Monte Carlo Event Generators — ❷

Peter Skands — Monash University

❶

General Introduction

Event Simulation 1: Dynamics of Confinement

❷

Event Simulation 2

Perturbative Aspects ➤ **Formal Theory**

Perturbative Uncertainties

This Lecture

The bad news:

Things will get a bit more technical (e.g., NNLO)

The good news:

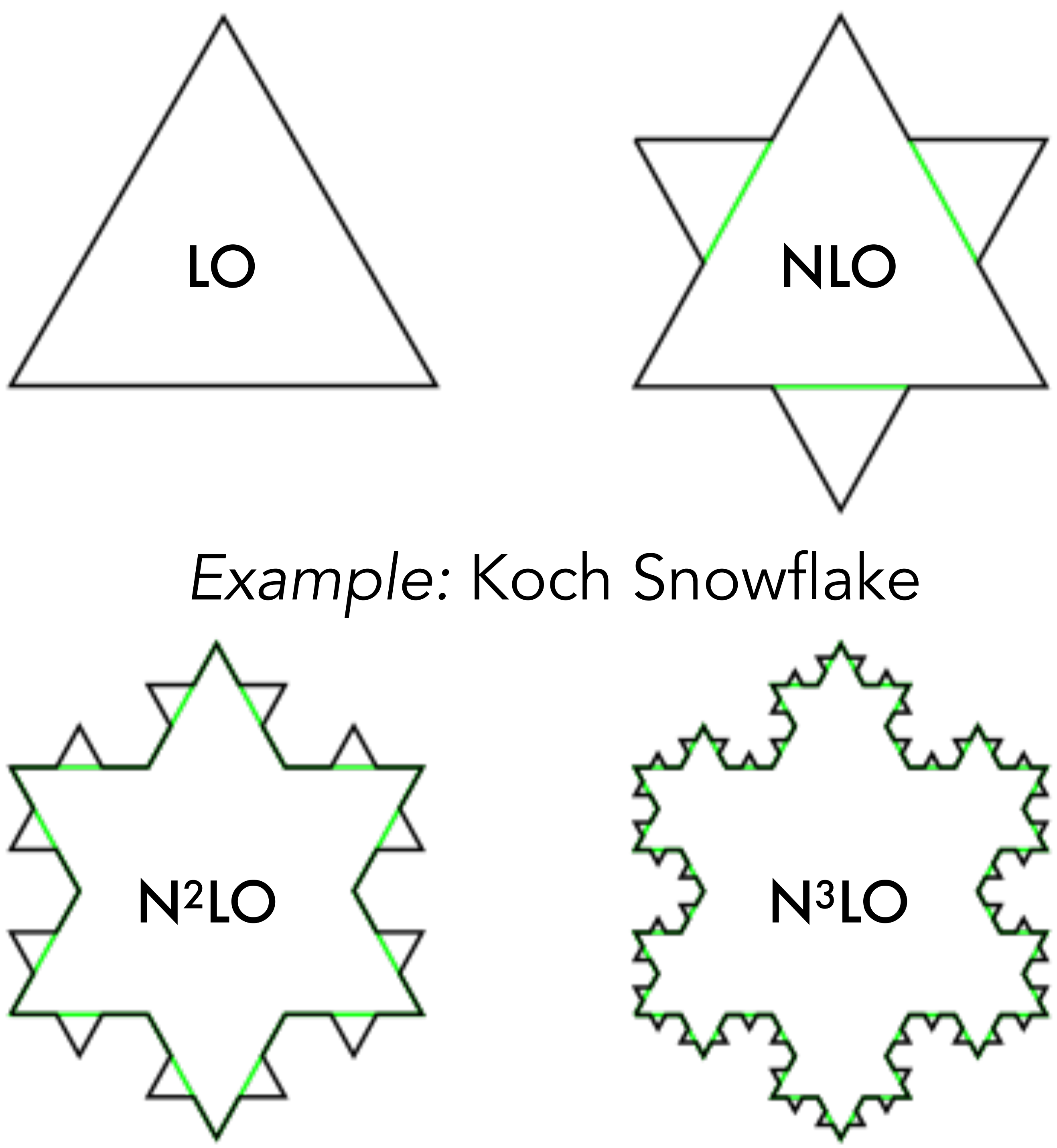
You can look forward to **percent-level accurate MCs** for HL-LHC and future colliders

Perturbation Theory

~ Calculate the area of a shape ($d\sigma$) with higher and higher detail

Difference from exact area $\propto \alpha^{n+1}$

Fixed Order



Example: Koch Snowflake

Note: (over)simplified analogy, mainly for IR structure. More at each order than shown here.

Perturbation Theory

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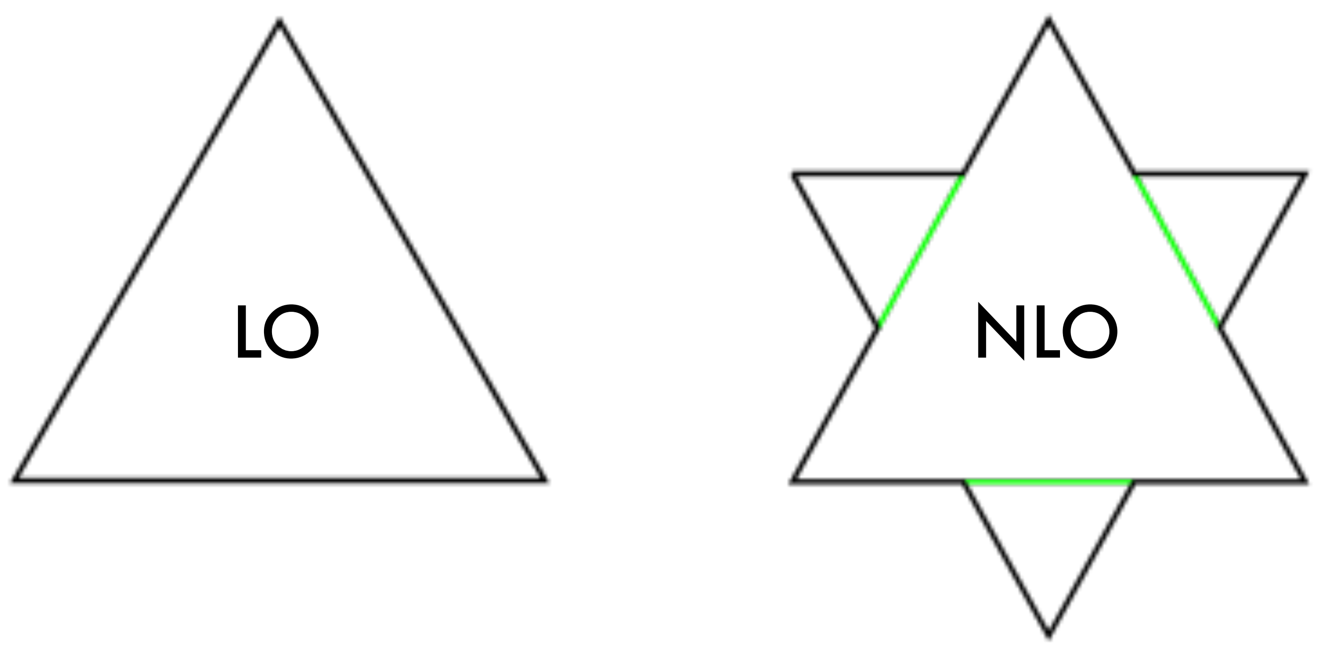
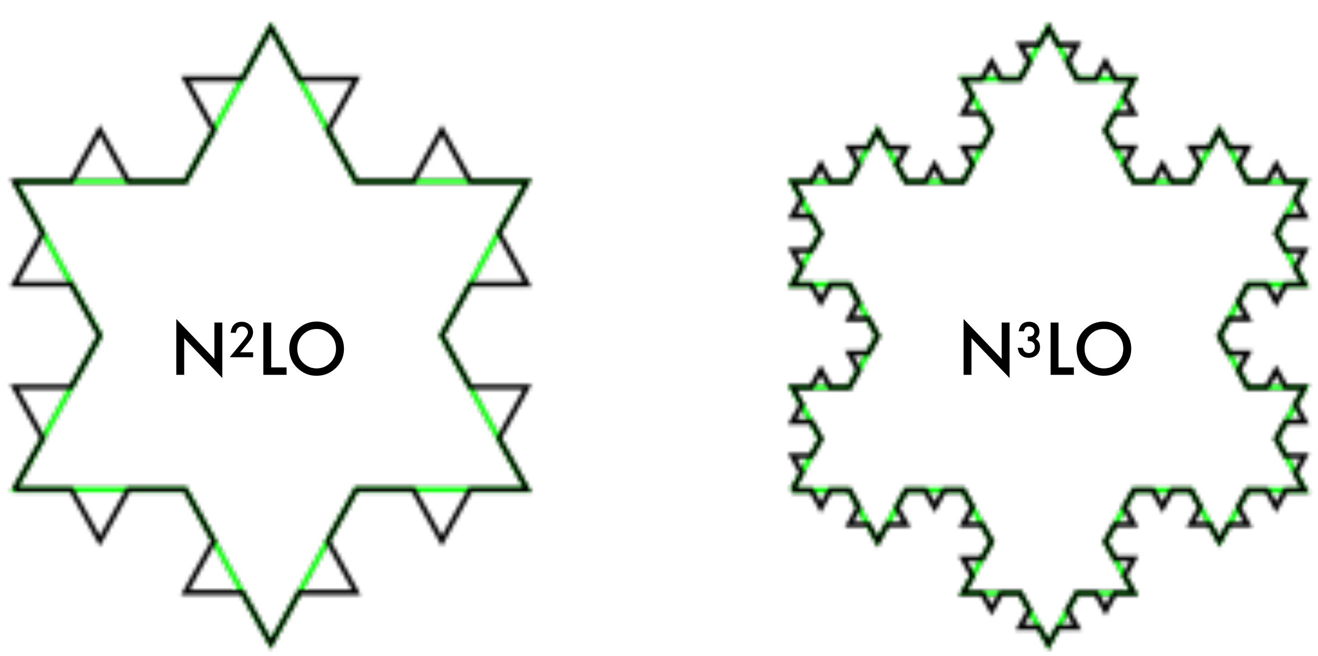
Fixed Order



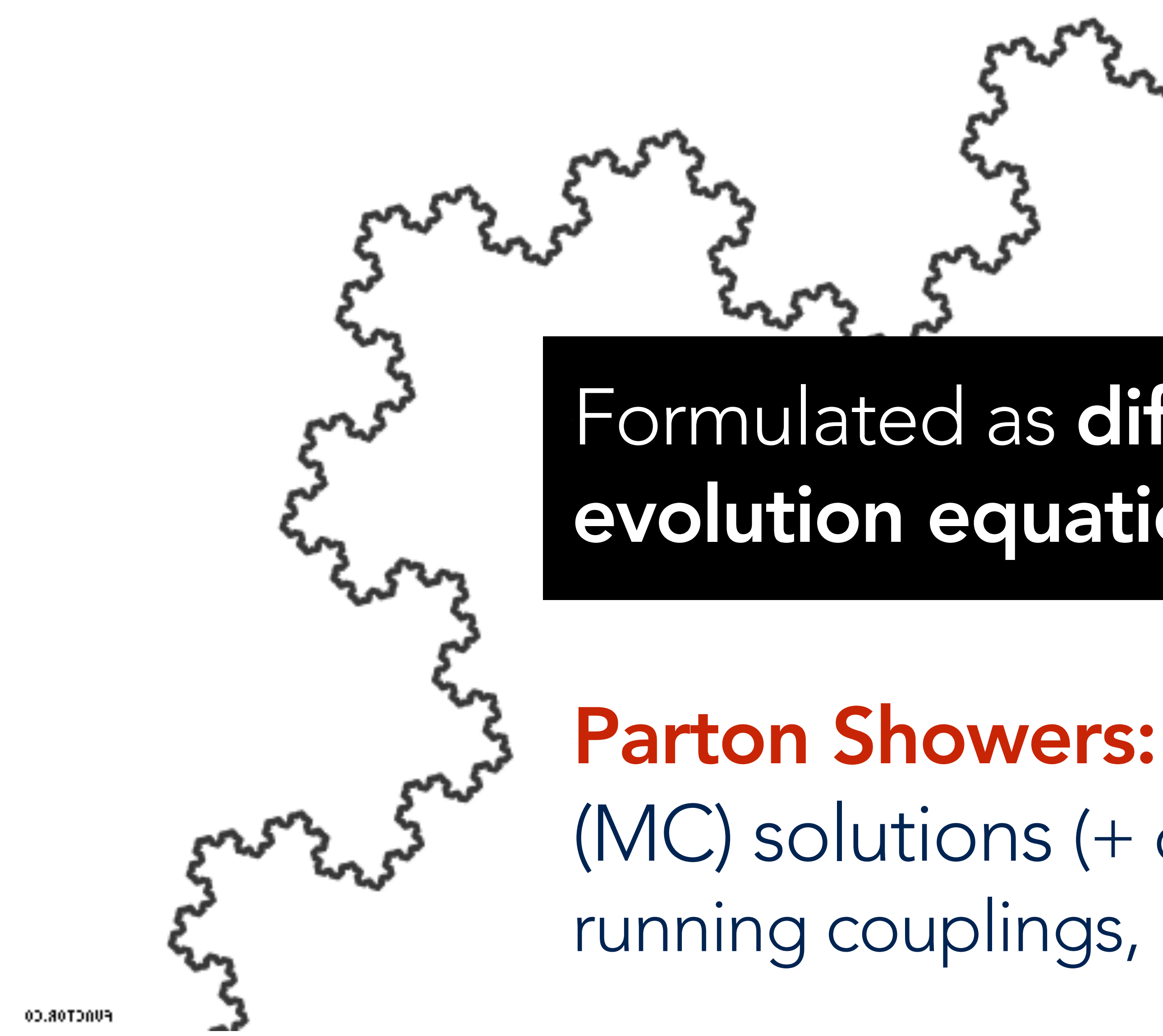
Example: Koch Snowflake



Resummation / Parton Showers

Massless gauge theories

Scale invariance ➜ *fractal* substructure



Formulated as **differential evolution equations**

Parton Showers: stochastic (MC) solutions (+ can build in running couplings, masses)

Note: (over)simplified analogy, mainly for IR structure. More at each order than shown here.

Why go beyond **Fixed-Order** perturbation theory?

Simple example of a multi-scale observable:

Fraction of events that pass a **jet veto** (for arbitrary hard process $Q_{\rm hard} \gg 1\,{\rm GeV}$)

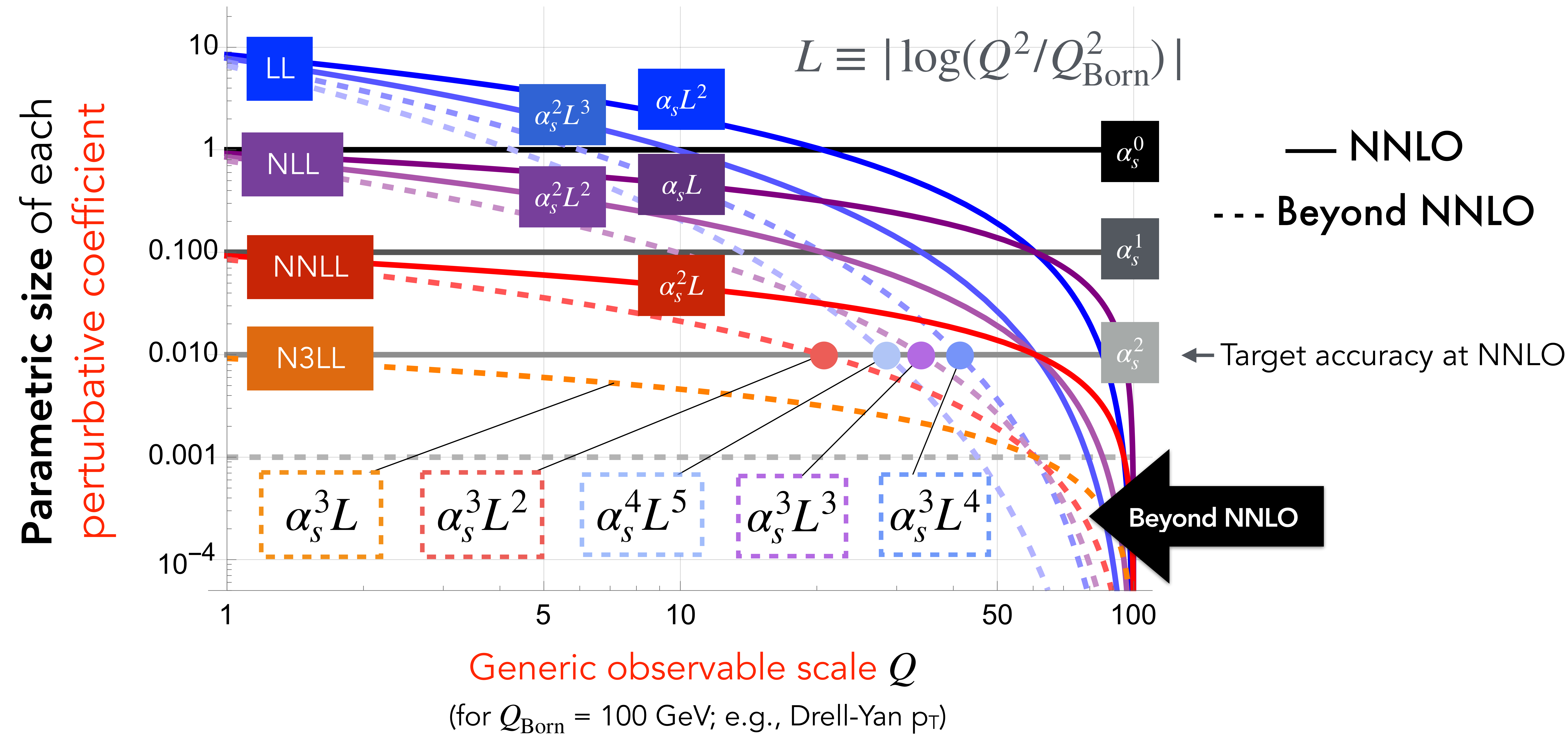
(i.e., **no additional jets** resolved above $Q_{\rm veto}$):

$$\overbrace{1}^{\rm LO} \; - \; \overbrace{\alpha_s(L^2 + L + F_1)}^{\rm NLO} \; + \; \overbrace{\alpha_s^2(L^4 + L^3 + L^2 + L + F_2)}^{\rm NNLO} + \; \dots$$

$$L \propto \ln(Q^2_{\rm veto} / Q^2_{\rm hard})$$

$$\left(\text{Logs arise from integrals over propagators} \propto \frac{1}{q^2} \right)$$

The Case for **Combining** Fixed-Order Calculations with **Resummations**



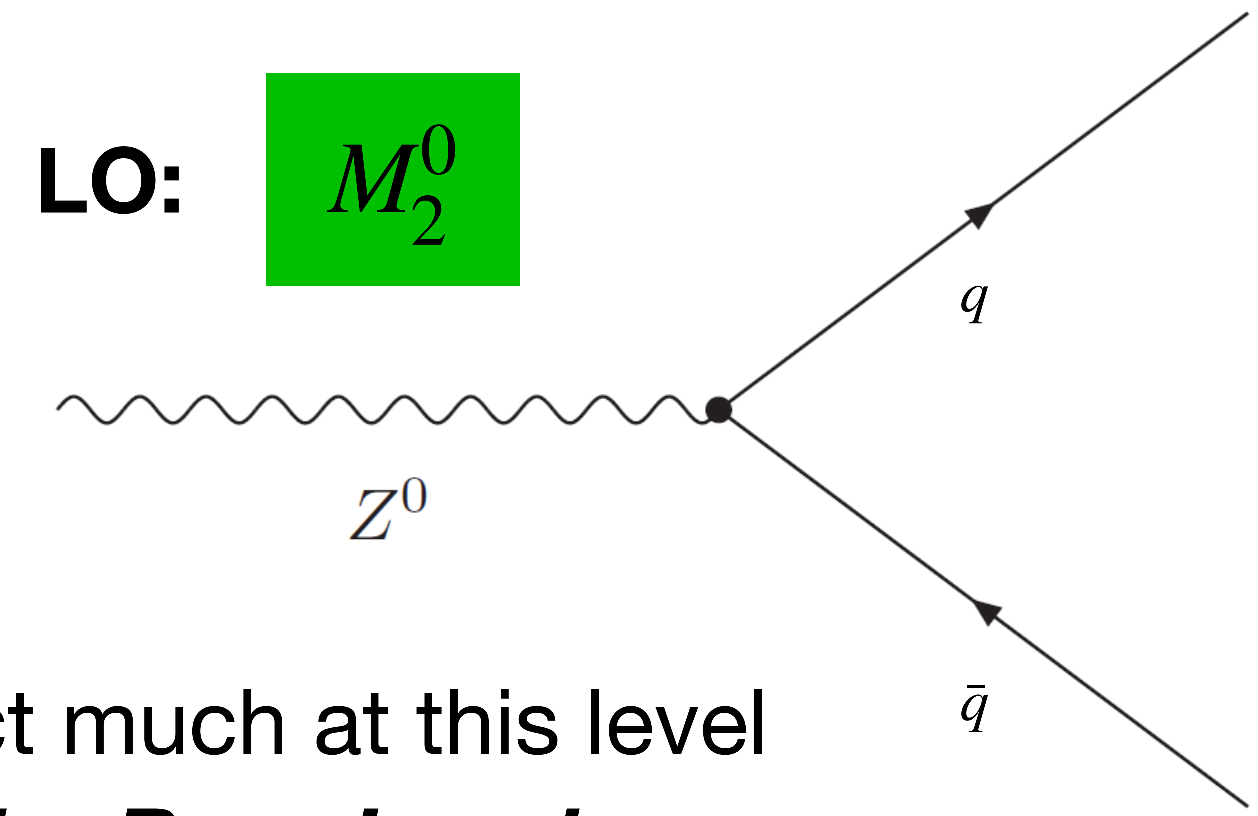
Resummation (*e.g.*, by showering) extends domain of validity of perturbative calculations

Jet Rates at Fixed Order

Consider $Z \to q\bar{q}$

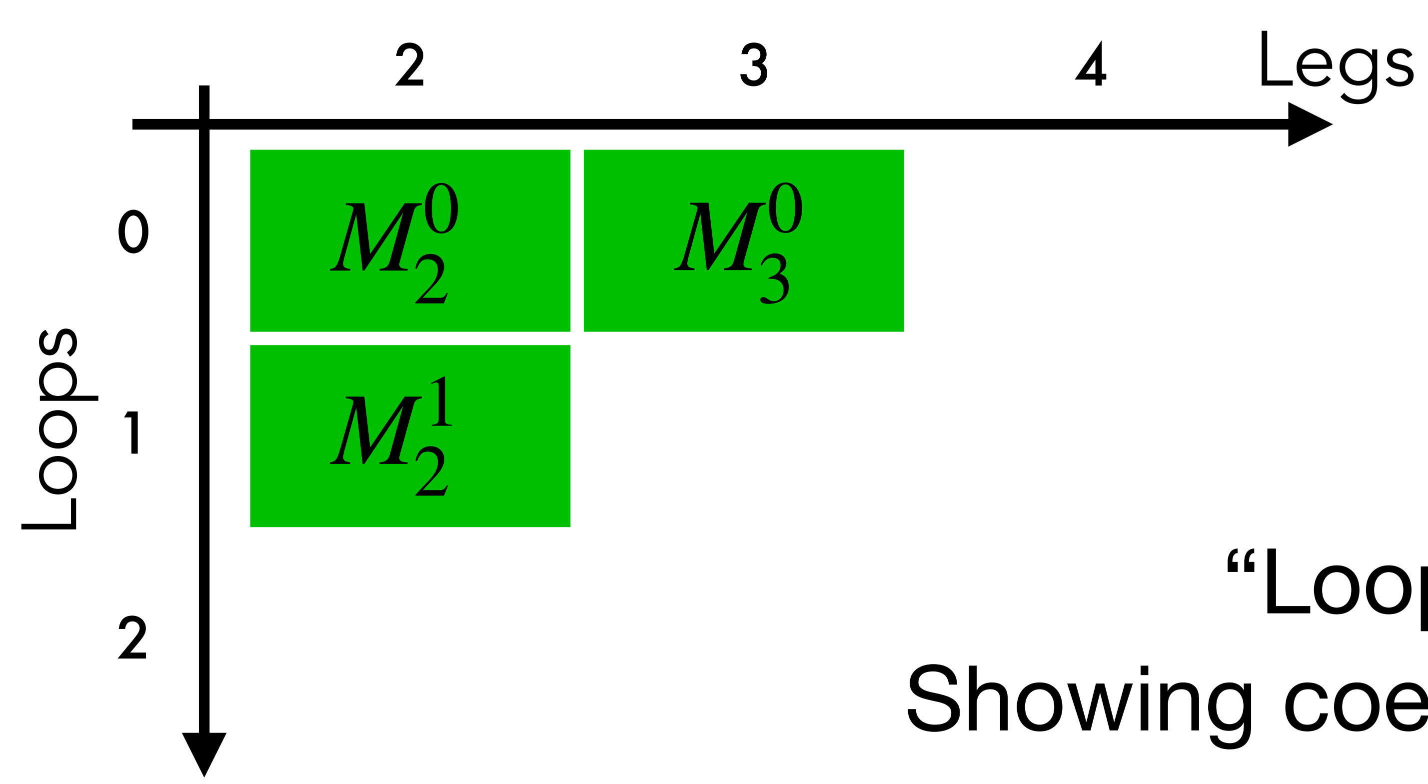
M_n^ℓ = QFT amplitude for n legs, ℓ loops

LO: M_2^0



Can't predict much at this level
a.k.a. ***the Born Level***

NLO:



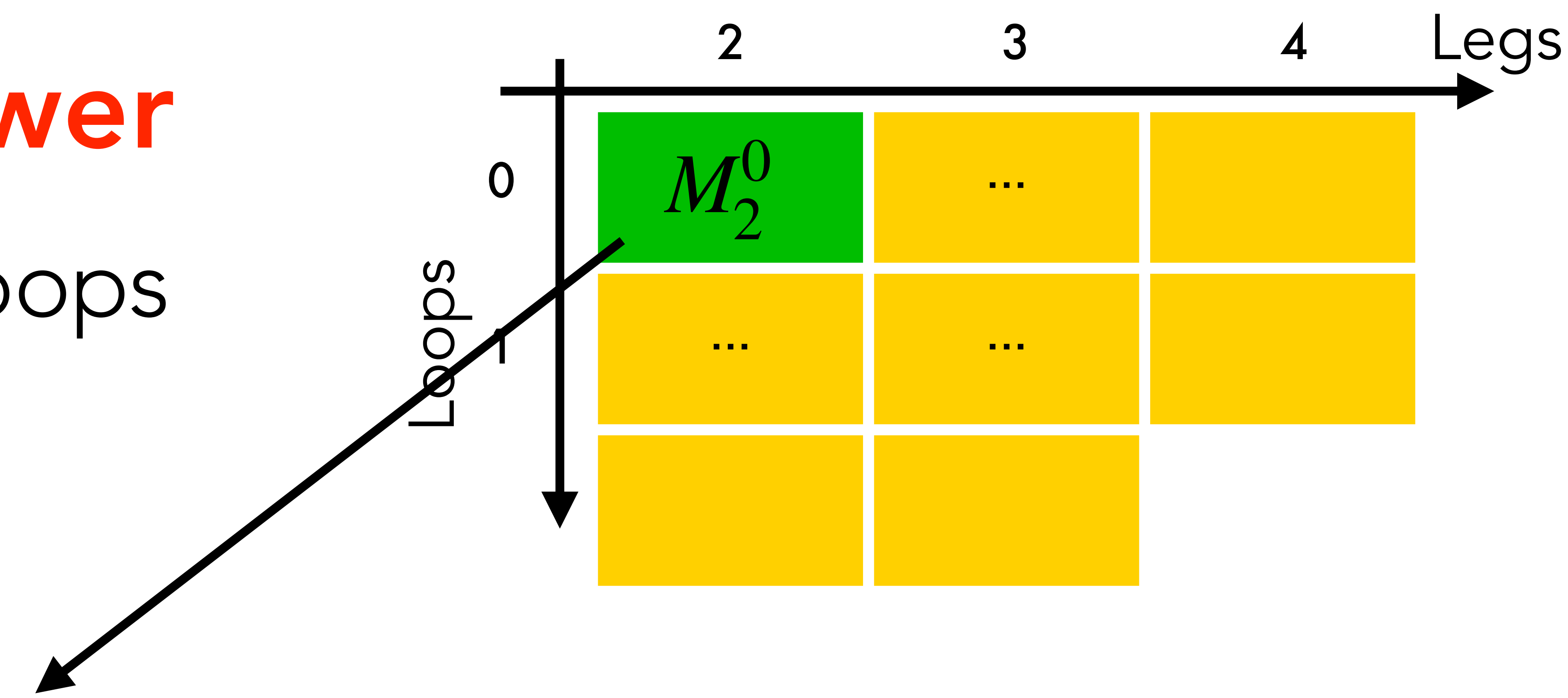
"Loops and Legs" diagram
Showing coefficients of perturbative series

Leading Order + Parton Shower

Consider $Z \to q\bar{q}$ @ LO $\otimes$ shower

M_n^ℓ = QFT amplitude for n legs, ℓ loops

… = Shower approximation



Starting density of states in Φ_2:

$$\frac{m_Z}{8\pi^4}\frac{\mathrm{d}^2\Gamma}{\mathrm{d}\Phi_2} = |M_2^0|^2$$

Act on each of these states with a **shower evolution operator** $\mathcal{S}$

$$|M_2^0|^2\,\mathcal{S}(\Phi_2)$$

$\mathcal{S}(\Phi_n)$ is an operator that **stochastically** evolves an n-parton state ~ zooming the fractal

Normally defined to be strictly unitary: can only change **properties** of state but not normalisation

Constructed to generate **approximate** (LL, NLL, …?) all-orders real **and** virtual corrections.

Perturbation Theory as a Markov Chain

$\mathcal{S}$: Stochastic differential evolution in "hardness" scale

~ Sliding **factorisation** scale ~ quantum **resolution** scale ~ jet resolution scale ~ momentum transfer ~ formation time ~ **characteristic wavelength**

(Determines which specific logs are resummed. Many showers use a scale ∝ $p_\perp$)

Differential cross section for a **generic observable "O"**:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}O} = \int \mathrm{d}\Phi_2 \overbrace{|M_2^0|^2}^{\text{Born-Level "Matching Coefficient"}} \overbrace{\mathcal{S}(\Phi_2, O)}$$

Shower operator ➜ next slide

We want to evaluate the observable O on the state **after** showering.
(Could also define the observable as an operator acting from the right)

A Simple Parton Shower

With only (iterated) $n \to n+1$ branchings

Shower operator

Evaluate O on Φ_n

$$\mathcal{S}_{+1}(\Phi_n, O) \;=\; \text{“Nothing happens”}\; \overbrace{\delta\left(\hat{O}(\Phi_n) - O\right)}^{\text{Evaluate } O \text{ on } \Phi_n}$$

Branching Kernel

$$+ \;\text{“Something happens”}\; \mathcal{S}_{+1}(\Phi_{n+1}, O)$$

MARKOV CHAIN

Unitarity: if nothing doesn’t happen, then something happens

$\Longrightarrow$ Probability for “Something happens” $= \dfrac{-\mathrm{d}\text{"Nothing Happens"}}{\mathrm{d}p_\perp^2}$

A Simple Parton Shower

With only (iterated) $n \to n+1$ branchings

Shower operator

'Sudakov Factor'

Evaluate O on Φ_n

$$\mathcal{S}_{+1}(\Phi_n, O) = \Delta\left(\Phi_n, Q_{\mathrm{IR}}\right) \, \delta\left(\hat{O}(\Phi_n) - O\right)$$

"Nothing happens"

Sudakov expansions
➜ "virtuals"

Branching Kernel

Branchings
➜ "reals"

$$+ \; \text{"Something happens"} \; \mathcal{S}_{+1}(\Phi_{n+1}, O)$$

"Something happens"

MARKOV CHAIN

UNITARITY

Sudakov Factor $\Delta(\Phi_n, Q) = \exp\left(- \int_{Q^2}^{Q_n^2} d\Phi_{+1} \frac{d\mathcal{P}_{n \to n+1}}{d\Phi_{+1}} \right)$

Branching Kernel

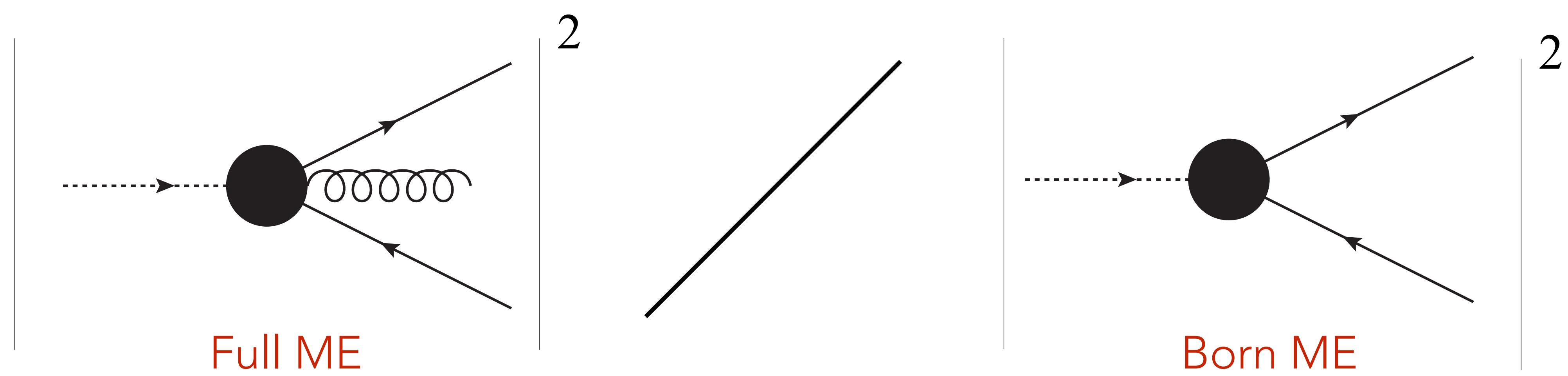
Soft-Collinear Approximations or tree-level MEs (MECs)

NB: partition of phase space and branching probabilities onto different terms not shown here

Examples of Branching Kernels (for single branchings)

Factorisation of (squared) amplitudes in IR singular limits

(leading colour)



Full ME (modulo nonsingular terms)

DGLAP

ij-collinear limit

jk-collinear limit

$$\frac{P_{q\to qg}(z_i)}{s_{qg}} + \frac{P_{q\to qg}(z_k)}{s_{g\bar{q}}}$$

One term for each **parton**

Requires **angular ordering** to get soft limits right

Antenna

$$\frac{2s_{q\bar{q}}}{s_{qg}s_{g\bar{q}}} + \frac{1}{s}\left(\frac{s_{g\bar{q}}}{s_{qg}} + \frac{s_{qg}}{s_{g\bar{q}}}\right)$$

eikonal term

collinear terms

partitioning of eikonal

One term for each colour-connected pair of partons

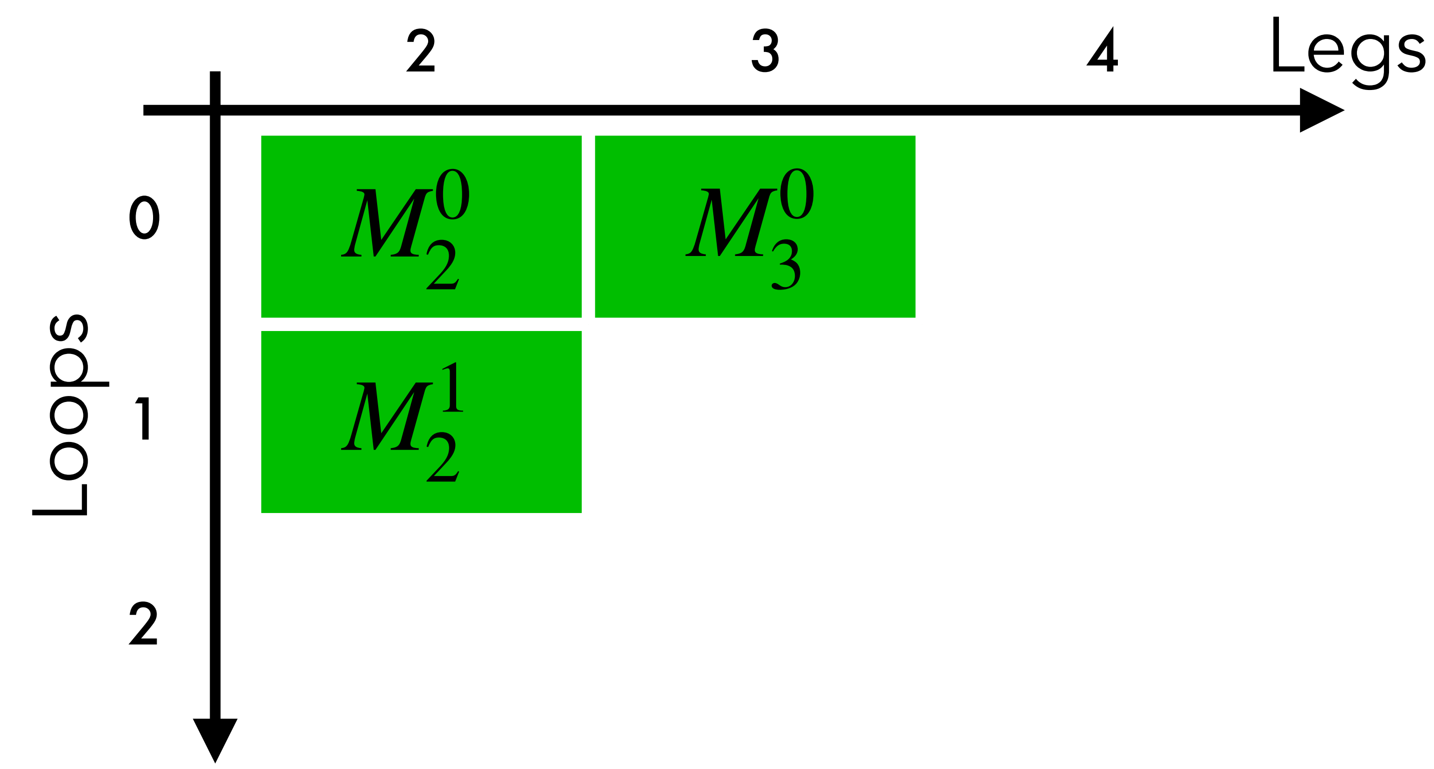
Dipole (CS/Partitioned)

$$\frac{\mathscr{K}_{qg,\bar{q}}(z_q)}{s_{qg}} + \frac{\mathscr{K}_{\bar{q}g,q}(z_{\bar{q}})}{s_{g\bar{q}}}$$

Two terms for each colour-connected pair of partons

Note: this is (intentionally) oversimplified. Many subtleties (recoil strategies, gluon parents, global vs sector, colour factors, initial-state partons, mass terms) not shown.

Jet Rates at NLO



Example: $Z \to q\bar{q}$ **@ NLO**

M_n^ℓ = QFT amplitude for n legs, ℓ loops

Fully-differential **NLO 2-jet rate:**

$$\frac{m_Z}{8\pi^4}\frac{\mathrm{d}^2\Gamma}{\mathrm{d}\Phi_2} = |M_2^0|^2 \ + \ 2\mathrm{Re}[M_2^1 M_2^{0*}] + \int \mathrm{d}\Phi_3 \, |M_3^0|^2 \, \delta^{(2)}\left(\Phi_2 - \hat{\Phi}_2(\Phi_3)\right)$$

+ also incorporates **LO 3-jet rate:**

$$\frac{m_Z}{8\pi^4}\frac{\mathrm{d}^5\Gamma}{\mathrm{d}\Phi_3} = |M_3^0|^2$$

Note: relative accuracy in general varies across domain

Most observables are **not** clear-cut n-jet observables.

E.g., "event shapes" sensitive to different multiplicities across their ranges

NLO combined with Parton Showers

Example: $Z \to q\bar{q}$ @ **NLO** $\otimes$ **shower**

M_n^ℓ = QFT amplitude for n legs, ℓ loops

… = Shower approximation

Loops \ Legs	2	3	4
0	M_2^0	M_3^0	…
1	M_2^1	…	…
2	…	…	…

MC@NLO and POWHEG (+ a few more recent proposals)

Differ in their approximate M_3^1 and M_2^2 & beyond: **vary $\leftrightarrow$ uncertainties!**

Note: can also start from $Z \to 3$ @ NLO

Divergent for 2-jet observables

NLO for 3-jet observables/regions

LO for 4-jet observables/regions

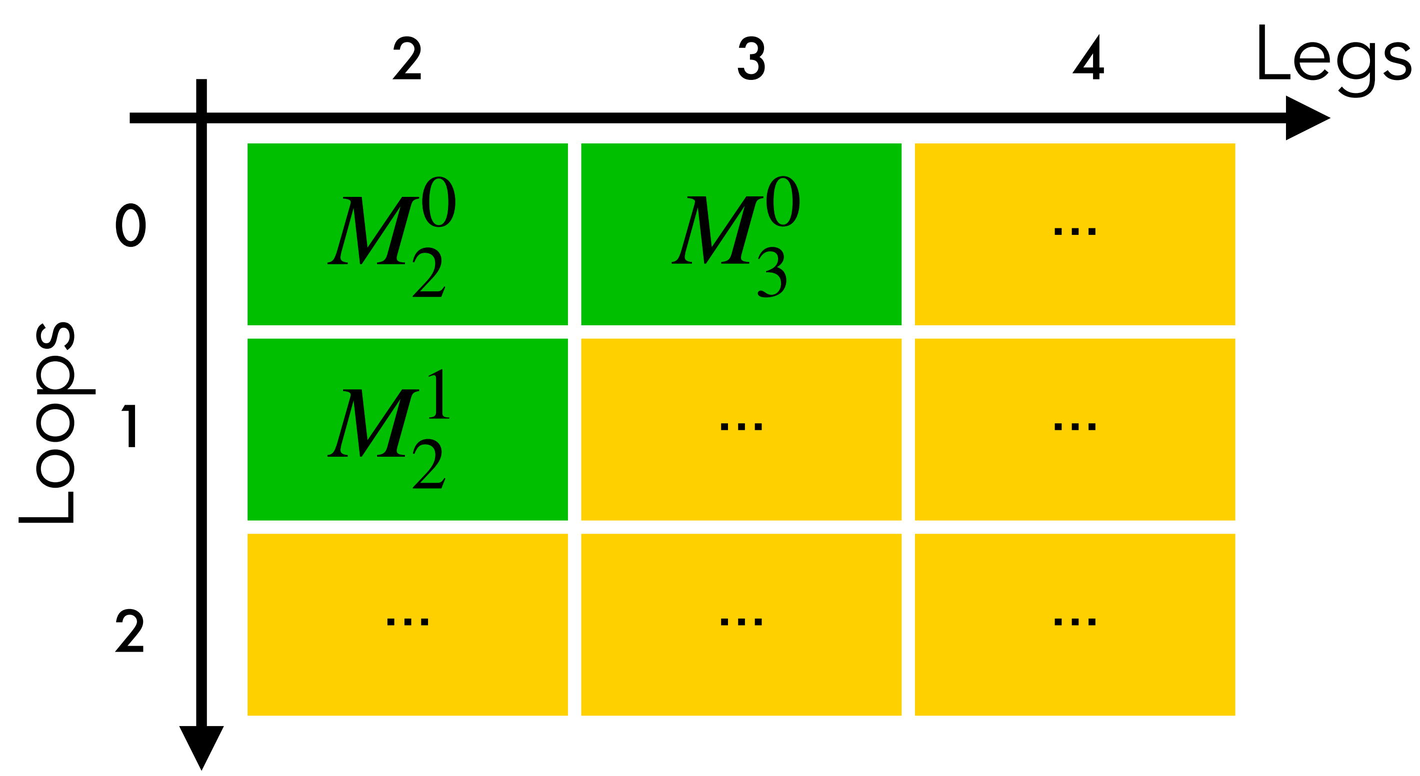
Loops \ Legs	2	3	4	5
0	∞	M_3^0	M_4^0	…
1	∞	M_3^1	…	…
2	∞	…	…	…

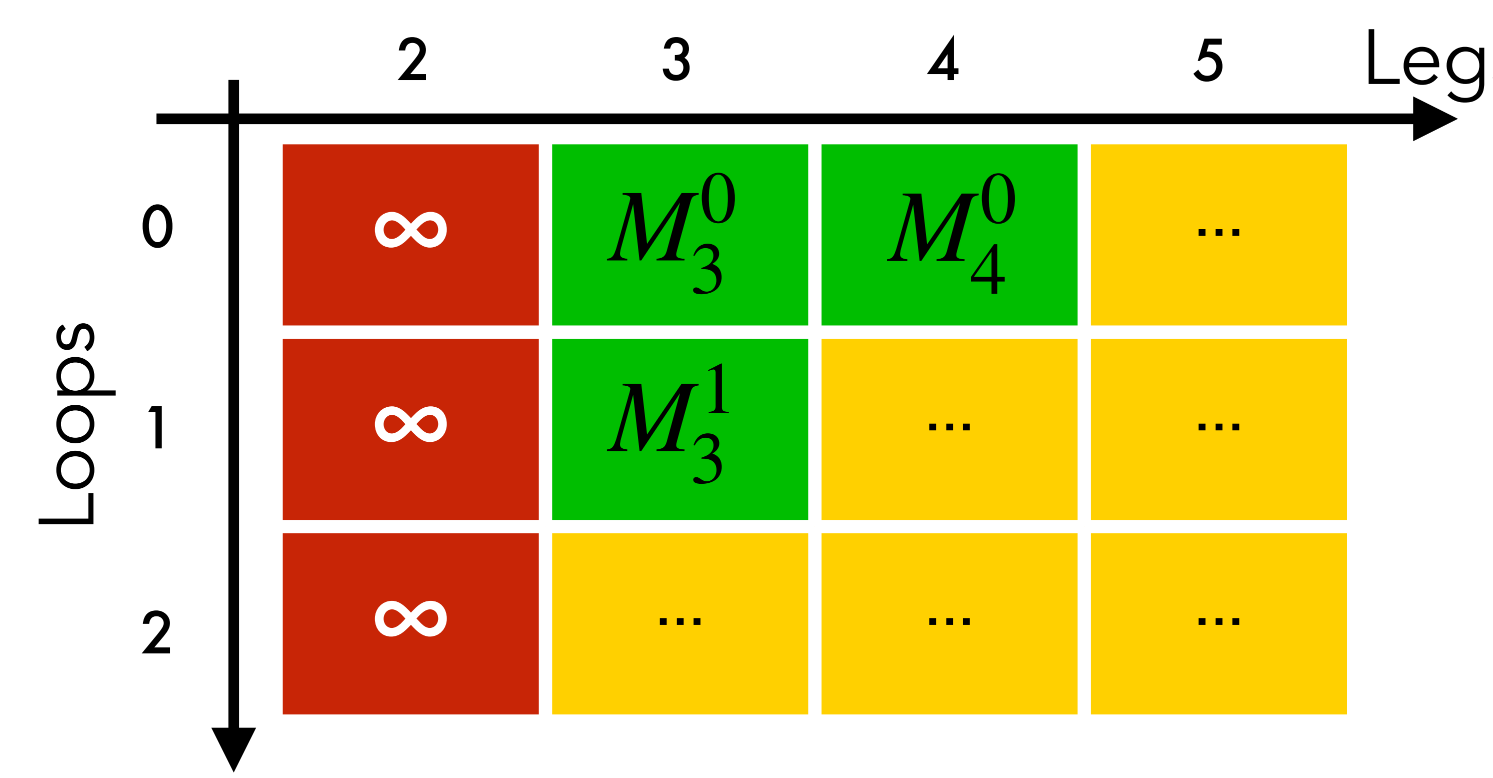
Matching and Merging

Matching:

One fixed-order calculation matched to a resummation (as, e.g., on previous slide)

E.g.: **EITHER** $Z \to 2$ @ NLO + Shower **OR** $Z \to 3$ @ NLO + Shower





Merging:

Combine **several** matched calculations (consistently!)

Generally achieved with **phase-space (jet) cuts**

E.g.: **IF $p_{T3} < p_{Tcut}$**, use $Z \to 2$ @ NLO + Shower, **ELSE** use $Z \to 3$ @ NLO + Shower

Important to ensure (and validate) smooth transition! (Devil is in the details.)

State of the Art: **NNLO + Showers**

Example: VinciaNNLO

(see also: GENEVA, MiNNLO$_{PS}$, NNLOPS)

Goal:

Loops \ Legs	2	3	4	5
0	M_2^0	M_3^0	M_4^0	...
1	M_2^1	M_3^1	...	...
2	M_2^2	...	...	...

So far swept under rug:

M_n^ℓ divergent for $\ell \geq 1$

$\Longrightarrow$ Change notation:

$$\mathrm{B}_n = |M_n^0|^2$$

$$\mathrm{V}_n = 2\mathrm{Re}[M_n^0 M_n^{1*}] + \int \mathrm{d}\Phi_{+1} |M_{n+1}^0|^2$$

$$\mathrm{W}_n = |M_n^1|^2 + 2\mathrm{Re}[M_n^2 M_n^{0*}] + \int \mathrm{d}\Phi_{+1} \mathrm{V}_{n+1}$$

B_n, V_n, W_n **are all finite**
(for n resolved partons)

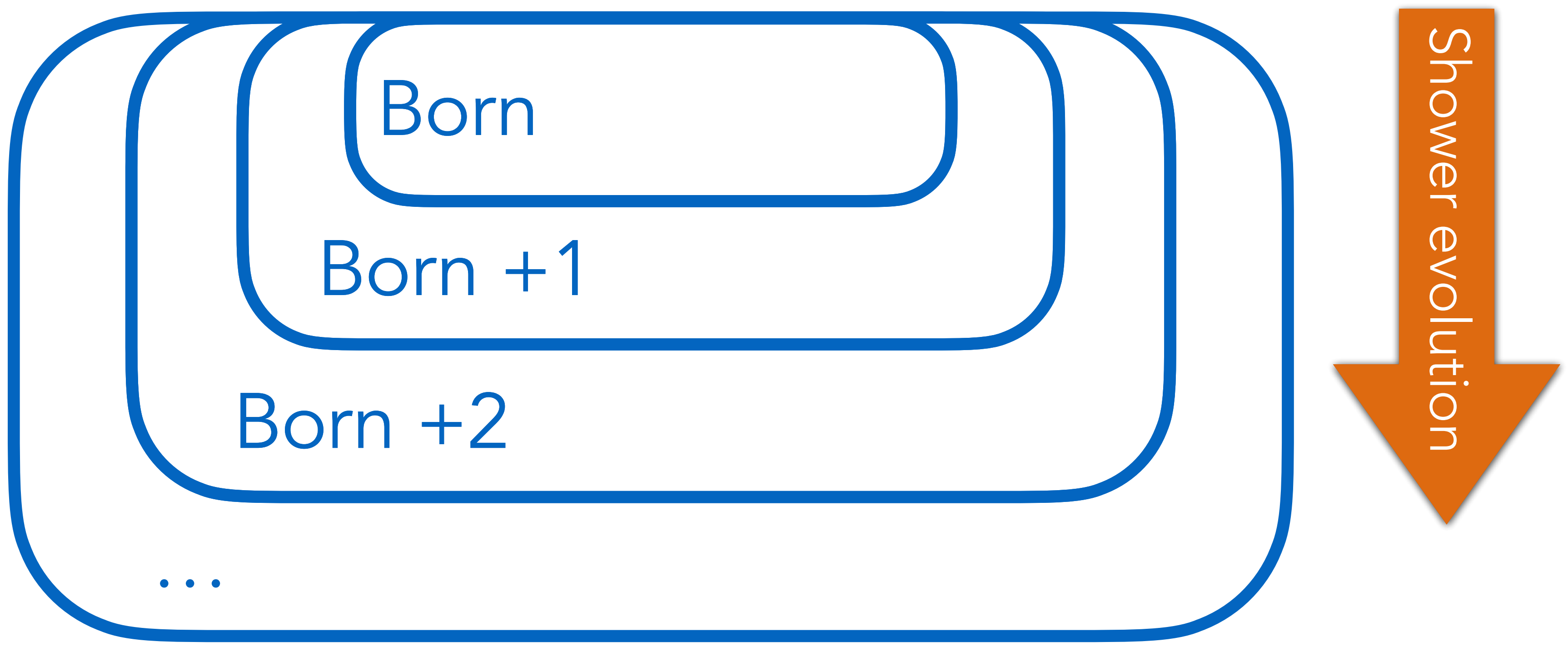
Separates **how to match them** from **how to calculate them**
(latter → a "clean" fixed-order problem)

Using Amplitudes as Branching Kernels

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

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

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



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

OK, let's get started

Start from $Z \to 2$ normalised to NNLO rate:

VINCIA NNLO

$$\frac{M_Z}{8\pi^4}\frac{d^2\Gamma}{d\Phi_2} = \overbrace{(\mathrm{B}_2 + \mathrm{V}_2 + \mathrm{W}_2)}^{\text{Born-Level Matching Coefficients : E.g., } \mathrm{V}_2 = (\alpha_s/\pi)\mathrm{B}_2} \underbrace{\mathcal{S}(\Phi_2; Q_{\mathrm{IR}})}_{\text{Shower operator}}$$

Disclaimer:

Will try to make it look a little easier than it actually is. Don't want to bury you in technical details.; see arXiv:2412.14242.

From $\mathcal{S} \implies$ Differential inclusive 3-jet rate:

$$\frac{M_Z}{8\pi^4}\frac{d^5\Gamma}{d\Phi_3} = (\mathrm{B}_2 + \mathrm{V}_2 + \mathrm{W}_2)\left(\underbrace{\Delta_2(M_Z, t_3) A_{2\mapsto 3}}_{\text{Ordinary } 2\mapsto 3 \text{ branchings}} + \overbrace{\int_{t_4 > t_3} d\Phi_{+1} \Delta_2(M_Z, t_4) A_{2\mapsto 4}}^{\textbf{New: } \text{“Direct” } 2\mapsto 4 \text{ branchings (only for “unordered” } t_4 > t_3)} \right)$$

t_3 : jet resolution scale of 3-jet configuration $\equiv \dfrac{s_{qg}s_{g\bar{q}}}{M_Z^2}$

$A_{2\mapsto 3}$: probability density for 3-jet configurations $\equiv \dfrac{\mathrm{B}_3}{\mathrm{B}_2} + \mathcal{O}(\alpha_s^2)$

$\Delta_2(M_Z, t_3)$: Sudakov no-branching probability $\equiv \exp\left(-\int_{t_3}^{M_Z^2} d\Phi_{+1} A_{2\mapsto 3} + \mathcal{O}(\alpha_s^2) \right)$

NNLO matching $\implies$ match this coefficient to the $\mathcal{O}(\alpha_s^2)$ fixed-order result

(& using same here to preserve unitarity)

3-jet Matching at $\mathcal{O}(\alpha_s^2)$

[see arXiv:2412.14242]

Equate fixed-order and shower 3-jet rates:

$$\mathrm{B}_3 + \mathrm{V}_3 + \mathcal{O}(\alpha_s^3) = (\mathrm{B}_2 + \mathrm{V}_2 + \mathrm{W}_2)\left(\Delta_2(M_Z, t_3) A_{2\mapsto 3} + \int_{t_4 > t_3} \mathrm{d}\Phi_{+1} \Delta_2(M_Z, t_4) A_{2\mapsto 4} \right)$$

Expand right-hand side through $\mathcal{O}(\alpha_s^2)$ and solve for $A_{2\mapsto 3}$:

$$\mathrm{B}_3 + \mathrm{V}_3 = (\mathrm{B}_2 + \mathrm{V}_2) A^0_{2\mapsto 3} + \mathrm{B}_2 A^1_{2\to 3} - \mathrm{B}_2 A^0_{2\mapsto 3} \int_{t_3}^{M_Z^2} \mathrm{d}\Phi_{+1} A^0_{2\mapsto 3} + \int_{t_4 > t_3} \mathrm{d}\Phi_{+1} \mathrm{B}_4$$

Assuming shower is matched to B_4

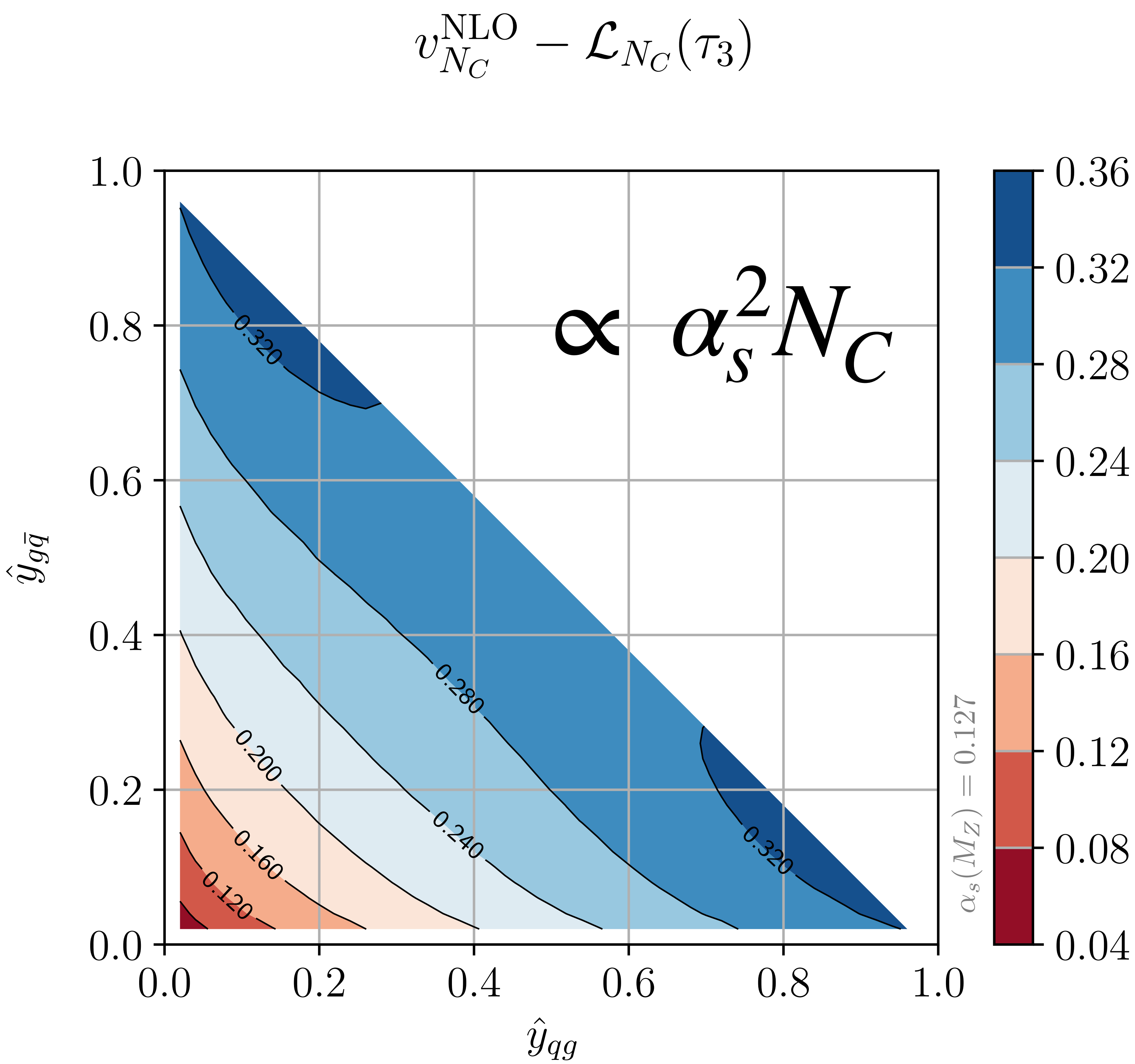
$$\mathcal{O}(\alpha_s^1) \implies A^0_{2\mapsto 3} = \frac{\mathrm{B}_3}{\mathrm{B}_2}$$

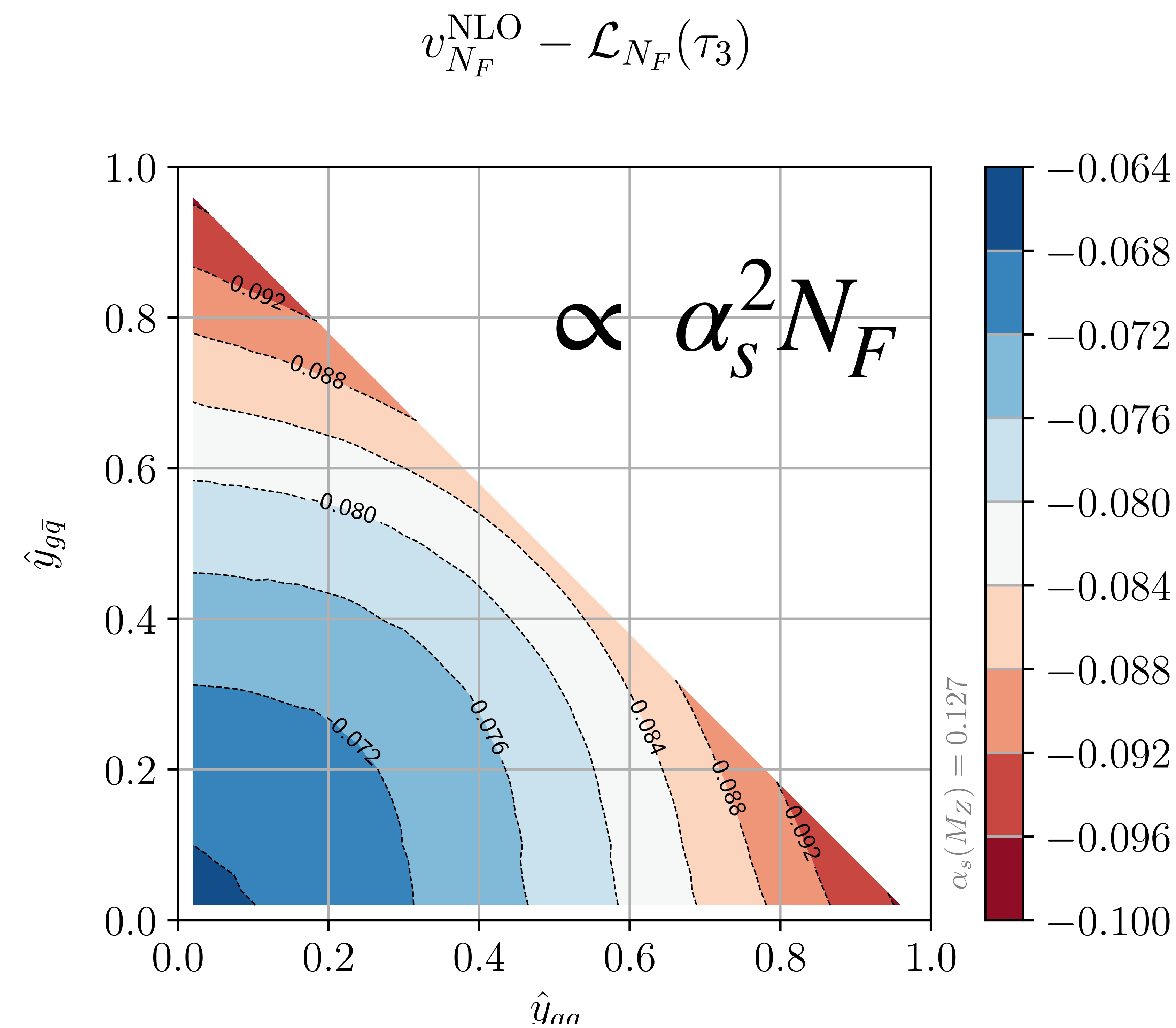
Shower off V_2 | "Sudakov on top" | Direct $2 \to 4$ branchings

$$\mathcal{O}(\alpha_s^2) \implies A^1_{2\mapsto 3} = \frac{\mathrm{V}_3 - \mathrm{V}_2 A^0_{2\mapsto 3}}{\mathrm{B}_2} + \frac{\mathrm{B}_3 \int_{t_3}^{M_Z^2} \mathrm{d}\Phi_{+1} A_{2\mapsto 3} - \int_{t_4 > t_3} \mathrm{d}\Phi_{+1} \mathrm{B}_4}{\mathrm{B}_2} \quad (+\ \mu_R \text{ term})$$

$\mathcal{O}(\alpha_s^2)$ Corrections to the 3-jet density

Dalitz Plots of the $\mathcal{O}(\alpha_s^2)$ correction terms:





Note: subleading-colour corrections $\propto \alpha_s^2/N_C^2$ left to future work

Summary of NNLO Matching

Several efforts breaking ground towards general NNLO matching

MiNNLO$_{PS}$, GENEVA, and now VinciaNNLO

\+ expect to combine with efforts to develop (N)NLL parton showers *(e.g., PanScales, ALARIC, …)*

Expect these to eventually define a new state of the art for High-Lumi LHC & Future Colliders

Message: expect **percent-level perturbative uncertainties** from MCs @ NNLO + (N)NLL accuracy in ~ few years

Current Status of VinciaNNLO:

First method to achieve a *fully-differential* matching in each of the respective phase spaces.

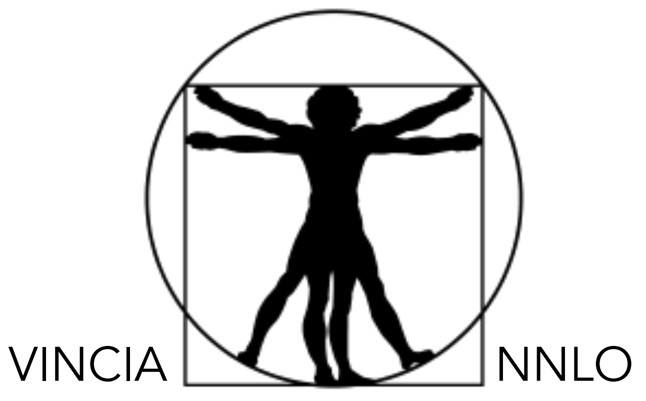
Proof of concepts so far only for colour-singlet decays to quarks *(e.g., ee colliders: $Z \to q\bar{q}$, $H \to s\bar{s}$)*

Full-fledged implementation underway in PYTHIA 8; coming in 2025.

Future Directions

NNLO MC for $H \to gg$, DIS, Drell-Yan, $e^+e^- \to WW$, and **LHC processes**

NNLO merging, and matching at N3LO



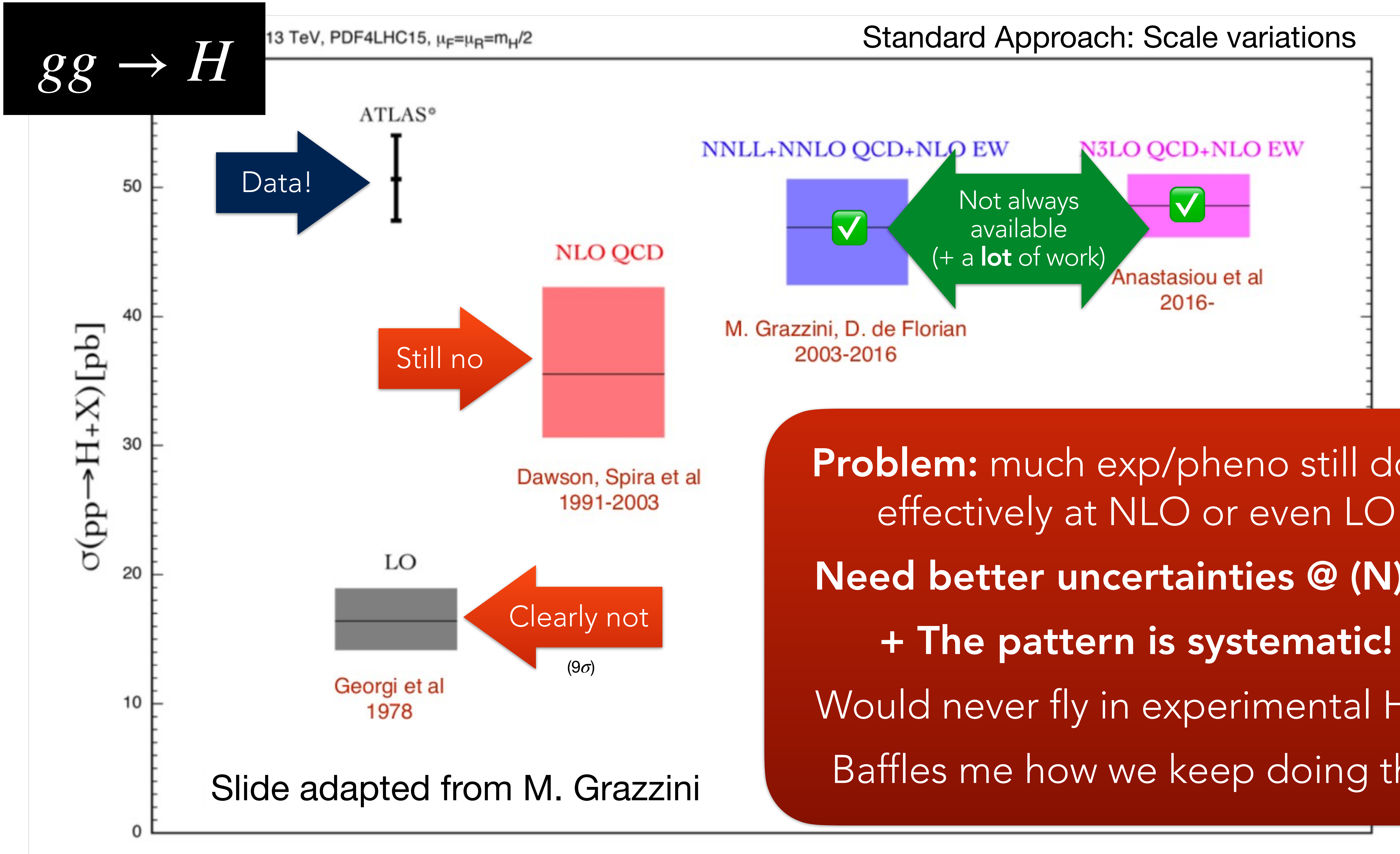
Uncertainties

Any prediction is
only as good as its
uncertainty estimate

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…

Are **scale variations** good enough?



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

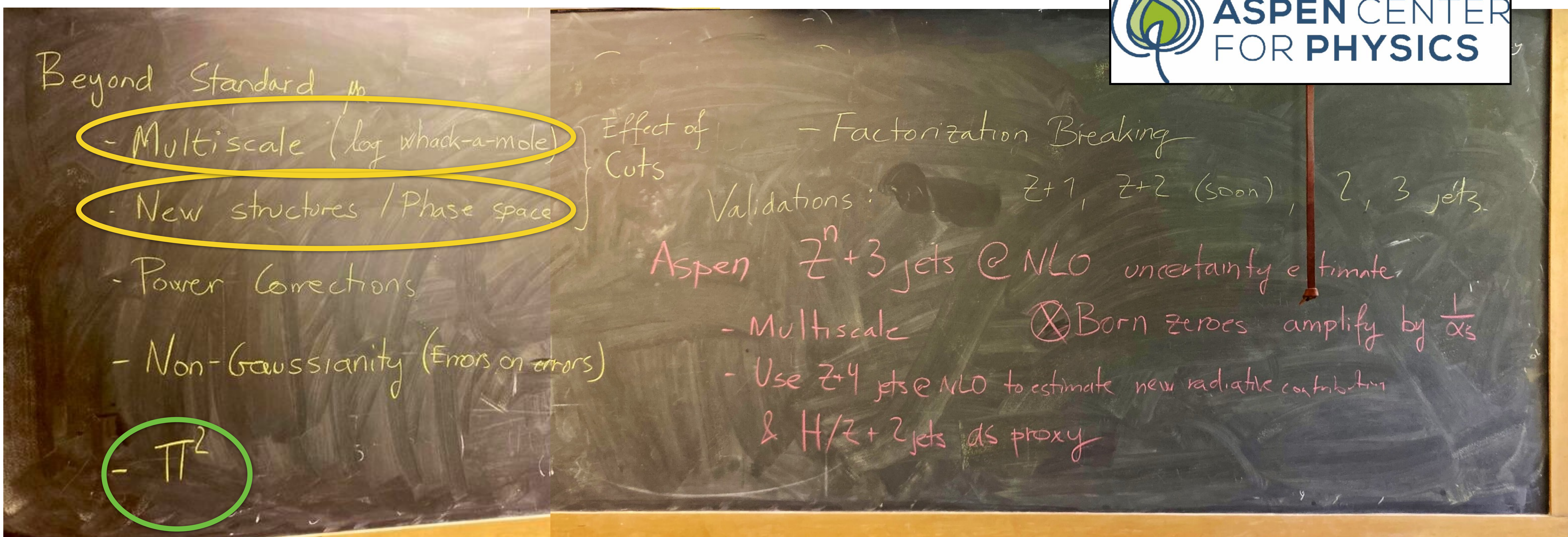
Beyond Scale Variations?

Some 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!*

Let's at least have a look …



Quantum Field Theory

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

between two different scales q_1 and q_2

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

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

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

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**

$\longrightarrow$ **quantitative uncertainty estimates?**

3) Initial-Initial Form Factors

General amplitude structures from Glauber-type gauge bosons:

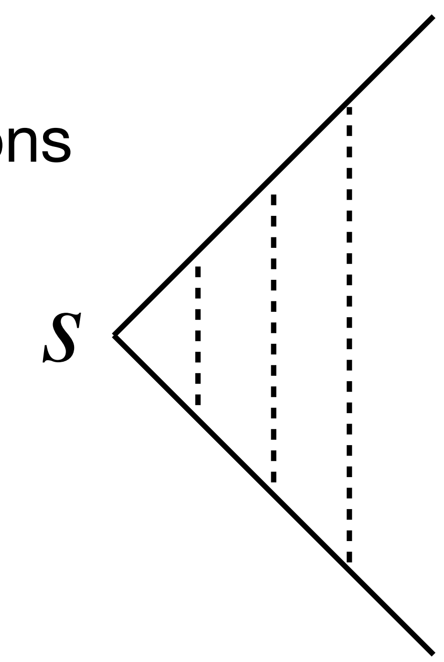
(Note: only aim here is getting lower bound on uncertainties from known amplitude structures, not discussing whether these terms should be resummed or not.)

Final-state parton pairs

Initial-state parton pairs

At all orders:

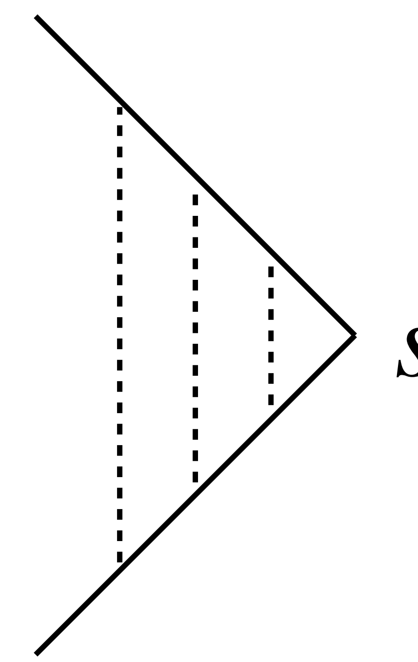
Loop corrections



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

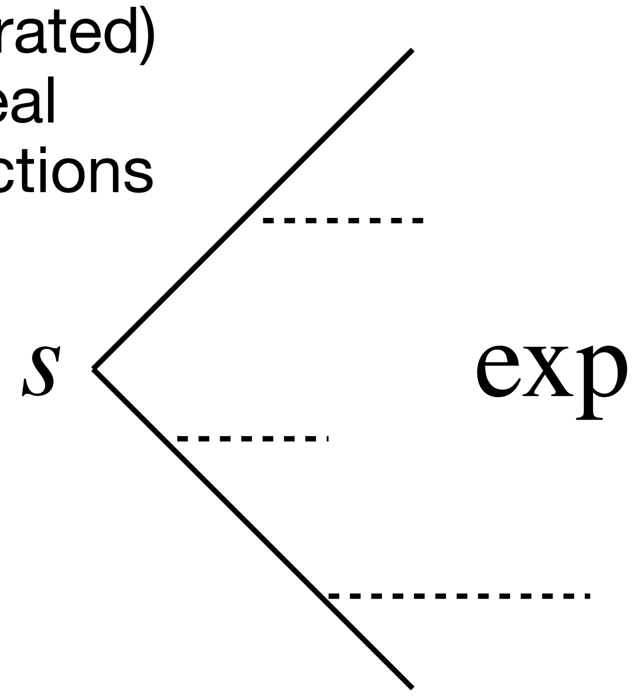
Colour factor = C_A = 3 for gluons, C_F = 4/3 for quarks

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



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

(Integrated) Real corrections



Cancel against $2 \rightarrow n$ in inclusive sums

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

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

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

Cancel

No Cancellation

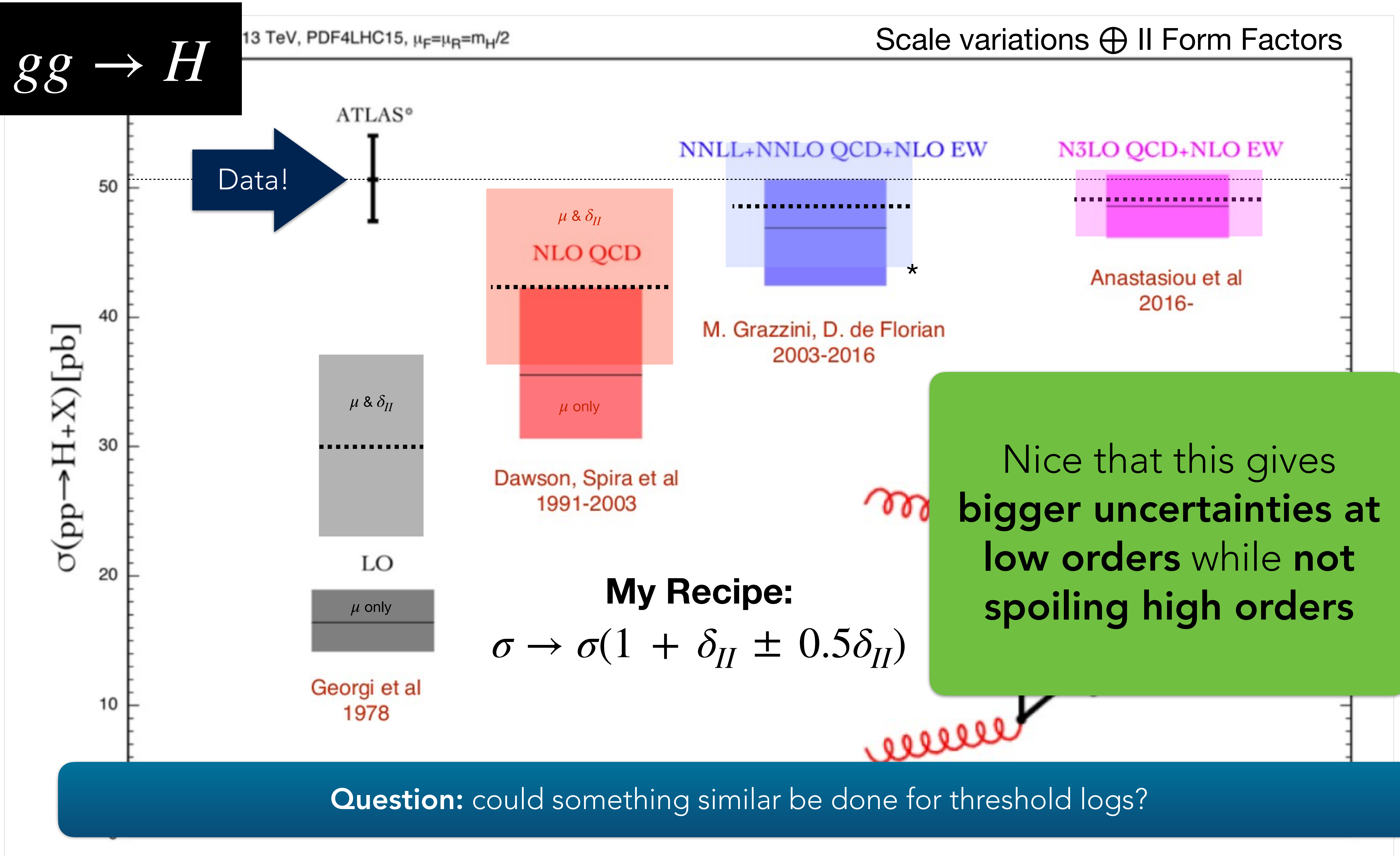
II Form Factors: Numerical Results

δ_{II}	ggH	V	VV	V+j_{100}	$t\bar{t}$	jj_{50}	jj_{200}
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



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**

Question: could something similar be done for threshold logs?

Uncertainties in Parton Showers

Standard for Shower Uncertainties: Renormalization-scale variations

Example: PYTHIA's DGLAP-based shower

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

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-singular terms** (dominate far from singular limits),
- **Non-trivial colour factors** outside collinear limits,
- **Higher-order log terms** not captured exactly by $\Delta_n(t_n, t_{n+1})$

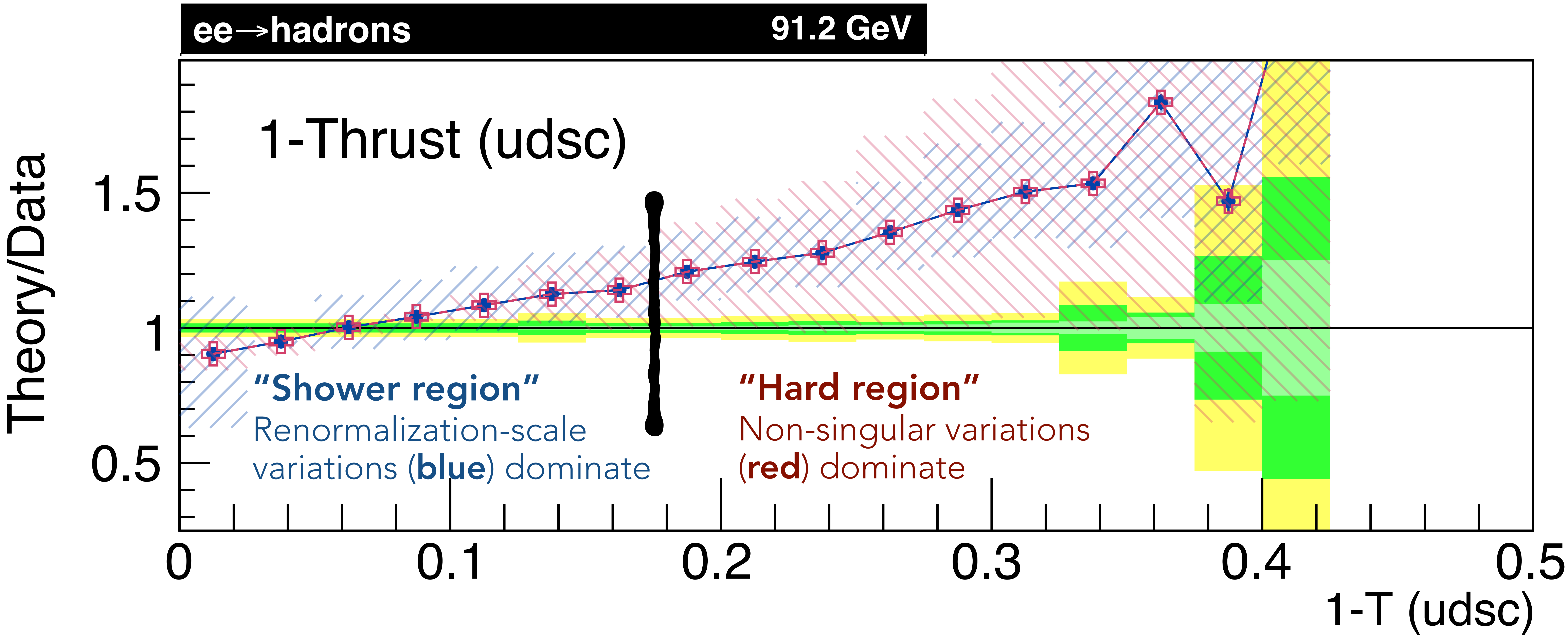
} *Vary μ_R **and** these*

[Hartgring, Laenen, PS JHEP 10 (2013) 127]

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

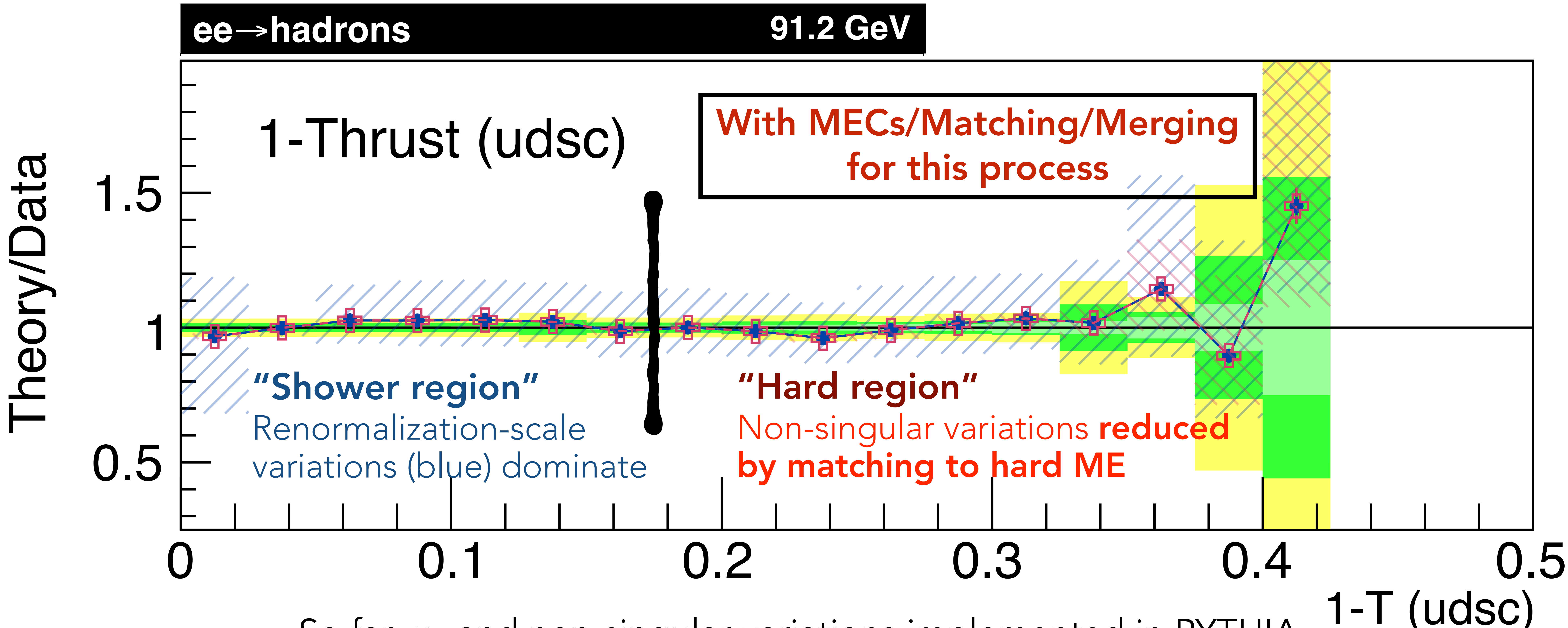


Note: ME corrections were switched off for illustration here. Would reduce **red** band, but not **blue**.

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



So far, μ_R and non-singular variations implemented in PYTHIA

Being re-implemented in VINCIA. Plan to add colour and Sudakov variations as well.

Lecture 2 Summary: From Amplitudes ➤ Events

4 communities, each with own specialisations, techniques, & problems

Scattering Amplitudes & Fixed Orders

MC Event Generators & Parton Showers

Resummation & PDFs

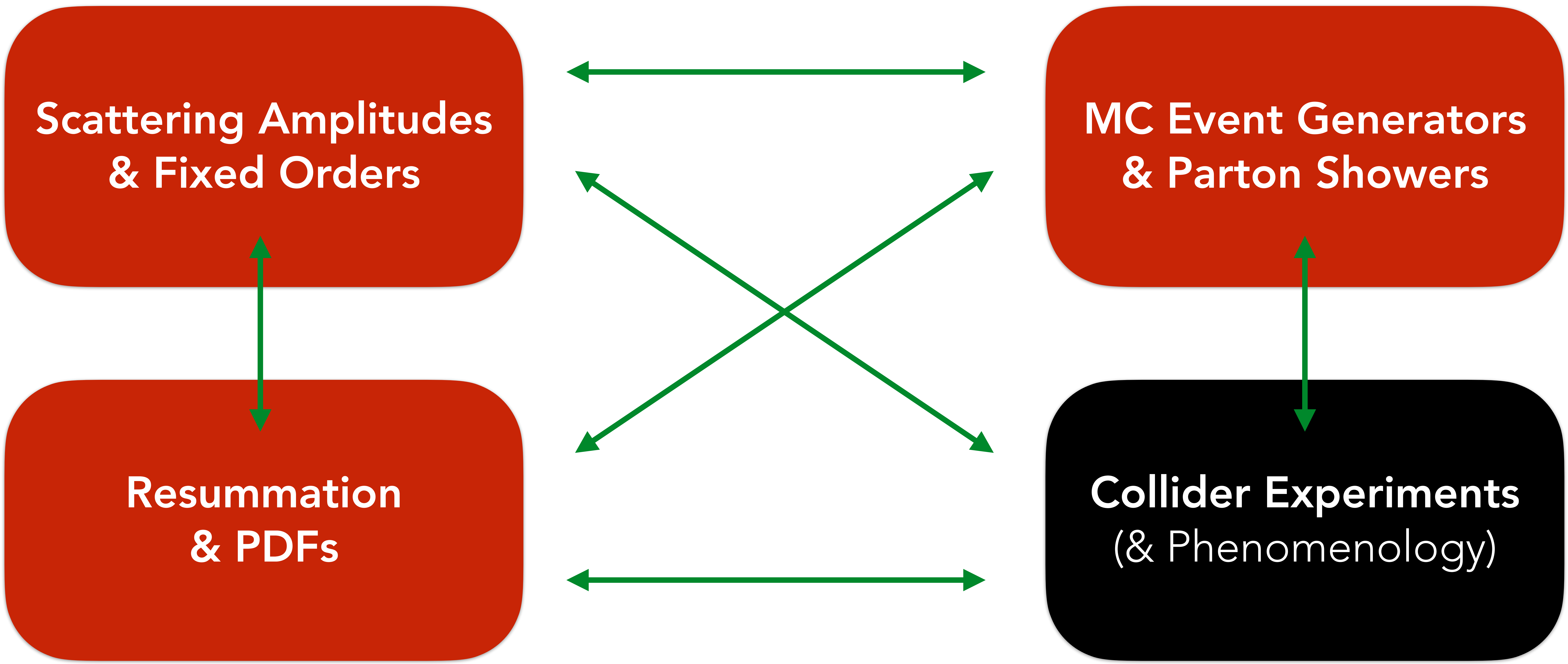
Collider Experiments (& Phenomenology)

- Phase-Space Integrations
- Speed, Efficiency
- Numerical Stability
- Accuracy
- Codes/Interfaces
- Combinations
- Uncertainties
- …

Lecture 2 Summary: From Amplitudes ➤ Events

4 communities, each with own specialisations, techniques, & problems

I think we will be ganging up to produce the calculations for the future



Final Words

MCs *can* be treated as black boxes, without knowing what's in them.

Best Case: Limited Sophistication

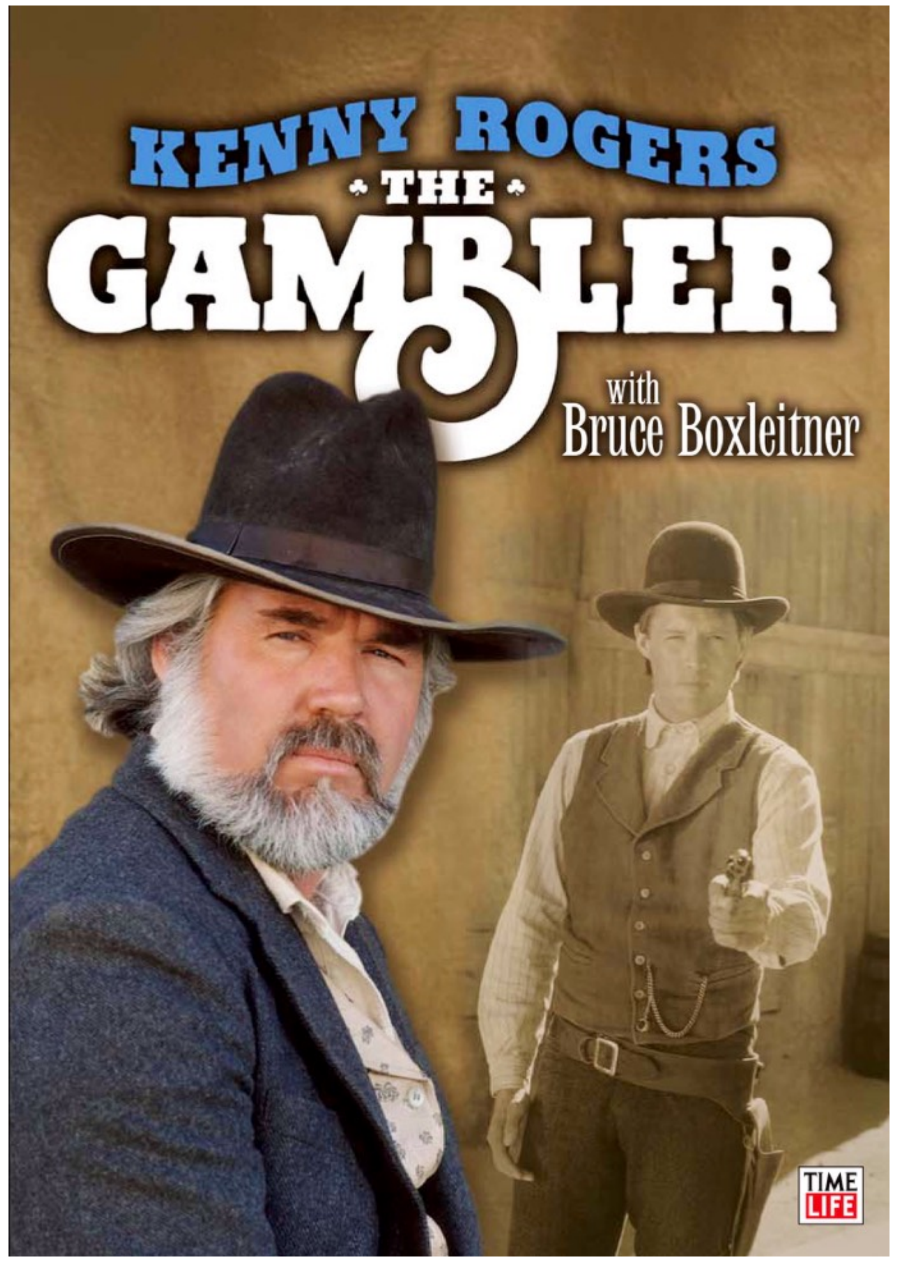
Worst Case: Not your lucky day

The key to successful Monte Carlo:

In the words of Kenny Rogers

Knowing what to throw away

Knowing what to keep



Kenny Rogers "The Gambler", first recorded in 1978

Same year as the first version of PYTHIA (JETGEN)