

Conceptual & Technical Challenges

in the matching of parton showers to higher-order calculations

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Australian Government

Australian Research Council



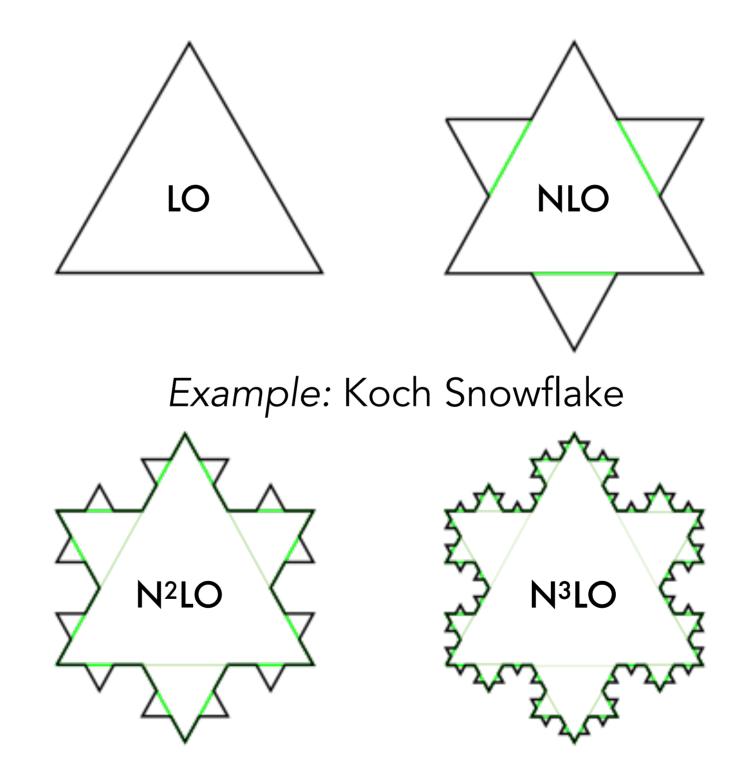




Perturbation Theory

Calculate $d\sigma$ with higher and higher detail ~ effective area of a shape

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



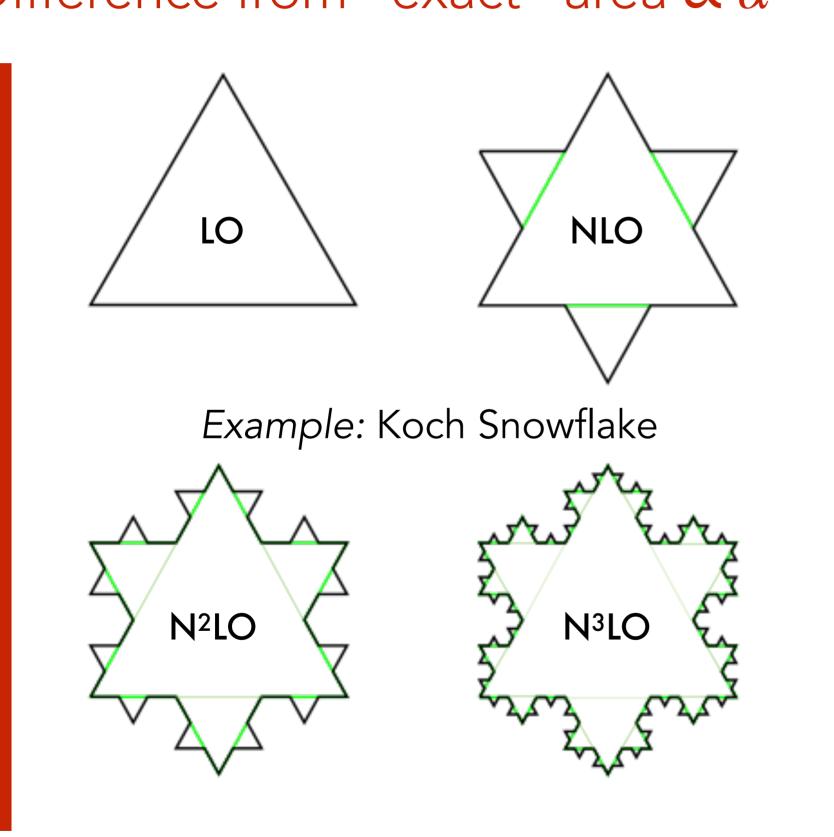
Note: (over)simplified analogy, mainly for IR structure. More at each order than shown here.

Fixed Order

Perturbation Theory

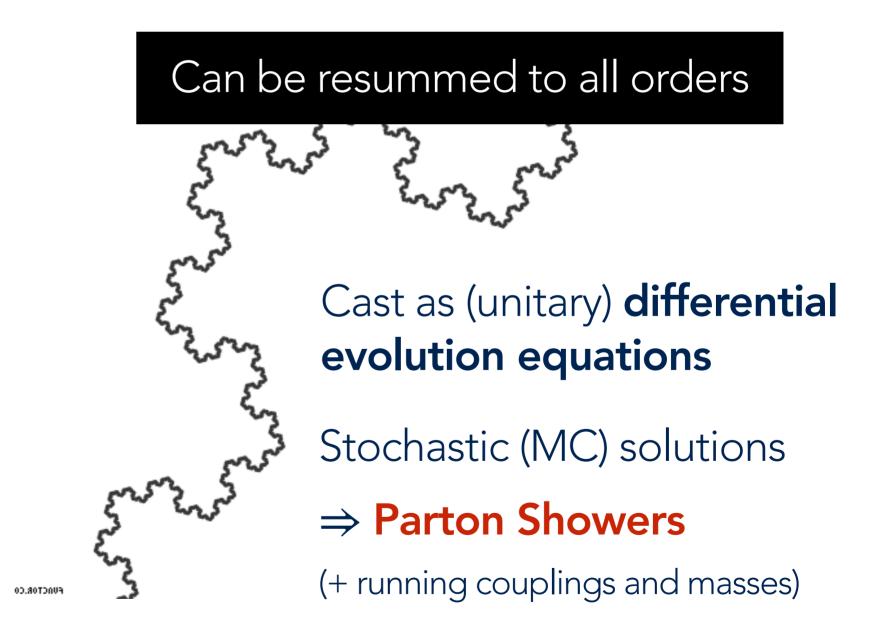
Showers

Calculate $d\sigma$ with higher and higher detail ~ effective area of a shape Difference from "exact" area $\propto \alpha^{n+1}$



Massless gauge theories

Scale invariance → fractal substructure

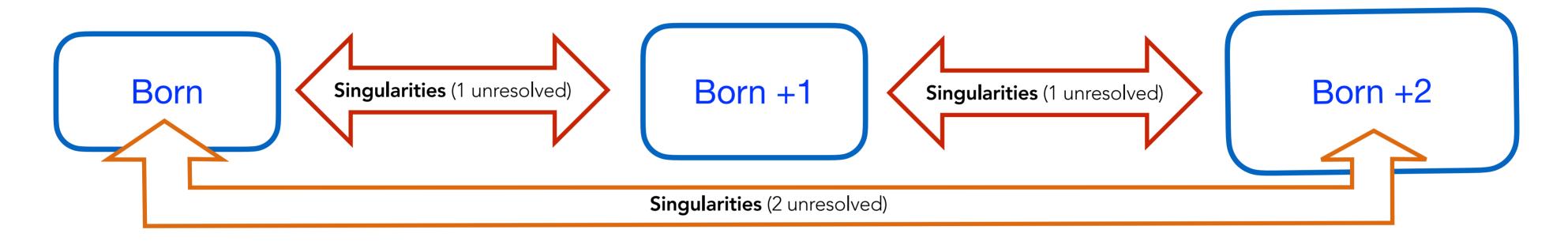


Note: (over)simplified analogy, mainly for IR structure. More at each order than shown here.

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Physical $d\sigma \Rightarrow$ Phase-Space Integrals

Fixed Order: each phase space treated separately (e.g., VEGAS)



Challenge: ensuring **finite** $d\sigma_i$ at each order \Leftrightarrow **unitarity**

$$\begin{array}{lll} & B_0 = |M_0^0|^2 \\ & V_0 = 2 \mathrm{Re}[M_0^{1*} M_0^0] + \int_{1 \mapsto 0} B_1 \\ & W_0 = |M_0^1|^2 + 2 \mathrm{Re}[M_0^{2*} M_0^0] + \int_{1 \mapsto 0} V_1 \end{array} \qquad \begin{array}{ll} B_1 = |M_1^0|^2 \\ & V_1 = 2 \mathrm{Re}[M_1^{1*} M_1^0] + \int_{2 \mapsto 1} B_2 \end{array} \qquad B_2 = |M_2^0|^2$$

Notation for **amplitudes**: M_n^{ℓ} : Born + n partons @ ℓ loops

Squared amplitudes: $(B_n V_n W_n)$: (LO, NLO, NNLO) for n partons

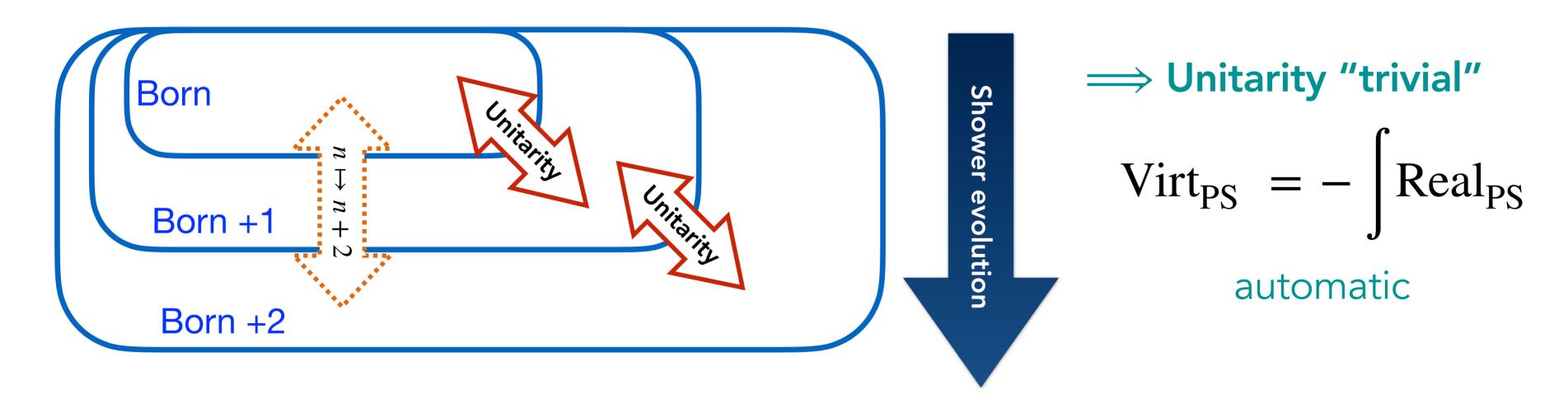
Physical $d\sigma \rightarrow$ Phase-Space Integrals

Showers: higher phase spaces *nested* inside lower ones (cf., SUNSHINE)

Unitary $n \mapsto n+1$ evolution operator $\propto a_{n+1}^{\dagger} a_n$

To **create** (n + 1)-parton state, **destroy** n-parton state (+ higher-order generalisations)

 \Rightarrow **Positive** correction to (n + 1) partons \leftrightarrow **Negative** correction to n partons



Challenges: recoil effects in $n \mapsto n + m$ mappings; (ordered) phase-space coverage; subleading pole structures; non-singular terms (matching?); tractable expansions.

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Multi-scale Problems

Simple example of a multi-scale observable:

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

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

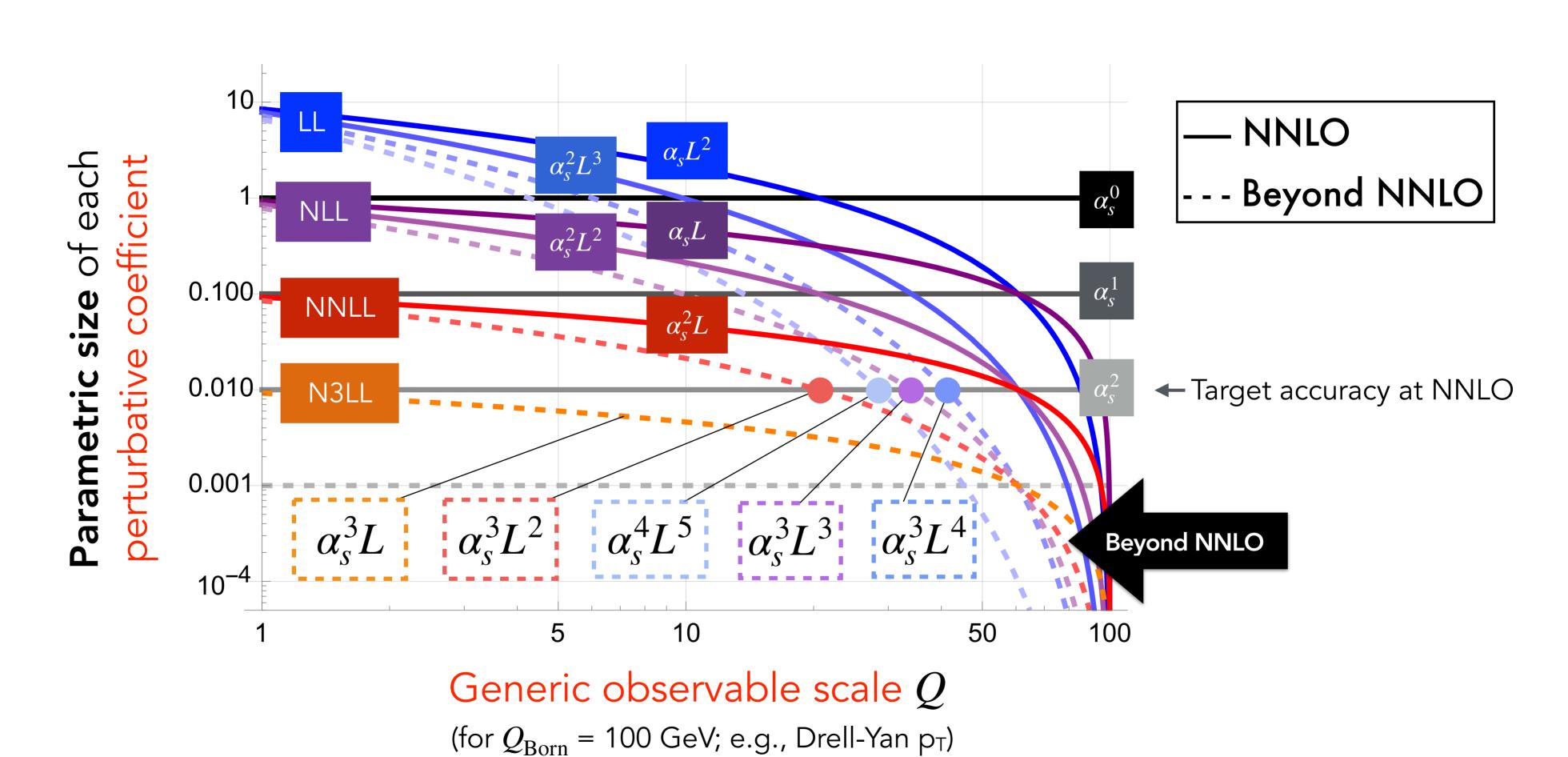
$$\frac{\text{NNLO}}{1} - \alpha_s(L^2 + L + F_1) + \alpha_s^2(L^4 + L^3 + L^2 + L + F_2) + \dots$$

$$L \propto \ln(Q_{\text{veto}}^2 / Q_{\text{hard}}^2)$$

(Arise from integrals over propagators $\propto \frac{1}{q^2}$)

Fixed-Order + Resummation

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

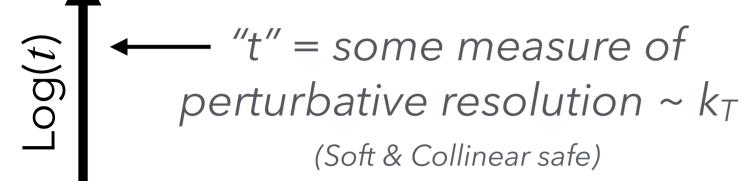


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NLO

 (t_0)

 (t_1, y_1)



Fixed-Order Coefficients

$$B_{0,1} = |M_{0,1}^0|^2$$

$$V_0 = 2\text{Re}[M_0^{1*}M_0^0] + \int_{1\mapsto 0} B_1$$



$$d\sigma_0 = (B_0 + V_0) d\Phi_0$$

Born + 1-jet Rate (LO):

$$d\sigma_1 = B_1 d\Phi_1 \rightarrow \alpha_s \ln^2(t_0/t_1)$$



"Lund Plane"

Powheg (box) - Schematic

 (t_0)

 (t_1, y_1)



 $t := t^{PW} = Powheg-box k_T$

Fixed-Order Coefficients

$$B_{0,1} = |M_{0,1}^0|^2$$

$$V_0 = 2\text{Re}[M_0^{1*}M_0^0] + \int_{1 \to 0} B_1$$



$$d\sigma_0 = (B_0 + V_0) d\Phi_0$$

Unitarity $\rightarrow d\sigma_0$ conserved

Born + 1-jet Rate (matched):

$$d\sigma_1 = d\sigma_0 \frac{B_1}{B_0} \Delta_0^{PW}(t_0, t_1^{PW}) \frac{d\Phi_1}{d\Phi_0}$$

Unitarity:
$$\Delta_0^{\text{PW}} = \exp\left(-\int_{1\mapsto 0} \frac{B_1}{B_0}\right)$$

All-orders summation $\longrightarrow \alpha$

"Lund Plane"

Powheg (box) — Schematic

 (t_0)

 (t_1, y_1)

 (t_2, y_2)

mentions



 $t := t^{PW} = Powheg-box k_T$

Fixed-Order Coefficients

$$B_{0,1} = |M_{0,1}^0|^2$$

$$V_0 = 2\text{Re}[M_0^{1*}M_0^0] + \int_{1 \to 0} B_1$$

Born Inclusive Rate (NLO):

$$d\sigma_0 = (B_0 + V_0) d\Phi_0$$

Unitarity $\rightarrow d\sigma_0$ conserved

Born + 1-jet Rate (matched):

$$d\sigma_1 = d\sigma_0 \frac{B_1}{B_0} \Delta_0^{PW}(t_0, t_1^{PW}) \frac{d\Phi_1}{d\Phi_0}$$

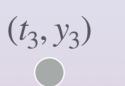
Unitarity:
$$\Delta_0^{PW} = \exp\left(-\int_{1\mapsto 0} \frac{B_1}{B_0}\right)$$

All-orders summation $\longrightarrow \alpha$

Subtleties:

- 2. Recoil effects $(d\Phi_{+1}^S)$ Addressed in other talks
- 3. New processes beyond LO _____ Brief
- 4. Initial-state colours

5. → NNLO ← Some detail

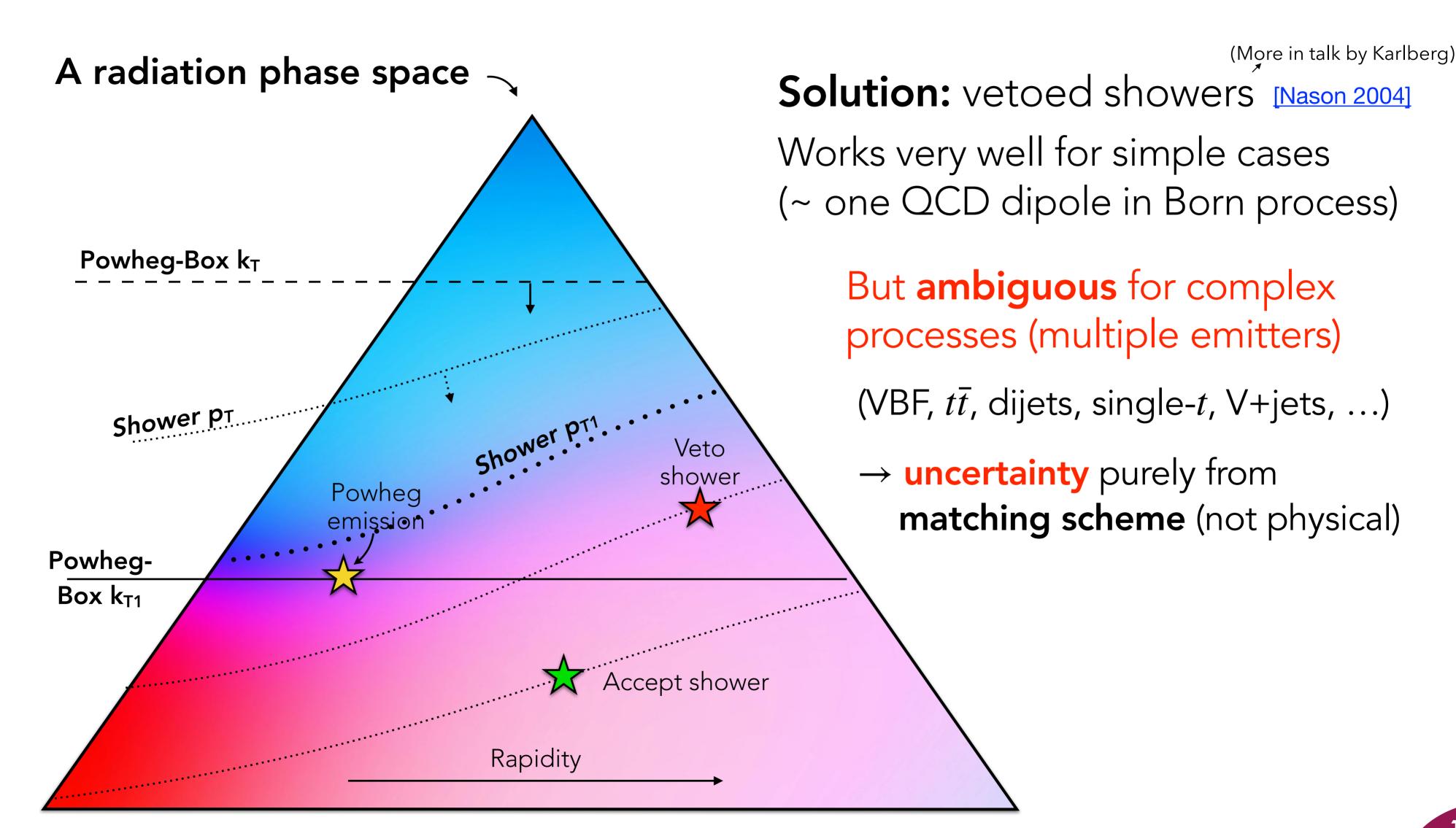


Born + n-jet Rate ($d\sigma_1 \otimes$ shower):

$$\frac{\mathrm{d}\sigma_n}{\mathrm{d}\sigma_{n-1}} = P_{+1}^{\mathrm{S}} \Delta_{n-1}^{\mathrm{S}}(t_{n-1}^{\mathrm{S}}, t_n^{\mathrm{S}}) \,\mathrm{d}\Phi_{+1}^{\mathrm{S}}$$

"Lund Plane"

1. Shower $p_{\perp} \neq \text{Powheg } p_{\perp}$



Extreme Case! VBF: $qq \rightarrow q'q'H$

[Jäger et al., 2020] [Buckley et al., 2021] [Höche et al., 2022]

Strong IF coherence effects Multiple emitters

→ several overlapping phase spaces

Many possible p_T definitions:

 $p_{\perp}(i \mapsto jk)$ symmetric or not in $j \leftrightarrow k$

 p_{\perp} with respect to the beam

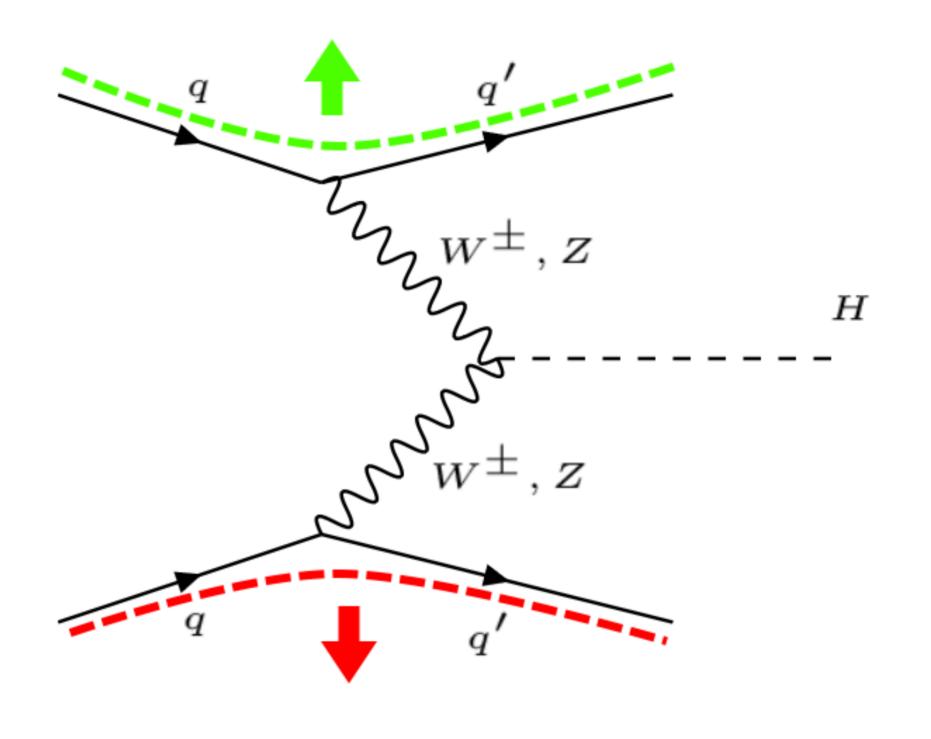
 p_{\perp} with respect to the IF dipoles

(How) is **mass** treated in the scale definition(s): p_{\perp}^2 vs $m_{\perp}^2=m^2+p_{\perp}^2$?

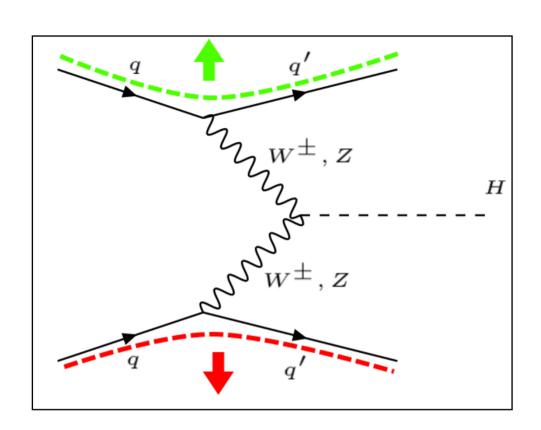
 p_{\perp} (or m_{\perp} ?) with respect to either of the final-state jets? With respect to Higgs?

Combinations of the above ...

(+ PYTHIA defines a problematic FF dipole → coherence issues)



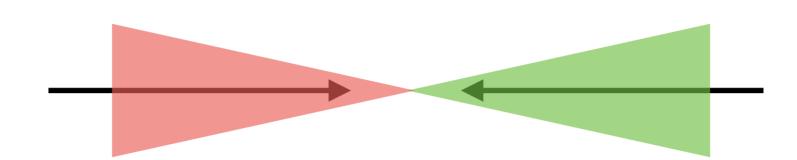
Why does it matter?



Many possible p_T definitions:

 $p_{\perp}(i\mapsto jk)$ symmetric or not in $j\leftrightarrow k$ p_{\perp} with respect to the beam p_{\perp} with respect to the IF dipoles

Coherence



Both IF dipoles are highly boosted

Throwing an emission back to $y \sim 0$ requires a highly energetic and backwards emission.

Should count as a high-scale hard emission – even at relatively low p_T with respect to the beam

(How) is **mass** treated in the scale definition(s): p_{\perp}^2 vs $m_{\perp}^2=m^2+p_{\perp}^2$?

 p_{\perp} (or m_{\perp} ?) with respect to either of the final-state jets? With respect to Higgs?

Combinations of the above ...

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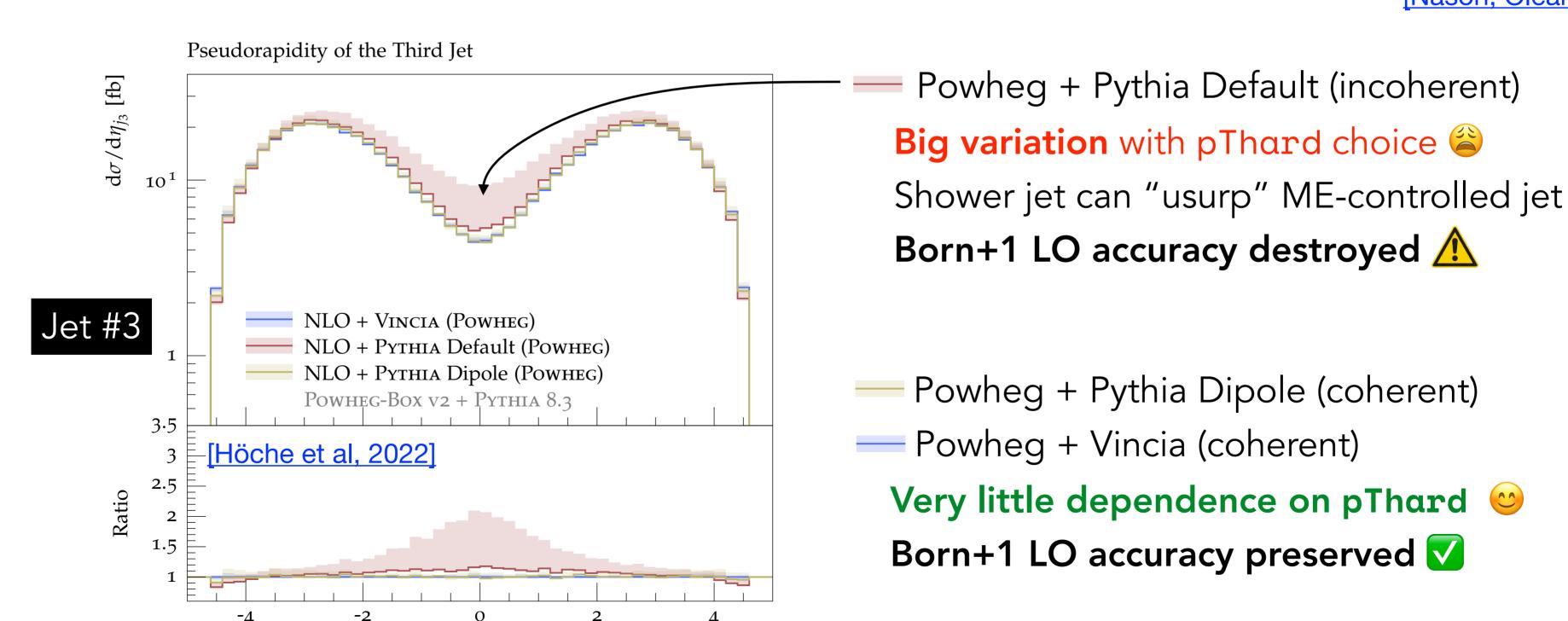


Consequences?

Varying the POWHEG-BOX \leftrightarrow PYTHIA/VINCIA hardness-scale ambiguity

POWHEG:pThard = 0 #Veto at $p_{\perp j;i}^{\text{POWHEG}}$ = SCALUP = scale at which POWHEG emitted this parton "Naive", Def \leq 8.310 POWHEG:pThard = 1 #Veto at $\min_i(p_{\perp i:i}^{\text{POWHEG}})$ = smallest scale at which POWHEG **could** have emitted this **parton**

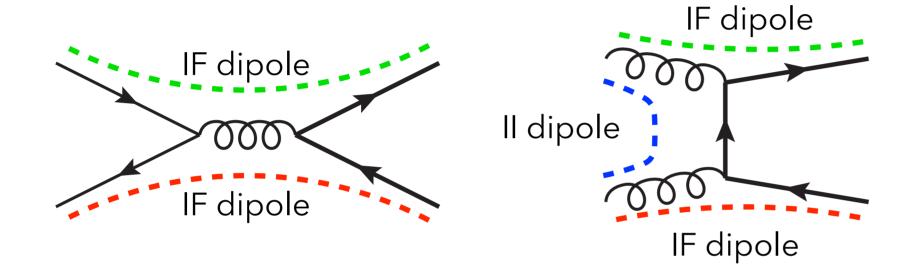
POWHEG: pThard = 2 # Veto at $\min_{i,j} (p_{\perp j;i}^{\text{POWHEG}})$ = smallest scale at which POWHEG **could** have produced this **event**[Nason, Oleani 2013]



Analogy in $t\bar{t}$ (but probably less severe)

Complex process = multiple emitters

→ several overlapping phase spaces

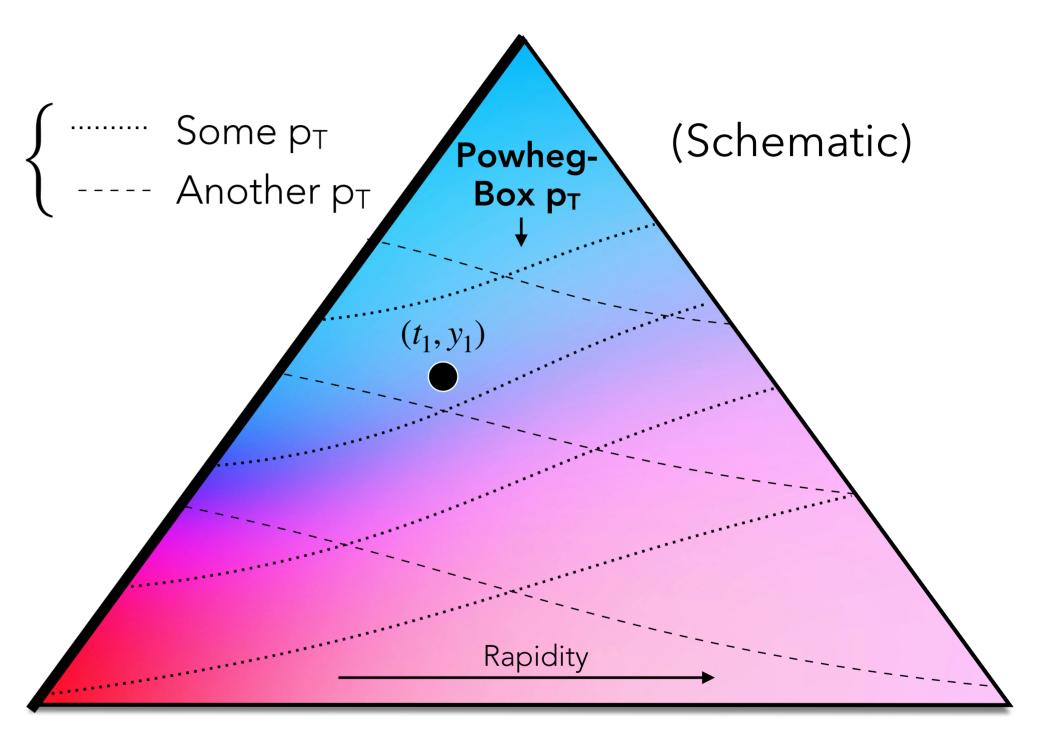


Many possible scale definitions

Interplay between colour flow, $d\Phi_{+1}^{S}$, and p_{T} scales (boosted dipoles)

IF flows can be either forward or backward

Coherent showers generate a p_T -dependent forward-backward asymmetry at Tevatron [PS, Webber, Winter, 2012]



POWHEG-Box generates 1st emission

= the one it judges to be the "hardest" according to its p_T definition

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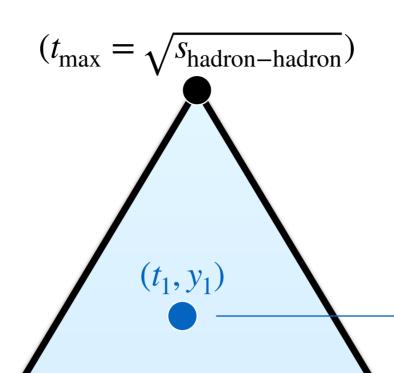
Hadron Collisions: More Challenges

(not exhaustive)

Log(t)

3. Often \exists significant phase space *above* the scale of the "Born" process

4. Initial-Initial colour flows



E.g., 13 TeV

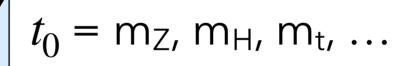
New phase-space region @ NLO

Jets with $t_1 > t_0$

FOPT:

- 3. If $t_0 \ll t_{\text{max}}$, multi-scale problem may be unavoidable (logs)
- 4. Large K factors from Initial-Initial form factors (log(-1)²)

 [Ahrens et al., 2009]



Matching:

Not all (hard) 1-jet events come from Born ones

"Automatic" in MC@NLO [Frixione, Webber 2002]

Done in POWHEG via " h_{damp} " ~ $\mathcal{O}(t_0)$ [Nason 2004]

(break strict unitarity) \Rightarrow d $\sigma_1 < k_{\rm Born}^{\rm NLO} \; {\rm B_1} \; {\rm d}\Phi_1$

5. NNLO



- "t" = some measure of perturbative resolution $\sim k_T$ (Soft & Collinear safe)

Fixed-Order Coefficients:

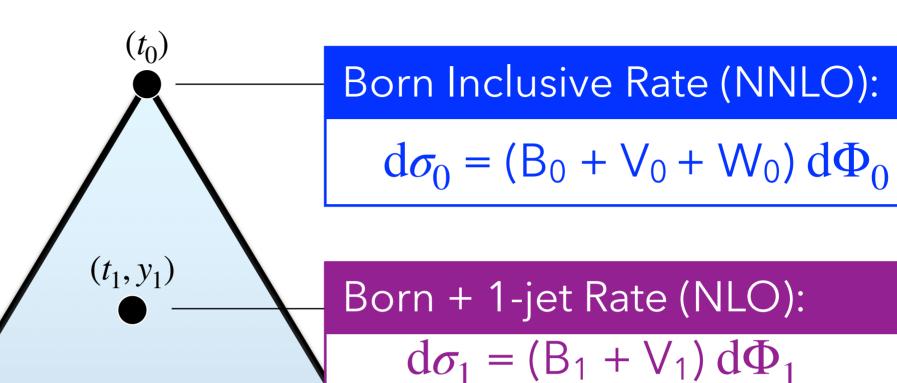
$$B_{0,1,2} = |M_{0,1,2}^{0}|^{2}$$

$$V_{0} = 2\operatorname{Re}[M_{0}^{1*}M_{0}^{0}] + \int_{1\mapsto 0} B_{1}$$

$$V_{1} = 2\operatorname{Re}[M_{1}^{1*}M_{1}^{0}] + \int_{2\mapsto 1} B_{2}$$

$$W_{0} = |M_{0}^{1}|^{2} + 2\operatorname{Re}[M_{2}^{0*}M_{0}^{0}]$$

$$+ \int_{1\mapsto 0} V_{1}$$



Born + 2-jet Rate (LO): $d\sigma_2 = B_2 d\Phi_2$ Truncation errors:



 $lpha_s^3 L^4$ $lpha_s^3 L^3$ $lpha_s^4 L^5$ $lpha_s^3 L^2$

Log(t)

NNLO MECS (VINCIA)

[El-Menoufi et al., 2024] [Campbell et al., 2023] [Li, PS, 2017] [Hartgring, Laenen, PS 2013] [Giele, Kosower, PS, 2011]

(→ talk later by B. El-Menoufi)

Nested shower cross sections:

$$d\sigma_0$$

$$d\sigma_0^{\text{ex}}(t_0, t_1) = d\sigma_0 \Delta_0(t_0, t_1)$$

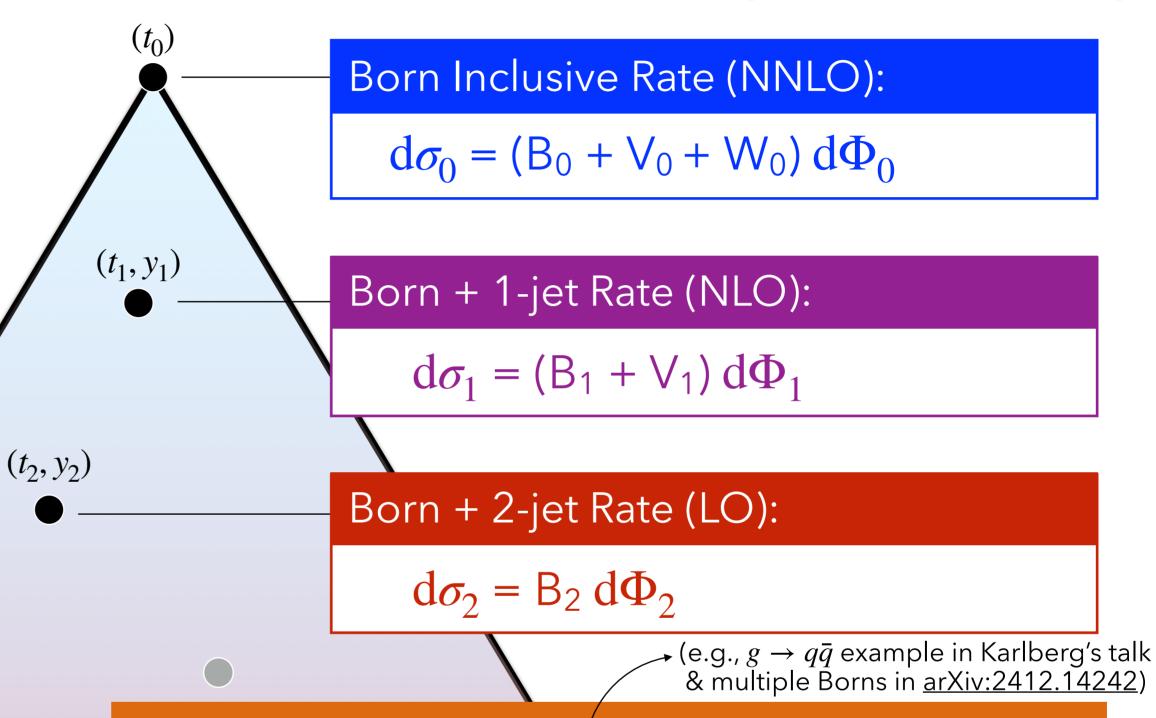
$$d\sigma_1 = d\sigma_0 \frac{d\Delta_{0\mapsto 1}(t_0, t)}{dt} \Big|_{t_1} d\Phi_{+1}^{S}$$

$$d\sigma_1^{\text{ex}}(t_1, t_2) = d\sigma_1 \Delta_1(t_1, t_2)$$

$$d\sigma_2 = d\sigma_1 \frac{d\Delta_{1\mapsto 2}(t_1, t)}{dt} \bigg|_{t_2} d\Phi_{+1}^{S}$$

$$+ d\sigma_0 \frac{d\Delta_{0\mapsto 2}(t_0, t)}{dt} \bigg|_{t_2} d\Phi_{+2}^{S}$$

→ Expand to 2nd order and construct matching conditions



Challenges:

- 1. Resolution choice(s), t
- 2. Sum over histories -
- 3. μ_R scheme and scales
- 4. $\mathcal{O}(\alpha_s^2)$ pole structure
- 5. Phase-space coverage
- 6. Preserving accuracy

Additional Inputs:

NNLL Sudakov Factor

$$\Delta_0^{\mathrm{NNLL}}(t_0, t_1)$$
: tames $t_1 \to 0$

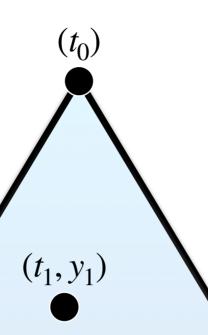
NNLO Normalisation:

$$d\sigma_0 = (B_0 + V_0 + W_0) d\Phi_0$$

Set scales as you would in merging (MiNLO)

Ansatz for diff. distribution of extra (NNLO) contributions

 t^{PW} vs t^{PS} ambiguity from POWHEG (but complexity now @ Born + 1) + now also a further t in Δ_0^{NNLL}



 (t_2, y_2)

Starting Point: Powheg for Born + 1

$$d\sigma_1 = (B_1 + V_1) d\Phi_1 \qquad \triangle t_1 \to 0$$



Born + 2-jet Rate (matched):

$$d\sigma_2 = d\sigma_1 \frac{B_2}{B_1} \Delta_1^{PW}(t_1, t_2^{PW}) \frac{d\Phi_2}{d\Phi_1}$$

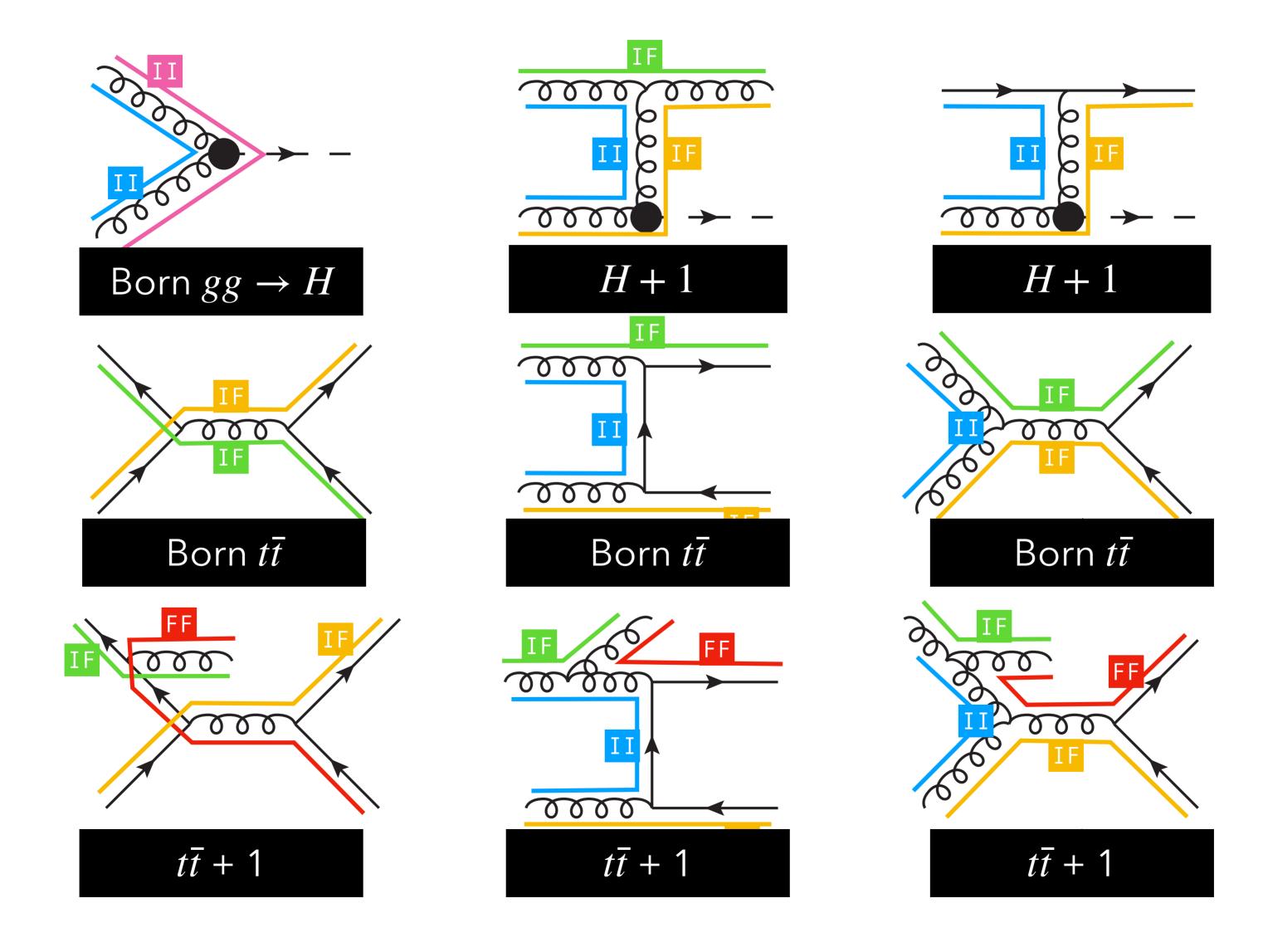
Unitarity*:
$$\Delta_1^{\text{PW}} = \exp\left(-\int_{2\mapsto 1} \frac{B_2}{B_1}\right)$$

*subject to $h_{\rm damp}$

Challenges:

- 1. Resolution choice(s), t
- 2. Sum over histories
- 3. μ_R scheme and scales
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Shower phase-space setups @ Born + 1



A very complex process: $t\bar{t}$



ATLAS PUB Note

ATL-PHYS-PUB-2023-029 22nd September 2023 The new approach is based on the Pythia 8 parton-shower matching parameter $p_{\rm T}^{\rm hard}$. It is designed to surpass the previous method, which involved comparing two generator setups to cover the uncertainty. The old method entangled all differences between the two setups in a single uncertainty while the new prescription implements a focused uncertainty that avoids double-counting with other uncertainties on the modelling of the top processes.

Production: Top quark (and $t\bar{t}$) p_T

Not well modelled by baseline Powheg+PYTHIA Improved @ NNLO QCD

⇒ take difference between nominal and reweighting to NNLO+NNLL as uncertainty

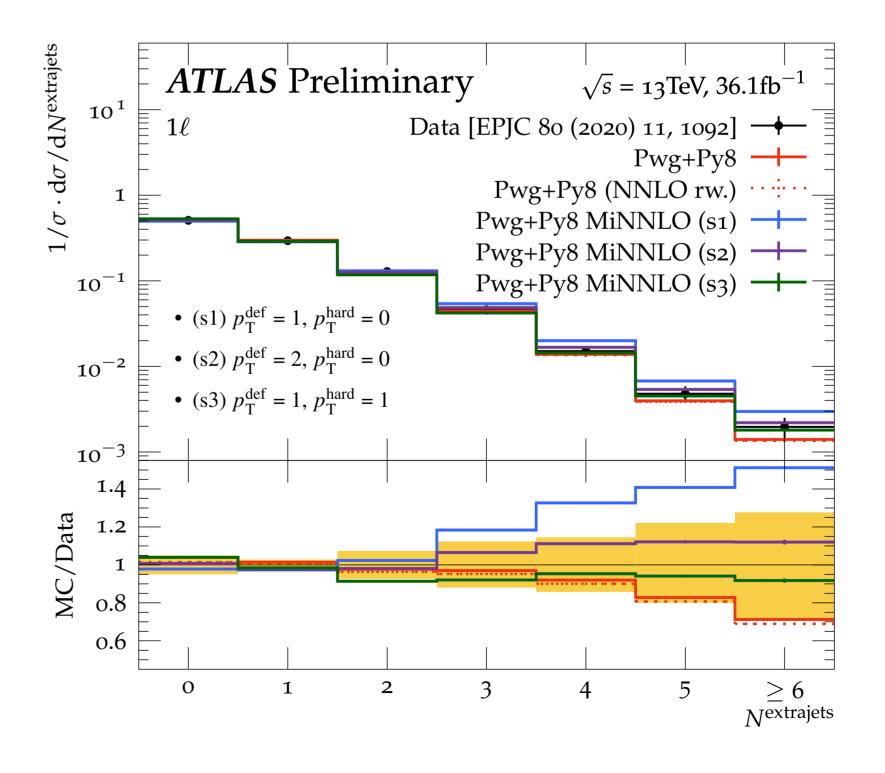
Could be improved upon by MC reaching that accuracy natively

[Mazitelli et al., 2112.12135]

First steps exploring MiNNLO_{PS} for $t\bar{t}$

→ Improvement (but still has **pThard** ambiguity)

Important testing ground



Fully-differential schemes require Born-local subtraction terms?

[Campbell, Hoche, Li, Preuss, PS, 2023; El-Menoufi, Preuss, Scyboz, PS, 2024]

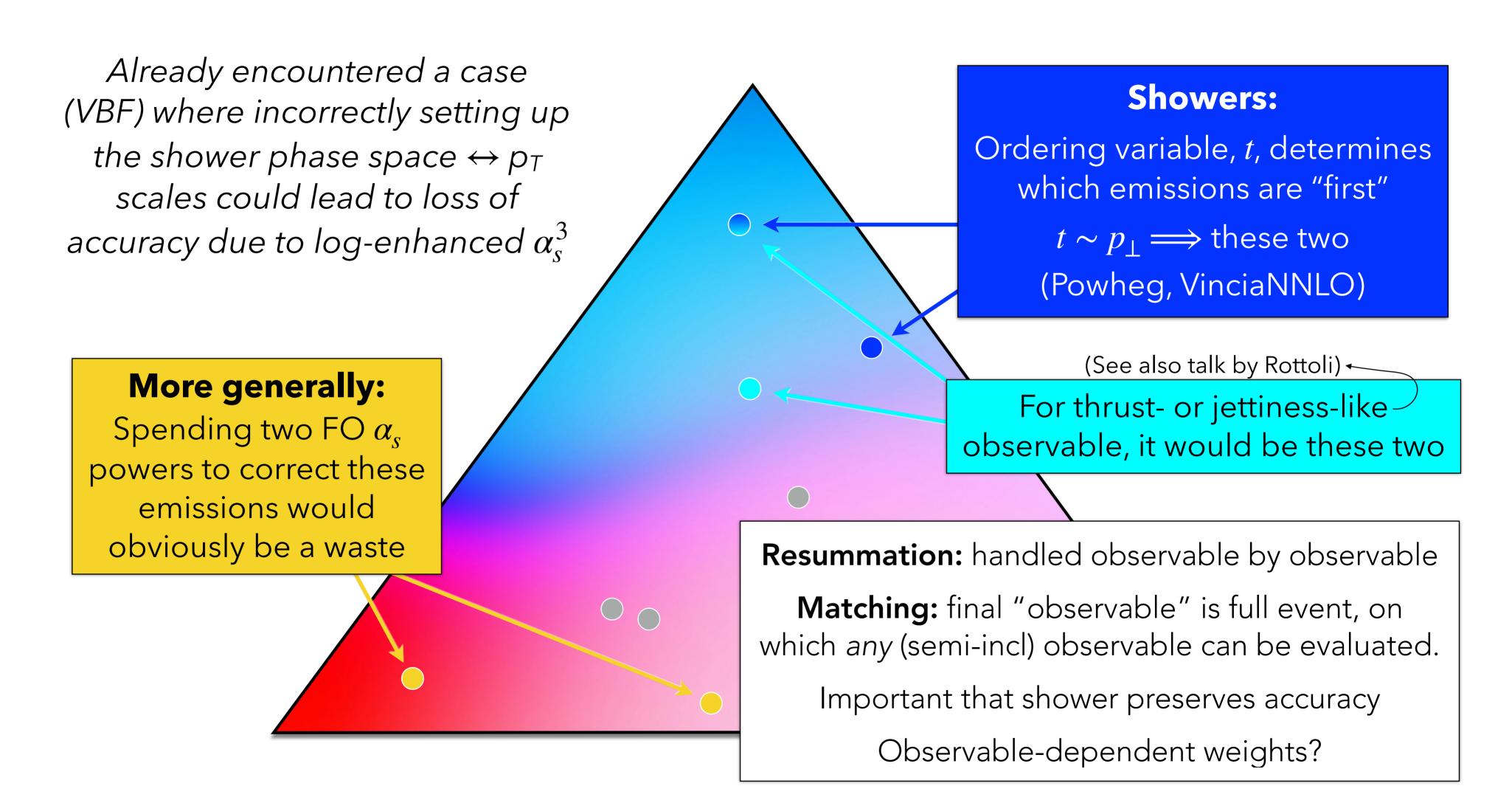
$$k_{\mathrm{NNLO}}(\Phi_2) = 1 + \frac{\mathrm{V}(\Phi_2)}{\mathrm{B}(\Phi_2)} + \frac{\mathrm{I}_{\mathrm{N}}^{\mathrm{NLO}}(\Phi_2)}{\mathrm{B}(\Phi_2)} + \frac{\mathrm{V}\mathrm{V}(\Phi_2)}{\mathrm{B}(\Phi_2)} + \frac{\mathrm{I}_{\mathrm{T}}(\Phi_2)}{\mathrm{B}(\Phi_2)} + \frac{\mathrm{I}_{\mathrm{S}}(\Phi_2)}{\mathrm{B}(\Phi_2)} + \frac{\mathrm{I}_{\mathrm$$

Not an immediate issue: trivial for decays; simple for colour-singlet production.

In general simple if shower kinematics preserve $\Phi_{\rm Born}$ variables. Or compute "sector jet rates"? Do matching using recent fully local subtraction schemes? E.g., [Caola, Melnikov, Röntsch, 2017]

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Spending our hard-earned α_{s} powers



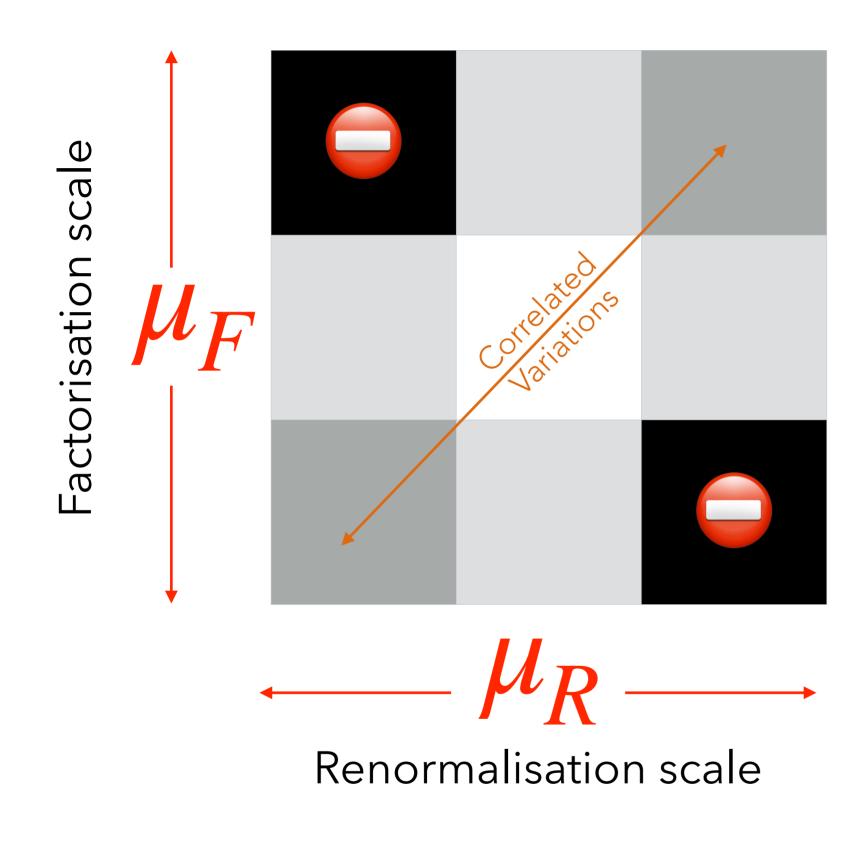
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One last thing!



Uncertainties!

Current Standard for Scale Variations: 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 recipe



Physical Scales, Fastest Apparent Convergence, Least Sensitivity, Maximum Conformality, ...

Vary by factor ~2 in either direction Induces variations $\propto \ln 2$

 \bigcirc 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 ...

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Multiscale Whack-a-mole

Multiscale Problems

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

between two different scales q_1 and q_2

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

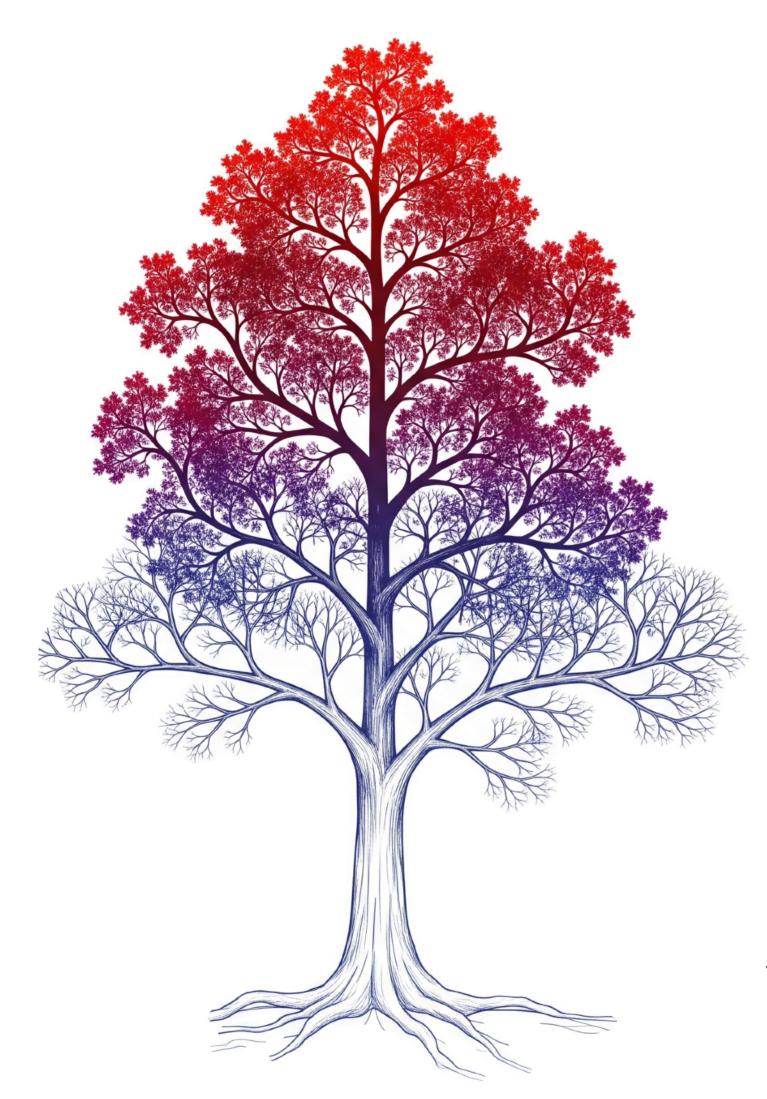
For complex processes involving multiple scales, say a few massive particles + a few jets:

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



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.



Further Discussion?

NNLO matching vs NLO merging?

NNLO matching with (N)LO merging?

Matching at N3LO?

Matching with new subtraction schemes?

Efficiency & Negative weights

Talk by Rottoli

+ Apologies to Geneva-NNLO

(I'm more familiar with MiNNLO_{PS} and VinciaNNLO; presume many challenges are similar, though manifestations may differ?)