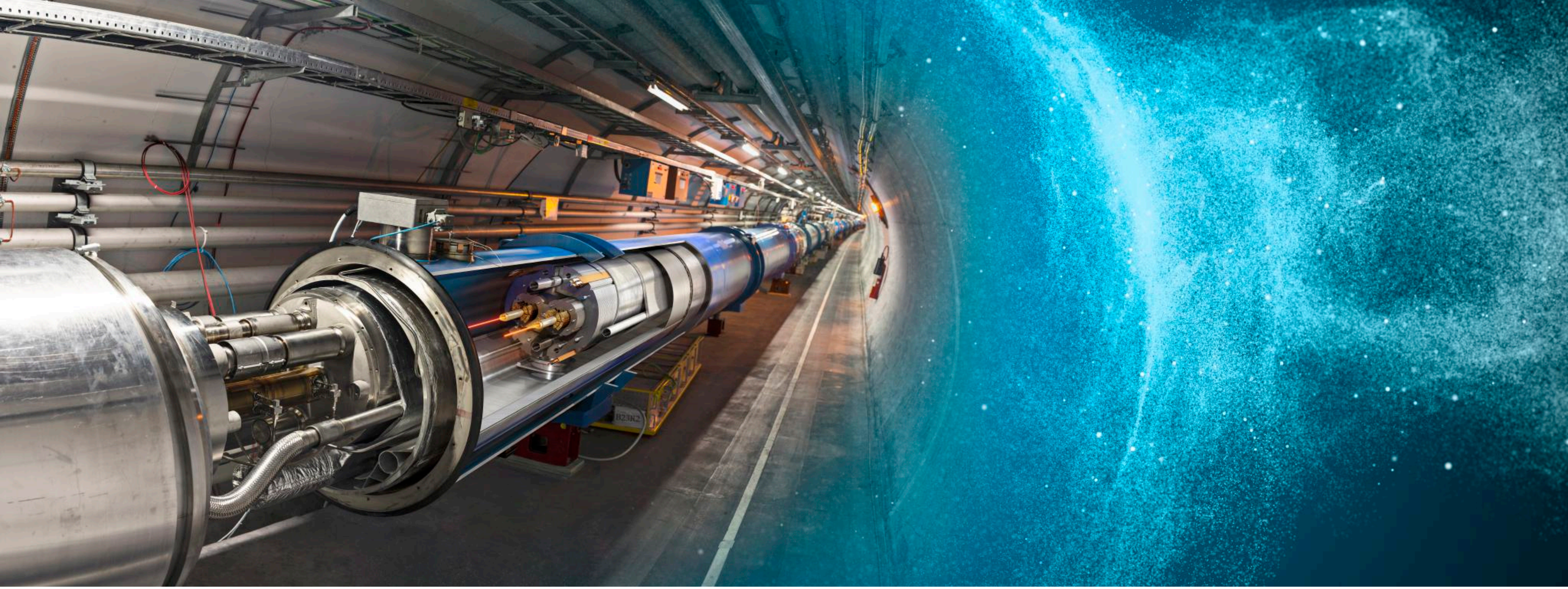


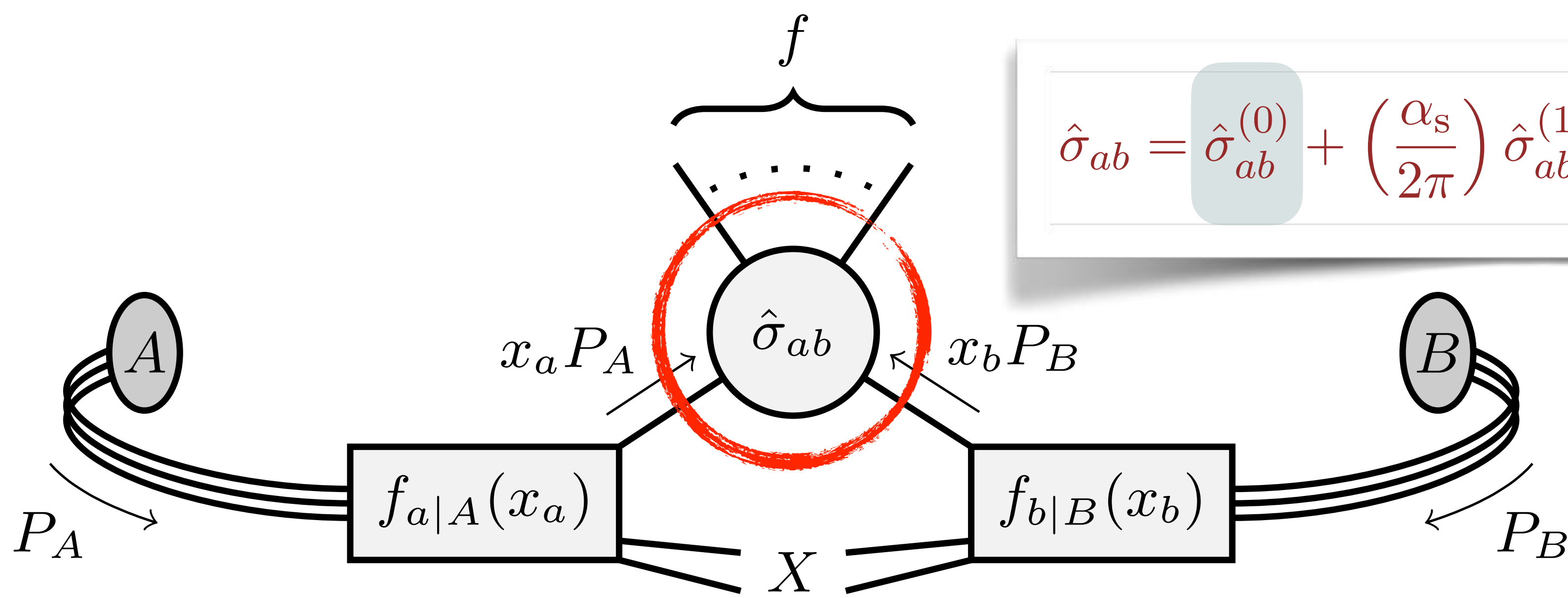
NUMERICAL CHALLENGES IN PRECISION CALCULATIONS

Alexander Huss

Workshop on generator & code acceleration — CERN, 14th November 2023

CERN

Hard Scattering — Perturbation Theory

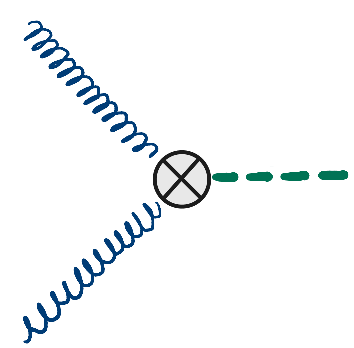


$$\hat{\sigma}_{ab} = \hat{\sigma}^{(0)}_{ab} + \left(\frac{\alpha_s}{2\pi}\right) \hat{\sigma}^{(1)}_{ab} + \left(\frac{\alpha_s}{2\pi}\right)^2 \hat{\sigma}^{(2)}_{ab} + \ldots$$

leading order (LO)

"tree level"

$$\int \mathrm{d}\Phi_n \Bigg($$



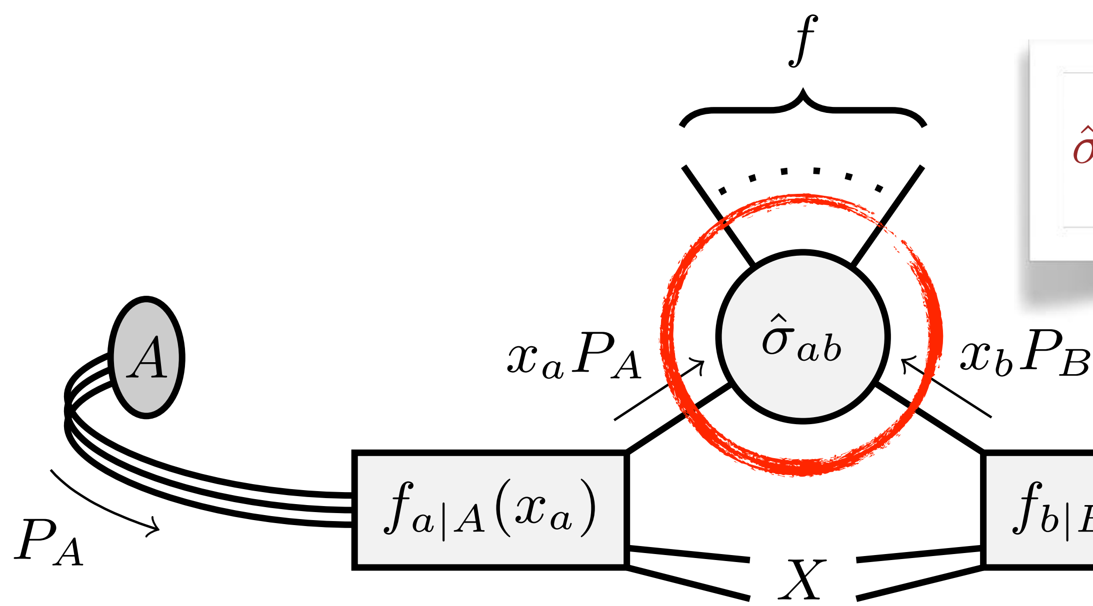
$$\Bigg)$$

no exceptional configurations

"simple" Matrix Elements

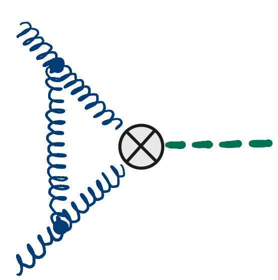
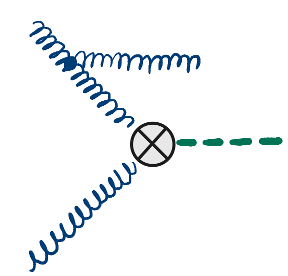
embarrassingly parallel problem with simple & well-behaved ingredients
⇒ well suited for parallelisation

Hard Scattering — Perturbation Theory



$$\hat{\sigma}_{ab} = \hat{\sigma}^{(0)}_{ab} + \left(\frac{\alpha_s}{2\pi}\right) \hat{\sigma}^{(1)}_{ab} + \left(\frac{\alpha_s}{2\pi}\right)^2 \hat{\sigma}^{(2)}_{ab} + \ldots$$

next-to-leading order (NLO)

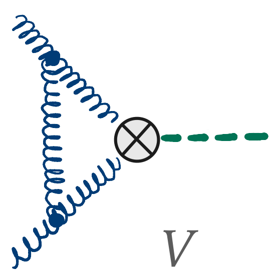
$\int \mathrm{d}\Phi_n \Big($  $\Big) + \int \mathrm{d}\Phi_{n+1} \Big($  $\Big)$

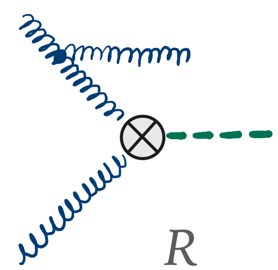
"virtual" (V) *"real" (R)*

why does it not extend simply to higher orders?
⇜⇝ singularities (individually ill-defined)

inclusive

SUBTRACTIONS — A TOY EXAMPLE

(

+ 

)

$$\frac{1}{\epsilon} + a$$

$$\int_0^1 \frac{1+bx}{x^{1+\epsilon}}\,\mathrm{d}x$$

$$\rightsquigarrow$$

$$-\frac{1}{\epsilon} + b$$

$$a + b$$

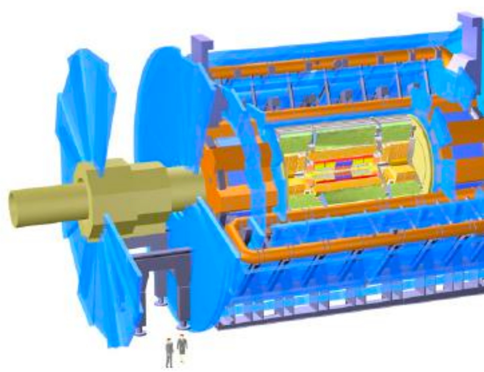
- *dimensionally regularized:*
  - $D = 4 - 2\epsilon$
  - everything up to $\mathcal{O}(\epsilon)$
- *emission "phase space":*
  - $x \in [0, 1]$
  - no emission $\leftrightsquigarrow$ $x \to 0$

Subtractions — A Toy Example

fiducial

$$\left(\frac{1}{\epsilon}+a\right)\mathcal{J}(0) \qquad \int_0^1 \frac{1+bx}{x^{1+\epsilon}}\,\mathcal{J}(x)\,\mathrm{d}x$$

- *measurement function* $\mathcal{J}(x)$
  - acceptance
  - jet algorithm
  - isolation
  - distributions
  - …



Very complicated / impossible(?) to do analytically

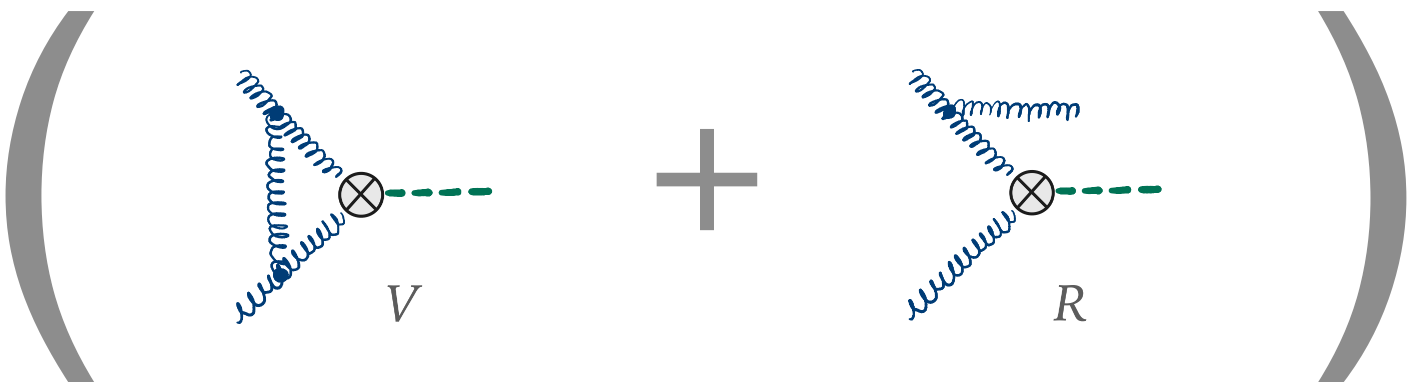
?

flexible *numerical* approach desired
↪ 2 strategies

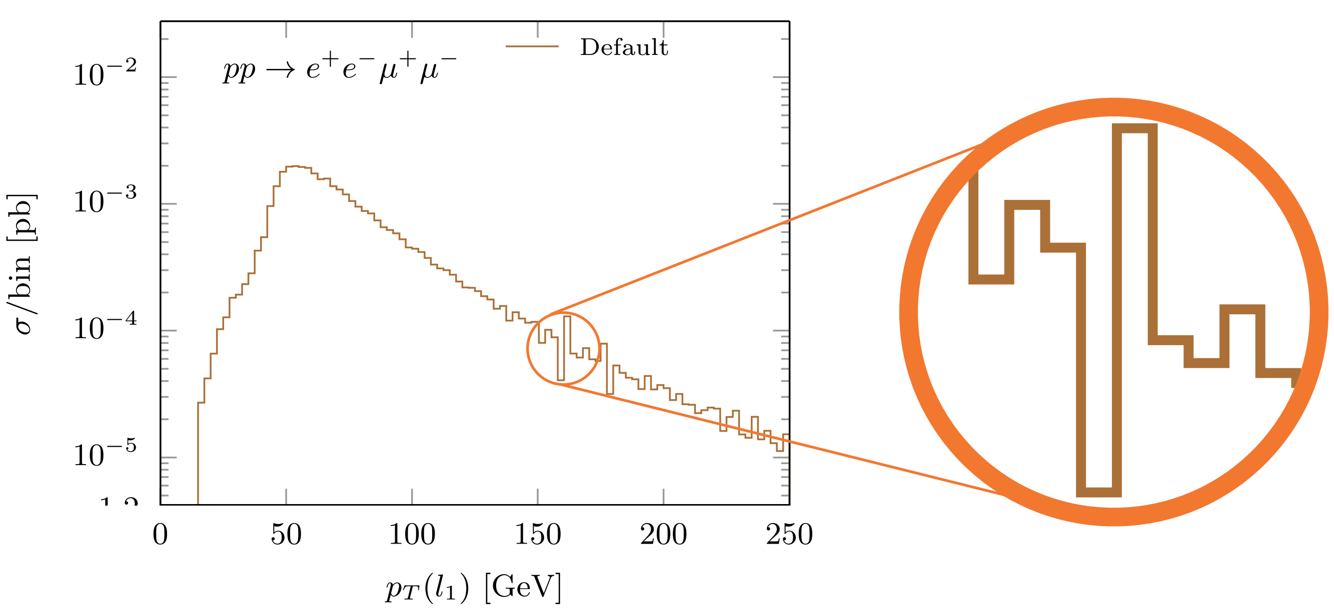
(notebook: indico "toy-nlo")

SUBTRACTIONS — A TOY EXAMPLE: SUBTRACTION

fiducial



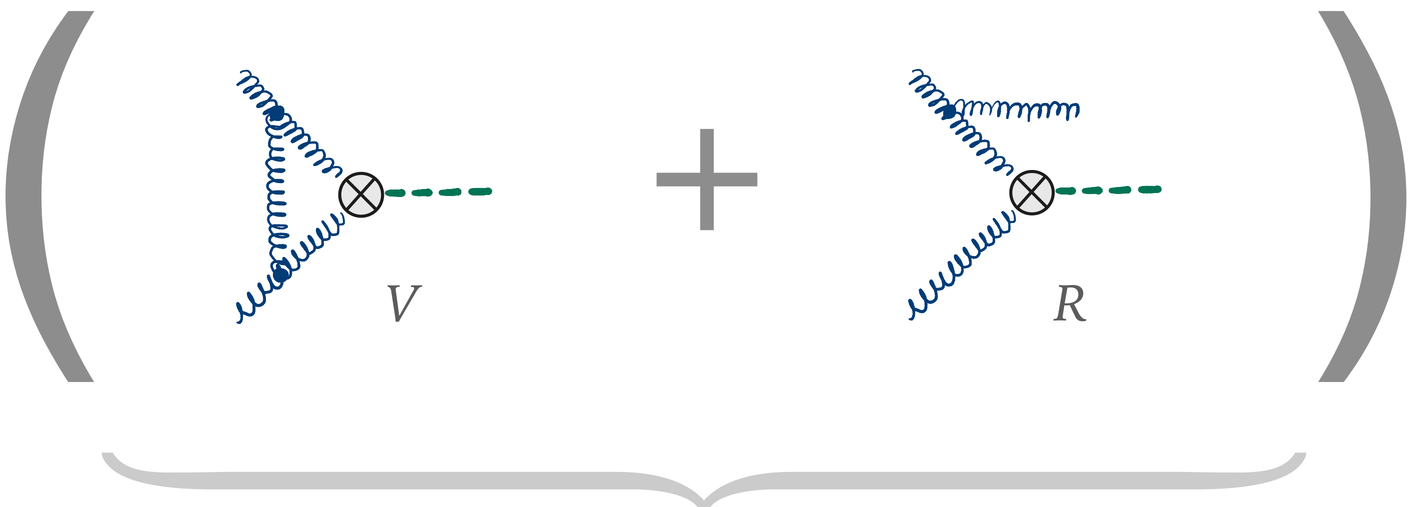
$$(a+b)\mathcal{J}(0) + \int_0^1 \frac{1+bx}{x}\left[\mathcal{J}(x)-\mathcal{J}(0)\right]\,\mathrm{d}x$$

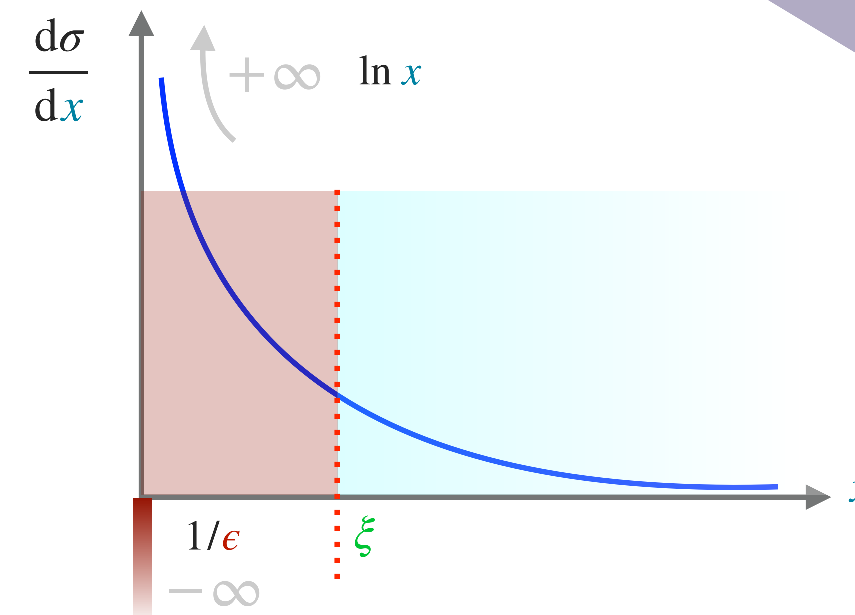


- *regulate divergence in the integrand*
  - can set $\epsilon = 0$
- *challenge: numerical cancellations*
  - floats not exact
  - outliers & “misbinning”

SUBTRACTIONS – A TOY EXAMPLE: SLICING

fiducial

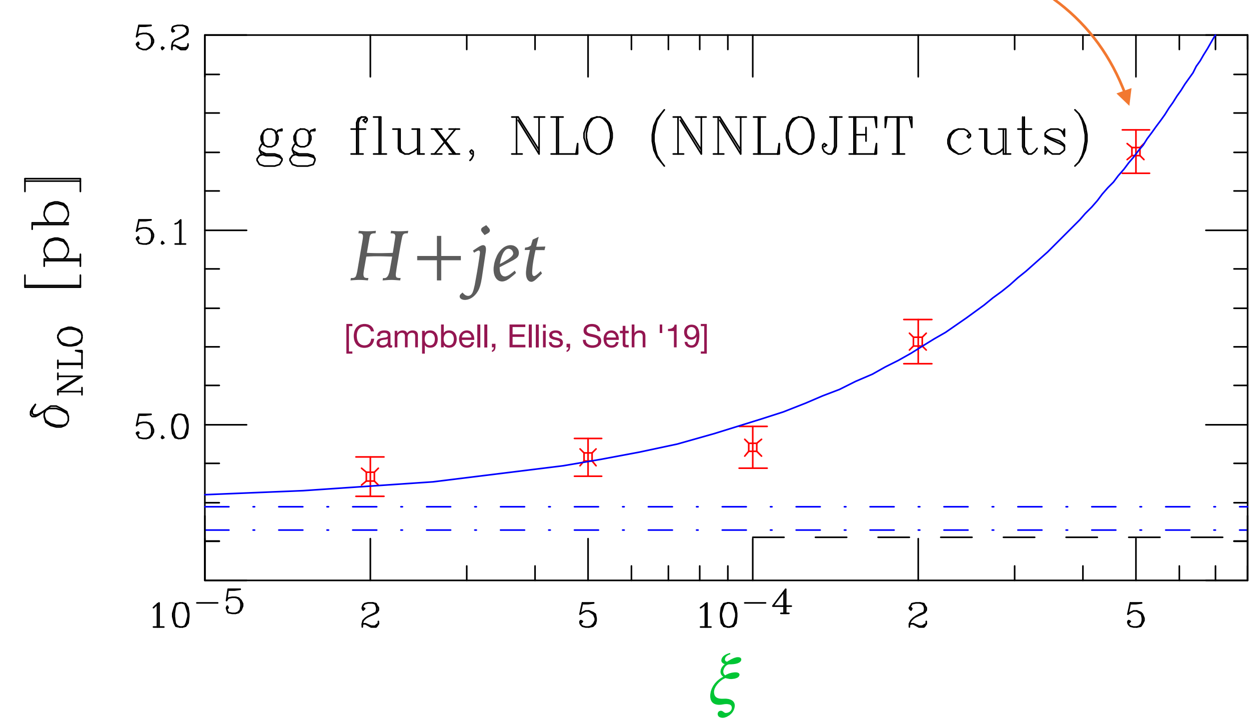




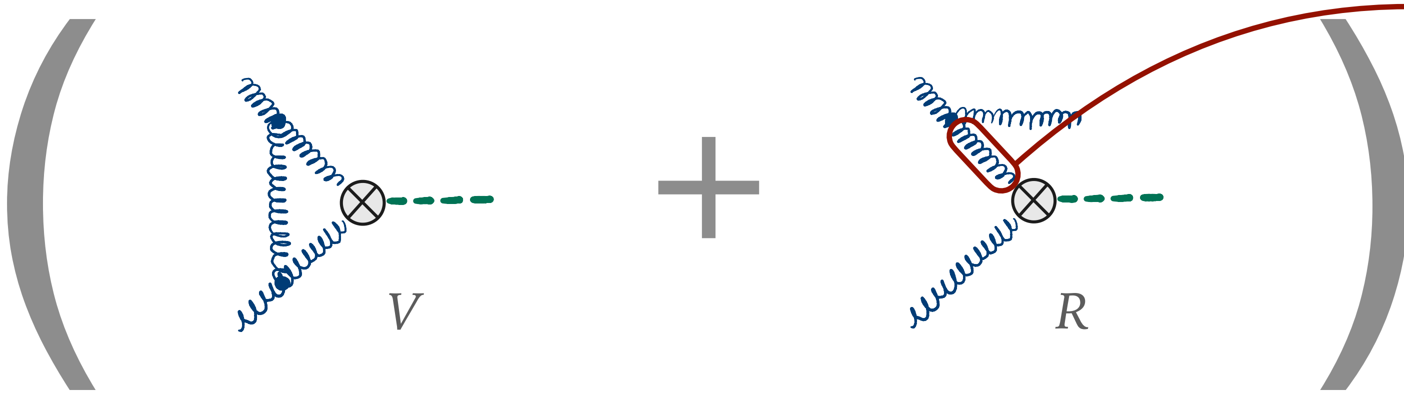
$$\left(a+\ln\xi\right)\mathcal{J}(0) + \int_{\xi}^{1} \frac{1+bx}{x}\,\mathcal{J}(x)\,\mathrm{d}x + \mathcal{O}(\xi^n)$$

need to control the error!

- *regulate divergence with cutoff*
  - error term $\mathcal{O}(\xi^n)$
- *challenge: numerical cancellations*
  - $\ln\xi$ cancels against 2nd term
  - higher target precision



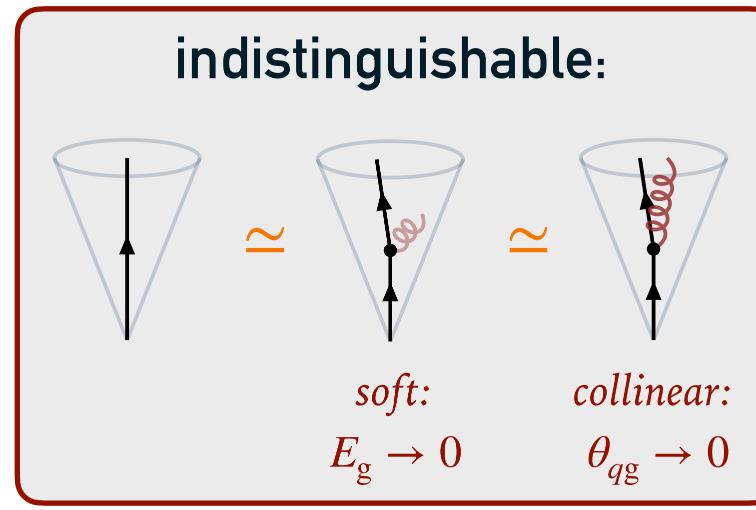
SUBTRACTIONS – NLO



$$\sim \frac{1}{(p_a - k_1)^2} \sim \frac{1}{p_{\mathrm{T},1}}$$

- *$1/\varepsilon^2$, $1/\varepsilon$*
- *single unresolved*

$p_{\mathrm{T}}^{\mathrm{H}} = p_{\mathrm{T},1} \to 0$



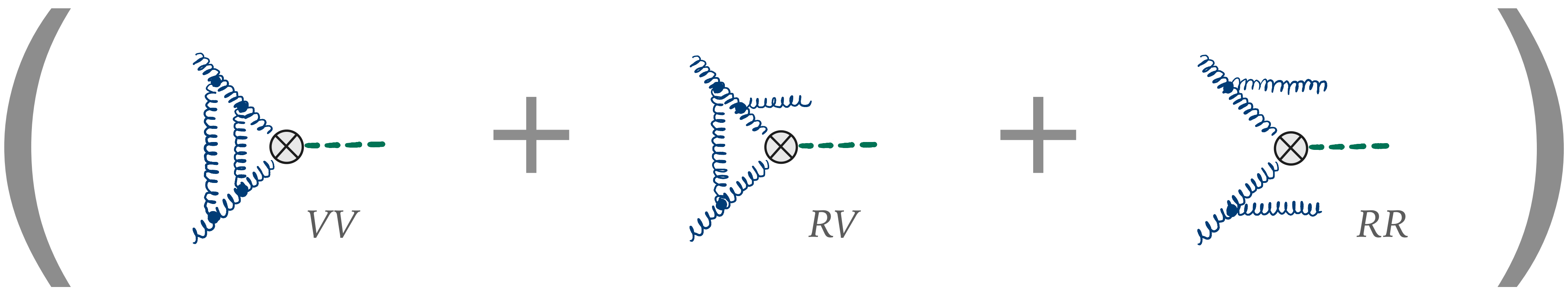
Infrared cancellation:

- subtraction: more complex integrands
  - correlated ME & counterterms
- slicing: higher precision target
  - non-local cancellations

conceptually solved:

CS dipoles, FKS, …

Subtractions – NNLO



- $1/\varepsilon^4,\ 1/\varepsilon^3,\ 1/\varepsilon^2,\ 1/\varepsilon$

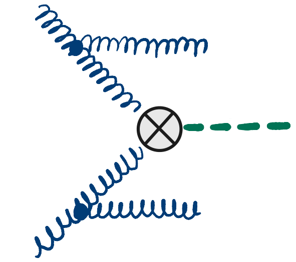
- $1/\varepsilon^2,\ 1/\varepsilon$
- *single unresolved*

- *single unresolved*
- *double unresolved*

single unresolved $\simeq$ H+jet @ NLO

fully unresolved $\simeq$ H @ NNLO

Subtractions – NNLO (Double-Real)



- conceptual challenge NLO ⇝ NNLO: overlapping singularities

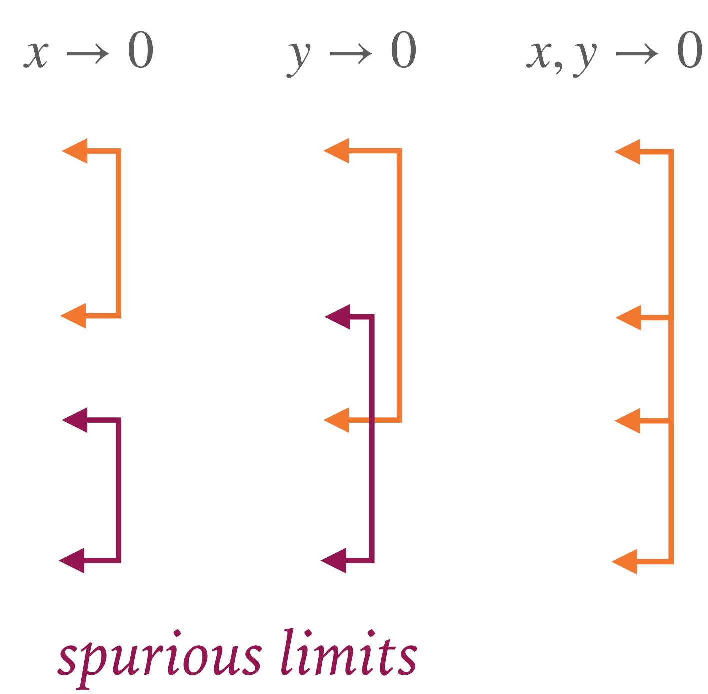
$$\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \, \frac{1 + bx + cy + dxy}{x^{1+\epsilon}\, y^{1+\epsilon}} \, \mathcal{J}(x,y)$$

(toy double real)

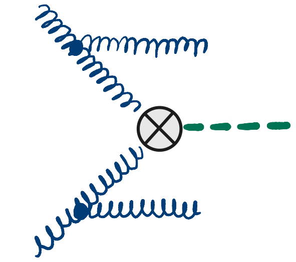
⇣ *local subtraction*

$$\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \, \frac{1}{x\,y} \Big[(1 + bx + cy + dxy)\, \mathcal{J}(x,y) - (1 + cy)\, \mathcal{J}(0,y) - (1 + bx)\, \mathcal{J}(x,0) + \mathcal{J}(0,0) \Big]$$

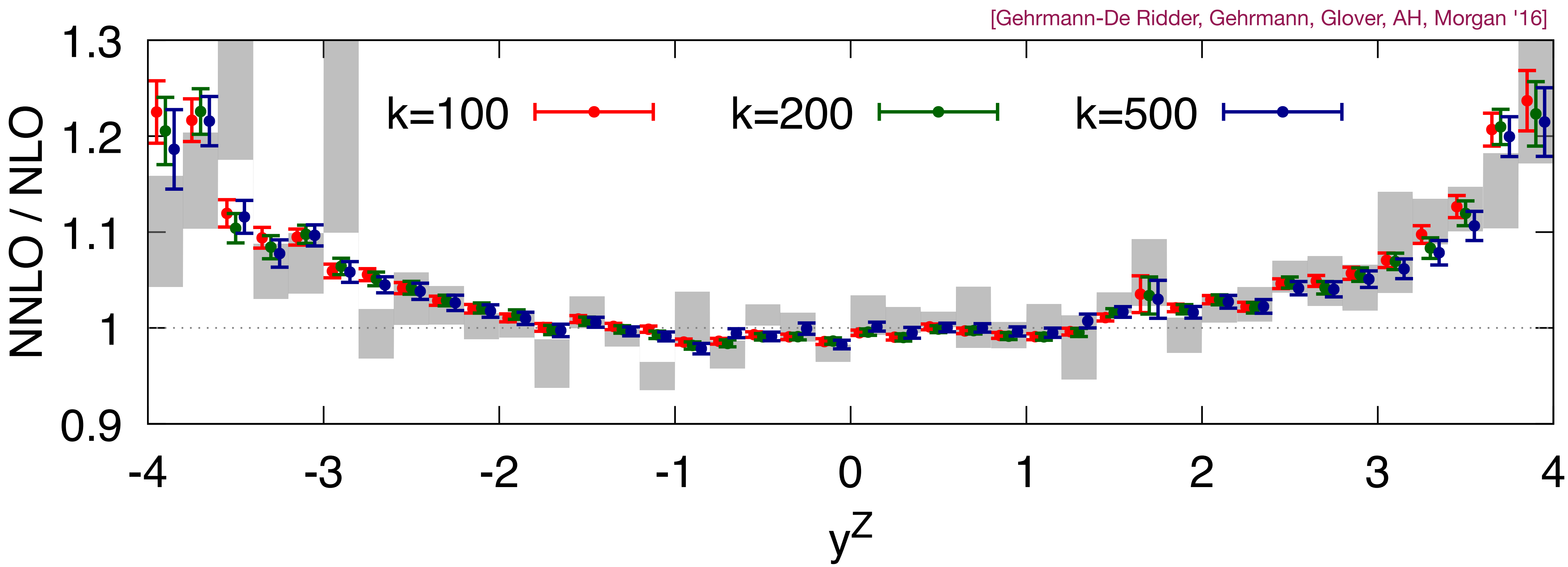
Sectors can disentangle counterterms but will induce large cancellations between integrated sectors



SUBTRACTIONS – NNLO (DOUBLE-REAL)

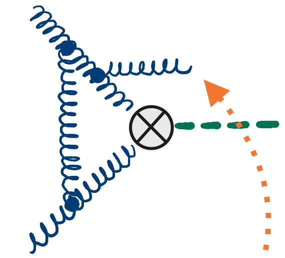


- impact from outliers: a subtle but important issue



- naive combination of raw data
- post-processing (outlier rejection / weighted avg.)

SUBTRACTIONS – NNLO (REAL-VIRTUAL)



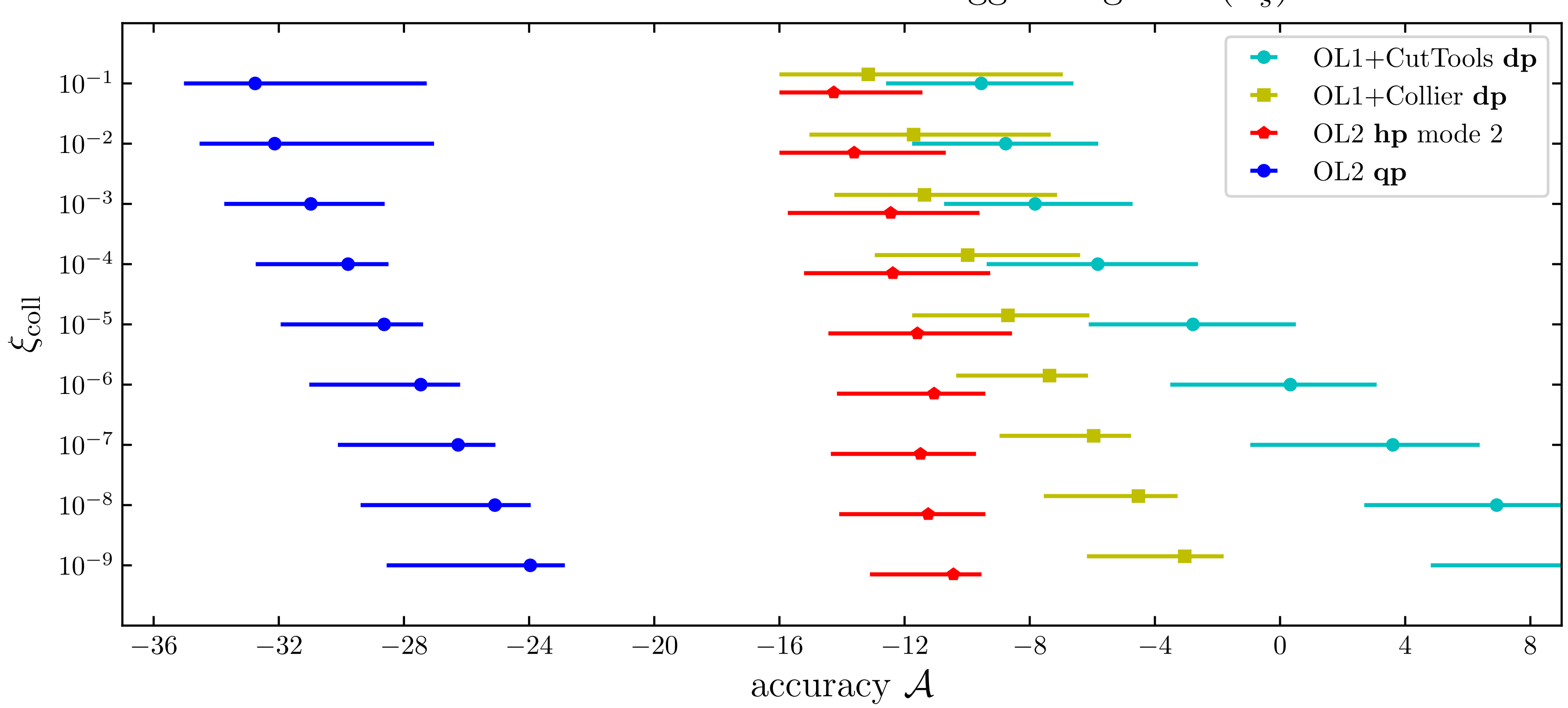
- automated one-loop providers:
  - MG5, OpenLoops, Recola, Gosam, NLOX, …

$E \to 0$,
$\cos\theta \to 1$

- new in context of NNLO (RV) ⇝ probe unresolved regions
  - numerical instabilities from e.g. spurious $1/\Delta$ singularities; $\Delta = \det(p_i \cdot p_j)$

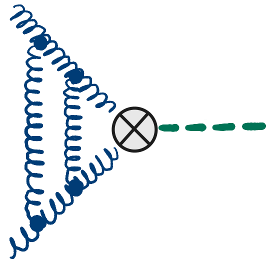
[Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller '19]

intial-state collinear radiation in gg $\to t\bar{t}g$ at $\mathcal{O}(\alpha_s^4)$



- *rescue system for numerical stability*
  - dp (f64) → hp (hybrid): $\times\, \mathcal{O}(2\text{–}10)$ penalty
  - dp (f64) → qp (f128): $\times\, \mathcal{O}(10\text{–}100)$ penalty

SUBTRACTIONS – NNLO (DOUBLE-VIRTUAL)



- among most challenging amplitudes so far: $2 \to 3$ (massless)
  - $\mathcal{O}$(few–100) seconds per phase-space point

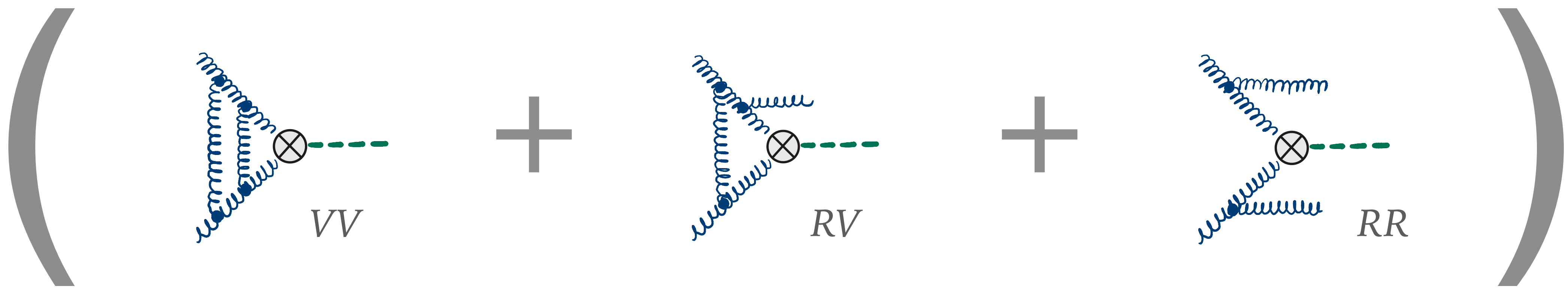
- pentagon functions (Feynman integrals)

[Chicherin, Sotnikov '21]

Precision	Correct digits	Timing (s)
double	13	2.5
quadruple	29	180
octuple	60	3900

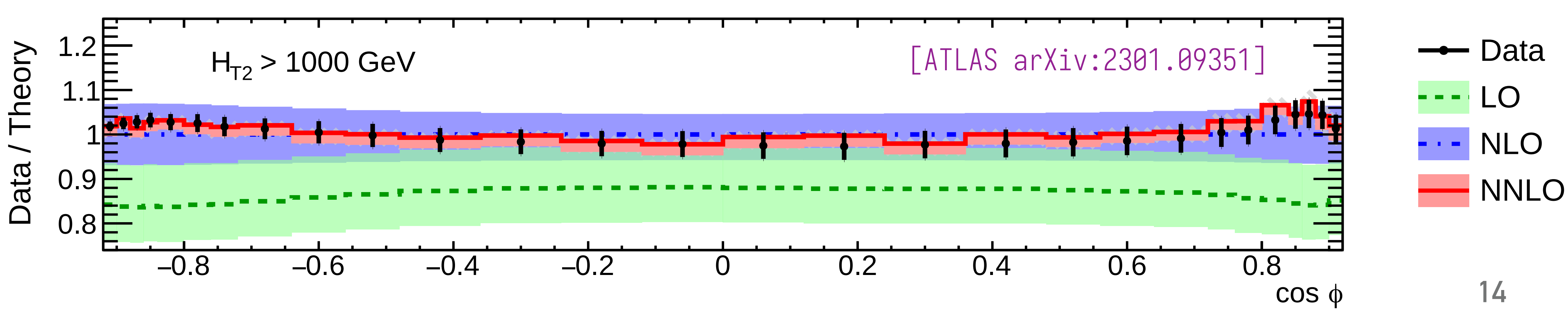
Talks by
D. Maitre,
S. Badger,
T. Gehrmann

Subtractions – NNLO



- typical runtime for $2 \to 2$ processes: $\mathcal{O}$(100k) CPU core hours
  - V+jet, di-jet, … ⇜⇝ VV:RV:RR ∼ 1:20:100 (CPU hours)
- an extreme $2 \to 3$ example: $\mathcal{O}$(100M) CPU core hours
  - tri-jet ⇜⇝ VV:RV:RR ∼ 1:100:200 (CPU hours)

$$\frac{1}{\sigma}\frac{\mathrm{d}\Sigma}{\mathrm{d}\cos\phi}$$



Subtractions – N^{3}LO

- $1/\varepsilon^6$, $1/\varepsilon^5$, …

- $1/\varepsilon^4$, $1/\varepsilon^3$, …
- *single unresolved*

- $1/\varepsilon^2$, $1/\varepsilon$
- *single unresolved*
- *double unresolved*

- *single unresolved*
- *double unresolved*
- *triple unresolved*

two methods for "2 → 1"

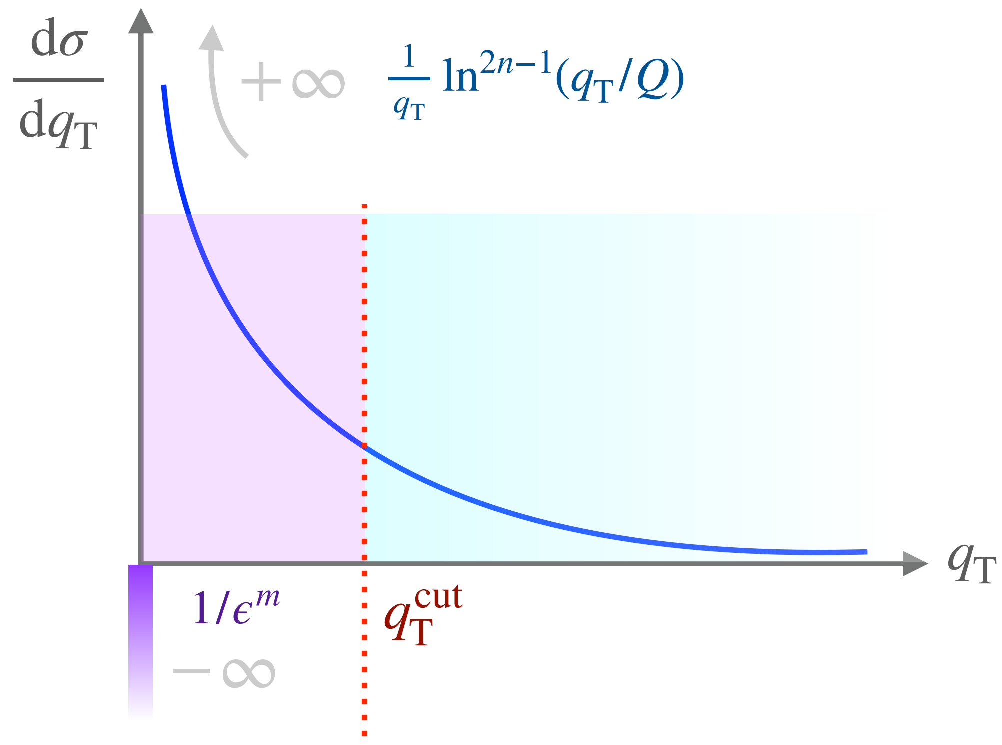
isolate "radiating" part

double unresolved $\simeq$ H+jet @ NNLO

fully unresolved $(\leftrightsquigarrow p_T^H \to 0)$ $\simeq$ H @ N^{3}LO

SUBTRACTIONS – N³LO: SLICING

[Chen, Gehrmann, Glover, AH, Yang Zhu '21]



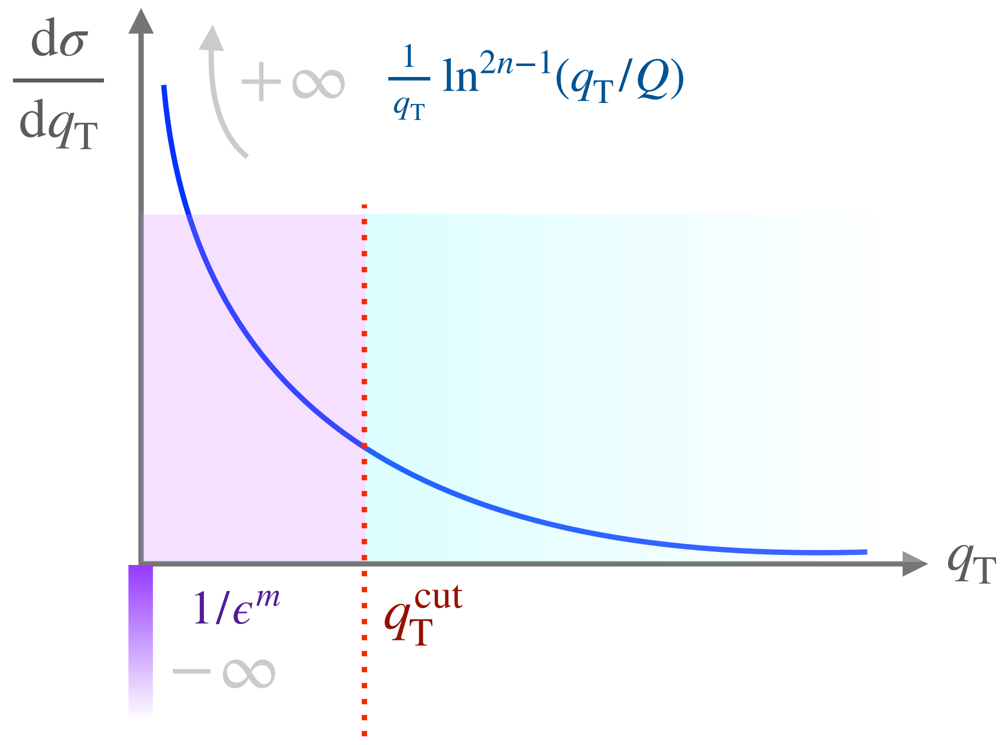
$$\delta\sigma^V_{\rm N^3LO}\Big|_{q_T<q_T^{\rm cut}} + \delta\sigma^V_{\rm N^3LO}\Big|_{q_T>q_T^{\rm cut}} + \mathcal{O}\left((q_T^{\rm cut}/Q)^n\right)$$

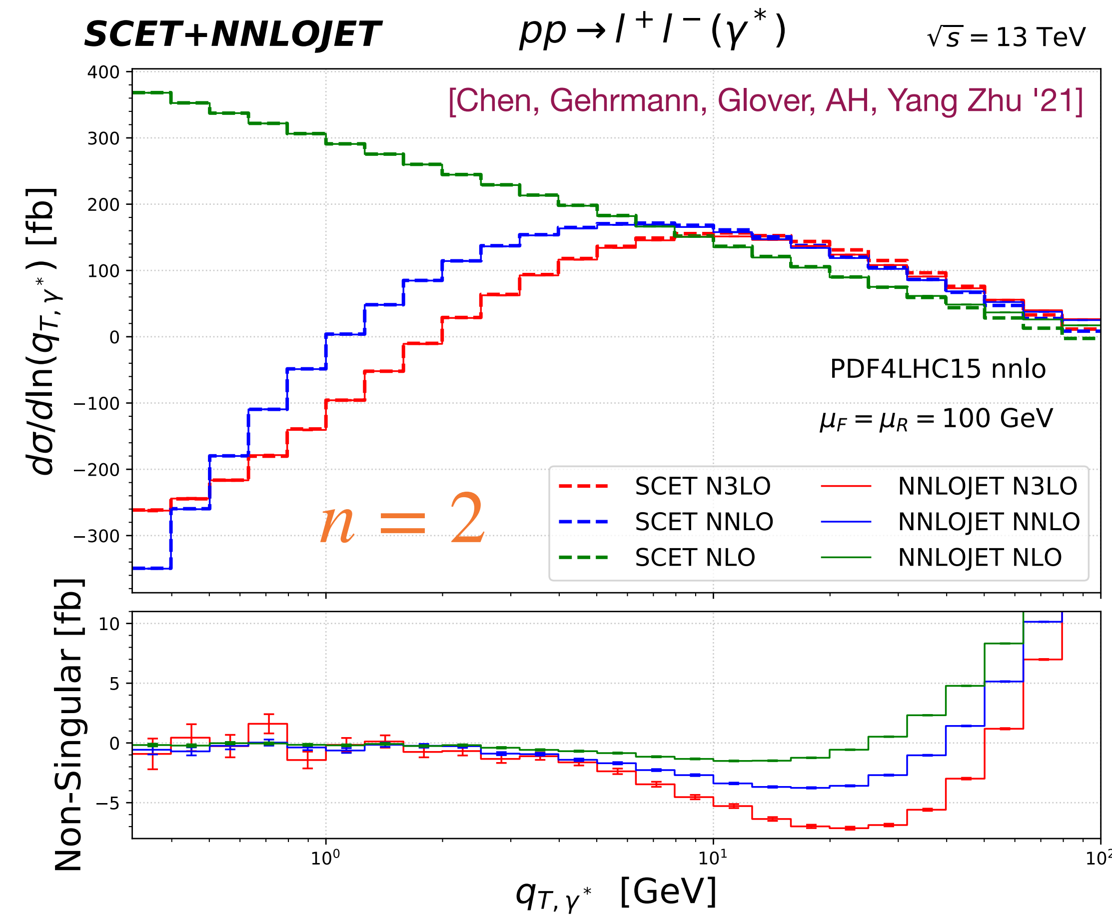
$\mathcal{O}(\epsilon)$ %   99.9… %   *(CPU cost)*

analytic   *V+jet calculation pushed to the limit*

- 2-loop amplitudes in single-unresolved limit
- 1-loop amplitudes in double-unresolved limits

Subtractions – N^3LO: Slicing





$$\delta\sigma^V_{N^3LO}\Big|_{q_T<q_T^{cut}} + \delta\sigma^V_{N^3LO}\Big|_{q_T>q_T^{cut}} + \mathcal{O}\left((q_T^{cut}/Q)^n\right)$$

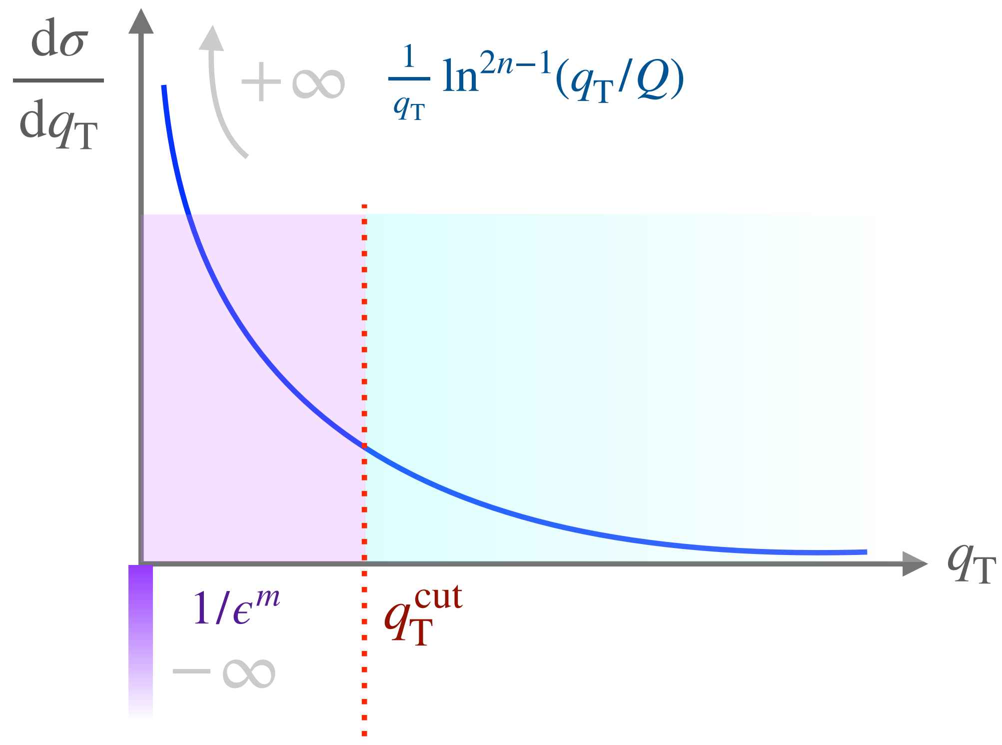
$$\mathcal{O}(150\,\text{fb}) - \mathcal{O}(150\,\text{fb}) \sim -8\,\text{fb}$$

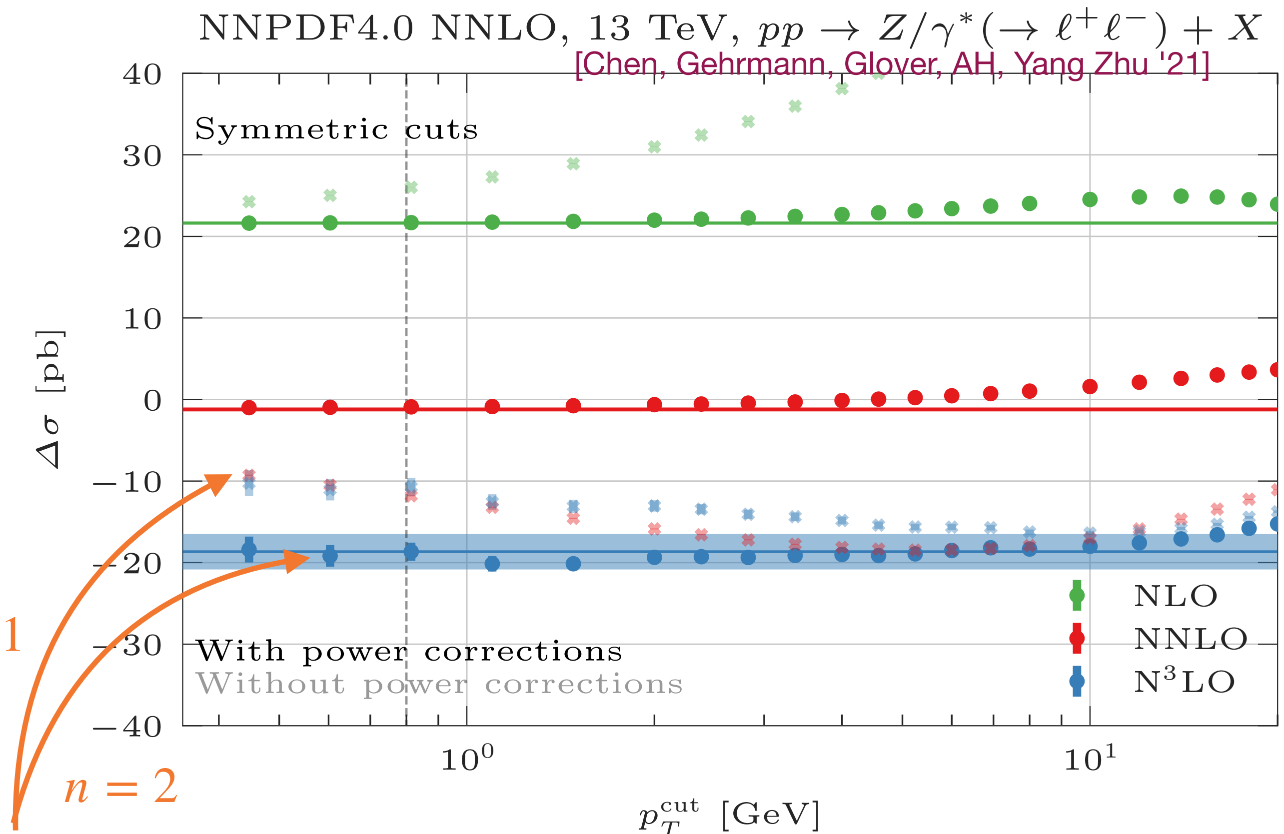
$\mathcal{O}(\epsilon)\,\%$ — 99.9… % — *(CPU cost)*

analytic — *V+jet calculation pushed to the limit*

- 2-loop amplitudes in single-unresolved limit
- 1-loop amplitudes in double-unresolved limits

SUBTRACTIONS – N³LO: SLICING





$n = 1$

$n = 2$

$$\delta\sigma^{V}_{\mathrm{N^3LO}}\Big|_{q_\mathrm{T}<q_\mathrm{T}^{\mathrm{cut}}} + \delta\sigma^{V}_{\mathrm{N^3LO}}\Big|_{q_\mathrm{T}>q_\mathrm{T}^{\mathrm{cut}}} + \mathcal{O}\left((q_\mathrm{T}^{\mathrm{cut}}/Q)^n\right)$$

impact of the error term

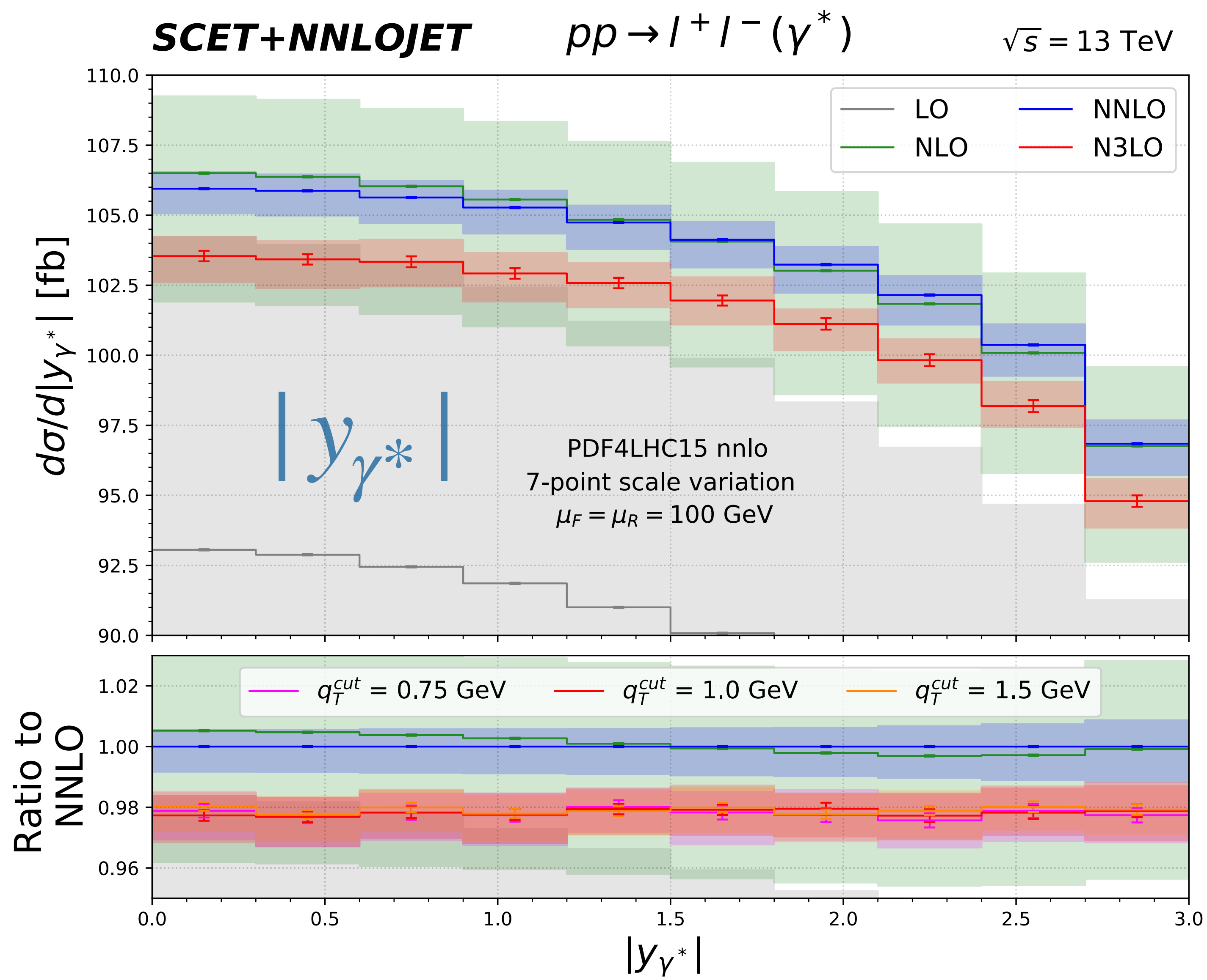
$\mathcal{O}(\epsilon)\,\%$ 99.9… % *(CPU cost)*

analytic *V+jet calculation pushed to the limit*

- 2-loop amplitudes in single-unresolved limit
- 1-loop amplitudes in double-unresolved limits

SUBTRACTIONS – N^{3}LO: SLICING

[Chen, Gehrmann, Glover, AH, Yang Zhu '21]

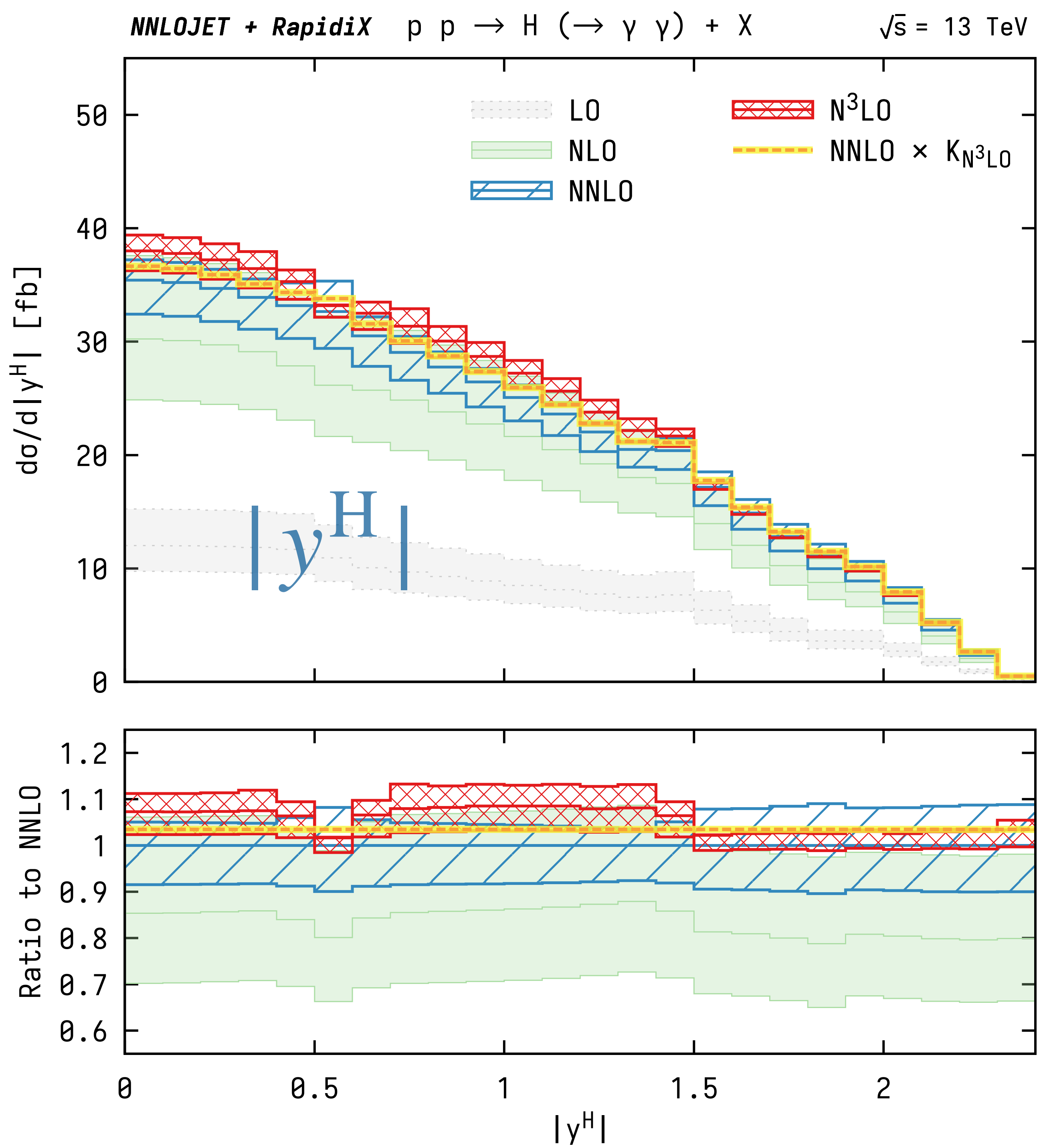


- investment:
  ↪ $\mathcal{O}$(5M) CPU core hours
- in principle, *fully differential*
- experiments can measure DY *triply-differentially* in $\mathcal{O}$(500) bins!
- in practice, extrapolated $\mathcal{O}$(100M) CPU core hours is getting problematic

SUBTRACTIONS – N³LO: SUBTRACTION

[Chen, Gehrmann, Glover, AH, Mistlberger, Pelloni '21]

- a *local subtraction* can significantly improve the performance
- requires inclusive prediction (so far only ggH @ LHC)
- reduce cost to underlying H+jet @ NNLO level:
  ↪ $\mathcal{O}$(100k) CPU core hours



Summary

- **Infrared singularities** — core bottle neck in precision calculations

⇒ both local & non-local approaches struggle with large numerical cancellations

- **higher orders:**
  - *more complex Matrix Elements — rescue system (quad?)*
  - *more complex integrand — whole collection of correlated MEs & counterterms each with separate measurement functions (branches) & scales (e.g.: α_s, PDFs), …*
  - *how realistic to put the full thing on e.g. GPUs?*
    ↪ *in the interim: attack smaller ingredients (ME, LIPS, …)?*

- **current paradigm:** "embarrassingly parallel" problem tackled using CPUs on large clusters
  - some NNLO $2 \to 3$ calculations reaching computing limits
    ↪ *more efficient method @ NNLO needed?*
  - N^{3}LO $2 \to 1$ with slicing — difficult to extrapolate to high-precision pheno.
    ↪ *compute power corrections? better observables? …*
  - N^{3}LO $2 \to 1$ with subtraction — good performance but relies on additional TH input

Summary

- **Infrared singularities** — core bottle neck in precision calculations

⇒ both local & non-local approaches struggle with large numerical cancellations

- **higher orders**:
  - *more complex Matrix Elements — rescue system (quad?)*
  - *more complex integrand — whole collection of correlated MEs & counterterms each with separate measurement functions (branches) & scales (e.g.: α_s, PDFs), …*
  - *how realistic to put the full thing on e.g. GPUs?*
    ↪ *in the interim: attack smaller ingredients (ME, LIPS, …)?*

- **current paradigm:** "embarrassingly parallel" problem tackled using CPUs on large clusters
  - some NNLO $2 \to 3$ calculations reaching computing limits
    ↪ *more efficient method @ NNLO needed?*
  - N^{3}LO $2 \to 1$ with slicing — difficult to extrapolate to high-precision pheno.
    ↪ *compute power corrections? better observables? …*
  - N^{3}LO $2 \to 1$ with subtraction — good performance but relies on additional TH input

Thank you!