Subtraction and Residual PDFs: heavy-quark treatments in global QCD analyses

Marco Guzzi

with

Pavel Nadolsky and Keping Xie

CTEQ

KENNESAW STATE UNIVERSITY

15th Conference on the Intersections of Particle and Nuclear Physics

CIPANP2025, University of Wisconsin-Madison, WI, June 9, 2025

WISCONSIN UNIVERSITY OF WISCONSIN–MADISON

Motivations

- Exp data at current and future colliders continue to extend on a wider range of collision energies and so do modern global analyses of proton PDFs

Towards new CTEQ (CT25) PDFs

Preliminary

NNLO fits with new data (nD) from LHC at 8 and 13 TeV

χ^2/N_{pt} for CT18A + new data (*vs.* CT18A at right) NNLO fits; 68% CL

ID	Experimental data set	N_{pt}	CT25prel	CT18A
	Drell-Yan pair production			
211	ATLAS 8 TeV W	22	$2.37^{+1.30}_{-0.68}$	$3.56^{+2.26}_{-1.65}$
212	CMS 13 TeV Z	12	$2.10^{+2.20}_{-0.38}$	$2.13^{+3.46}_{-0.30}$
214	ATLAS 8 TeV Z 3D	188	$1.14^{+0.10}_{-0.04}$	$1.21^{+0.32}_{-0.15}$
215	ATLAS 5.02 TeV W,Z	27	$0.70^{+0.27}_{-0.06}$	$0.74^{+0.31}_{-0.08}$
217	LHCb 8 TeV W	14	$1.36^{+0.37}_{-0.34}$	$1.47^{+0.43}_{-0.38}$
218	LHCb 13 TeV Z	16	$1.06^{+0.76}_{-0.38}$	$1.29^{+0.95}_{-0.44}$
	13 TeV $t\bar{t}$ production			
521	ATLAS all-hadronic $y_{t\bar{t}}$	12	$1.07^{+0.08}_{-0.05}$	$1.07^{+0.12}_{-0.07}$
528	CMS dilepton $y_{t\bar{t}}$	10	$1.10^{+0.56}_{-0.40}$	$1.13^{+0.85}_{-0.53}$
581	CMS lepton+jet $m_{t\bar{t}}$	15	$1.38^{+0.65}_{-0.40}$	$1.44^{+0.89}_{-0.56}$
587	ATLAS lepton+jet $m_{t\bar{t}} + y_{t\bar{t}} + y^B_{t\bar{t}} + H^{t\bar{t}}_T$	34	$0.94^{+0.13}_{-0.11}$	$0.94^{+0.28}_{-0.09}$
	Inclusive jet production			
553	ATLAS 8 IncJet	171	$1.54^{+0.09}_{-0.06}$	$1.57^{+0.12}_{-0.07}$
554	ATLAS 13 IncJet	177	$1.25^{+0.07}_{-0.03}$	$1.26^{+0.08}_{-0.04}$
555	CMS 13 IncJet	78	$1.11^{+0.13}_{-0.09}$	$1.10^{+0.21}_{-0.10}$

(fits with 1 new process, 'nProcces')

nDY

nTT

nIncJet

nD

(combined fit)

also dijet data, but don't (officially) know how to combine with inclusive jets

776 new data points from DY, $t\bar{t}$ and jets for CT25

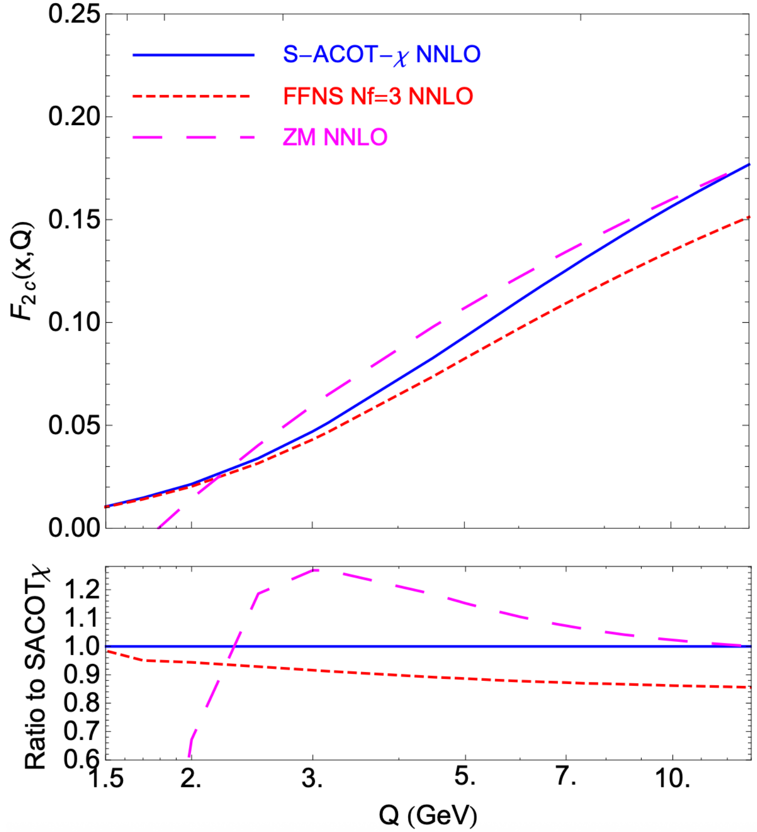
Motivations

- Exp data at current and future colliders continue to extend on a wider range of collision energies and so do modern global analyses of proton PDFs.

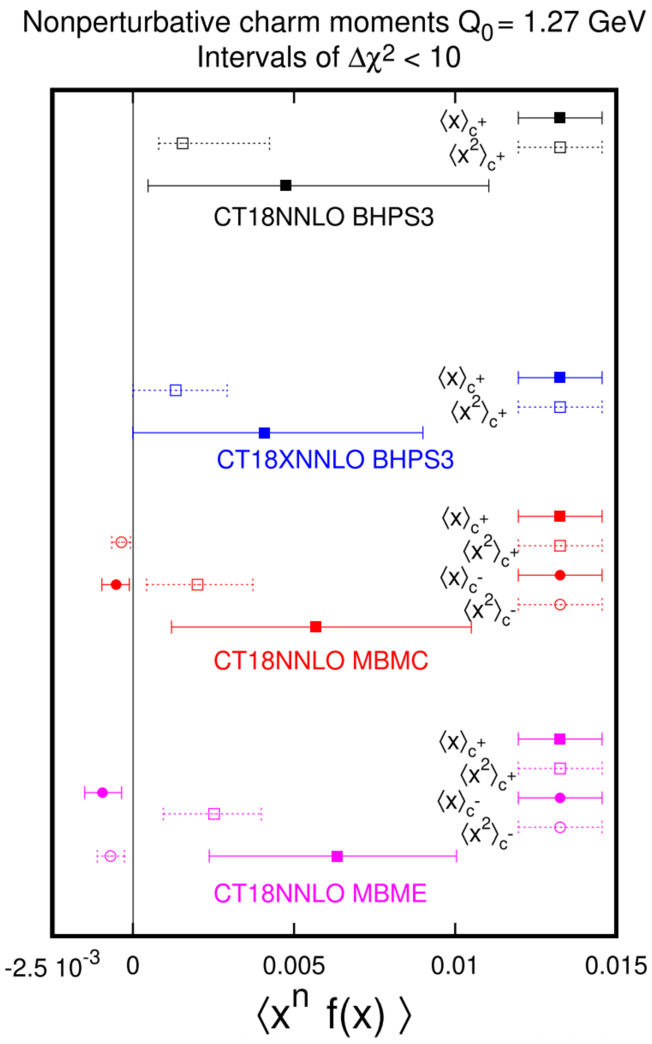
- Increased sensitivity to mass effects, e.g., phase-space suppression, large radiative corrections to collinear $Q\bar{Q}$ production: **magnitude comparable to $\boldsymbol{NNLO}$ and $\boldsymbol{N^3LO}$ corrections.** Need a consistent **General Mass Variable Flavor Number (GMVFN)** scheme

impact on many important observables

DIS structure Functions



MG, Nadolsky, Lai, Yuan, PRD 2012



MG, Hobbs, Xie, Nadolsky, Yuan, PLB 2023

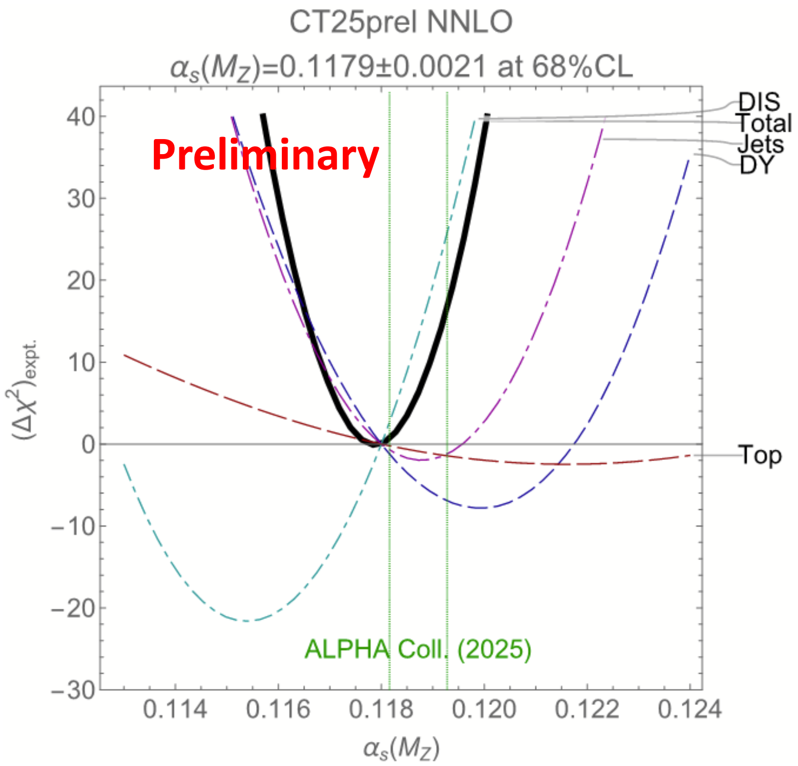


Figure by P. Nadolsky (2025)

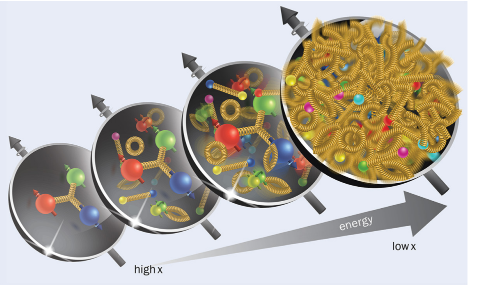
Motivations

- Exp data at current and future colliders continue to extend on a wider range of collision energies and so do modern global analyses of proton PDFs.

- Increased sensitivity to mass effects, e.g., phase-space suppression, large radiative corrections to collinear $Q\bar{Q}$ production: **magnitude comparable to $NNLO$ and N^3LO corrections**. Need a consistent **General Mass Variable Flavor Number (GMVFN)** scheme

- Natural to evaluate cross sections in a factorization (GMVFN) scheme, which assumes that the number of (nearly) massless quark flavors varies with energy, and at the same time includes dependence on heavy-quark masses in relevant kinematical regions.

- Particularly relevant for global PDF analyses



Outline/Goals

- ➢ Simplify GMVFN scheme implementations to improve PDFs extractions and phenomenology
- ➢ ACOT-like GMVFN schemes: extended to pp collisions using the concept of ***subtraction and residual PDFs.*** Applied to various processes of interest:

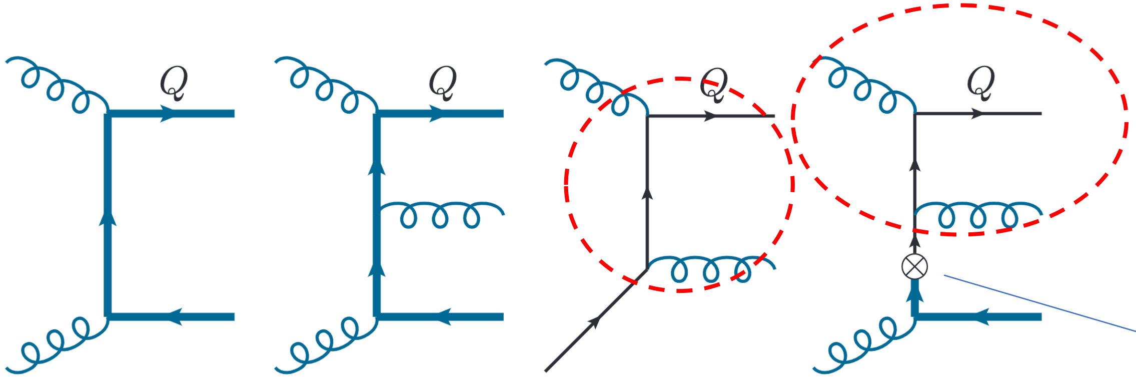
- pp→ $Z + b + X$ @NLO; MG, Nadolsky, Reina, Wackeroth, Xie, **PRD 2024**;
- pp→ $H + X$ @NNLO; Biello, Gauld, MG, Nadolsky, Sankar, Wiesemann, Xie, Zanderighi (In prog.);
- DIS: Extension of ACOT-like schemes to aN^3LO; MG, Nadolsky, Xie, (In prog.)

This effort is important to understand new high-precision data at colliders, and is connected to:

- Consistent treatment of HQ effects in PDFs (Intrinsic HQ, constrain HQ PDFs)
- DGLAP evolution @N^3LO
- NNLO → N^3LO transition

Subtraction and Residual PDFs: Basic idea

Inclusive production of a HQ in pp collisions as an example



LO FC   NLO FC   LO FE   Subtraction

Mass fully retained in $\hat{\sigma}$ and dPS

Mass fully retained in dPS

The subtraction term avoids double counting and cancels enhanced collinear contributions from FC when $\hat{s} \gg 4m_Q^2$ or $p_T \gg \ m_Q$

Collinear splitting $gg \to Q\bar{Q}$

S-ACOT-Massive-Phase-Space (S-ACOT-MPS)

$$\sigma = \mathrm{FC} \ + \mathrm{FE} - \mathrm{SB}.$$

Subtraction well defined also in the $p_T \to 0$ limit

allows us to get (FE-Subtraction) in one step

FE − Subtraction ➡ facilitated by introducing **Residual PDF:**

$$\delta f_Q(x,\mu^2) = f_Q(x,\mu^2) - \underbrace{\frac{\alpha_s}{2\pi}\log\left(\frac{\mu^2}{m_Q^2}\right)P_{Q\to g}(x)\otimes f_g(x,\mu^2)}_{\textbf{Subtraction PDF}}$$

Other details in: K. Xie, “Massive elementary particles in the standard model and its supersymmetric triplet Higgs extension.” https://scholar.smu.edu/hum_sci_physics_etds/7, 2019. PhD Thesis

GMVFN Theory framework (pp collisions)

The differential cross section for $p_A\, p_B \to F + X$ where F contains at least one HQ, can be written

$$\frac{\mathrm{d}\sigma(A+B\to F+X)}{\mathrm{d}\mathcal{X}} = \sum_{i,j}\int_{x_A}^{1}\mathrm{d}\xi_A \int_{x_B}^{1}\mathrm{d}\xi_B\, f_{i/A}(\xi_A,\mu) f_{j/B}(\xi_B,\mu)\frac{\mathrm{d}\widehat{\sigma}(i+j\to F+X)}{\mathrm{d}\mathcal{X}}$$

After dσ/dχ is UV renormalized, we identify its infrared-safe part d$\hat{\sigma}$/dχ by factoring out ``parton-level'' PDFs

$$G_{ij} \equiv \frac{\mathrm{d}\sigma(i+j\to F+X)}{\mathrm{d}\mathcal{X}} \text{ after UV renormalization},$$
$$H_{km} \equiv \frac{\mathrm{d}\widehat{\sigma}(k+m\to F+X)}{\mathrm{d}\mathcal{X}},$$

$$\widehat{x}_i \equiv x_i/\xi_i$$

$$\boxed{\begin{aligned} G_{ij}\left(x_A,x_B\right) &= \sum_{k,m}\int_{x_A}^{1}\mathrm{d}\xi_A\int_{x_B}^{1}\mathrm{d}\xi_B\, f_{k/i}(\xi_A) f_{m/j}(\xi_B) H_{km}\left(\widehat{x}_A,\widehat{x}_B\right) \\ &\equiv [f_{k/i}\rhd H_{km}\lhd f_{m/j}](x_A,x_B). \end{aligned}}$$

Convolution product with two variables

$$[f\rhd H]\left(x_A,x_B\right) \equiv \int_{x_A}^{1}\frac{\mathrm{d}\xi_A}{\xi_A} f(\xi_A) H(\widehat{x}_A,x_B),$$
$$[H\lhd f]\left(x_A,x_B\right) \equiv \int_{x_B}^{1}\frac{\mathrm{d}\xi_B}{\xi_B} H(x_A,\widehat{x}_B) f(\xi_B).$$

Convolution product with one variable

$$\int_x^1\frac{\mathrm{d}\xi}{\xi} f(\xi) g\left(\frac{x}{\xi}\right) = [f\rhd g]\left(x\right) = [g\lhd f]\left(x\right)$$

GMVFN Theory framework (pp collisions)

The perturbative expansion of terms leads to

$$G_{i,b}(x_A,x_B) = G^{(0)}_{i,b}(x_A,x_B) + a_s\,G^{(1)}_{i,b}(x_A,x_B) + a_s^2\,G^{(2)}_{i,b}(x_A,x_B) + \ldots,$$
$$H_{i,a}(\widehat{x}_A,\widehat{x}_B) = H^{(0)}_{i,a}(\widehat{x}_A,\widehat{x}_B) + a_s\,H^{(1)}_{i,a}(\widehat{x}_A,\widehat{x}_B) + a_s^2 H^{(2)}_{i,a}(\widehat{x}_A,\widehat{x}_B) + \ldots,$$
$$f_{a/b}(\xi) = \delta_{ab}\delta(1-\xi) + a_s\,A^{(1)}_{ab}(\xi) + a_s^2 A^{(2)}_{ab}(\xi) + a_s^3 A^{(3)}_{ab}(\xi) + \ldots,$$

$$\widehat{x} = x/\xi.$$

$A^{(k)}_{ab}$ $(k = 0,1,2,\ldots)$ operator-matrix elements (OMEs)

$A^{(1)}_{hg}(\xi) = 2P^{(1)}_{hg}(\xi)\,\ln(\mu^2/m_h^2)$ * for $g \to Q\bar{Q}$

Substituting these in the previous formula for G and solving for $H^{(k)}$ order by order in a_s one obtains

$$H^{(0)}_{ij}(x_A,x_B) = G^{(0)}_{ij}(x_A,x_B),$$

$$H^{(1)}_{ij}(x_A,x_B) = G^{(1)}_{ij}(x_A,x_B) - [A^{(1)}_{ki} \rhd H^{(0)}_{kj}](x_A,x_B) - [H^{(0)}_{im} \lhd A^{(1)}_{mj}](x_A,x_B)$$

$$\begin{aligned} H^{(2)}_{ij}(x_A,x_B) = {} & G^{(2)}_{ij}(x_A,x_B) - [A^{(1)}_{ki} \rhd H^{(1)}_{kj}](x_A,x_B) - [H^{(1)}_{im} \lhd A^{(1)}_{mj}](x_A,x_B) \\ & - [A^{(2)}_{ki} \rhd H^{(0)}_{kj}](x_A,x_B) - [H^{(0)}_{im} \lhd A^{(2)}_{mj}](x_A,x_B) \\ & - [A^{(1)}_{ki} \rhd H^{(0)}_{km} \lhd A^{(1)}_{mj}](x_A,x_B)\,, \end{aligned}$$

$$\begin{aligned} H^{(3)}_{ij}(x_A,x_B) = {} & G^{(3)}_{ij}(x_A,x_B) - [A^{(1)}_{ki} \rhd H^{(2)}_{kj}](x_A,x_B) - [H^{(2)}_{im} \lhd A^{(1)}_{mj}](x_A,x_B) \\ & - [A^{(2)}_{ki} \rhd H^{(1)}_{kj}](x_A,x_B) - [H^{(1)}_{im} \lhd A^{(2)}_{mj}](x_A,x_B) \\ & - [A^{(3)}_{ki} \rhd H^{(0)}_{kj}](x_A,x_B) - [H^{(0)}_{im} \lhd A^{(3)}_{mj}](x_A,x_B) \\ & - [A^{(1)}_{ki} \rhd H^{(1)}_{km} \lhd A^{(1)}_{mj}](x_A,x_B) \\ & - [A^{(2)}_{ki} \rhd H^{(0)}_{km} \lhd A^{(1)}_{mj}](x_A,x_B) - [A^{(1)}_{ki} \rhd H^{(0)}_{km} \lhd A^{(2)}_{mj}](x_A,x_B). \end{aligned}$$

....

Two forms for the OMEs

$$\begin{cases} A^{(n)}_{ij}(\xi,\mu^2) = \displaystyle\sum_{l=1}^{n} \left(\frac{1}{\epsilon}\right)^l P^{(n,l)}_{ij}(\xi) + \sum_{l=0}^{n} \ln^l\left(\frac{\mu^2}{\mu^2_{\rm IR}}\right) P'^{(n,l)}_{ij}(\xi) \\ A^{(n)}_{Qj}\left(\xi,\dfrac{\mu^2}{m_Q^2}\right) = \displaystyle\sum_{l=0}^{n} \ln^l\left(\frac{\mu^2}{m_Q^2}\right) a^{(n,l)}_{Qj}(\xi) \end{cases}$$

*Our convention for the splitting functions

$$P_{ij}(x,a_s) = a_s P^{(1)}_{ij}(x) + a_s^2 P^{(2)}_{ij}(x) + a_s^3 P^{(3)}_{ij}(x) + \ldots\,.$$

Subtraction PDFs

Once the $H_{ij}^{(k)}$ functions are determined, the hadronic cross section in pp collisions can be written as

$$\mathrm{d}\sigma = \sum_{i,j} f_{i/A} \triangleright \left[a_s H^{(1)} + a_s^2 H^{(2)} + a_s^3 H^{(3)} + \ldots\right]_{ij} \triangleleft f_{j/B}$$

Then, the various subtraction ("sub") terms can be collected as follows:

$$-\mathrm{d}\sigma_{\mathrm{sub}} = - a_s^2 \left[g \triangleright A_{Qg}^{(1)} \triangleright H_{Qg}^{(1)}\right] \triangleleft g - a_s^3 \left[\sum_{i,j=g,q,\bar{q}} f_i \triangleright A_{Qi}^{(2)} \triangleright H_{Qj}^{(1)}\right] \triangleleft f_j$$
$$- a_s^3 \left[\sum_{i,j=g,q,\bar{q}} f_i \triangleright A_{Qi}^{(1)} \triangleright H_{Qj}^{(2)}\right] \triangleleft f_j + (\mathrm{exch.})\,,$$

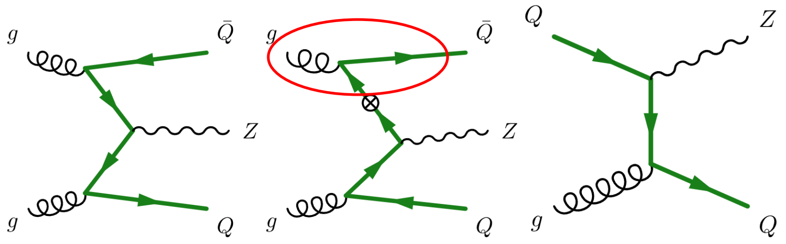
In DIS, one proceeds in a similar fashion to reshuffle the various contributions in the Wilson coefficient functions.

At this point we can define subtraction HQ PDFs $\tilde{f}_Q^{(1)} = a_s[A_{Qg}^{(1)} \triangleleft g]$, $\tilde{f}_Q^{(2)} = a_s^2 \sum_{i=g,q,\bar{q}} [A_{Qi}^{(2)} \triangleleft f_i]$

$$\tilde{f}_Q^{(\mathrm{NLO})}(x,\mu) \equiv \tilde{f}_Q^{(1)} + \tilde{f}_Q^{(2)}$$

$$\boxed{-\mathrm{d}\sigma_{\mathrm{sub}} = - a_s\, \tilde{f}_Q^{(\mathrm{NLO})} \triangleright H_{Qg}^{(1)} \triangleleft g - a_s^2 \sum_{i=g,q,\bar{q}} \tilde{f}_Q^{(1)} \triangleright H_{Qi}^{(2)} \triangleleft f_i}$$

Residual PDFs

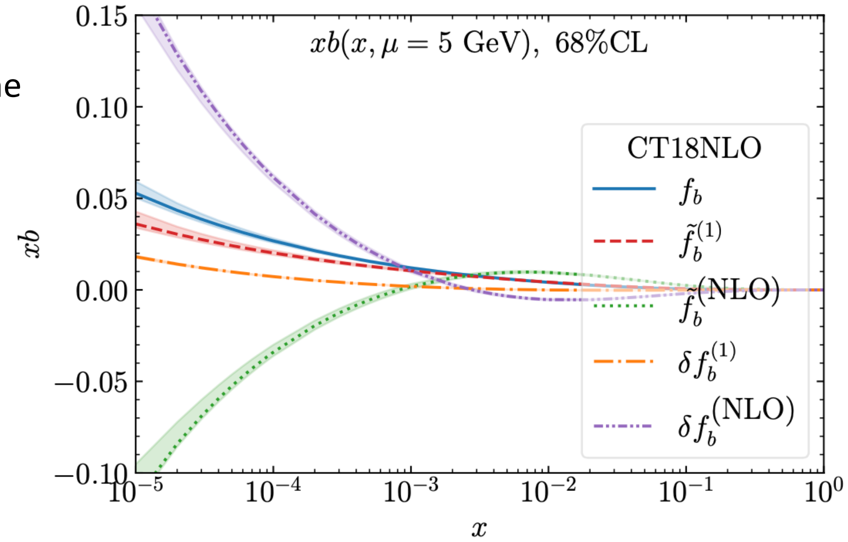


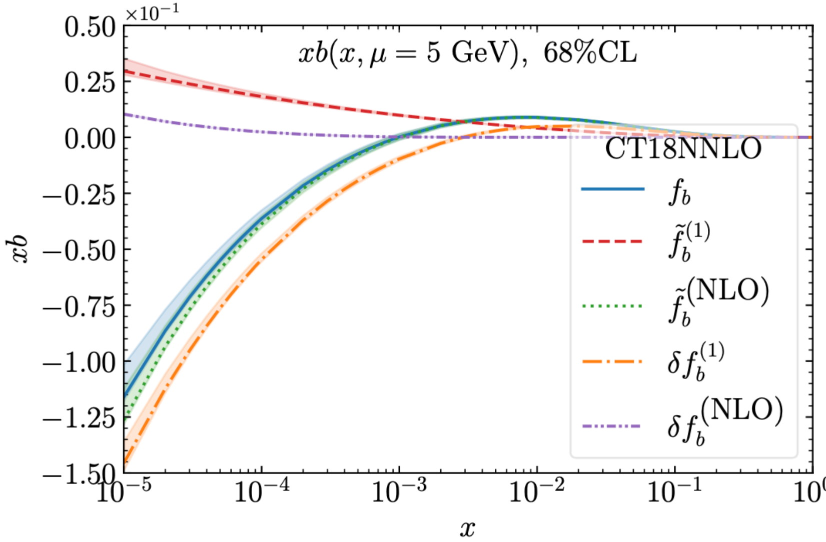
FE and SUB share the same matrix elements and can be combined in one piece in terms of residual PDFs!

$$\delta f_Q^{(1)} = f_Q - \tilde{f}_Q^{(1)}, \qquad \delta f_Q^{(\mathrm{NLO})} = f_Q - \tilde{f}_Q^{(\mathrm{NLO})}$$

$$\begin{aligned}
\mathrm{d}\sigma_{\mathrm{FE}} - \mathrm{d}\sigma_{\mathrm{sub}} =& a_s (f_Q - \tilde{f}_Q^{(\mathrm{NLO})}) \triangleright H_{Qg}^{(1)} \triangleleft g \\
&+ a_s^2 (f_Q - \tilde{f}_Q^{(1)}) \triangleright \left[H_{Qg}^{(2)} \triangleleft g + \sum_{i=q,\bar{q}} H_{Qq}^{(2)} \triangleleft f_i \right] + (\mathrm{exch.}) \\
=& a_s\, \delta f_Q^{(\mathrm{NLO})} \triangleright H_{Qg}^{(1)} \triangleleft g + a_s^2\, \delta f_Q^{(1)} \triangleright \left[H_{Qg}^{(2)} \triangleleft g + \sum_{i=q,\bar{q}} H_{Qq}^{(2)} \triangleleft f_i \right]
\end{aligned}$$

HQ, Subtraction and Residual PDFs near the b-quark threshold





Subtraction and Residual PDFs

Subtraction PDFs consist of convolutions between PDFs and universal operator matrix elements (OMEs). They are process independent.

(J. Blümlein is leading the effort in the calculation of the OMEs @N3LO. See Ablinger et al. *PLB*2024 and *NPB*2024 on $A_{Qg}^{(3)}$)

Subtraction and Residual PDFs are provided in the form of LHAPDF6 grids for phenomenology applications: https://sacotmps.hepforge.org/

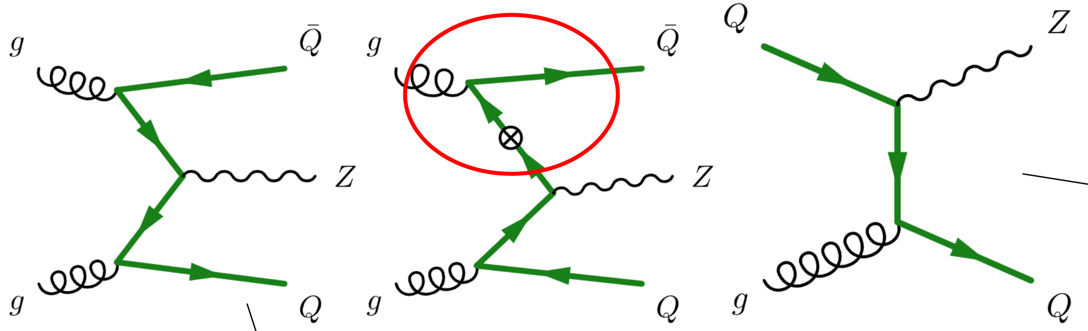
The next generation of CTEQ global analyses will use a module to generate Subtraction and Residual CT-PDFs

This recipe has been applied to reactions of interest:

1. pp $\to Z + Q + X$; $(Q = b$-quark) @NLO; M.G., Nadolsky, Reina, Wackeroth, Xie; **PRD2024**, 2410.03876

pp→Z+Q+X @LO: cancellation pattern

(for $pp \to Z + Q + X$ this is $O(\alpha_s^2)$)



FC term Sub FE term

$$H_{Qg}^{(1)}(x_A, x_B) = G_{Qg}^{(1)}(x_A, x_B)\Big|_{\mathrm{FE}}$$

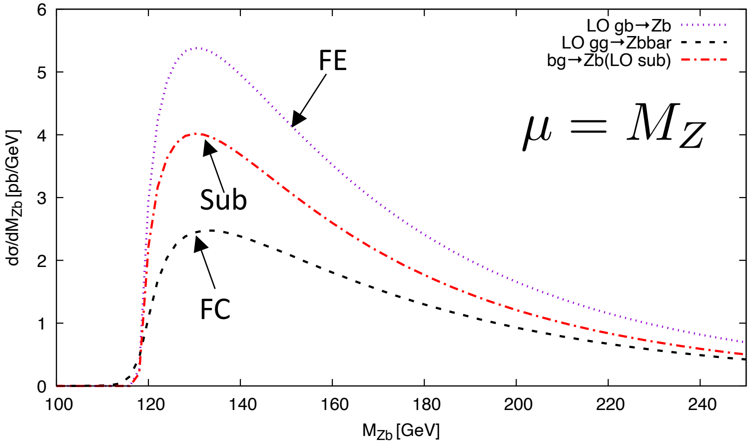
$$H_{gg}^{(2)}(x_A, x_B) = G_{gg}^{(2)}(x_A, x_B)\big|_{\mathrm{FC}} - \left[A_{Qg}^{(1)} \triangleright H_{Qg}^{(1)}\right](x_A, x_B) - \left[H_{gQ}^{(1)} \triangleleft A_{Qg}^{(1)}\right](x_A, x_B)$$

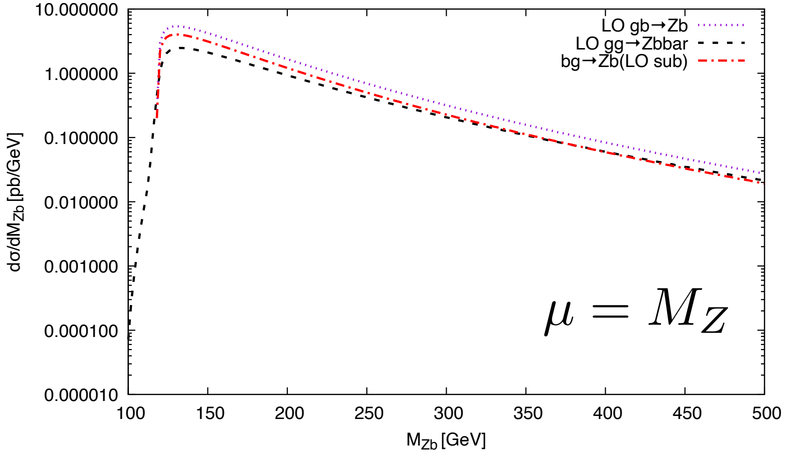
$$a_s H^{(1)} + a_s^2 H^{(2)} = a_s H_{Qg}^{(1)}(x_A, x_B) + a_s^2 H_{gg}^{(2)}(x_A, x_B) + a_s^2 H_{q\bar{q}}^{(2)}(x_A, x_B)$$

$$\mathrm{d}\sigma = \sum_{i,j} f_{i/A} \triangleright \left[a_s H^{(1)} + a_s^2 H^{(2)}\ \right]_{ij} \triangleleft f_{j/B}$$

Subtraction

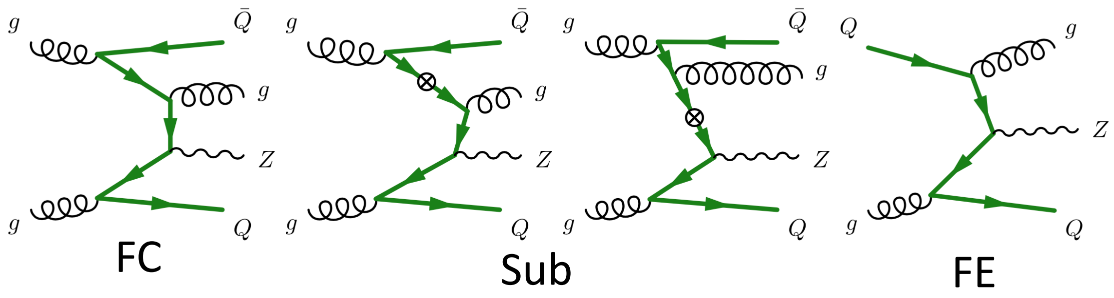
$$-\mathrm{d}\sigma_{\mathrm{sub}} = -\, a_s^2 \left[g \triangleright A_{Qg}^{(1)} \triangleright H_{Qg}^{(1)}\right] \triangleleft g + (\mathrm{exch.})$$



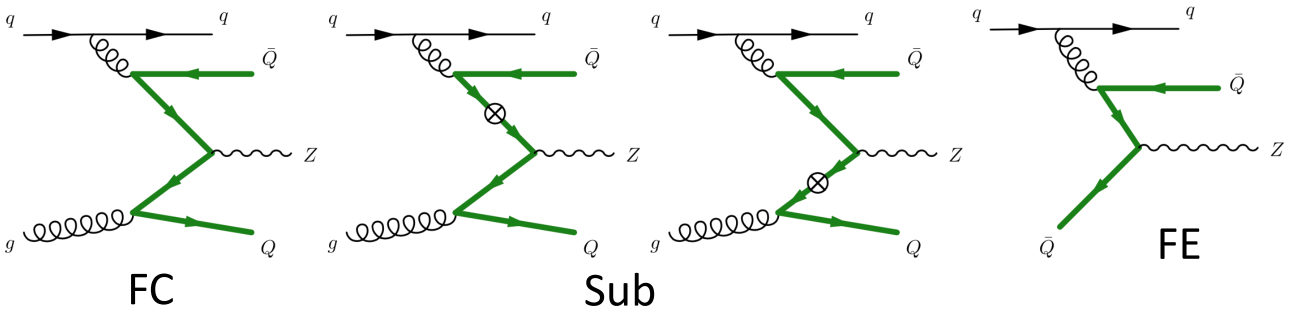


pp→Z+Q+X @NLO: cancellation pattern

(for $pp \to Z + b + X$ this is $O(\alpha_s^3)$)



gg-channel



qg-channel

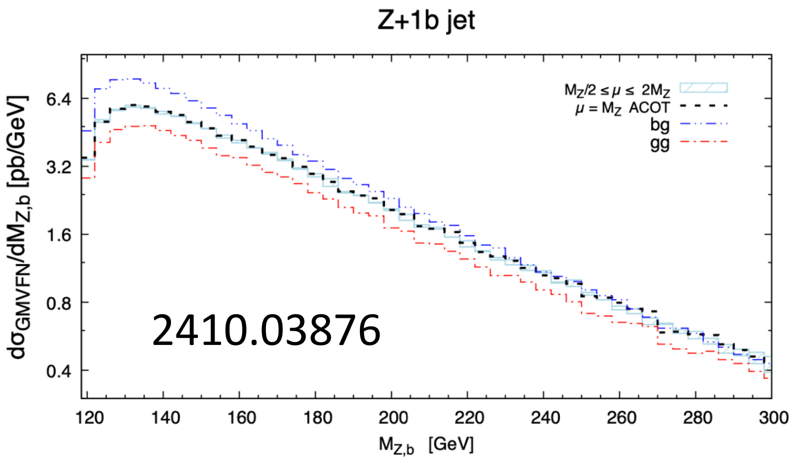
Virtual diagrams are not shown here, but are included in the calculation.

$$H_{Qi}^{(2)}(x_A, x_B) = \widehat{G}_{Qi}^{(2)}(x_A, x_B)\Big|_{\rm FE} \qquad \text{for } i = g, q, \bar{q}\,;$$

$$H_{ij}^{(3)}(x_A, x_B) = \widehat{G}_{ij}^{(3)}(x_A, x_B)\Big|_{\rm FC} - [A_{Qi}^{(1)} \triangleright H_{Qj}^{(2)}](x_A, x_B) - [H_{iQ}^{(2)} \triangleleft A_{Qj}^{(1)}](x_A, x_B)$$
$$- [A_{Qi}^{(2)} \triangleright H_{Qj}^{(1)}](x_A, x_B) - [H_{iQ}^{(1)} \triangleleft A_{Qj}^{(2)}](x_A, x_B) \qquad \text{for } i, j = g, q, \bar{q}\,;$$

$$H_{q\bar{q}}^{(3)}(x_A, x_B) = \widehat{G}_{q\bar{q}}^{(3)}(x_A, x_B)\Big|_{\rm FC} .$$

$$a_s H^{(1)} + a_s^2 H^{(2)} + a_s^3 H^{(3)} = a_s H_{Qg}^{(1)}(x_A, x_B) + a_s^2 H_{gg}^{(2)}(x_A, x_B) + a_s^2 H_{q\bar{q}}^{(2)}(x_A, x_B)$$
$$+ a_s^2 H_{Qg}^{(2)}(x_A, x_B) + a_s^2 H_{Qq}^{(2)}(x_A, x_B)$$
$$+ a_s^3 H_{gg}^{(3)}(x_A, x_B) + a_s^3 H_{qg}^{(3)}(x_A, x_B) + a_s^3 H_{q\bar{q}}^{(3)}(x_A, x_B)$$



GMVFN scheme Xsec for $pp \to Z + Q + X$ @NLO

$$d\sigma_{\rm FC}^{\rm NLO} = f_g \rhd \left[a_s^2\, d\widehat{\sigma}^{(2)}_{gg\to ZQ\bar{Q}} + a_s^3\, d\widehat{\sigma}^{(3)}_{gg\to ZQ\bar{Q}(g)}\right] \lhd f_g$$
$$+ \sum_{i=q,\bar{q}} f_i \rhd \left[a_s^2\, d\widehat{\sigma}^{(2)}_{q\bar{q}\to ZQ\bar{Q}} + a_s^3\, d\widehat{\sigma}^{(3)}_{q\bar{q}\to ZQ\bar{Q}(g)}\right] \lhd f_{\bar{i}}$$
$$+ a_s^3 \sum_{i=q,\bar{q}} \left[f_g \rhd d\widehat{\sigma}^{(3)}_{gq\to ZQ\bar{Q}(q)} \lhd f_i + f_i \rhd d\widehat{\sigma}^{(3)}_{qg\to ZQ\bar{Q}(q)} \lhd f_g\right]$$

$$d\sigma_{\rm FE}^{\rm NLO} = f_g \rhd \left[a_s\, d\widehat{\sigma}^{(1)}_{gQ\to ZQ} + a_s^2\, d\widehat{\sigma}^{(2)}_{gQ\to ZQ(g)}\right] \lhd f_Q$$
$$+ a_s^2 \sum_{i=q,\bar{q}} f_i \rhd d\widehat{\sigma}^{(2)}_{qQ\to ZQ(q)} \lhd f_Q + (\text{exch.});$$

$$d\sigma_{\rm sub}^{\rm NLO} = a_s\, f_g \rhd d\widehat{\sigma}^{(1)}_{gQ\to ZQ} \lhd \tilde{f}_Q^{(\rm NLO)} + a_s^2\, f_g \rhd d\widehat{\sigma}^{(2)}_{gQ\to ZQ(g)} \lhd \tilde{f}_Q^{(1)}$$
$$+ a_s^2 \sum_{i=q,\bar{q}} f_i \rhd d\widehat{\sigma}^{(2)}_{qQ\to ZQ(q)} \lhd \tilde{f}_Q^{(1)} + (\text{exch.})\,;$$

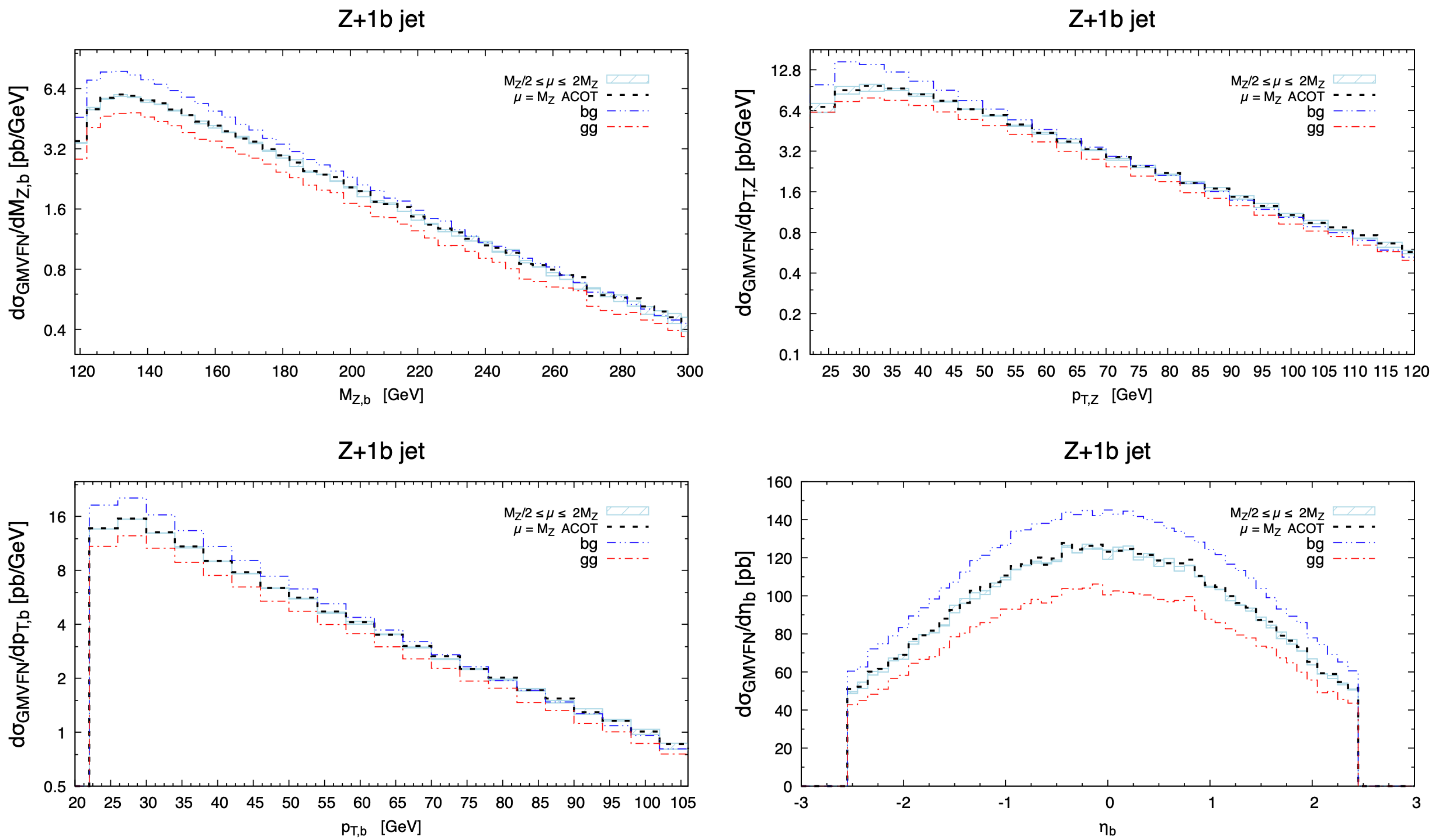
Equivalently, with the $d\sigma_{FE} - d\sigma_{sub}$ reorganized in terms of HQ PDF residuals we obtain a very simple form

$$d\sigma_{\rm GMVFN}^{\rm NLO} = d\sigma_{\rm FC}^{\rm NLO} + a_s\, f_g \rhd \left[d\widehat{\sigma}^{(1)}_{gQ\to ZQ}\right] \lhd \delta f_Q^{(\rm NLO)}$$
$$+ a_s^2\, f_g \rhd \left[d\widehat{\sigma}^{(2)}_{gQ\to ZQ(g)}\right] \lhd \delta f_Q^{(1)} + a_s^2 \sum_{i=q,\bar{q}} f_i \rhd \left[d\widehat{\sigma}^{(2)}_{qQ\to ZQ(q)}\right] \lhd \delta f_Q^{(1)} + (\text{exch.})$$

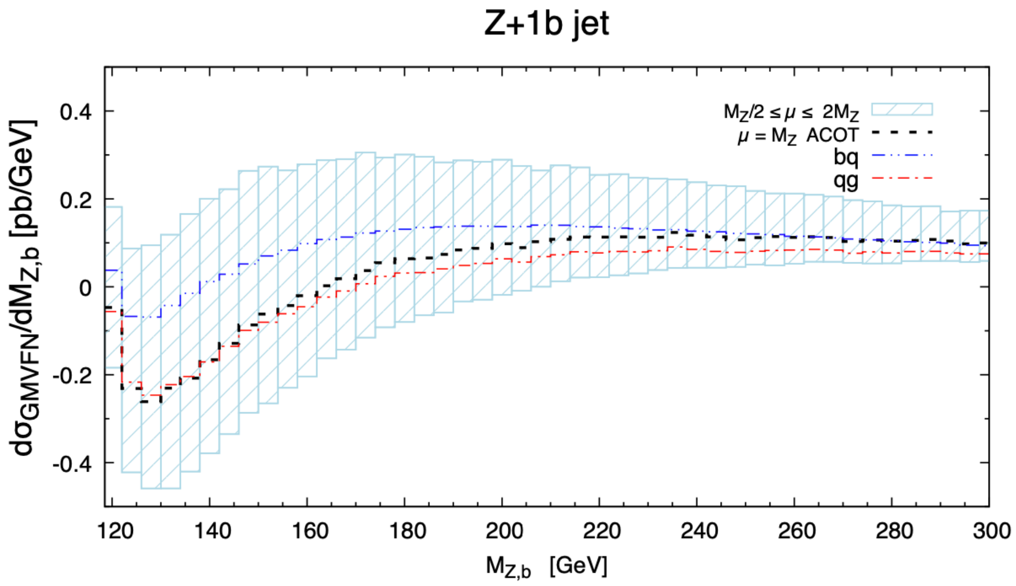
Lowest mandatory order" (LMO) representation at NLO in that it retains only the unambiguous terms up to order a_s^3 required by order-by-order factorization and scale invariance. Any ACOT-like scheme must contain such terms.

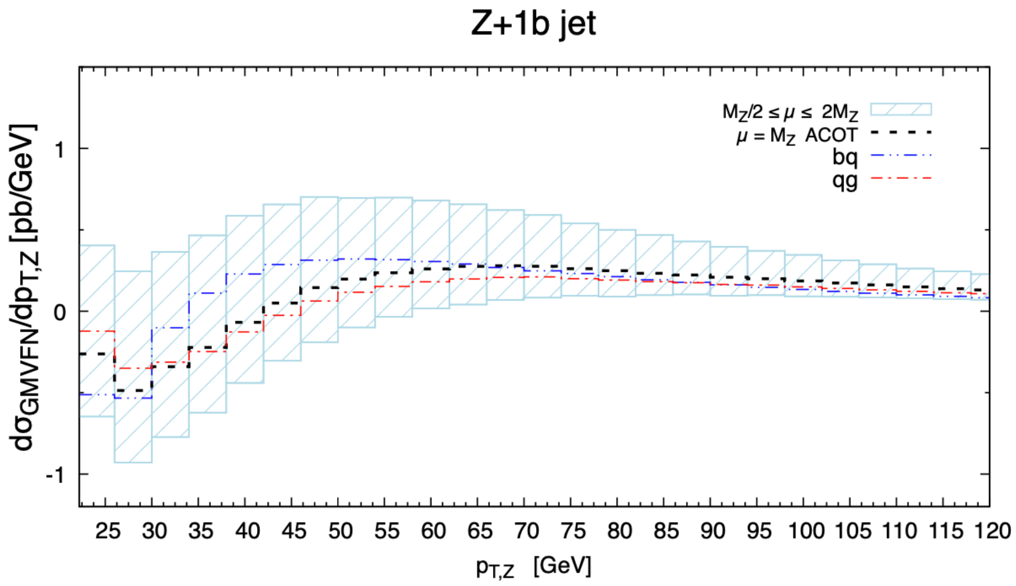
2410.03876, PRD 2024

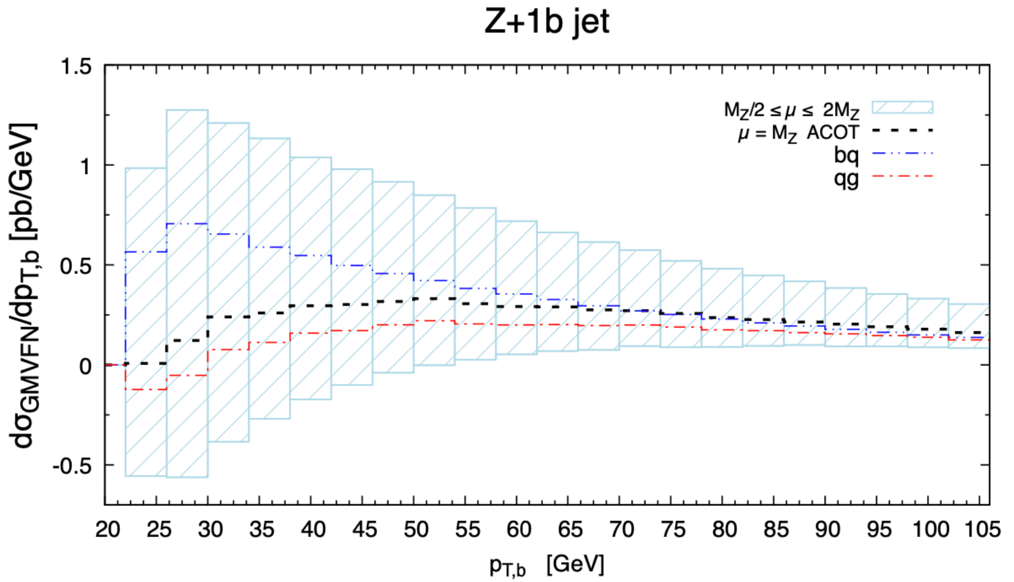
Results: Z+b differential distributions (gg channel)

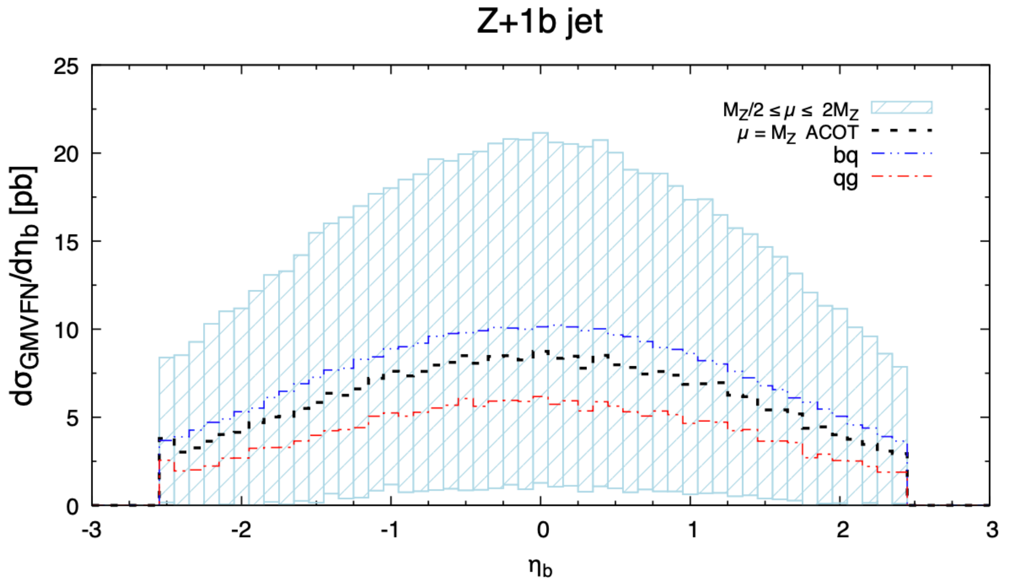


Results: Z+b differential distributions (qg channel)







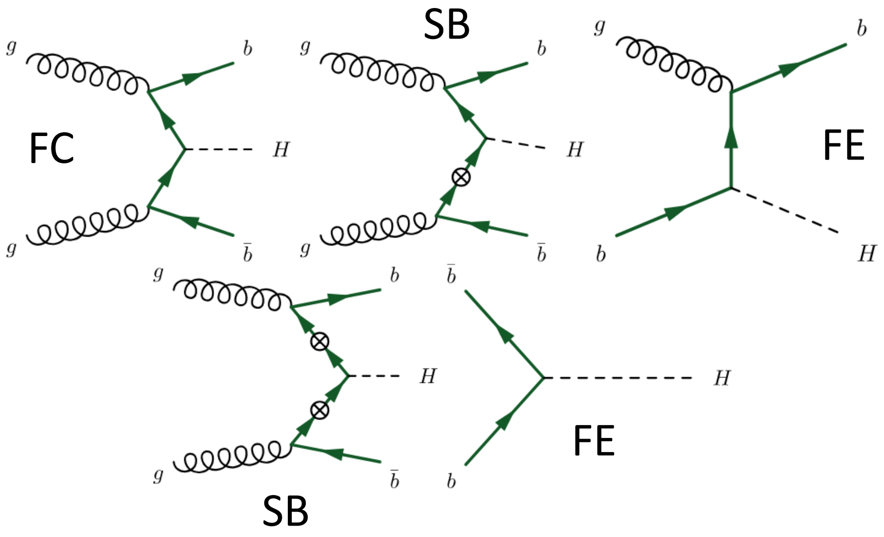


This recipe has been applied to physical processes of interest:

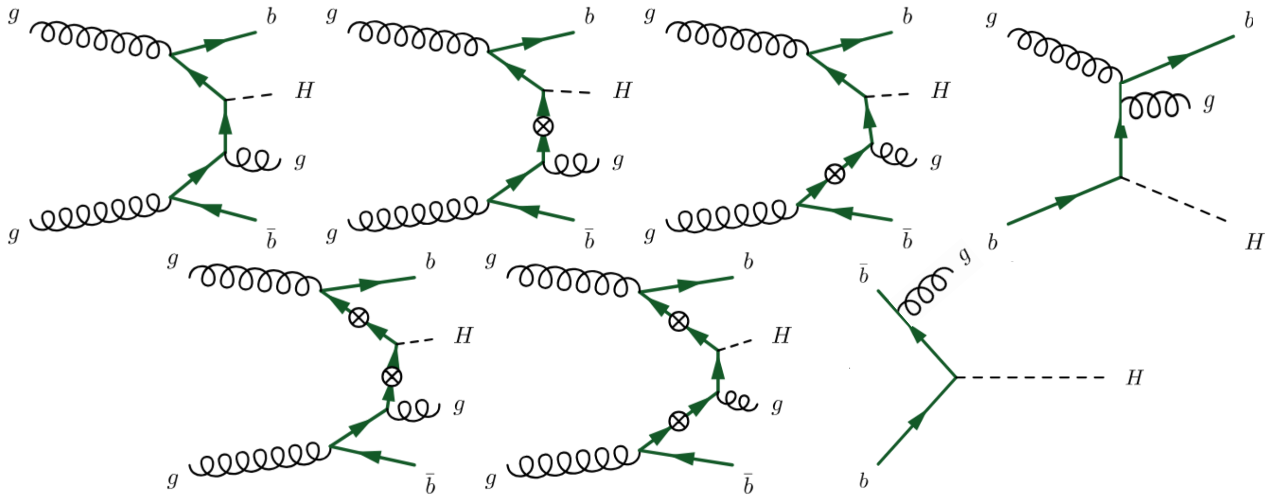
1. pp $\to Z + Q + X$; $(Q = b$-quark) @NLO; M.G., Nadolsky, Reina, Wackeroth, Xie; **PRD2024**, 2410.03876

2. pp $\to H + X$, $@\mathrm{NNLO}$; Biello, Gauld, MG, Nadolsky, Sankar, Wiesemann, Xie, Zanderighi (In progress)

pp→H+X @LO, NLO: cancellation patterns



$$H^{(2)}_{gg}(x_A,x_B) = \widehat{G}^{(2)}_{gg}(x_A,x_B)\Big|_{\mathrm{FC}} - \left[A^{(1)}_{Qg} \triangleright H^{(1)}_{Qg}\right](x_A,x_B) - \left[H^{(1)}_{gQ} \triangleleft A^{(1)}_{Qg}\right](x_A,x_B)$$
$$- \left[A^{(1)}_{Qg} \triangleright H^{(0)}_{Q\bar{Q}} \triangleleft A^{(1)}_{Qg}\right](x_A,x_B)\,.$$

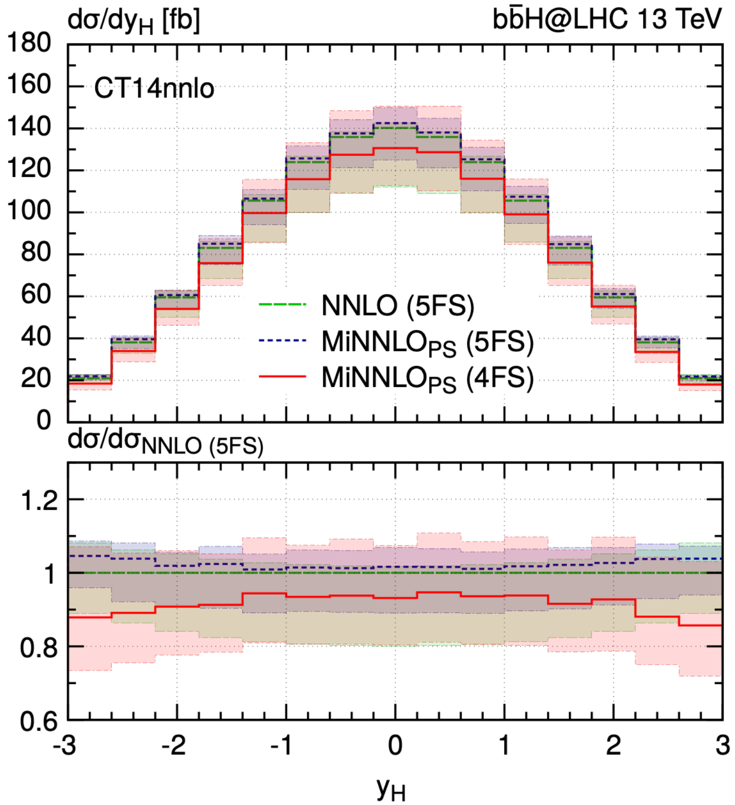


$$H^{(3)}_{gg}(x_A,x_B) = \widehat{G}^{(3)}_{gg}(x_A,x_B)\Big|_{\mathrm{FC}} - [A^{(1)}_{Qg} \triangleright H^{(2)}_{Qg}](x_A,x_B) - [H^{(2)}_{gQ} \triangleleft A^{(1)}_{Qg}](x_A,x_B)$$
$$- [A^{(2)}_{Qg} \triangleright H^{(1)}_{Qg}](x_A,x_B) - [H^{(1)}_{gQ} \triangleleft A^{(2)}_{Qg}](x_A,x_B)$$
$$- [A^{(1)}_{Qg} \triangleright H^{(0)}_{Q\bar{Q}} \triangleleft A^{(2)}_{Qg}](x_A,x_B) - [A^{(2)}_{Qg} \triangleright H^{(0)}_{Q\bar{Q}} \triangleleft A^{(1)}_{Qg}](x_A,x_B)$$
$$- [A^{(1)}_{Qg} \triangleright H^{(1)}_{Q\bar{Q}} \triangleleft A^{(1)}_{Qg}](x_A,x_B)$$

+ …

Flavor-scheme matching in $b\bar{b}H$

The calculation of NNLO corrections in $pp \to b\bar{b}H$, with parton shower matching in both massless (5FS) [2402.04025] and massive scheme (4FS) [2412.09510], opens new opportunities to study the flavour-scheme matching in bbH using subtracted and residual PDFs.



State-of-the-art

Only fully-inclusive matched results are known for $b\bar{b}H$ in different schemes:

- Santander matching [1112.3478]
- FONLL [1508.01529, 1607.00389] with current matching at $N^3LO_{5FS} + NLO_{4FS}$ [2004.04752]
- NLO + NNLLpart + $y_b\, y_t$ matching [1508.03288, 1605.01733]

Long-term goal

Matching of NNLO+PS 4FS and NNLO+PS 5FS using ACOT-like schemes with subtraction and residual PDFs at fully-differential level with parton-shower matching in the POWHEG fremework with the MiNNLOPS method.

Biello, Gauld, MG, Nadolsky, Sankar, Wiesemann, Xie, Zanderighi [in progress]

$b\bar{b}H$ at the first order

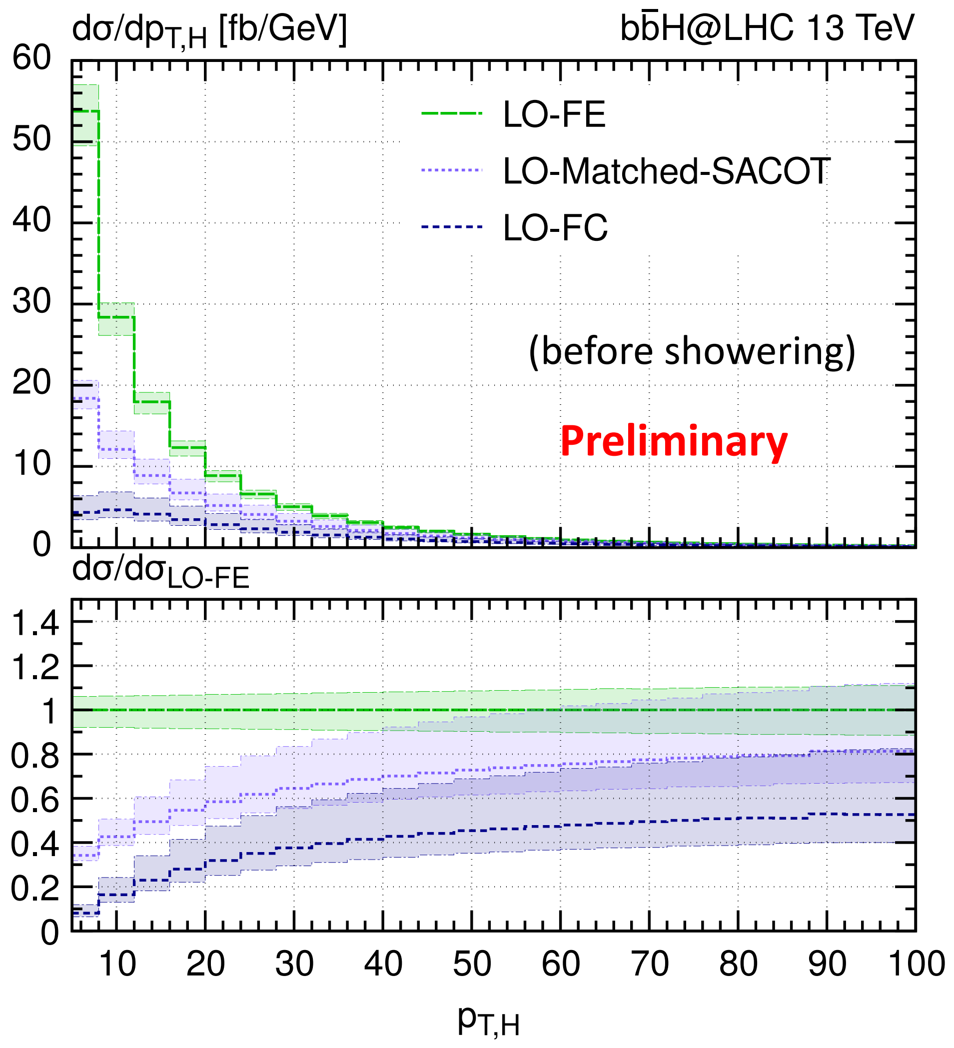
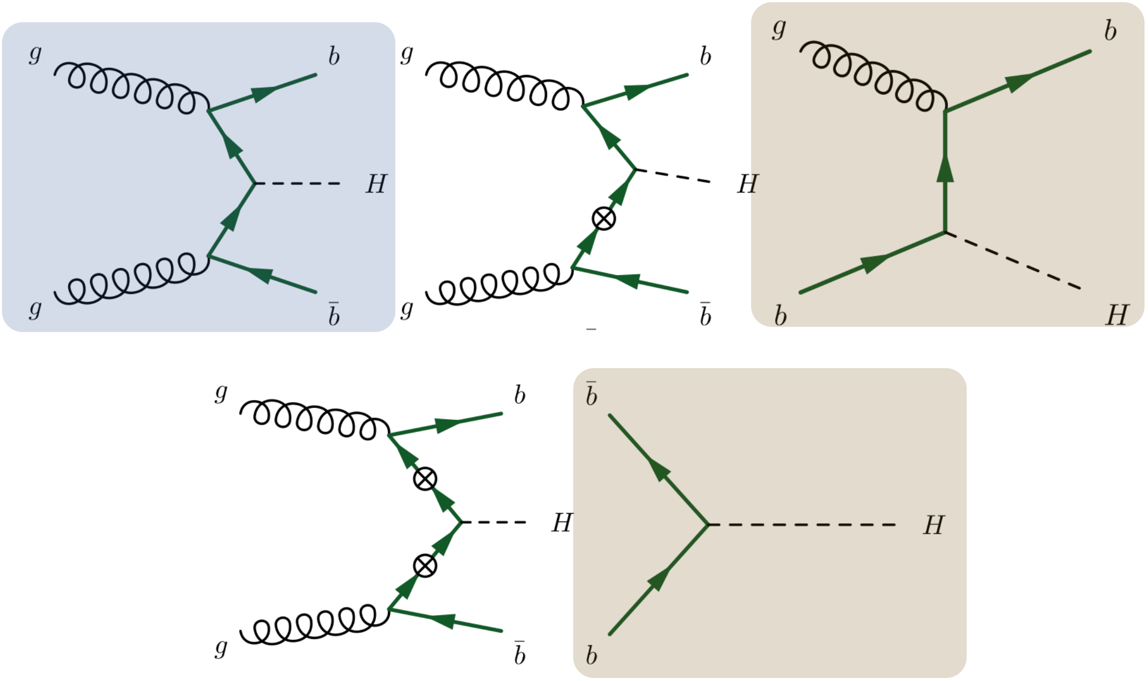


Figure by C. Biello and A. Sankar

We first performed the S-ACOT matching at the first order by combining:

- Flavor Creation (obtained using a LO_{PS} 4FS generator)
- Flavor Excitation and corresponding subtraction (obtained by modifying an NLO_{PS} 5FS generator with standard and subtracted PDFs)



$b\bar{b}H$ at the first order

Fully exclusive matched results interfaced with PYTHIA8 for the parton-shower simulation.

Setup:

CT18NLO+CT18NLOsub

$m_b = 4.75$ GeV

$m_H = 125$ GeV

$\overline{MS}$ bottom Yukawa with $m_b(m_b) = 4.18$ GeV and three-loop running

Standard scale variation via event reweighting in POWHEG.

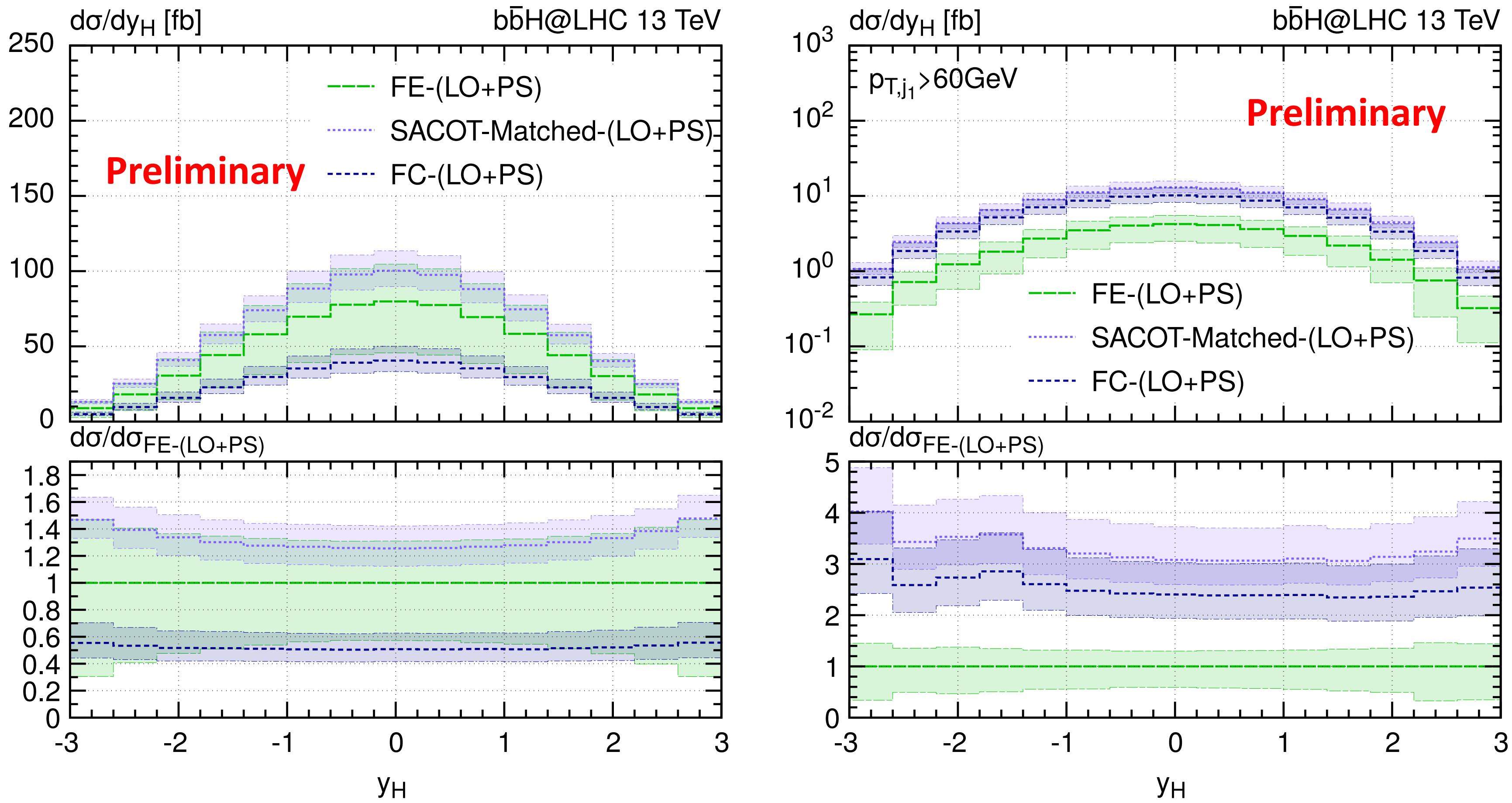


Figure by C. Biello and A. Sankar

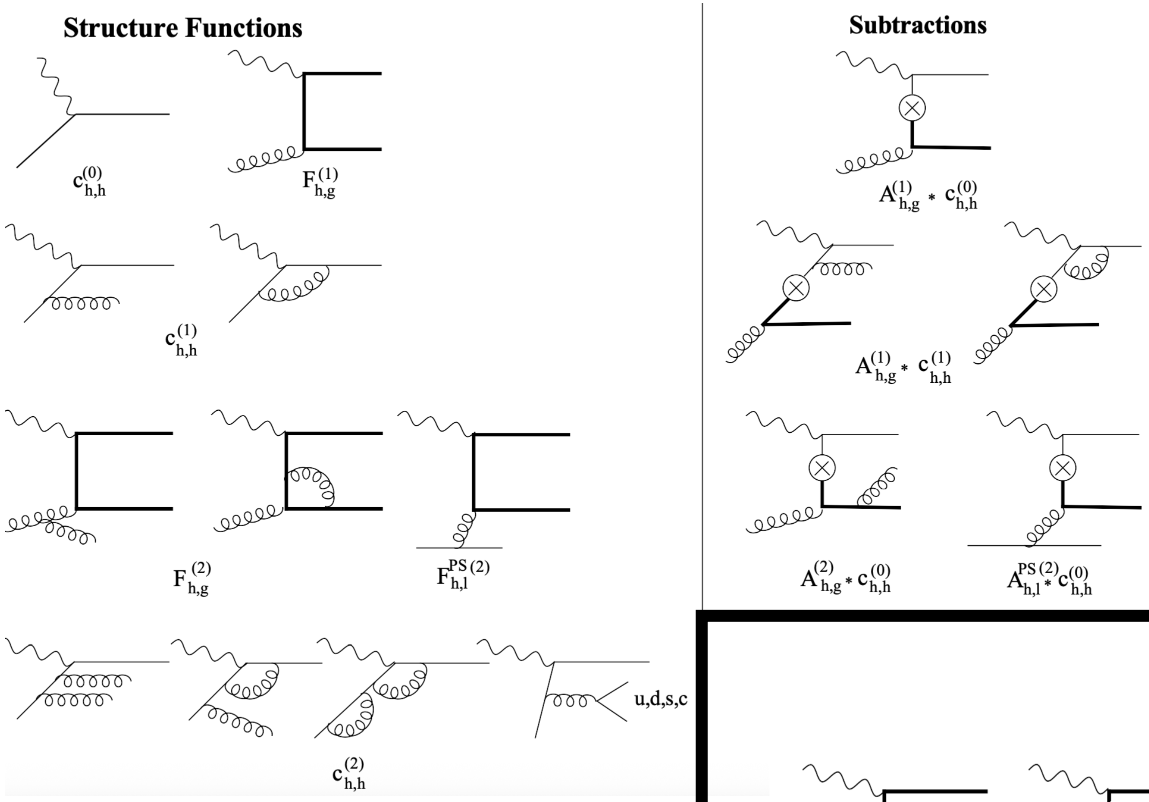
This recipe has been applied to physical processes of interest:

1. pp $\rightarrow Z\ + Q\ +\ X$; $(Q = b$-quark) @NLO; M.G., Nadolsky, Reina, Wackeroth, Xie; **PRD2024**, 2410.03876

2. pp $\rightarrow H + X$, $@\mathrm{NNLO}$; Biello, Gauld, MG, Nadolsky, Sankar, Wiesemann, Xie, Zanderighi (In progress)

3. DIS @N3LO in QCD MG, Nadolsky, Xie (In progress)

DIS @NNLO, @N^3LO: cancellation patterns



S-ACOT-χ @NNLO NC DIS, MG, Nadolsky, Lai, Yuan, PRD 2012

$$C^{(0)}_{h,a}(\widehat{x}) = \delta_{ha}\delta(1-\widehat{x});$$

$$C^{(1)}_{h,g} = F^{(1)}_{h,g} - C^{(0)}_{h,h} \otimes A^{(1)}_{hg}; \quad C^{(1)}_{h,l} = C^{(1)}_{l,h} = 0; \quad C^{(1)}_{h,h} = F^{(1)}_{h,h} - C^{(0)}_{h,h} \otimes A^{(1)}_{hh};$$

$$C^{(2)}_{h,g} = F^{(2)}_{h,g} - C^{(0)}_{h,h} \otimes A^{(2)}_{hg} - C^{(1)}_{h,h} \otimes A^{(1)}_{hg} - C^{(1)}_{h,g} \otimes A^{(1)}_{gg};$$

$$C^{(2)}_{h,l} = F^{PS,(2)}_{h,l} - C^{(0)}_{h,h} \otimes A^{PS,(2)}_{hl} - C^{(1)}_{h,g} \otimes A^{(1)}_{gl};$$

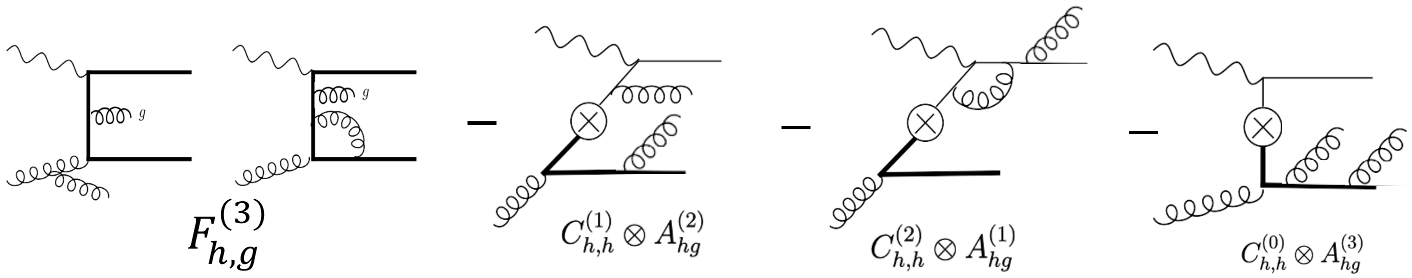
$$C^{(2)}_{h,h} = F^{(2)}_{h,h} - C^{(0)}_{h,h} \otimes A^{(2)}_{hh} - C^{(1)}_{h,h} \otimes A^{(1)}_{hh} - C^{(1)}_{h,g} \otimes A^{(1)}_{gh}.$$

Default GMVFN scheme for DIS in CTEQ PDF analyses

S-ACOT-χ @NNLO CC DIS
Phys.Rev.D 105 (2022), 2107.00460; Gao et al.

See also 2504.13317, by P. Risse et al.

At N^3LO we have (MG, Nadolsky, Xie, In prep.)



$$C^{(3)}_{h,g} = F^{(3)}_{h,g} - C^{(0)}_{h,h} \otimes A^{(3)}_{hg} - C^{(1)}_{h,h} \otimes A^{(2)}_{hg} - C^{(2)}_{h,h} \otimes A^{(1)}_{hg} - C^{(1)}_{h,g} \otimes A^{(2)}_{gg} - C^{(2)}_{h,g} \otimes A^{(1)}_{gg};$$

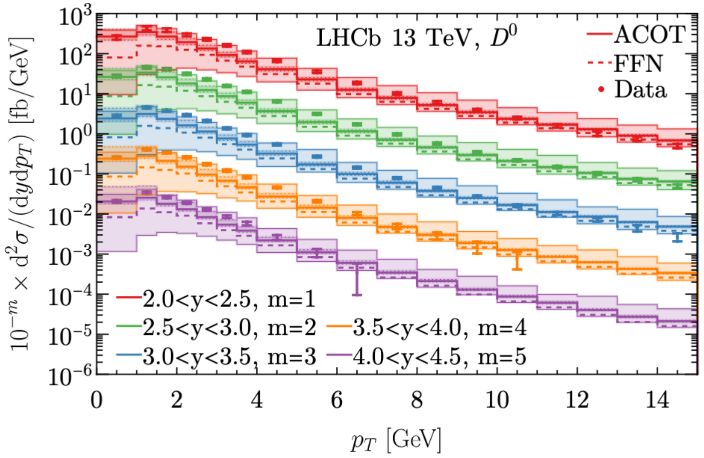
$$C^{(3)}_{h,l} = F^{PS,(3)}_{h,l} - C^{(0)}_{h,h} \otimes A^{PS,(3)}_{hl} - C^{(1)}_{h,h} \otimes A^{PS,(2)}_{hl} - C^{(2)}_{h,h} \otimes A^{(1)}_{hl} - C^{(1)}_{h,g} \otimes A^{(2)}_{gl} - C^{(2)}_{h,g} \otimes A^{(1)}_{gl}$$

$$C^{(3)}_{h,h} = F^{(3)}_{h,h} - C^{(0)}_{h,h} \otimes A^{(3)}_{hh} - C^{(1)}_{h,h} \otimes A^{(2)}_{hh} - C^{(2)}_{h,h} \otimes A^{(1)}_{hh} - C^{(1)}_{h,g} \otimes A^{(2)}_{gh} - C^{(2)}_{h,g} \otimes A^{(1)}_{gh}$$

Current bottlenecks for full implementation at NNLO and beyond in QCD

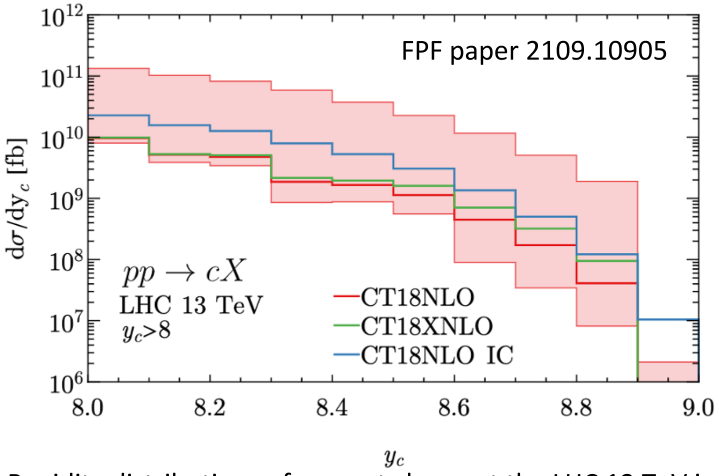
- 4-loop splitting functions
- 3-loop $A_{ij}^{(3)}$OMEs in the x space.

Other results using ACOT-like schemes



Transverse momentum at central rapidity at LHCb 13TeV (LHCb data from JHEP 03 (2016) 159).

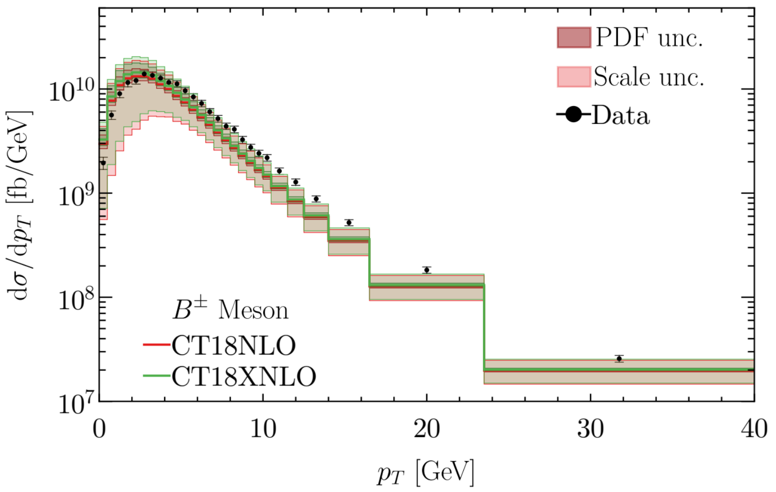
Error bands are scale uncertainties.

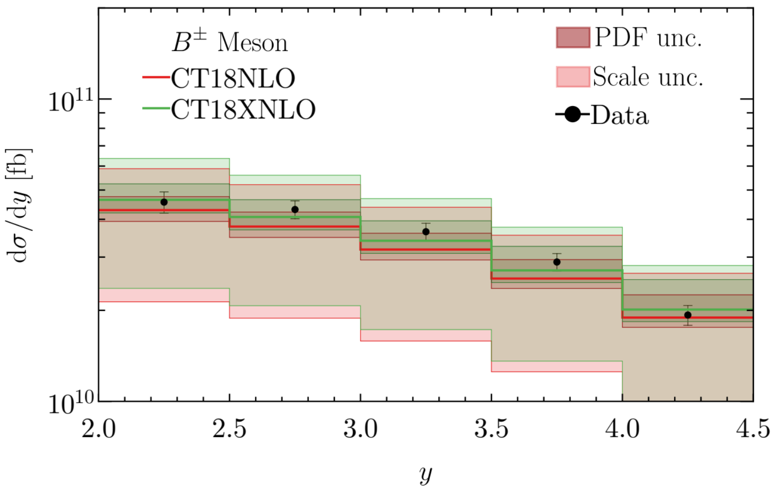


Rapidity distributions of prompt charm at the LHC 13 TeV in the very forward region (yc > 8). Error band represents the CT18NLO induced PDF uncertainty at 68% C.L.

Charm hadroproduction and Z + c production at the LHC can constrain the IC contributions. LHCb Z+c data deserve attention as they can potentially discriminate gluon functional forms at $x \geq 0.2$ and improve gluon accuracy.

For small x below 10^{-4}, higher-order QCD terms with $\ln(1/x)$ dependence grow quickly at factorization scales of order 1 GeV. FPF facilities like FASERν will access novel kinematic regimes where both large-x and small-x QCD effects contribute to charm hadroproduction rate. [arXiv:2109.10905]





NLO theory predictions for the pT and y distributions obtained with CT18NLO and CT18XNLO PDFs compared to $B^{\pm}$ production data from LHCb 13 TeV [arXiv:2203.06207]

Theoretical uncertainties at NLO are large (O(50%)) and mainly ascribed to scale variation. This can be improved by including higher-order corrections which imply an extension of the S-ACOT-MPS scheme to NNLO

Concluding Remarks

- Developed theory framework to extend ACOT-like GMVFN schemes to pp collisions based on collinear fact., and Subtraction and Residual PDFs.

- ACOT-like schemes used to describe Z+b production differentially @NLO in QCD

- Work is in progress for Higgs production @NNLO, and DIS @aN^3LO

- Important for PDF analyses and to improve current understanding of exp data

- Subtraction PDFs provided in the form of LHAPDF grids to for phenomenology

BACK UP

Operator Matrix Elements

$$\hat{\mathcal{F}}_{i,q}^{\rm NS}\Big(n_f, \frac{Q^2}{p^2}, \mu^2\Big) = A_{qq}^{\rm NS}\Big(n_f, \frac{\mu^2}{p^2}\Big) \otimes \mathcal{C}_{i,q}^{\rm NS}\Big(n_f, \frac{Q^2}{\mu^2}\Big) \,,$$

From mass factorization on DIS structure functions

$$\hat{\mathcal{F}}_{i,k}^{\rm S}\Big(n_f, \frac{Q^2}{p^2}, \mu^2\Big) = \sum_{l=q,g} A_{lk}^{\rm S}\Big(n_f, \frac{\mu^2}{p^2}\Big) \otimes \mathcal{C}_{i,l}^{\rm S}\Big(n_f, \frac{Q^2}{\mu^2}\Big) \,.$$

The $A_{ij}^{(k)}$ represent the renormalized operator-matrix elements (OME's) which are defined by

$$A_{lk}\Big(n_f, \frac{\mu^2}{p^2}\Big) =< k(p)|O_l(0)|k(p) > \,, \qquad (l, k = q, g)$$

where O_l are the renormalized operators which appear in the operator-product expansion of two electromagnetic currents near the light cone.

Further simplifications in ACOT-type schemes

$\delta f_Q^{(NLO)}$?

$$
\begin{aligned}
\mathrm{d}\sigma^{\mathrm{NLO}}_{\mathrm{GMVFN}} = d\sigma^{\mathrm{NLO}}_{\mathrm{FC}} &+ a_s\ f_g \rhd \left[\mathrm{d}\widehat{\sigma}^{(1)}_{gQ\to ZQ}\right] \lhd \delta f_Q^{(\mathrm{NLO})} \\
&+ a_s^2\ f_g \rhd \left[\mathrm{d}\widehat{\sigma}^{(2)}_{gQ\to ZQ(g)}\right] \lhd \delta f_Q^{(1)} + a_s^2 \sum_{i=q,\bar{q}} f_i \rhd \left[\mathrm{d}\widehat{\sigma}^{(2)}_{qQ\to ZQ(q)}\right] \lhd \delta f_Q^{(1)} + (\mathrm{exch.})
\end{aligned}
$$

Lowest mandatory order" (LMO) representation at NLO in that it retains only the unambiguous terms up to order a_s^3 required by order-by-order factorization and scale invariance. Any ACOT-like scheme must contain such terms.

Further simplifications in ACOT-type schemes

One generally can augment $\mathrm{d}\sigma^{\mathrm{NLO}}_{\mathrm{GMVFN}}$ with extra radiative contributions from higher orders with the goal to improve consistency with the specific GMVFN scheme adopted in the fit of the used PDFs. The GMVFN scheme assumed for determination of CTEQ-TEA PDFs with up to 5 active flavors is closely matched with the following additional choices:

1. Evolve αs(μ) and PDFs fi(ξ,μ) with Nf = 5 at μ ≥ mb. The hard cross sections are also evaluated with Nf = 5 in virtual loops both for massive and massless channels. If the virtual contributions are obtained in the Nf = 4 scheme, they should be converted to the Nf = 5 scheme by adding known terms to the hard cross sections.

2. The sums over initial-state light quarks and antiquarks in $\mathrm{d}\sigma^{\mathrm{NLO}}_{\mathrm{GMVFN}}$ are extended to also include the b-quark PDF via the introduction of the singlet PDF $\Sigma \equiv \sum_{i=1}^{5}(f_i + \bar{f}_i)$

3. replace $\tilde{f}_Q^{(1)}$ in $\mathrm{d}\sigma^{\mathrm{NLO}}_{\mathrm{sub}}$ and $\delta f_Q^{(1)}$ in $\mathrm{d}\sigma^{\mathrm{NLO}}_{\mathrm{GMVFN}}$ by f^(NLO) and δf^(NLO), respectively.

4. The αs and PDFs must be evolved at least at NLO, although evolution at NNLO is acceptable or even desirable in some contexts.

5. In the hard cross sections inside dσFE − dσsub, dependence on the HQ mass can be eliminated altogether or simplified, producing a difference only in higher-order terms.

Further simplifications in ACOT-type schemes

With the simplifications discussed above, we obtain

$$\tilde{f}_Q^{(1)} = a_s \left[A_{Qg}^{S,(1)} \lhd g \right], \quad \tilde{f}_Q^{(2)} = a_s^2 \left[A_{Qq}^{\mathrm{PS},(2)} \lhd \Sigma + A_{Qg}^{S,(2)} \lhd g \right]$$

$$\tilde{f}_Q^{(\mathrm{NLO})}(x,\mu) \equiv \tilde{f}_Q^{(1)} + \tilde{f}_Q^{(2)} \qquad \delta f_Q^{(\mathrm{NLO})} = f_Q - \tilde{f}_Q^{(\mathrm{NLO})}$$

$$\boxed{\begin{aligned} \mathrm{d}\sigma_{\mathrm{ACOT}}^{\mathrm{NLO}} = \mathrm{d}\sigma_{\mathrm{FC}}^{\mathrm{NLO}} + \Bigg(& a_s\ f_g \rhd \mathrm{d}\widehat{\sigma}_{gQ\to ZQ}^{(1)} \\ & + a_s^2\, f_g \rhd \mathrm{d}\widehat{\sigma}_{gQ\to ZQ(g)}^{(2)} + a_s^2\, \Sigma \rhd \mathrm{d}\widehat{\sigma}_{qQ\to ZQ(q)}^{(2)} \Bigg) \lhd \delta f_Q^{(\mathrm{NLO})} + (\mathrm{exch.})\,. \end{aligned}}$$

Z+b: ACOT vs S-ACOT