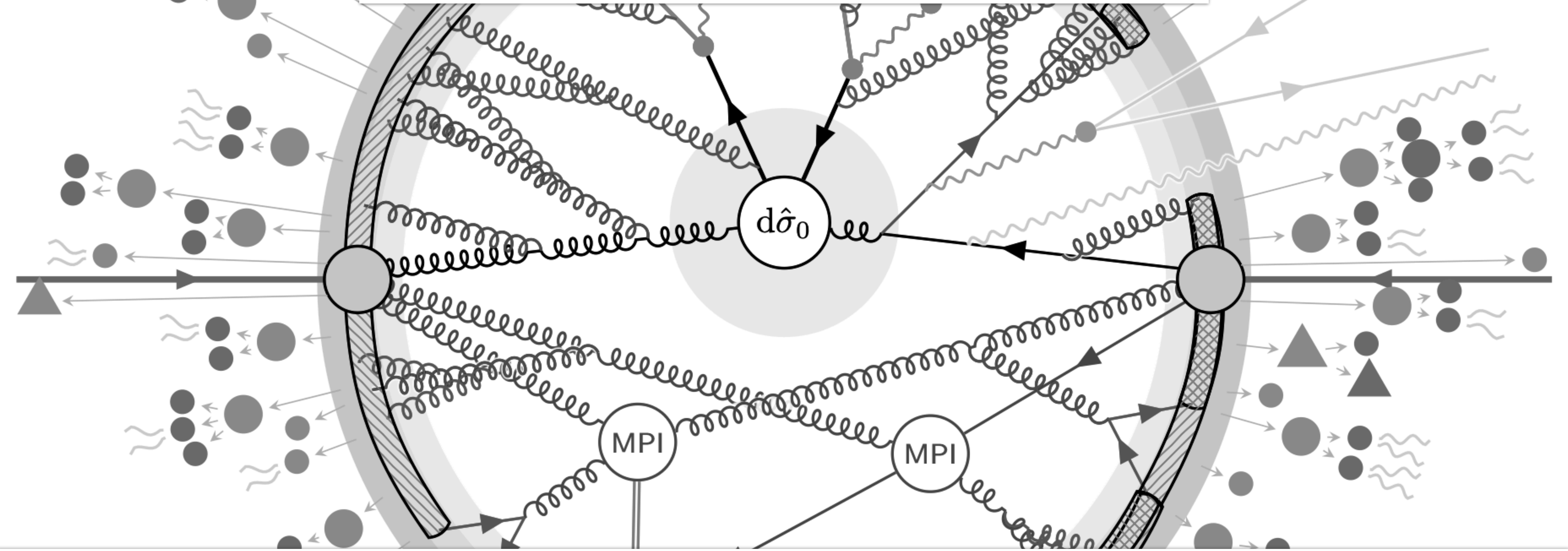
Modelling of LHC Collisions in PYTHIA
Physics and Uncertainties

Peter Skands — University of Oxford & Monash University



Overview

Introduction: The structure of LHC collisions (in PYTHIA)

Recent Studies (focus on SM precision environments ↔ BSM backgrounds)

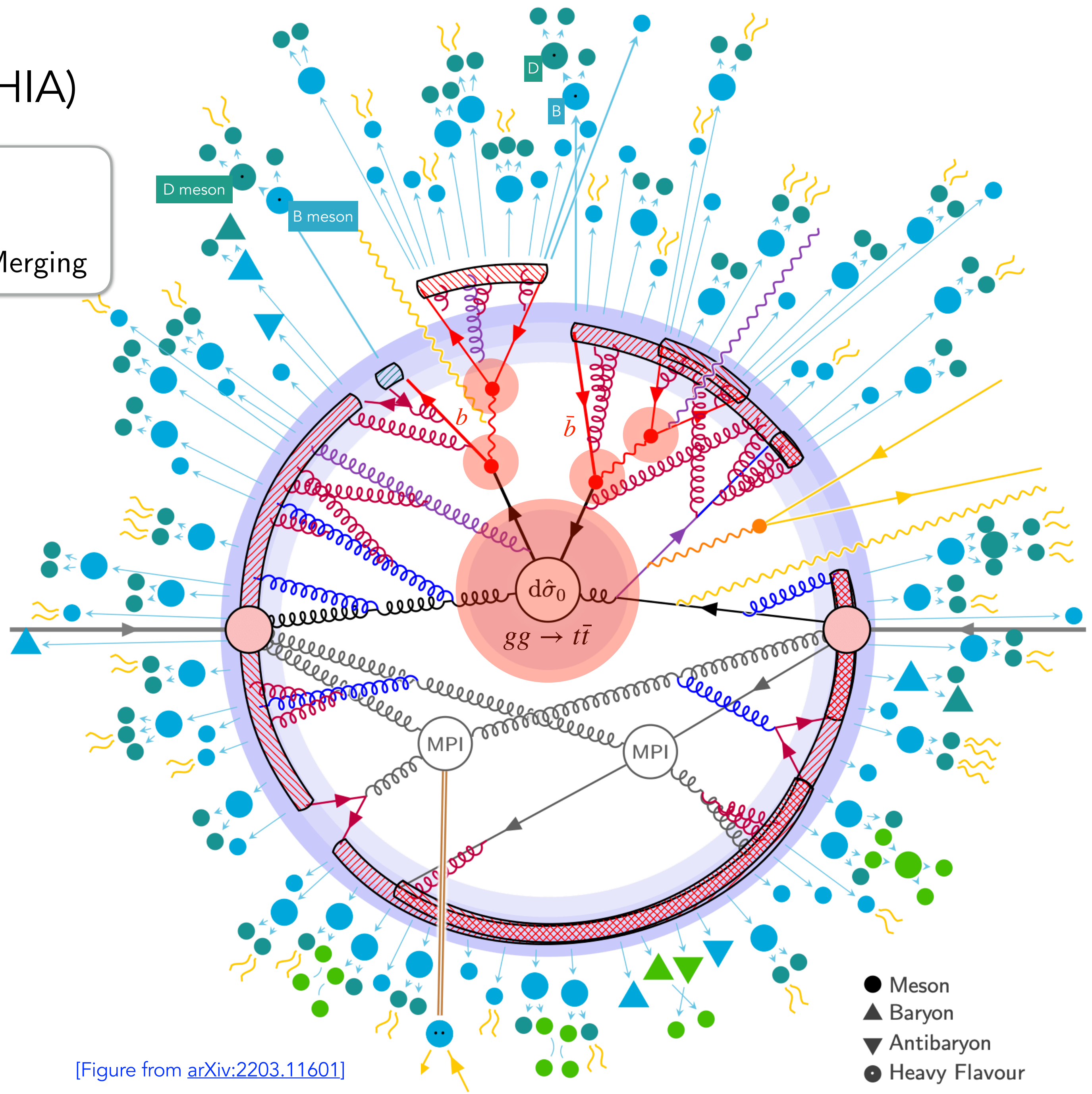
1. **NLO** Matching Systematics with POWHEG-Box *(examples: VBF, $t\bar{t}$)*
2. From NLO to **NNLO** *(examples: $t\bar{t}$, V, H, VH, VV, …)*
3. The computational bottleneck in **ME merging** *(example: V+jets)*
4. New Discoveries in **Hadronization** *(examples: HF baryons, JES)*

NB: want to address/explain state of the art & systematics in real contexts → a bit theory heavy

An LHC collision (in PYTHIA)

Hard Process

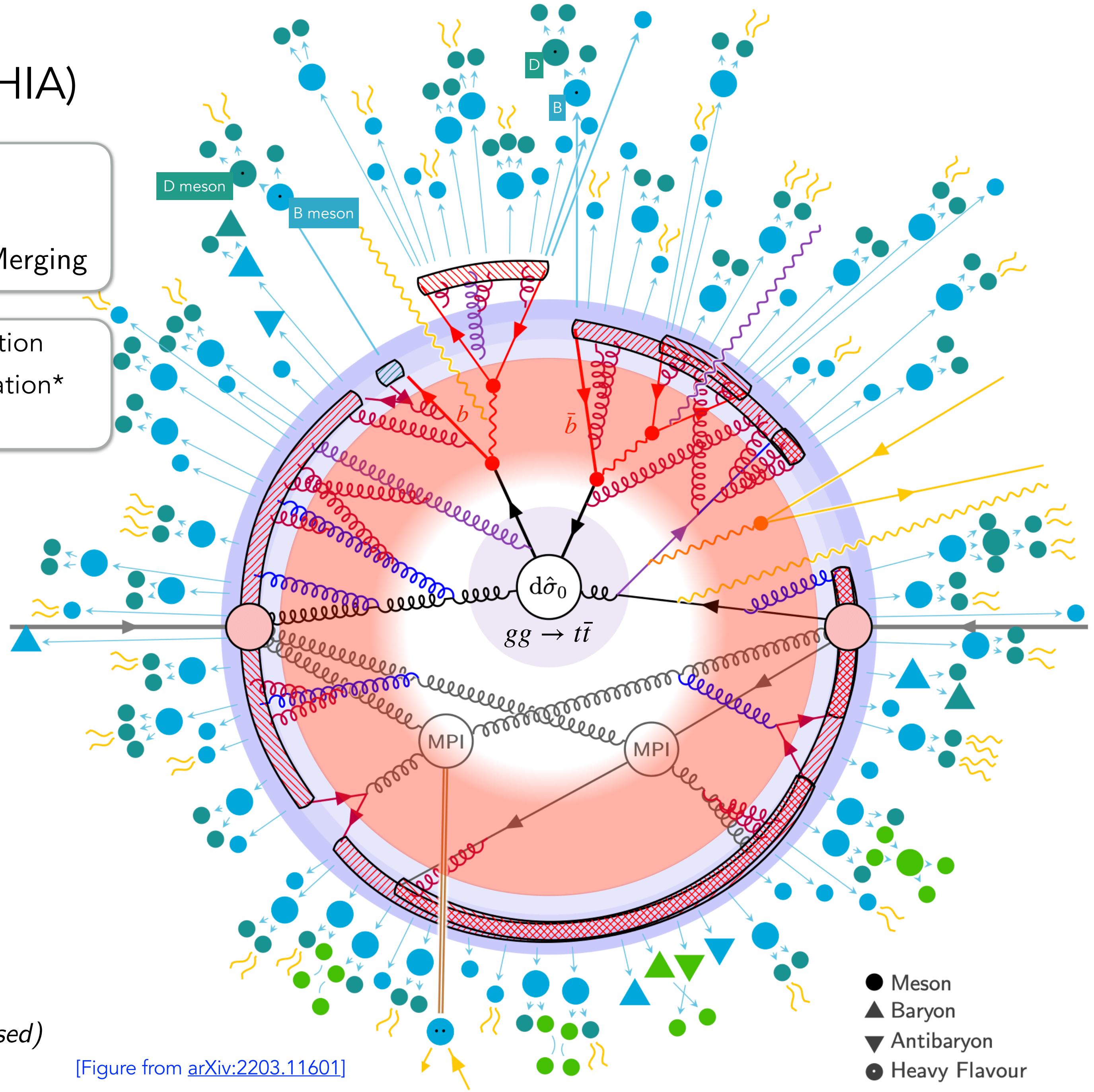
- ◯ Hard Interaction
- ● Resonance Decays
- ■ MECs, Matching & Merging



[Figure from arXiv:2203.11601]

An LHC collision (in PYTHIA)

Hard Process	◯ Hard Interaction ● Resonance Decays ■ MECs, Matching & Merging	
Parton Showers	■ QCD Final-State Radiation ■ QCD Initial-State Radiation* ■ Electroweak Radiation	



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- ○ Multiparton Interactions
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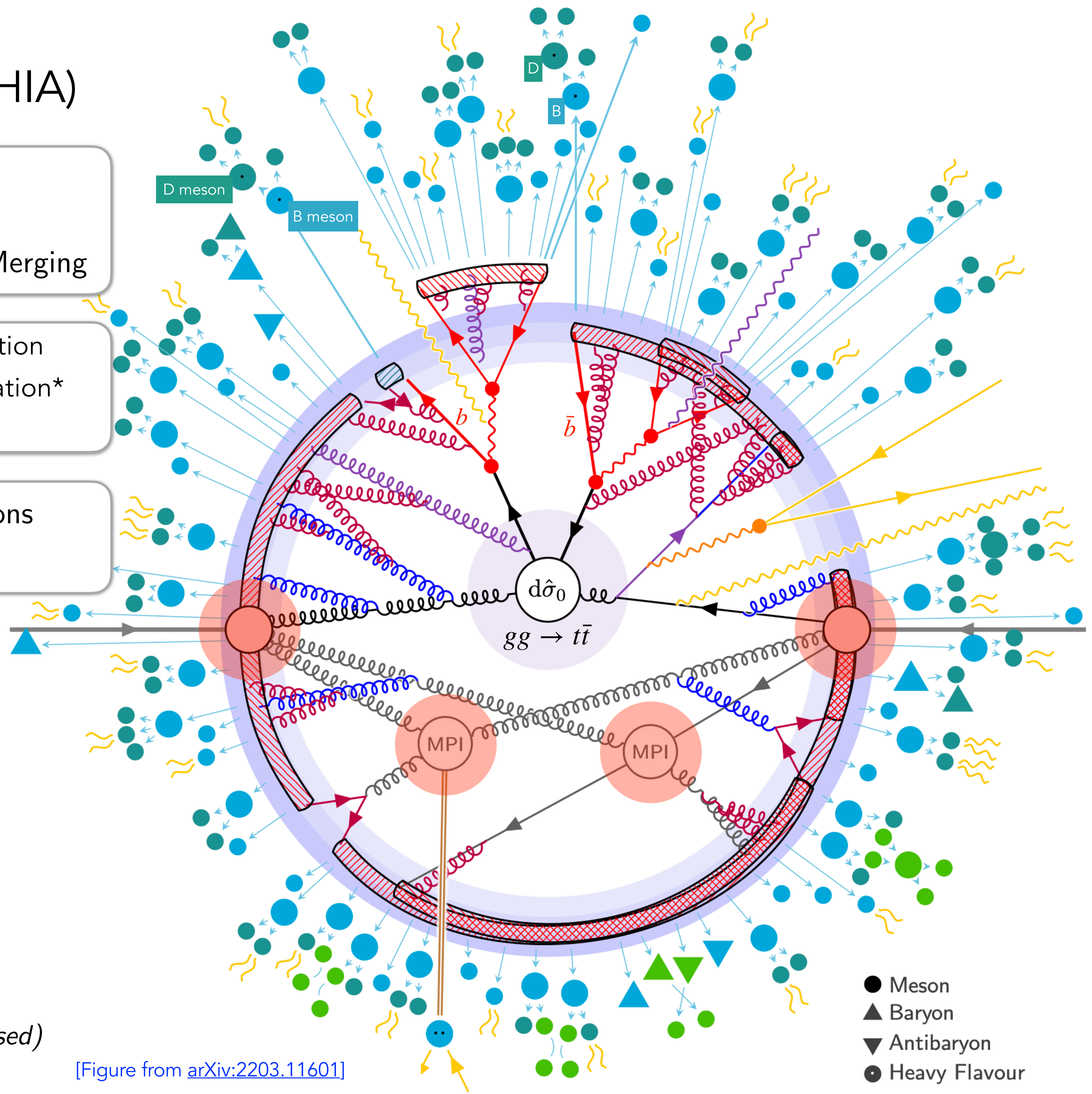

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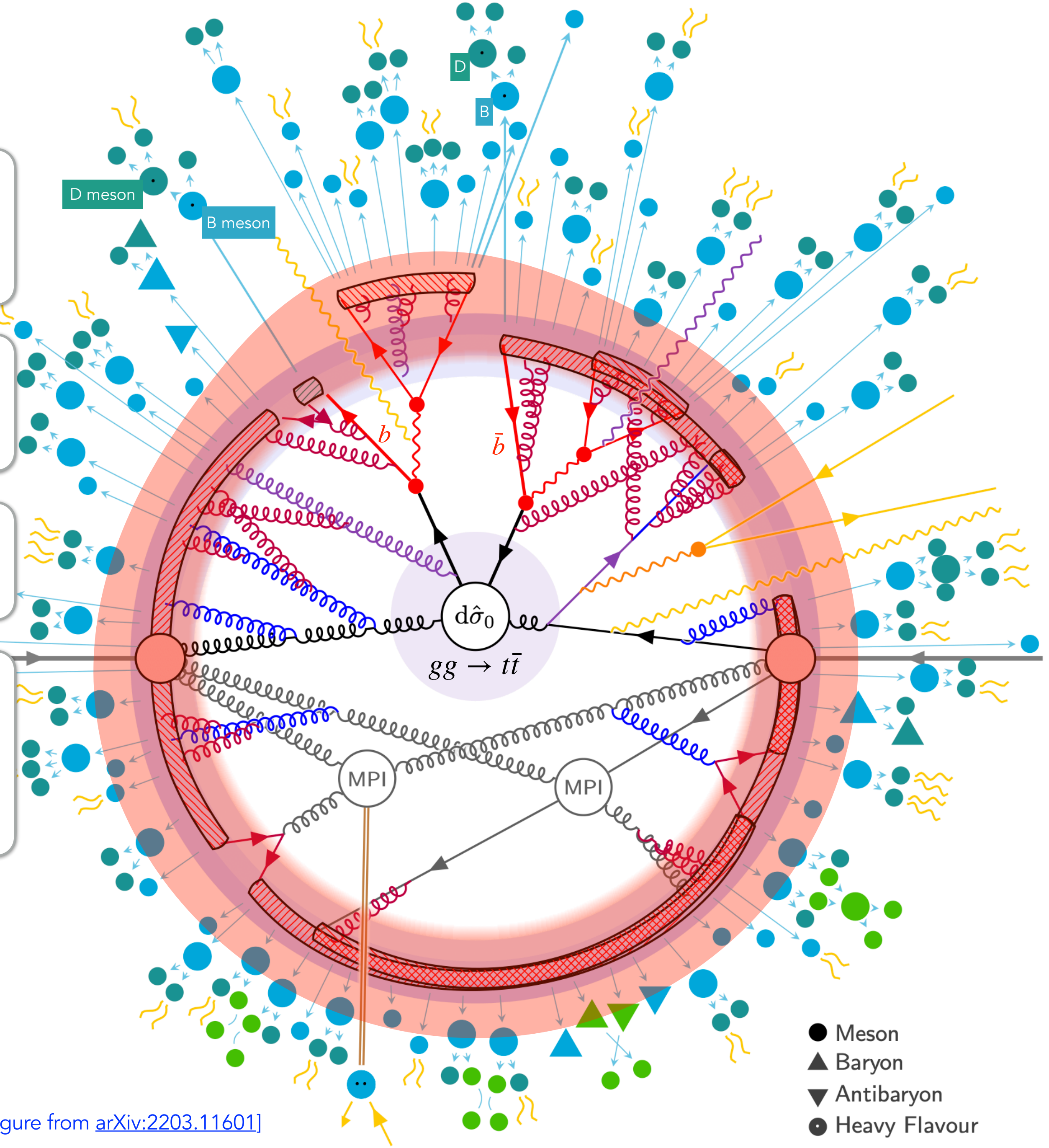
Hadronization
- Strings
- Colour Reconnections
- String Interactions
- Bose-Einstein & Fermi-Dirac



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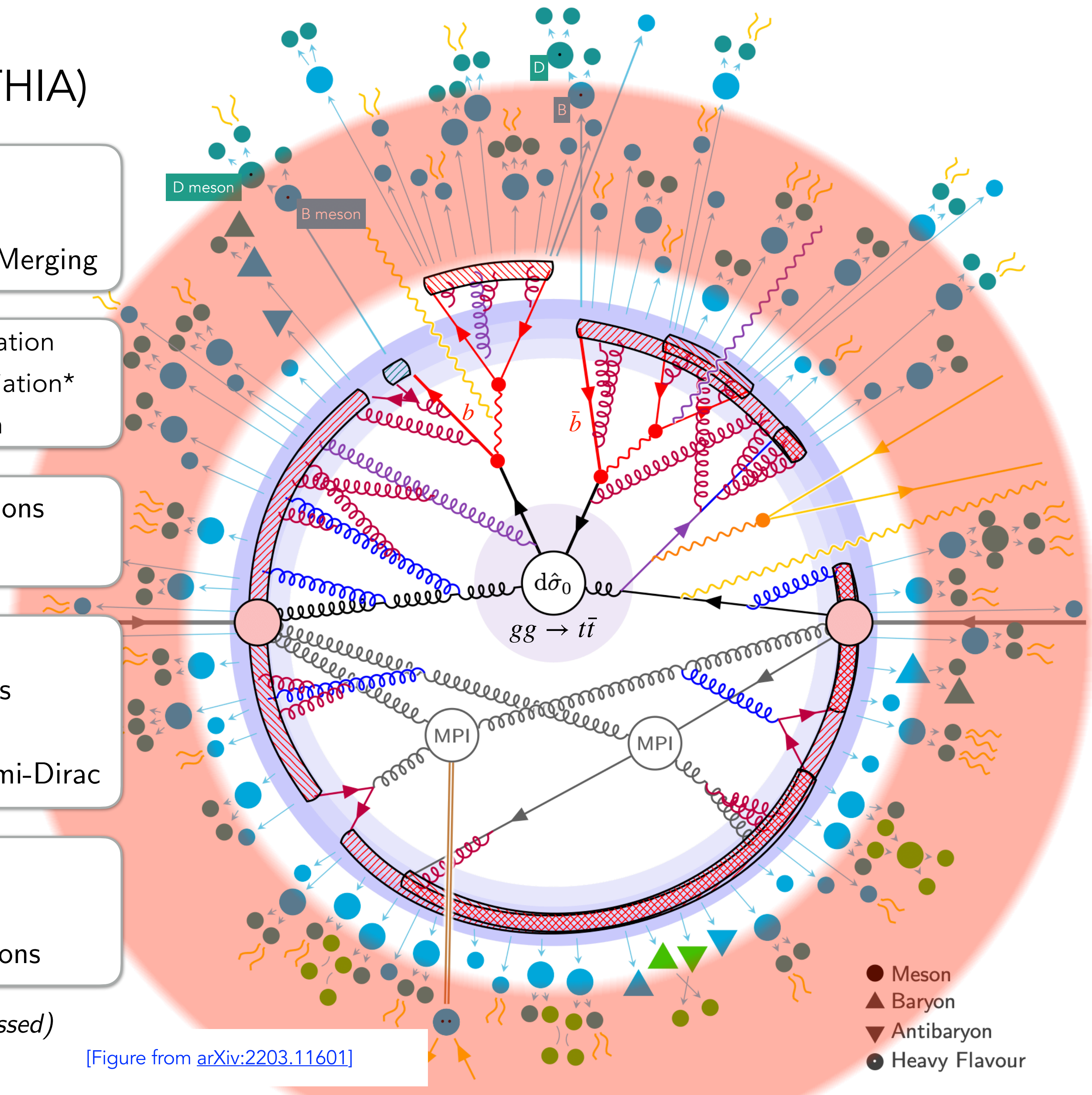
Hadron (& τ) Decays	■ Primary Hadrons ■ Secondary Hadrons ■ Hadronic Reinteractions	

(: incoming lines are crossed)*



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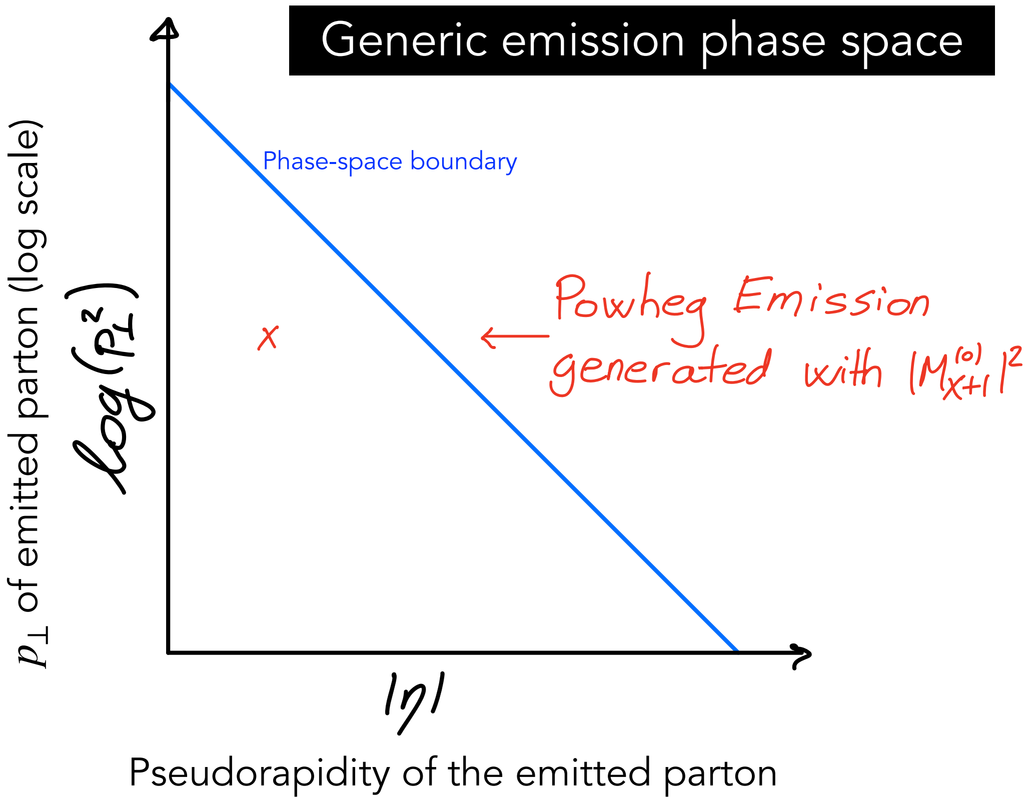
1. NLO Radiation in POWHEG

Generate hardest emission with (exact) tree-level matrix element $|M^{(0)}_{X+1}|^2$

(instead of with approximate parton-shower kernel)

Arbitrary Hard Process

Superscript (0) means tree level



1. Radiation in POWHEG — in a nutshell

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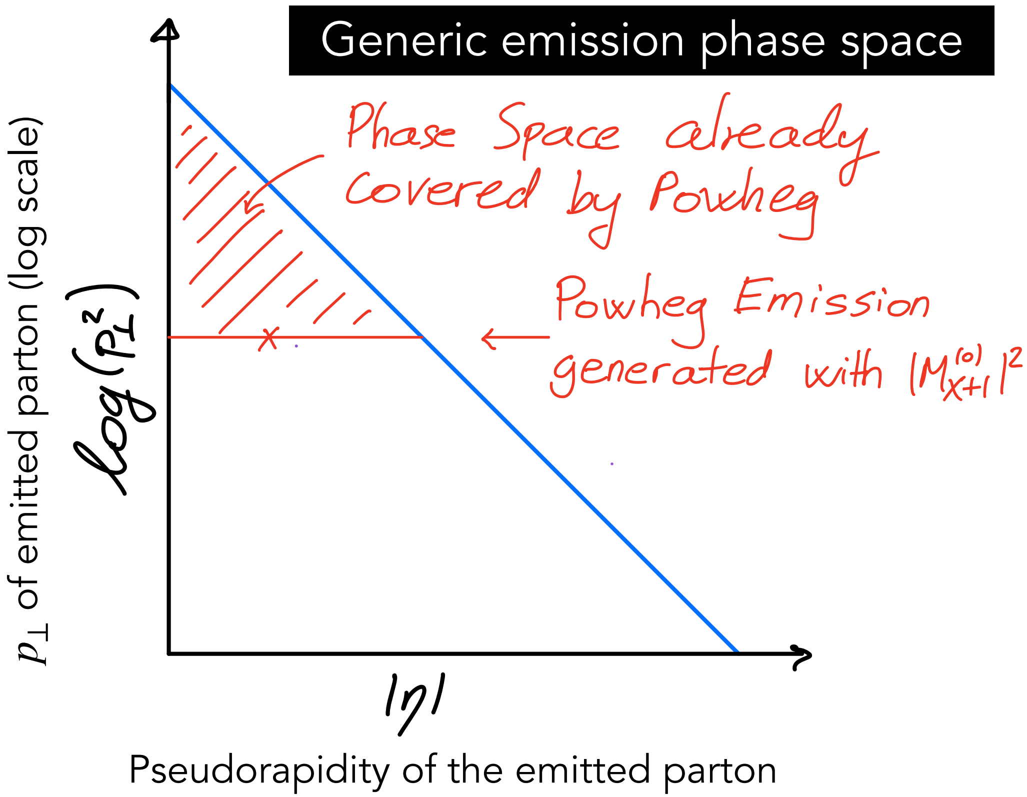

POWHEG emissions are generated in a shower-like manner (MECs)

Combines Matrix-Element Corrections (MEC) [Bengtsson & Sjöstrand 1987 + …]

with NLO Born-Level Normalization [Nason 2004; Fixione, Nason, Oleari 2007]

Sweeping over the phase space, from high to low p_T

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Generate hardest emission with (exact) tree-level matrix element $|M^{(0)}_{X+1}|^2$

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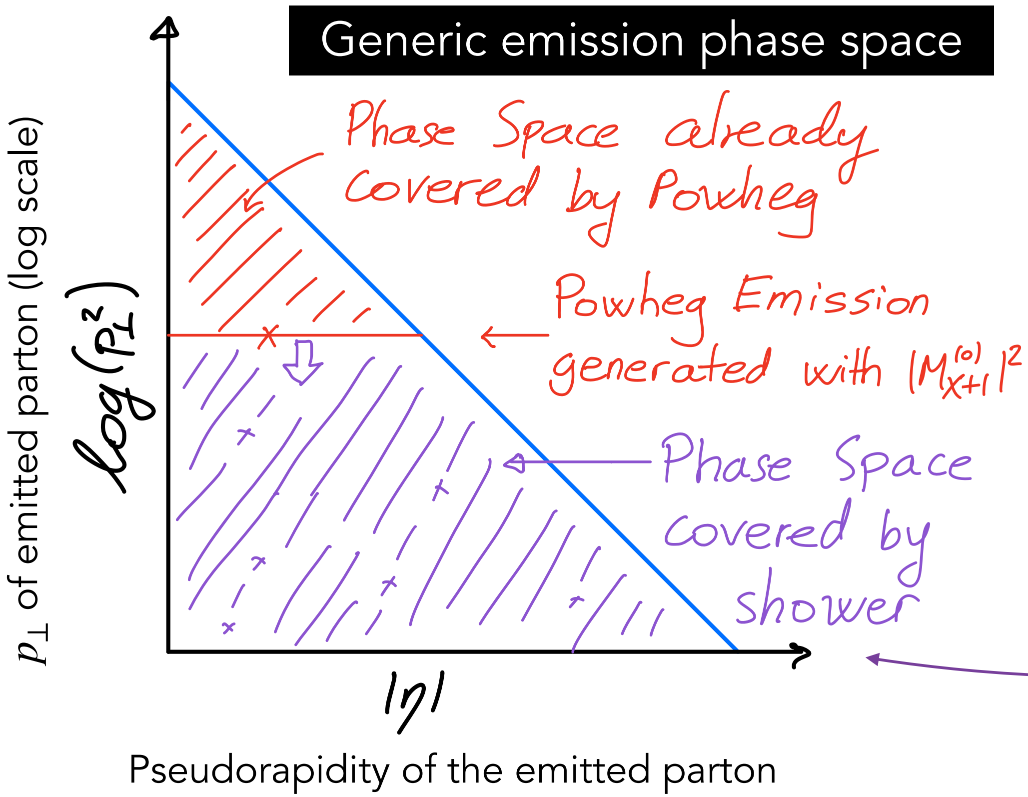
Then let parton shower take over for all further emissions.



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Sweeping over the phase space, from high to low p_T

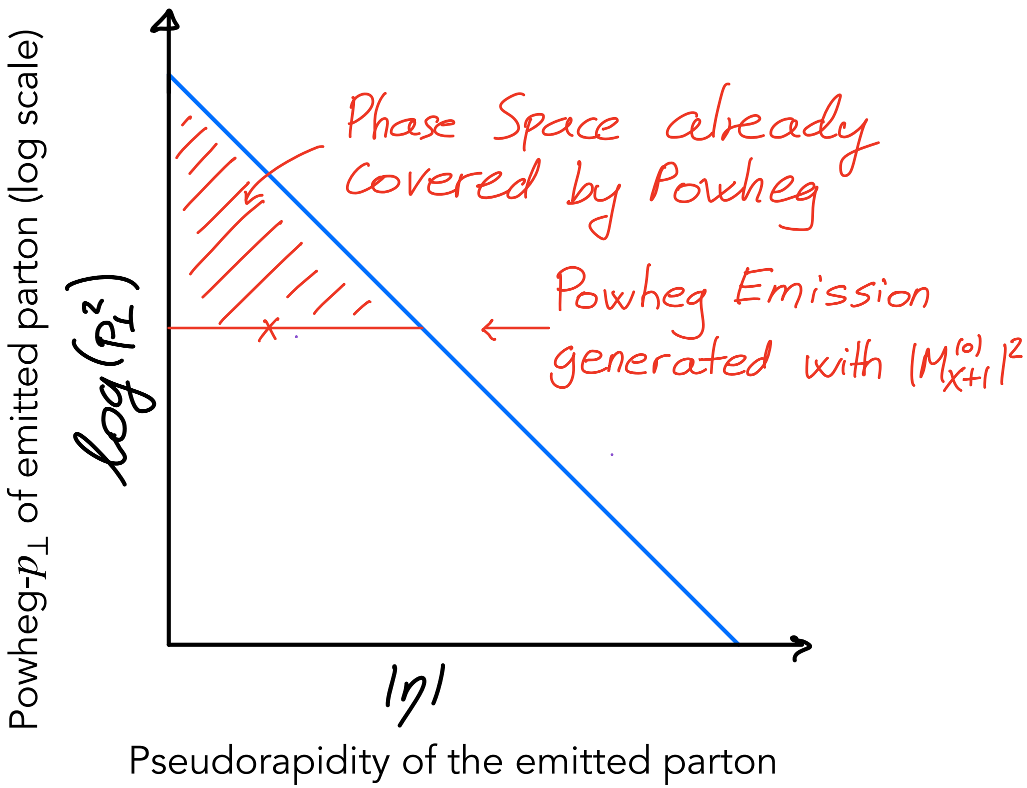
This is how it is supposed to work

POWHEG-Box [Alioli et al, 2010]

PowHeg-Box: independent of shower generator

Convenient: can be used with **any shower**

Caveat: must use its own definition of "p_T" ≠ shower's p_T



Naive POWHEG Matching

Continue the shower starting from the POWHEG p_T scale

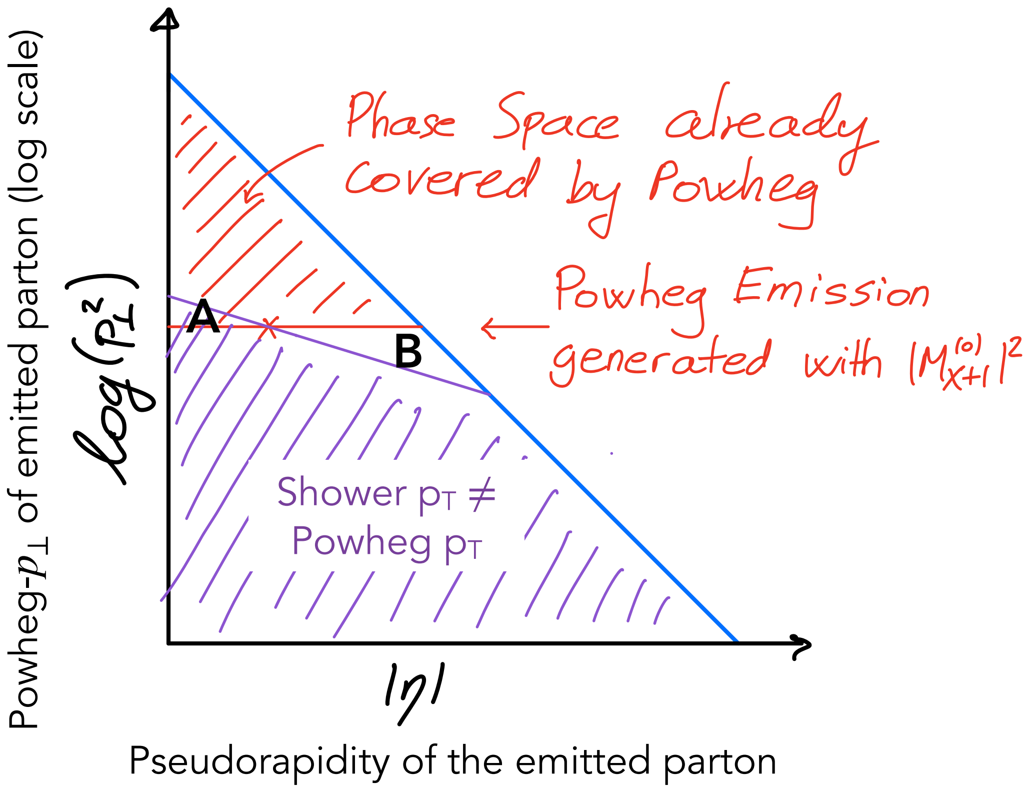
(Saved in LHEF SCALUP value)

POWHEG-Box [Alioli et al, 2010]

PowHeg-Box: encodes its own phase-space generator for 1st emission

Output via LHEF. Convenient: can be used with **any parton shower**

Caveat: must use its own definition of "p_T" ≠ shower's p_T



Naive POWHEG Matching

Continue the shower starting from the POWHEG-Box p_T scale

(Saved in LHEF SCALUP value)

FAILS!

Region **A** is double-counted

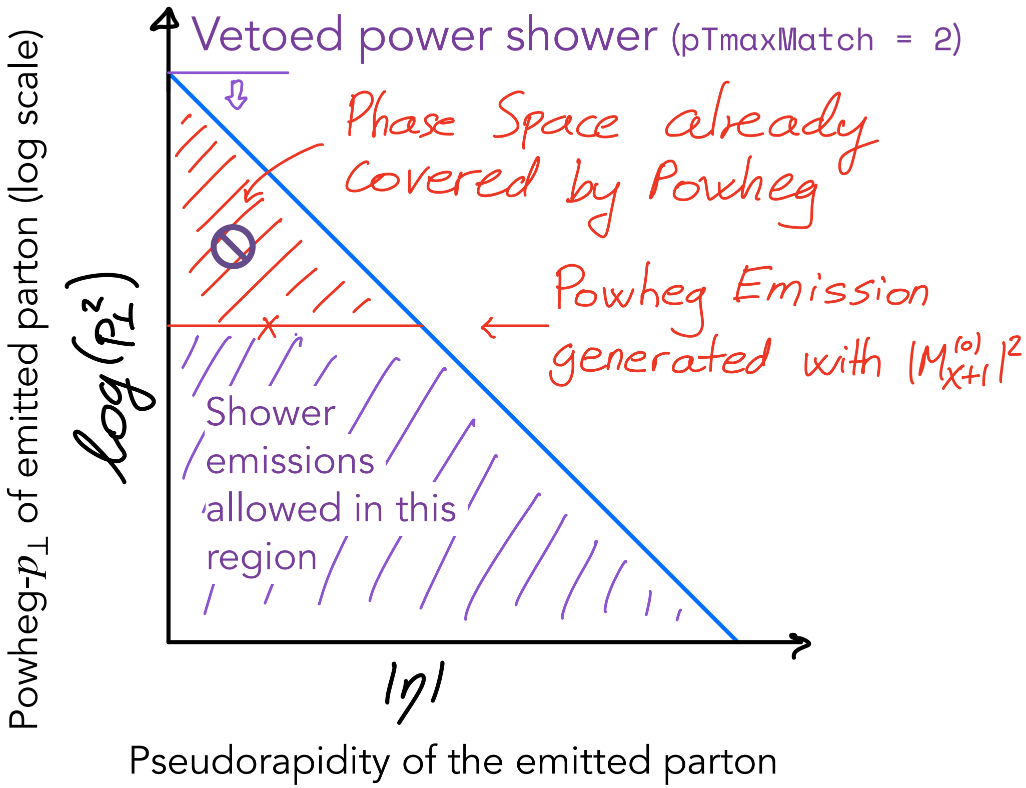
Region **B** is left empty

Current best practice

Vetoed "Power Showers" — with PYTHIA's POWHEG hooks (`POWHEG:veto = 1`)

Let shower fill **all** of phase space (⇒ lots of double counting but at least no holes)

Eliminate double counting: for each shower emission, compute the would-be $p_{\perp i}^{\mathrm{Powheg}}$ and veto any that would double-count $p_{\perp 1}^{\mathrm{Powheg}}$



Vetoed Power Showers

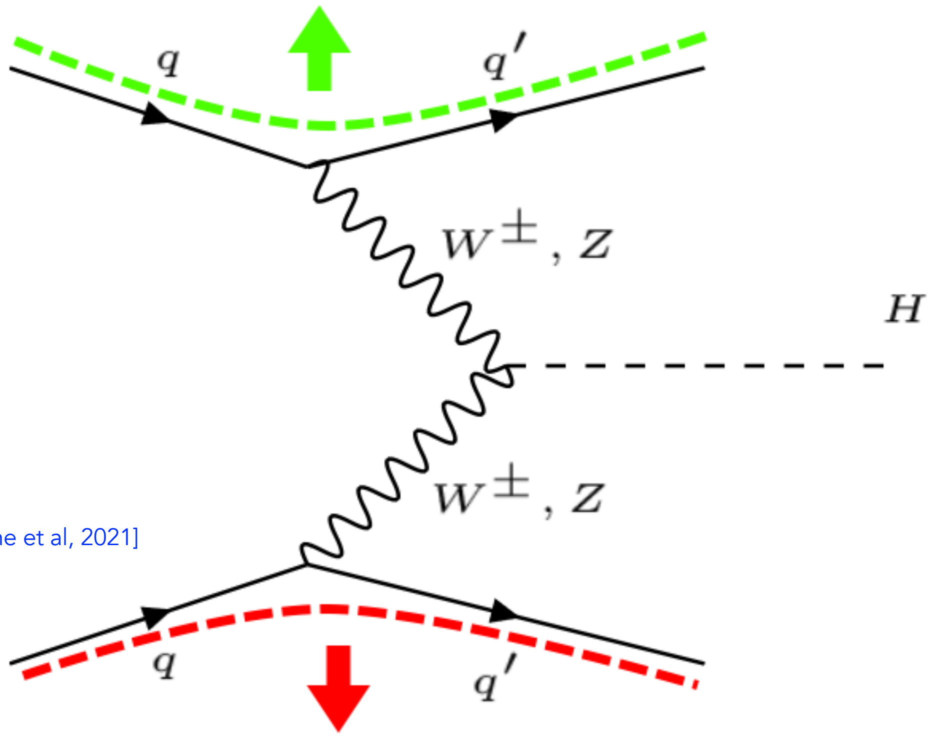
Work very well for **simple processes** (like Drell-Yan)

But the ambiguities can be much more severe for more complex processes.

Especially ones involving initial-final colour flows

A More Complex Process

Vector boson fusion, $qq \to q'q'H$



[Höche et al, 2021]

Multiple emitters
$\rightsquigarrow$ several overlapping phase spaces

And many possible p_T definitions:

$p_\perp$ with respect to the beam

$p_\perp$ with respect to the final-state q' partons

$p_\perp$ with respect to either of the $(q_* q')$ dipoles (crossed)

$p_\perp$ with respect to the H?

(+ PYTHIA defines a problematic $(q'q')$ dipole)

+ Interpolations/combinations of the above …

Again, POWHEG-Box generates the first emission, which it judges to be the "hardest" according to its own p_T definition

Note: similar concerns for any process with coloured partons in the final state at Born level

$t\bar{t}$ (& $t \to bW$), $V/H + \text{jet(s)}$, *dijets, trijets, …*

POWHEG-Box Matching Systematics

Varying the POWHEG-Box ↔ PYTHIA hardness-scale ambiguity

POWHEG:pThard = 0 # Veto at $p_{\perp j;i}^{\mathrm{POWHEG}}$ = **SCALUP** = scale at which POWHEG says it emitted this parton

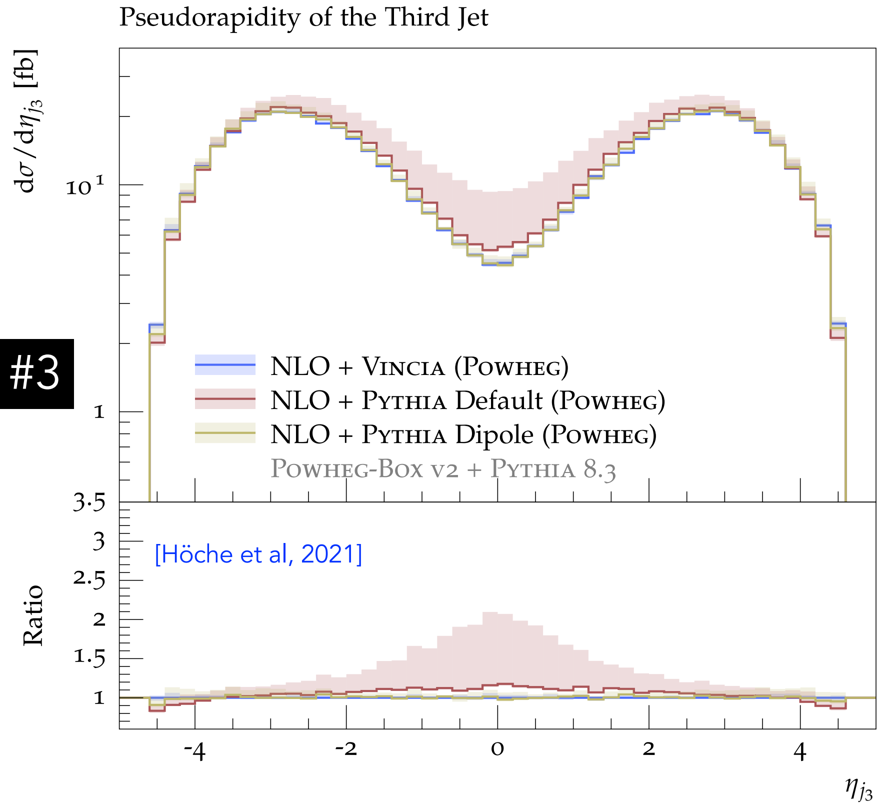
POWHEG:pThard = 1 # Veto at $\min_i (p_{\perp j;i}^{\mathrm{POWHEG}})$ = smallest scale at which POWHEG **could** have emitted this **parton**

POWHEG:pThard = 2 # Veto at $\min_{i,j} (p_{\perp j;i}^{\mathrm{POWHEG}})$ = smallest scale at which POWHEG **could** have produced this **event**

[Nason, Oleari 2013]

Less radiation

Jet #3



Powheg + Pythia Default

Big variation with pThard choice ☹️

Tends to fill in the rapidity gap **even for the 3rd jet** (which **should** be under control in POWHEG VBF)

Powheg + Pythia Dipole

Powheg + Vincia

Very little dependence on pThard 😊

Born-Level **NLO accuracy preserved** ✅

VBF: 4th Jet = First Pure-Shower Emission

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Less radiation ↓

[Nason, Oleari 2013]

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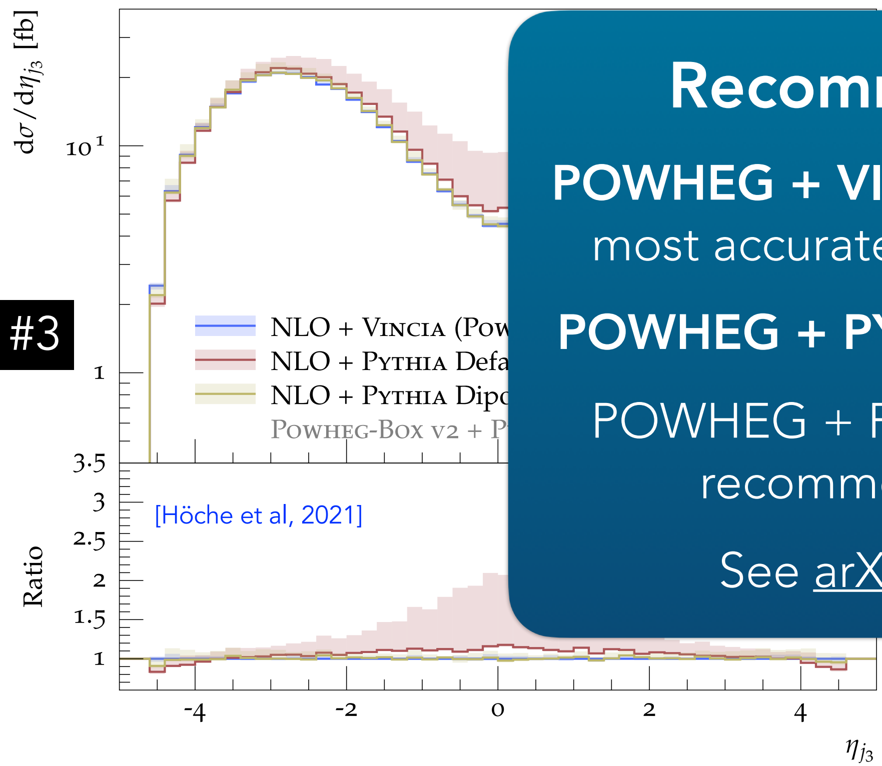
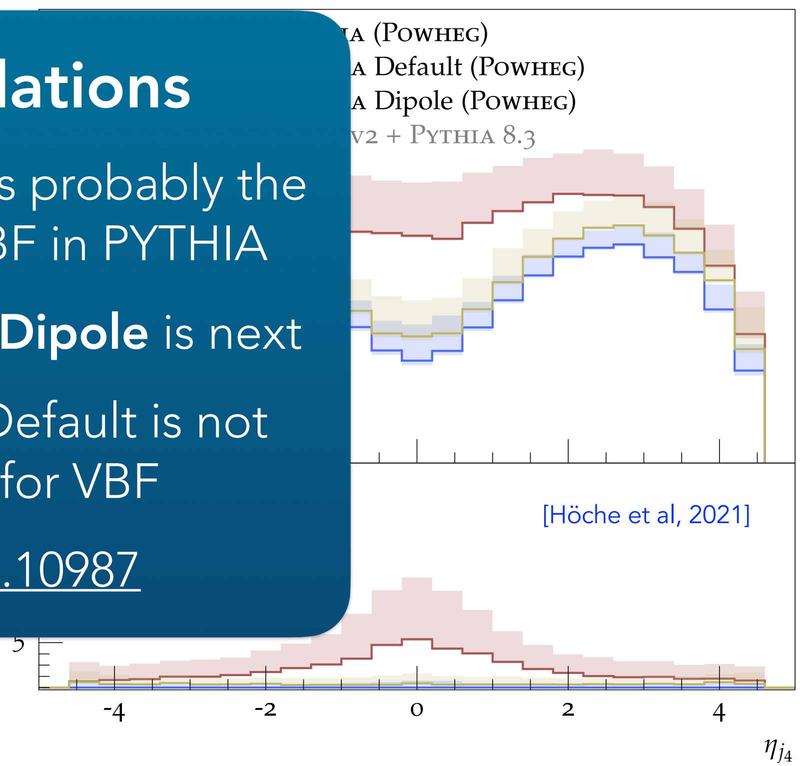


Jet #4



Recommendations

POWHEG + VINCIA is probably the most accurate for VBF in PYTHIA

POWHEG + PYTHIA Dipole is next

POWHEG + Pythia Default is not recommended for VBF

See arXiv:2106.10987

2. From NLO to NNLO

Fixed-Order State of the Art is becoming NNLO → few-% precision

Applying such calculations in a collider context requires **NNLO matching**

MiNNLO$_{PS}$ builds on (extends) POWHEG NLO for X + jet [Hamilton et al. 1212.4504, Monni et al. 1908.06987]

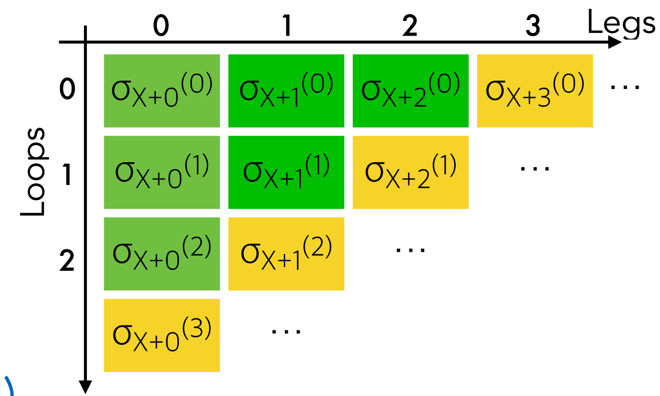
Allow the first jet to approach $p_\perp \to 0$ ~ X + 0

Tame divergence with analytic (NNLL) Sudakov

(introduces additional hardness scale = resummation scale)

Normalize inclusive $\mathrm{d}\sigma_X$ to NNLO

(ambiguity on "spreading" new contributions in phase space.)



Probably the best you can do with current off-the-shelf parton showers

But is approximate; introduces several new (unphysical) ambiguities:

$p_\perp^{\mathrm{Shower}}$ vs $p_\perp^{\mathrm{Powheg}}$ vs $Q_{NNLL}^{\mathrm{resummation}}$ & differential NNLO spreading

MiNNLOPS inherits some issues from POWHEG-Box

Large dependence on pThard scale

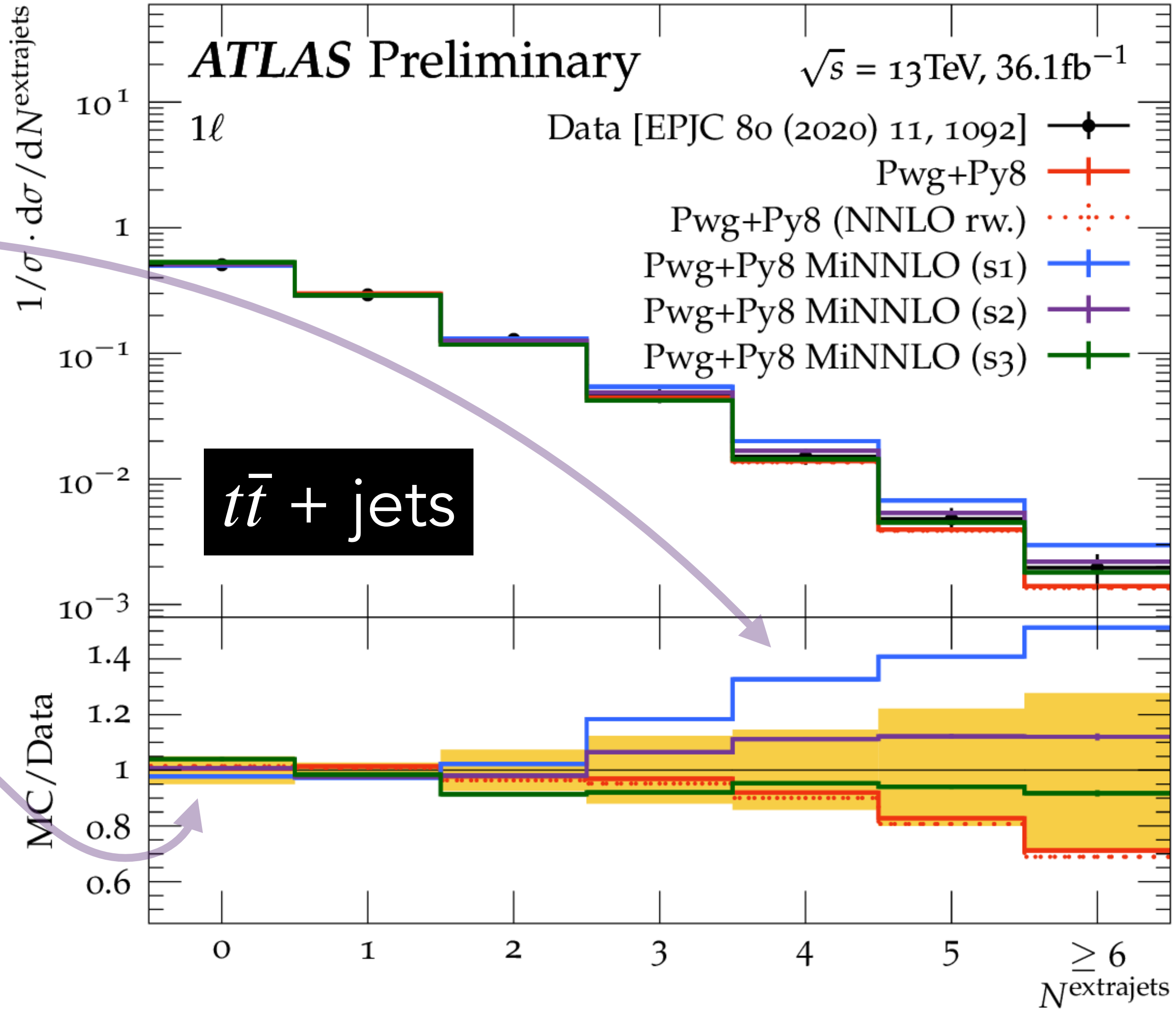
Big variations in predictions for further jets

Calculation "anchored" in NLO for X+jet

$\Longrightarrow$ Also big variations for Born-level (0-jet) observable.

Not the pattern one expects of an NNLO calculation

ATL-PHYS-PUB-2023-029. September 2023.



Recommendations to Users of these Calculations

MiNNLO$_{PS}$ is an *approximate* matching scheme

Does not "match" shower to NNLO point by point in phase space

(Impossible to do so with LL showers.)

Does not (always) do vetoed showers

(This can in principle be done.)

Depends on several auxiliary scales

(Intrinsic to scheme. Physical observables should not depend on them → *vary!*)

Comprehensive variations mandatory to estimate scheme uncertainties

Cannot blindly trust the NNLO label

Nor is the subsequent shower *guaranteed* to preserve accuracy

E.g., Regular POWHEG + proper vetoed showers may do "better" for some observables?

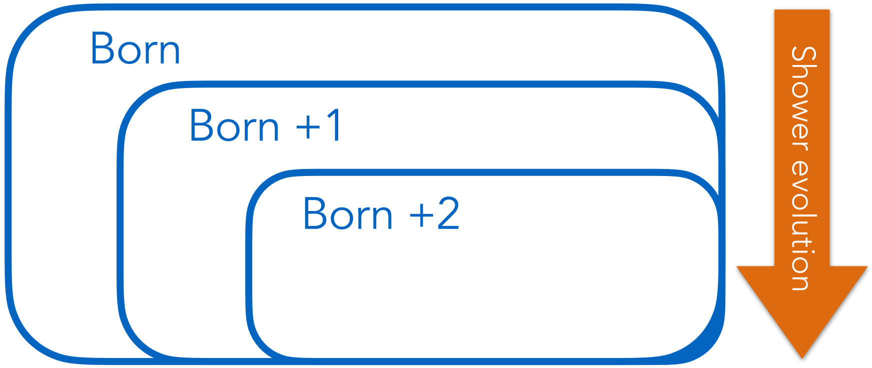
Towards True NNLO Matching

VINCIA NNLO

Idea: Use (nested) Shower Markov Chain as NNLO Phase-Space Generator

Harnesses the power of showers as efficient phase-space generators for QCD

Pre-weighted with the (leading) QCD singular structures = soft/collinear poles



Different from conventional Fixed-Order phase-space generation (eg VEGAS)

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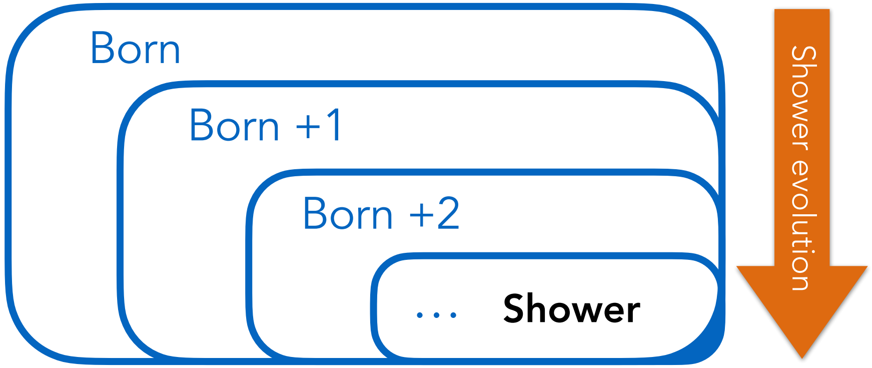

Simply continue shower afterwards

No unphysical scales ⇒ small matching systematics

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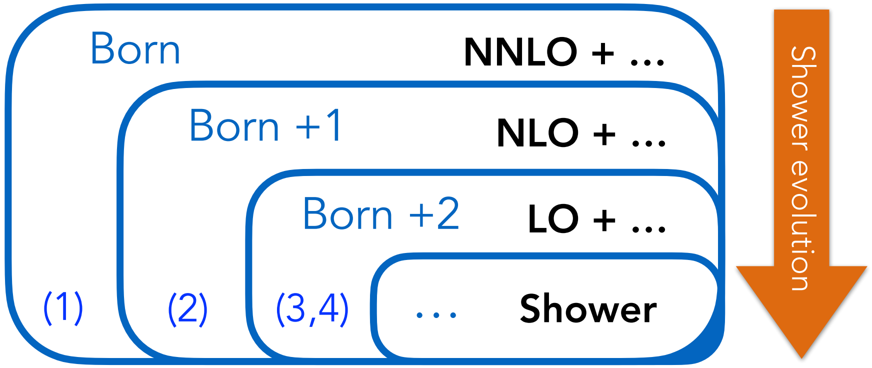


Need:

(1) Born-local NNLO K-factors: $k_{\mathrm{NNLO}}(\Phi_2)$

(2) NLO MECs in the first $2 \mapsto 3$ shower branching: $w^{\mathrm{NLO}}_{2\mapsto 3}(\Phi_3)$

(3) LO MECs for second (iterated) $2 \mapsto 3$ shower branching: $w^{\mathrm{LO}}_{3\mapsto 4}(\Phi_4)$

(4) Direct $2 \mapsto 4$ branchings for unordered sector with LO MECs: $w^{\mathrm{LO}}_{2\mapsto 4}(\Phi_4)$

NEW

→ Friday

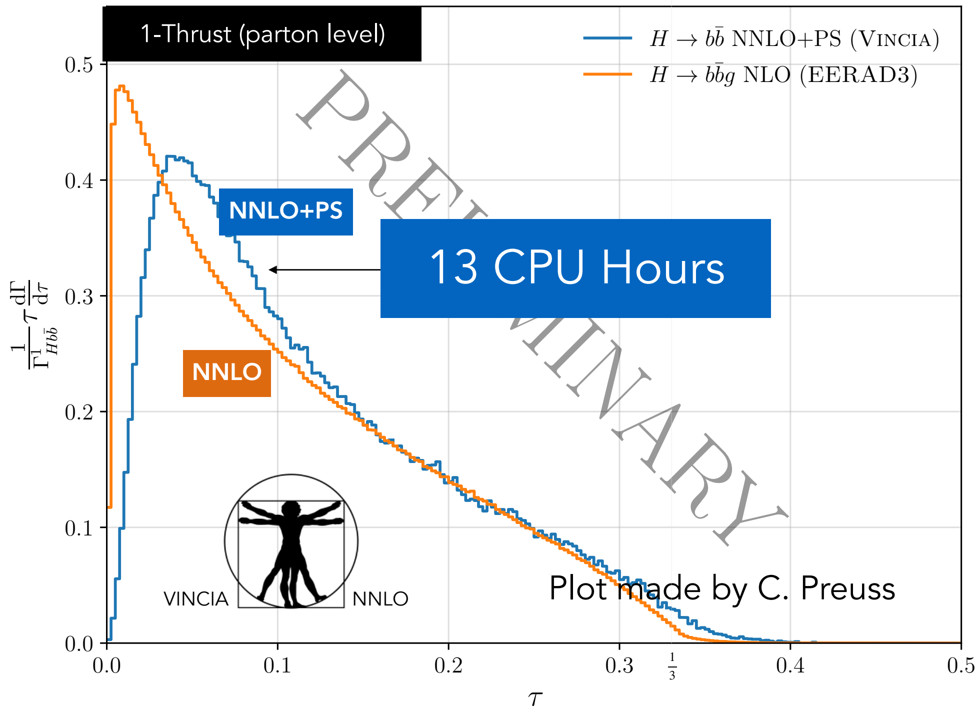
Simply continue shower afterwards

No unphysical scales ⇒ small matching systematics

(arXiv:2108.07133 & arXiv:2310.18671)

Preview: VINCIA NNLO+PS for $H \to b\bar{b}$

VINCIA NNLO

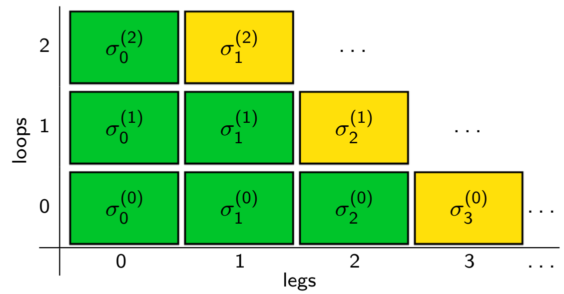


Note:

NNLO Reference = **EERAD3** NLO $H \to b\bar{b}g$

[Coloretti, Gehrmann-de Ridder, Preuss, JHEP 06 (2022) 009]

NNLO accuracy in $H \to 2j$ implies **NLO correction in first emission** and **LO correction in second emission.**



So for Thrust, NNLO $H \to b\bar{b}$ is effectively

NLO for $\tau < 1/3$

LO for $\tau > 1/3$

VINCIA NNLO+PS: shower as phase-space generator: efficient & no negative weights!

➤ Looks ~ 5 x ***faster*** than **EERAD3** (for equivalent unweighted stats)

+ is **matched to shower** + can be **hadronized**

Proof of concepts now done for $Z/H \to q\bar{q}$; work remains for pp (& for N^{n}LL accuracy)

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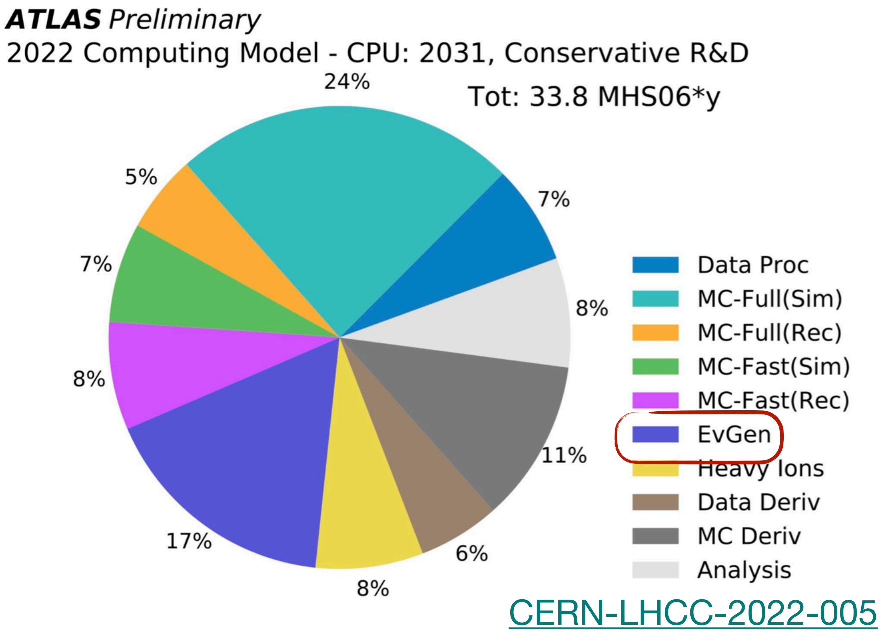
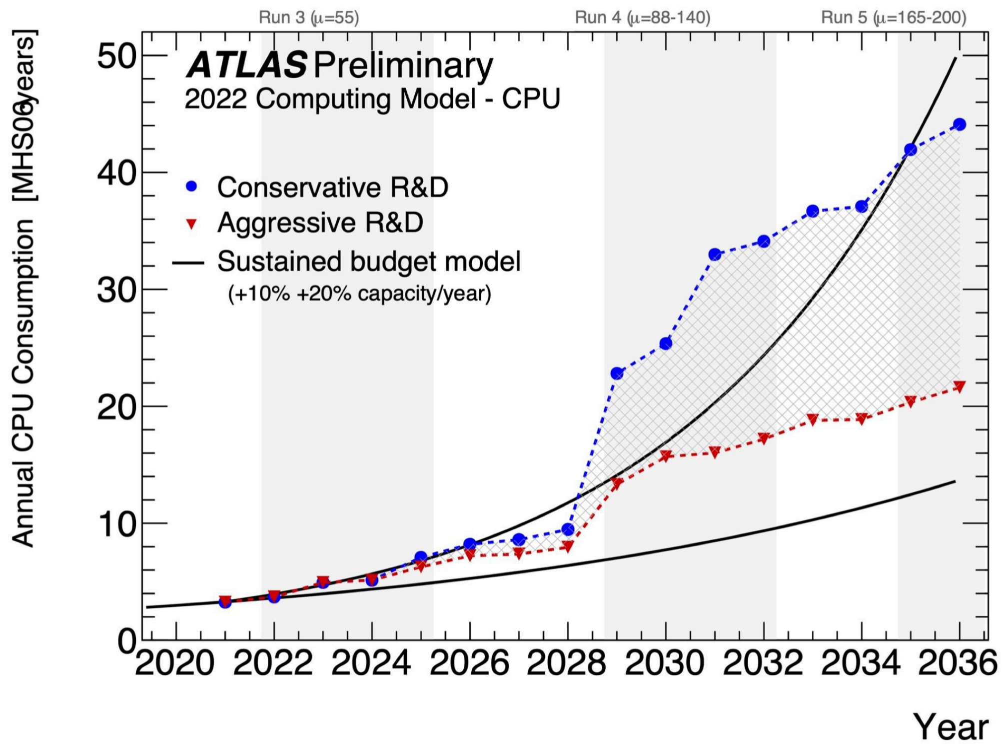
The Computational Bottleneck in ME Merging

Condensed remarks from talk by T. Moskalets (ATLAS) at CERN Workshop Nov 2023





- **Largest fraction of EvGen CPU time is taken by generation of multi-leg MC predictions**
  - namely, multijet merged Sherpa V+jets

Matrix-Element Merging — The Complexity Bottleneck

For CKKW-L style merging: (incl UMEPS, NL3, UNLOPS, …)

Need to take **all contributing shower histories into account**.

In conventional parton showers (Pythia, Herwig, Sherpa, …)

Each phase-space point receives contributions from many possible branching "histories" (aka "clusterings")

# of histories grows ~ # of Feynman Diagrams, **faster than factorial**

Number of Histories for n Branchings

Starting from a single $q\bar{q}$ pair	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$
CS Dipole	2	8	48	384	3840	46080	645120

Bottleneck for merging at high multiplicities (+ high code complexity)

Sector Showers (without maths)

NEW

VINCIA's shower is unique in being a "Sector Shower"

PS & Villarejo JHEP 11 (2011) 150
Brooks, Preuss, **PS** JHEP 07 (2020) 032

Partition N-gluon Phase Space into N "sectors" (using step functions).

Each sector ↔ one specific gluon being the "softest" in the event

Inside each sector, only one kernel contributes (the most singular one)!

Sector Kernel = the eikonal for the soft gluon and its collinear DGLAP limits for $z > 0.5$.

➜ Unique properties: shower operator becomes **bijective** and is a **true Markov chain**

The crucial aspect:

Only a **single history** contributes to each phase-space point !

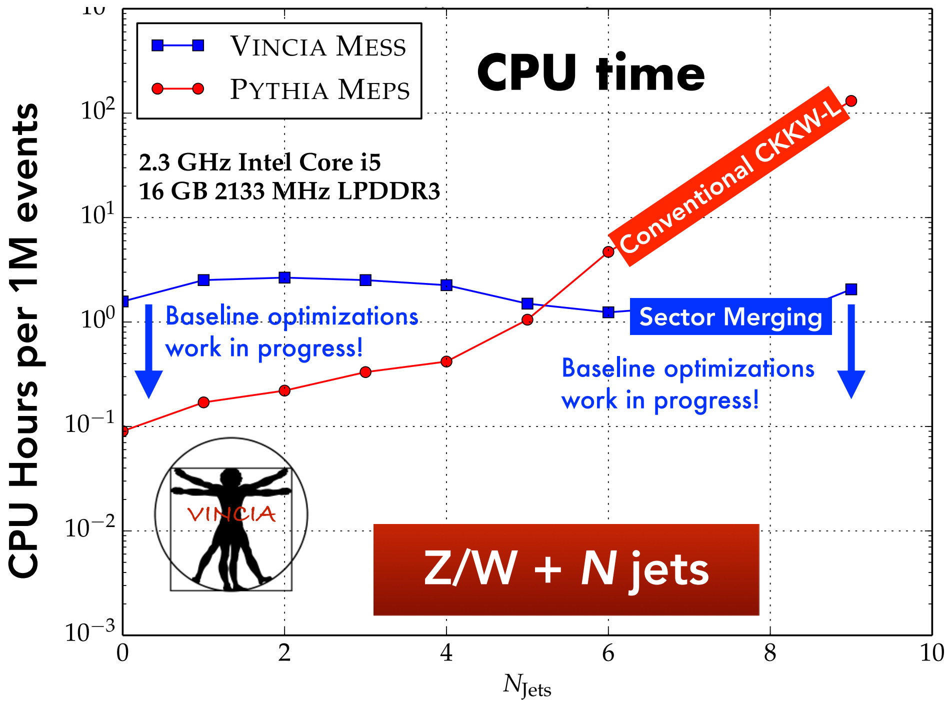
$\Longrightarrow$ **Factorial growth of number of histories reduced to constant!**

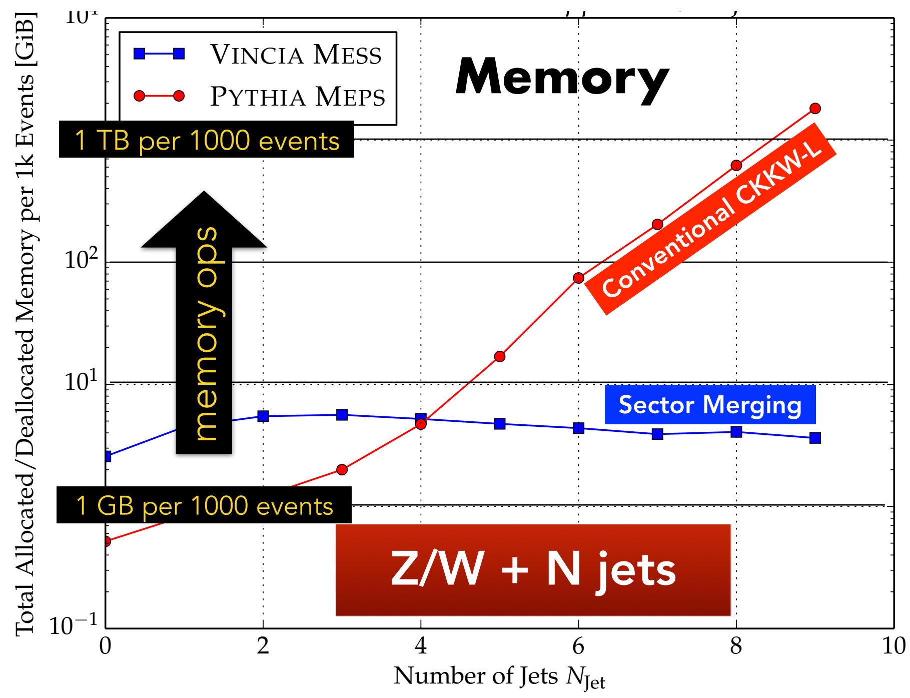
(And the number of sectors only grows linearly with the number of gluons)

($g \to q\bar{q}$ ➜ leftover factorial in number of same-flavour quarks; not a big problem)

Sectorized CKKW-L Merging publicly available from Pythia 8.306

Brooks & Preuss, "Efficient multi-jet merging with the VINCIA sector shower", arXiv:2008.09468





Demonstrated constant scaling with multiplicity. Extensions now pursued:

Optimisations of baseline algorithm

Sectorized **iterated tree-level ME corrections** (demonstrated in PS & Villarejo arXiv:1109.3608)

Sectorized **multi-leg merging at NLO** (active research grants, with **C. Preuss, Wuppertal**)

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New Discoveries in Hadronization

NEW

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

Not predicted by default Pythia (Monash)

Very exciting!

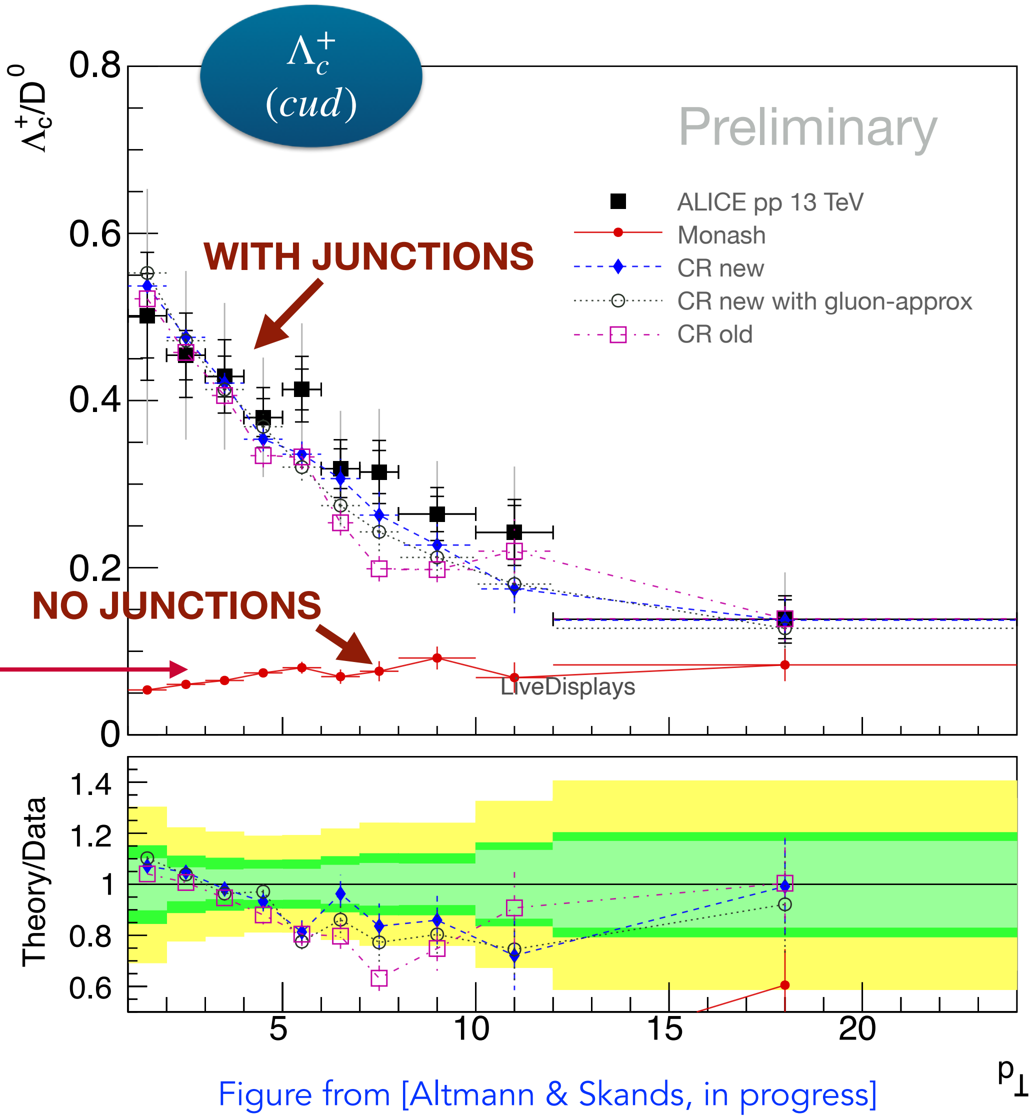


Figure from [Altmann & Skands, in progress]

LHCb: also in Bottom

Λ_b asymmetry

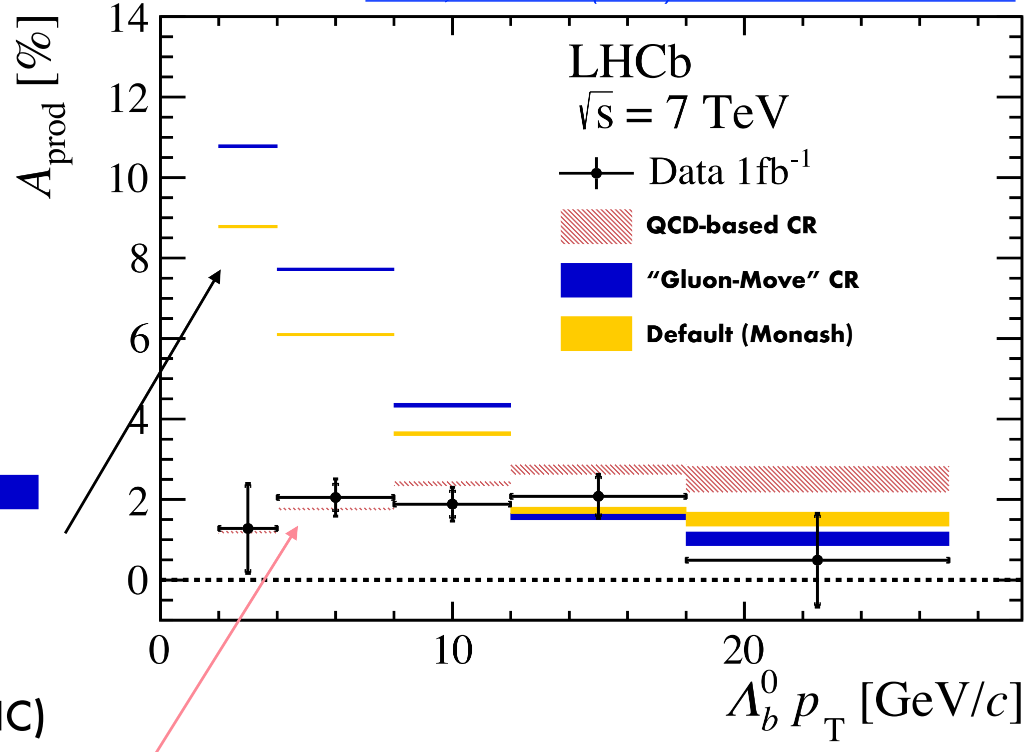
$$A = \frac{\sigma(\Lambda_b^0) - \sigma(\overline{\Lambda}_b^0)}{\sigma(\Lambda_b^0) + \sigma(\overline{\Lambda}_b^0)}$$

Baseline Expectations: &

b quark combines with the proton beam remnant $\Longrightarrow$ Λ_b production

Not possible for $\bar{\Lambda}_b$ (no $\bar{p}$ remnant at LHC)

[LHCb, JHEP 10 (2021) 060 • arXiv: 2107.09593](https://arxiv.org/abs/2107.09593)

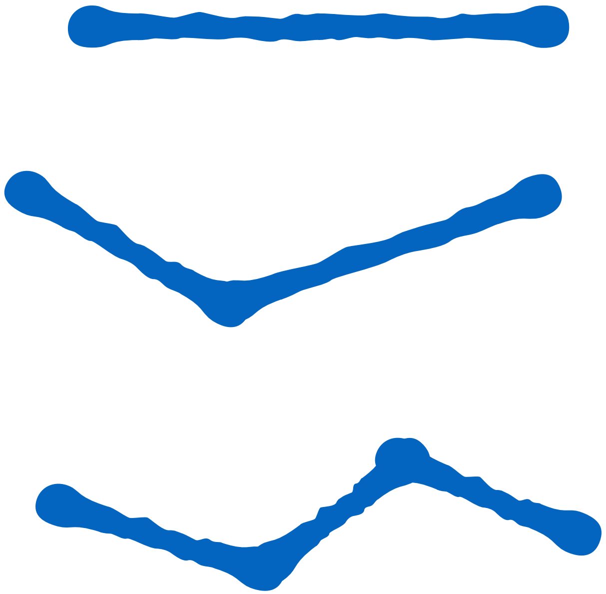


QCD CR with "string junctions" [Christiansen & Skands JHEP 08 (2015) 003]

Adds large amount of low-p_T Λ_b and $\bar{\Lambda}_b$, in equal amounts. Dilutes asymmetry!

What are String Junctions?

Open Strings

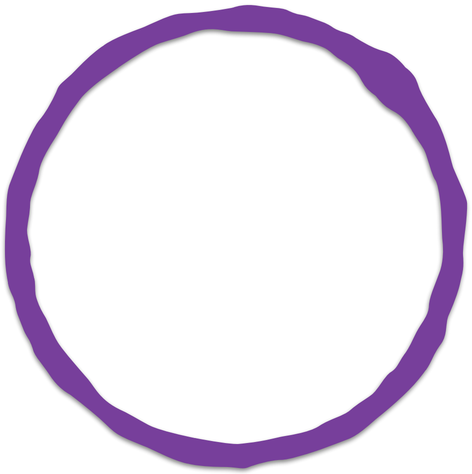


$q\bar{q}$ strings (with gluon kinks)

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

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

Closed Strings

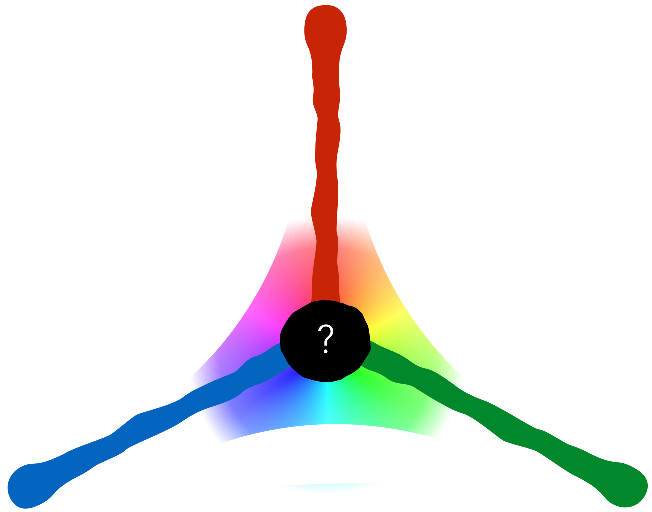


Gluon rings

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

$\Upsilon \to ggg$ + shower

SU(3) String Junction



Open strings with $N_C = 3$ endpoints

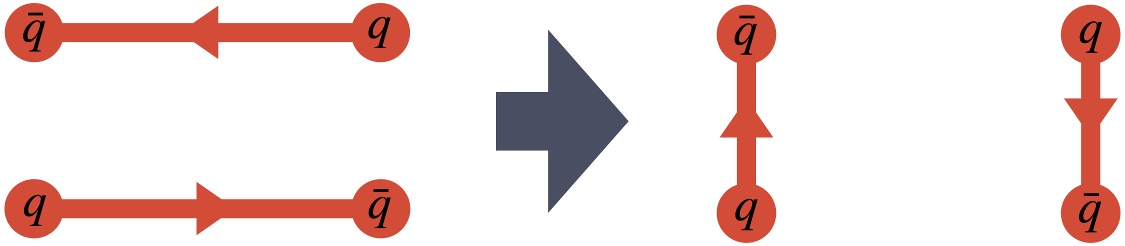
E.g., Baryon-Number violating neutralino decay $\tilde{\chi}^0 \to qqq$ + shower

How do QCD Colour Reconnections Create String Junctions?

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

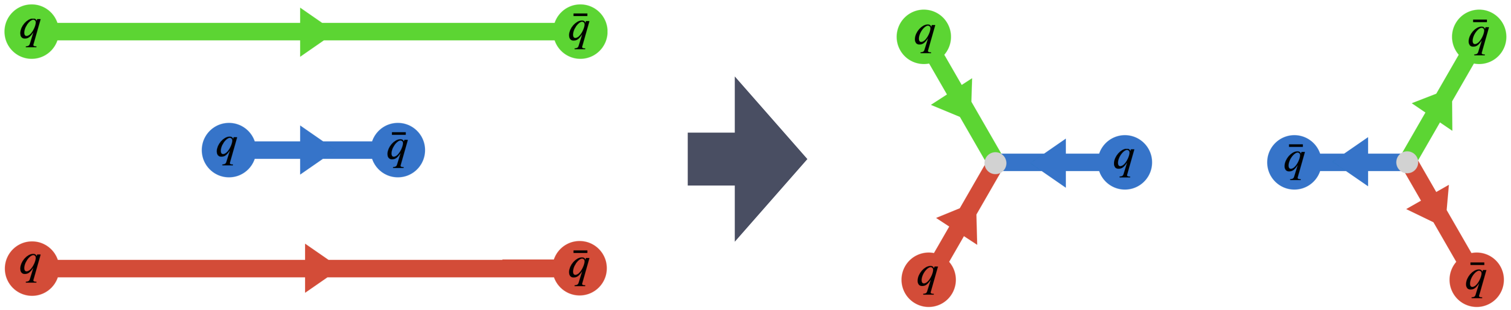
[Christiansen & **PS** JHEP 08 (2015) 003]

➢ Allows for reconnections to minimise string lengths



Dipole-type reconnection

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

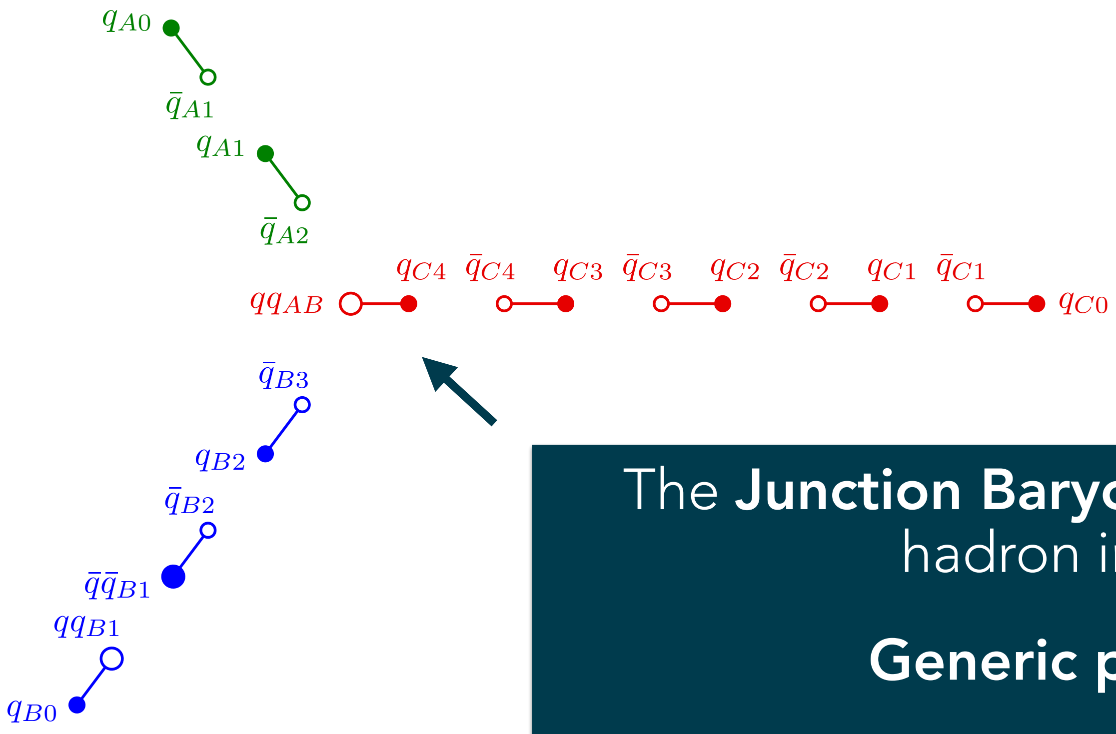


Junctions!

What do String Junctions do?

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

➤ No new string-fragmentation parameters



[Sjöstrand & **PS**, NPB 659 (2003) 243]

[+ J. Altmann & **PS**, in progress]

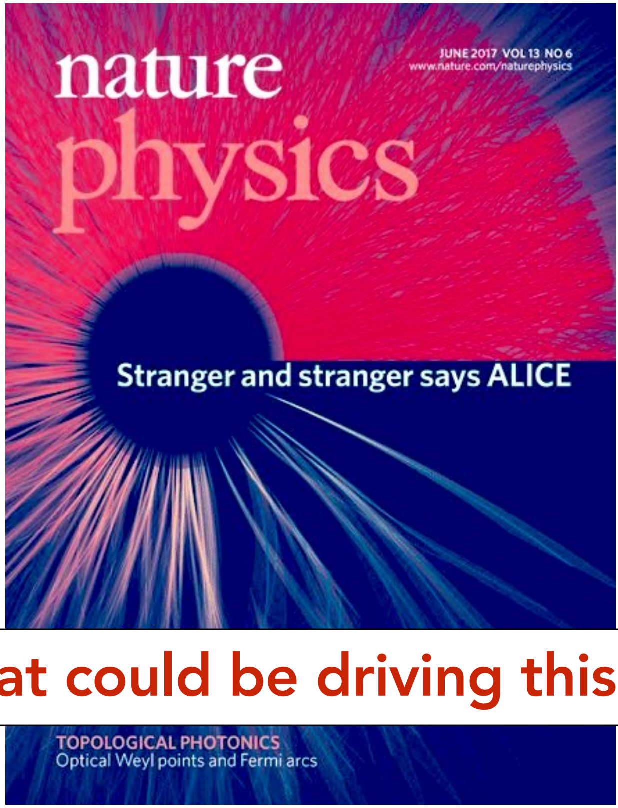
The **Junction Baryon** is the most "subleading" hadron in all three "jets".

Generic prediction: low p_T

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

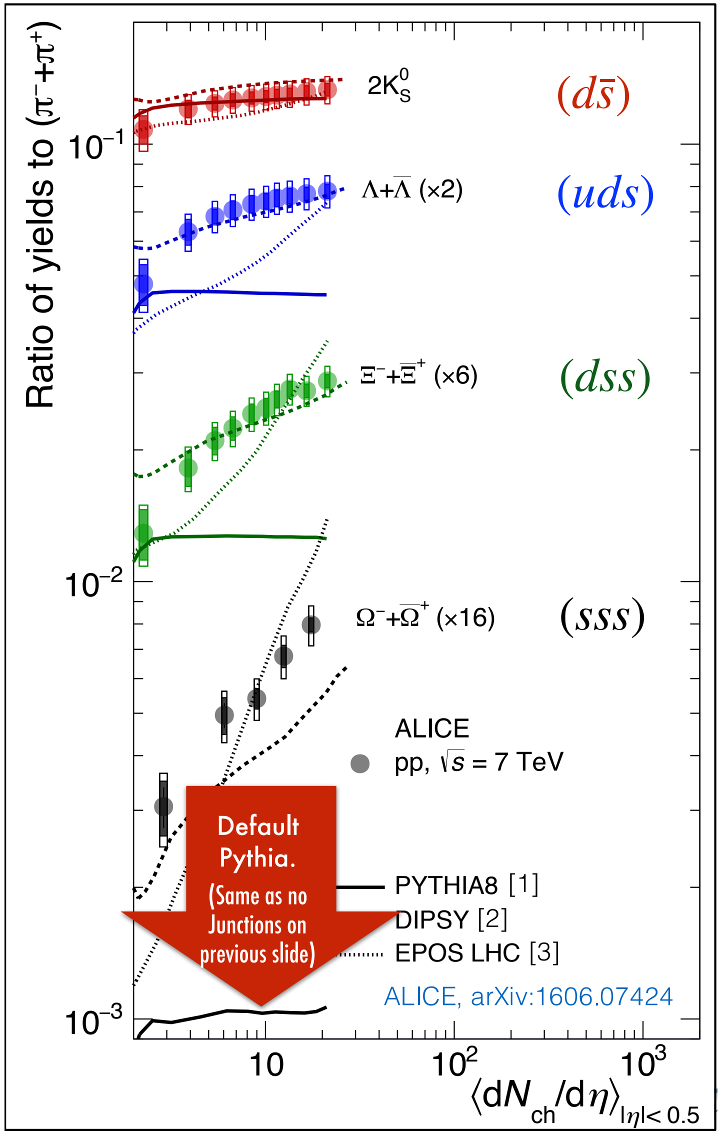
What a **strange** world we live in, said Alice

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



June 2017

What could be driving this?



NEW In Progress: Strangeness Enhancement from Close-Packing

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

Close-packing

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

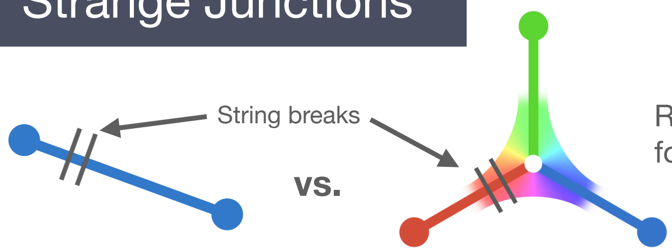
$p = 2$, $q = 0$ $\quad C_6 = 2.5 C_F$

Dense string environments

→ Casimir scaling of **effective string tension**

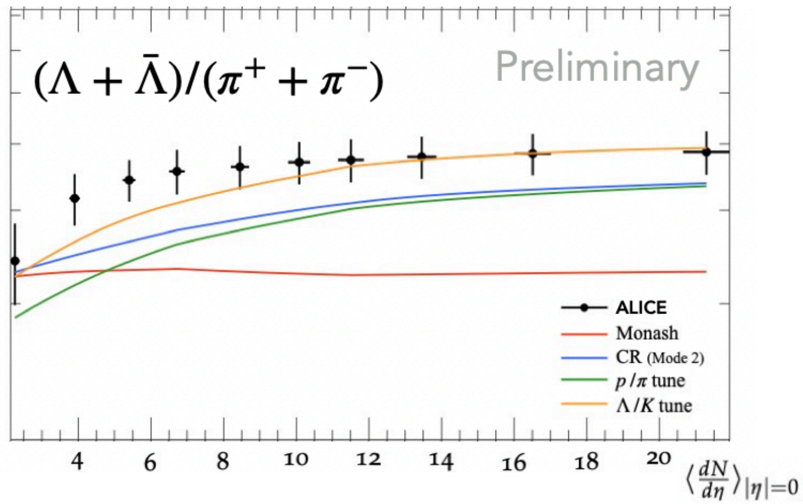
→ Higher probability of strange quarks

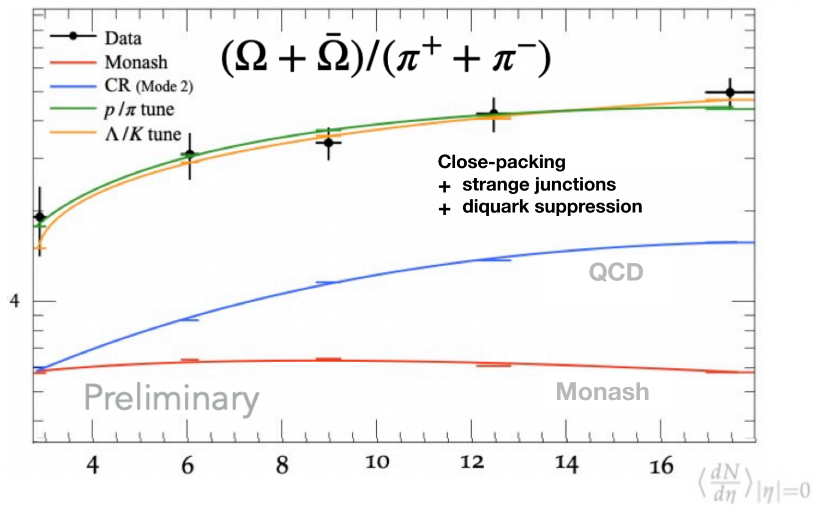
Strange Junctions



Results in strangeness enhancement focused in baryon sector

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





Particle Composition: Impact on Jet Energy Scale

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 & Outlook

State of the art for perturbation theory: NNLO (→ N3LO)

Matching to showers + hadronization mandatory for collider studies (+ resummation extends range)

Now: can use off-the-shelf showers with MiNNLO$_{PS}$

Based on POWHEG-Box + Analytical Resummation + NNLO normalisation

Approximate method; depends on several auxiliary unphysical scales → can exhibit large variations

Work in progress: VinciaNNLO ⇢ **Friday**

Based on nested shower-like phase-space generation with second-order MECs

True NNLO matching → Expect small matching systematics

So far only worked out for colour-singlet decays.

(Also developing extensions towards NLL, NNLL showers …)

Beautiful Strings

New discoveries at LHC on particle composition, esp. **baryons and strangeness**

New research grant with LHCb (Warwick) focusing on strings with b-quark endpoints

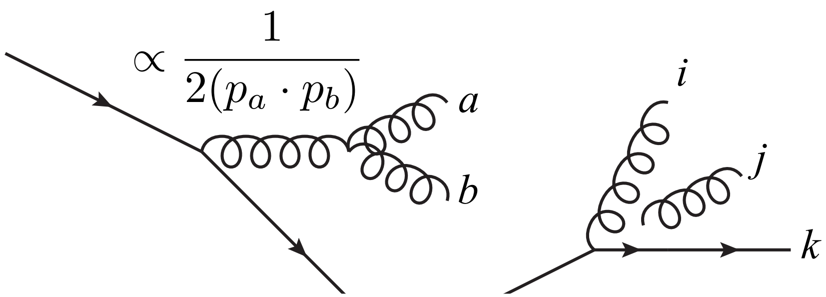
And QED corrections in B decays

Extra Slides

Parton Showers: Theory

see e.g PS, *Introduction to QCD*, TASI 2012, arXiv:1207.2389

Most bremsstrahlung is driven by divergent propagators → simple structure



Mathematically, **gauge amplitudes factorize** in **singular limits**

Partons ab → **collinear**:

$$|\mathcal{M}_{F+1}(\ldots,a,b,\ldots)|^2 \overset{a||b}{\to} g_s^2 \mathcal{C} \frac{P(z)}{2(p_a \cdot p_b)} |\mathcal{M}_F(\ldots,a+b,\ldots)|^2$$

$P(z)$ = **DGLAP splitting kernels**", with $z = E_a/(E_a+E_b)$

Gluon j → **soft**:

$$|\mathcal{M}_{F+1}(\ldots,i,j,k\ldots)|^2 \overset{j_g\to 0}{\to} g_s^2 \mathcal{C} \frac{(p_i \cdot p_k)}{(p_i \cdot p_j)(p_j \cdot p_k)} |\mathcal{M}_F(\ldots,i,k,\ldots)|^2$$

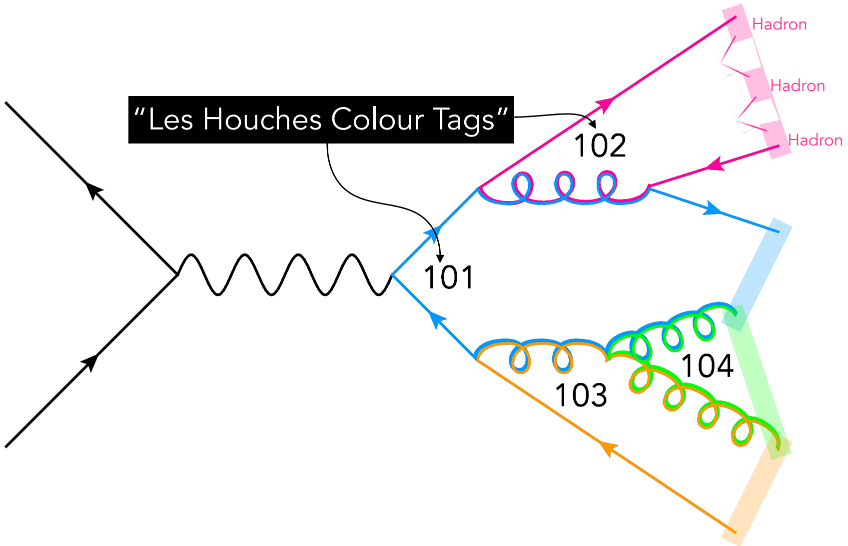
Coherence → Parton j really emitted by (i,k) "dipole" or **"antenna" (eikonal factors)**

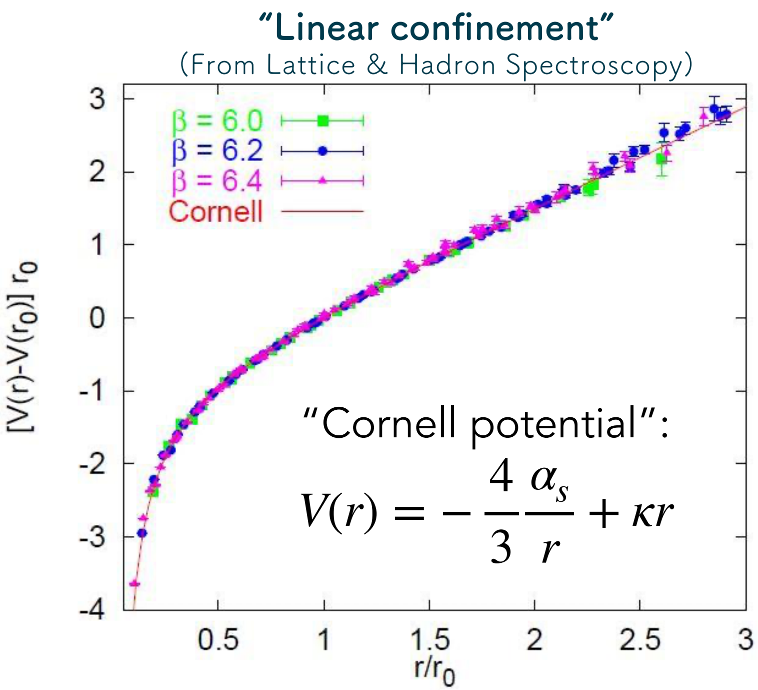
These are the **building blocks of parton showers** (DGLAP, dipole, antenna, …)

(+ running coupling, unitarity, and explicit energy-momentum conservation.)

Confinement in PYTHIA: *The Lund String Model*

Simplified (leading-N$_C$) **"colour flow"** ➜ determine between which partons to set up confining potentials





Map from Partons to Strings:

Quarks ➡ string endpoints; gluons ➡ transverse "kinks"

System then evolves as a string world sheet

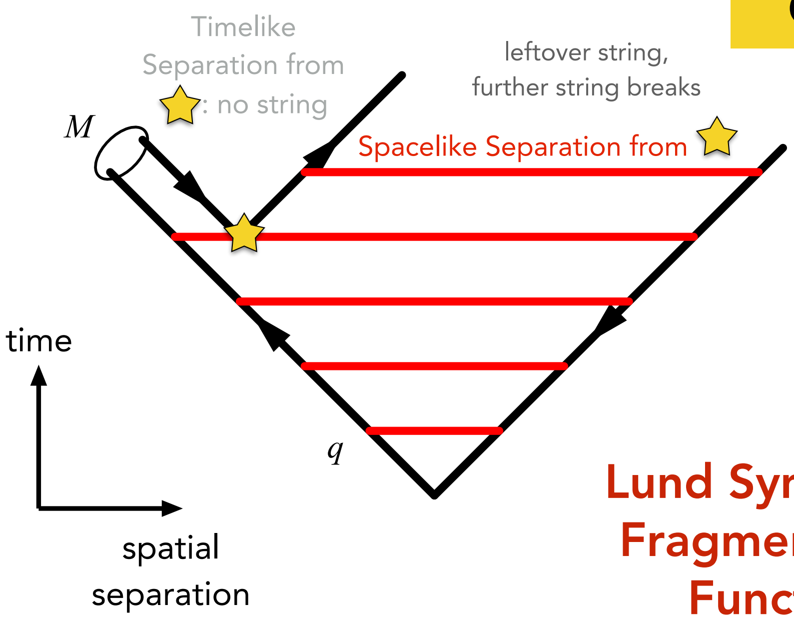
+ **String breaks** via spontaneous $q\bar{q}$ pair creation ("Schwinger mechanism") → **hadrons**

The String Fragmentation Function

Consider a string break ⭐, producing a meson M, and a leftover string piece

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

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

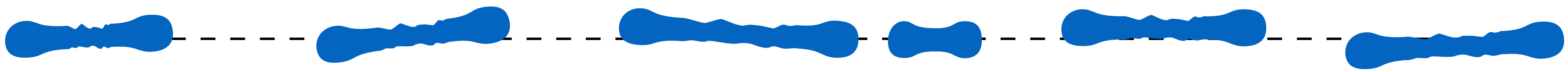
↑ Supresses high-z hadrons

↑ Supresses low-z hadrons

Automated Hadronization Uncertainties

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 **different?**

Would this particular final state become **more likely** $(w' > 1)$? Or **less likely** $(w' < 1)$

Crucially: **maintaining unitarity** $\Longrightarrow$ inclusive cross section remains unchanged!

August 2023: 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

Pythia 8.311

Demonstration

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

Example: Longitudinal Fragmentation Function (Lund Symmetric FF)

$f(z)$ ~ ***scaled*** **light-cone hadron momentum fraction**

$$\propto \frac{1}{z^{1+r_Q b m_Q^2}} (1-z)^a \exp\left(-\frac{b m_\perp^2}{z}\right)$$

variations

Reweighting Methodology:

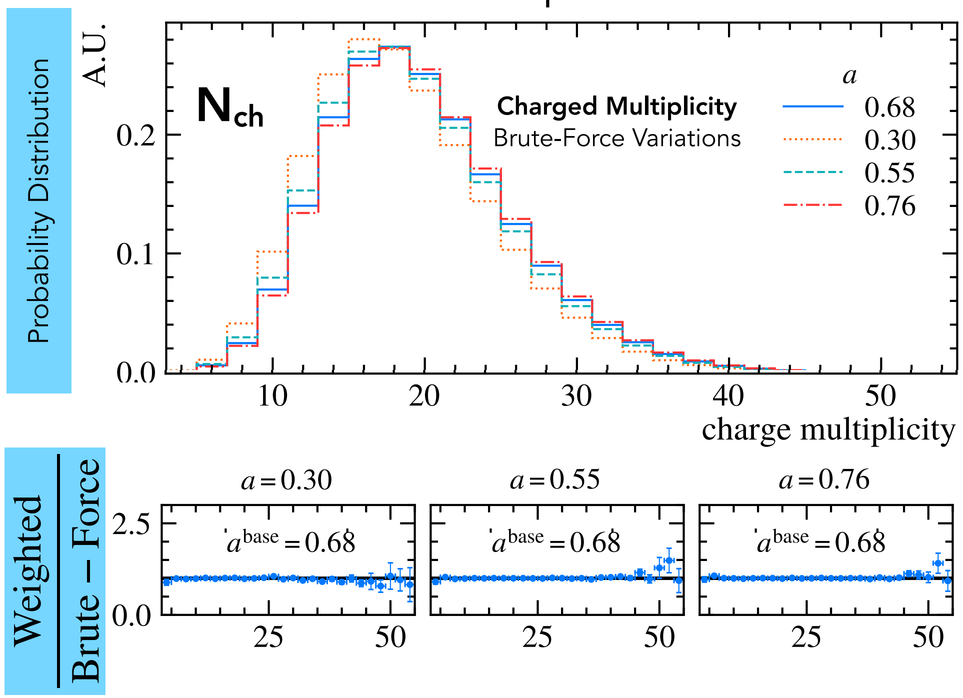
Accept-Reject Algorithm (analogous to shower variations):

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

with

$$R'_{\text{accept}}(z) = \frac{P'_{\text{accept}}(z)}{P_{\text{accept}}(z)} \qquad R'_{\text{reject}}(z) = \frac{P'_{\text{reject}}(z)}{P_{\text{reject}}(z)} = \frac{1 - P'_{\text{accept}}(z)}{1 - P_{\text{accept}}(z)}$$

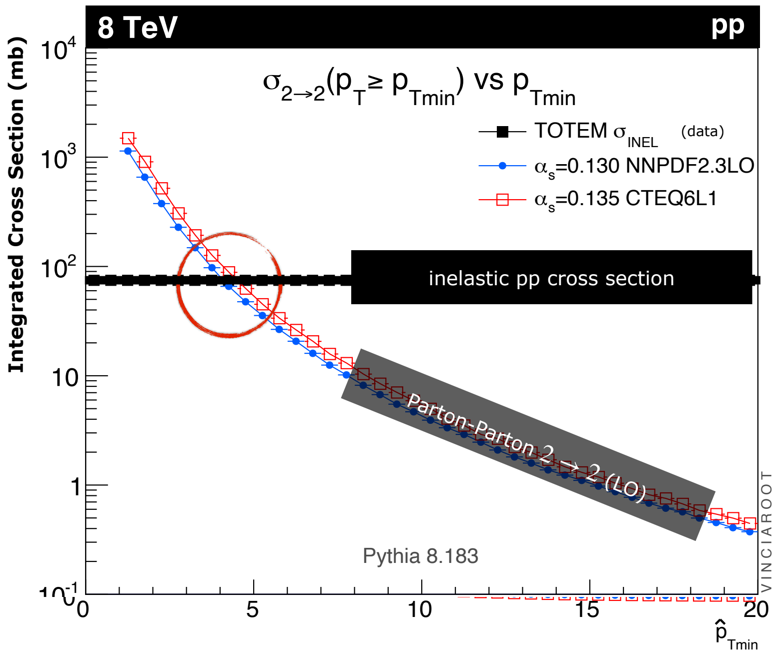
Example



A Brief History of MPI in PYTHIA

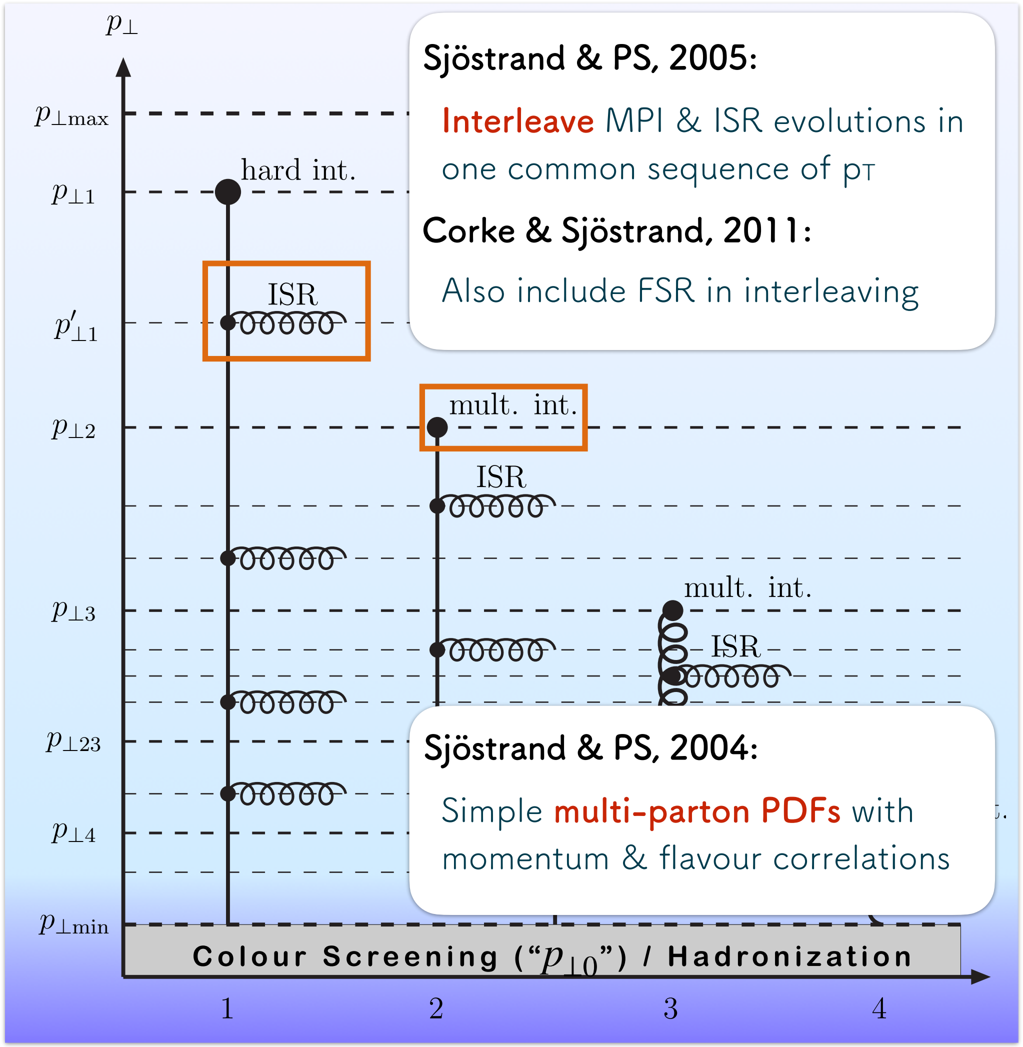
$$\frac{\sigma_{\text{parton-parton}}(\hat{p}_\perp)}{\sigma_{\text{hadron-hadron}}} > 1$$

$\Longrightarrow$ 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