High Precision for Hard Processes
Turin, 10/9-13/9 2024

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

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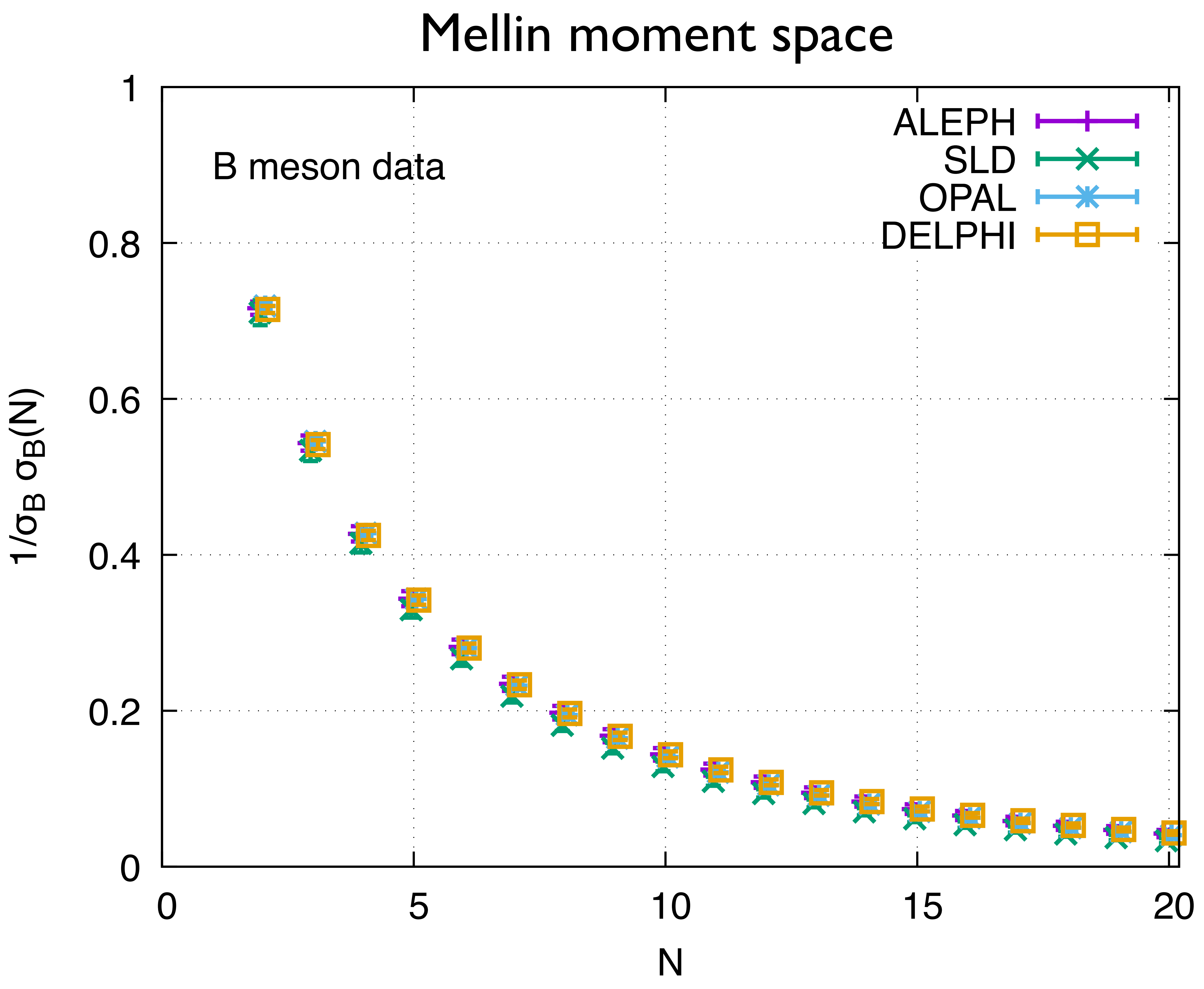
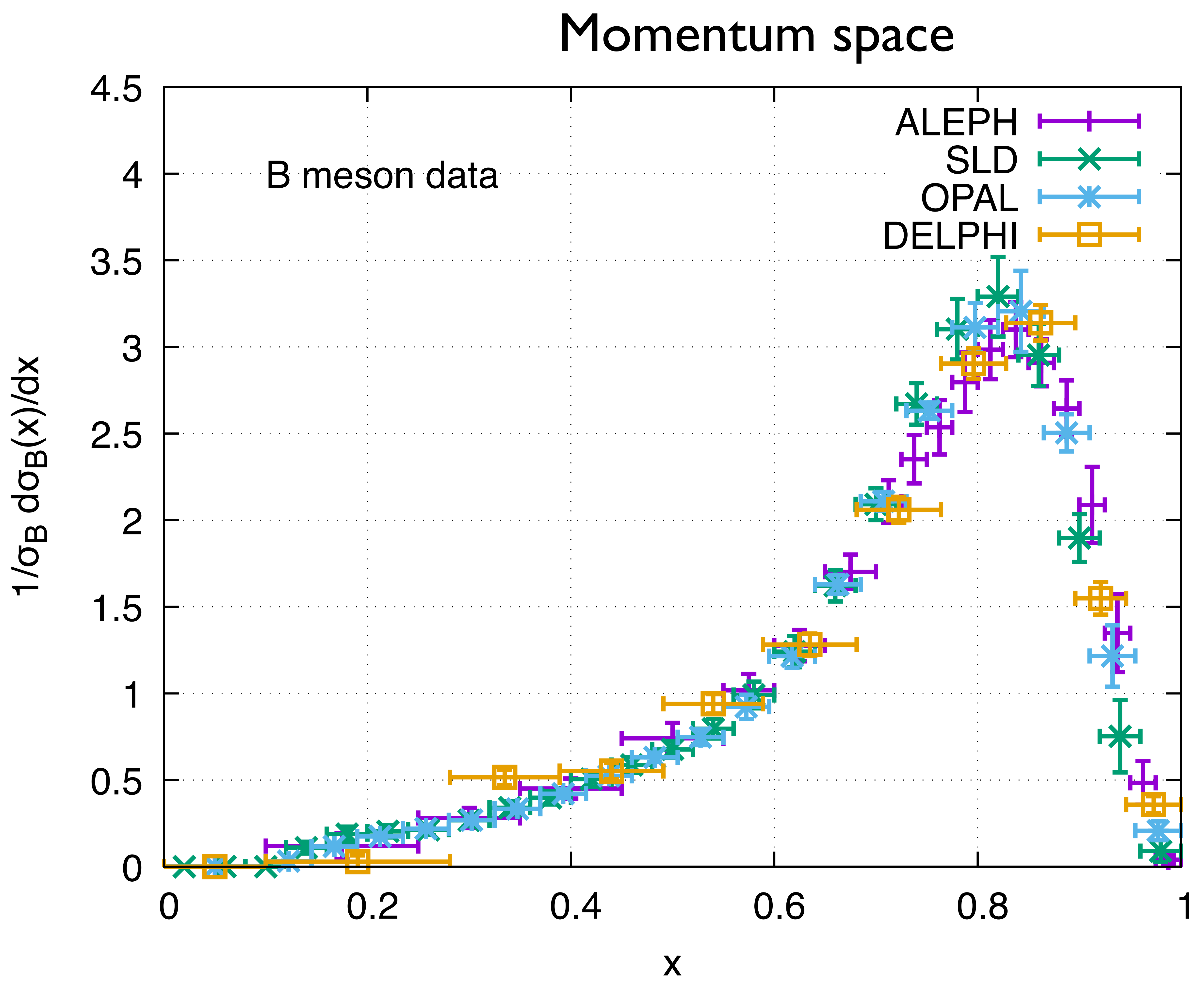
with Leonardo Bonino and Giovanni Stagnitto

LEP and SLC data





Approximate relation : 1-x ~ 1/N

The problem

Hard interaction at some large scale,
observation of a heavy hadron with a given momentum

Multiple scales : at least the **large scale Q**, the **heavy quark mass m**, the momentum of the heavy hadron (which can constrain the **energy of emitted gluons**), the **non-perturbative scale Λ** of the hadronisation of the heavy quark into the heavy hadron

Problem addressed multiple times, using multiple languages:
phenomenological models, pQCD, renormalons, effective coupling, HQET, SCET, bHQET,…

e+e- to heavy quark fragmentation

Heavy quark discovery

Bjorken
Suzuki

Peterson, Schlatter, Schmitt and Zerwas

Dokshitzer, Khoze, Troyan

Jaffe, Randall

Mele, Nason

Rijken, van Neerven

MC, Nason, Oleari

Melnikov, Mitov

MC, Gardi

MC, Catani

Aglietti, Corcella, Ferrera

Corcella, Ferrera

Mitov, Moch
Blümlein, Ravindran

Neubert

Gardi

Flickinger, Fleming, Kim, Mereghetti

Czakon, Generet, Mitov, Poncelet

Ridolfi, Ubiali, Zaro

Maltoni, Ridolfi, Ubiali, Zaro

Bonino, MC, Stagnitto

1974 1977 1982 1991 1993 1995 1996 2001 2003 2004 2005 2006 2007 2016 2019 2022 2023 2024

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Bjorken and Suzuki, 1977

involving the same produced partons (with the same momenta), but not involving a cascade decay. (ii) For neutrino production, electroproduction, and e^+e^- annihilation, at energies far above threshold, the inclusive momentum distribution of a stable hadron H containing the Q peaks near the maximum momentum, i.e., at values of the scaling variable $z \sim 1$. (iii) For events containing a nonleptonic decay of Q into ordinary quarks

Bjorken

A model is presented to describe hadron fragmentation off light and heavy partons. Fragmentation functions are parametrized by onc variable. When a heavy parton of a new flavour fragments, a heavy hadron tends to carry away most of the parton momentum, leaving light hadron (π and K) spectra softer than those from light partons.

Suzuki

A heavy quark to heavy hadron
fragmentation function f(z) will be peaked near z=1:

$$\langle z \rangle \simeq 1 - \frac{1\ GeV}{m}$$

e+e- to heavy quark fragmentation

Heavy quark discovery

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Bonino, MC, Stagnitto

1974 1977 1982 1991 1993 1995 1996 2001 2003 2004 2005 2006 2007 2016 2019 2022 2023 2024

Mele, Nason, 1991

Nuclear Physics B361 (1991) 626–644
North-Holland

THE FRAGMENTATION FUNCTION FOR HEAVY QUARKS IN QCD

B. MELE

CERN, Geneva, Switzerland

P. NASON

INFN, Gruppo Collegato di Parma, Parma, Italy

Received 13 February 1991
(Revised 26 March 1991)

An erratum in 2017, almost 30 years later

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Nuclear Physics B 921 (2017) 841–842
www.elsevier.com/locate/nuclphysb

Corrigendum

Corrigendum to "The fragmentation function for heavy quarks in QCD" [Nucl. Phys. B 361 (1991) 626–644]

B. Mele [a,*], P. Nason [b]

[a] *INFN, Sezione di Roma, Rome, Italy*
[b] *INFN, Sezione di Milano Bicocca, Milan, Italy*

Received 11 May 2017; accepted 11 May 2017
Available online 24 May 2017

(no worry, just some typos)

Mele, Nason, 1991

Mele-Nason systematise **perturbative QCD evolution** of the e+e- fragmentation function to full next-to-leading accuracy, and also resum soft logarithms with leading accuracy

More importantly, they introduce the concept of a **universal and perturbatively calculable "initial condition"**:

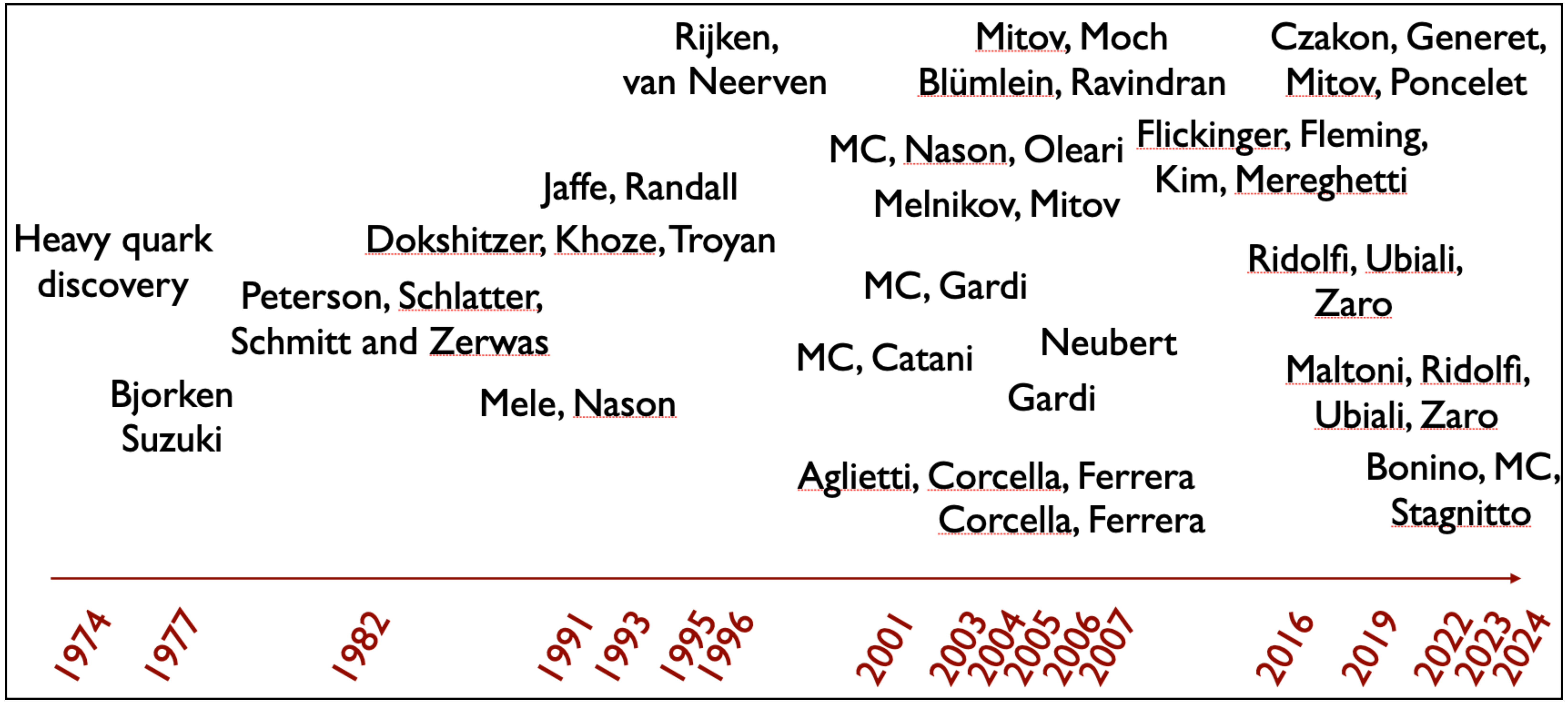
$$\sigma_N(Q) = \hat{\sigma}_N(Q,\mu)\exp\left\{P_N^{(0)}t + \frac{1}{4\pi^2 b_0}\left(\alpha_S(\mu_0) - \alpha_S(\mu)\right)\left(P_N^{(1)} - \frac{2\pi b_1}{b_0}P_N^{(0)}\right)\right\}\underline{\hat{D}_N^{[1]}(\mu_0,m)}$$

Perturbatively calculable
initial condition
(or fragmentation function) : pFF

$$\hat{D}^{[1]}(x,\mu,m) = \delta(1-x) + \frac{\alpha_S C_F}{2\pi}\left[\frac{1+x^2}{1-x}\left(\log\frac{\mu^2}{m^2} - 2\log(1-x) - 1\right)\right]_+$$

Overall accuracy: NLO + NLL_{coll} + LL_{soft}

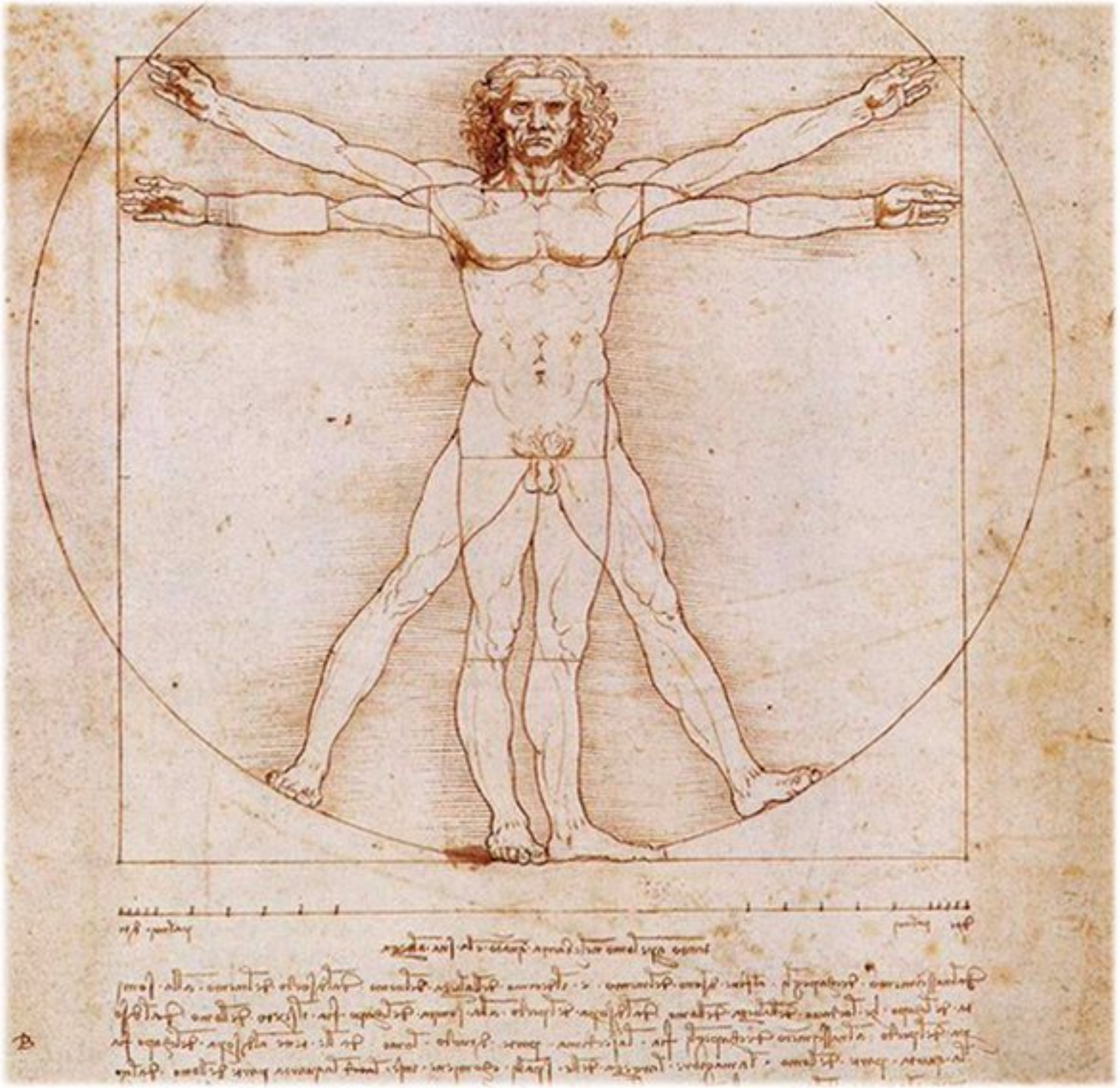
e+e- to heavy quark fragmentation

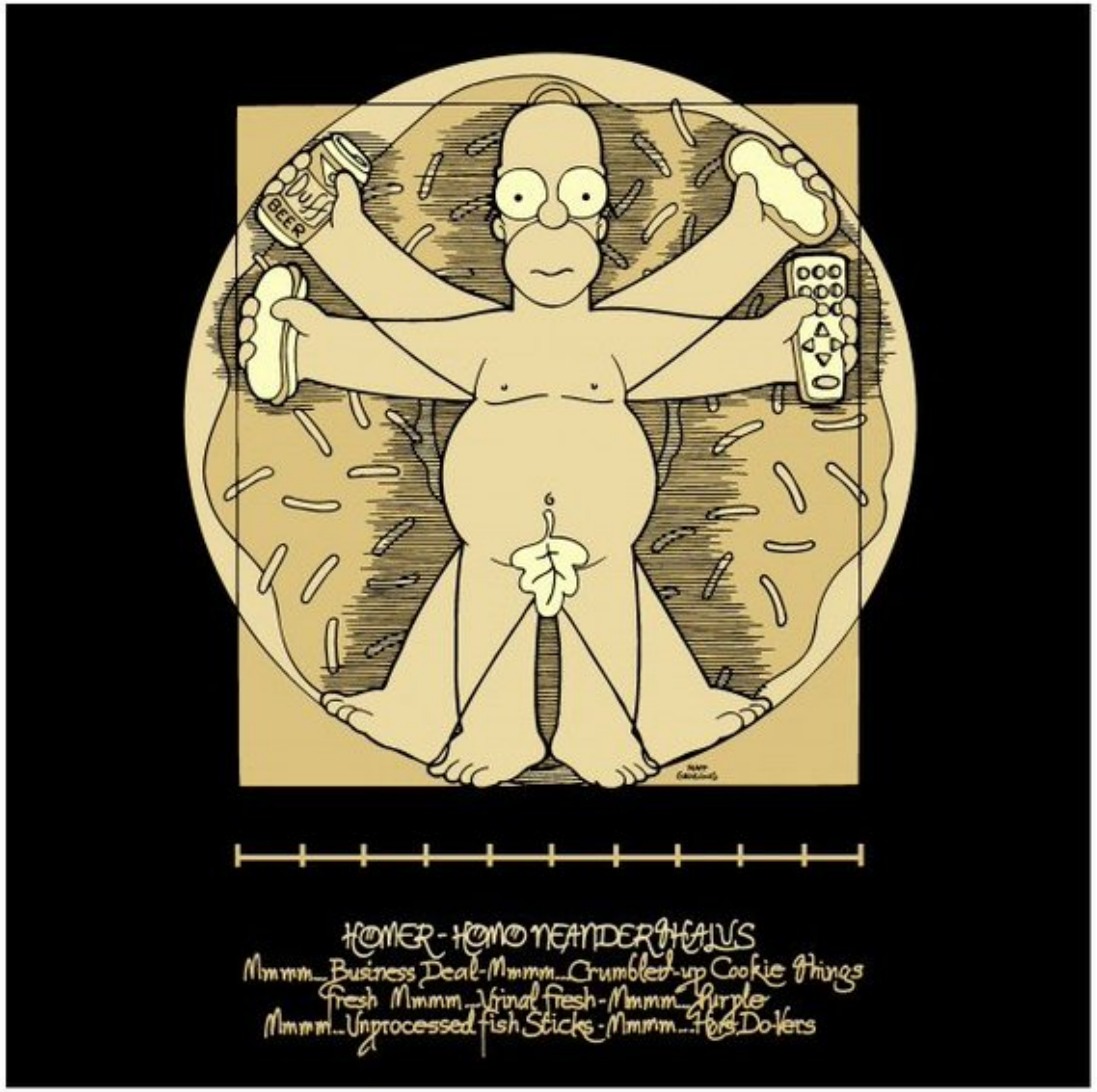


Thanks to these and many other papers, we can now try pushing the overall accuracy to **N**NLO + **N**NLL$_{coll}$ + **NN**LL$_{soft}$

What kind of precision do we expect ?

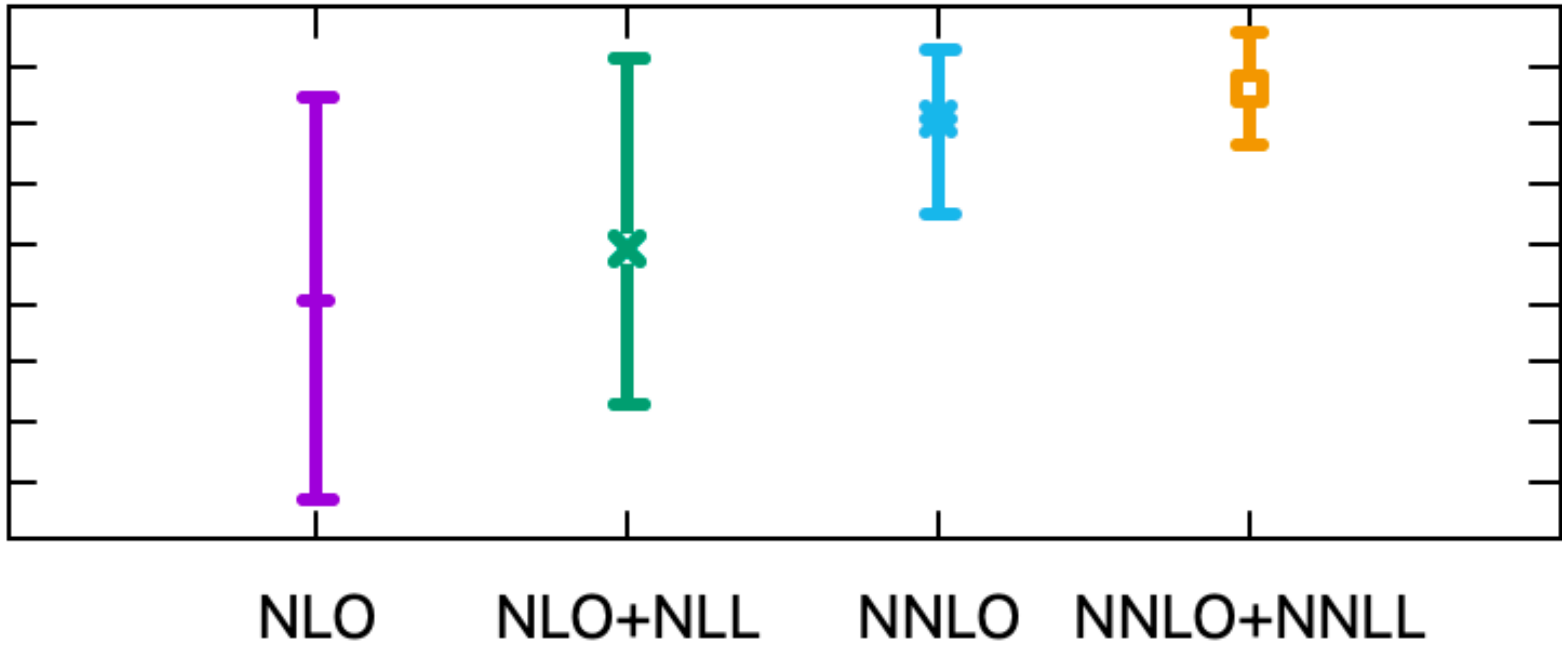
Expectation | Reality



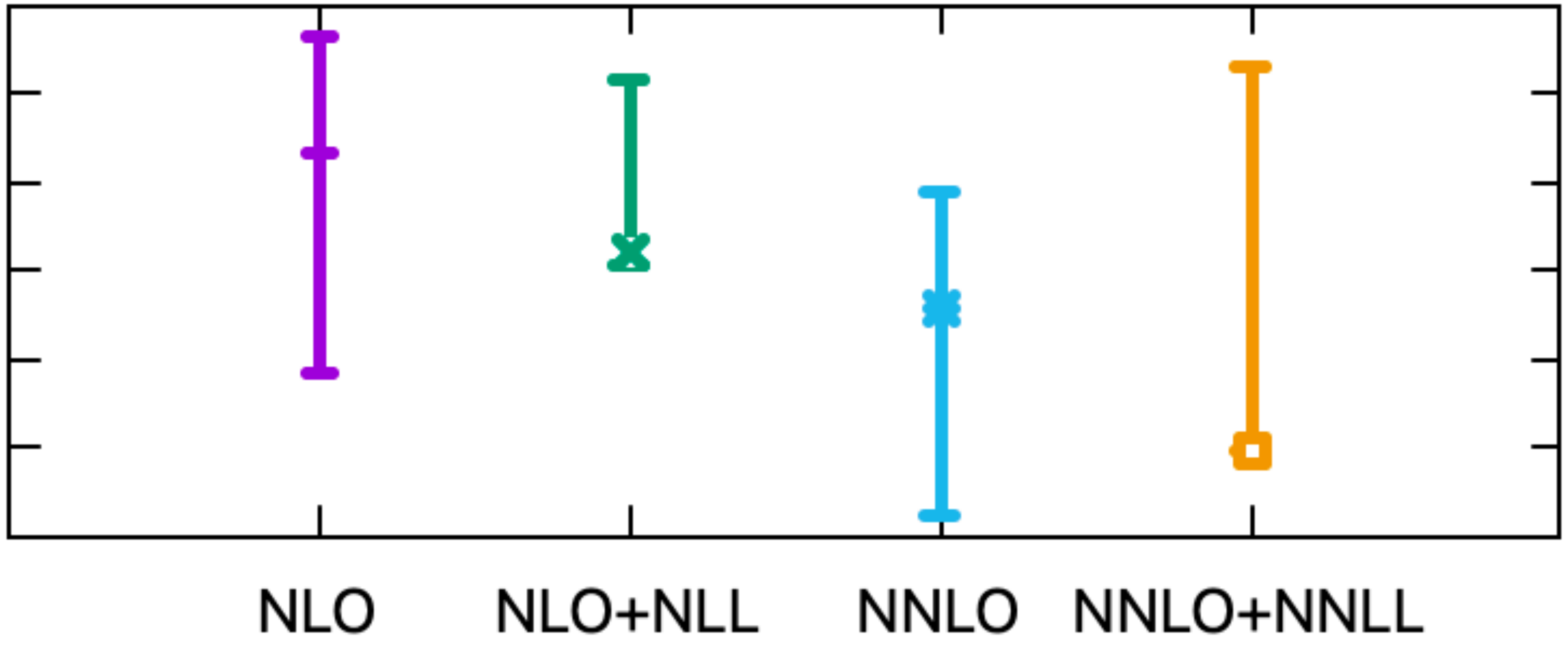


https://x.com/biosystkuleuven/status/1103313156674330624

Expectation



Reality



Putting it all together

Bonino, MC, Stagnitto, 2312.12519

$$e^+e^- \to \gamma, Z \to H_Q + X$$

- Up to NNLO coefficient function
- Up to NNLO initial condition (= decay function = pFF = FF = …)
- Up to NNLL collinear resummation
- Up to NNLL soft resummation → matching to fixed order
  - Landau pole regularisations
- Phenomenological non-perturbative fragmentation functions
- Modular and (eventually) public C++ library
  - Mellin moments and x-space results
  - Fits to experimental data

The cross section

$$\frac{d\sigma_H}{dx}(x,\sqrt{s}) \simeq \underline{\frac{d\sigma_Q}{dx}(x,\sqrt{s},m)} \otimes \underline{D^{np}_{Q\to H}(x,\{\text{params}\})}$$

Perturbative (with resummations)

Non-perturbative

Moments or x-space distribution

$$\sigma_Q(\sqrt{s},m) = \underline{\hat{\sigma}_i(\sqrt{s},\mu_F,\mu_R)} \otimes \underline{E_{ij}(\mu_F,\mu_{F0})} \otimes \underline{D_{j\to Q}(m,\mu_{F0},\mu_{R0})}$$

Coefficient functions

DGLAP evolution (MELA)

Initial conditions (Decay functions) (Fragmentation functions)

Thanks to Moch, De Florian, Maltoni, Ridolfi, Ubiali, Zaro, for providing Fortran implementations of the NNLO coefficient functions and initial conditions

Labeling

The components of σ_Q, the **coefficient functions** $\hat{\sigma}_i$ and the **initial conditions** $D_{j\to Q}$, are calculated to a given **perturbative order**, with or without **soft resummation matched** to the fixed order, with or without **Landau pole regularisation**

$$\sigma_Q^{fo+res,match,reg}(\cdot, \sqrt{s}, \mu_R, \mu_F, \mu_{0R}, \mu_{0F}, m)$$

The final result also has residual factorisation and renormalisation scale dependence

Additive

$$D_{i\to Q}^{fo+res\,\boxed{\mathrm{add}}\,reg} = D_{i\to Q}^{fo} + D_{i\to Q}^{res,reg} - [D_{i\to Q}^{res(,reg)}]_{\alpha_s^p}$$

log-R

$$\log D_{i\to Q}^{fo+res\,\boxed{\mathrm{logR}}\,reg} = \log D_{i\to Q}^{fo} + \log D_{i\to Q}^{res,reg} - [\log D_{i\to Q}^{res(,reg)}]_{\alpha_s^p}$$

Landau pole

Moments of soft-resummed coefficient functions and initial conditions have poles respectively at

$$N^L = \exp\left(\frac{1}{b_0 \alpha_s(\mu^2)}\right) \qquad \text{and} \qquad N_0^L = \exp\left(\frac{1}{2b_0 \alpha_s(\mu_0^2)}\right)$$

~ 7 for charm
~ 30 for bottom

- Signal of onset of non-perturbative physics
- Perturbative moments unphysical beyond the Landau poles
- x-space distributions (with Minimal Prescription) highly irregular near x=1

Landau pole regularisation

An ad hoc regularisation allows one to make the resummed moments better behaved, i.e. more physical-looking (though not necessarily more physical or "accurate")

CNO

MC, Oleari, Nason 05

$$N \to N \frac{1 + f/N_0^L}{1 + fN/N_0^L}$$

Rescale N so as to shift the pole to higher moments

$$D_{i\to Q}^{fo+res,match,\mathrm{CNO(f)}}$$

CGMP

Czakon, Generet, Mitov, Poncelet 23

$$\begin{aligned}
&\exp\left[\ln N g_0^{(1)}(\lambda_0) + g_0^{(2)}(\lambda_0) + \alpha_s g_0^{(3)}(\lambda_0)\right] \\
&\quad \simeq g_2^{(1)}\alpha_s \ln^2(N) + g_3^{(1)}\alpha_s^2 \ln^3(N) + g_4^{(1)}\alpha_s^3 \ln^4(N) + g_5^{(1)}\alpha_s^4 \ln^5(N) + g_6^{(1)}\alpha_s^5 \ln^6(N) \\
&\quad + g_1^{(2)}\alpha_s \ln(N) + g_2^{(2)}\alpha_s^2 \ln^2(N) + g_3^{(2)}\alpha_s^3 \ln^3(N) + g_4^{(2)}\alpha_s^4 \ln^4(N) \\
&\quad + g_1^{(3)}\alpha_s^2 \ln(N) + g_2^{(3)}\alpha_s^3 \ln^2(N)\,.
\end{aligned}$$

Expand and truncate the Sudakov exponential

$$D_{i\to Q}^{fo+res,match,\mathrm{CGMP}}$$

The (as yet nameless) code

Bonino, MC, Stagnitto, 2312.12519

Calculate the N=2 moment of the bottom fragmentation function in e+e- at 91.2 GeV to NNLO+NNLL, with log-R matching and CNO Landau pole regularisation

```
> ./ffexe -bottom -n 2 -Q 91.2 -m 4.75 -NNLO -NNLL -logR -CNO

# bottom fragmentation function at 91.2, calculated with e+e- CoefficientFunction at NNLO with NNLL soft
resummation (with log-R matching and CNO(f=1.25) Landau pole regularisation) in the nf-flavours (including
the heavy quark) scheme with nf = 5 flavours, using the photon-only bottom LO EW cross section (normalised
to the bottom LO EW cross section and QCD corrections to NNLO, with massless heavy quark thresholds),
calculated with hard scale = 91.2, muR = 91.2, muF = 91.2, alphas(muR) = 0.118 evolved using MELA
evolution (TRN solution) to NNLO in the VFNS scheme [with max 5 flavours and thresholds at 1.5, 4.75,
1e+10], using alphas_ref(Qref=91.2) = 0.118 -------, InitialCondition for bottom quark at NNLO with NNLL
soft resummation (with log-R matching and CNO(f=1.25) Landau pole regularisation) in the nl-flavours
(nl=nf-1, light flavours only) scheme with nf = 5 flavours, calculated with hard scale = 4.75, muR = 4.75,
muF = 4.75, alphas(muR) = 0.21593775 evolved using MELA evolution (TRN solution) to NNLO in the VFNS
scheme [with max 5 flavours and thresholds at 1.5, 4.75, 1e+10], using alphas_ref(Qref=91.2) = 0.118 [VFNS
coupling corrected to FFNS near threshold using full FFNS evolution from alphas_VFNS(m)] -------, evolved
with MELA evolution (TRN solution) to NNLO in the VFNS scheme [with max 5 flavours and thresholds at 1.5,
4.75, 1e+10], using alphas_ref(Qref=91.2) = 0.118, initial scale = 4.75 [alphas = 0.215938], final scale =
91.2 [alphas = 0.118]

2 0.787945433
```

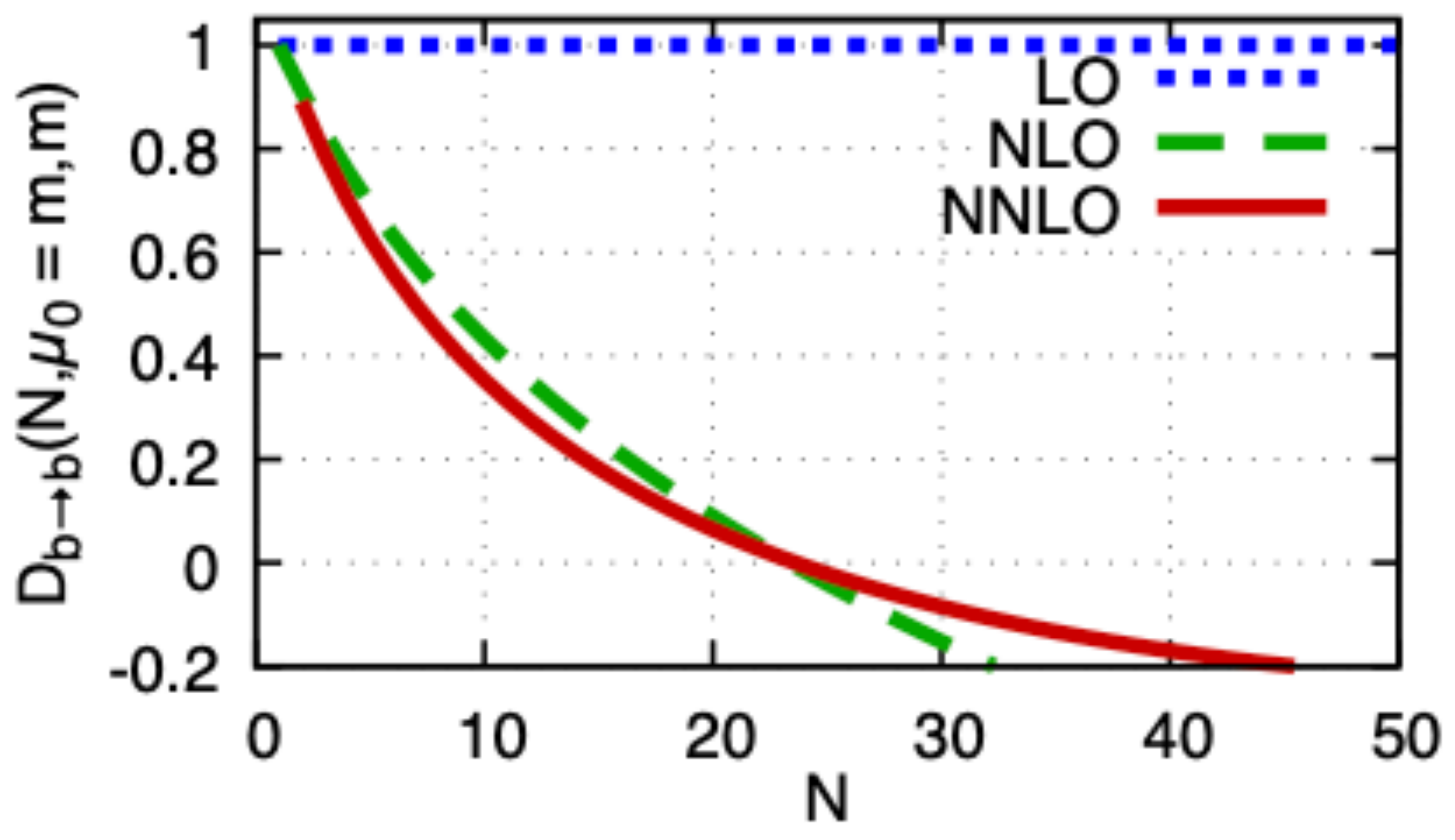
Bottom initial condition

bottom initial condition, m=4.75 GeV

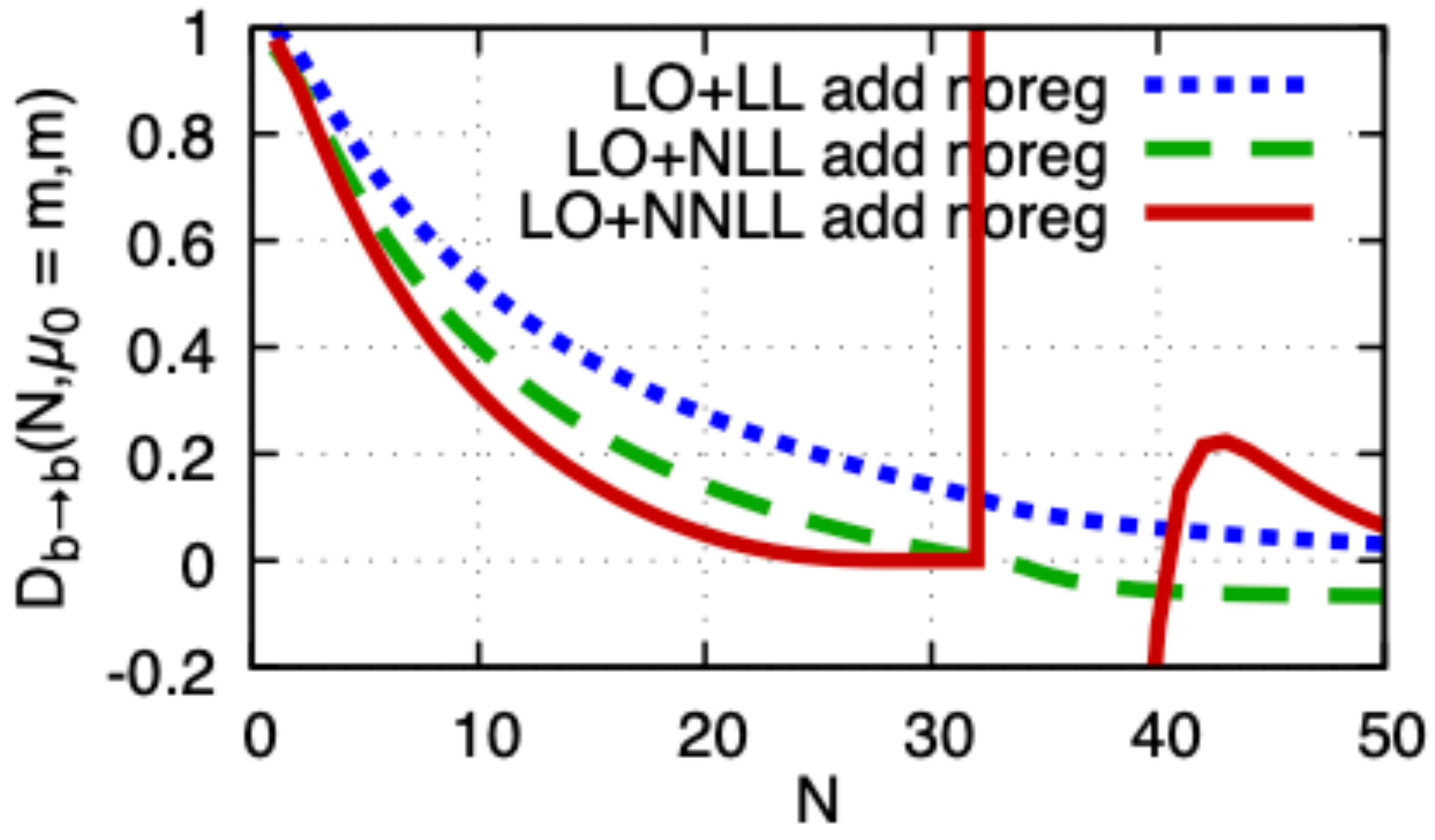
$\mu_0 = \mu_{0R} = \mu_{0F} = m$

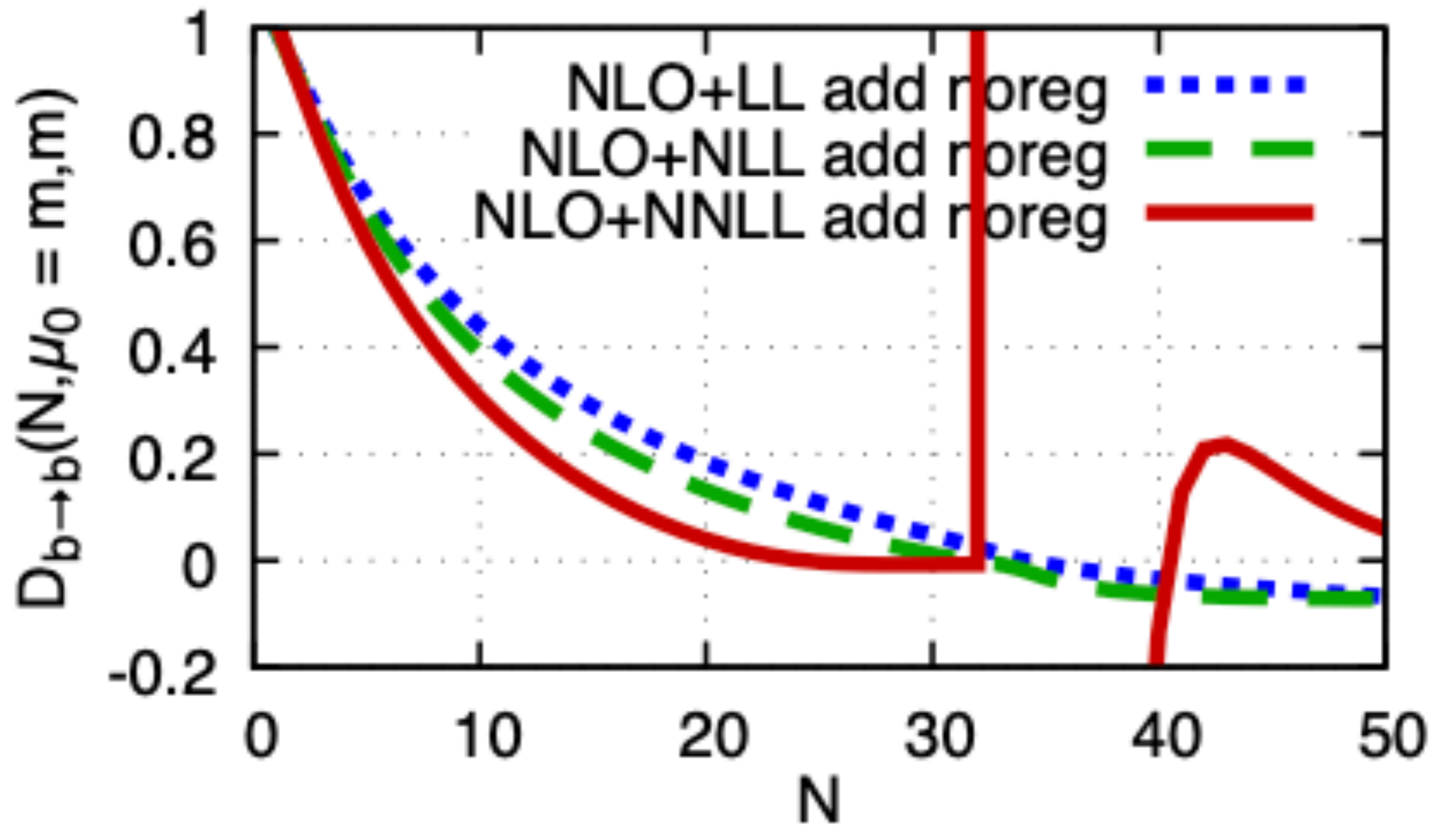
$\alpha_S(Q=91.2 \text{ GeV}) = 0.118$

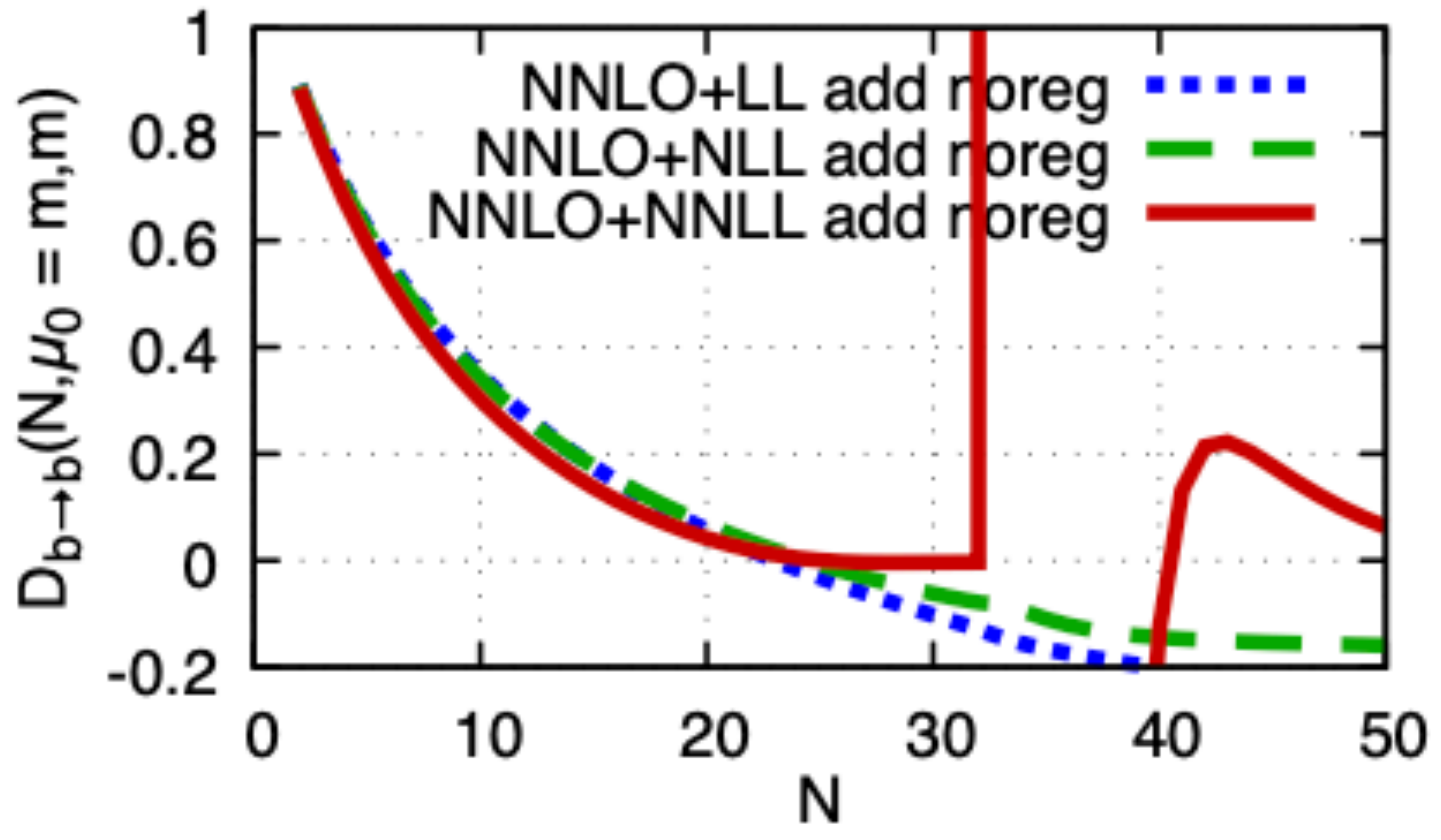
$\alpha_S(m) = 0.21593775$



Fixed order







Additive matching, no Landau pole regularisation

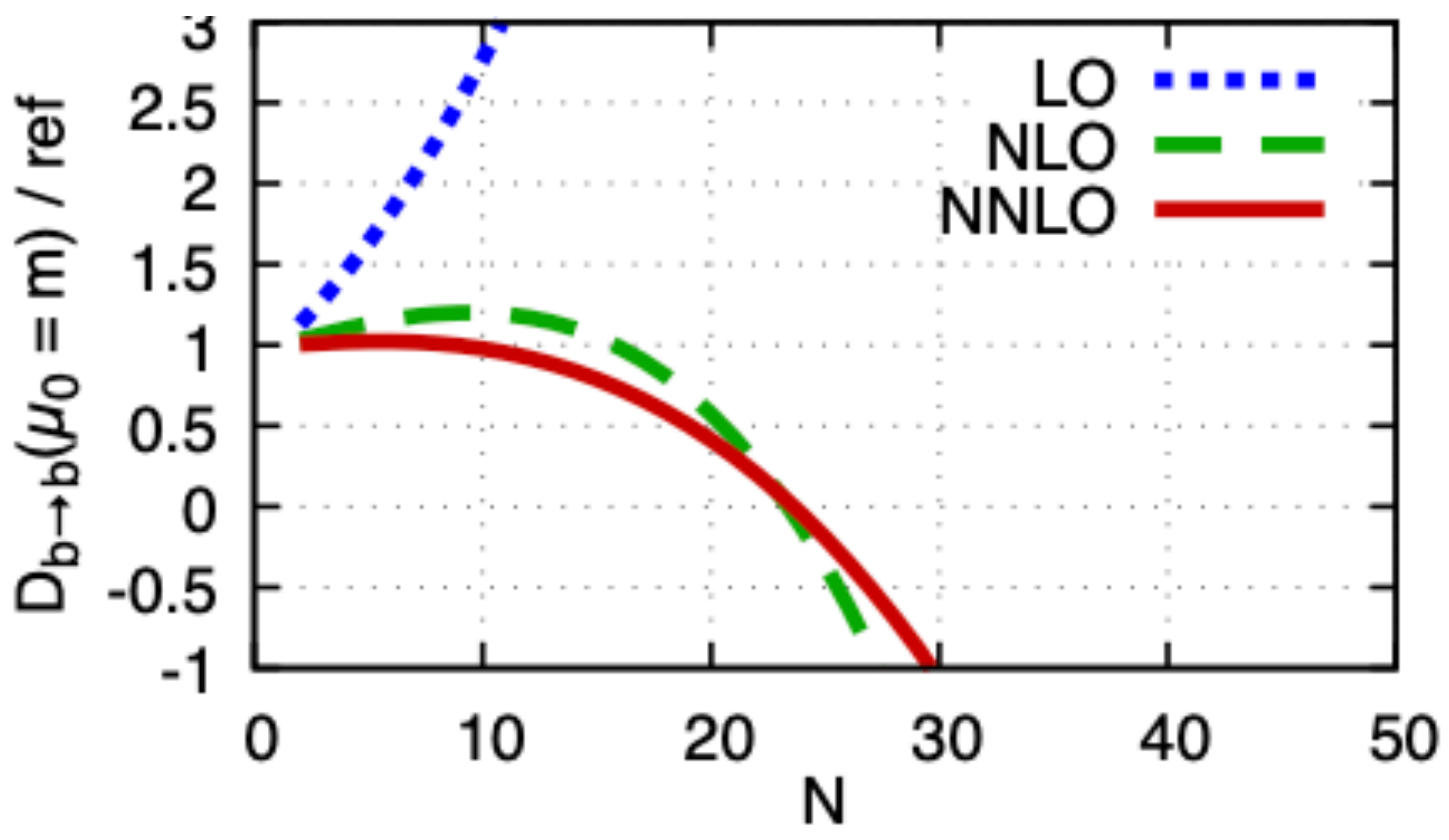
Bottom initial condition

bottom initial condition, m=4.75 GeV

$\mu_0 = \mu_{0R} = \mu_{0F} = m$

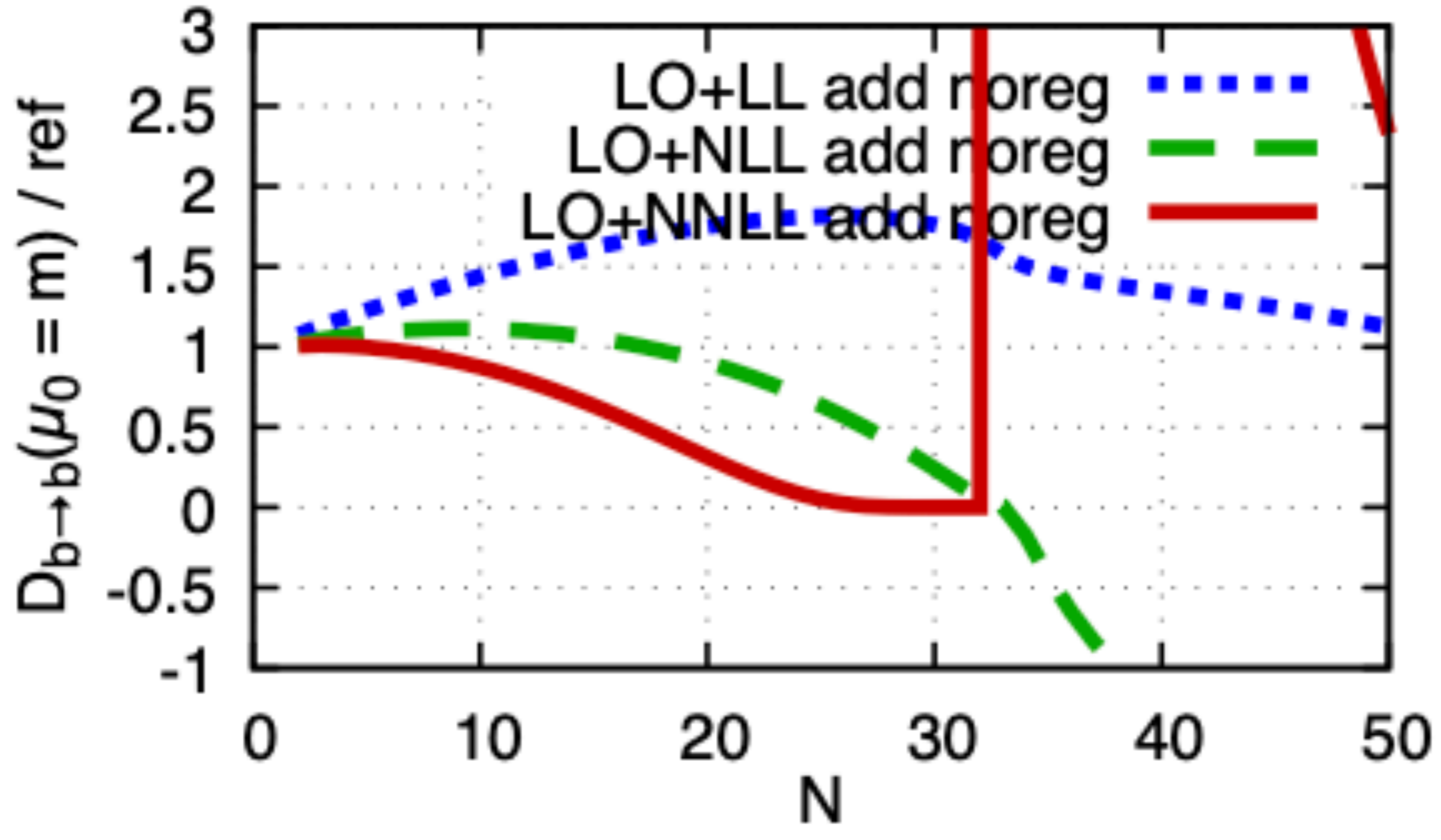
$\alpha_S(Q=91.2 \text{ GeV}) = 0.118$

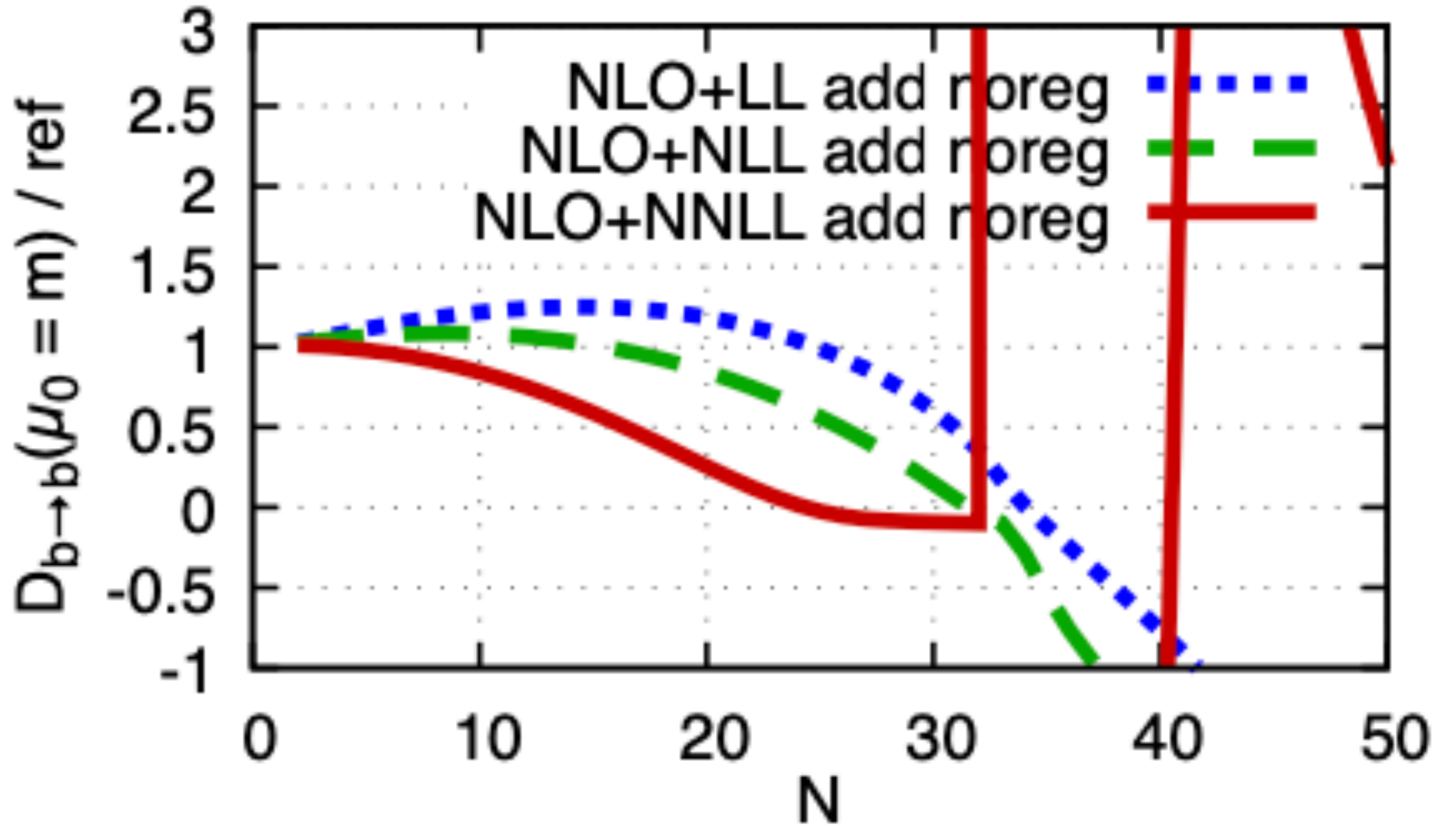
$\alpha_S(m) = 0.21593775$

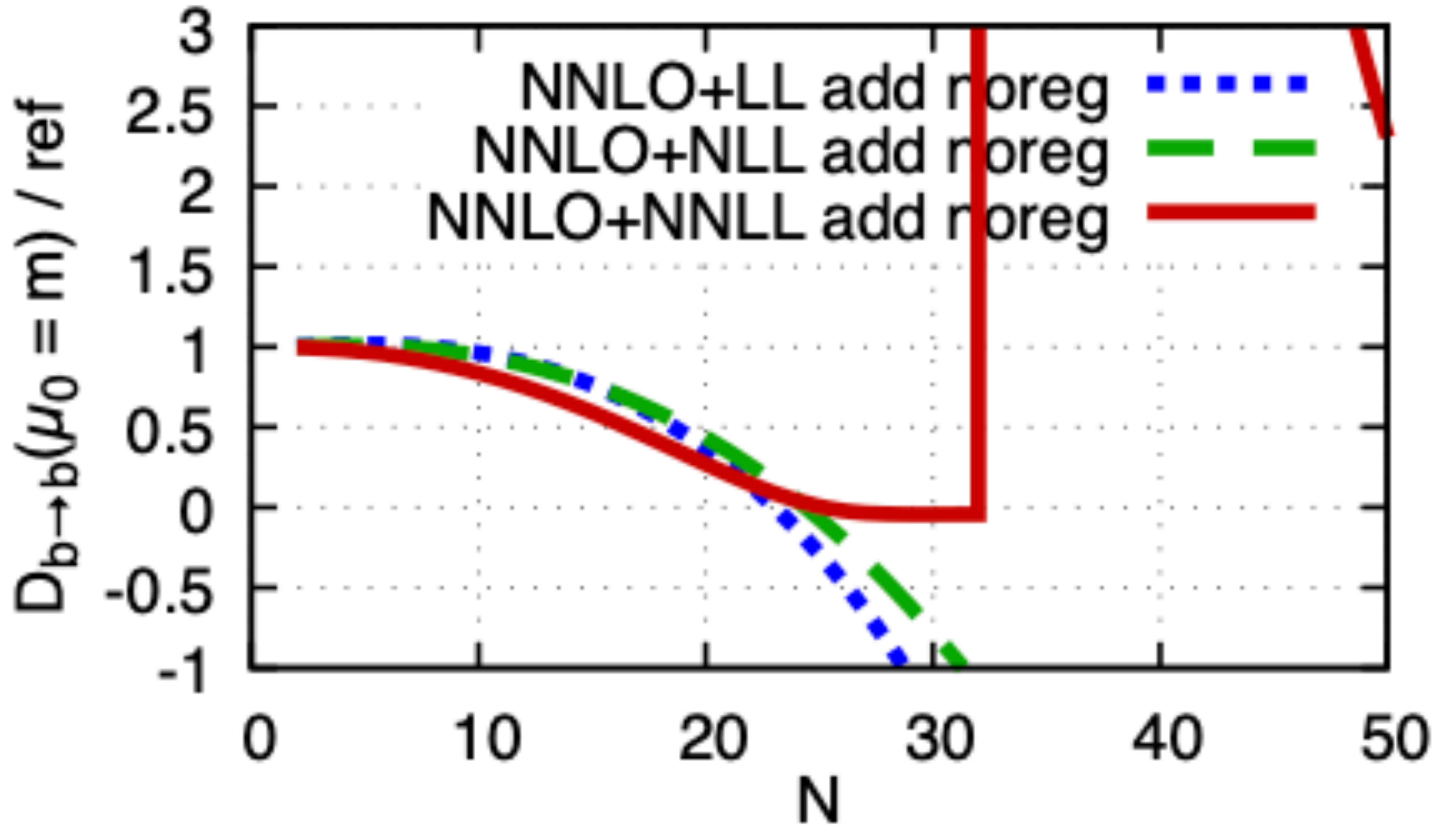


Ratio to a single curve

ref = 'NNLO+NNLL logR CNO(1.25)'

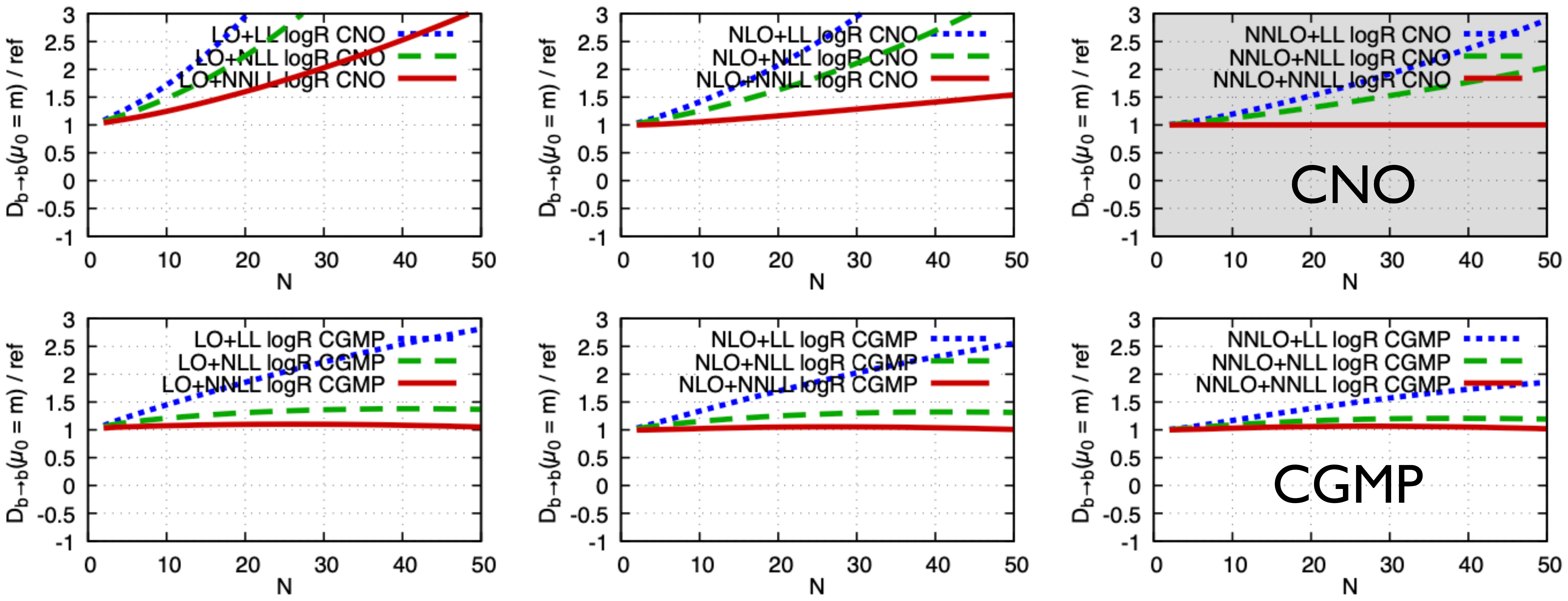






No obvious perturbative hierarchy NNLL < NLL < LL

Bottom initial condition



'log-R CGMP' displays the expected hierarchy: NNLL < NLL < LL

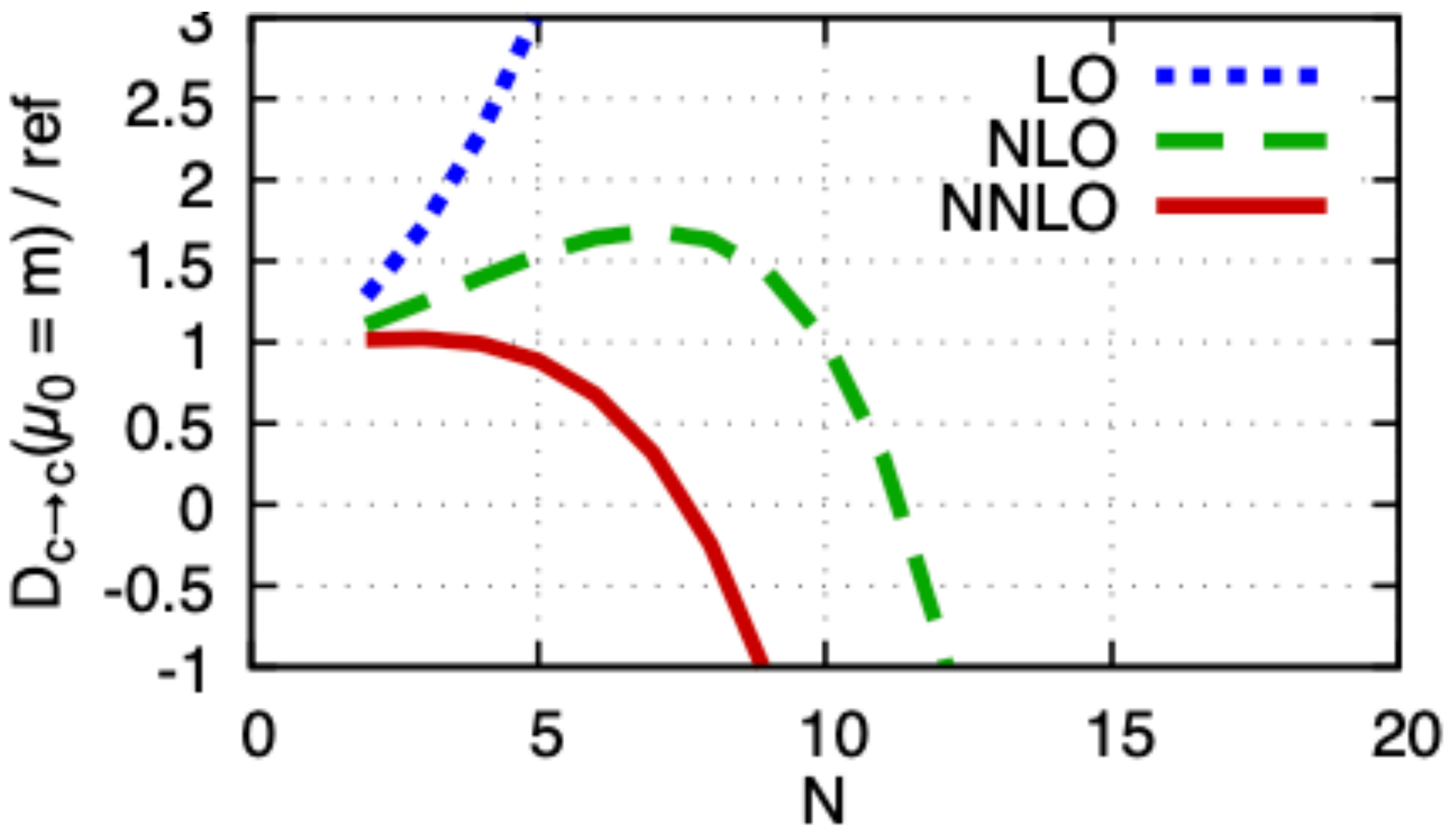
Charm initial condition

charm initial condition, m=1.5 GeV

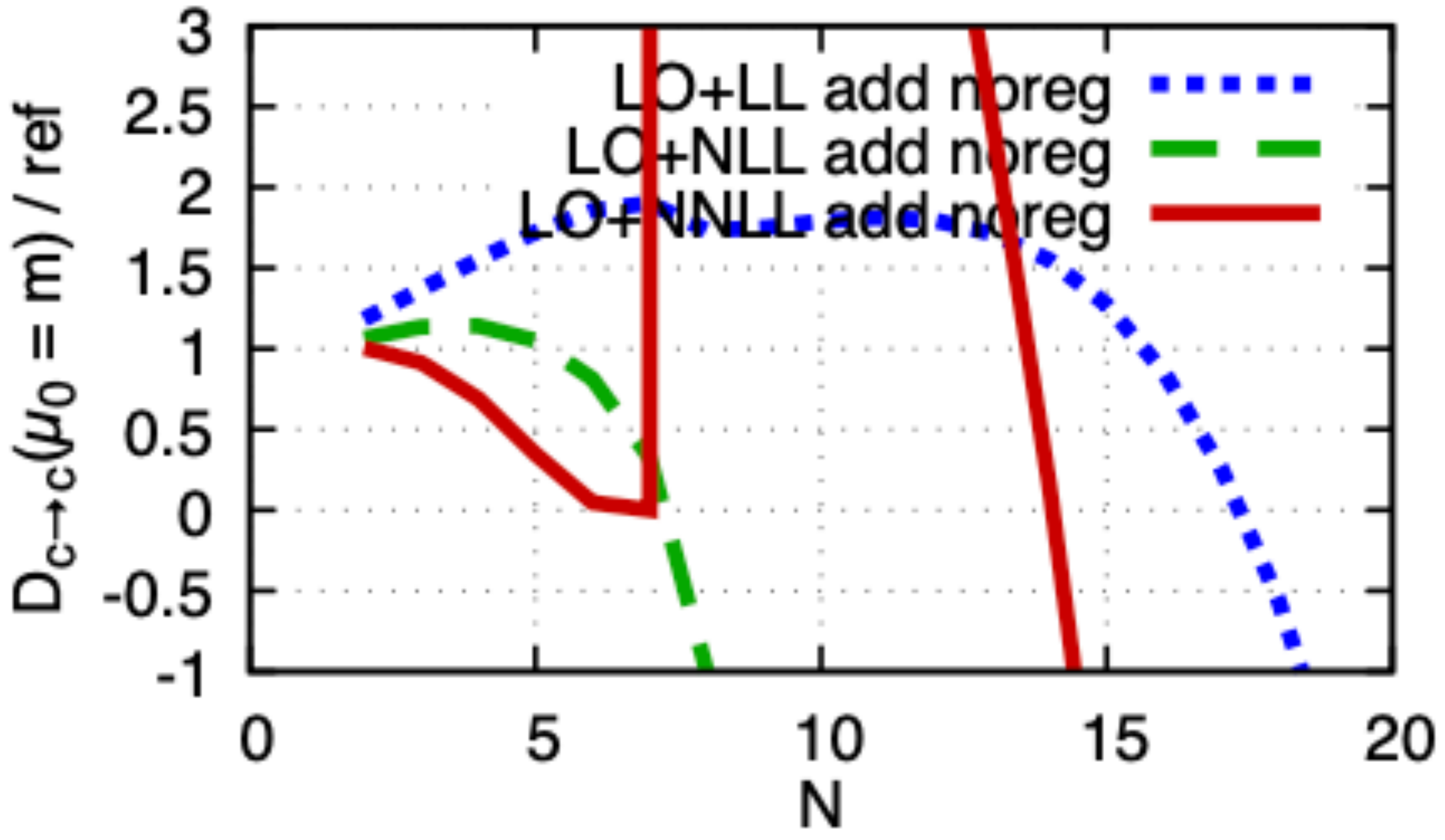
$\mu_0 = \mu_{0R} = \mu_{0F} = m$

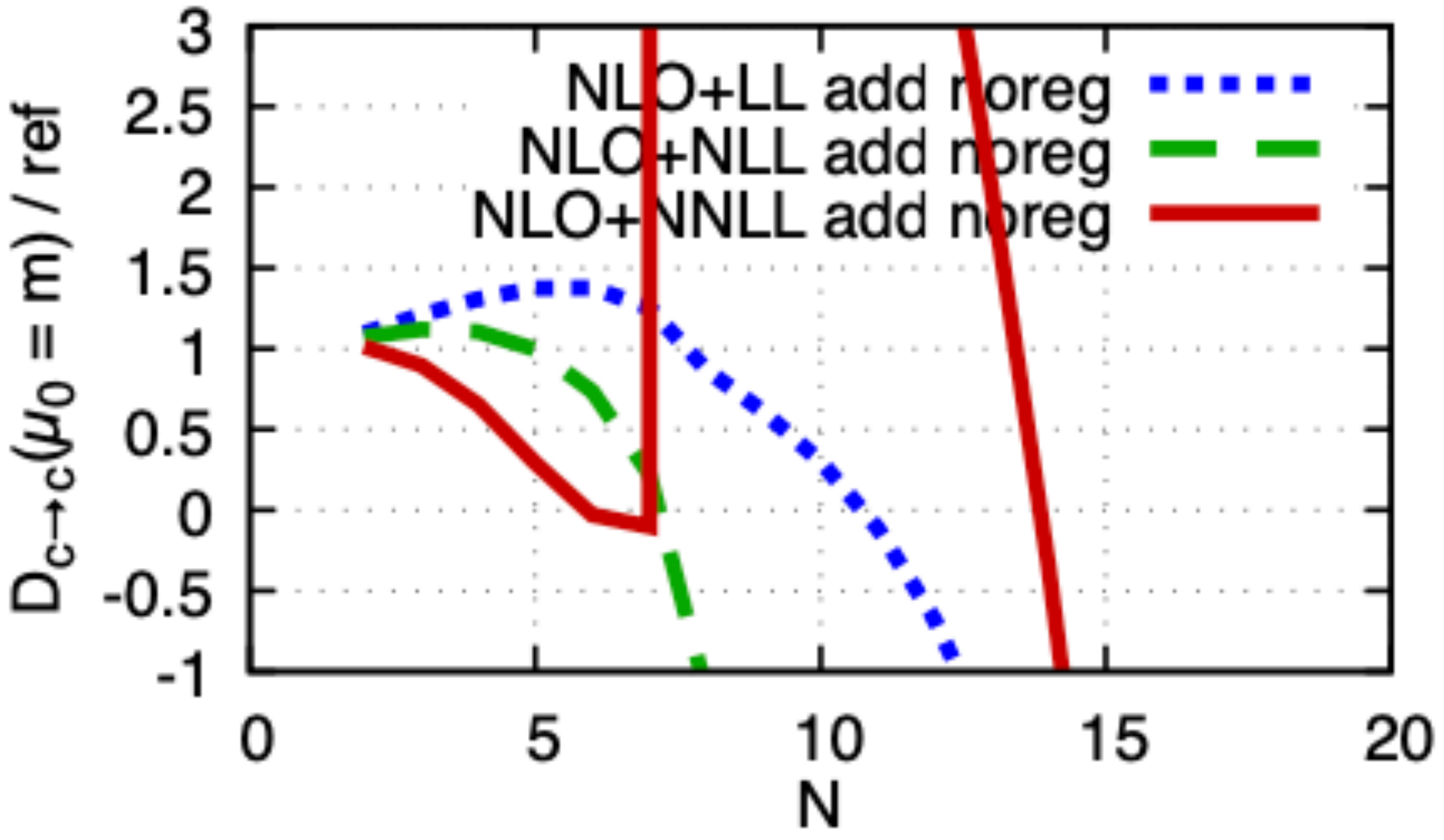
$\alpha_S(Q{=}91.2\ \mathrm{GeV}) = 0.118$

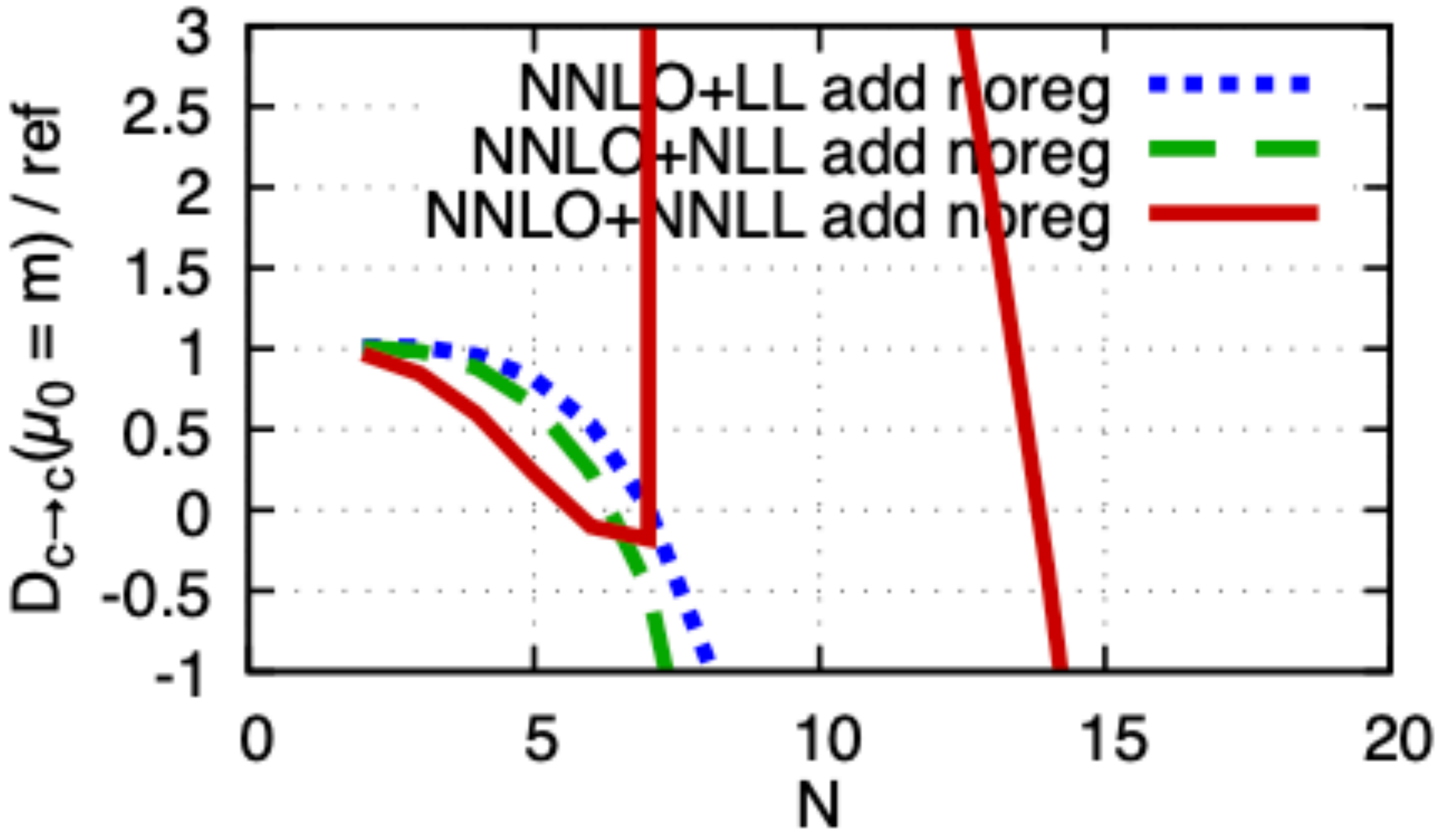
$\alpha_S(m) = 0.34731228$



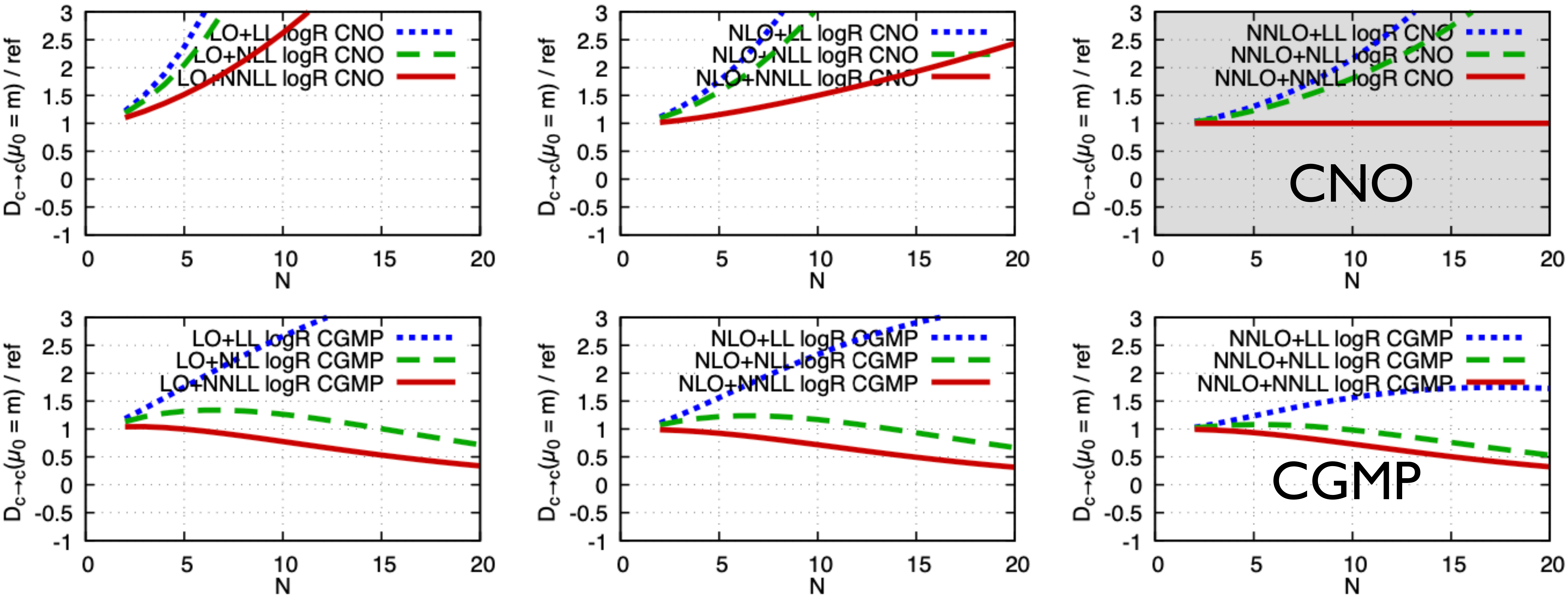
ref = 'NNLO+NNLL logR CNO(1.25)'



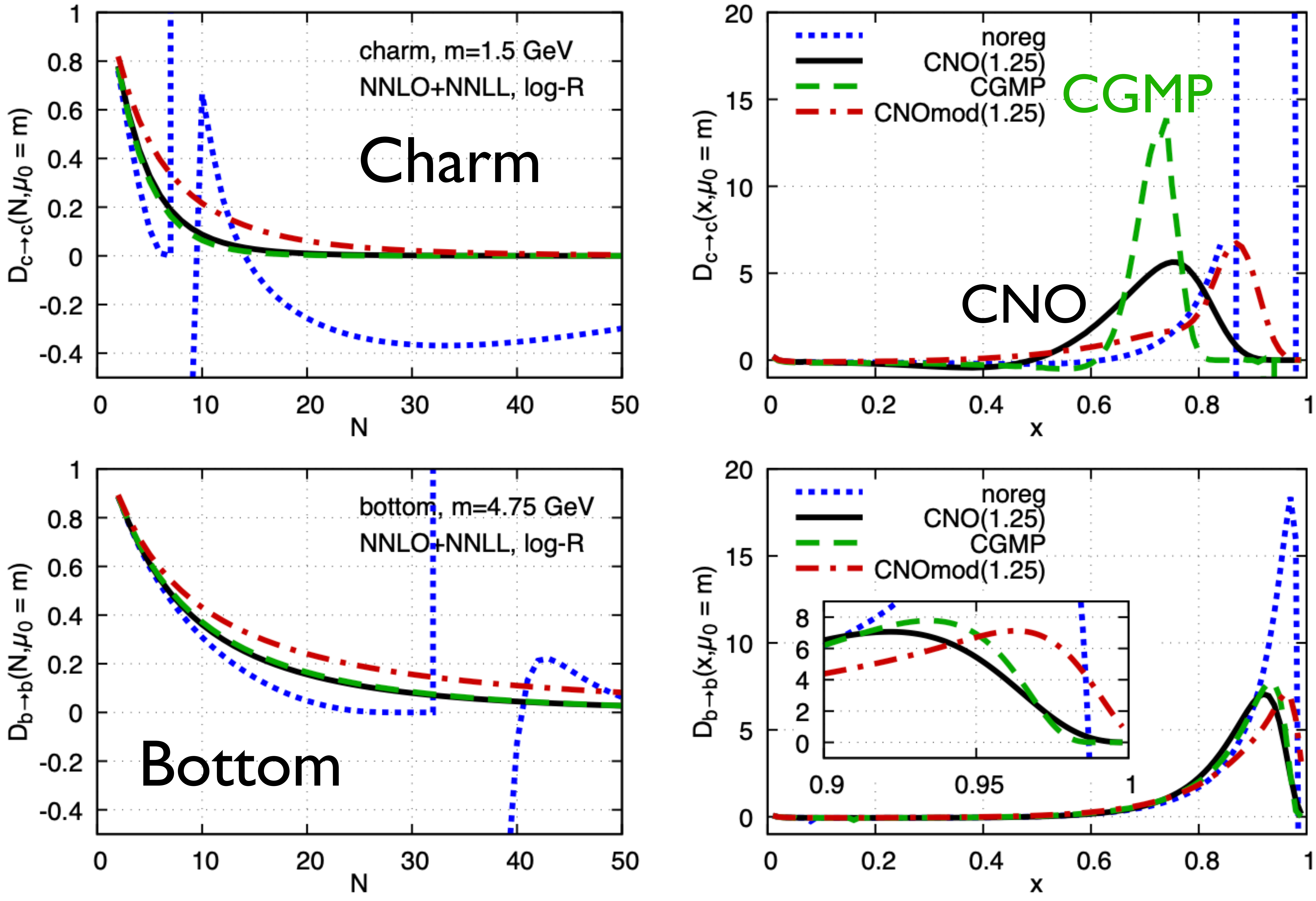




Charm initial condition



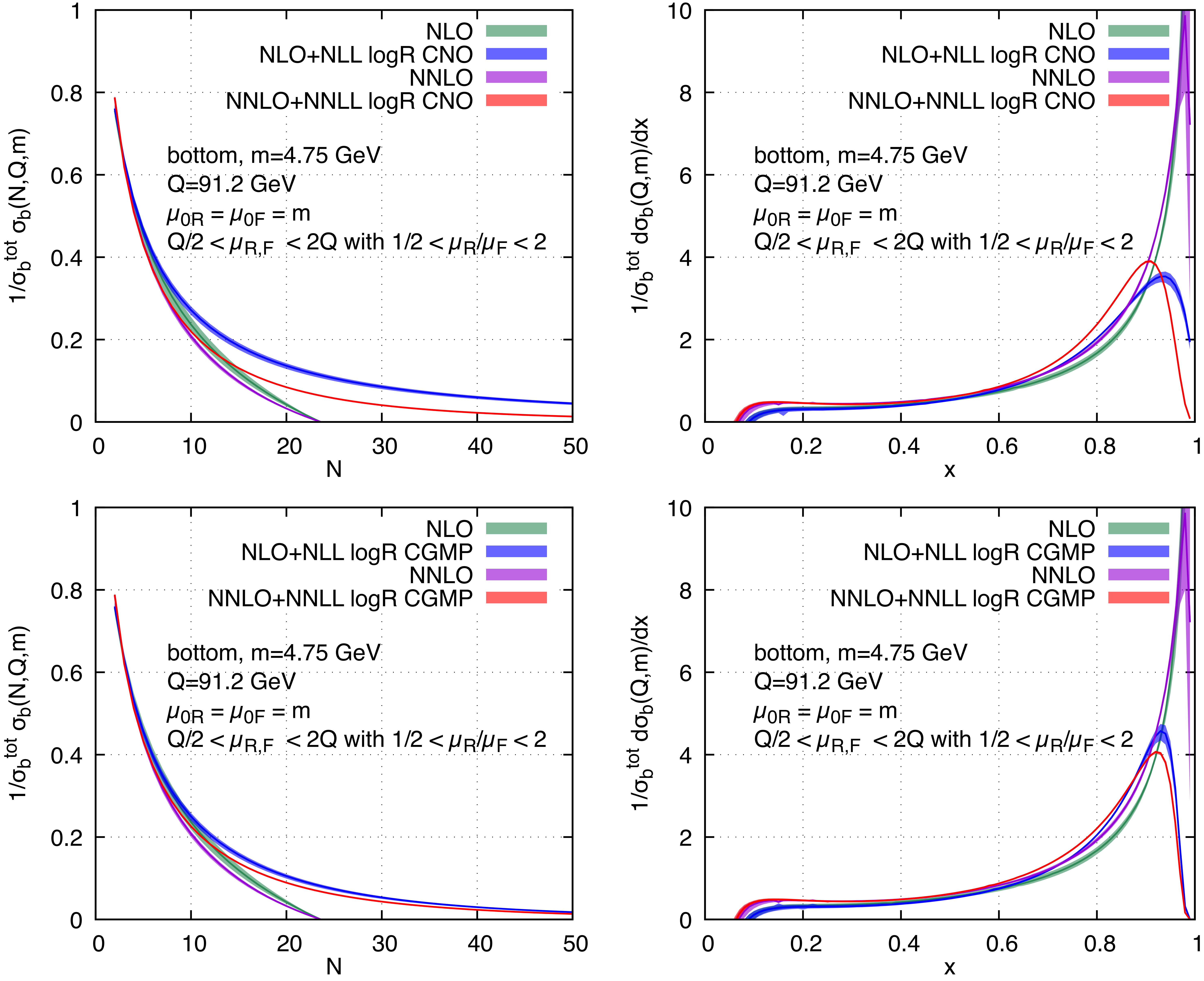
Charm v. Bottom initial conditions



CNO and, to a larger extent, CGMP problematic for charm (too rapid fall-off)

Both CGMP and CNO well behaved for bottom

Bottom e+e- FF: **final** scales variations

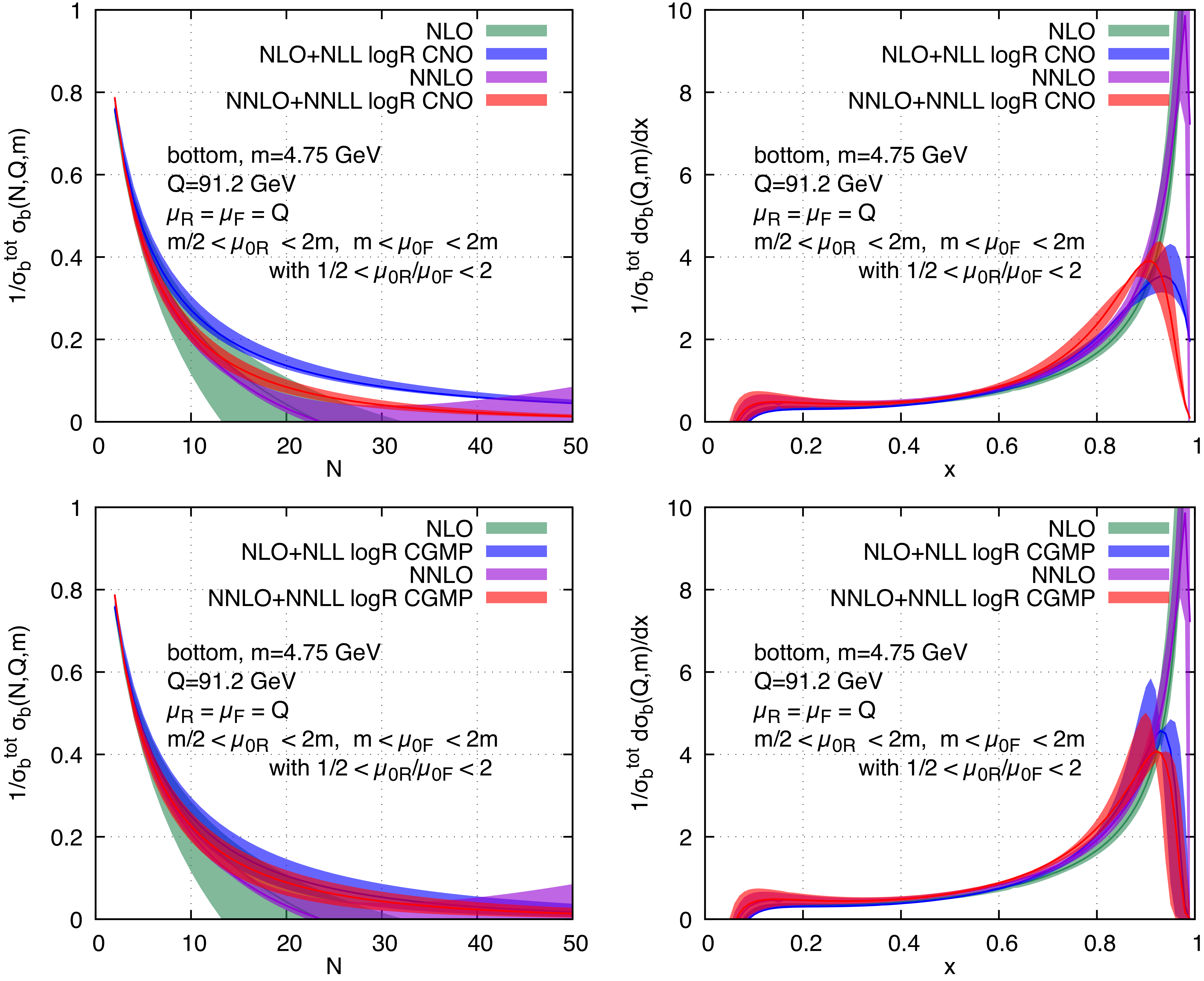


CNO

CGMP

Bands shrink as expected at higher orders, but do not always overlap

Bottom e+e- FF: **initial** scales variations

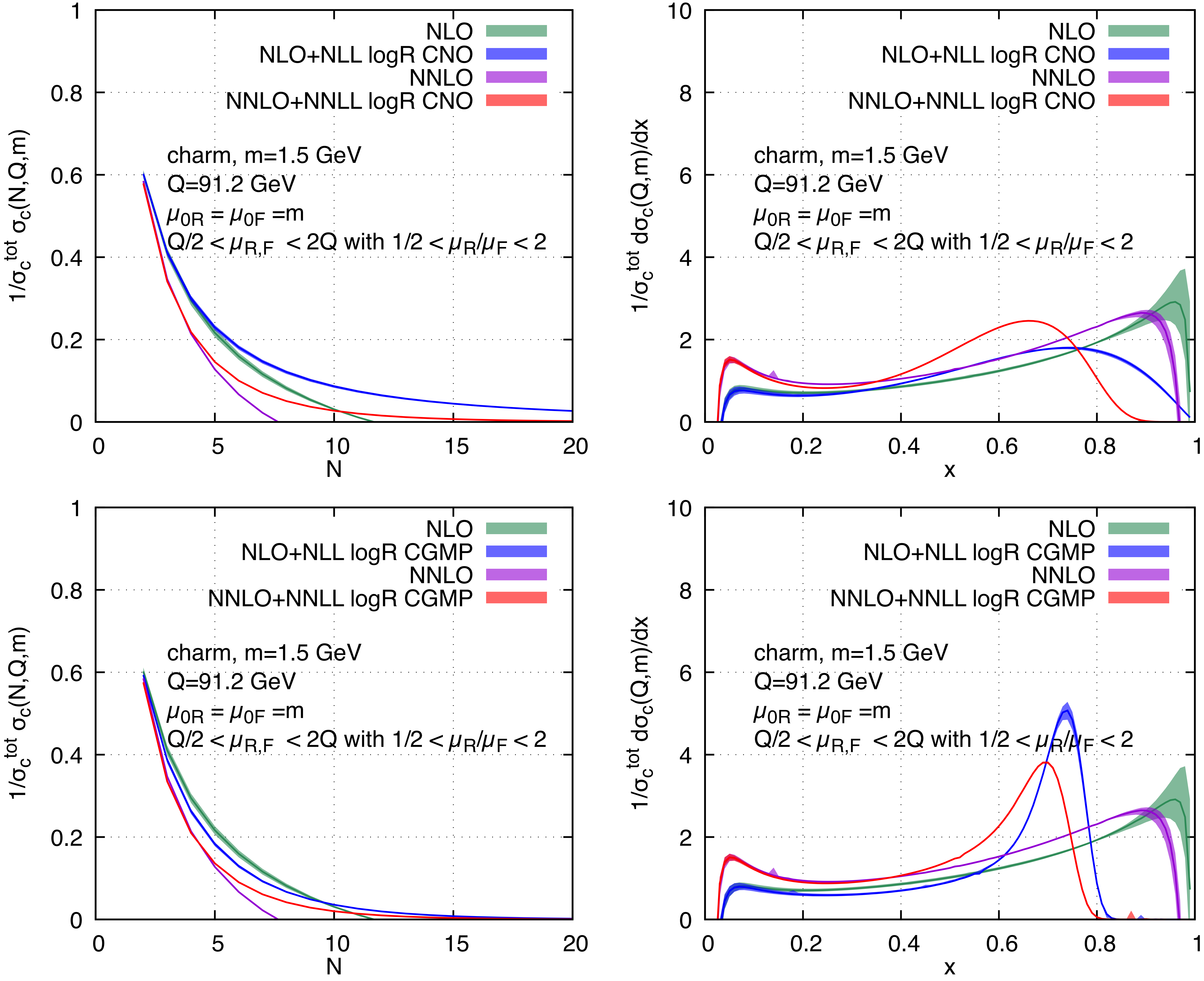


CNO

CGMP

Bands shrink as expected at higher orders, but do not always overlap

Charm e+e- FF: **final** scales variations

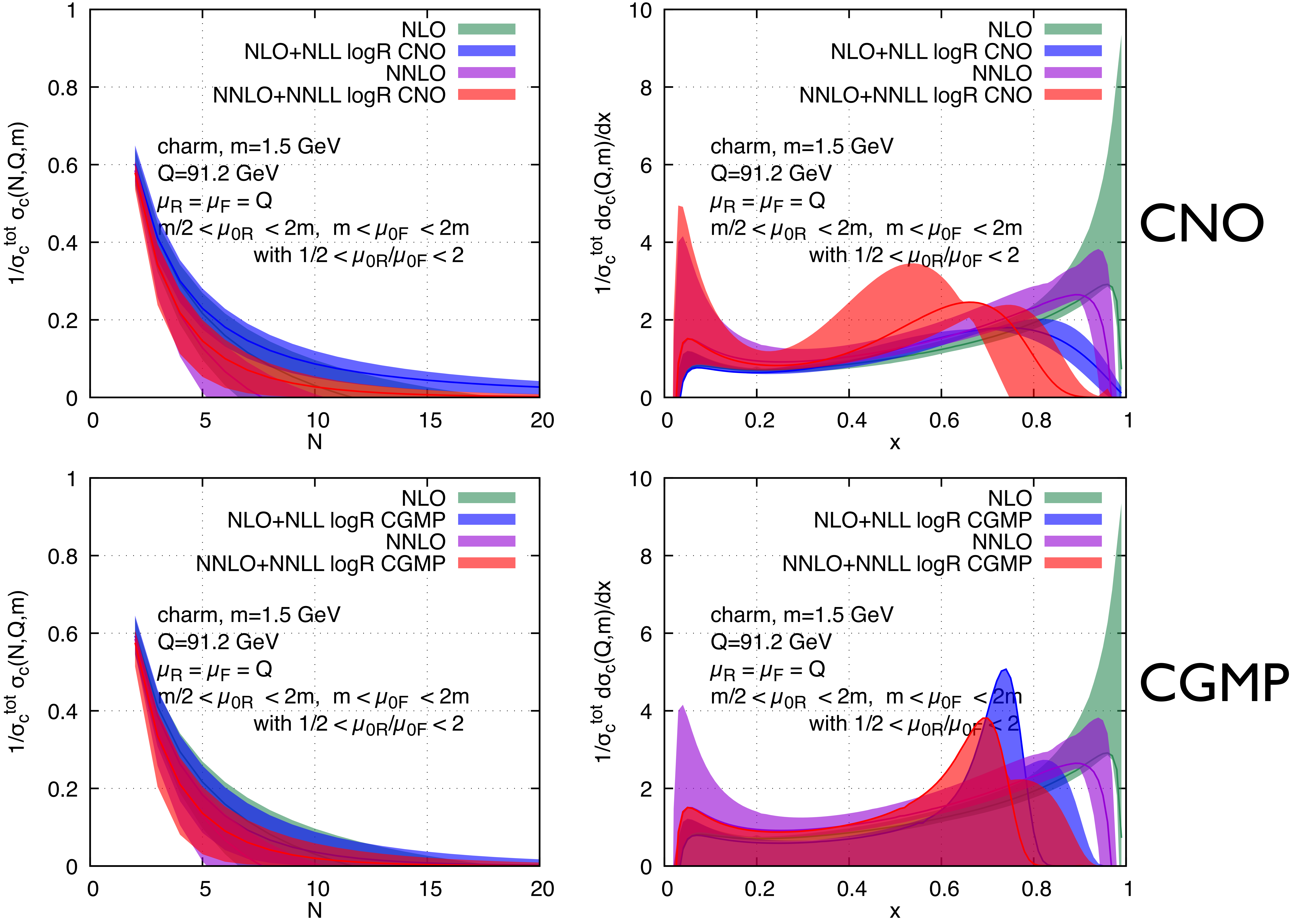


CNO

CGMP

Bands a bit all over the place

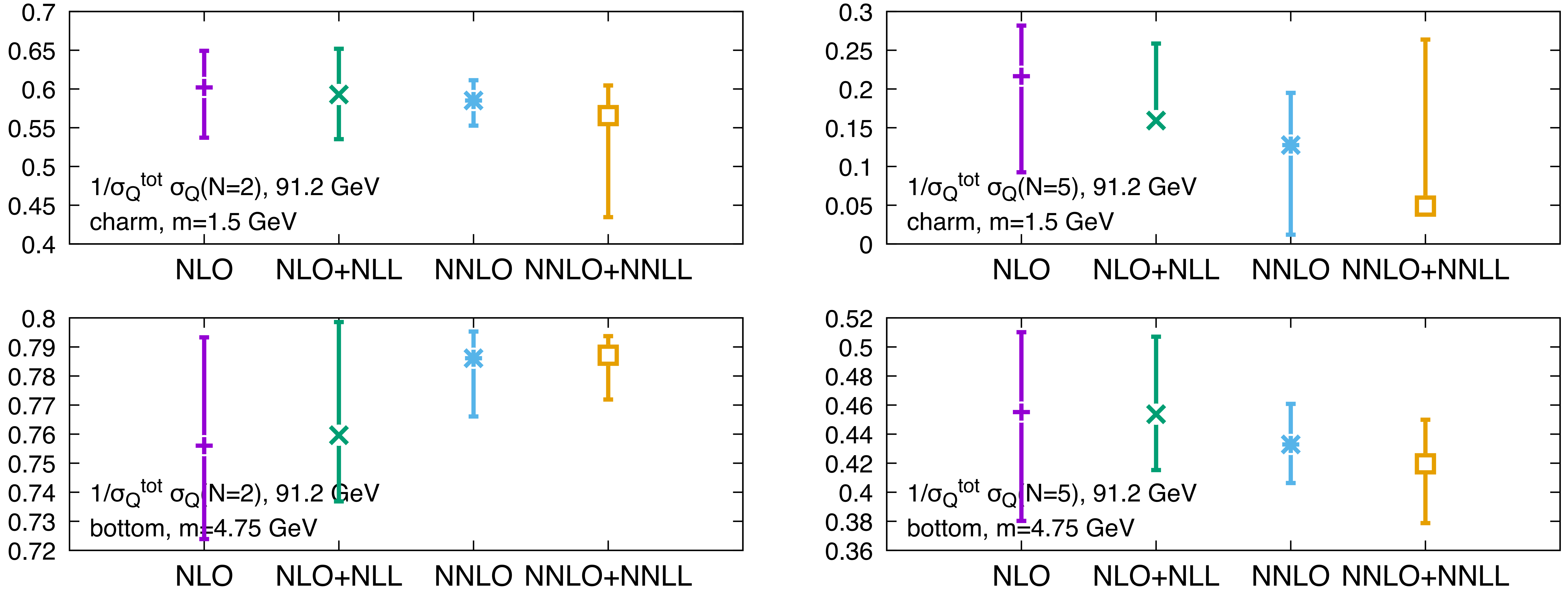
Charm e+e- FF: **initial** scales variations



Bands a bit all over the place

Convergence (or lack thereof)

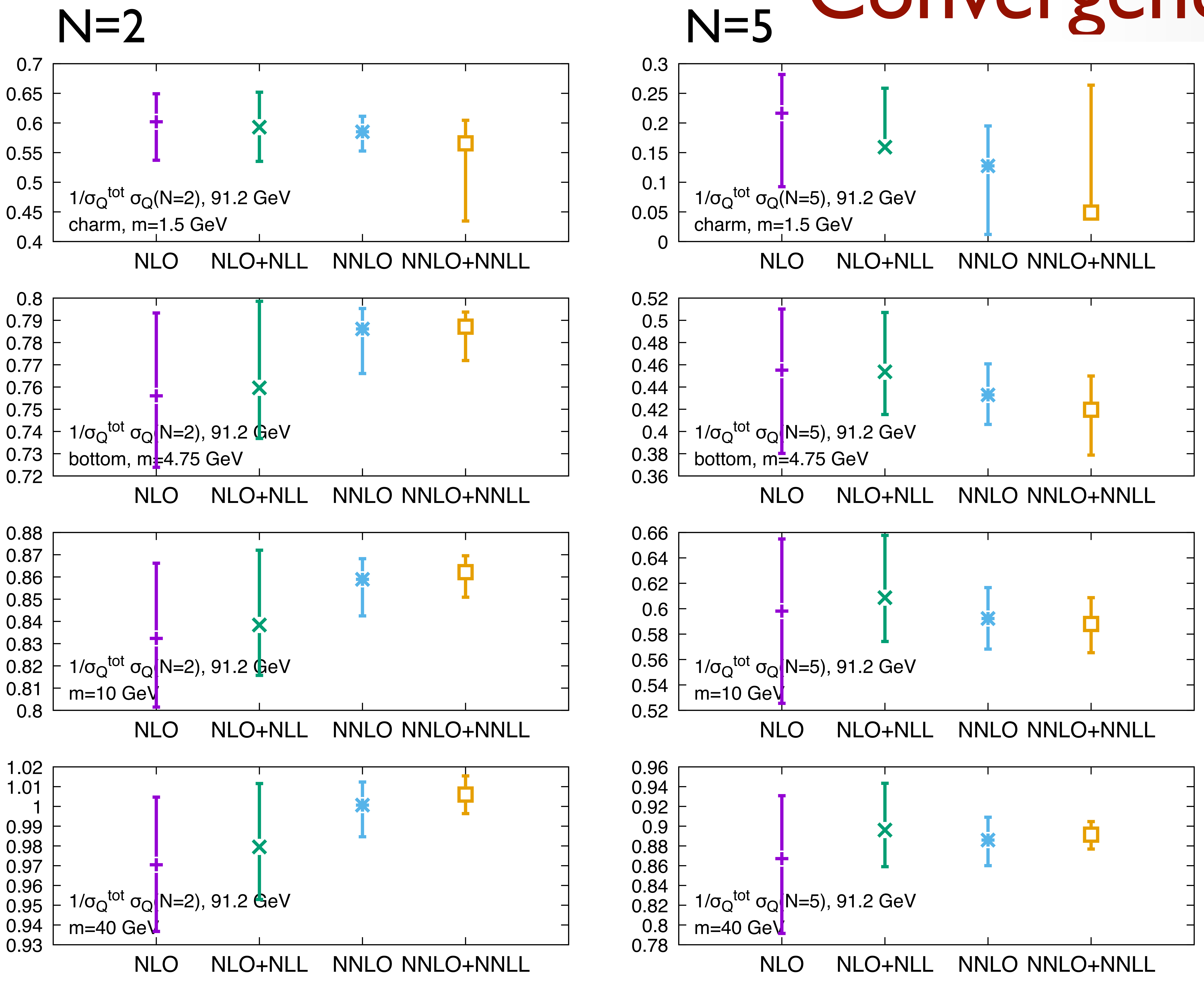
N=2 N=5



Charm

Bottom

Convergence (or lack thereof)



Charm

Bottom

m=10 GeV

m=40 GeV

Nothing wrong with NNLO or NNLL.

It's just that bottom to a certain extent, and certainly charm, are quite light.

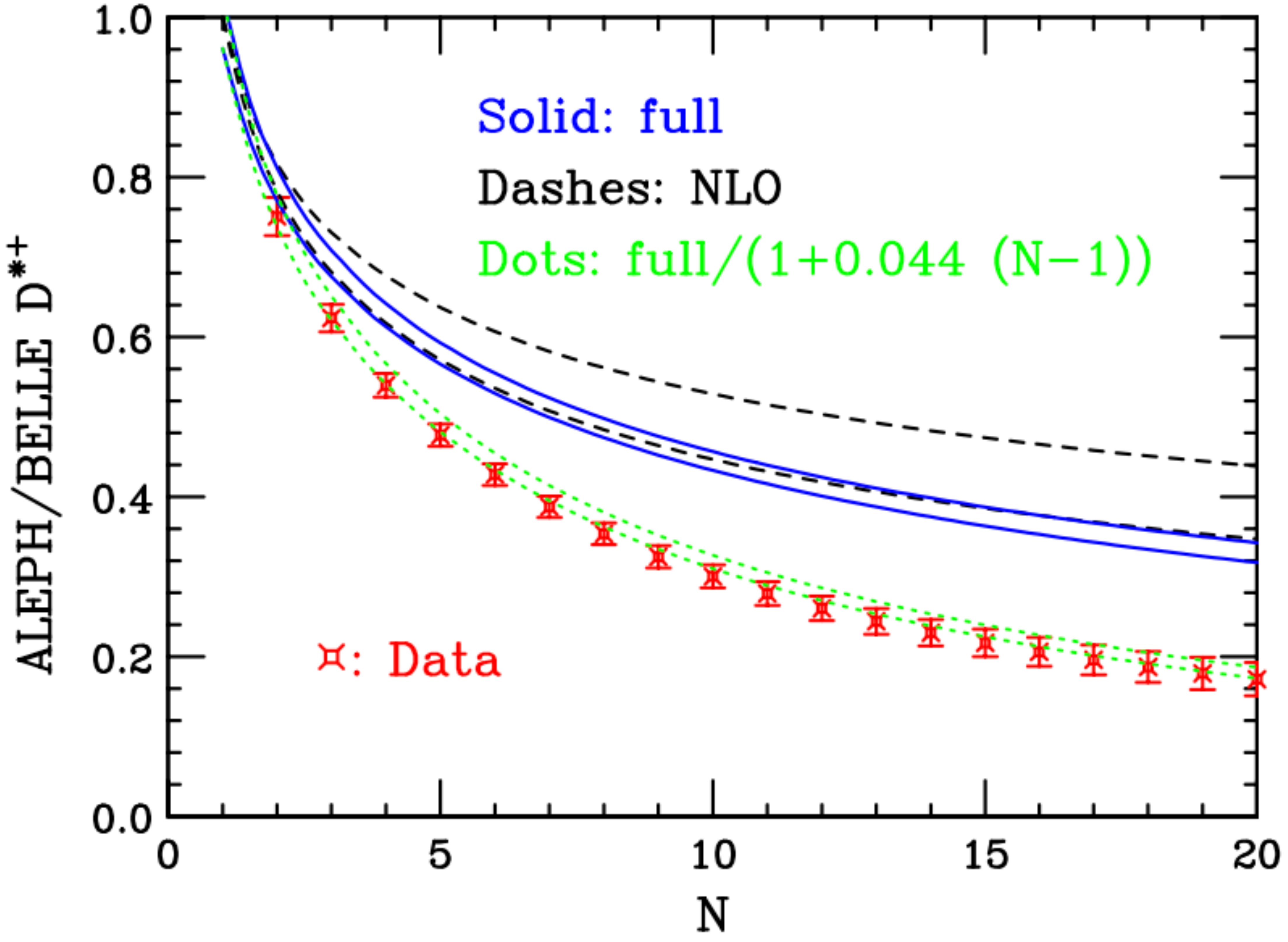
A first observable: charm ratio

$$R_D(N, Q_i, Q_f) \equiv \frac{\sigma_D(N, Q_f = 91.2, m = 1.5, \text{np pars})}{\sigma_D(N, Q_i = 10.6, m = 1.5, \text{np pars})}$$

Ratio of moments of D meson data at two different energies

Essentially independent of non-perturbative and low scales physics.
It tests factorisation and DGLAP evolution from 10.6 GeV to 91.2 GeV

MC, Oleari, Nason 05



Previously calculated at NLO+NLL and compared to data

Sizeable discrepancy observed, likely beyond perturbative uncertainties.

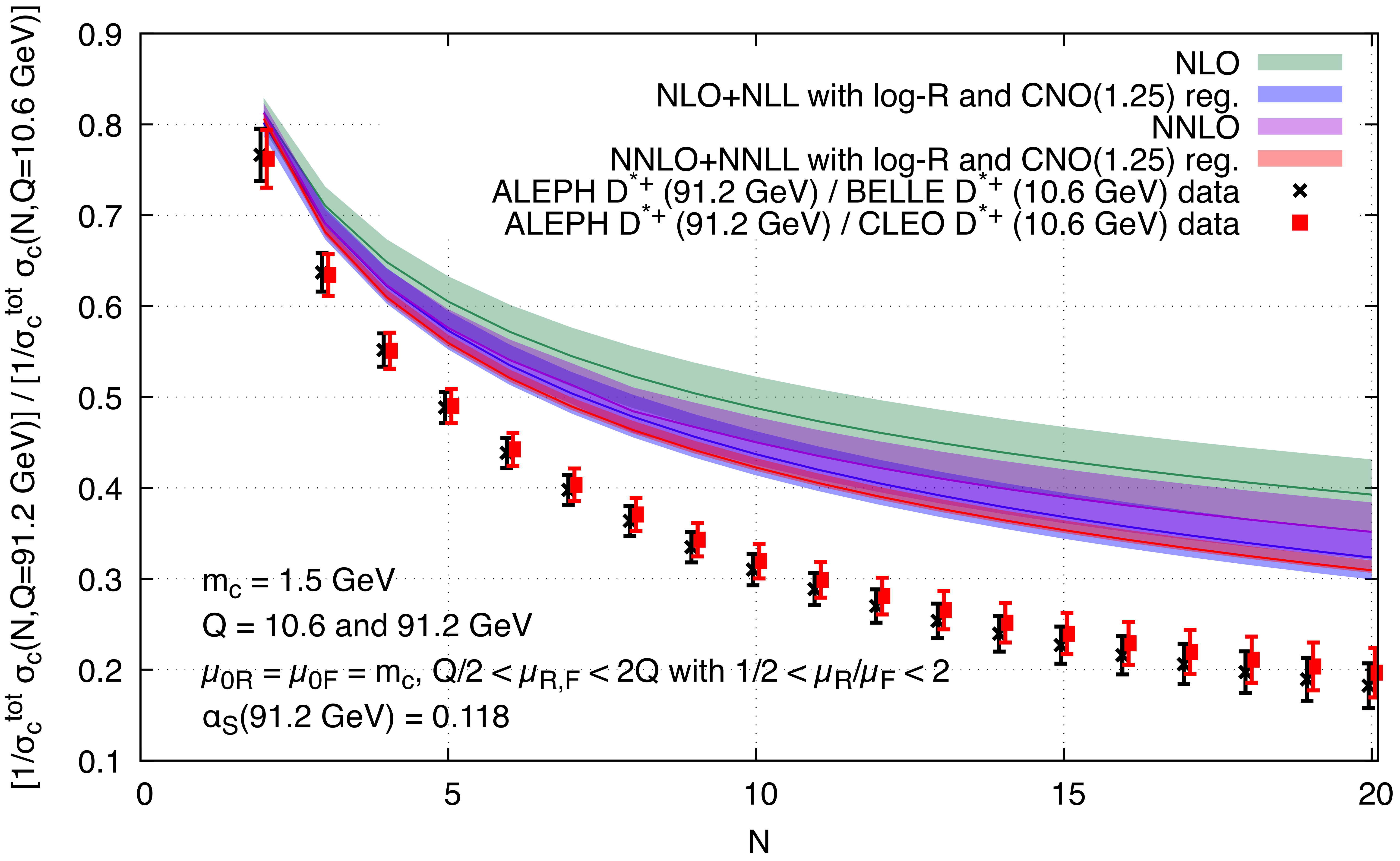
A sign of power corrections at 10.6 GeV ?

A very big coefficient to a $1/Q^2$ correction, or a reasonably-sized coefficient to an (unexpected) $1/Q$ correction would fit the data

A first observable: charm ratio

$$R_D(N, Q_i, Q_f) \equiv \frac{\sigma_D(N, Q_f = 91.2, m = 1.5, \mathrm{np\ pars})}{\sigma_D(N, Q_i = 10.6, m = 1.5, \mathrm{np\ pars})}$$

Ratio of moments of D meson data at two different energies



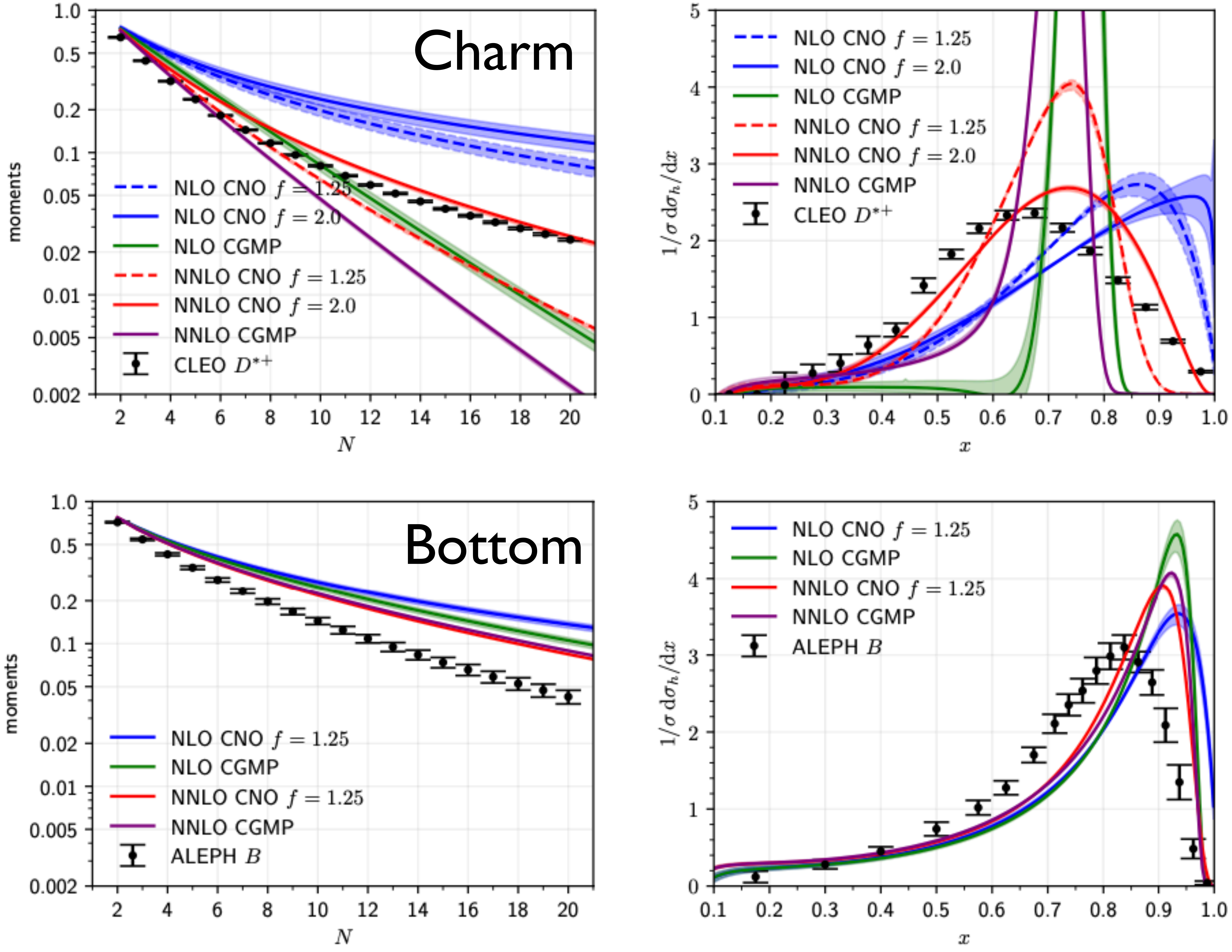
New evaluation at NNLO+NNLL

As expected, perturbatively compatible with NLO+NLL

Discrepancy with data unchanged

Things improve a bit when considering mass corrections in resummation
[MC, Ghira, Marzani, Ridolfi, 2406.04173]
See talk by Andrea Ghira later today

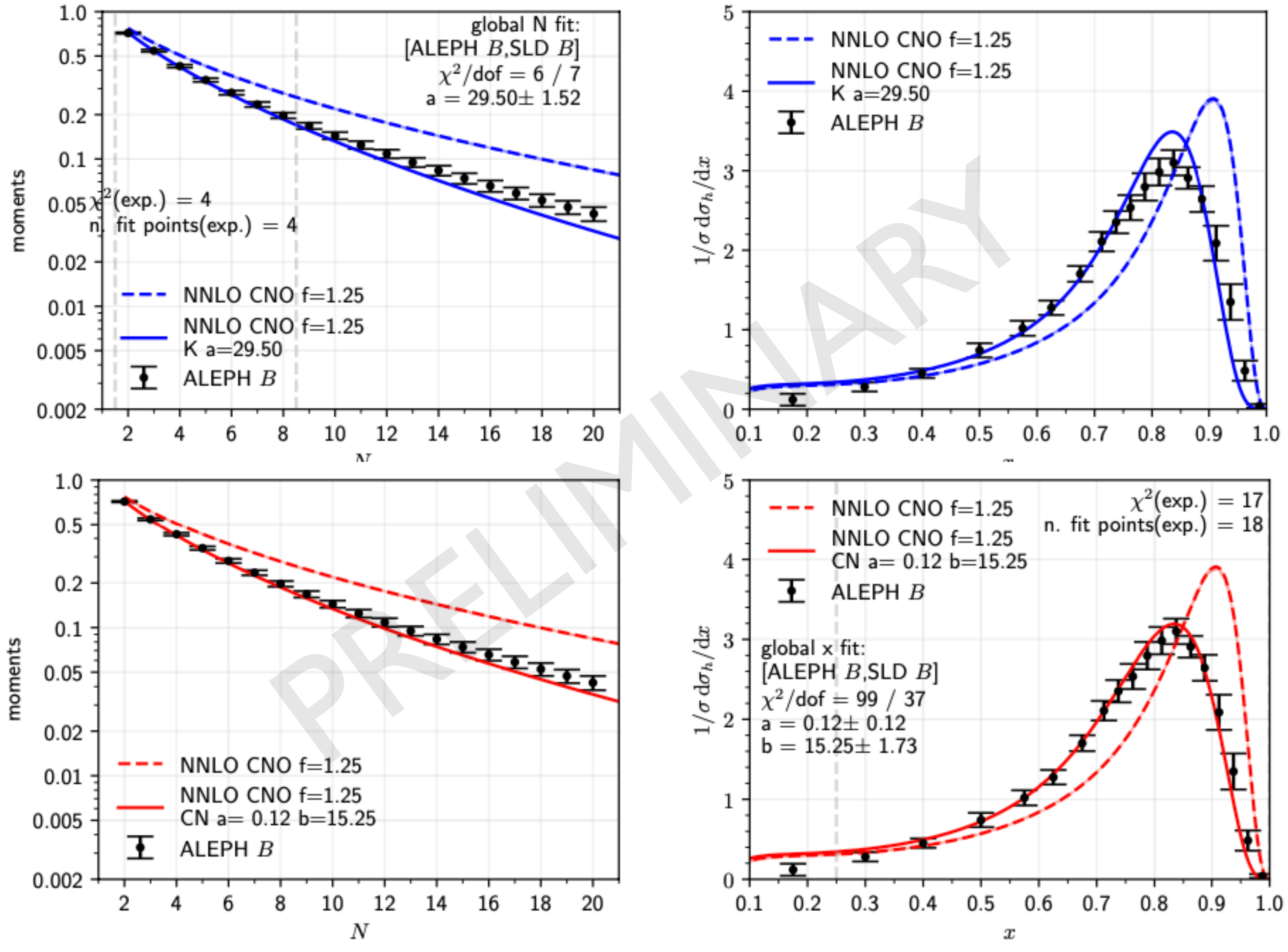
Comparisons to data



pQCD + Landau regularisation only

Challenge of describing data from this baseline clearly larger for charm. The shape of the pQCD+Landau regularisation curve can make fits impossible with a simple non-perturbative parameterisation
=> CNO f=2 needed for charm

Global fits to ALEPH+SLD bottom data



Fit in N-space with

$$D_{\rm NP}^{K}(x) = (a+1)(a+2)x^a(1-x)$$

(Kartvelishvili et al.)

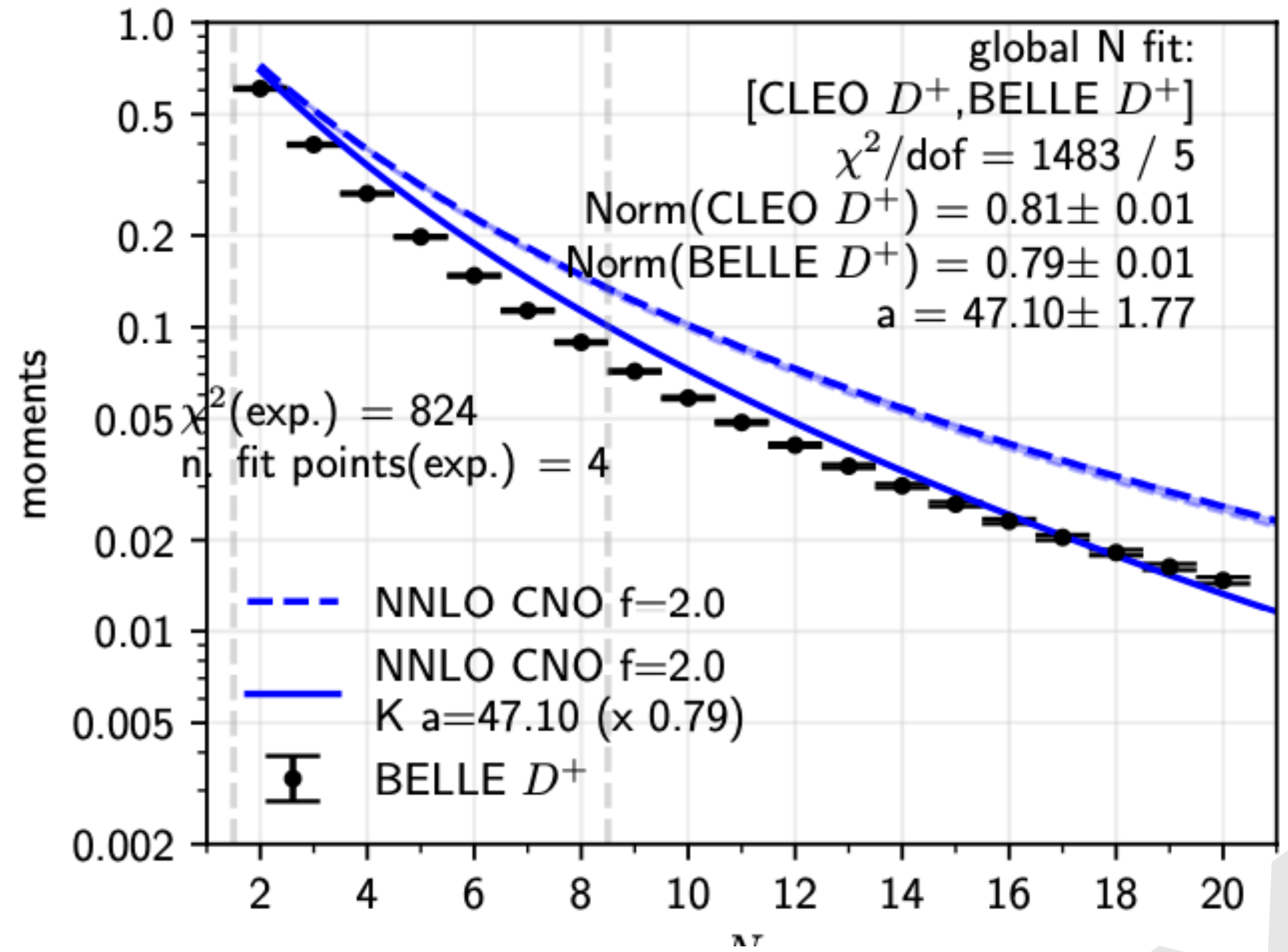
Fit in x-space with

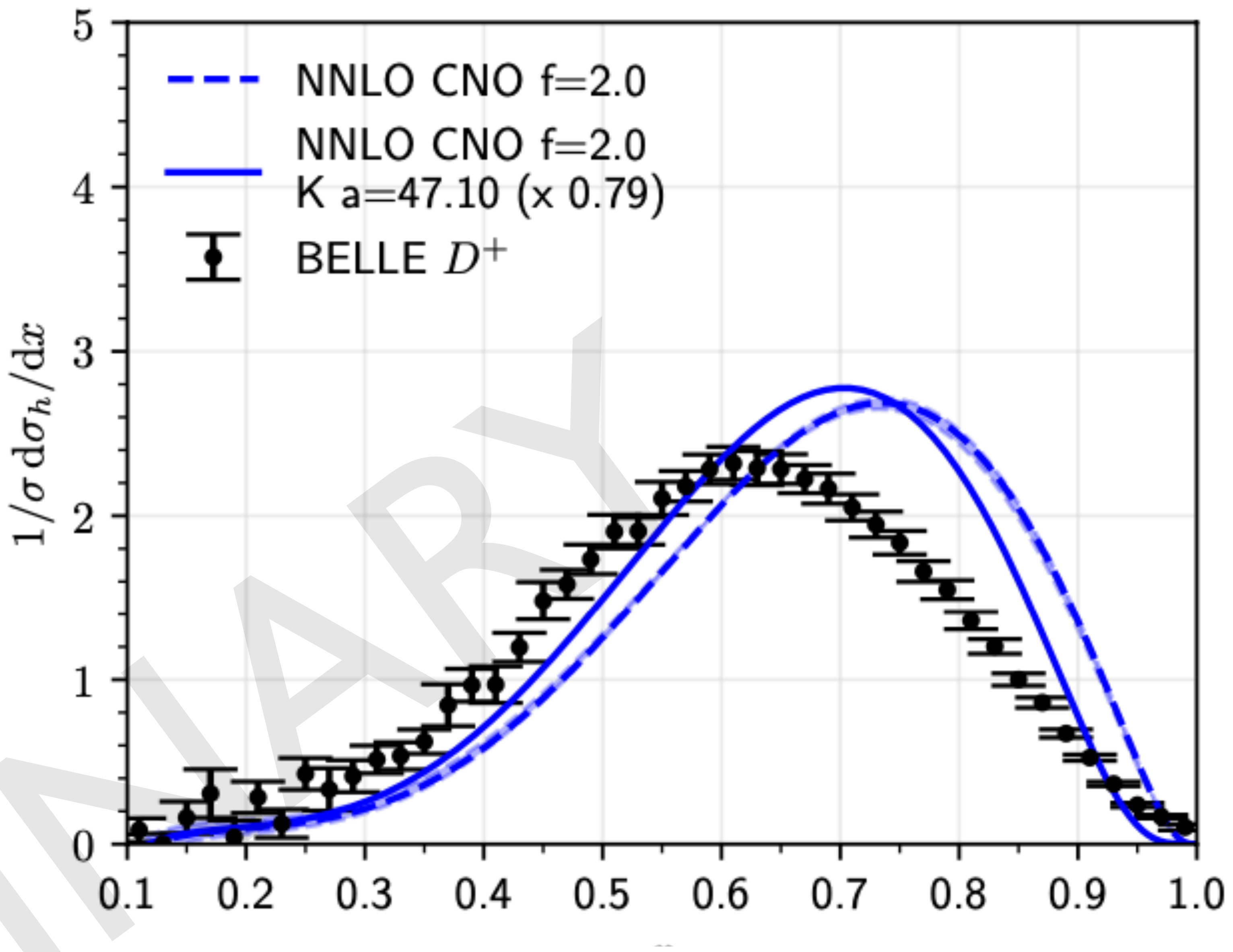
$$D_{\rm NP}^{CN}(x) = \frac{\Gamma(a+b+2)}{\Gamma(a+1)\Gamma(b+1)}\,(1-x)^a x^b$$

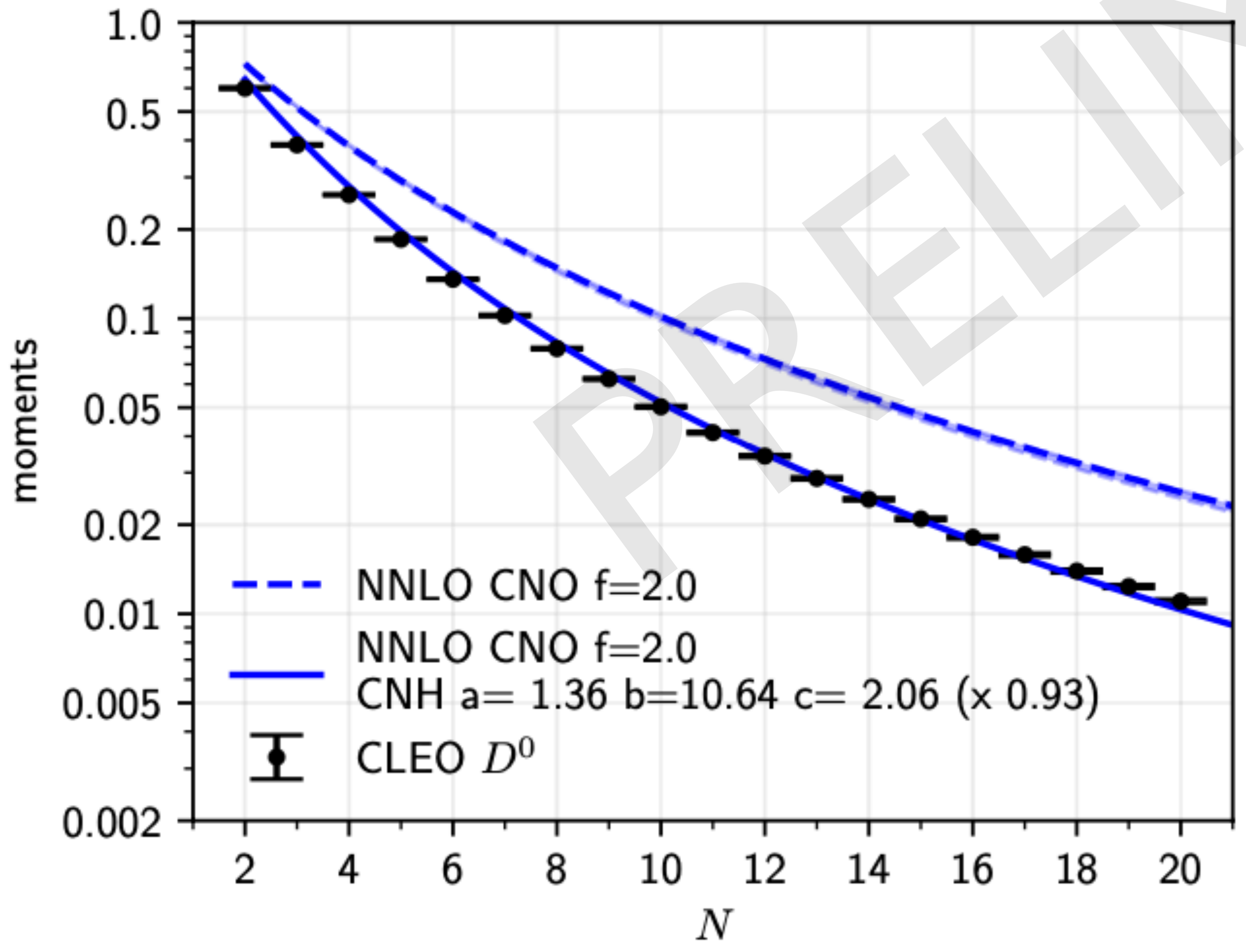
(Colangelo-Nason)

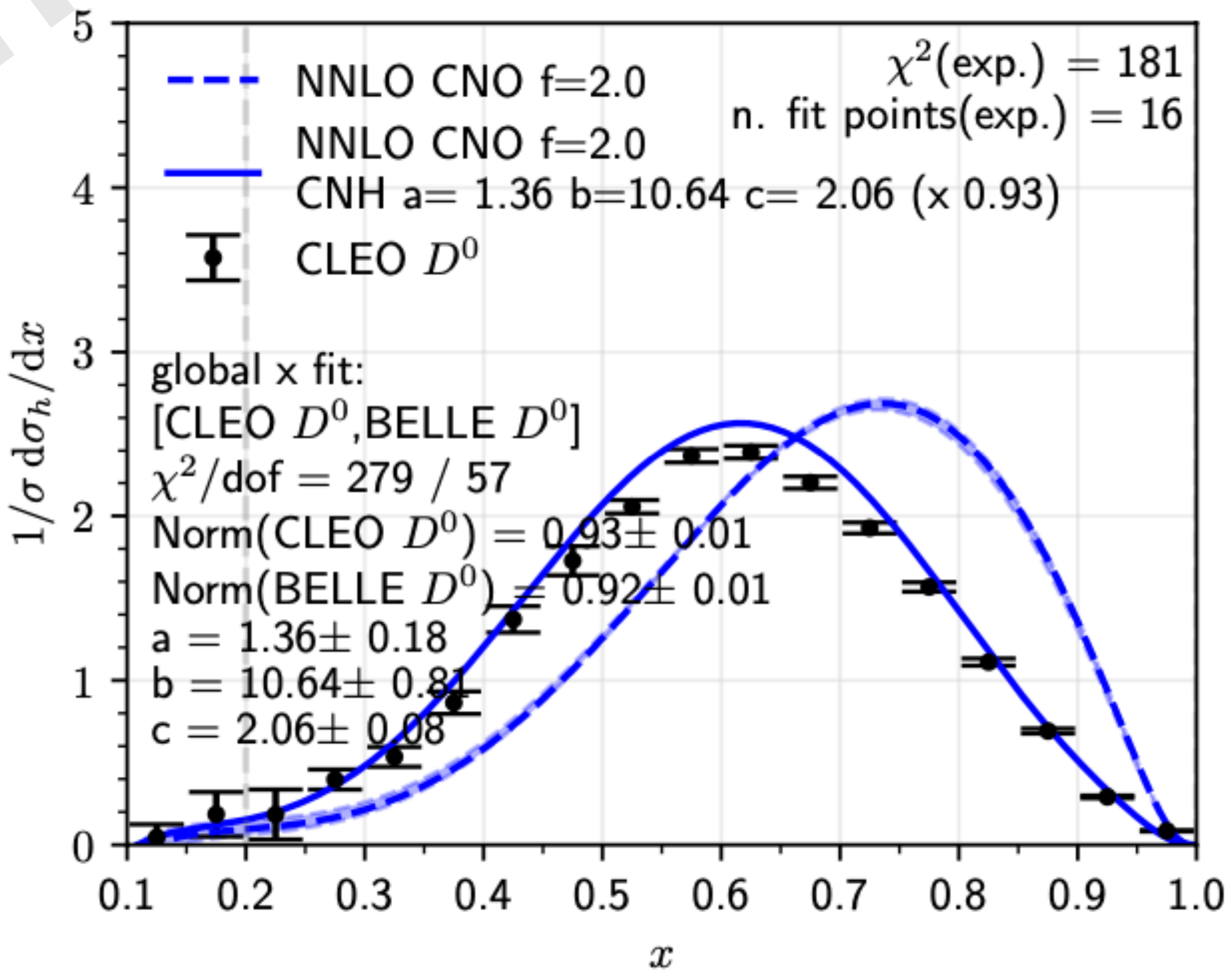
Reasonably good fits can be obtained with few parameters and ‘legacy’ Landau pole regularisation

Global fits to CLEO+Belle charm data









PRELIMINARY

Fit in N-space with

$$D^K_{\rm NP}(x) = (a+1)(a+2)x^a(1-x)$$

(Kartvelishvili et al.)

Fit in x-space with

$$D^{CNH}_{\rm NP}(x) = \frac{1}{1+c}\left[\delta(1-x) + cN^{-1}_{a,b}(1-x)^a x^b\right]$$

(Colangelo-Nason + hard component)

Good fits harder to come by, more parameters and tweaks to Landau pole regularisation needed

Conclusions

- Long history of heavy quark fragmentation
  - Renewed recent interest
  - Multiple implementations available, at least at NNLO+NNLL accuracy

- Our own work does not seem to show a systematic improvement going from NL to NNL accuracy. Sometimes, especially for charm, it’s quite the contrary.

- A strong dependence on the choice of the regularisation procedure of the Landau pole is observed. This also affects the perturbative convergence of the resummed predictions

- Perspectives:
  - Best case (but unlikely….) scenario: petition for the existence of a new heavy quark with 30 GeV mass
  - Realistic scenario: the interface between the perturbative and non-perturbative regions, and how it affects phenomenology, likely deserves further study