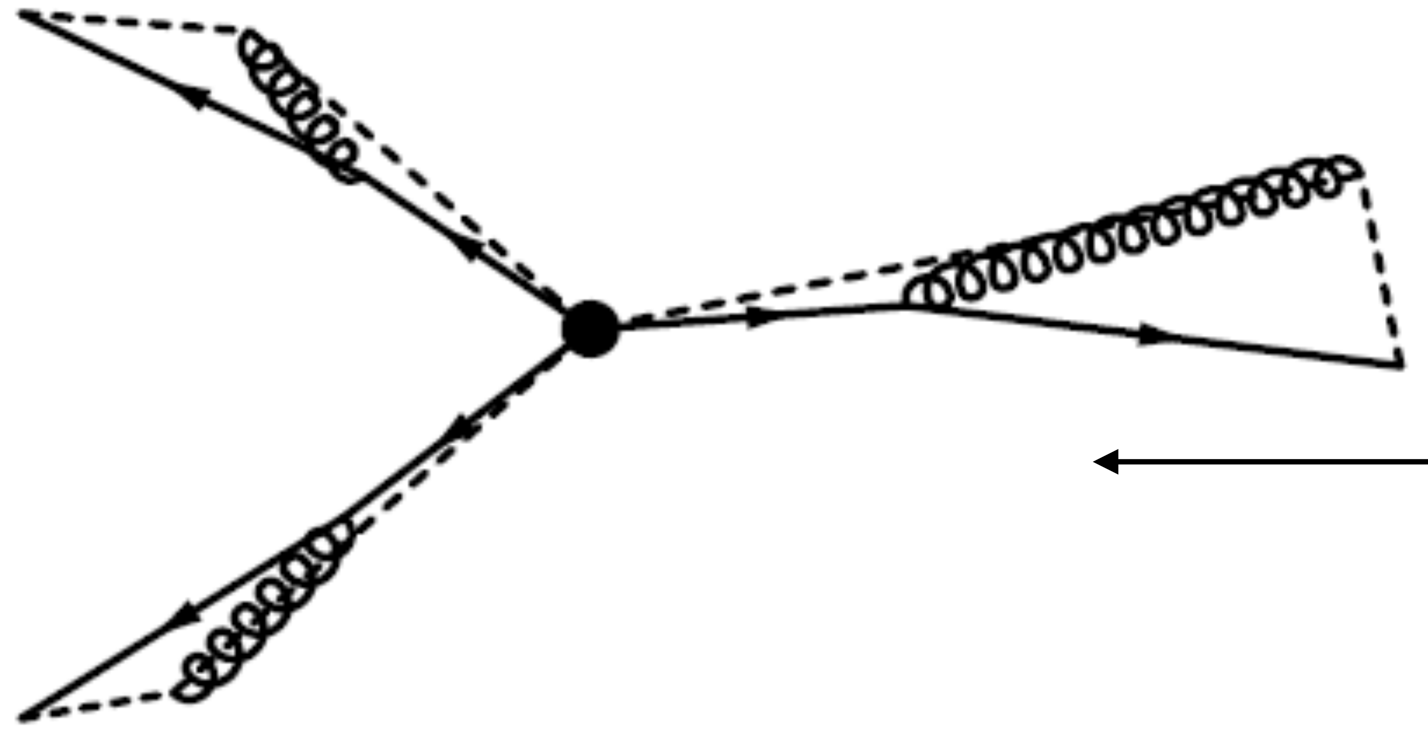
1st String-Junction Fragmentation Model Sjöstrand & **PS**, *Nucl.Phys.B* 659 (2003) 243

Focused on hard BNV processes: $\tilde{\chi} \to q_i q_j q_k,\ \tilde{t}_i^* \to q_j q_k,\ \ldots$

Fun (but a bit of a long shot …)



(Junction strings can also have kinks):



Would love to tell you ***this*** has been seen at LHC

But then you probably wouldn't be hearing about it from me

However, **string junctions** *may* have been seen!

Predicting the Junction Baryon Spectrum

The Junction Baryon = smoking gun of String Junctions

Predicting the movement of the string junction is crucial!

To make solid predictions for Junction Baryon spectra, we use a trick: Sjöstrand & **PS**, *Nucl.Phys.B* 659 (2003) 243

Find the Lorentz frame in which the string **junction is at rest (JRF)**

Inverse boost (+ $\mathcal{O}(\Lambda_{\mathrm{QCD}})$ kicks) $\Longrightarrow$ junction baryon spectrum

Junction = Topological Feature of Confinement Field

$V(r) = \kappa r$

$\Longrightarrow$ each "leg" (string piece) acts on the other two with **constant force**

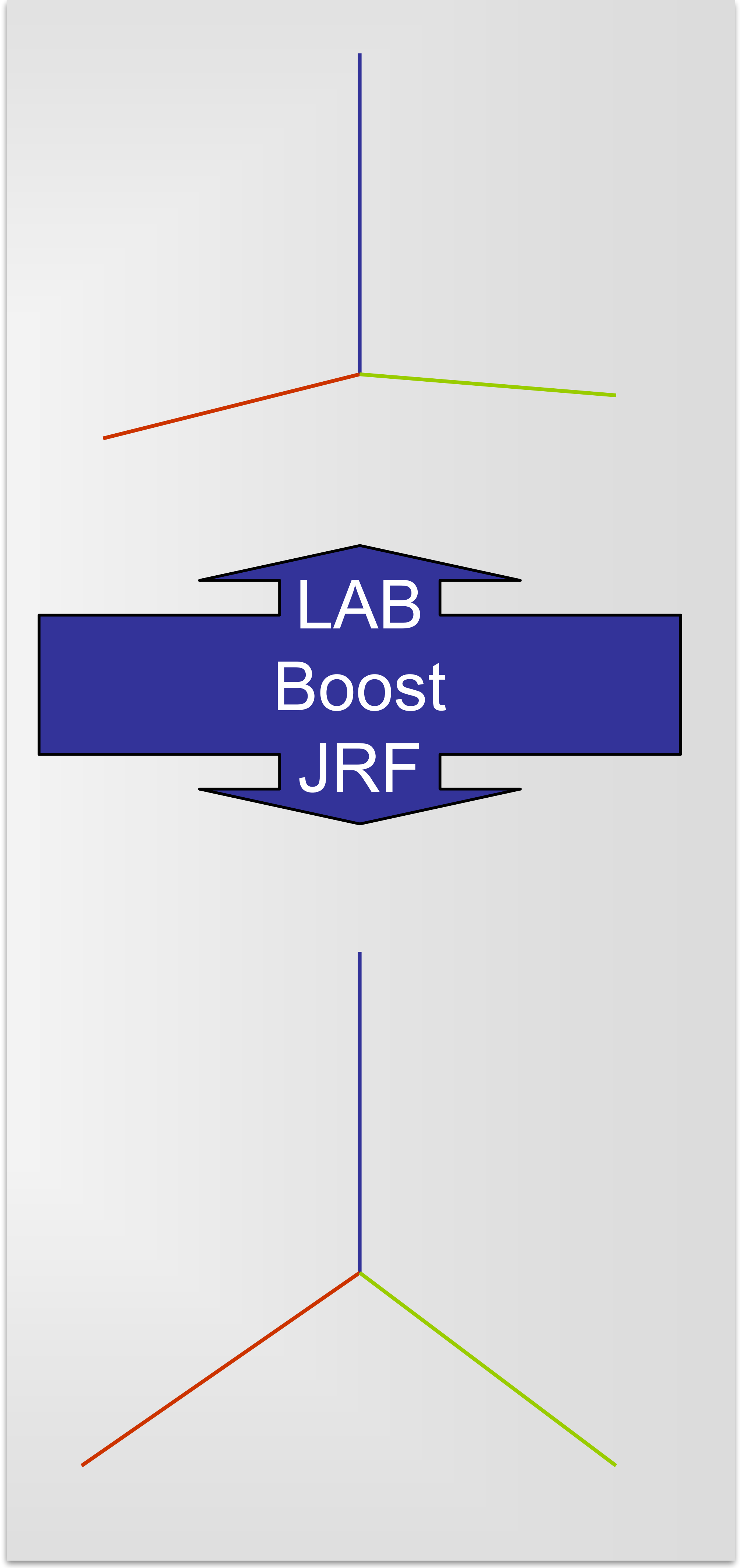
$\vec{F} = \kappa \vec{e}_r$.

$\Longrightarrow$ In "Mercedes Frame", the angle is $120°$ between the legs

Massless legs: exact solution. **Mercedes Frame = Junction Rest Frame (JRF).**

Massive legs (eg heavy flavours or ones with lots of kinks!) => Iterative algorithm.

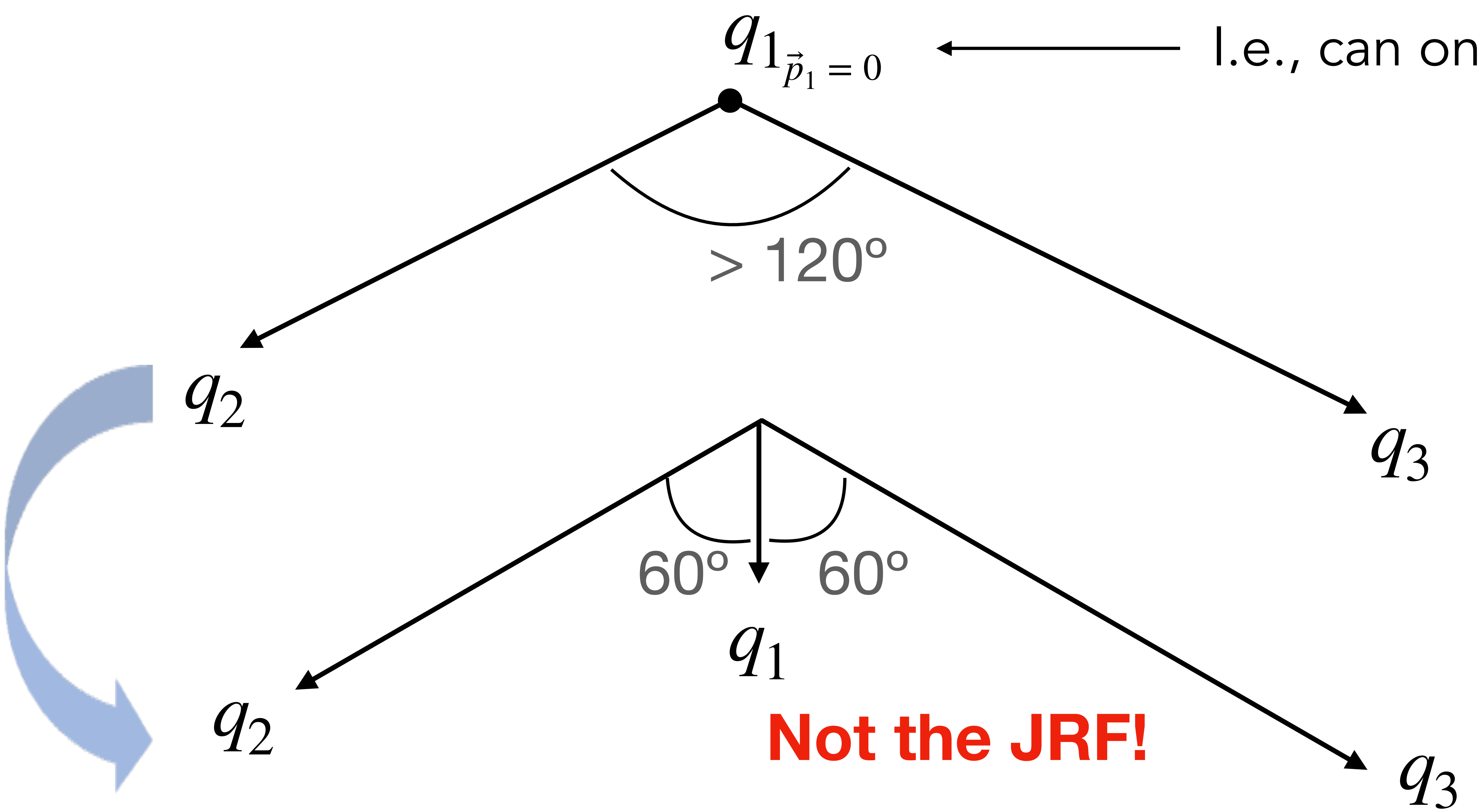
But org algorithm often broke down (failed to converge) for "soft legs"



Does a Boost to the Mercedes Frame Always Exist?

Consider the following kinematic case

In the **rest frame of one of the partons**, and the angle between the other two is **greater than 120 degrees** (not considered in org algorithmic implementation)



I.e., can only happen for massive partons

Not the JRF!

Org algorithm failed to converge

Slide adapted from J. Altmann

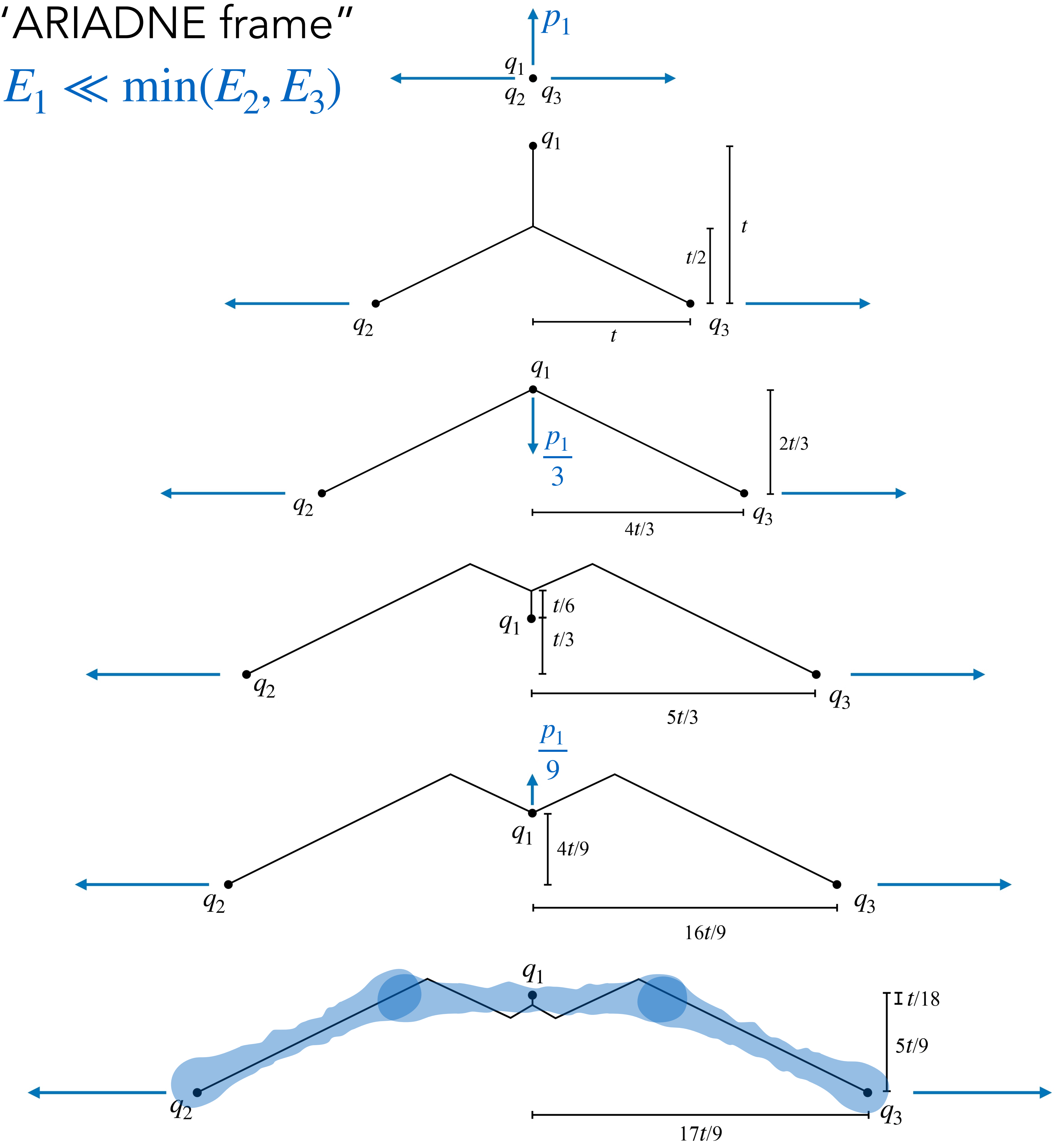
NEW

The case of a **heavy slow endpoints**: Pearl on a String

String Motion: Soft Massless Case

"ARIADNE frame"

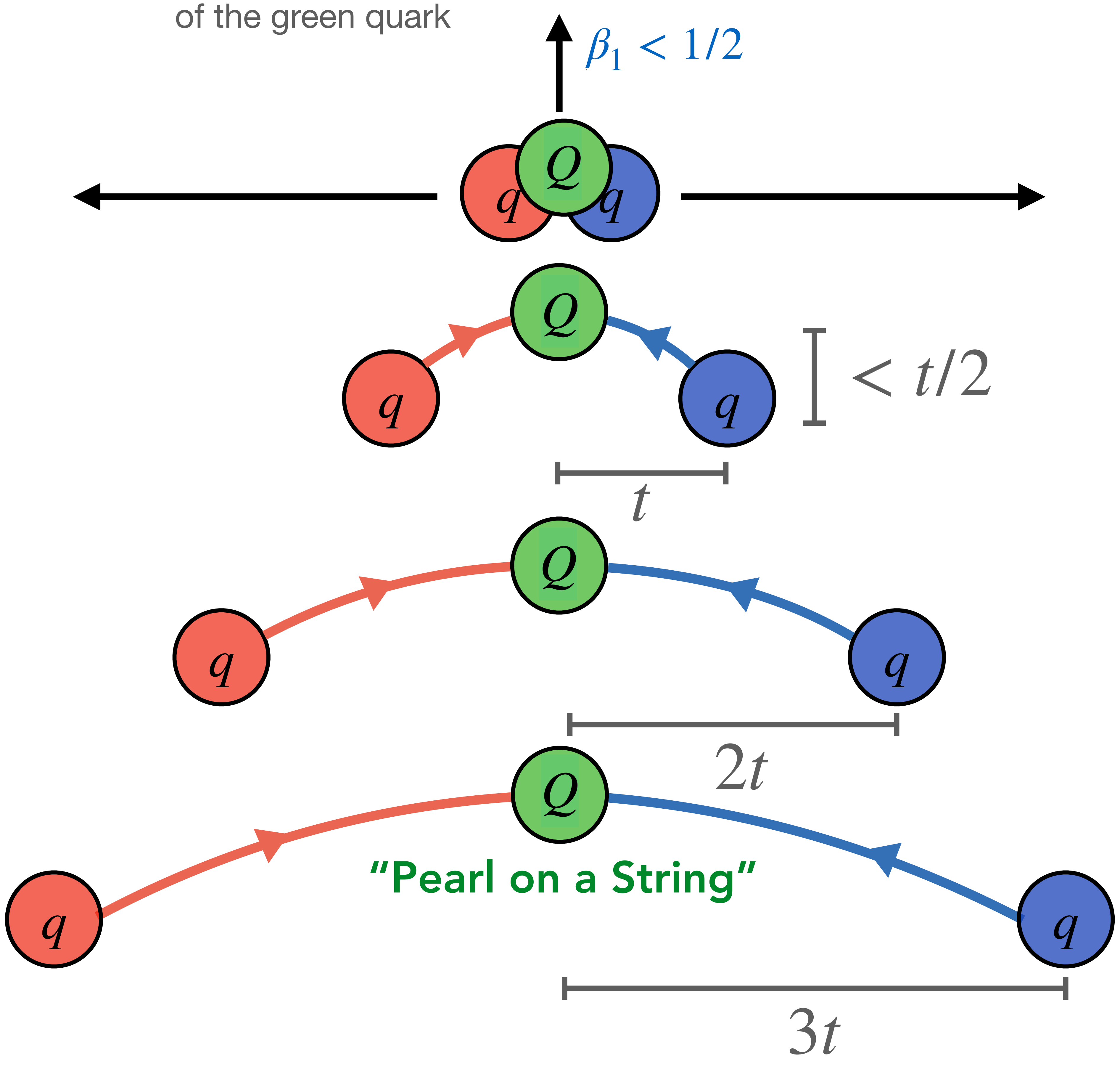
$E_1 \ll \min(E_2, E_3)$



Similar to a mesonic string with a gluon kink

String Motion: Slow Massive Case

Example of pearl-on-a-string viewed in the Ariadne frame of the green quark



"Pearl on a String"

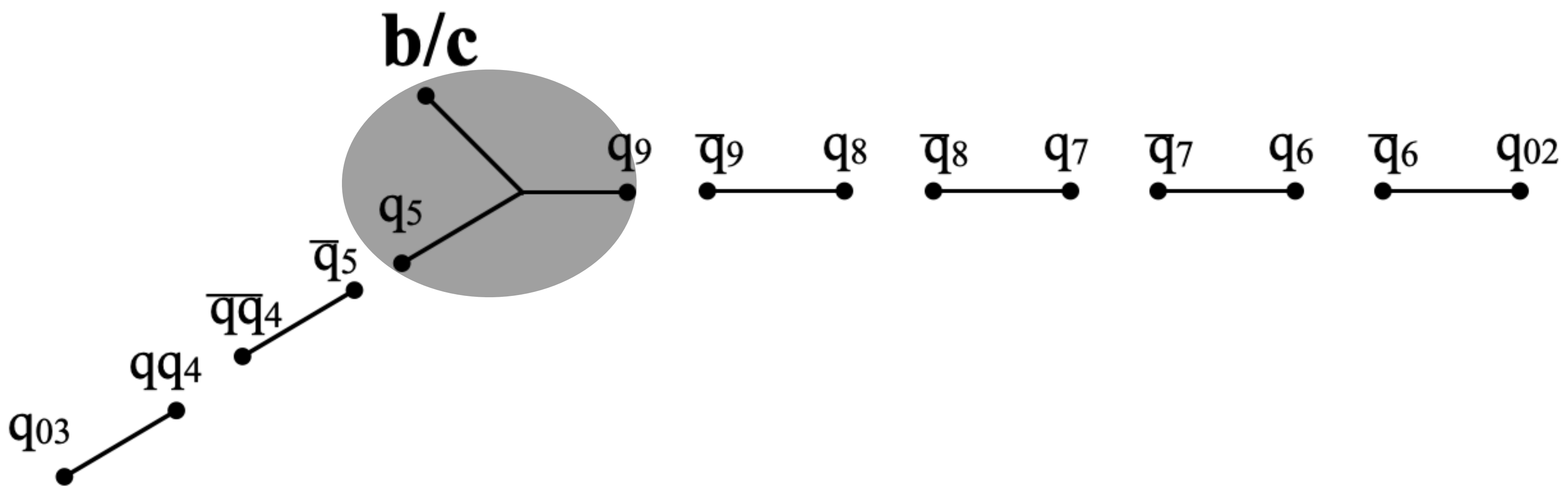
With thanks to G. Gustafson. Slide adapted from J. Altmann

New: the case of a **heavy slow endpoint**: **Pearl on a String**

The **junction gets "stuck"** to the soft quark, which we call a **pearl-on-a-string**

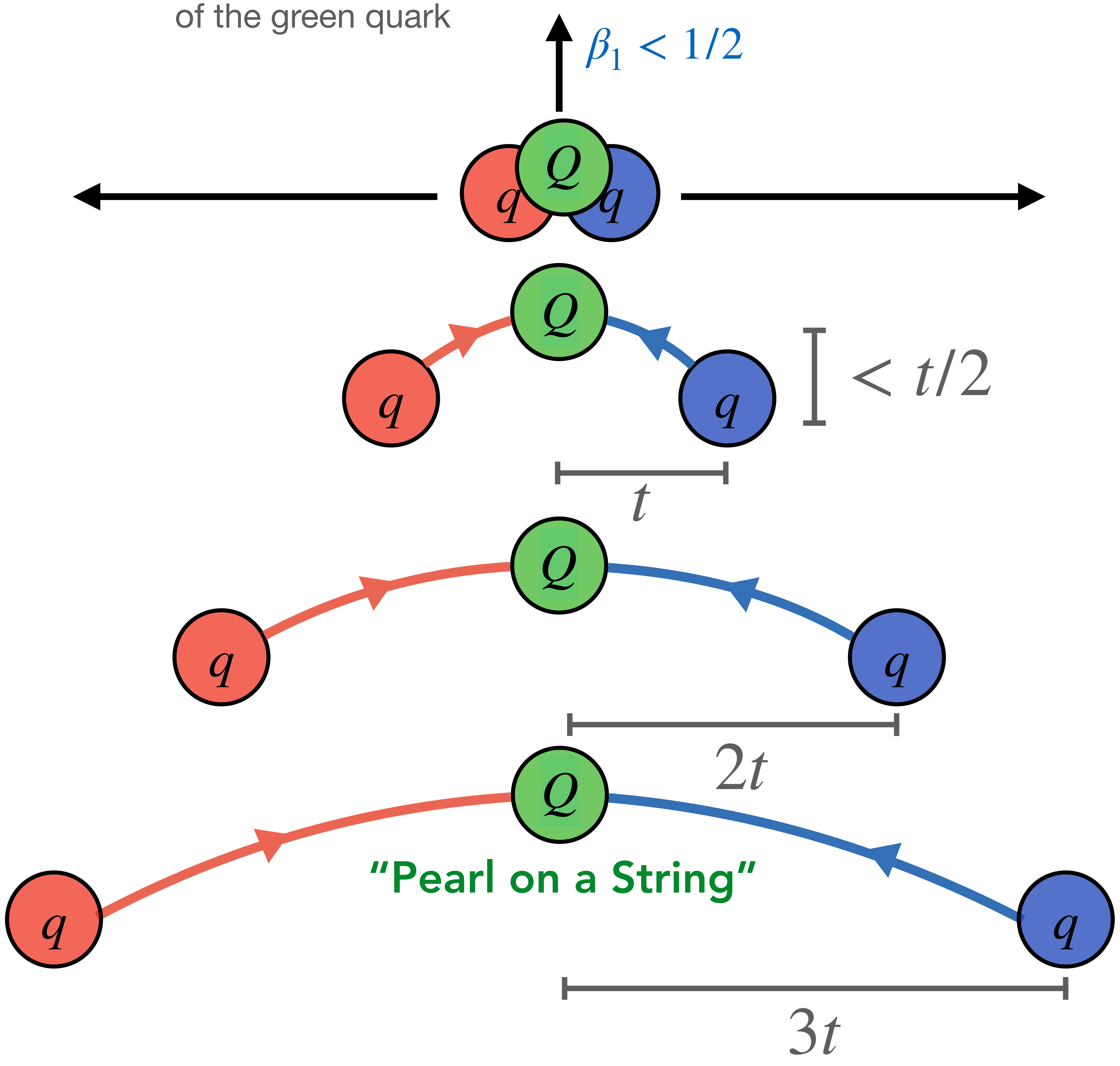
More likely to occur for junctions with heavy flavour endpoints

For a string junction to make a **heavy baryon**, the junction leg with the heavy quark can't "break" (*i.e.* a "soft" junction leg) = **pearl-on-a-string!**



String Motion: Slow Massive Case

Example of pearl-on-a-string viewed in the Ariadne frame of the green quark



"Pearl on a String"

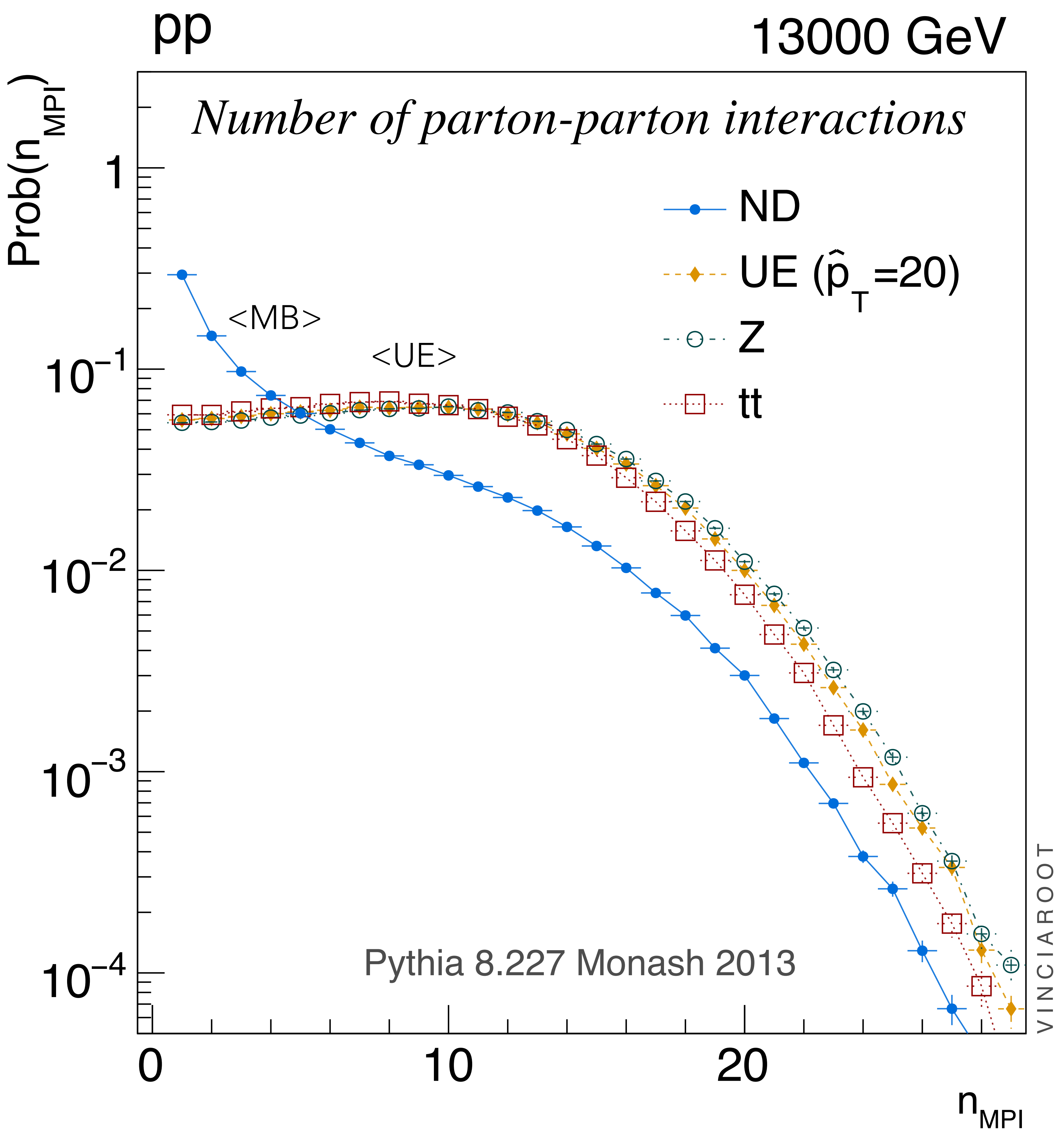
Slide adapted from J. Altmann

How many MPI are there? *

Example for pp collisions at 13 TeV — PYTHIA's default MPI model

Averaged over all pp impact parameters

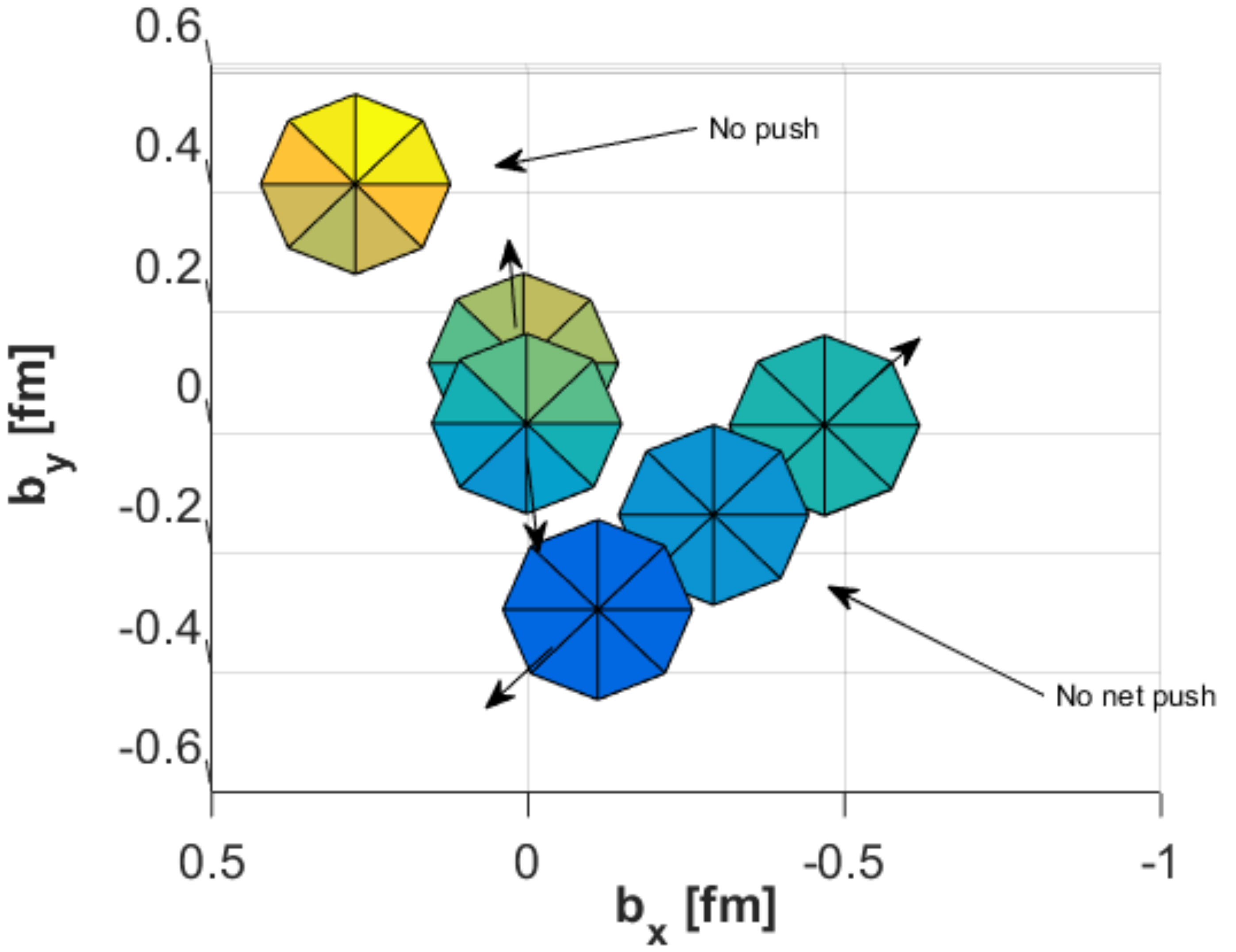
(Really: averaged over all pp overlap enhancement factors)



*note: can be arbitrarily soft

Collective Flow in PYTHIA: *String Shoving*

Bierlich, Chakraborty, Gustafson, Lönnblad, arXiv:1710.09725, 2010.07595



Strings should push each other transversely

Colour-electric fields ➜ Classical force

Model string radial shape & shoving physics

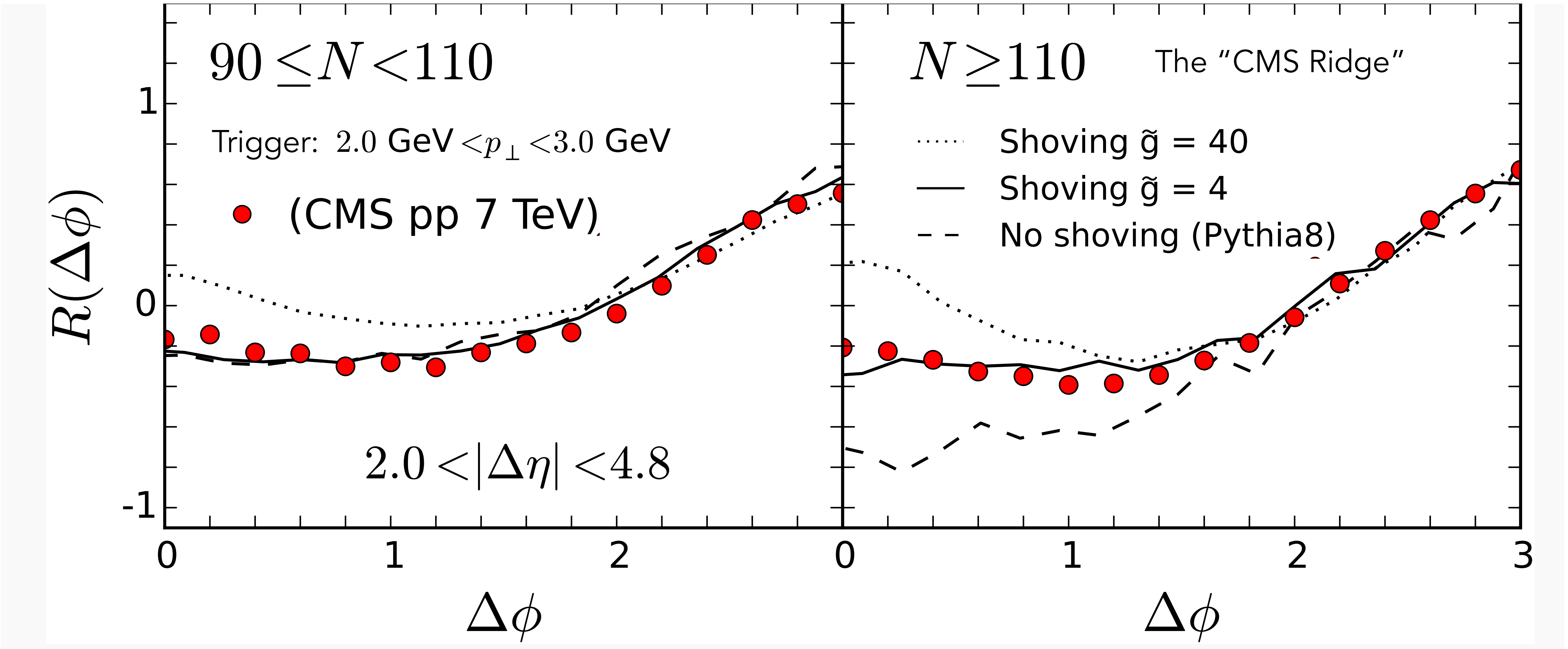
$$\Longrightarrow \text{force} \quad f(d_\perp) = \frac{g\kappa d_\perp}{R^2}\exp\left(-\frac{d_\perp^2}{4R^2}\right)$$

g: fraction of energy in chromo-electric field (as opposed to in condensate or magnetic flux)

$d_\perp$: transverse distance (in string-string "shoving frame")

R: string radius

κ: string tension ~ $1\,\mathrm{GeV/fm}$



CMS 1009.4122. Also: ATLAS 1906.08290, ALICE 2101.03110