New Developments in Theory Uncertainties

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[Sibyll Trelawney, Harry Potter and the Prisoner of Azkaban, Warner Bros.]

Predictions are only as good as their uncertainty estimates

Overview

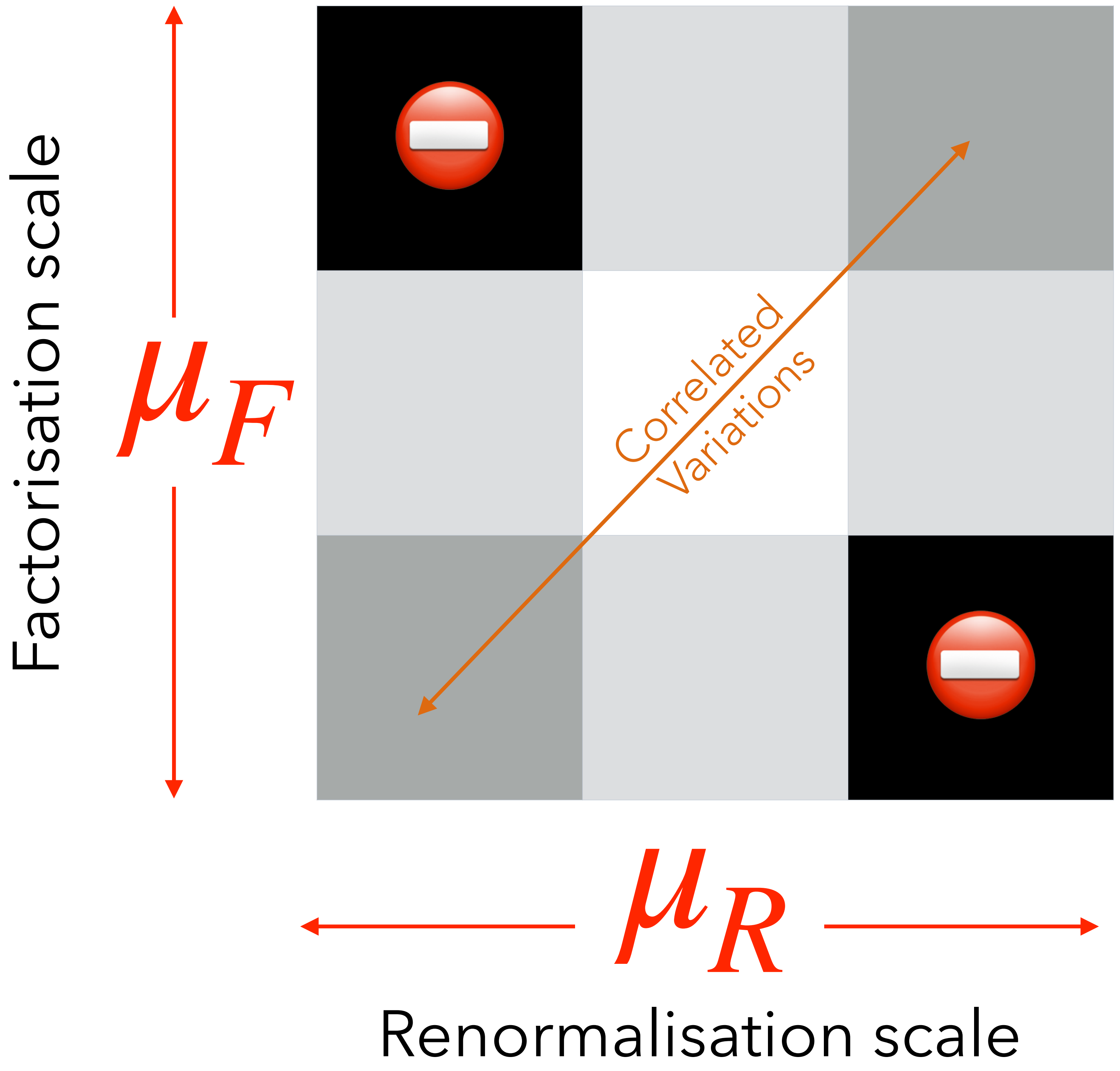
1. ME Uncertainties
2. Shower Uncertainties
3. Matching Uncertainties
4. Nonperturbative Uncertainties

Disclaimer: I am not offering solutions to all the issues I will mention

But we should acknowledge them, and think about how to deal with them…

❶ ME Uncertainties

Current Standard: 7-Point Variations



Strong coupling evaluated at $\alpha_s(\mu_R)$

PDFs evaluated at $f(x, \mu_F)$

Pick **central values** according to  your favourite (theory friend's) recipe

- Physical Scales, Fastest Apparent Convergence, Least Sensitivity, Maximum Conformality, …

Vary by factor ~2 in either direction

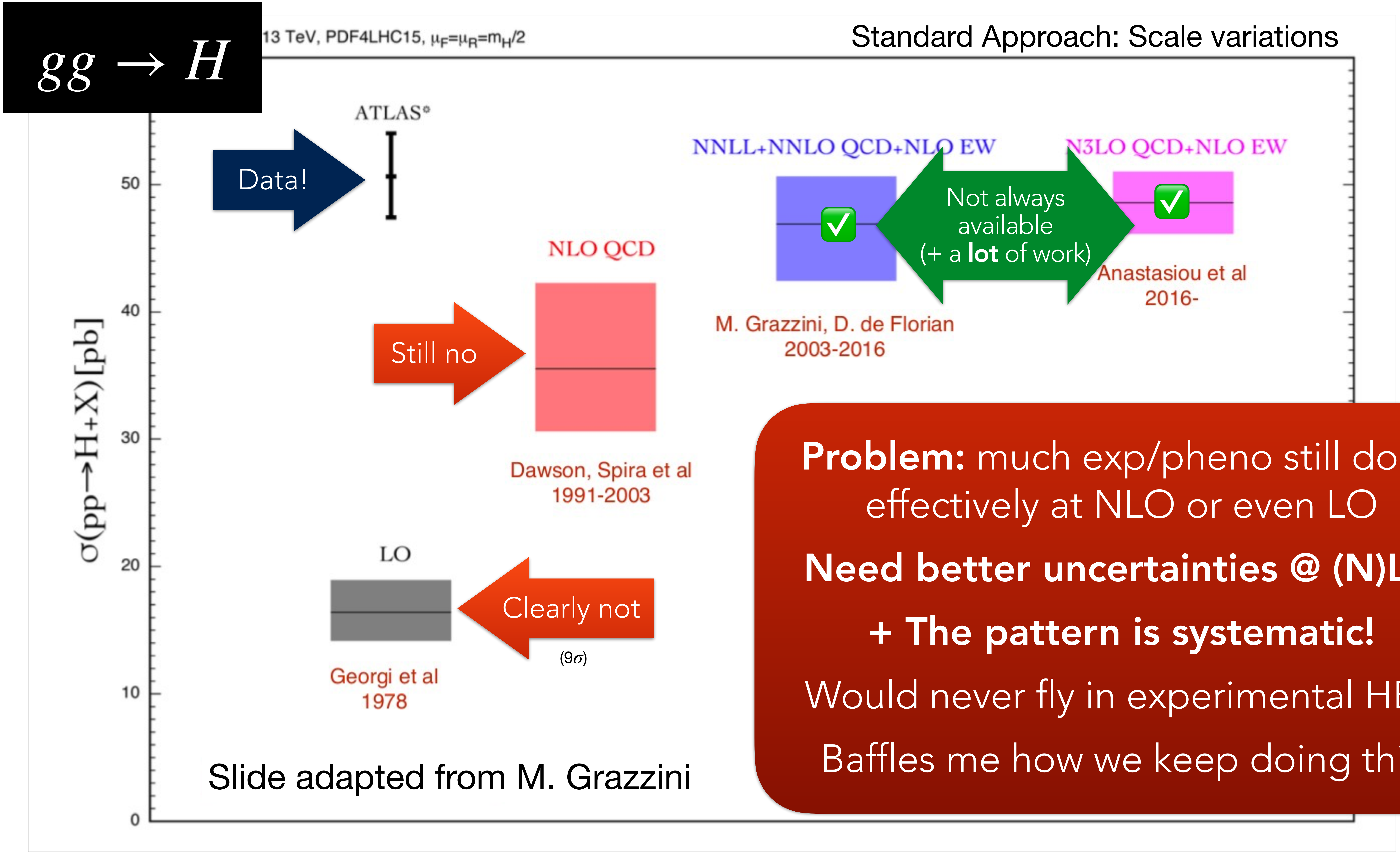
- Induces variations $\propto \ln 2$
- ⛔ drop anti-correlated ones $\propto (\ln 2)^2 = \ln 4$

I think many people suspect this is unsatisfactory and unreliable

Problem: little **explicit** guidance on what else to do …

Are **scale variations** good enough?

$gg \to H$



Standard Approach: Scale variations

Data!

Still no

Clearly not

(9σ)

Not always available
(+ a **lot** of work)

✓

✓

Slide adapted from M. Grazzini

Problem: much exp/pheno still done effectively at NLO or even LO

Need better uncertainties @ (N)LO

+ The pattern is systematic!

Would never fly in experimental HEP

Baffles me how we keep doing this

Beyond Scale Variations?

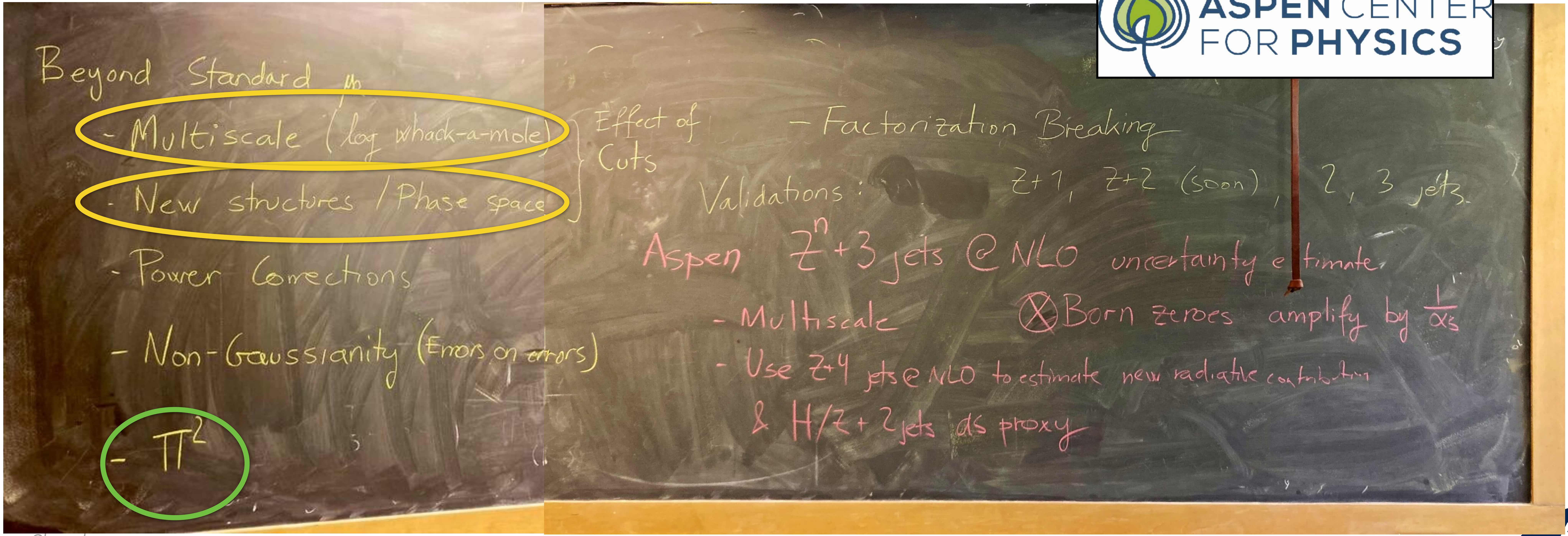
Interesting recent proposals have added "nuisance parameters"

May be the best you can do if you know nothing else.

But we ***do*** know some things! *Scientia Potentia Est!* [Hobbes, *Leviathan*, Latin Version, 1668]

Let's at least have a look …

ASPEN CENTER FOR PHYSICS



Beyond Standard μ
- Multiscale (log whack-a-mole)
- New structures / Phase space
- Power Corrections
- Non-Gaussianity (Errors on errors)
- π^2

Effect of Cuts

– Factorization Breaking

Validations: Z+1, Z+2 (soon), 2, 3 jets.

Aspen Z^n+3 jets @ NLO uncertainty estimate
- Multiscale
- ⊗ Born zeroes amplify by $\frac{1}{\alpha_s}$
- Use Z+4 jets @ NLO to estimate new radiative contribution & H/Z+2 jets as proxy

1) Multiscale Problems ~ Log Whack-a-Mole

Quantum Field Theory

Integrating propagators $\propto \frac{1}{q^2}$

between two different scales q_1 and q_2

$$\Longrightarrow \ln\left[\frac{q_1}{q_2}\right]$$

For **complex processes** involving **multiple scales**, say a few massive particles + a few jets:

$$\Longrightarrow \ln\left[\frac{\mu}{M_i}\right] , \ln\left[\frac{\mu}{p_{\perp i}}\right] , \ldots$$

Whack-a-mole

No single scale choice can absorb all the logs (best you can do is a geometric mean)
Nor can any factor-2 variation around such a scale (if the hierarchies are greater than factor-2)

At the very least, need to vary the *functional form* of the scale choice, for the problem at hand.

2) Higher Orders ➢ New Structures

Common to all of these is that they are not accessed at all by scale variations

- New helicity structures (e.g., relief of Born-level helicity suppression)
- New phase-space regions (e.g., accessing scales higher than μ_F)
- New colour structures
- New flavour structures
- Interference with other Born states

Often possible to **predict their presence** (or absence) on **general grounds**

⟶ **quantitative uncertainty estimates?**

3) Initial-Initial Form Factors

General amplitude structures from Glauber-type gauge bosons:

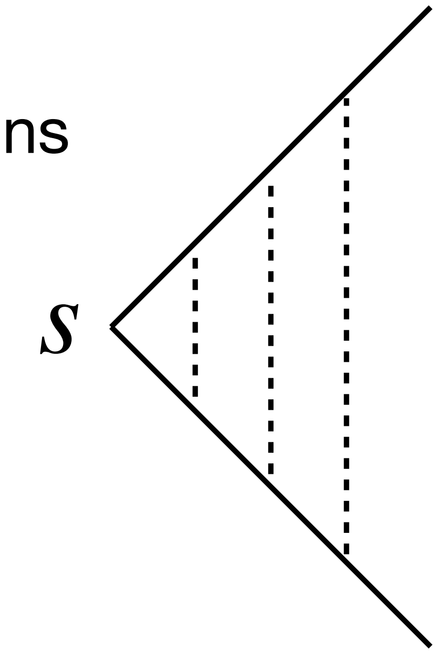
(Note: only aim here is getting lower bound on uncertainties from known amplitude structures, not discussing whether these terms should be resummed or not.)

Final-state parton pairs

At all orders:

Initial-state parton pairs

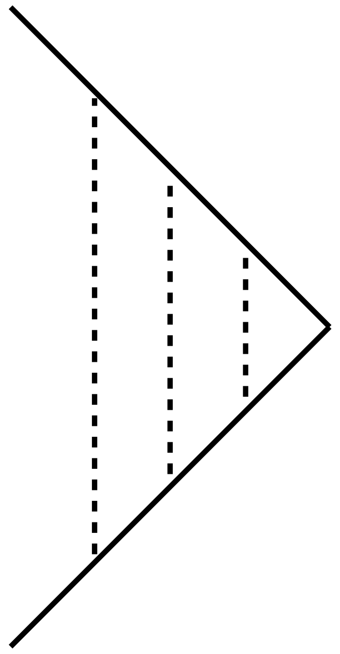
Loop corrections



$$\exp\left[-\frac{\alpha_s(\mu_F^2)}{2\pi}\mathscr{C}\ln^2(-\mu_F^2/s)\right]$$

Colour factor = C_A = 3 for gluons, C_F = 4/3 for quarks

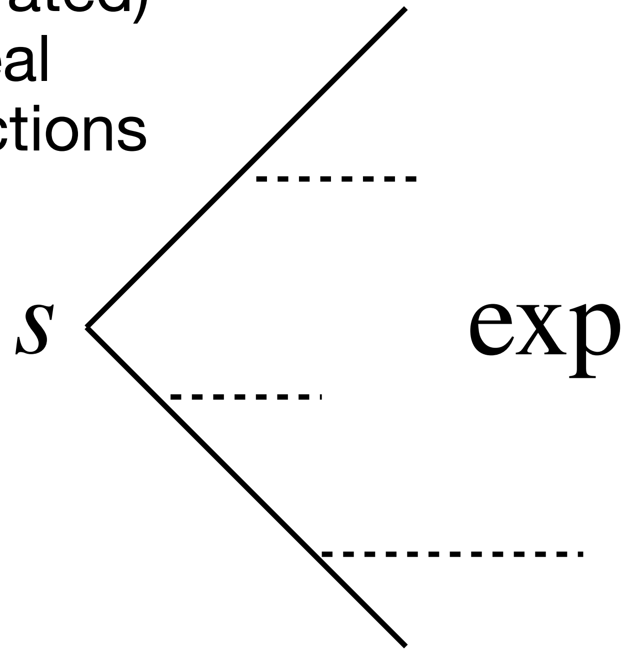
$\ln^2(-1) = -\pi^2$



$\mu^2 \sim s$

$$s \rightarrow \exp\left[\frac{\alpha_s(\mu_F^2)\pi}{2}\mathscr{C}\right]$$

(Integrated) Real corrections



Cancel against $2 \rightarrow n$ in inclusive sums

$$\exp\left[\frac{\alpha_s(\mu_F^2)}{2\pi}\mathscr{C}\ln^2(-\mu_F^2/s)\right]$$

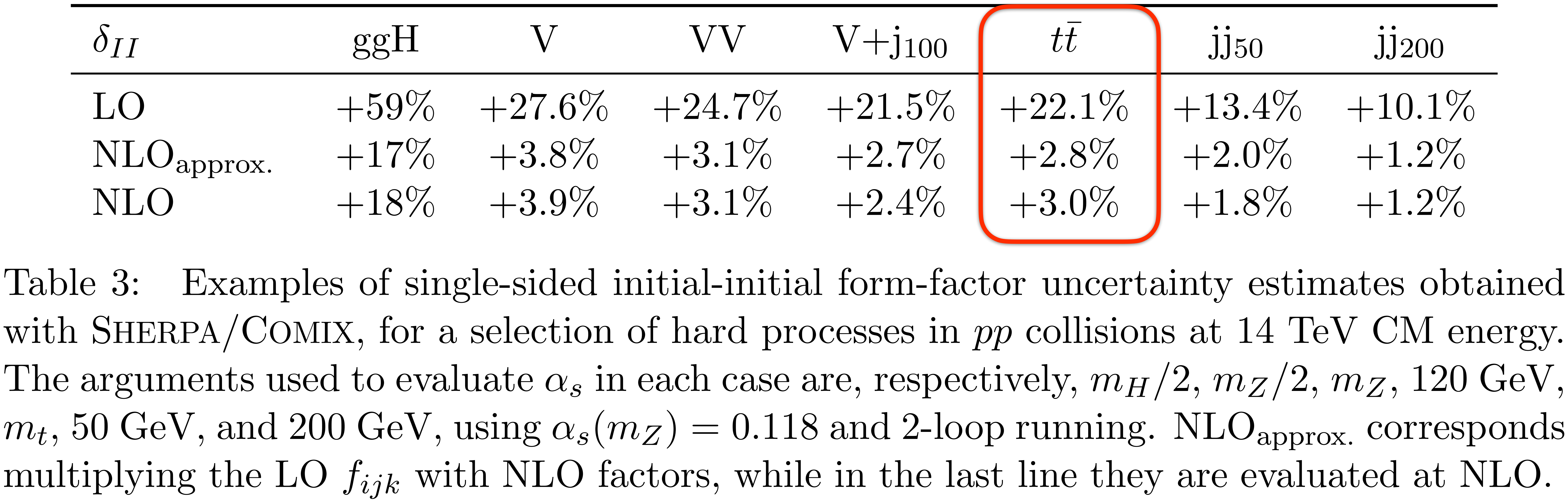
Cancel

~~We are not summing inclusively over $n \rightarrow 2$~~

No Cancellation

Use 1st uncontrolled order of this as additional uncertainty estimate for processes involving colour annihilation?

II Form Factors: Numerical Results



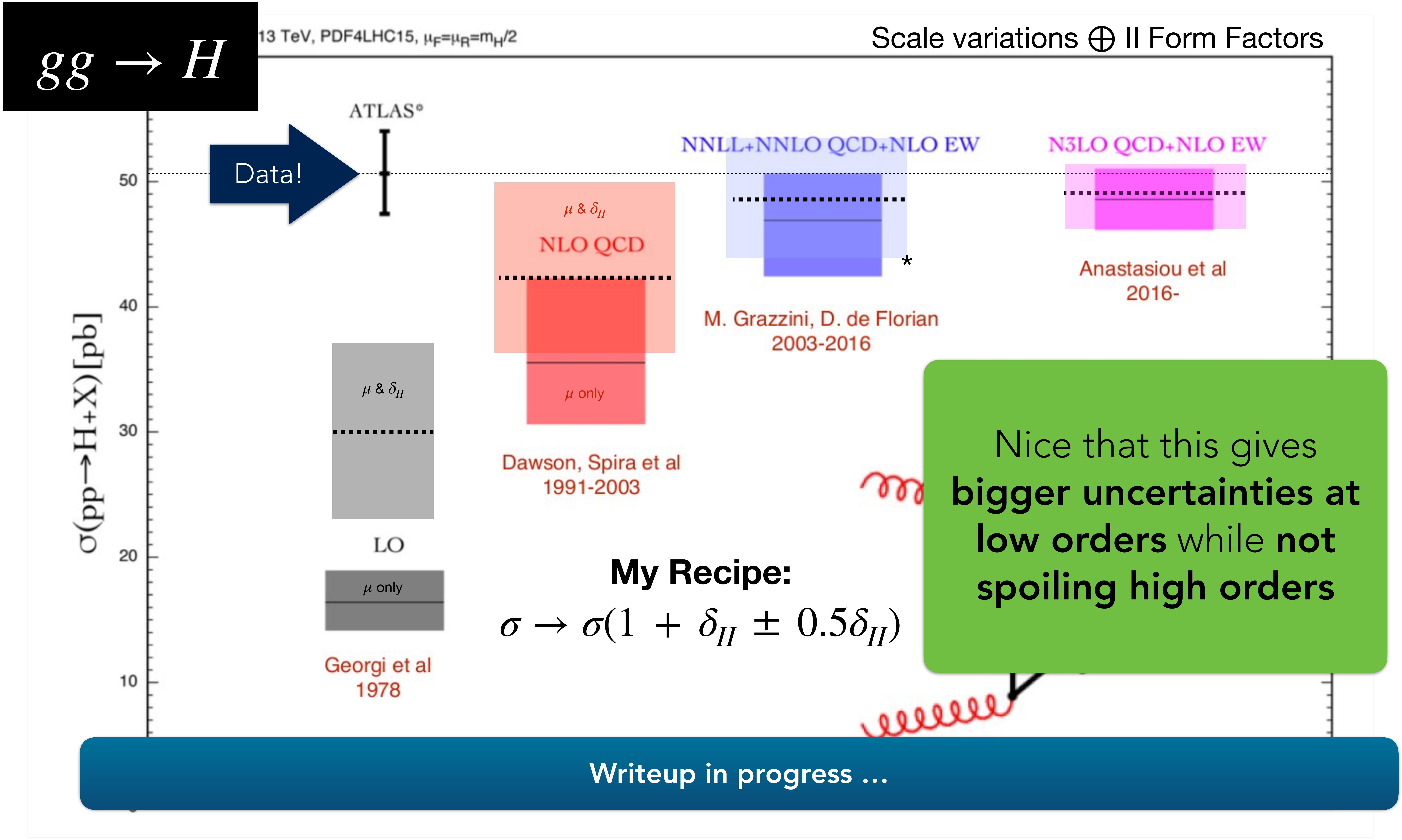
δ_{II}	ggH	V	VV	V+j100	$t\bar{t}$	jj50	jj200
LO	+59%	+27.6%	+24.7%	+21.5%	+22.1%	+13.4%	+10.1%
$\text{NLO}_{\text{approx.}}$	+17%	+3.8%	+3.1%	+2.7%	+2.8%	+2.0%	+1.2%
NLO	+18%	+3.9%	+3.1%	+2.4%	+3.0%	+1.8%	+1.2%

Table 3: Examples of single-sided initial-initial form-factor uncertainty estimates obtained with SHERPA/COMIX, for a selection of hard processes in *pp* collisions at 14 TeV CM energy. The arguments used to evaluate α_s in each case are, respectively, $m_H/2$, $m_Z/2$, m_Z, 120 GeV, m_t, 50 GeV, and 200 GeV, using $\alpha_s(m_Z) = 0.118$ and 2-loop running. $\text{NLO}_{\text{approx.}}$ corresponds multiplying the LO f_{ijk} with NLO factors, while in the last line they are evaluated at NLO.

Calculations by D. Reichelt for Aspen study

Adding Single-Sided II Form Factors

$gg \to H$



Data!

My Recipe:

$$\sigma \to \sigma(1 + \delta_{II} \pm 0.5\delta_{II})$$

Nice that this gives **bigger uncertainties at low orders** while **not spoiling high orders**

Writeup in progress …

❷ Shower Uncertainties

Uncertainties in Parton Showers

Standard for Shower Uncertainties: Renormalization-scale variations

Example: DGLAP-based shower (e.g., PYTHIA):

$$|M_{n+1}|^2 \sim \sum_{i\in\text{partons}} \underbrace{\frac{\alpha_s^{\rm MC}(\mu_i^2)}{4\pi}}_{\mu_i^2 \,\propto\, p_{\perp i}^2} \underbrace{\mathscr{C}_i}_{\substack{2C_F \text{ for quark,} \\ C_A \text{ for gluon}}} \underbrace{\left(\frac{P_i(z)}{Q_i^2}\right)}_{\substack{\text{DGLAP Splitting Kernel} \\ \text{(Or dipole/antenna/...)}}} |M_n|^2 \underbrace{\Delta_n(t_n, t_{n+1})}_{\text{Sudakov factor}}$$

t is the shower evolution/ ordering variable

Varying μ_i only induces terms proportional to the shower splitting kernels

Actual higher-order MEs also have:

Non-trivial colour interferences outside collinear limits,

Non-singular terms (dominate far from singular limits),

Higher-order log terms not captured exactly by $\Delta_n(t_n, t_{n+1})$

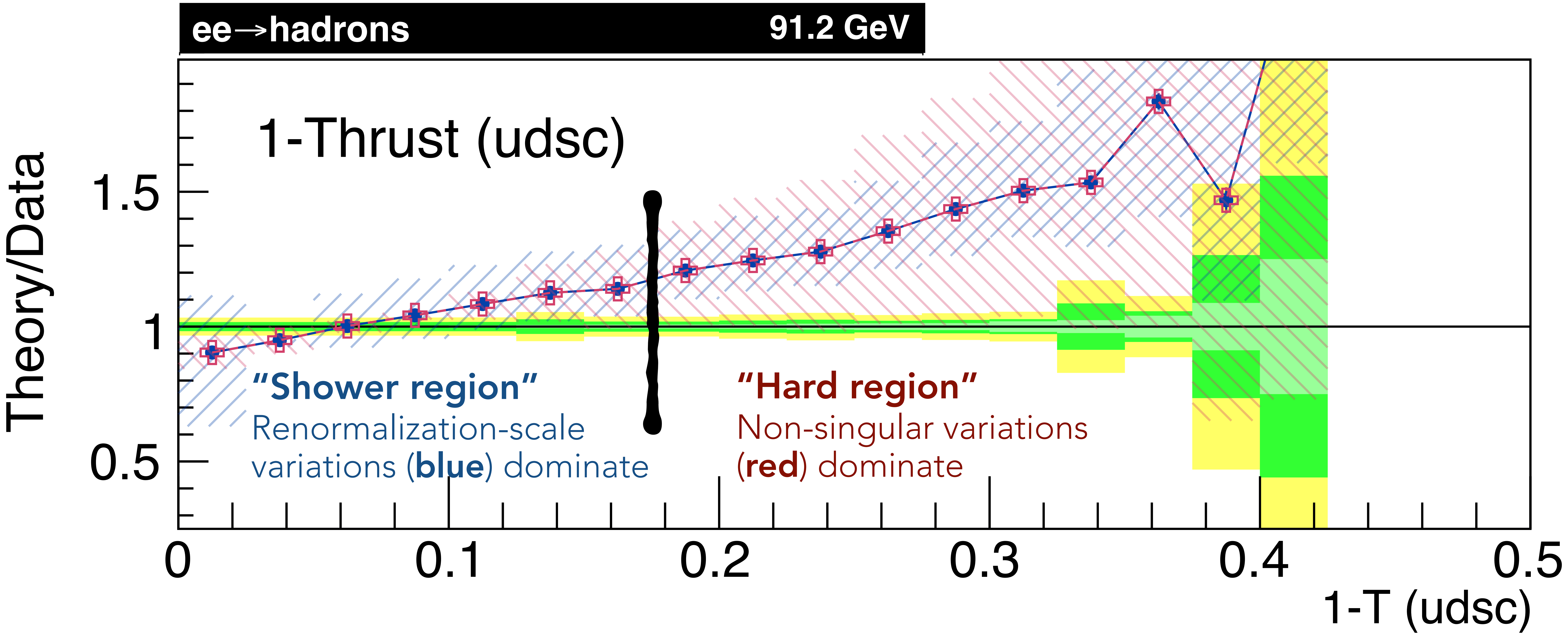
Vary these too!
[Hartgring, Laenen, PS JHEP 10 (2013) 127]

Implemented in PYTHIA 8 (`cNS`) [Mrenna, PS, PRD94 (2016) 7]

Non-Singular Variations: Example

Example from Mrenna & PS, “Automated Parton-Shower Variations in Pythia 8”, PRD 94 (2016) 7

Can vary **renormalisation-scale** and **non-singular terms** independently



“Shower region”
Renormalization-scale variations (**blue**) dominate

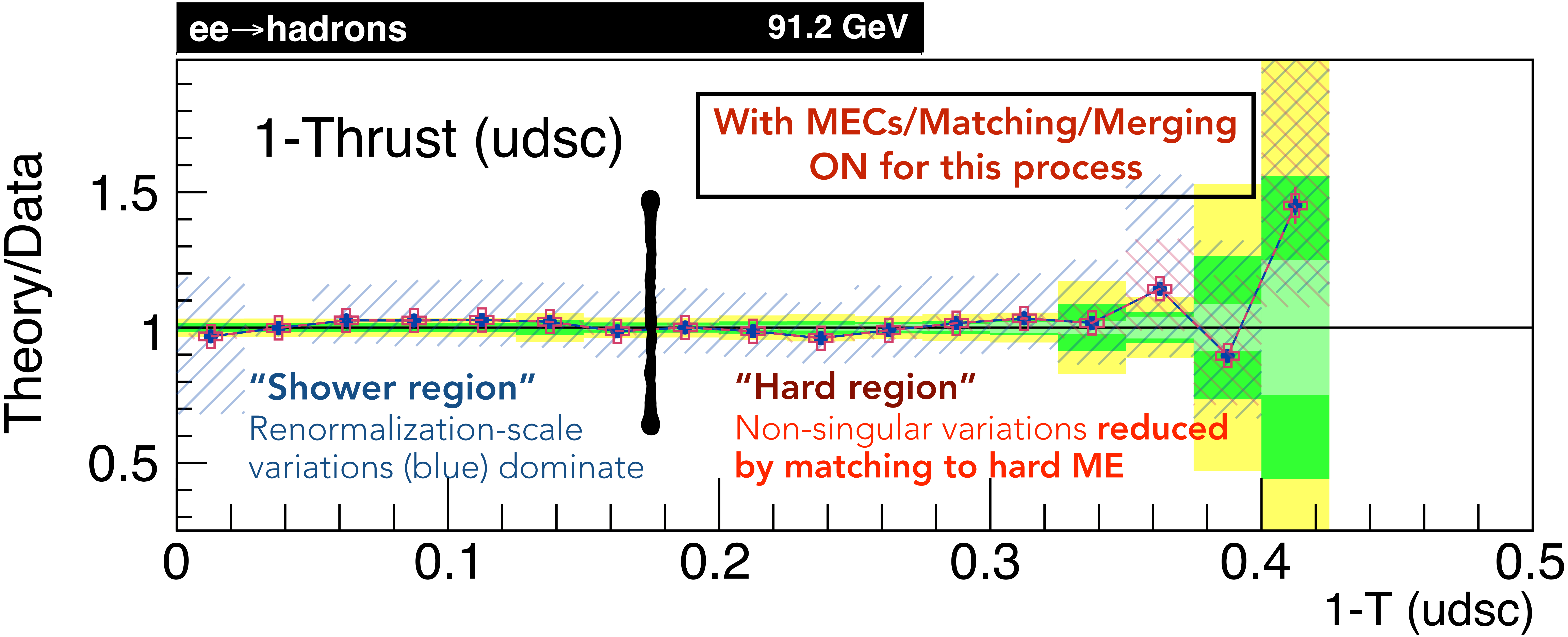
“Hard region”
Non-singular variations (**red**) dominate

Note: ME corrections were switched off for illustration here. Would reduce **red** band, but not **blue**.

Effect of Matching to Matrix Elements

Example from Mrenna & PS, "Automated Parton-Shower Variations in Pythia 8", PRD 94 (2016) 7

Can vary **renormalisation-scale** and **non-singular terms** independently



With MECs/Matching/Merging ON for this process

"Shower region"
Renormalization-scale variations (blue) dominate

"Hard region"
Non-singular variations **reduced by matching to hard ME**

Note also: in the context of merging, consistent scale choices can be important: EPJC 72 (2012) 2078

❸ Matching Uncertainties

Powheg Box — A Subtlety

[Alioli et al, 2010]

Industry Standard: "Powheg Box"

Exploits having its own definition of "p_T"

≠ shower's definition of p_T

Con: breaks clean matching

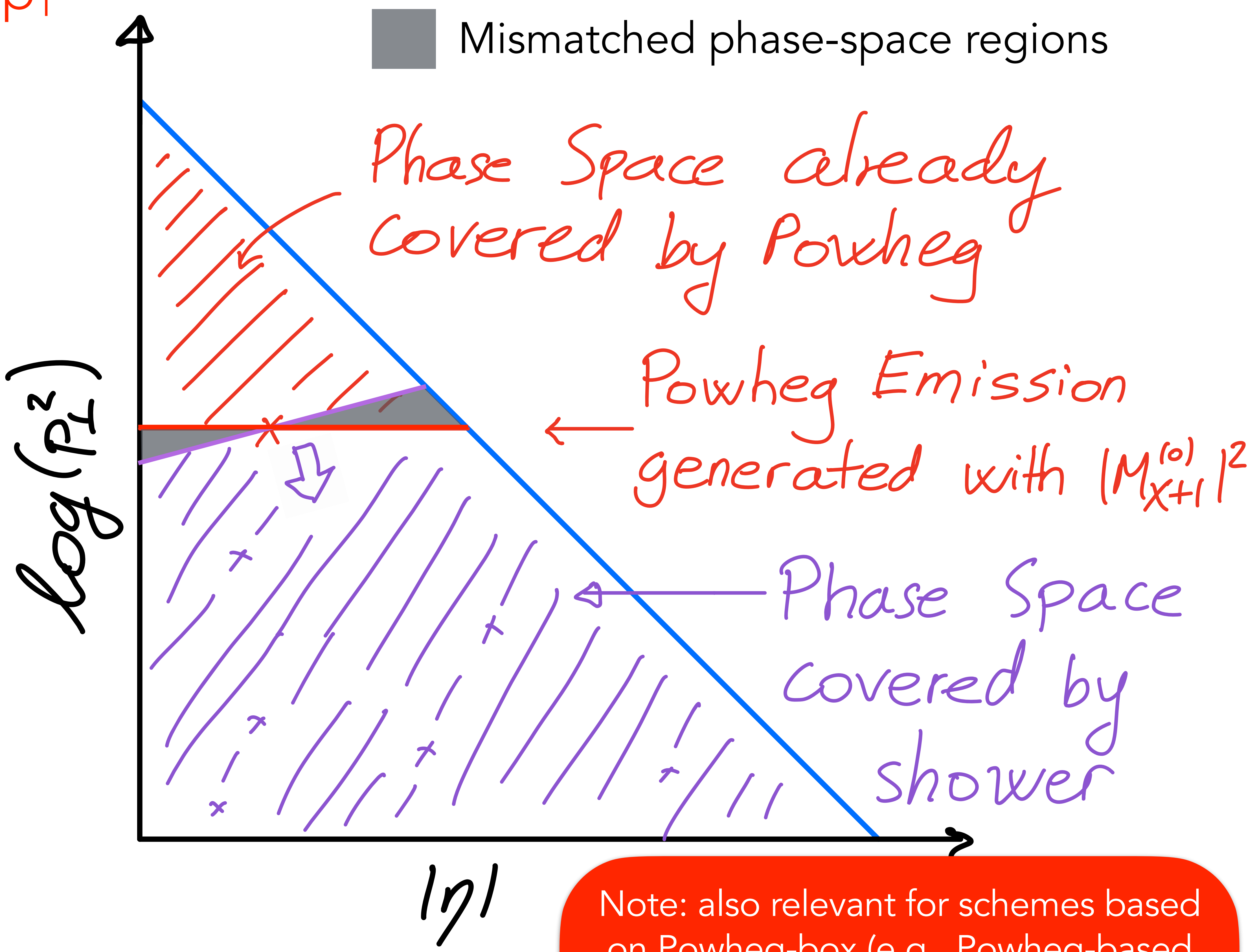
Solution: Vetoed Showers

(+ truncated showers)

Works very well for simple cases

Induces an uncertainty/ambiguity

Purely associated with the matching scheme (not physical)



Can be important for complex / multi-scale processes.

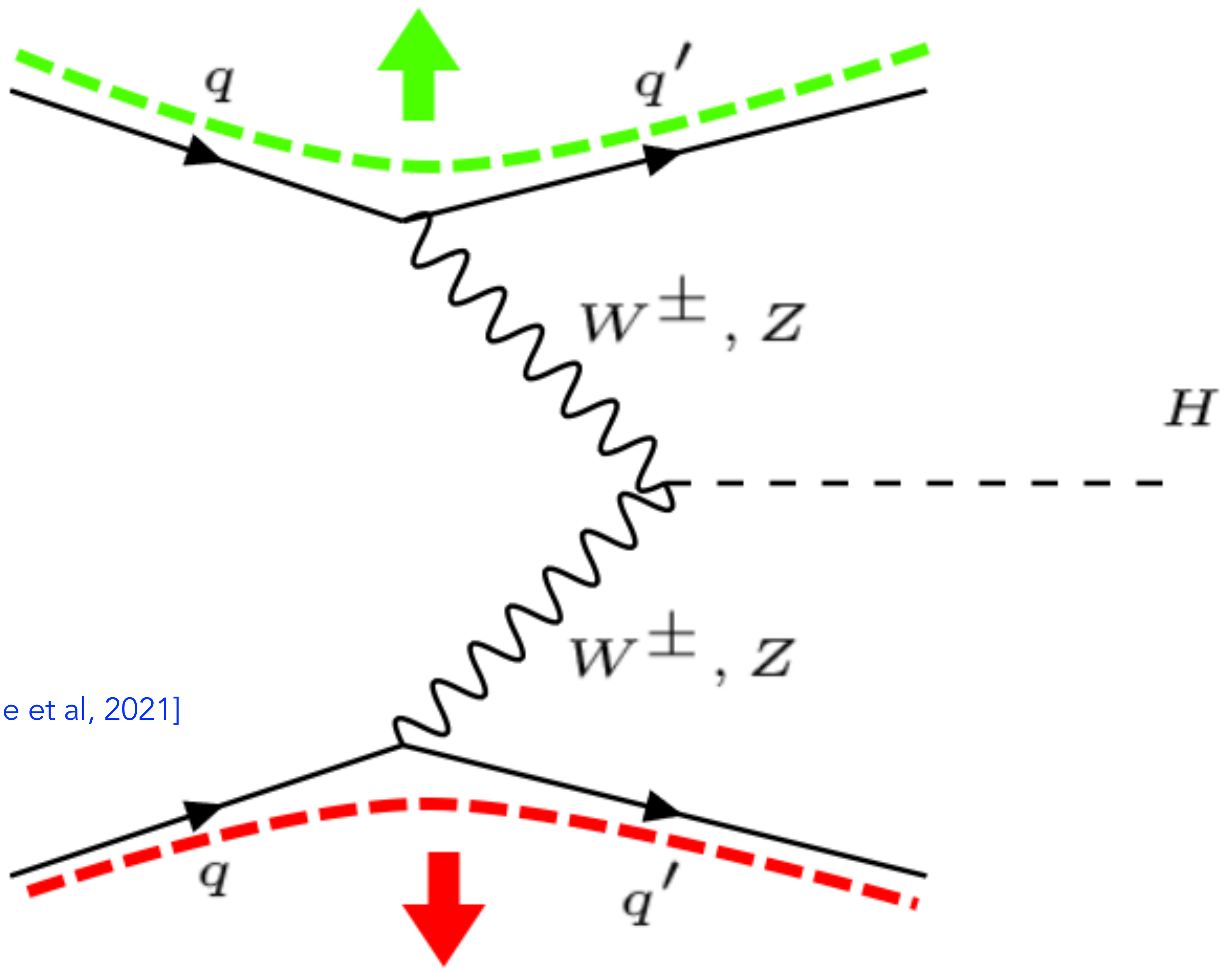
E.g., Nason, Oleari arXiv:1303.3922

VBF: [Höche et al., SciPost Phys. 12 (2022) 1](SciPost Phys. 12 (2022) 1)

Note: also relevant for schemes based on Powheg-box (e.g., Powheg-based merging, MiNNLOPS)

A More Complex Process

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



[Höche et al, 2021]

Multiple emitters
⤳ 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

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

POWHEG-Box Matching Systematics

Varying the POWHEG-Box ↔ PYTHIA hardness-scale ambiguity

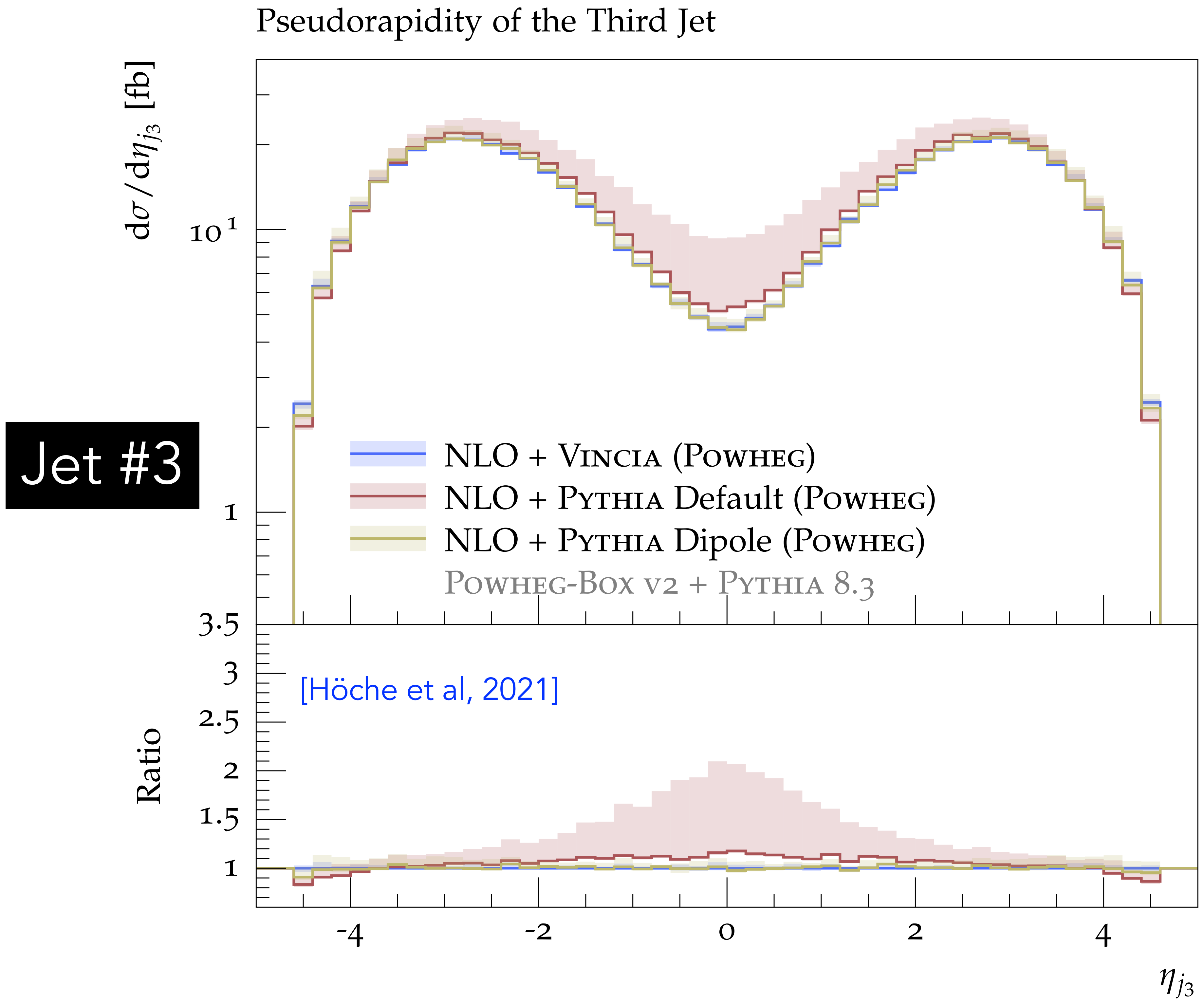
`POWHEG:pThard = 0` # Veto at $p_{\perp j;i}^{\mathrm{POWHEG}}$ = **SCALUP** = scale at which POWHEG says it emitted this parton

`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



▬ 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

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

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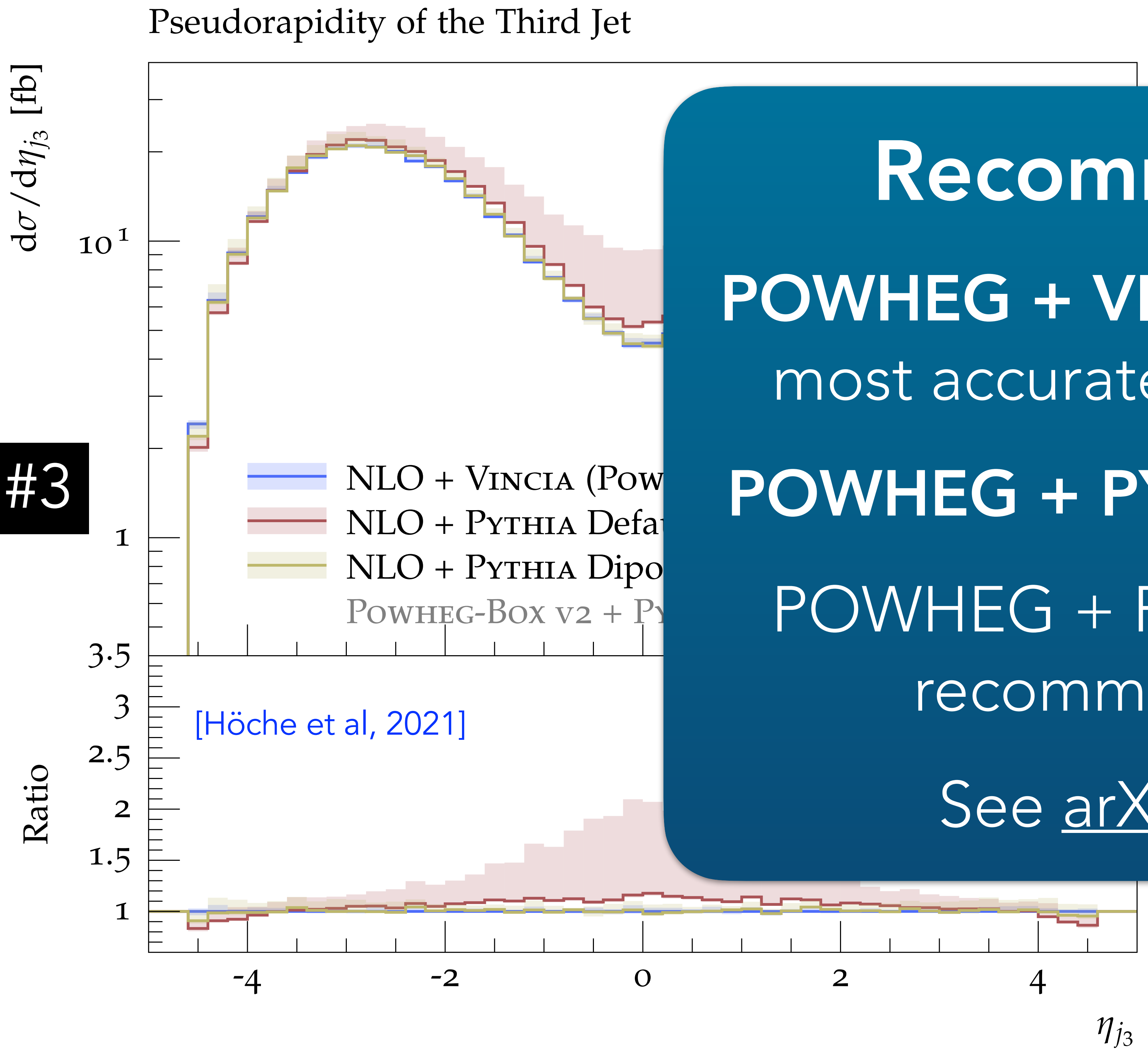
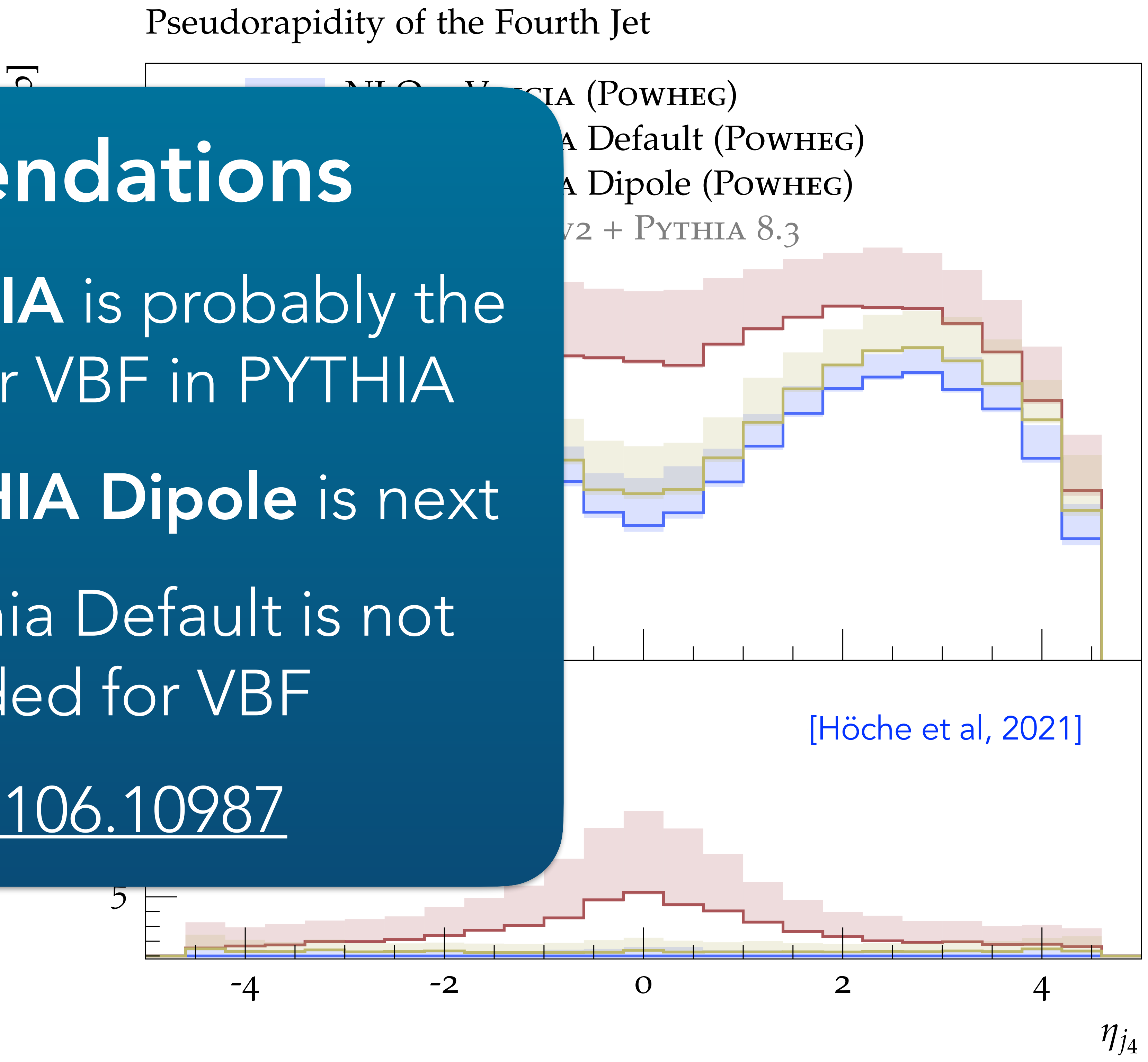
[Nason, Oleari 2013]

Less radiation ↓

Jet #3





Jet #4

Recommendations

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

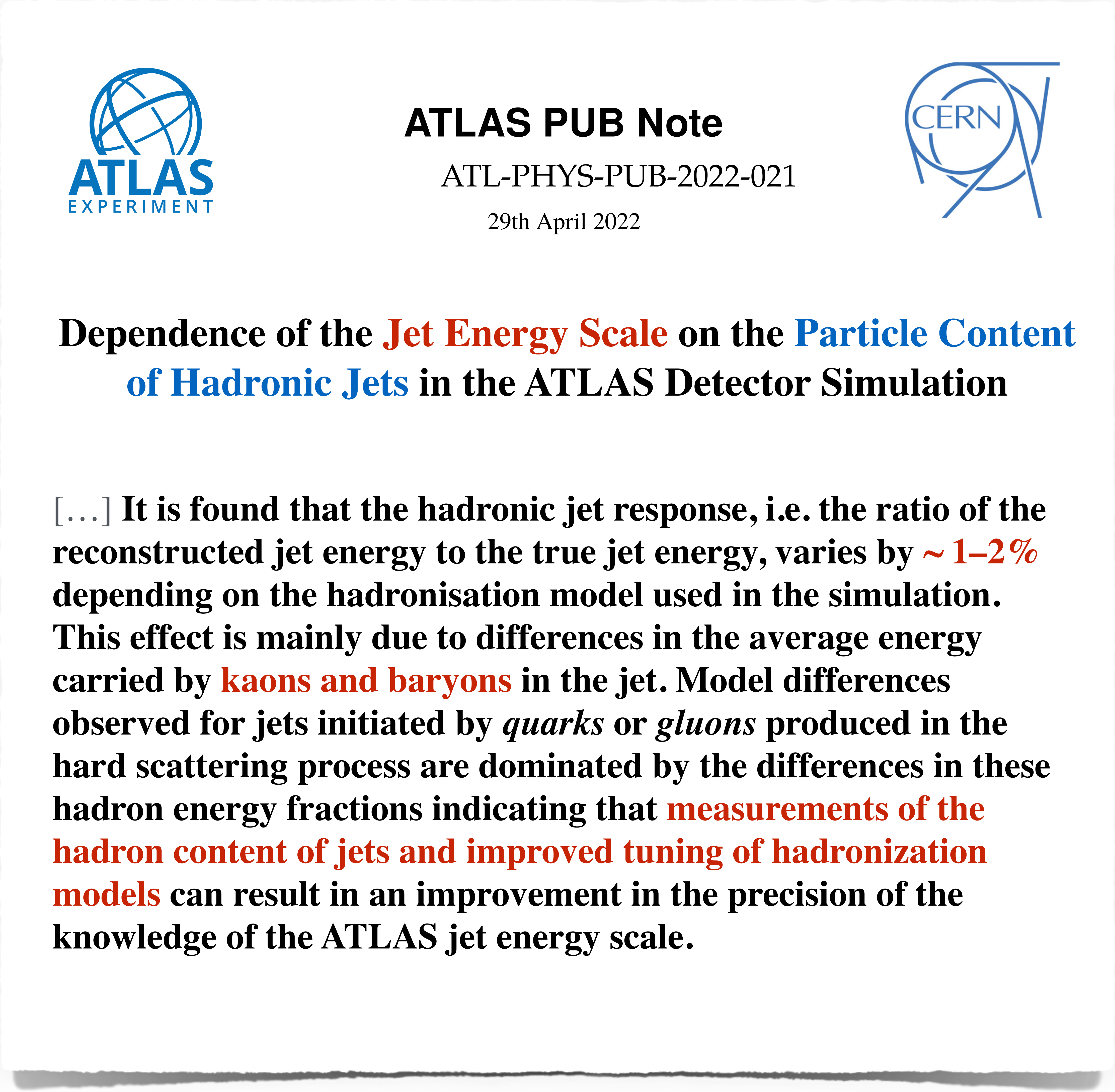
POWHEG + PYTHIA Dipole is next

POWHEG + Pythia Default is not recommended for VBF

See arXiv:2106.10987

④ Non-Perturbative Uncertainties

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

[…] **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 E_T carried by baryons (& 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!

➪ Careful Modelling & Constraints

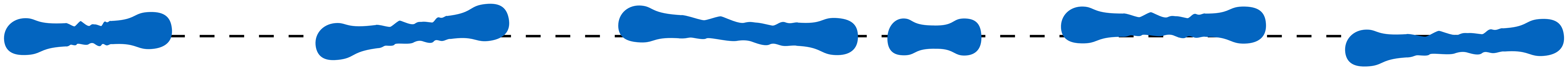
- Interplay with advanced UE models
- In-situ constraints from LHC data
- Revisit comparisons to LEP data w PID

NEW

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 → **PYTHIA 8.311**

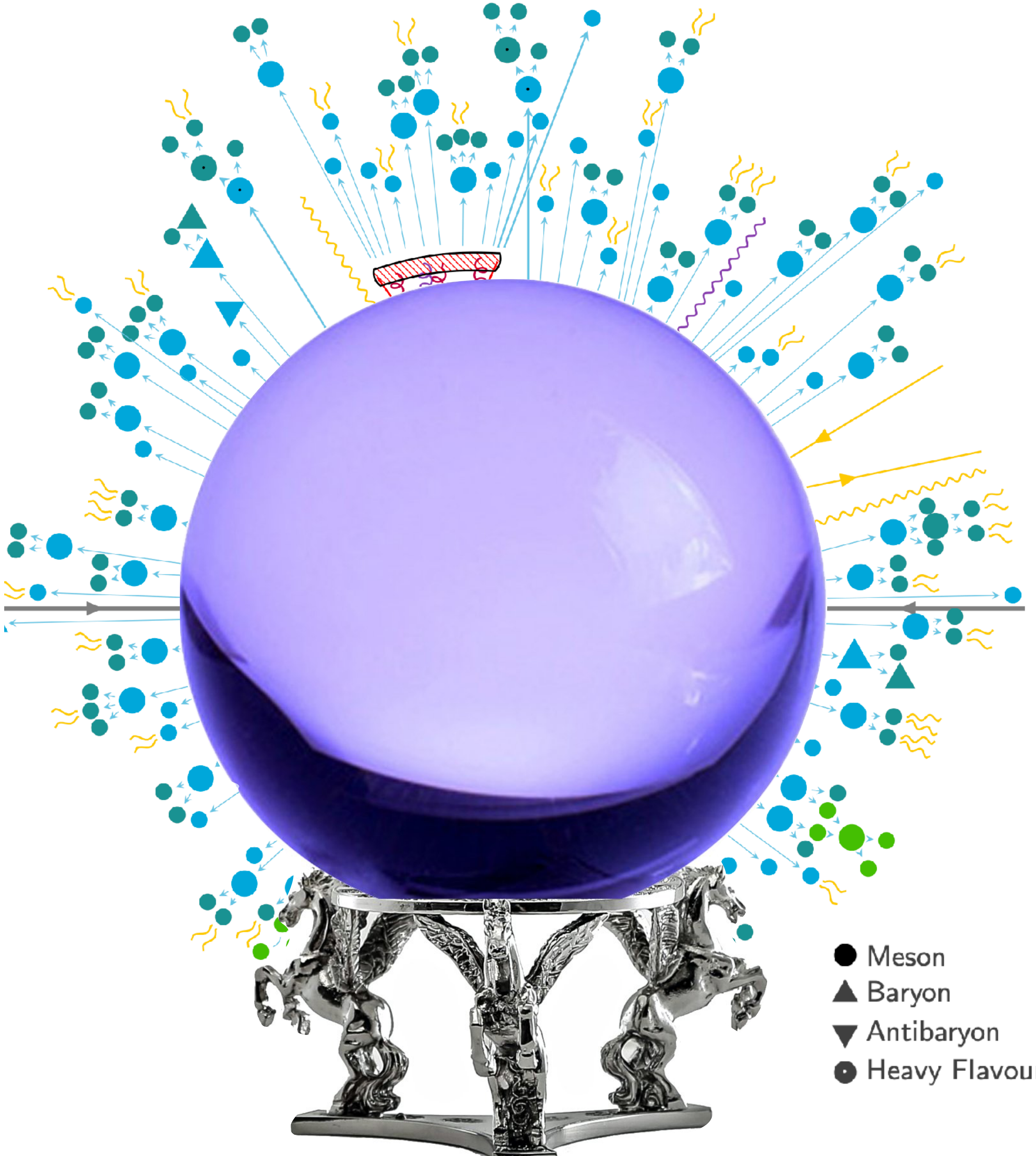
+ Flavour variations (still experimental, writeup in progress) → **PYTHIA 8.313**

Note: automated (weight) variations not available for MPI (UE) or Colour Reconnections (CR)

Outlook

- ○ Hard Interaction
- ● Resonance Decays
- 🟪 MECs, Matching & Merging
- 🟥 FSR
- 🟦 ISR*
- 🟨 QED
- 🟧 Weak Showers
- 🟫 Hard Onium
- ○ Multiparton Interactions
- ☐ Beam Remnants*

(: incoming lines are crossed)*



- ▨ Strings
- ▨ Ministrings / Clusters
- ☐ Colour Reconnections
- ☐ String Interactions
- ☐ Bose-Einstein & Fermi-
- 🟦 Primary Hadrons
- 🟩 Secondary Hadrons
- 🟩 Hadronic Reinteraction

- ● Meson
- ▲ Baryon
- ▼ Antibaryon
- ⊙ Heavy Flavour