

# Heavy Quark Fragmentation in $e^+e^-$ Collisions to NNLO+NNLL Accuracy in Perturbative QCD

**BOOST Genova - 30/07/2024**



**Universität  
Zürich<sup>UZH</sup>**



**Swiss National  
Science Foundation**

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[2312.12519] with Matteo Cacciari (LPTHE) and Giovanni Stagnitto (UniMiB)

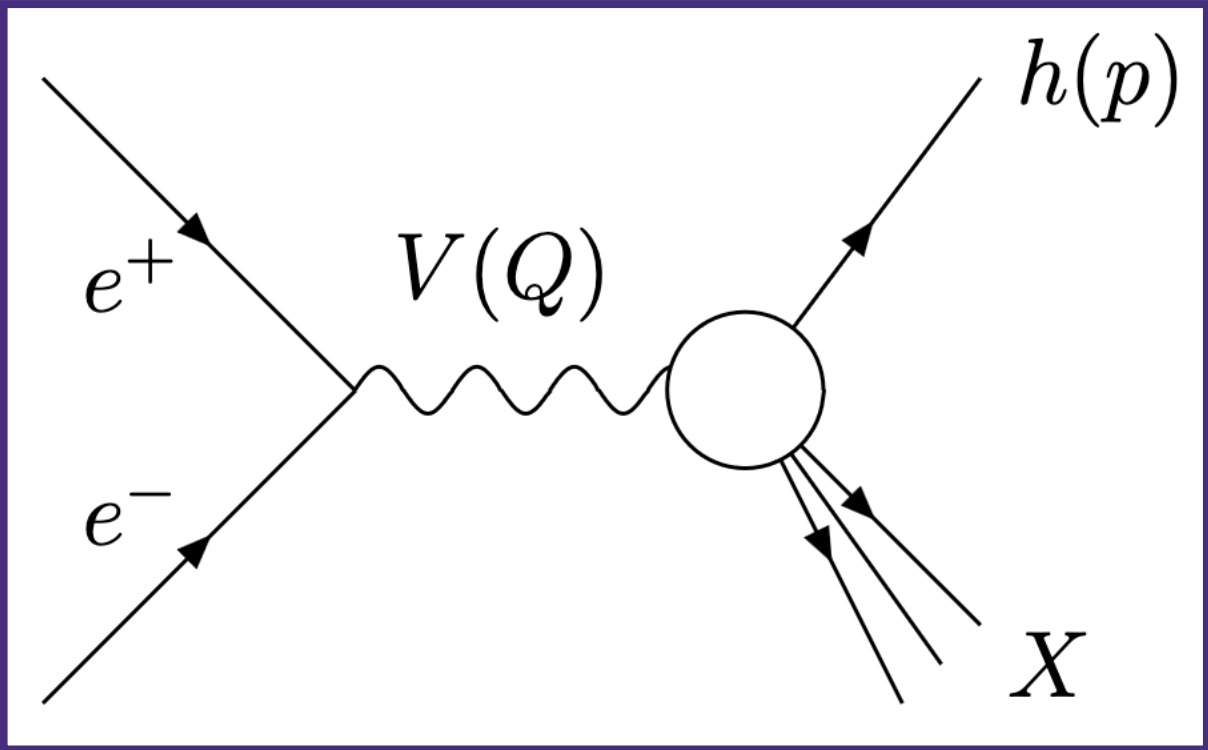
# Introduction

## Fragmentation function formalism

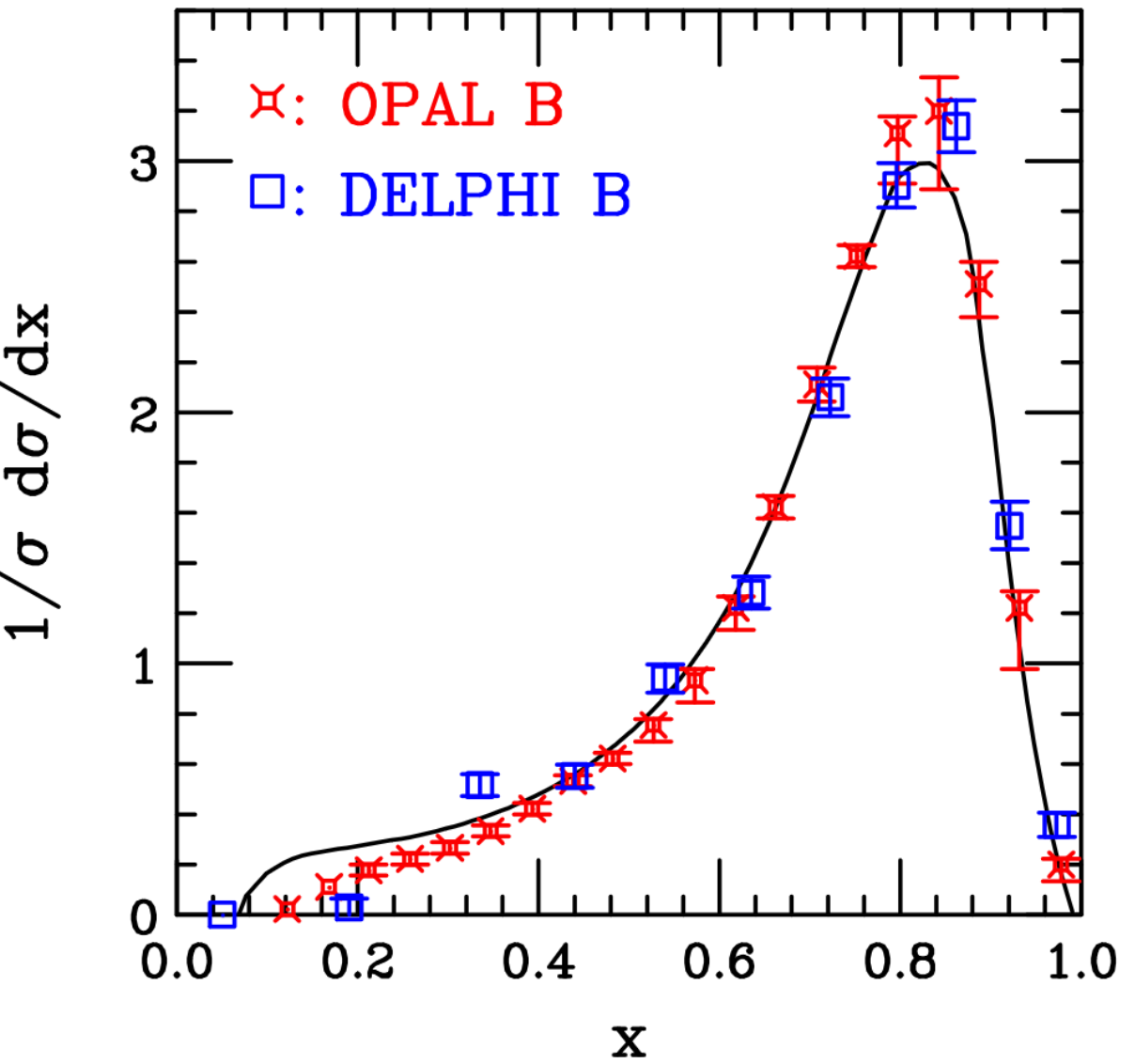
- Goal: describe fragmentation of heavy quarks ( $c$  and  $b$ ) into hadrons
- Process:  $e^+e^- \rightarrow V(Q) \rightarrow h(p) + X$
- Tool: QCD perturbative fragmentation function formalism
  - Factorisation  $\rightarrow$  hadron cross section  $\sigma_h(x, Q)$ 

$$\sigma_h(x, Q) \simeq \sigma_Q(x, Q, m) \otimes D_{Q \rightarrow h}^{np}(x, \{\text{par}\})$$
  - Fully perturbative cross section for heavy quark  $Q$  of mass  $m$ 

$$\sigma_Q(x, Q, m) = \hat{\sigma}_i(x, Q, \mu_F) \otimes D_{i \rightarrow Q}(x, \mu_F, m) + \mathcal{O}((m/Q)^p)$$
 [Mele, Nason '91]
  - Fragmentation functions are universal (process independent)
- Mellin space: convolution  $\rightarrow$  simple product



[Cacciari et al. '05]




$x = E_h/E_{\text{beam}}$   
 $Q = 2E_{\text{beam}}$   
 $\mu_F$ : factorisation scale

# Introduction

## Perturbative ingredients

$$\bullet \frac{1}{\sigma_Q^{tot}} \sigma_Q(Q, m) = \frac{1}{\sigma_Q^{tot}} \sigma^{(0)} \sum_{i,j} C_i(Q, \mu, \mu_F) E_{ij}(\mu_F, \mu_{0F}) D_{j \rightarrow Q}(\mu_{0F}, m)$$

2 factorisation scales:  
 $\mu_F$  and  $\mu_{0F}$

- Initial conditions  $D_{j \rightarrow Q}$  @ NNLO [Melnikov, Mitov '04] [Mitov '04] [Maltoni et al. '22]
- DGLAP Evolution (ZM-VFNS @ NLO)  $E_{ij}$  with MELA [Bertone et al. '15] [Ridolfi et al. '19] 
- Coefficient functions  $C_i$  @ NNLO [Rijken, van Neerven '97] [Blümlein, Ravindran '06] [Mitov, Moch '06]
- Poor behaviour in large- $N$  ( $x \rightarrow 1$ ) region (Sudakov region)
  - Need resummation @ NNLL in initial conditions and coefficient functions [Cacciari, Catani '01] [Aglietti et. al '06] [Maltoni et al. '22] [Czakon et al. '22]

# Theory overview

## Soft-gluon resummation

- Sudakov-resummed **initial conditions**

- Constant large- $N$  limit of fixed order result & Sudakov factor

$$D_{Q \rightarrow Q}^{res} = [D_{Q \rightarrow Q}]_c \exp \left[ \ln N g_{ini}^{(1)}(\lambda_0) + g_{ini}^{(2)}(\lambda_0) + \alpha_S g_{ini}^{(3)}(\lambda_0) \right]$$

- Different **matchings** to fixed order result (e.g.  $\log R$ )

$$\log D_{i \rightarrow Q}^{fo+res, \log R, reg} = \log D_{Q \rightarrow Q}^{fo} + \log D_{Q \rightarrow Q}^{res, reg} - [\log D_{Q \rightarrow Q}^{res, (reg)}]_{\alpha_s^p}$$

- **Landau pole** in  $g_{ini}^{(i)}(\lambda_0) : \lambda_0 = 1/2 \rightarrow N_0^L = \exp(1/(2b_0\alpha_s))$

- $N_0^L \sim 7$  for **charm** &  $N_0^L \sim 32$  for **bottom**  $\rightarrow$  (many) **prescriptions**

- “**CNO**” (Cacciari-Nason-Oleari): shift in  $N$  in  $D_{Q \rightarrow Q}^{res}$  and  $[D_{Q \rightarrow Q}^{res}]_{\alpha_s^p}$  : parameter  $f$  [Cacciari et al. '05]

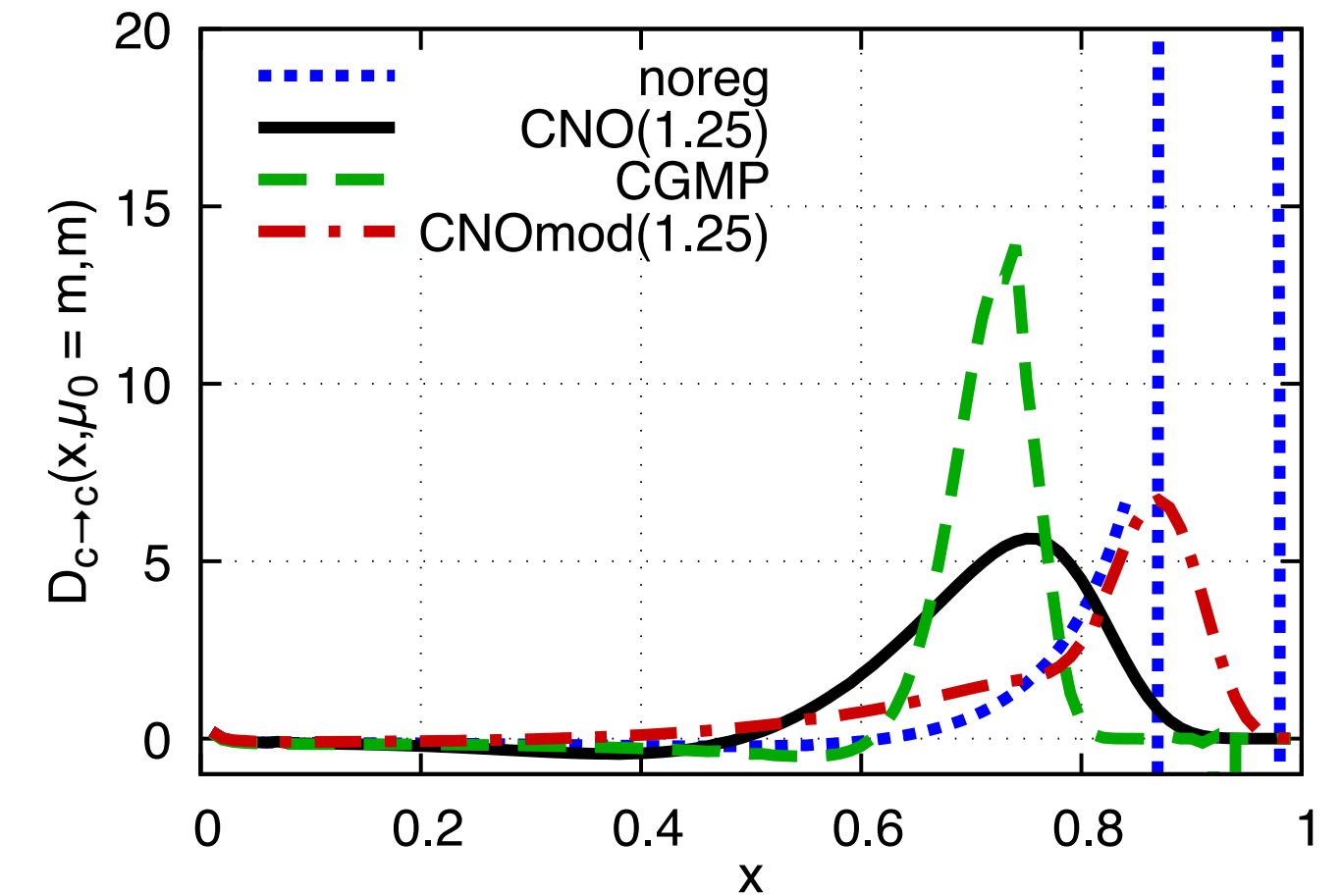
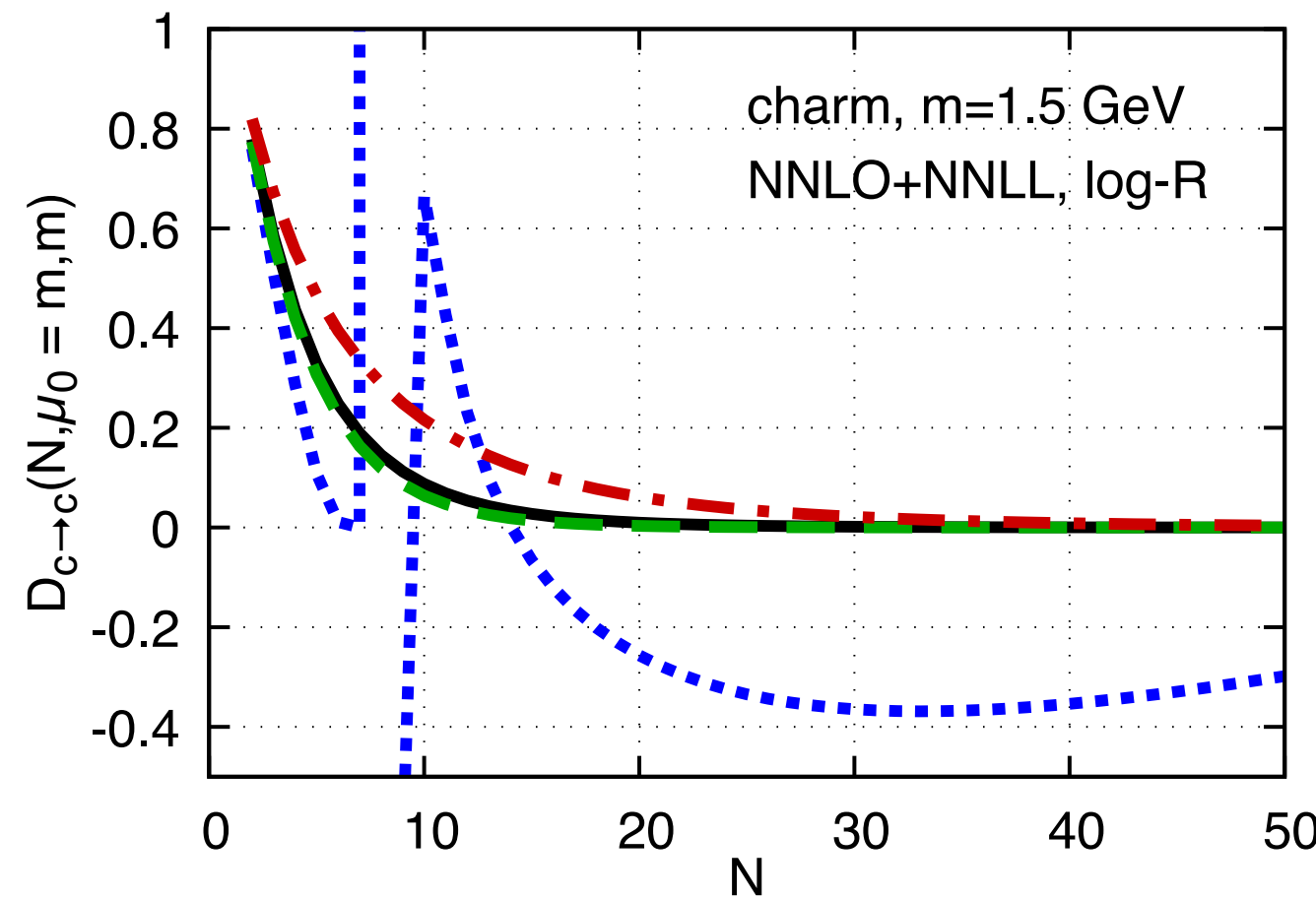
- “**CGMP**” (Czakon-Generet-Mitov-Poncelet): truncation of Sudakov factor [Czakon et al. '22]

- “**CNOmod**” (Cacciari-Nason-Oleari + Czakon-Generet-Mitov-Poncelet): shift in  $N$  only in  $D_{Q \rightarrow Q}^{res}$  [Czakon et al. '22]

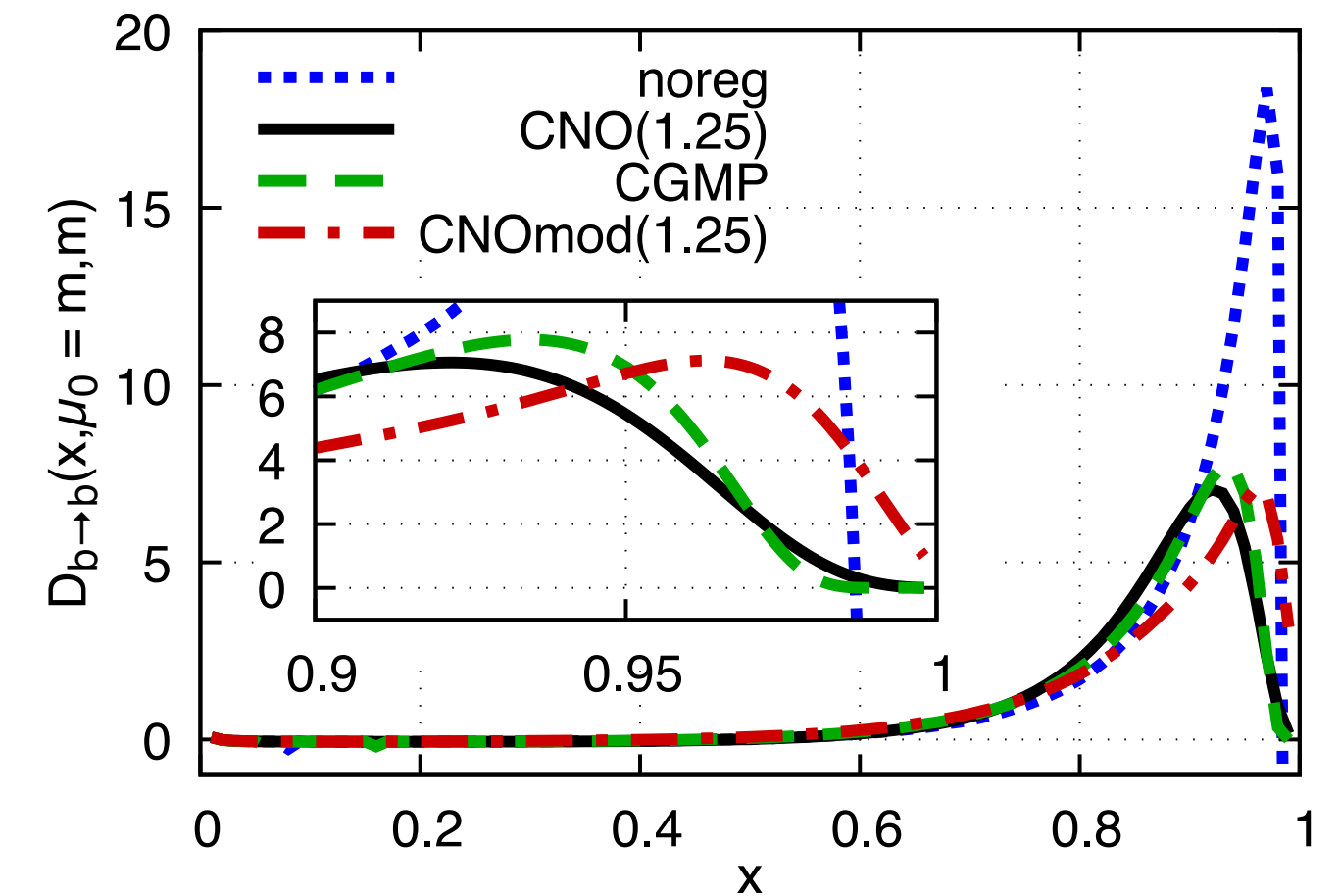
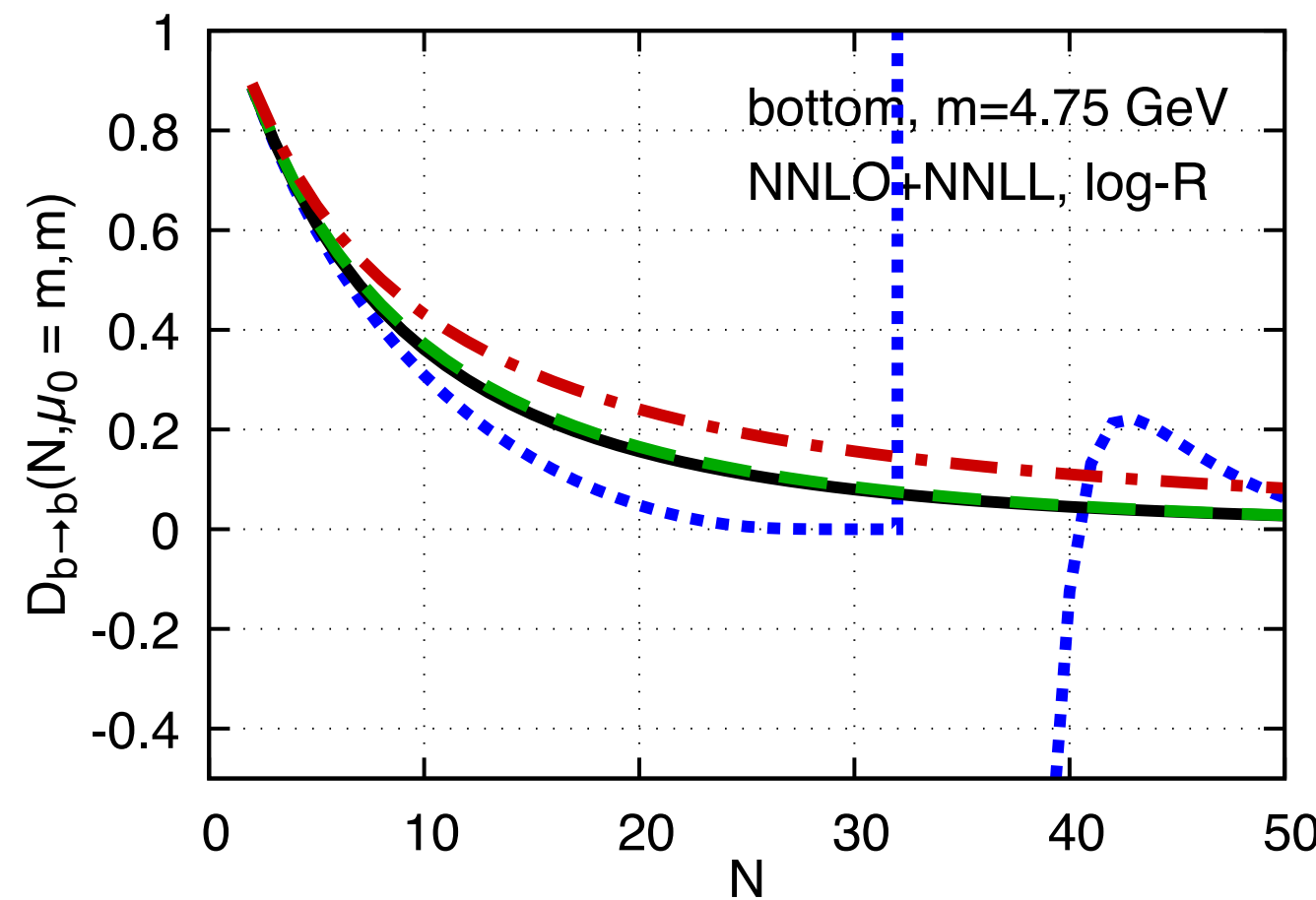
# Numerical results

## Heavy quark initial condition: NNLO + NNLL logR

- $D_{Q \rightarrow Q}^{fo+res,match,reg}(\cdot, Q, \mu_R, \mu_F, \mu_{0R}, \mu_{0F}, m)$
- Prescription chosen for Landau pole (*reg*) has huge impact
- Some shapes not suited for fits
  - NNLO+NNLL log-R CNO (default)
- Lower mass  $\rightarrow$  more sensitivity to Landau
- Evolution and convolution do not help ...



Charm



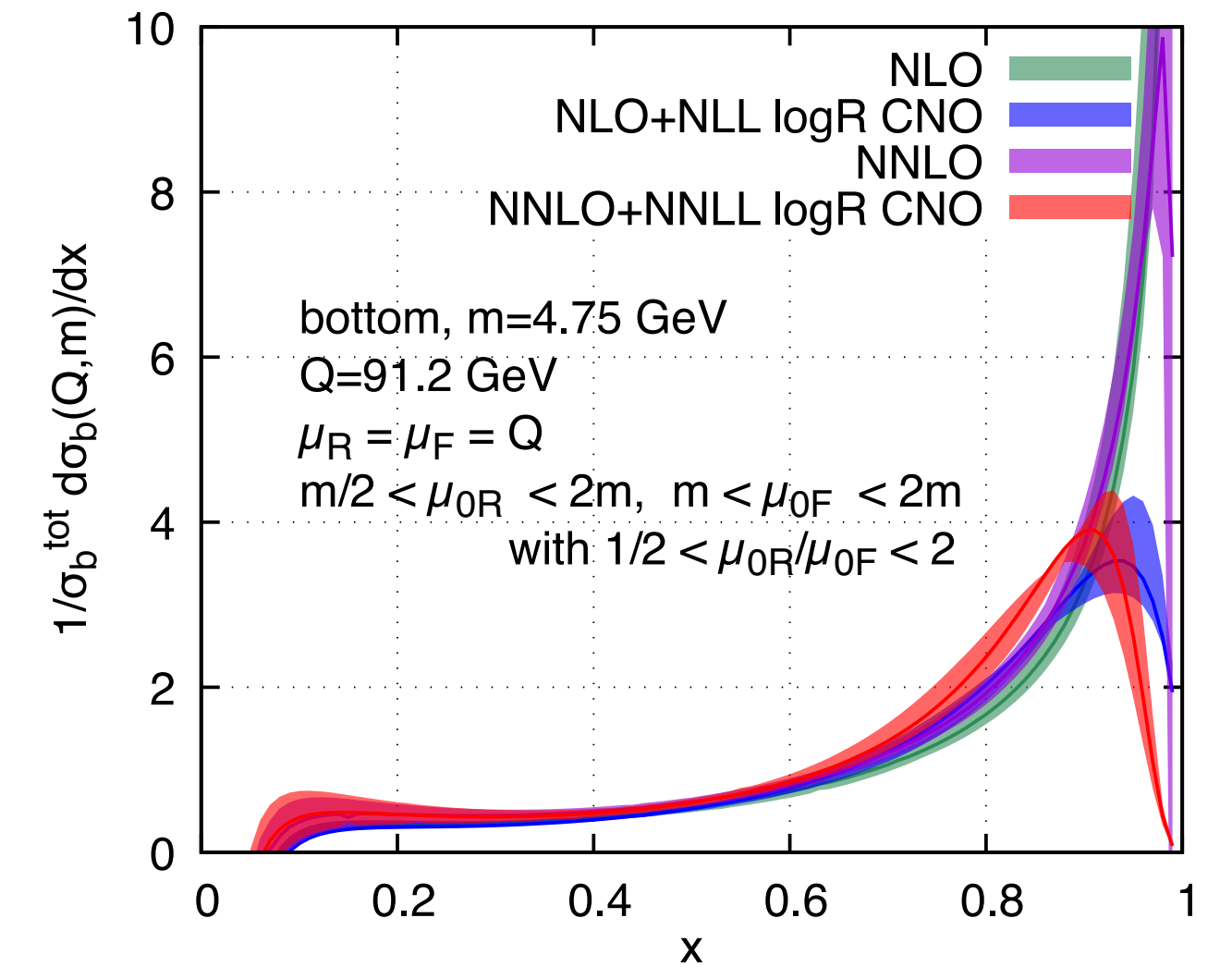
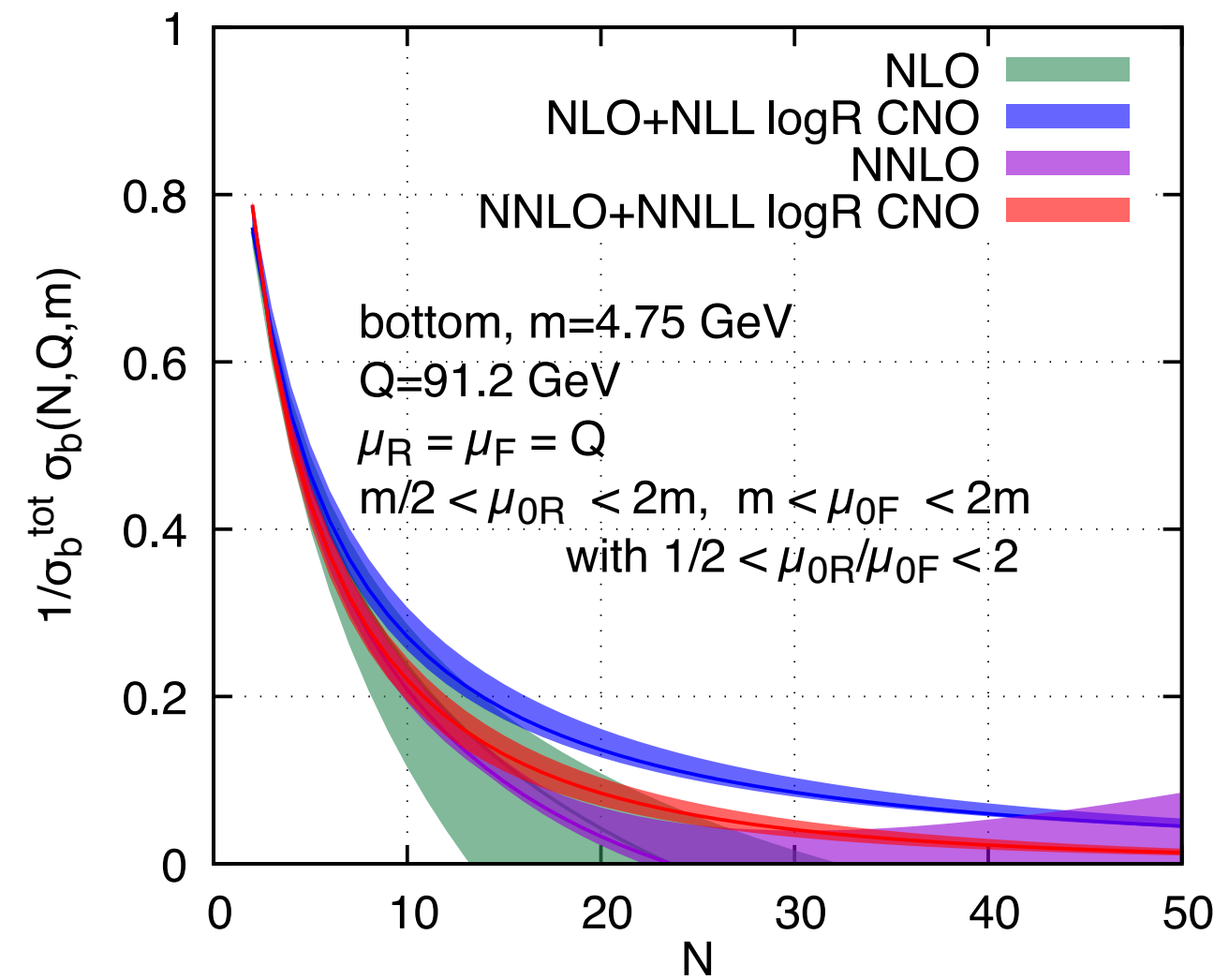
Bottom

# Numerical results

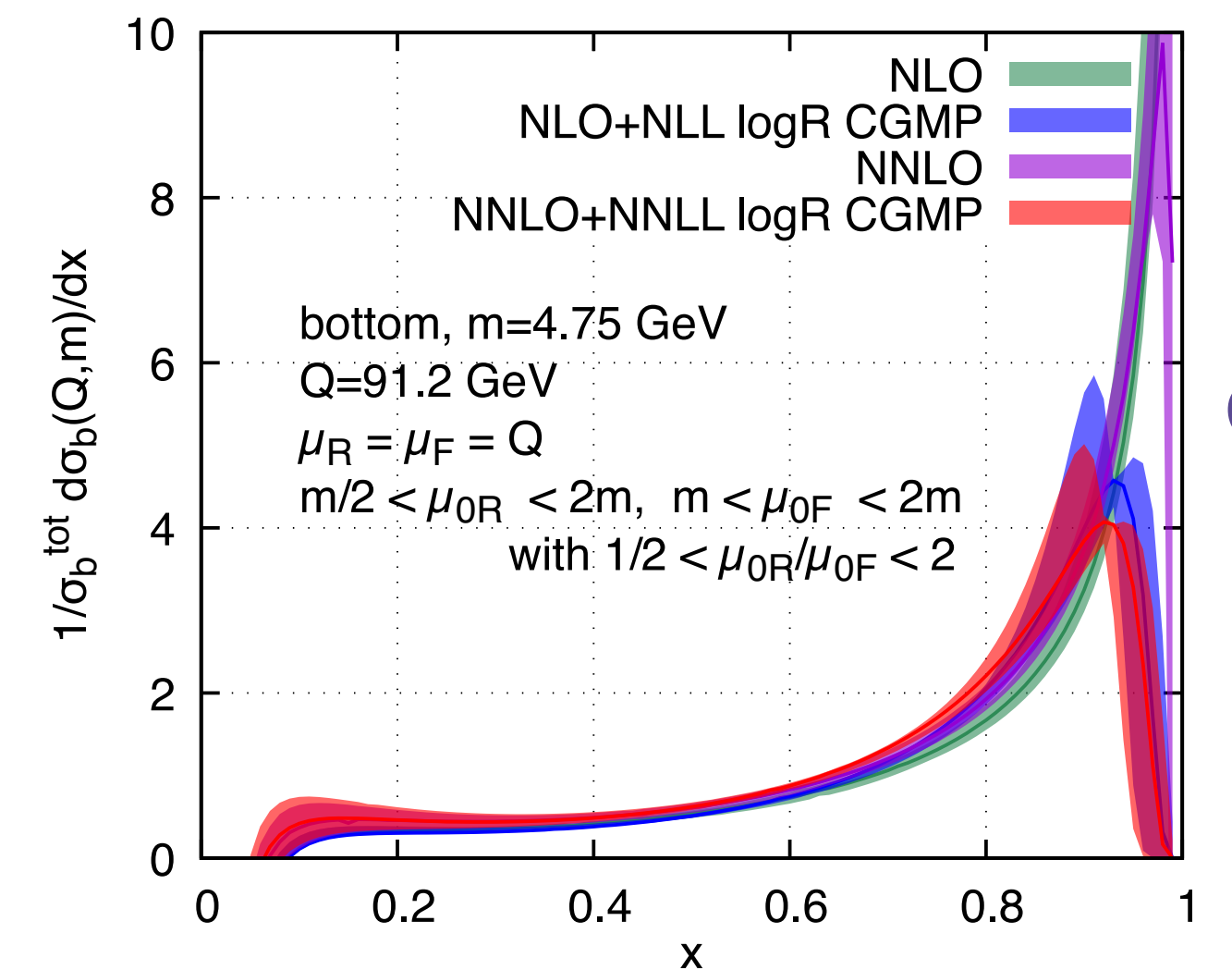
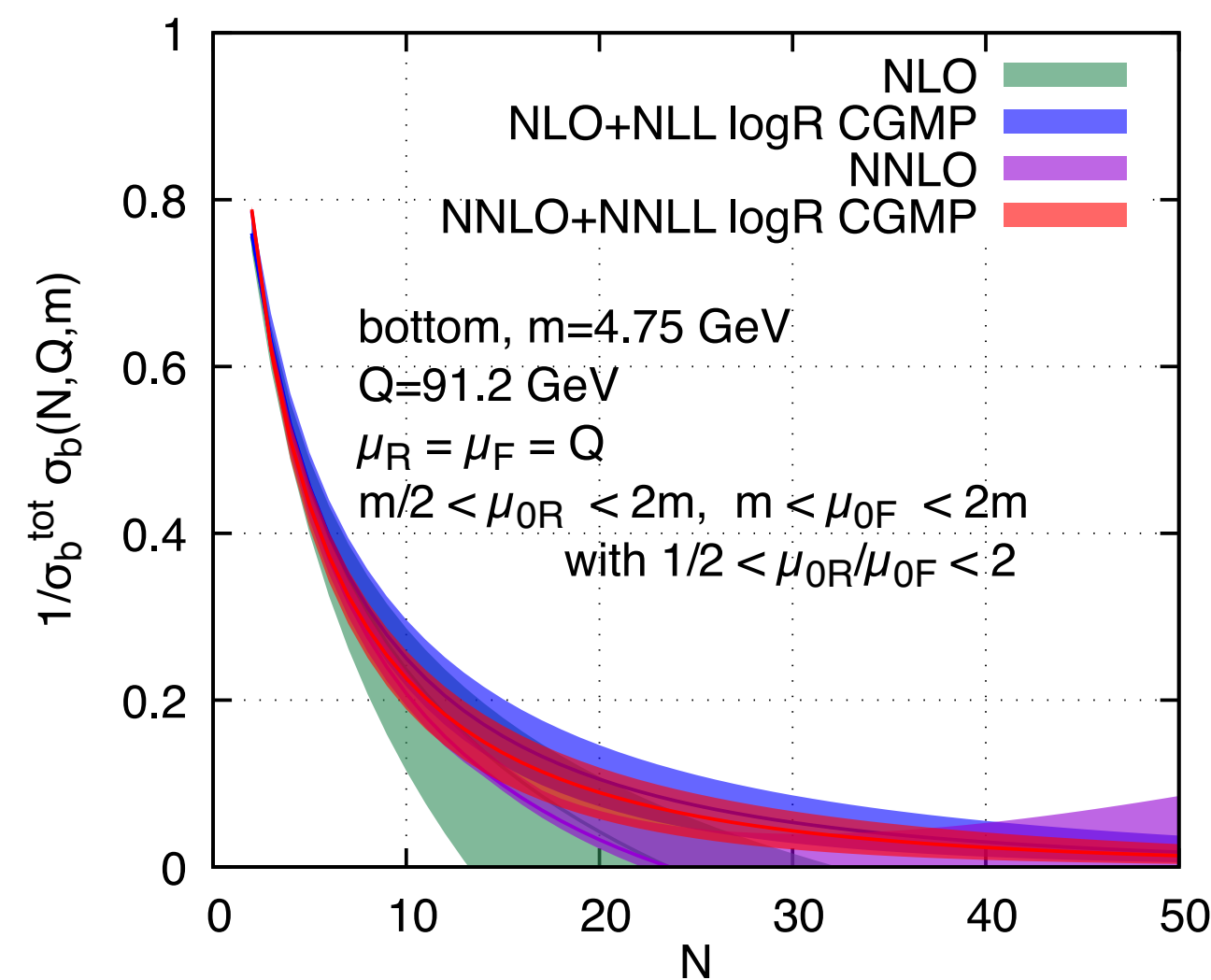
## Full $e^+e^-$ fragmentation function

- $\sigma_Q^{fo+res,logR,reg}(\cdot, Q, \mu_R, \mu_F, \mu_{0R}, \mu_{0F}, m)$
- Uncertainty bands for  $\mu_{0R}$  and  $\mu_{0F}$  5-point scale variation in initial conditions (around  $m$ )
  - NNLO+NNLL band (red) **not** much narrower than NLO+NLL one (blue)
  - Bands do not overlap  $\rightarrow$  **poor convergence** of perturbative series (CNO)
- Drastic dependence on Landau pole regularisation
- Charm: **worse**

Bottom



CNO



CGMP

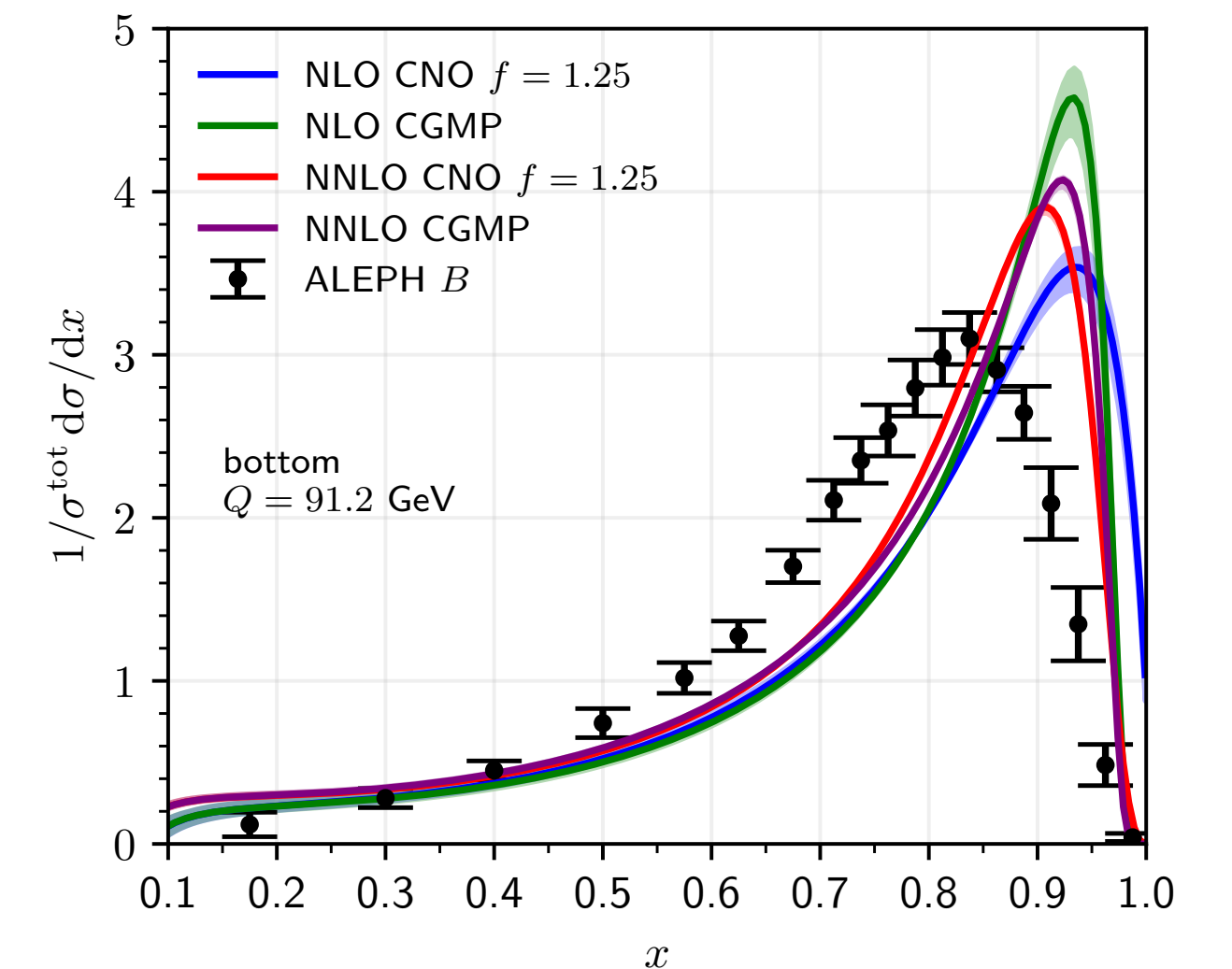
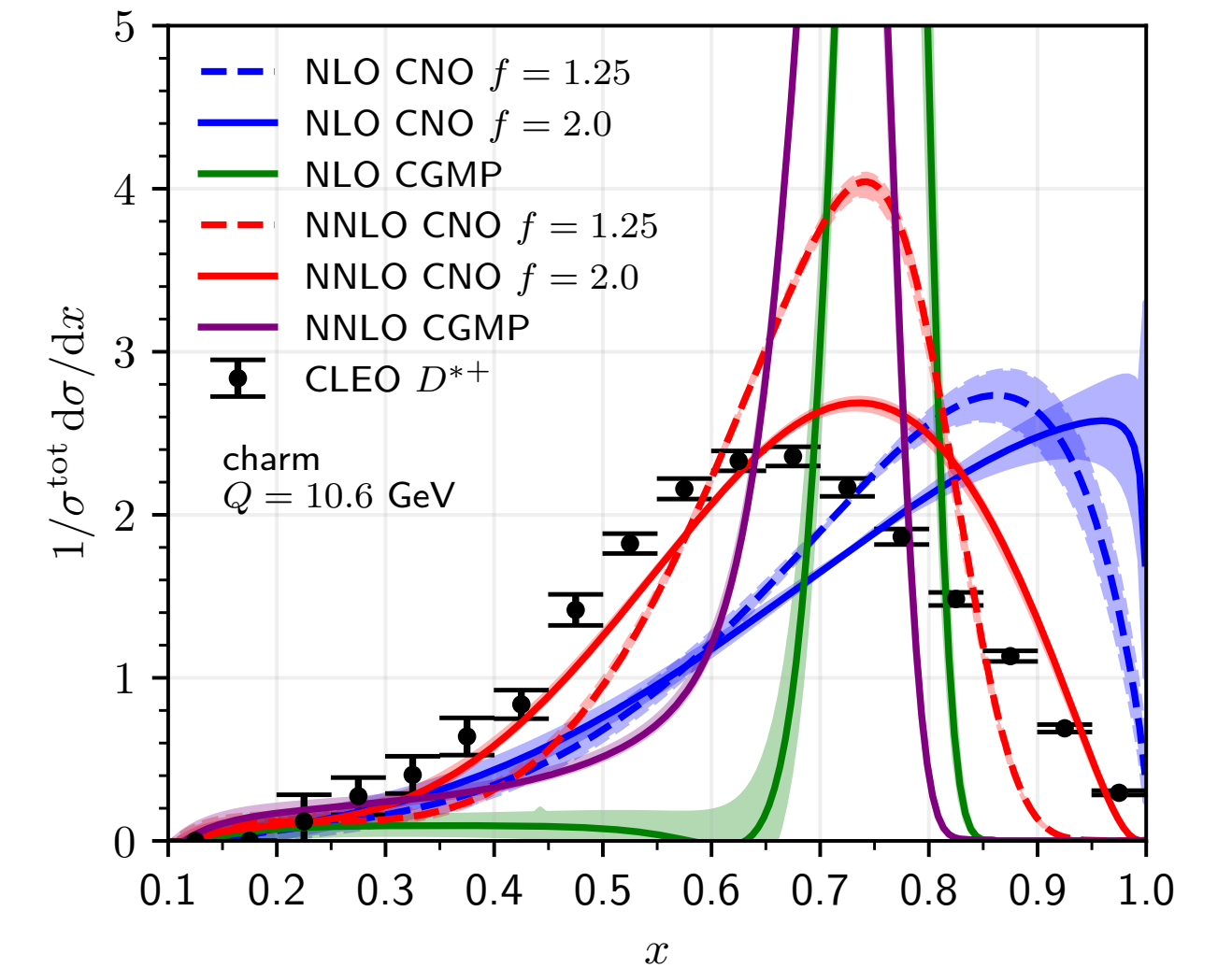
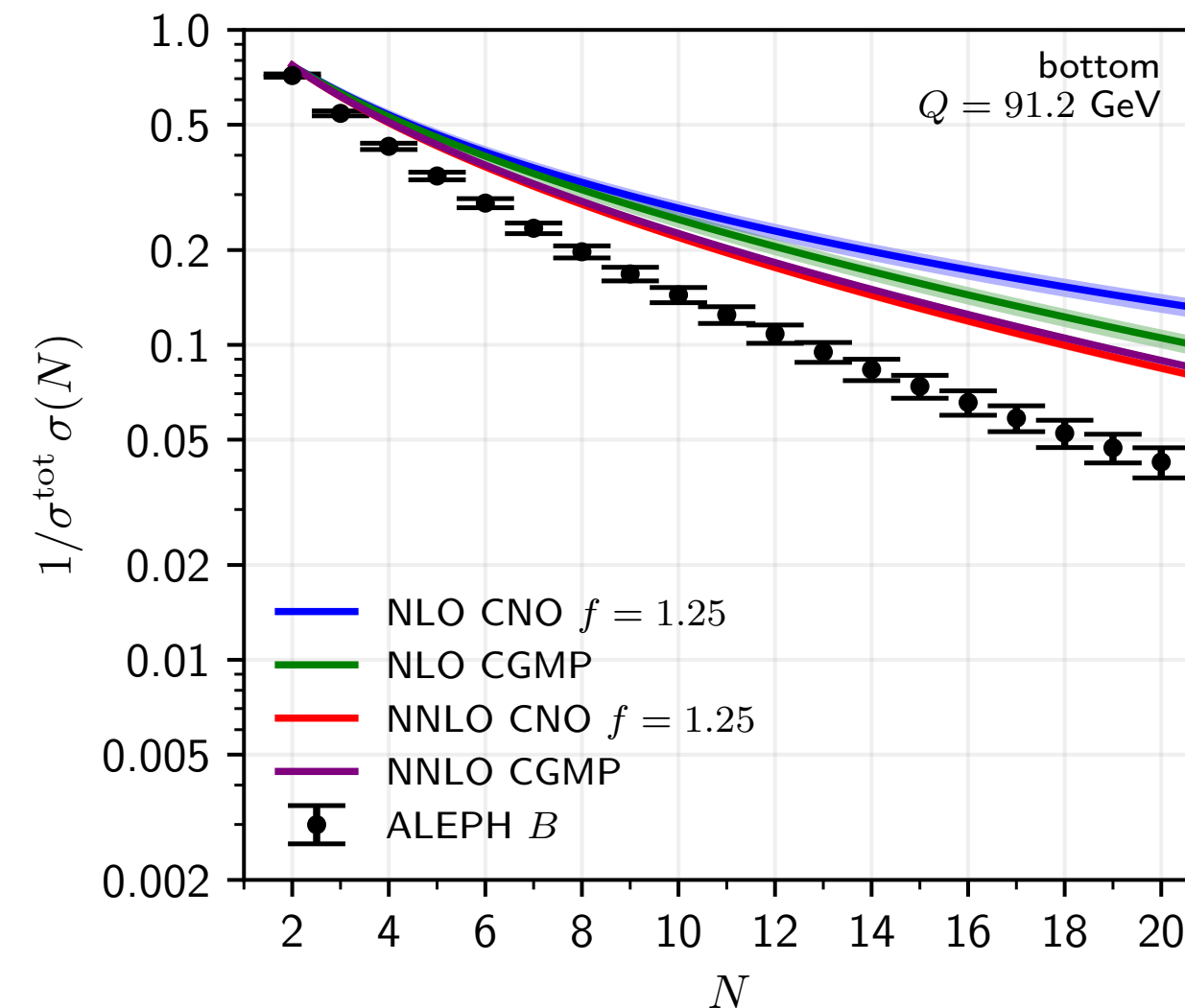
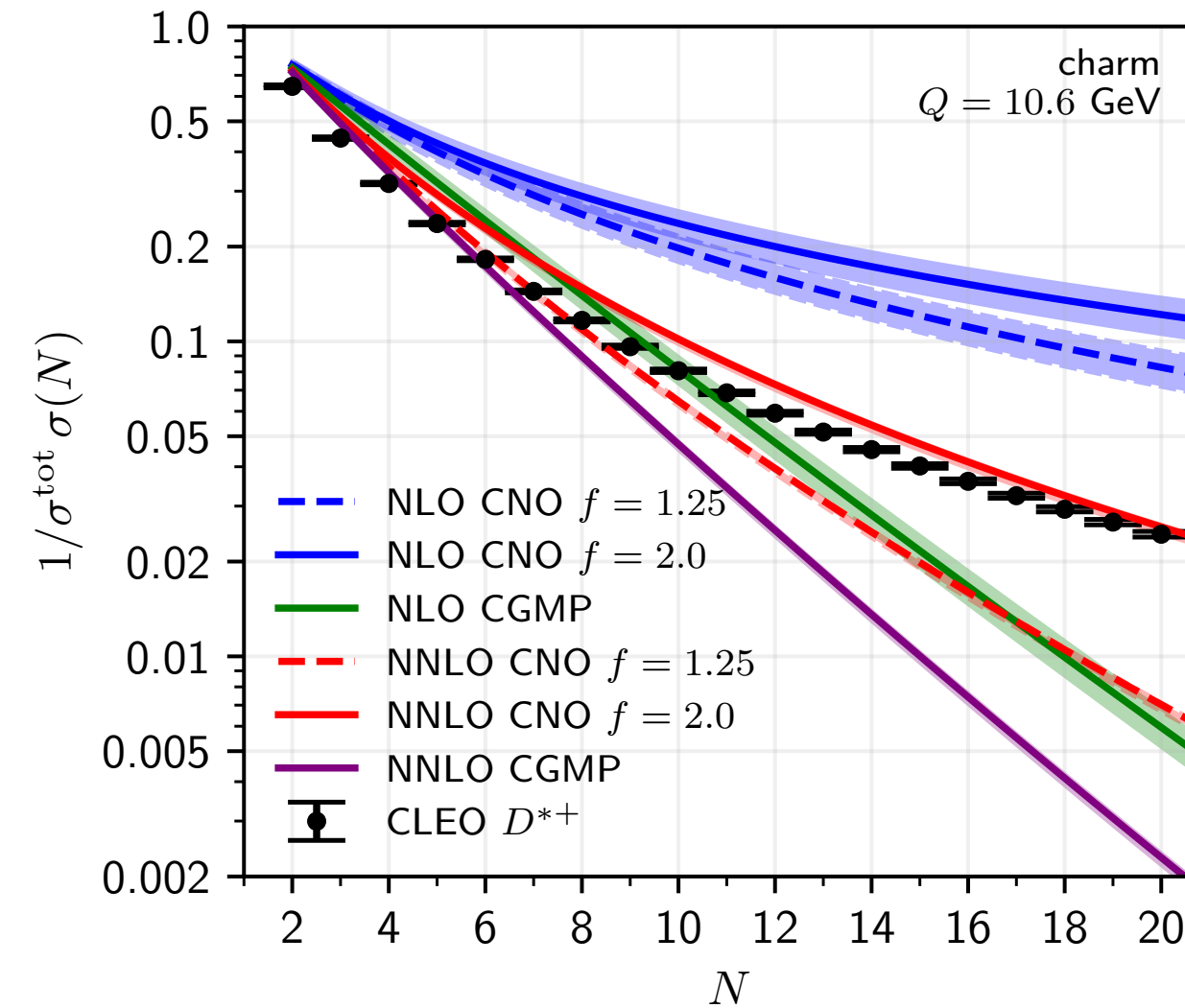
# Towards phenomenology

## pQCD at comparison with data

$$\sigma_h(N, Q) = \sigma_Q(N, Q, m) D_{Q \rightarrow h}^{np}(N, \{\text{par}\})$$

- **Bottom:** all prescriptions can be used for fits
- **Charm:** most NNLO+NNLL curves dip below data at  $N \gtrsim 6$
- $D^{np}$  can only “lower” theoretical prediction
  - Bottom: NNLO+NNLL logR CNO ( $f=1.25$ )
  - Charm: NNLO+NNLL logR CNO ( $f=2.0$ )
- Single-moment and single-parameter “fits”

$f$ : CNO regularisation parameter



Charm

Bottom

# Single-point fits

## CNO bottom single-point fits up to NNLO + NNLL

Bottom

- Recall: non-perturbative FF factorised

$$\sigma_h(N, Q) = \sigma_Q(N, Q, m) D_{Q \rightarrow h}^{np}(N, \{\text{par}\})$$

- Our take: as simple as possible

- Single parameter non-perturbative function

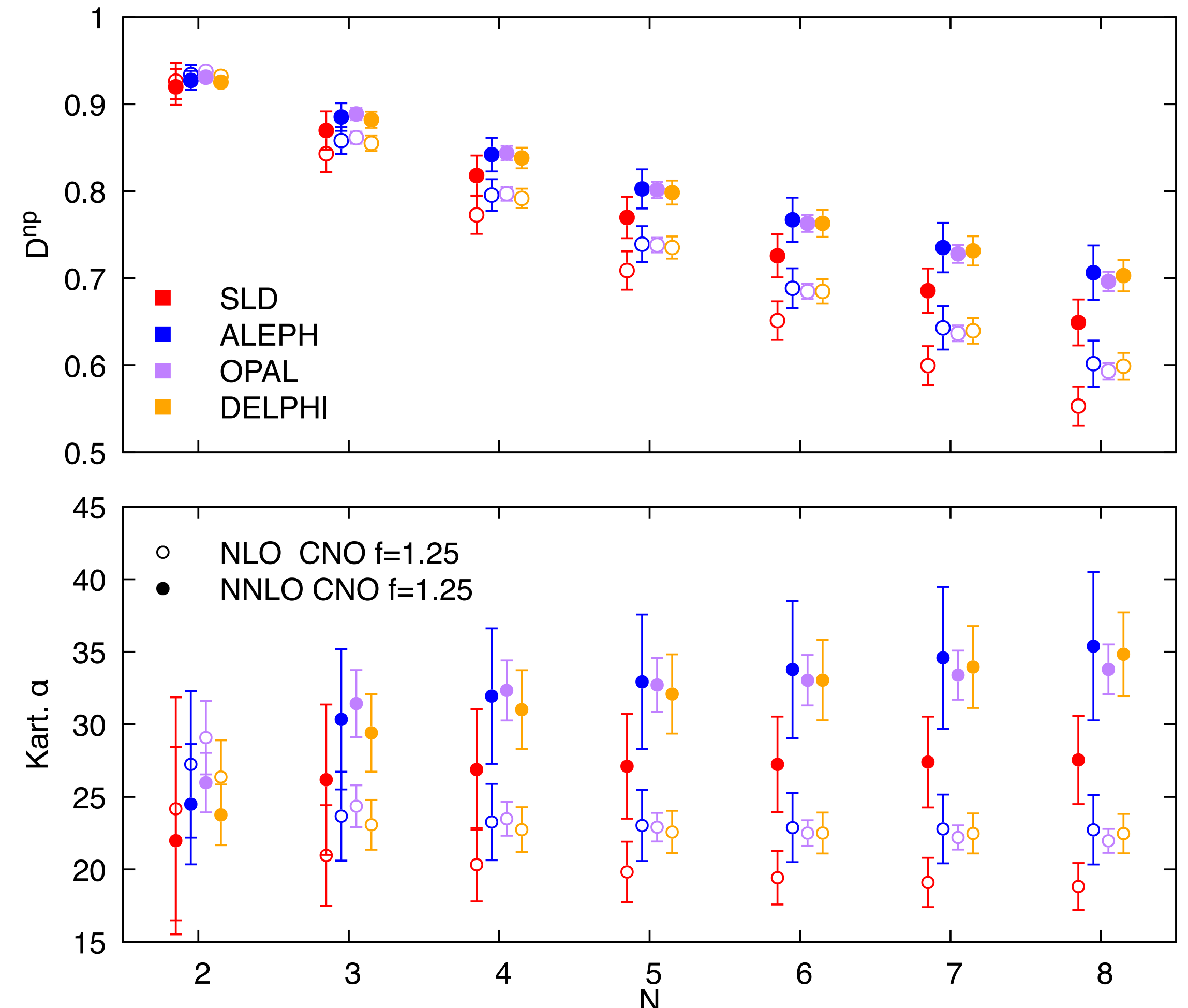
$$D_K^{np}(x) = (\alpha + 1)(\alpha + 2)x^\alpha(1 - x) \text{ [Kartvelishvili et al. '78]}$$

- “Fit” moments between 2 and 8 (relevant for hadronic collisions)

- $D^{np} = \text{data}/(\text{pert. theo})$

- $\alpha$  values stable in  $N$

- NNLO+NNLL results closer to data  $\rightarrow$  smaller non-perturbative component





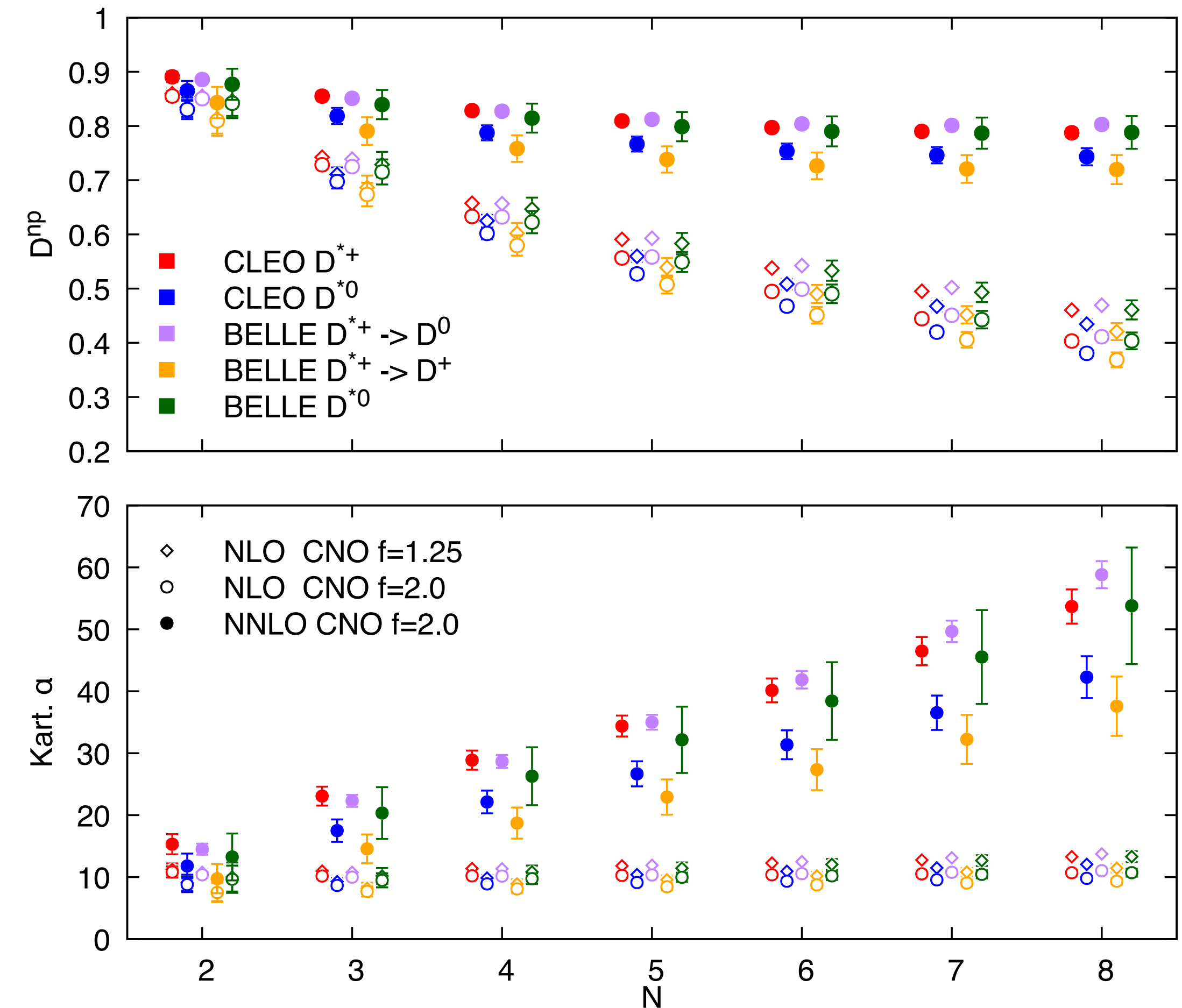
# Single-point fits

## CNO charm single-point fits up to NNLO + NNLL

Charm

- @ NLO+NLL
  - $\alpha$  values stable in  $N$
  - Stable under variation of  $f$
- @ NNLO+NNLL
  - large dependency of  $\alpha$  on  $N$
  - $f = 2.0$  mandatory choice

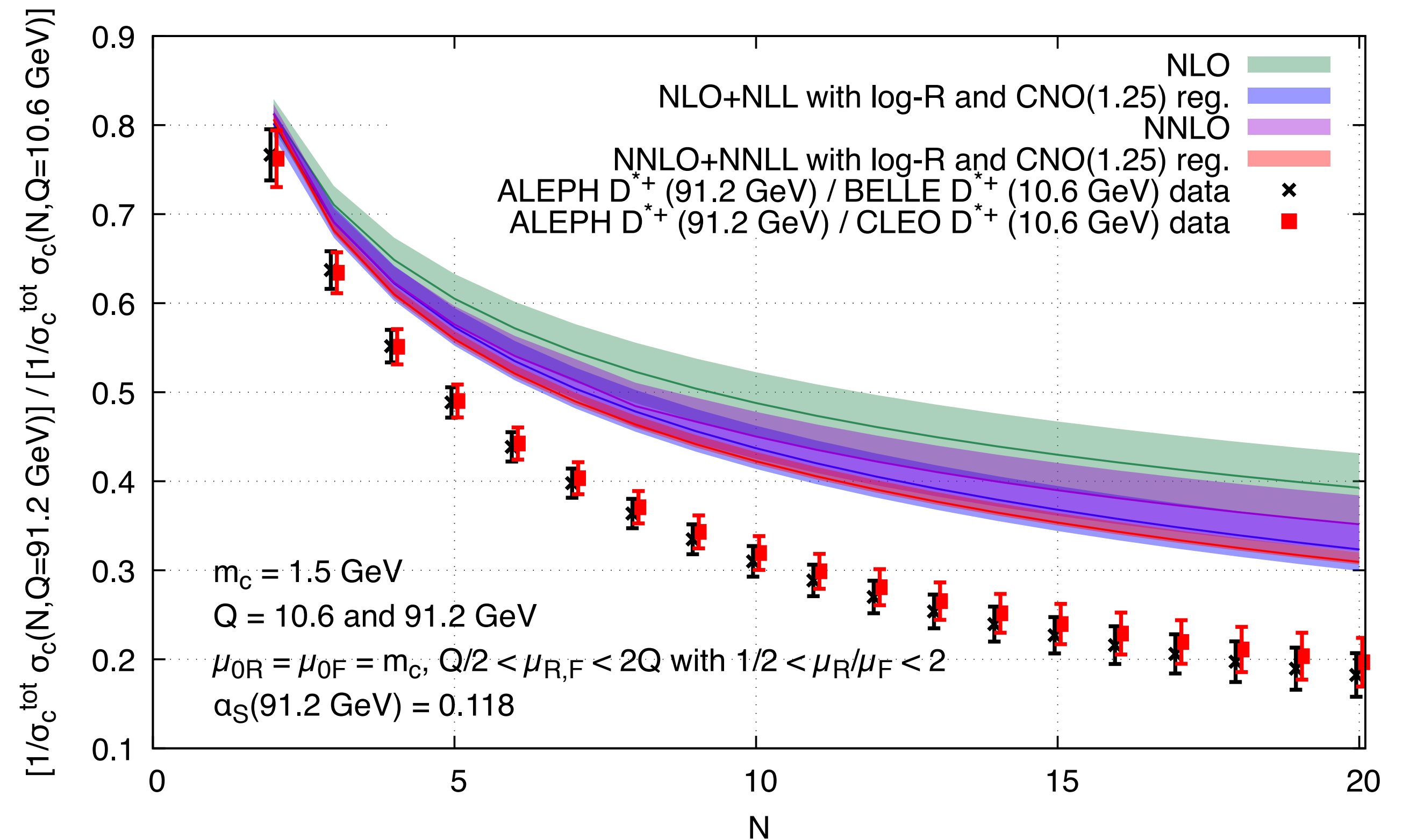
$f$ : CNO regularisation parameter



# Charm ratio

## A perturbative observable

- Ratio of ALEPH (91.2 GeV) and BELLE/ CLEO (10.6 GeV) moments for  $D^{*+}$
- Non-perturbative and low-scales effects largely cancel in theory prediction  $\rightarrow$  entirely perturbative
- Data undershoot pure QCD prediction
- Large power suppressed effects in coefficient functions?
- Discrepancy reduced if heavy-quark threshold effects also in resummed coefficient functions [Cacciari et al. 2406.04173]



$$\frac{\sigma_Q(M_Z, m)}{\sigma_Q(M_\Upsilon, m)} \simeq \frac{C_q(M_Z, \mu_Z)}{\sigma_Q^{\text{tot}}(M_Z)} E(\mu_Z, \mu_\Upsilon) \frac{\sigma_Q^{\text{tot}}(M_\Upsilon)}{C_q(M_\Upsilon, \mu_\Upsilon)}$$

# Matching conditions at NNLO

based on [2407.07623] in  
collaboration with  
Christian Biello (MPP)

## Towards a ZM-VFNS at NNLO

- $\frac{1}{\sigma_Q^{tot}} \sigma_Q(Q, m) = \frac{1}{\sigma_Q^{tot}} \sigma^{(0)} \sum_{i,j} C_i(Q, \mu, \mu_F) E_{ij}(\mu_F, \mu_{0F}) D_{j \rightarrow Q}(\mu_{0F}, m) \rightarrow$  crossing heavy flavour thresholds ( $\mu \sim m$ )

- need **time-like thresholds** matching conditions (ZM-VFNS)

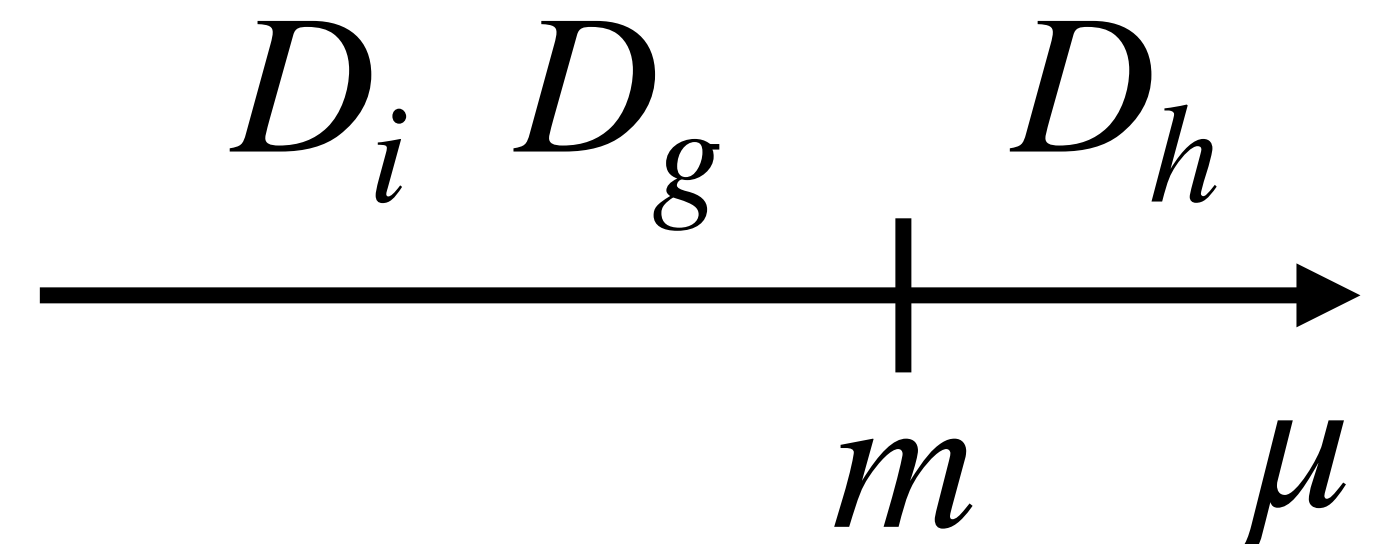
- NLO matching conditions for  $D_h$  and  $D_g$  [Cacciari et al. '05]

- NNLO  $D_i$  (NNLO corrections to  $D_h D_g$  still missing) [Biello, Bonino '24]

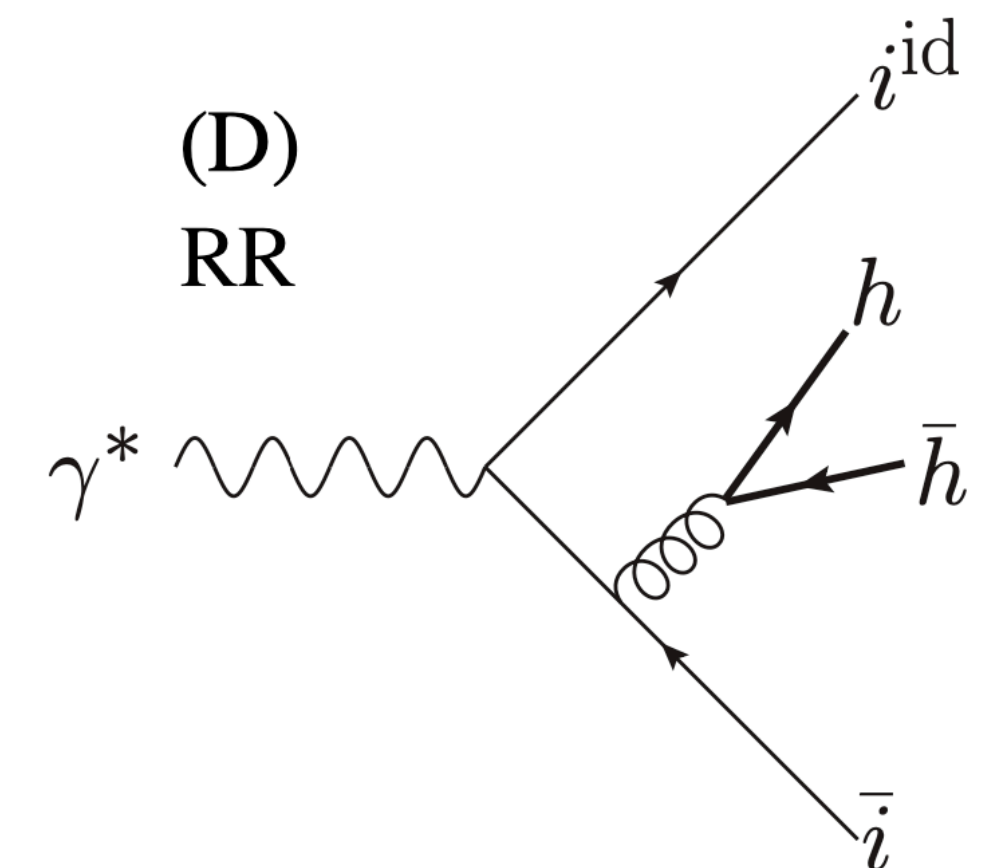
- $\mu \ll m \rightarrow$  **decoupling scheme**: only massless flavours FFs + mass effects in XS ( $d\sigma$ )

$$\frac{d\sigma^H}{dx} = \int_x^1 \frac{dz}{z} \left\{ \sum_{j \in \mathbb{L}_n} D_j^{(n_L)} \frac{d\sigma_j}{dz} + D_g^{(n_L)} \frac{d\sigma_{h\bar{h}g^{id.}}}{dz} + \sum_{i \in \mathbb{L}_{n_L-g}} D_i^{(n_L)} \frac{d\sigma_{h\bar{h}i^{id.\bar{i}}}}{dz} \right\}$$

- $\mu \gg m \rightarrow$  full massless  $\overline{MS}$  scheme  $\frac{d\sigma^H}{dx} = \int_x^1 \frac{dz}{z} \left\{ \sum_{k \in \mathbb{L}_n} D_k^{(n)} \frac{d\hat{\sigma}_k}{dz} \right\}$



$\mu = \mu_F =$  factorization scale



# Matching conditions at NNLO

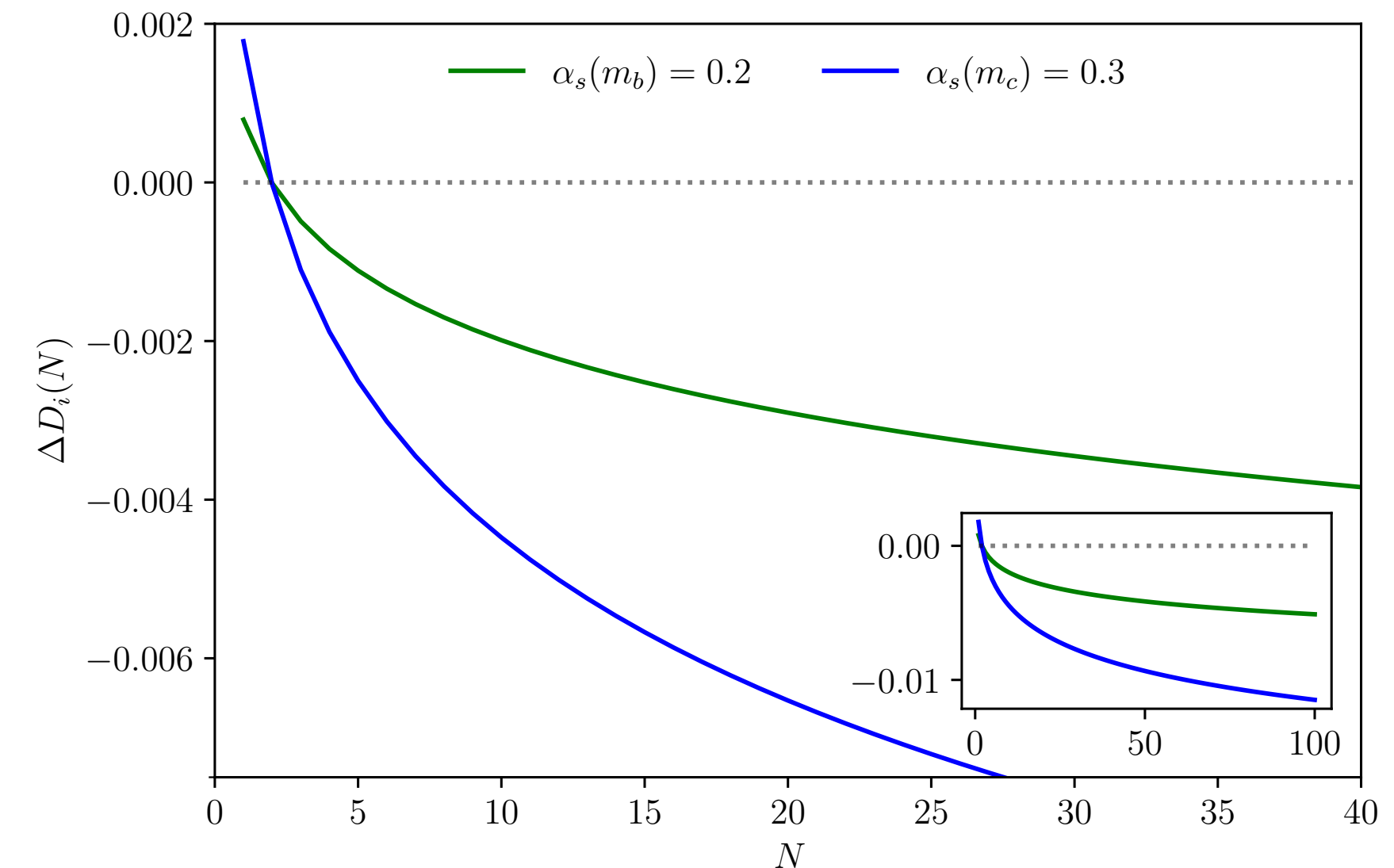
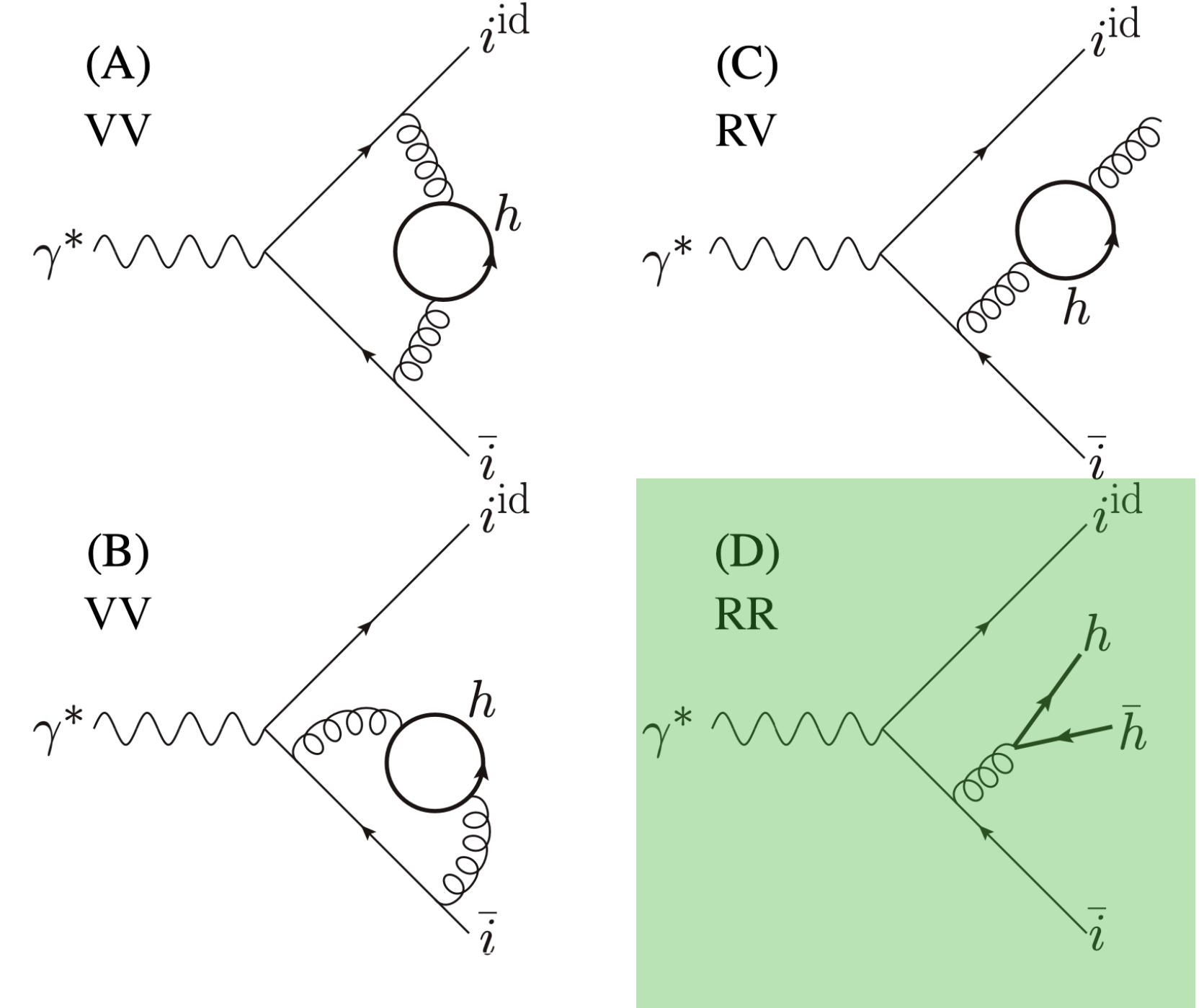
## The light flavour matching condition

- NNLO matching conditions for **light flavour** (Mellin space)

$$D_i^{(n)}(N, \mu) = \left\{ 1 + \frac{1}{\sigma_{i\bar{i}}} \mathcal{M}_{(N,z)} \left[ \delta_{D_i}^i(z) \right] \right\} D_i^{(n_L)}(N, \mu)$$

- Takes **RR** [Gehrmann Stagnitto '22] [Bonino et al. '24] **RV** and **VV** [Blümlein et al. '16] **massive** and **massless** corrections

$$\begin{aligned} D_i^{(n)}(N, \mu) = & \left\{ 1 + \left( \frac{\alpha_s}{2\pi} \right)^2 C_F \frac{1}{N^3(N+1)^3} \left[ -\frac{2}{3} N^3(N+1)^3 S_{1,2}(N) - \frac{2}{3} N^3(N+1)^3 S_{2,1}(N) + \frac{1}{3} N^3(N+1)^3 S_3(N) \right. \right. \\ & + \frac{5}{9} N^3(N+1)^3 S_2(N) + S_1(N) \left( \frac{2}{3} N^3(N+1)^3 S_2(N) - \frac{28}{27} N^3(N+1)^3 \right) - \frac{4}{3} N^3(N+1)^3 \zeta_3 \\ & + \left( \frac{9307}{1296} - \frac{29}{108} \pi^2 \right) N^6 + \left( \frac{9307}{432} - \frac{29}{36} \pi^2 \right) N^5 + \left( \frac{3281}{144} - \frac{29}{36} \pi^2 \right) N^4 + \left( \frac{10939}{1296} - \frac{29}{108} \pi^2 \right) N^3 - \frac{5}{54} N^2 - \frac{1}{9} N + \frac{1}{6} \\ & - \frac{8}{9} N^3(N+1)^3 \log^3 2 + \frac{29}{9} N^3(N+1)^3 \log^2 2 + \frac{1}{54} (12\pi^2 - 359) N^3(N+1)^3 \log 2 \\ & + \left( \frac{10}{9} N^3(N+1)^3 S_1(N) - \frac{2}{3} N^3(N+1)^3 S_2(N) - \frac{1}{36} N (3N^5 + 9N^4 + 53N^3 + 67N^2 + 8N - 12) \right) \log \left( \frac{\mu^2}{m^2} \right) \\ & \left. + \left( \frac{1}{12} N^2(N+1)^2 (3N^2 + 3N + 2) - \frac{1}{3} N^3(N+1)^3 S_1(N) \right) \log^2 \left( \frac{\mu^2}{m^2} \right) \right] + \mathcal{O}(\alpha_s^3) \left. \right\} D_i^{(n_L)}(N, \mu). \end{aligned}$$



# Conclusions

- NNLO + NNLL reached for bottom & charm
  - Open question on Landau pole regularisation
    - Can we do better?
    - Current limit on theoretical precision
  - Interesting developments on charm-ratio
- 1 out of 3 of the NNLO matching conditions ✓
- Results important for  $pp$ –phenomenology

# Backup: Landau pole regularisations

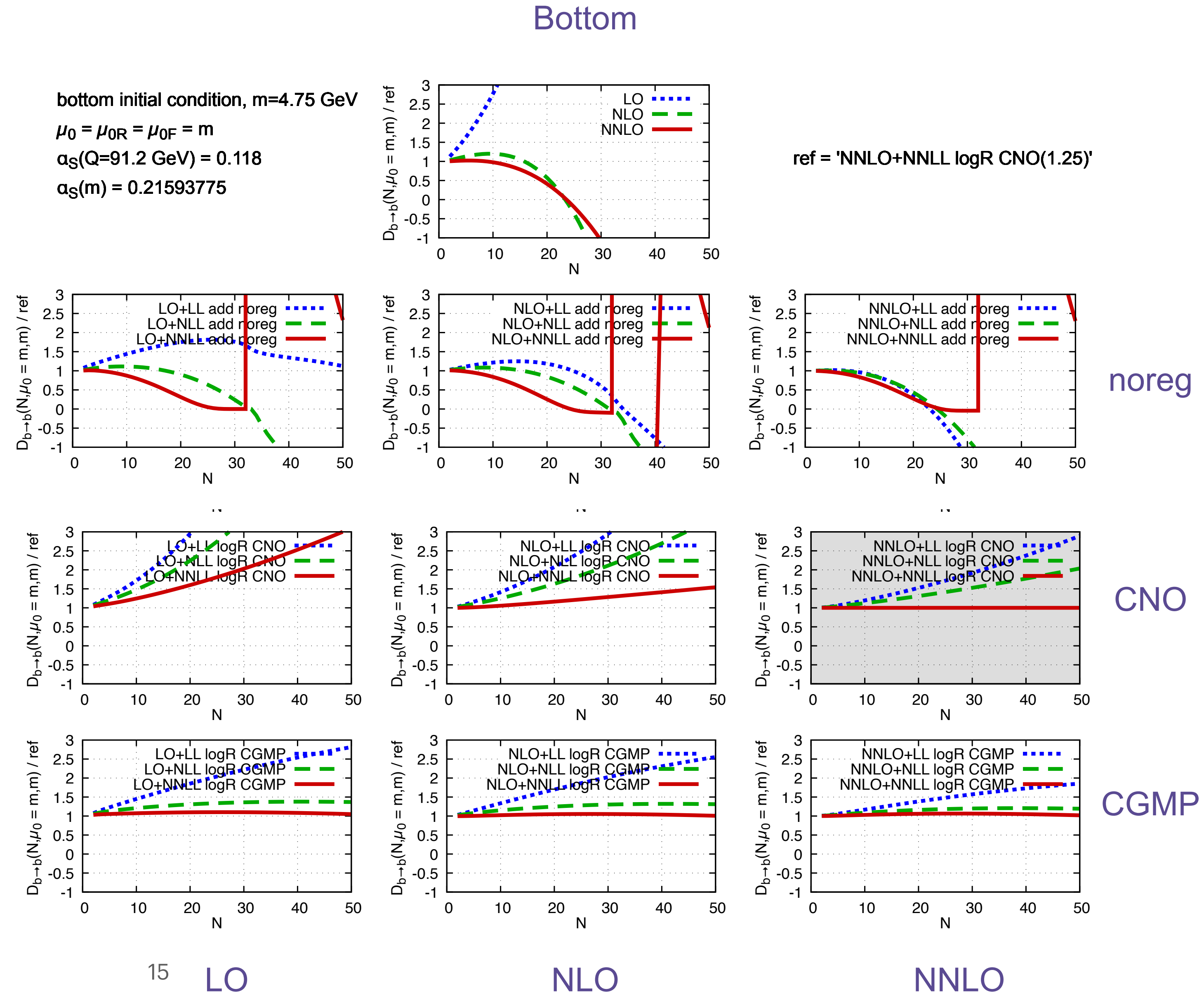
## CNO & CGMP prescription

- “CNO” (Cacciari-Nason-Oleari): shift in  $N$  [Cacciari et al.\_0510032]  $N \rightarrow N \frac{1 + f/N^L}{1 + fN/N^L}$ 
  - Consistent with all known perturbative results ✓
  - Yields physically acceptable results ✓
  - Does not introduce power corrections larger than generally expected for the process in question:  $N\Lambda_{QCD}/m$  for IC and  $N\Lambda_{QCD}^2/Q^2$  for CF ✓
- “CGMP” (Czakon-Generet-Mitov-Poncelet): truncation in the **exponent** of Sudakov factor [Czakon et al.\_2210.06078]
  - introduces power corrections larger than generally expected

# Numerical results

## Heavy quark initial condition

- Full range of perturbative orders
  - Ratio to **NNLO+NNLL log-R CNO**
- No obvious perturbative hierarchy  $NNLL < NLL < LL$
- No systematic convergence
  - But for log-R CGMP
- **NNLO+NNLL log-R CNO** (default)

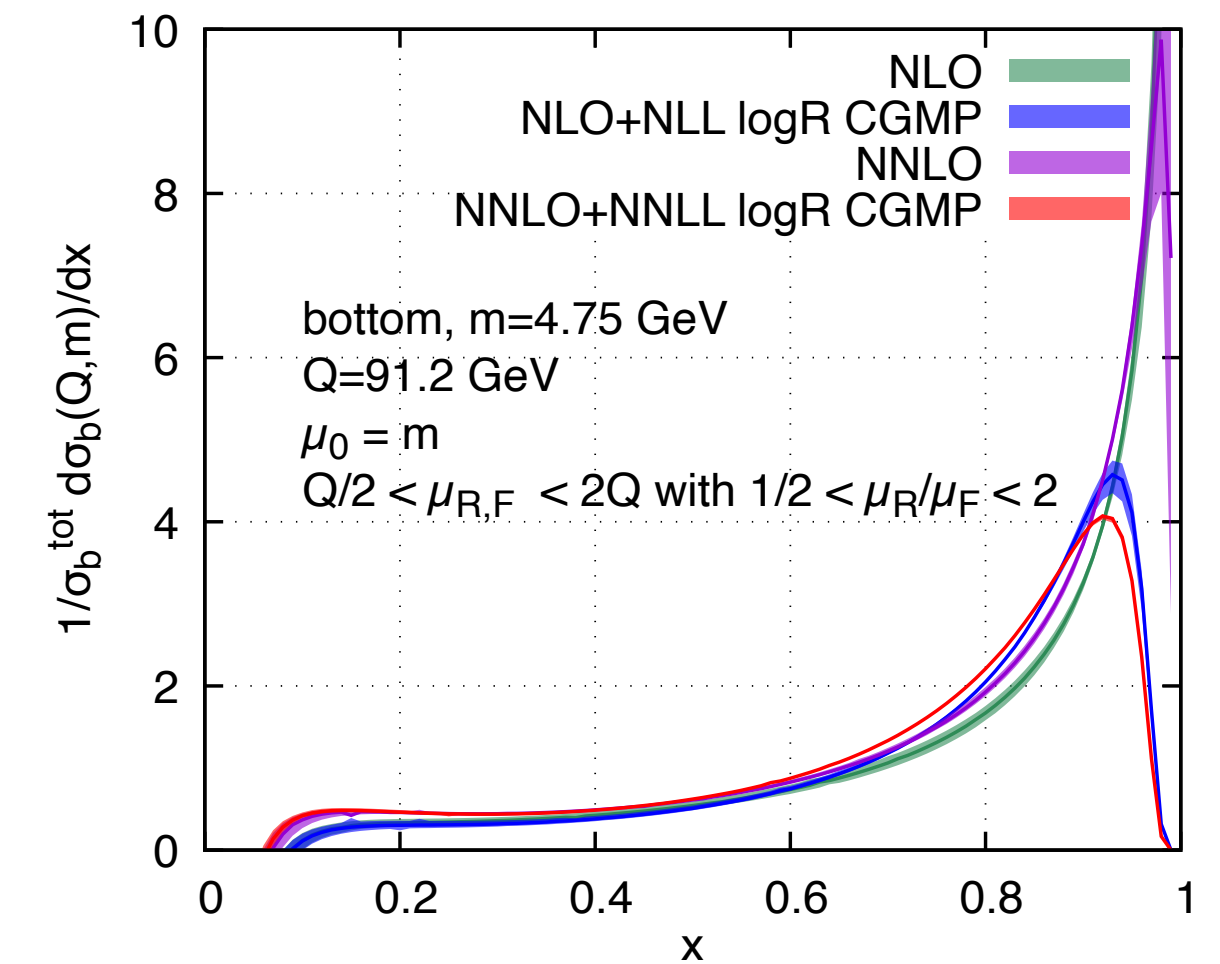
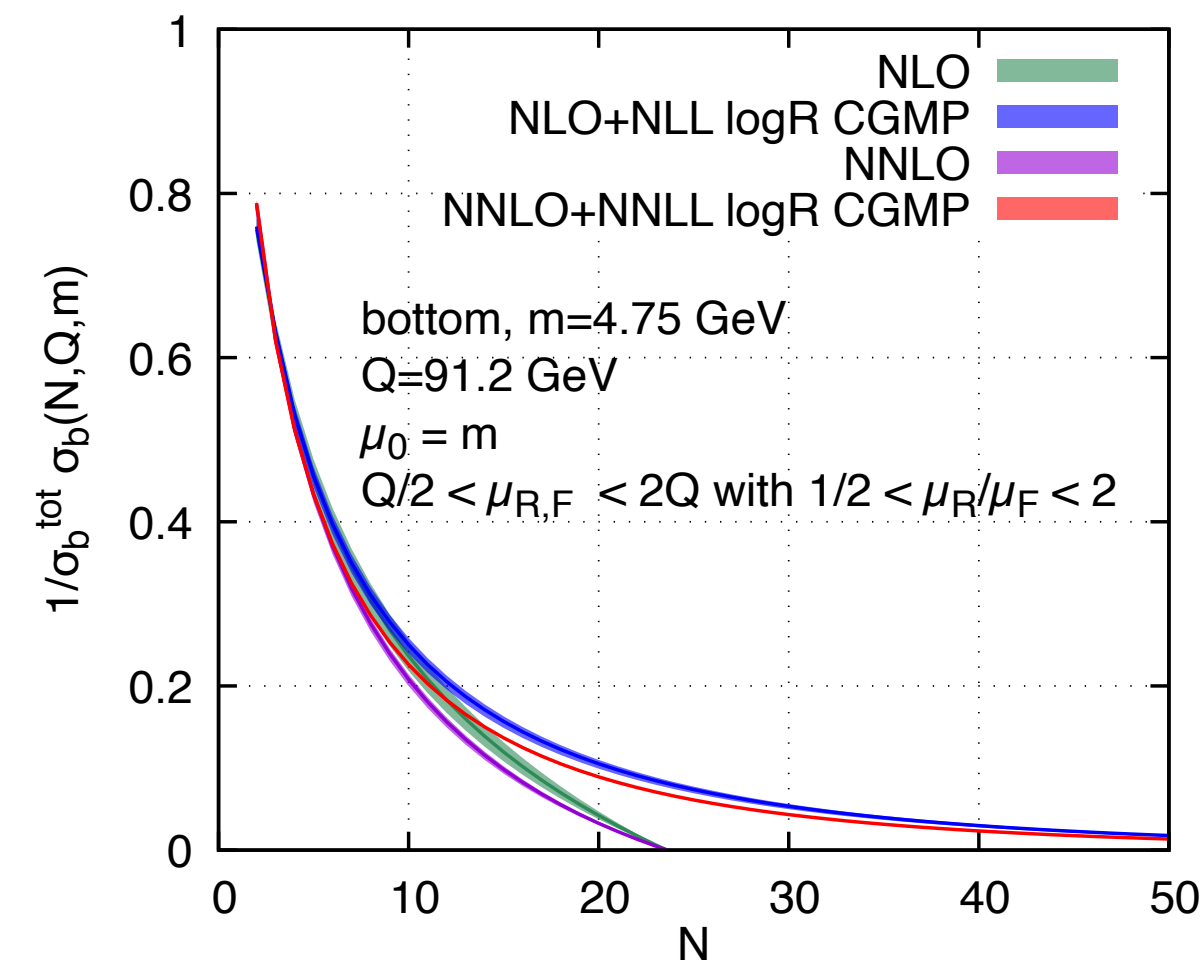
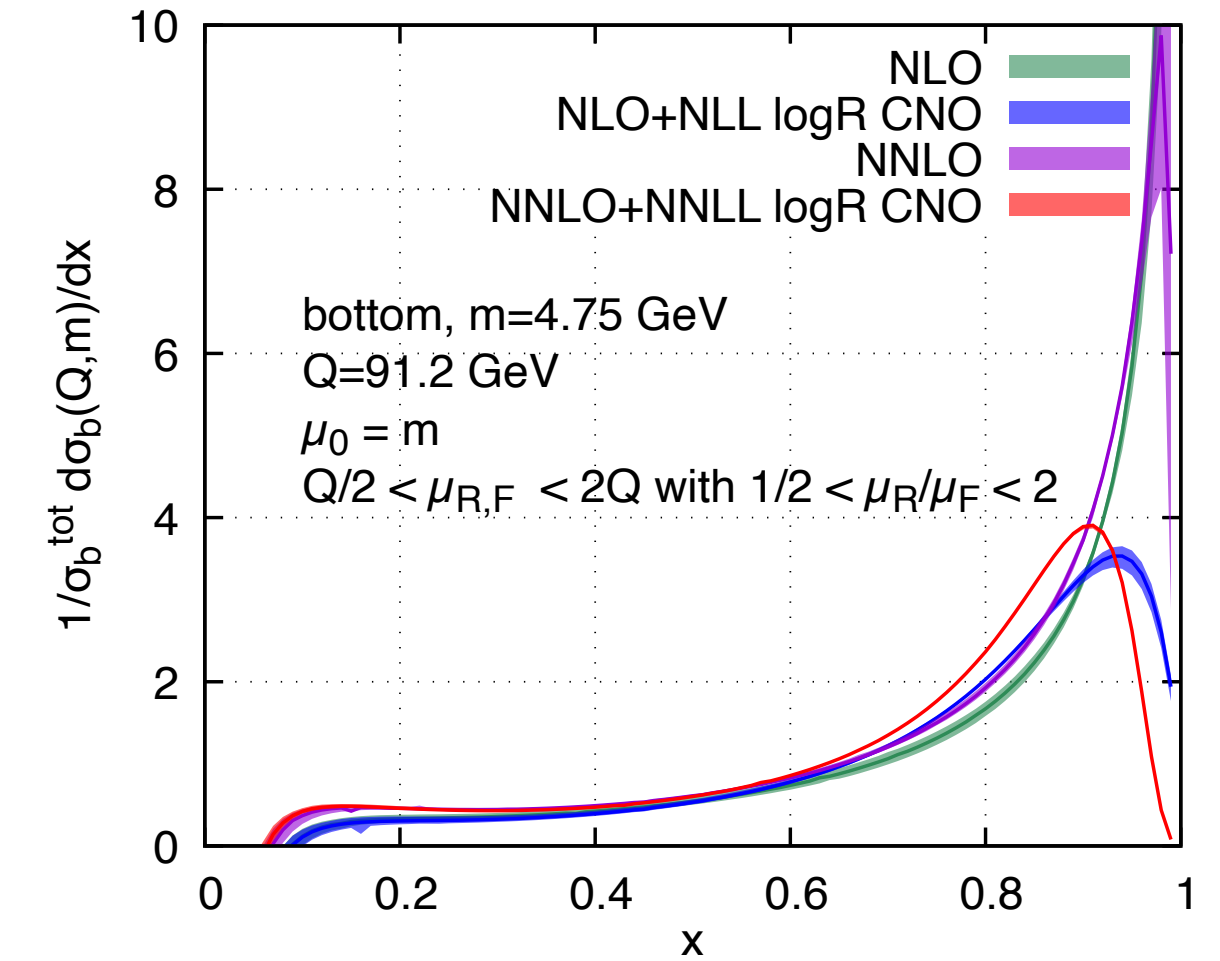
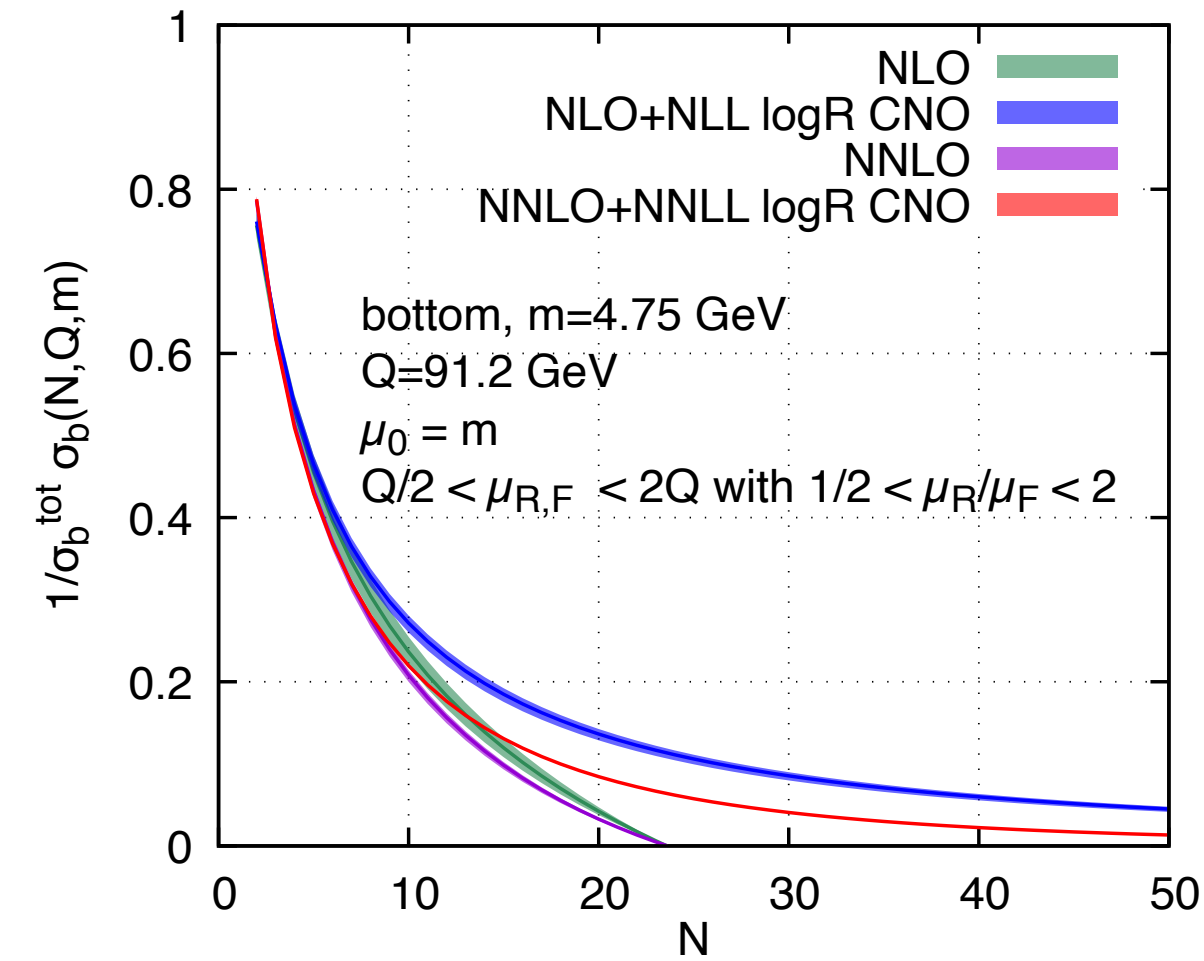


# Backup: numerical results

Bottom

## Full $e^+e^-$ fragmentation function

- Perturbative hierarchy **better** respected for  $\mu_R$  and  $\mu_F$  variations around  $Q$



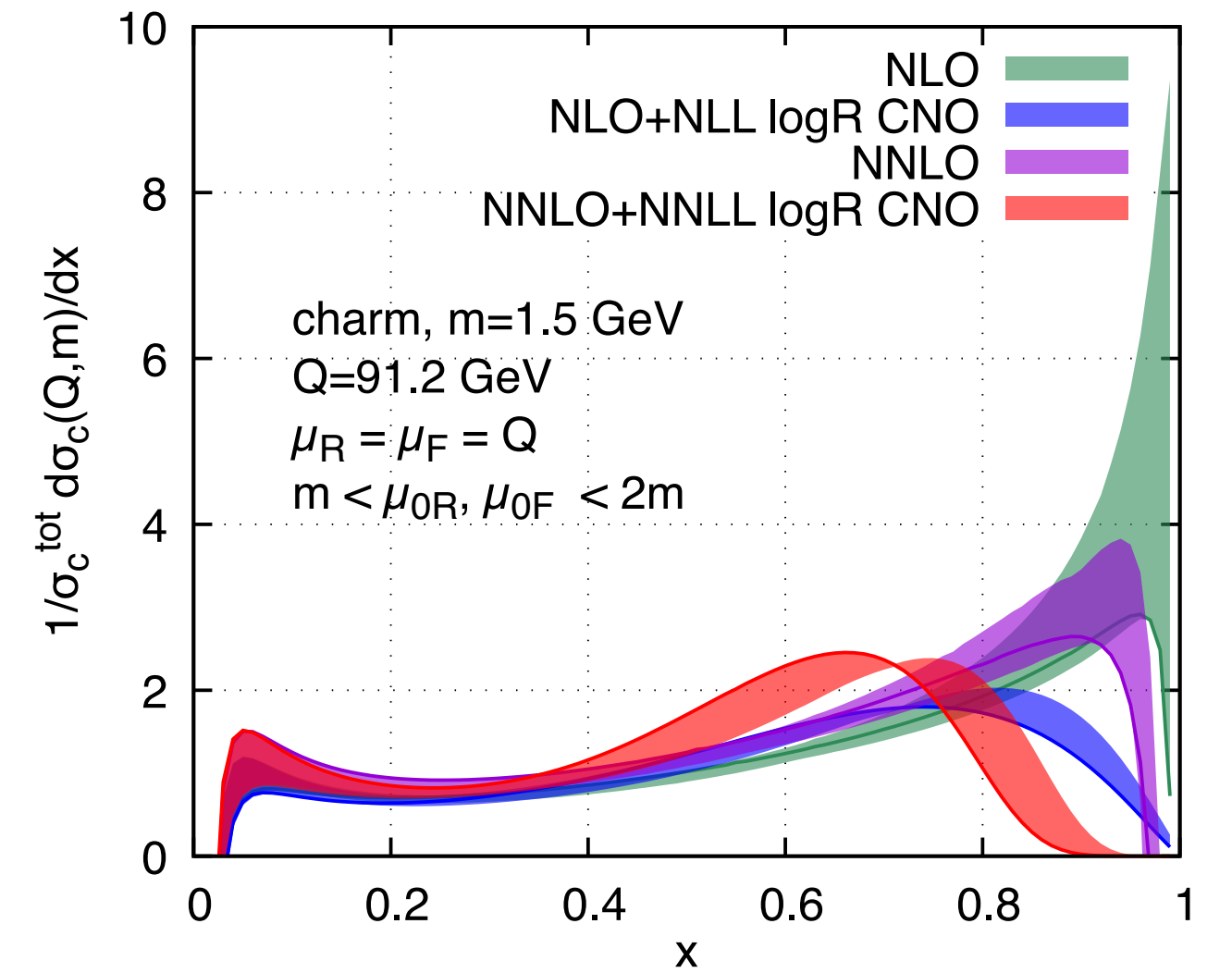
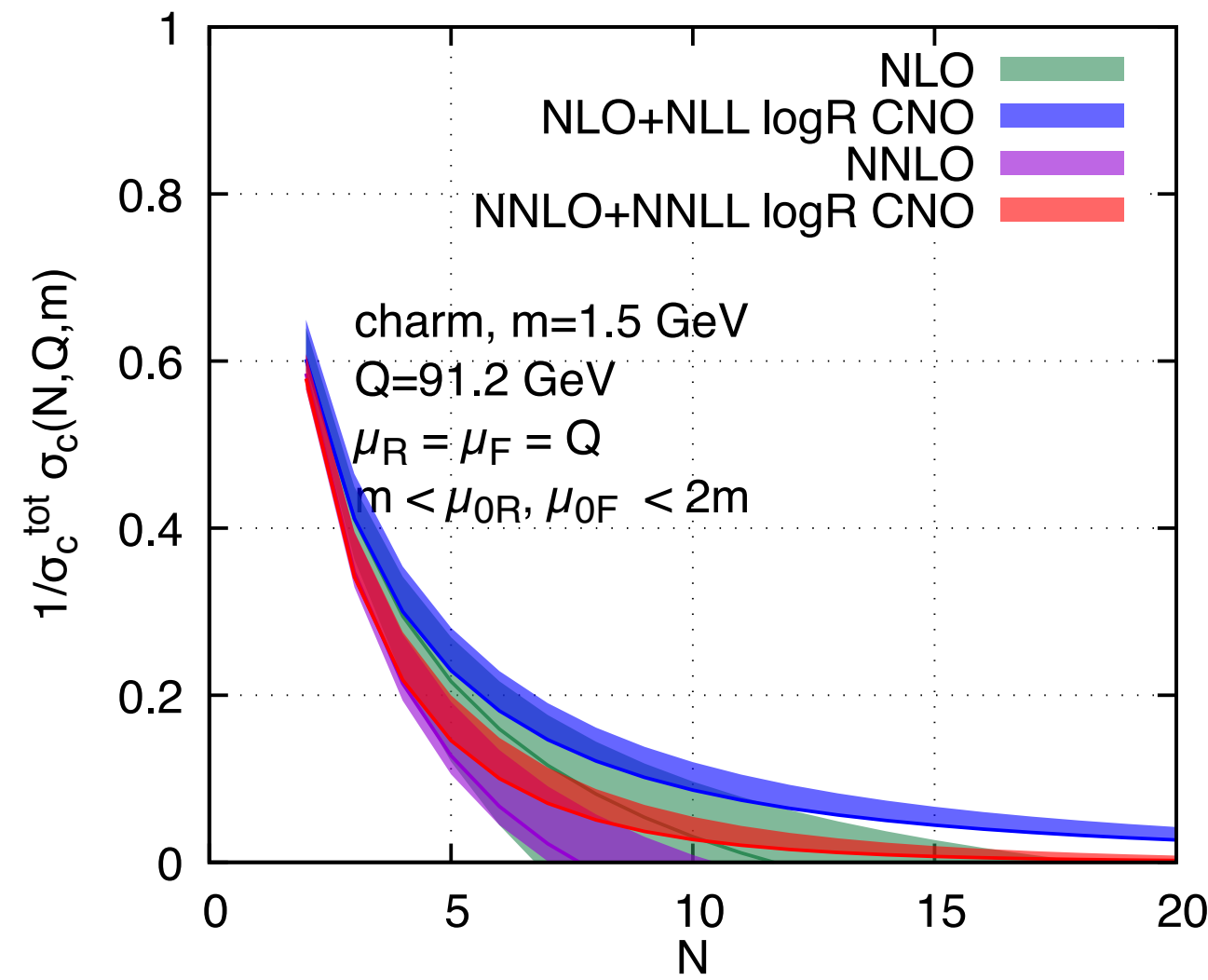


# Numerical results

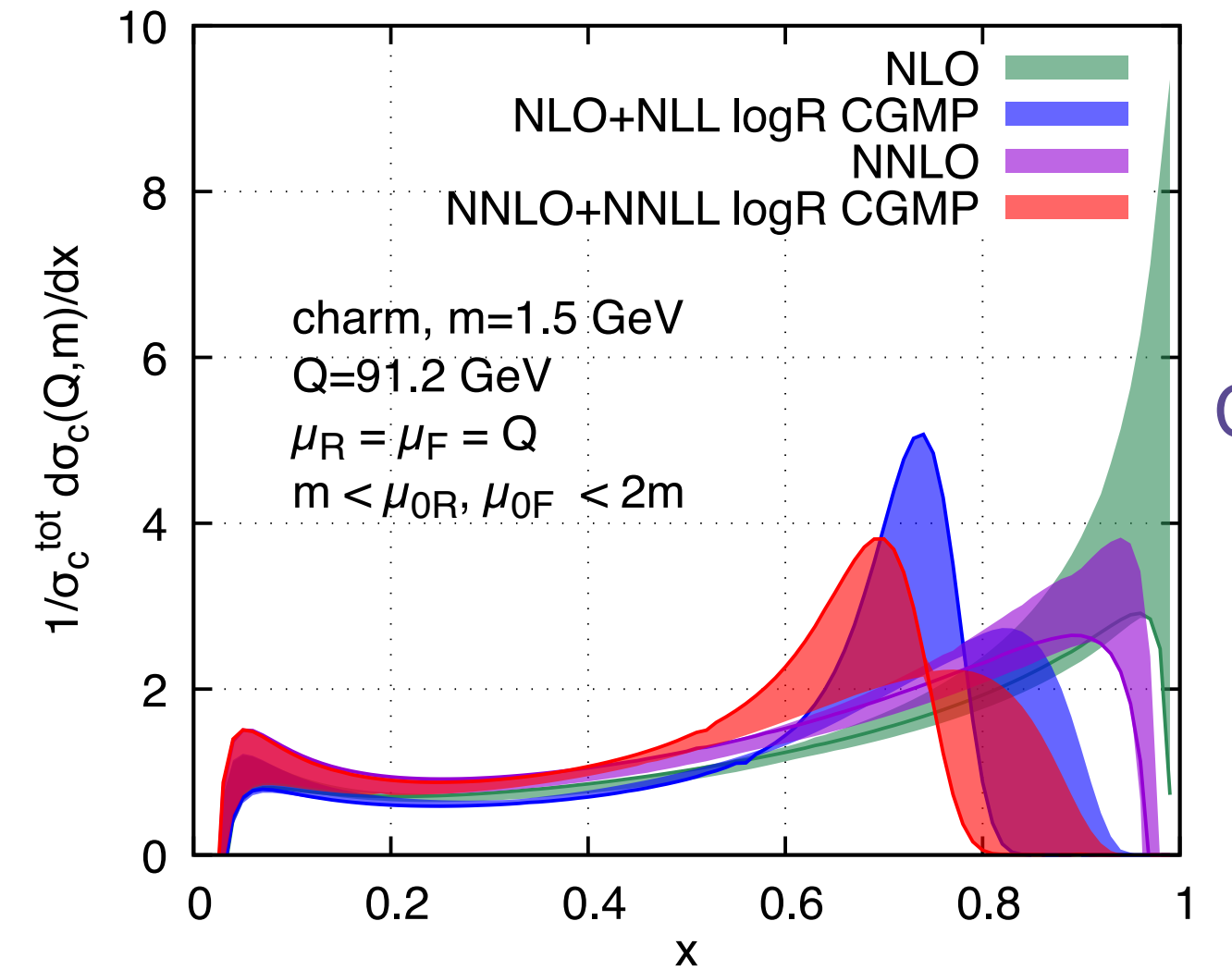
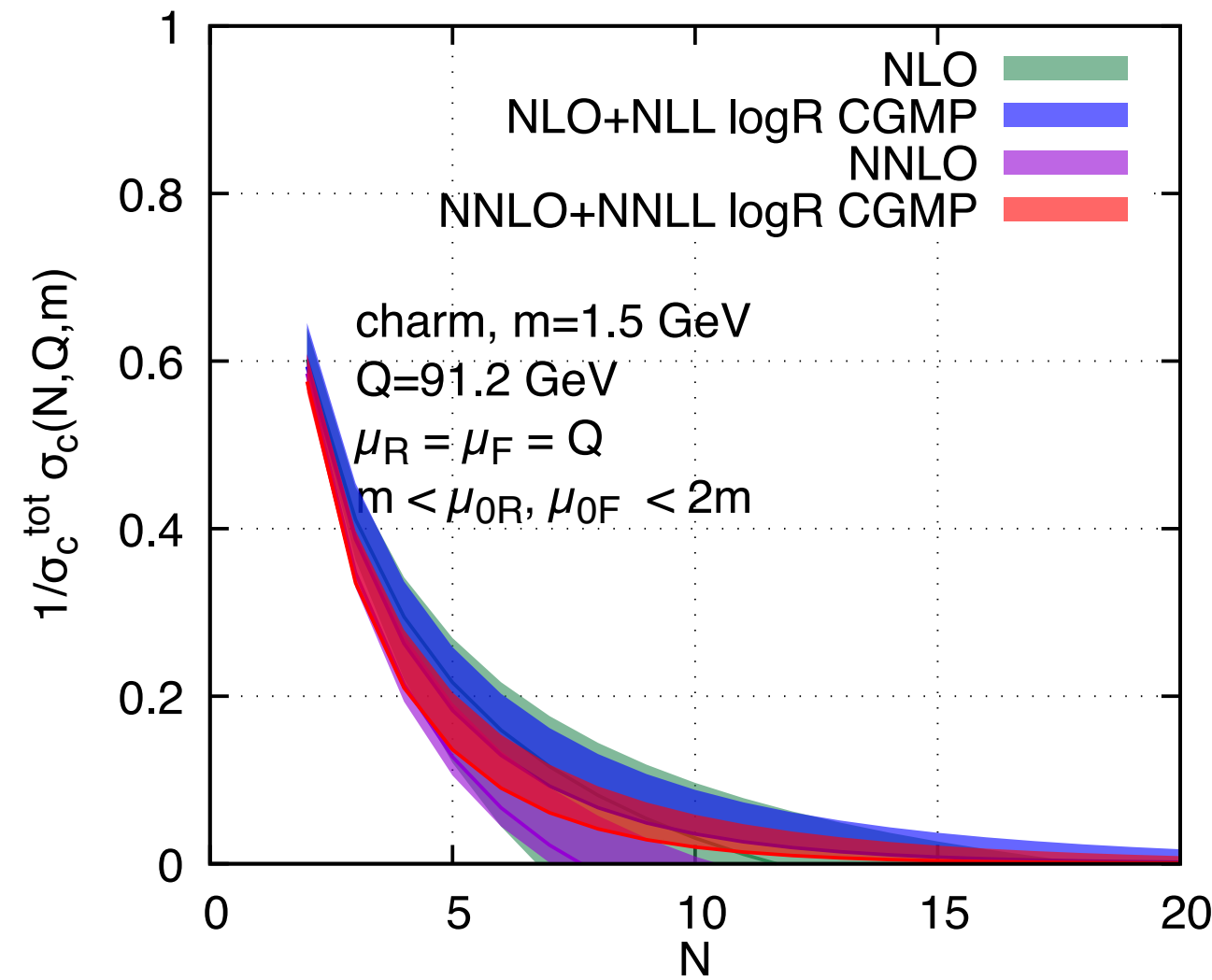
## Full $e^+e^-$ fragmentation function

- Scale variation around  $m$ 
  - Wider bands than bottom case
  - Any perturbative hierarchy essentially lost
- Larger sensitivity to Landau pole regularisation than bottom
- Can we still compare with the data?

Charm



CNO



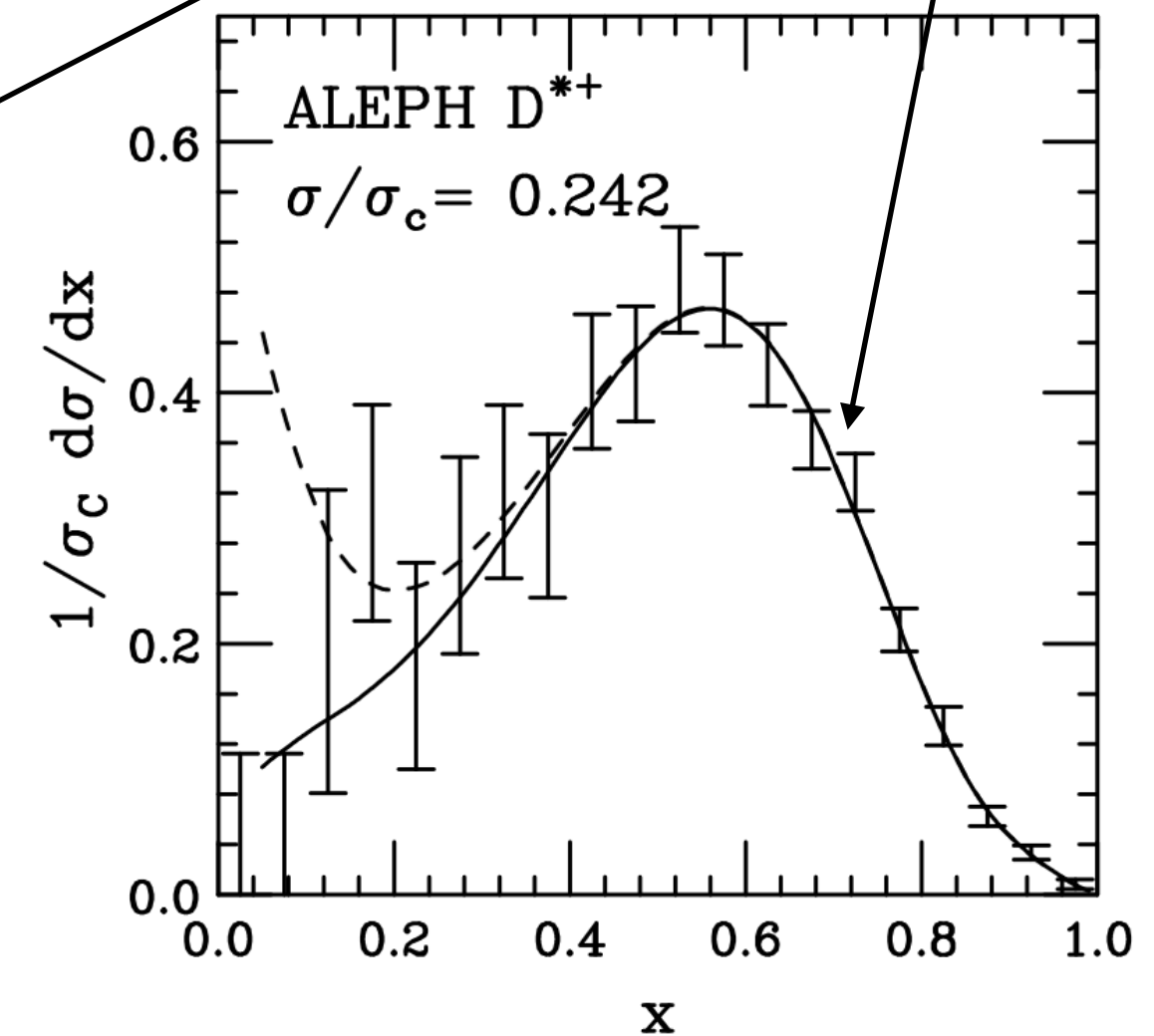
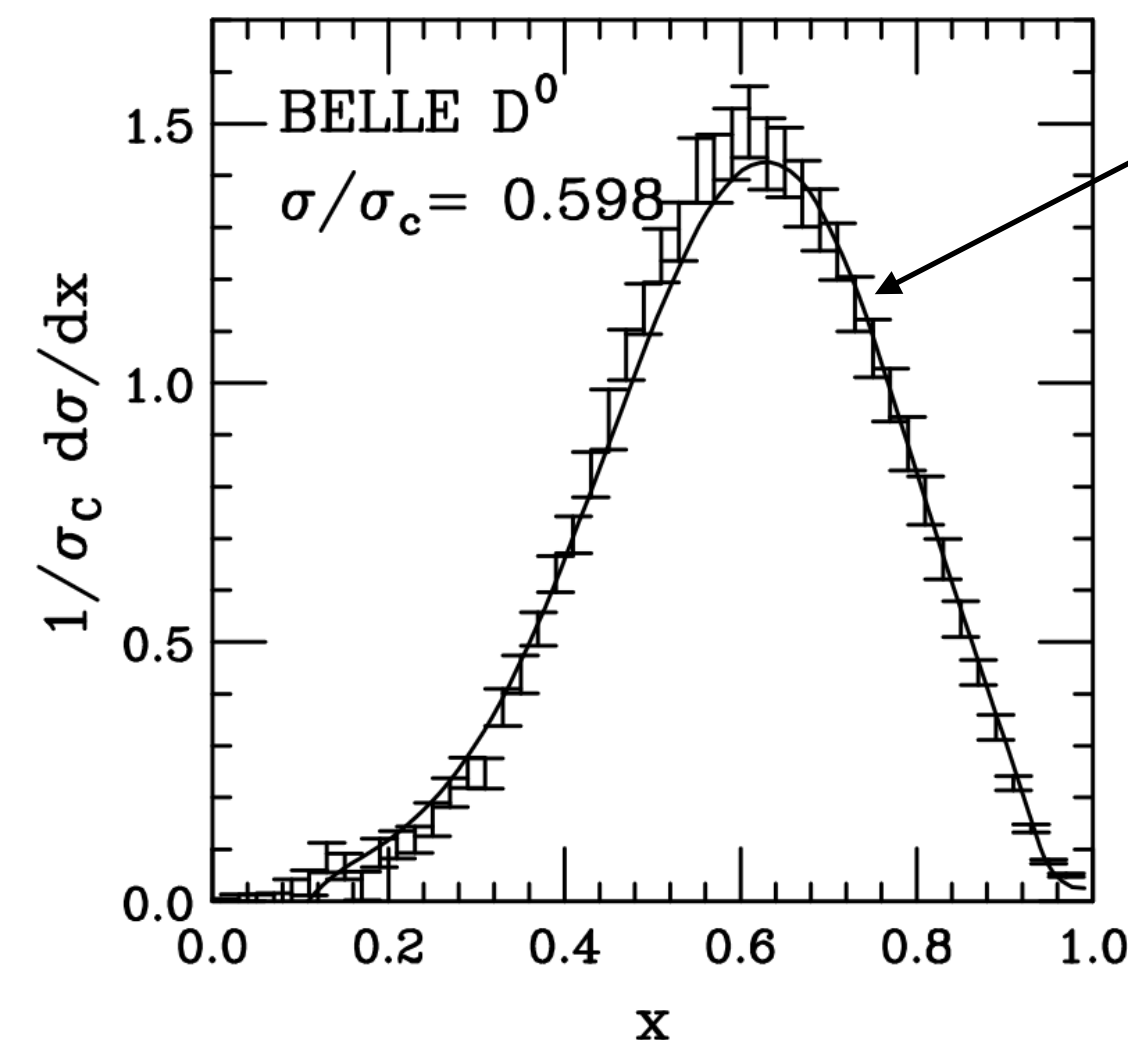
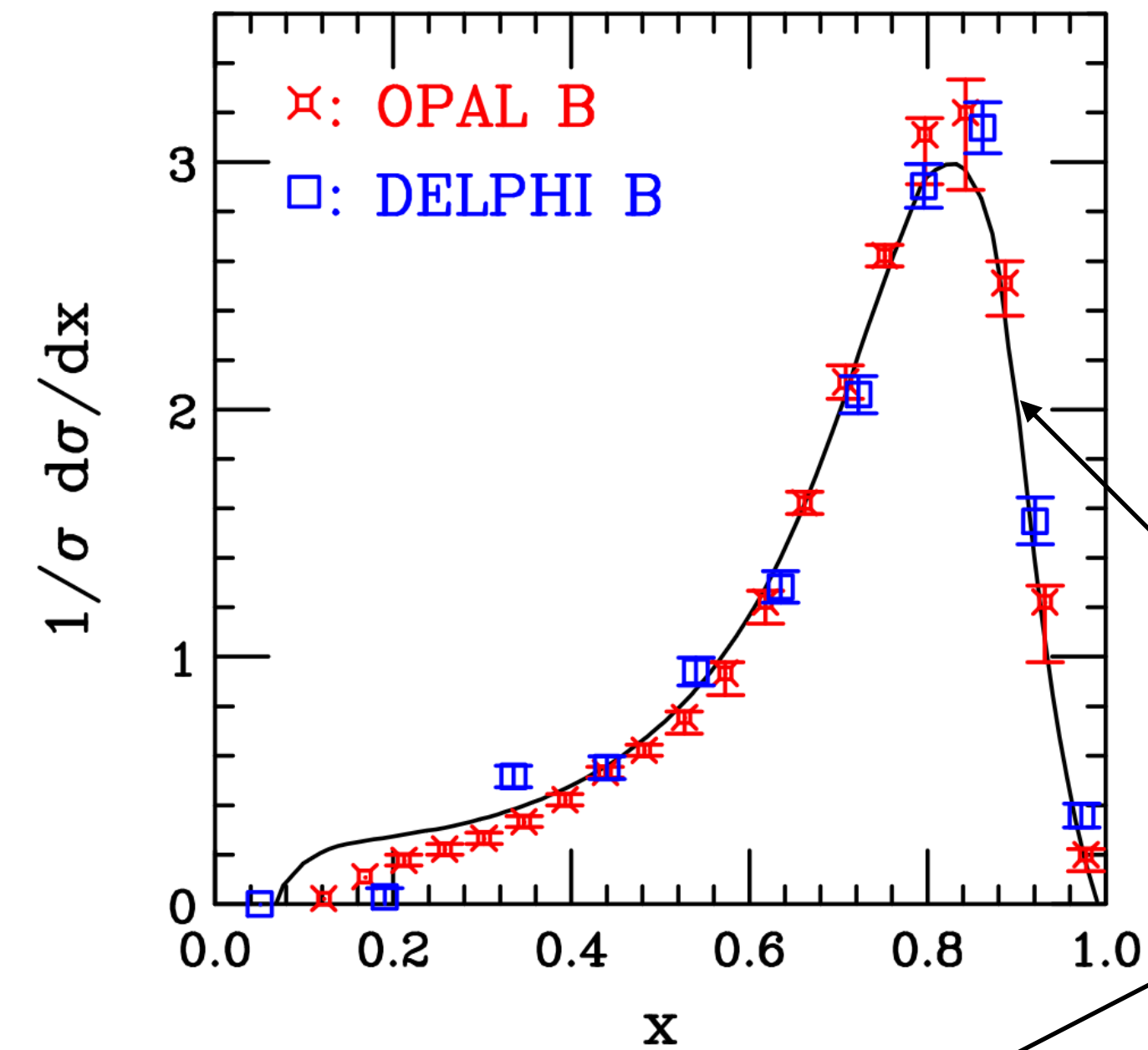
CGMP

# Backup: the data

## At $e^+e^-$ colliders

- Compare with the data, what do we have?
- Many data comprising bottom and charm
- $B$  mesons @ 91.2 GeV ( $Z^0$ -peak):
  - ALEPH (mesons) [ALEPH\_0106051], SLD [SLD\_0202031], OPAL [OPAL\_0210031], DELPHI (some baryons as well) [DELPHI\_002-069 CONF 603]
- $D$  mesons, 2 energies:
  - ALEPH @ 91.2 GeV [ALEPH\_9909032], BELLE [Belle\_0506068], CLEO @ 10.6 GeV (ISR-corrected) [CLEO\_0402040] [CLEO\_9707018]

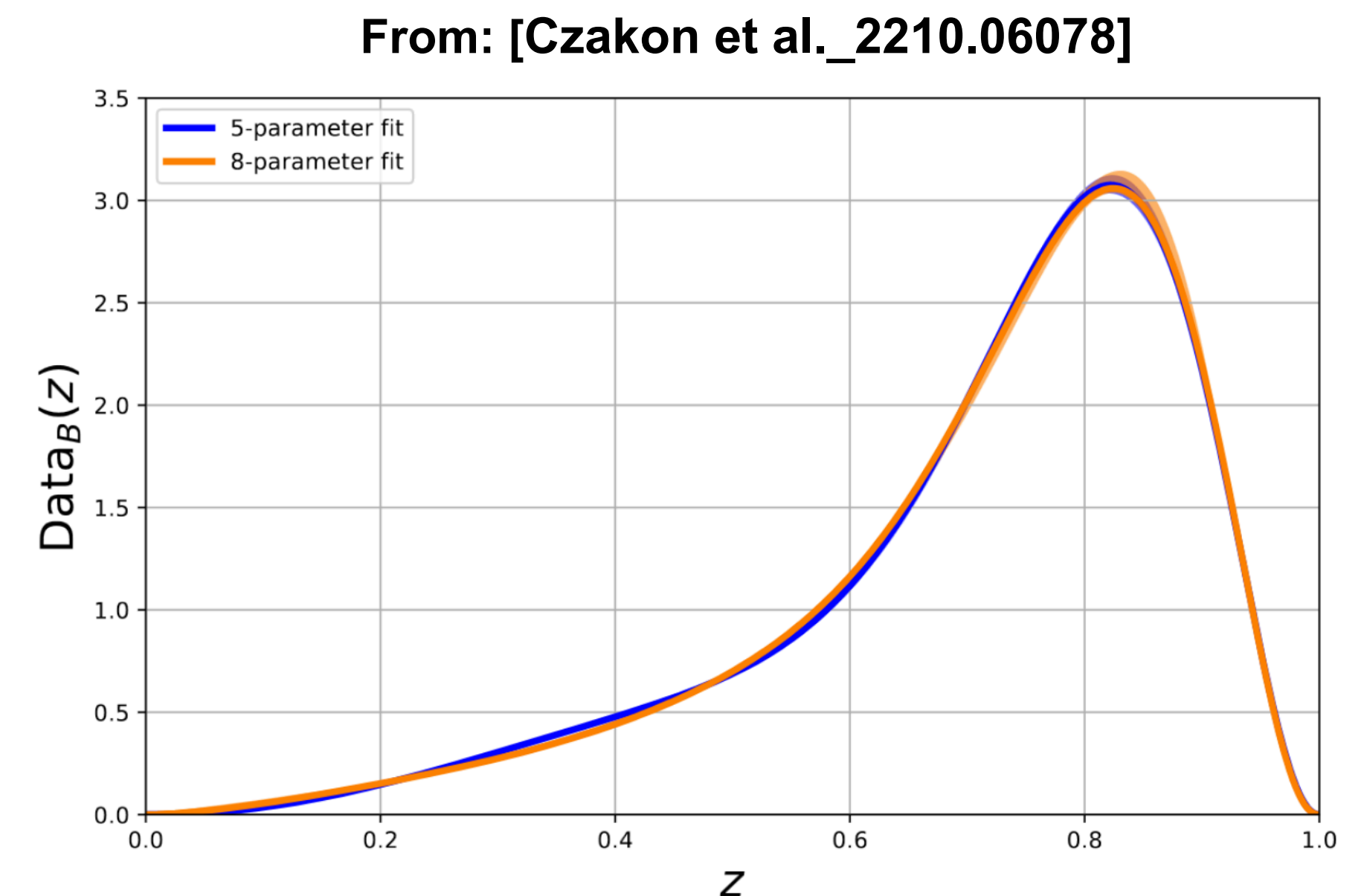
From: [Cacciari et al.\_0510032]



# Backup:state of the art for fits

## New results on bottom fragmentation

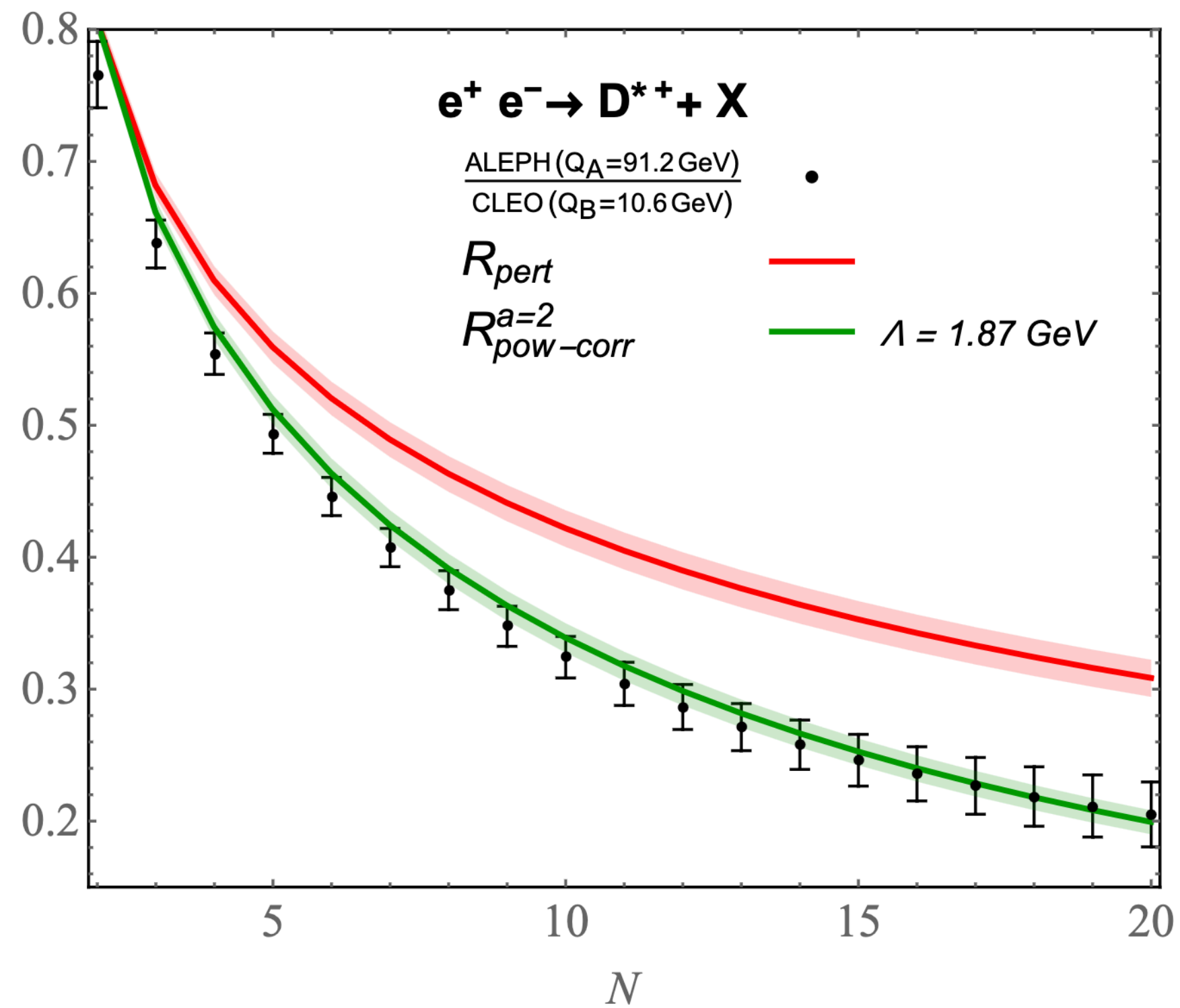
- Cacciari-Nason-Oleari 2005 → bottom & charm fits @ NLO + NLL
  - Good fits to  $D$  and  $B$  mesons fragmentation spectra
- Aglietti-Corcella-Ferrera 2007 → bottom & charm @ NLO + NNLL
  - Effective  $\alpha_S$ : call for full NNLO analysis [Aglietti et. al\_0610035] [Corcella, Ferrera\_0706.2357]
- Czakon-Generet-Mitov-Poncelet 2022 → bottom @ NNLO + NNLL
  - Fits to  $D^{np}$  with 5-8 parameters
- Our contribution:
  - Charm @ NNLO + NNLL through  $b$ -threshold → fits to charm
  - Public code!



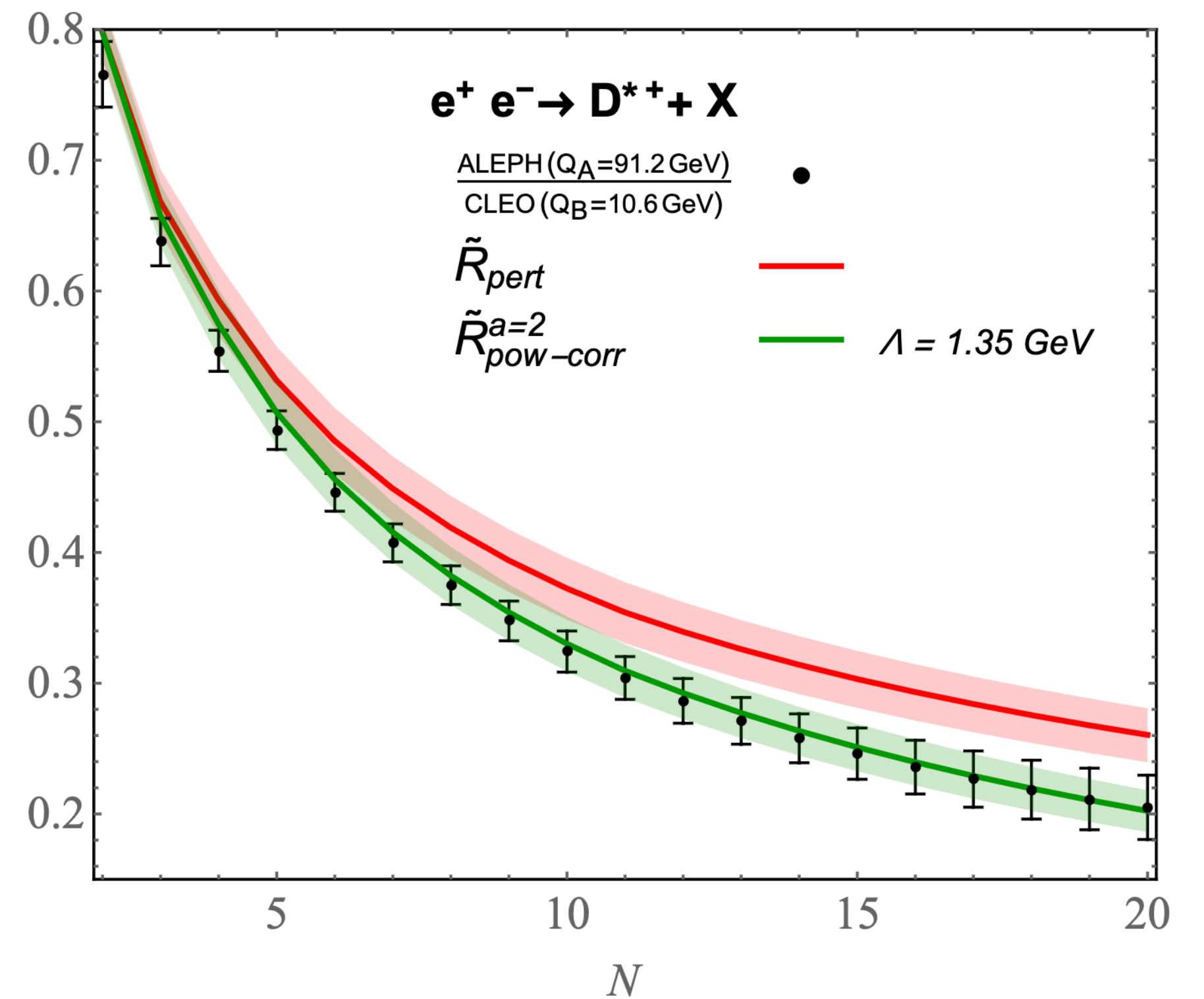
# Improved charm ratio

## Power corrections and/or mass effects

NNLO+NNLL



K-factor at NLL



$$R_{pow-corr}^a = R_{per} \times \frac{1 + \frac{\Lambda^a}{Q_A^a} \mathcal{C}(N)}{1 + \frac{\Lambda^a}{Q_B^a} \mathcal{C}(N)}, \quad a = 2, \quad \mathcal{C}(N) = N - 1$$

$$\tilde{R}_{pert} = R_{pert} \times K_{th}$$

# Matching conditions at NNLO

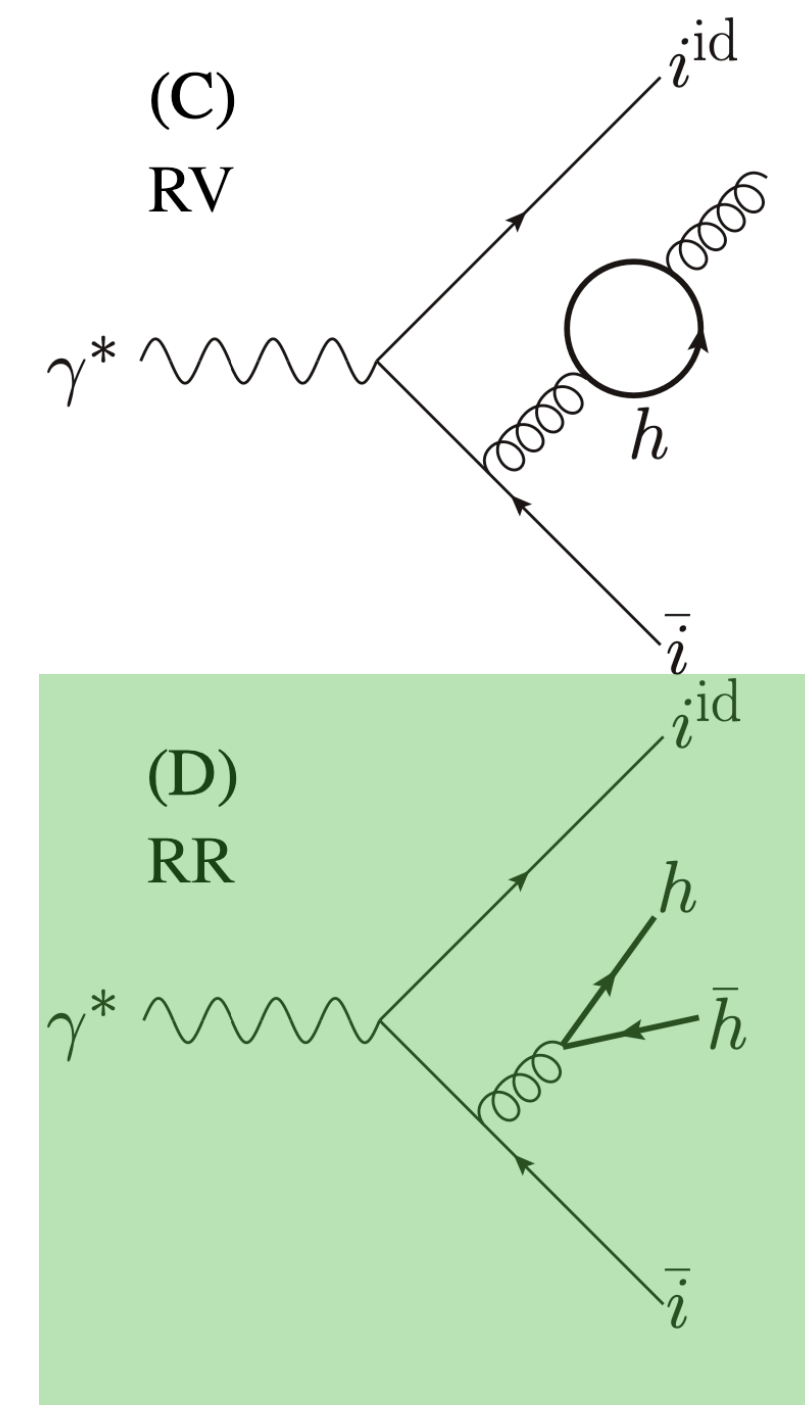
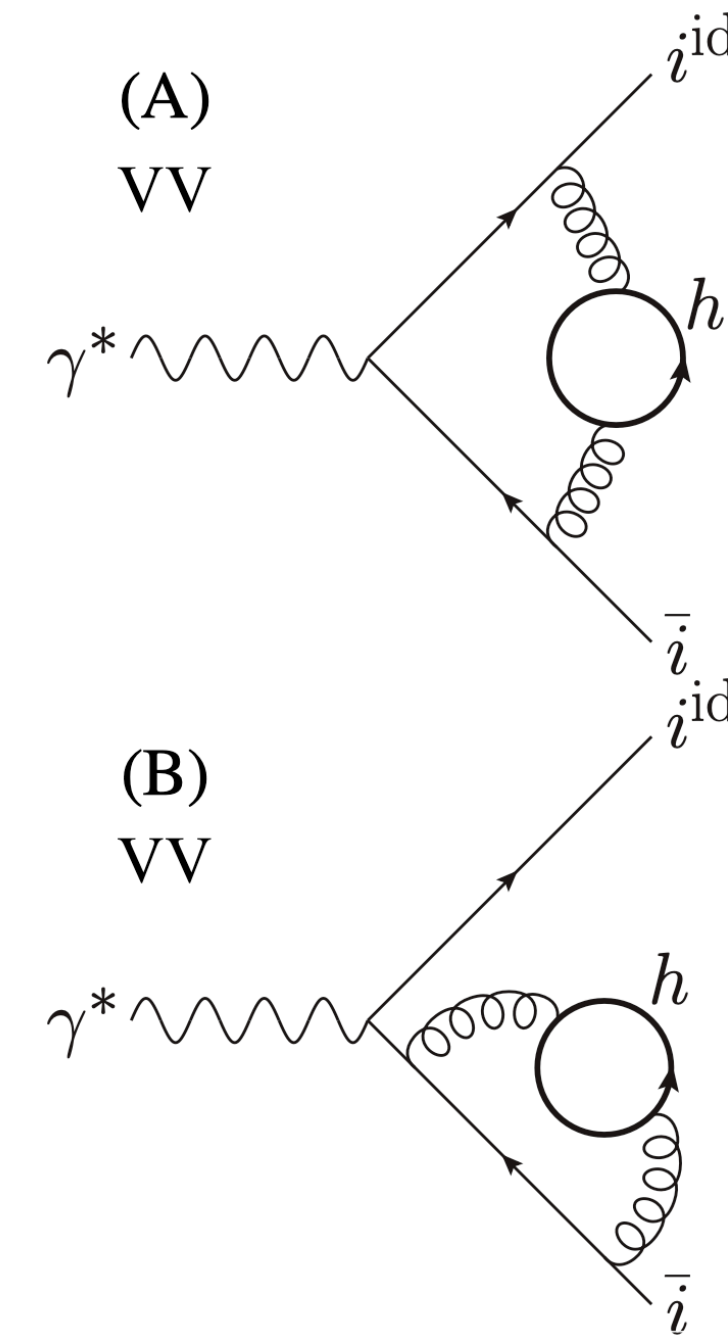
## The light flavour matching condition

- NNLO matching conditions for **light flavour** (Mellin space)

$$D_i^{(n)}(N, \mu) = \left\{ 1 + \frac{1}{\sigma_{i\bar{i}}} \mathcal{M}_{(N,z)} \left[ \delta_{D_i}^i(z) \right] \right\} D_i^{(n_L)}(N, \mu)$$

- Takes **RR** [Gehrmann Stagnitto '22] [Bonino et al. '24] **RV** and **VV** [Blümlein et al. '16] **massive** and

massless corrections  $\delta_{D_i}^i := \frac{d\sigma_{h\bar{h}i^{\text{id}}\bar{i}}^{Q_i}}{dz} - \frac{d\hat{\sigma}_{h\bar{h}i^{\text{id}}\bar{i}}^{Q_i}}{dz} + \frac{d\sigma_{i,f}}{dz} - \frac{d\hat{\sigma}_{i,f}}{dz} + \delta_{\alpha_s}$



$$\begin{aligned} \bar{\mathcal{B}}_{ih\bar{i}}^{0,\text{id},i}(z) = & \frac{1}{216(z-1)} \left[ -18(z^2+1) \log^2 \frac{m^2}{Q^2} + 6(-13z^2 + 6(z^2+1) \log(1-z) + 6(z^2+1) \log(z) - 16) \log \frac{m^2}{Q^2} \right. \\ & + 36(z^2+1) \text{Li}_2 \left( \frac{z-1}{z} \right) + 6\pi^2(z^2+1) - 18(z^2+1) \log^2(1-z) + 6 \log(1-z) (13z^2 - 6(z^2+1) \log(z) + 16) \\ & \left. - z(115z+72) + 12(z(8z+3) + 8) \log(z) - 172 \right] + \mathcal{O} \left( \frac{m}{Q} \right). \end{aligned} \quad (\text{C.25})$$