A determination of $\alpha_s(m_Z)$ at aN^{3}LO$_{\text{QCD}}\otimes$NLO$_{\text{QED}}$ from NNPDF4.0

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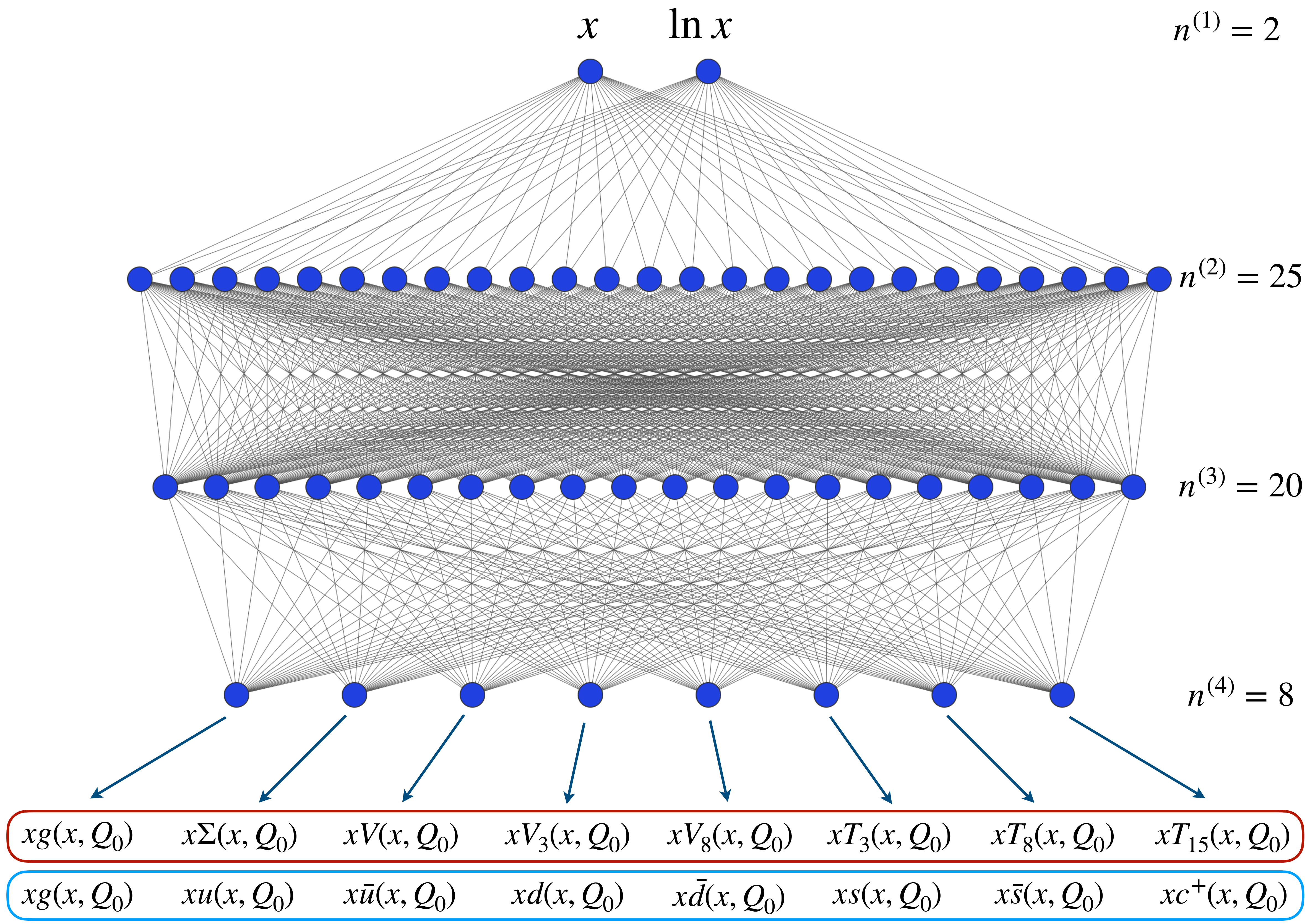
Stony Brook, 7 May 2025

- Updates since α_s from NNPDF3.1

α_s from NNPDF4.0

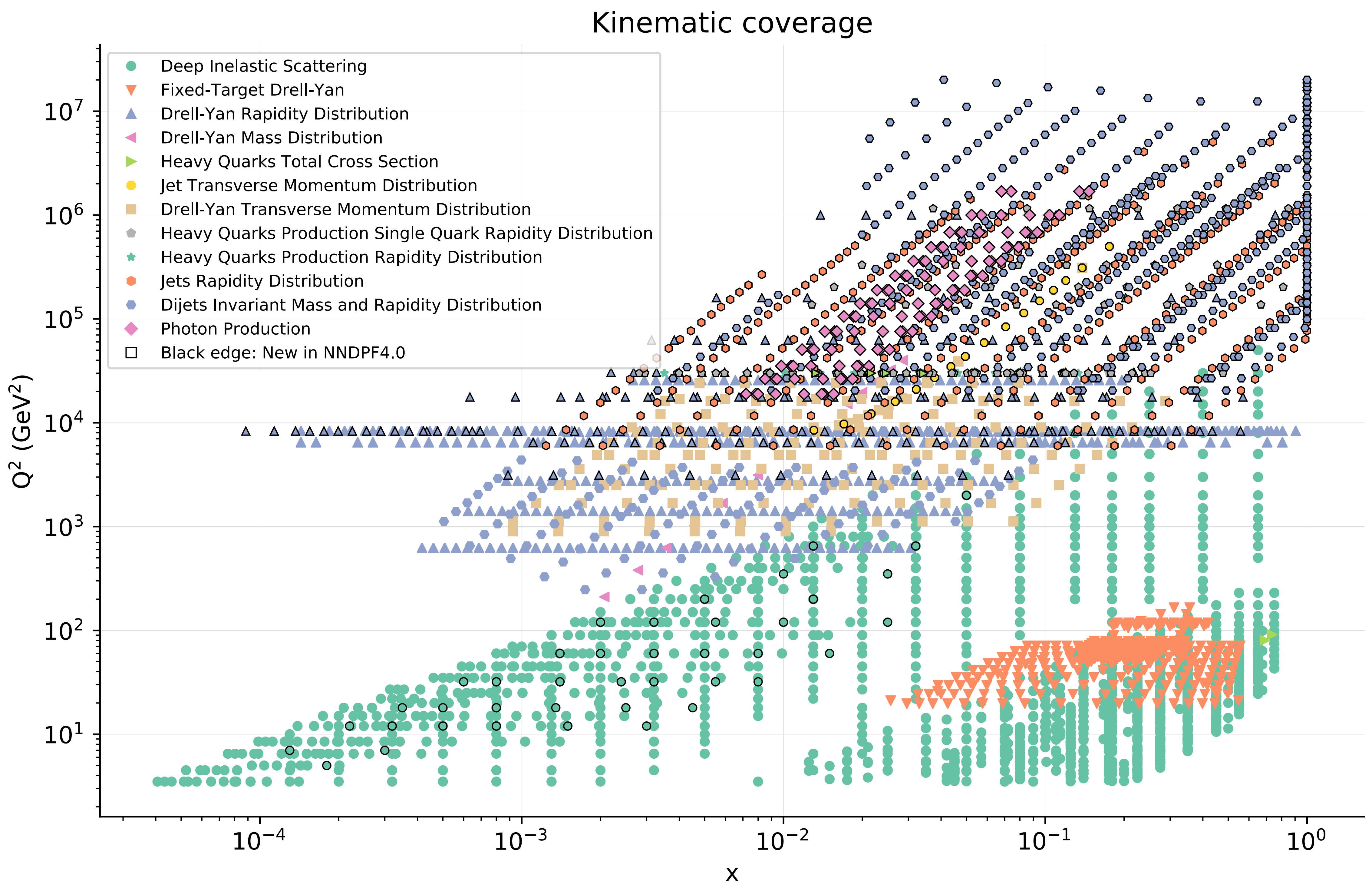
Last determination was based on NNPDF3.1. Lost of progress since then:

- Updated Machine Learning methodology [NNPDF:2109.02653]
  - Stochastic gradient descent
  - Hyperoptimization
  - Validated with closure tests
- NNPDF4.0 global dataset [NNPDF:2109.02653]
  - ~400 more datapoints, mostly from the LHC
  - Many new processes
- Missing higher order uncertainties at the level of the fit [NNPDF, 2401.10319]
- NLO QED and photon PDF [NNPDF:2401.08749]
- aN3LO QCD [NNPDF:2402.18635]



Big impact due to new treatment of theory uncertainty

- In NNPDF3.1 the **dominant source of uncertainty** was from **missing higher orders (MHOU)**:
  $\alpha_s(m_Z) = 0.1185(5)^{\mathrm{PDF}}(1)^{\mathrm{meth}}\boxed{(11)^{\mathrm{MHOU}}} = 0.1185(12)$
- Obtained from NNLO-NLO shift
  $$\Delta\alpha_s^{\mathrm{MHOU}} \equiv \frac{1}{2}\left|\alpha_s^{\mathrm{NNLO}} - \alpha_s^{\mathrm{NLO}}\right| = 0.0011$$
- Include a **theory covariance matrix from scale variations** at the level of the fit leads to much reduced uncertainty:
  NNPDF4.0 methodology, NNPDF3.1-like data: $\alpha_s(m_Z) = 0.1188(6)^{\mathrm{PDF+MHOU}}$



Theory uncertainties in PDFs

- To account for theory uncertainties we treat the theory covmat on the same footing as the experimental covmat: $C_{\rm exp} \rightarrow C_{\rm exp} + C_{\rm th}$
- The theory covmat can be constructed as follows:

$$C_{\mathrm{MHOU},ij} \propto \sum_{\kappa_f,\kappa_r} \Big(T_i(\kappa_f,\kappa_r) - T_i(0,0)\Big)\Big(T_j(\kappa_f,\kappa_r) - T_j(0,0)\Big)$$

Fit without theory uncertainties **Fit with theory uncertainties**

$$\chi^2 = \left(-\frac{1}{2}(T-D)^T C_{\rm exp}^{-1}(T-D)\right) \longrightarrow \chi^2 = \left(-\frac{1}{2}(T-D)^T (C_{\rm exp}+C_{\rm th})^{-1}(T-D)\right)$$

PDFs at approximate N^{3}LO

DGLAP evolution from EKO: github.com/NNPDF/eko

DIS coefficients from Yadism: github.com/NNPDF/yadism

A PDF fit requires several theory inputs:

- **DGLAP splitting functions**
  small-x and large-x limits
  Mellin moments
- **Matching conditions for variable flavor number schemes**
  Now exactly known but original aN3LO publications use approximations
- **DIS coefficient functions**
  Massless known, massive limits known
- **Hadronic cross-section**
  Not much is known

Strategy:

- When N^{3}LO theory is known, it is **used**
- When partial information is available, use it while accounting for **parametrisation uncertainty**
- When it is unknown account for **missing higher order uncertainty**

N^{3}LO QCD corrections in PDF determination

Splitting Functions (information is partial)

Singlet (P_{qq}, P_{gg}, P_{gq}, P_{qg})
- large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
- small-x limit [JHEP 06 (2018) 145]
- large-x limit [NPB 832 (2010) 152; JHEP 04 (2020) 018; JHEP 09 (2022) 155]
- 5 (10) lowest Mellin moments [PLB 825 (2022) 136853; ibid. 842 (2023) 137944; ibid. 846 (2023) 138215]

Non-singlet ($P_{NS,v}$, $P_{NS,+}$, $P_{NS,-}$)
- large-n_f limit [NPB 915 (2017) 335; arXiv:2308.07958]
- small-x limit [JHEP 08 (2022) 135]
- large-x limit [JHEP 10 (2017) 041]
- 8 lowest Mellin moments [JHEP 06 (2018) 073]

DIS structure functions (F_L, F_2, F_3)
- DIS NC (massless) [NPB 492 (1997) 338; PLB 606 (2005) 123; NPB 724 (2005) 3]
- DIS CC (massless) [Nucl.Phys.B 813 (2009) 220]
- massive from parametrisation combining known limits and damping functions [NPB 864 (2012) 399]

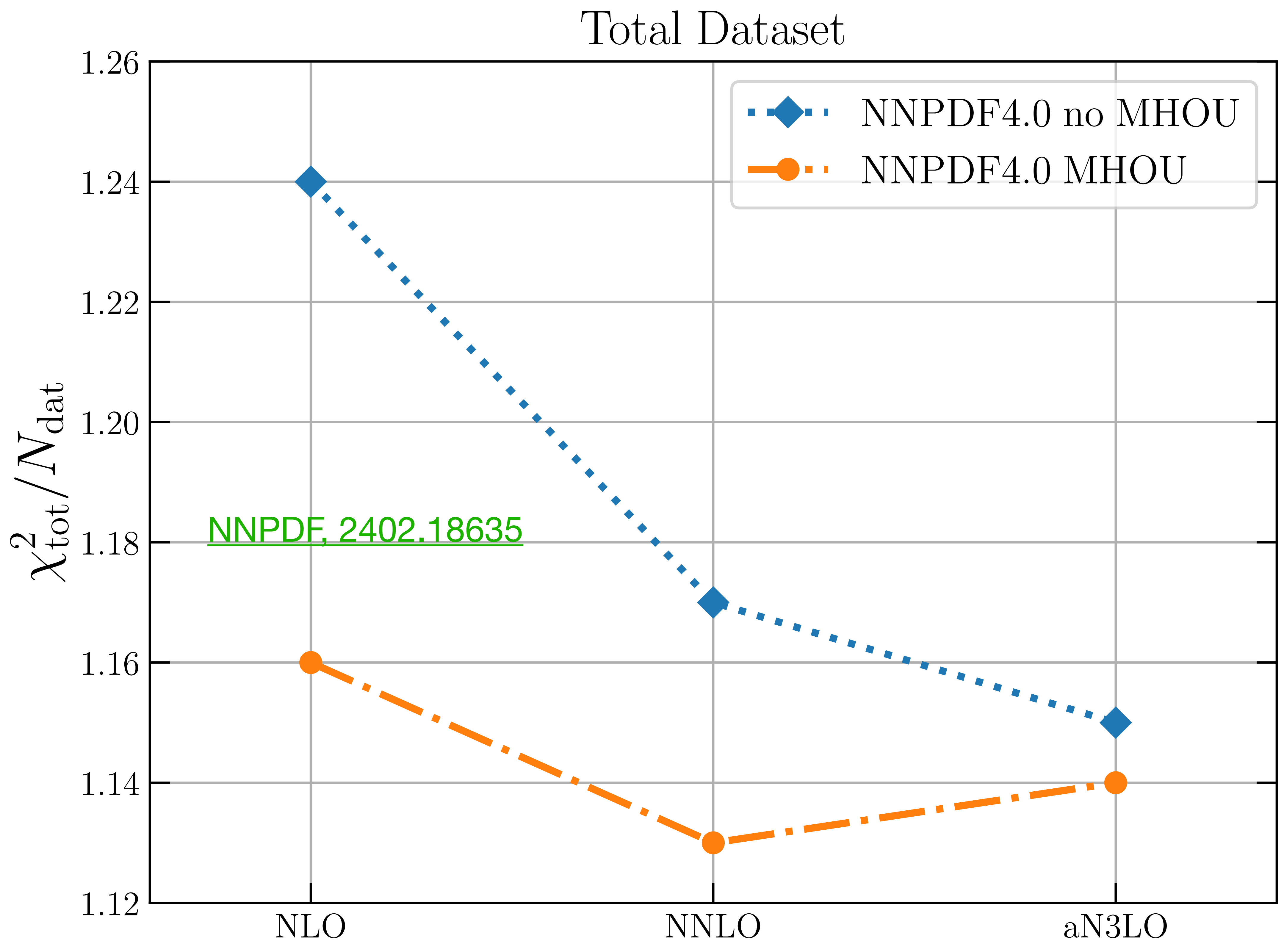
PDF matching conditions
- all known except for $a_{H,g}^3$ [NPB 820 (2009) 417; NPB 886 (2014) 733; JHEP 12 (2022) 134]

Coefficient functions for other processes
- DY (inclusive) [JHEP 11 (2020) 143]; DY (y differential) [PRL 128 (2022) 052001]

Emanuele R. Nocera (UNITO) | Progress from NNPDF | 5 August 2024 | 12 / 25

E. Nocera, Workshop on Hadron Physics and Opportunities Worldwide
Dalian, China, August 2024
(More is known today!)

Fit quality



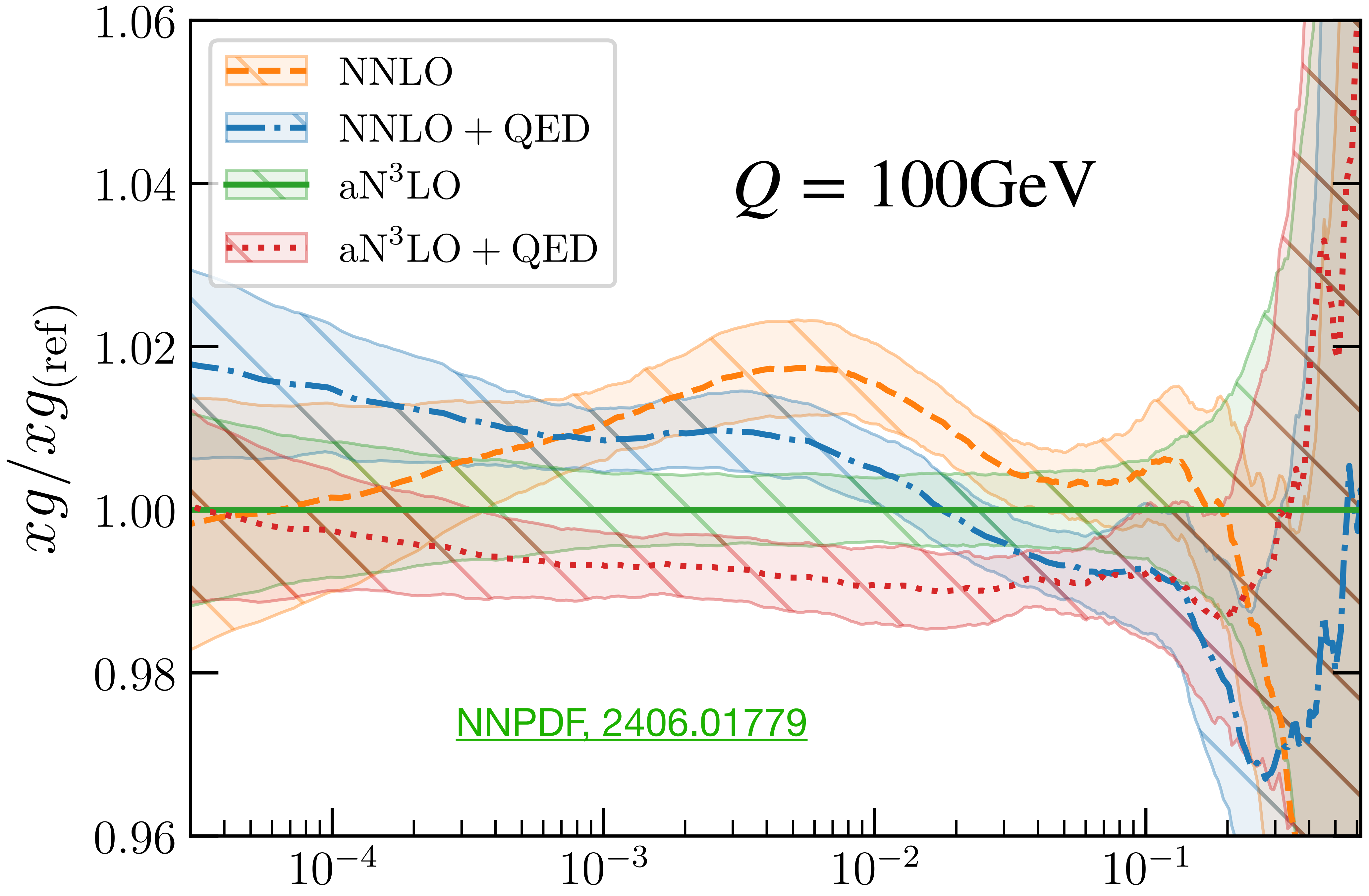
- Without MHOUs the fit improves (lower χ^2) with increasing perturbative order for both NNPDF and MSHT
- With MHOUs the fit depends only weakly on the perturbative order
- At N^{3}LO MHOUs have a small impact on the χ^2

QED corrections and photon PDF

NNPDF4.0QED means:

- NLO QED corrections
  $P = P_{QCD} + P_{QCD\otimes QED}$
  $P_{QCD\otimes QED} = \alpha_{em} P^{(0,1)} + \alpha_{em}\alpha_s P^{(1,1)} + \alpha_{em}^2 P^{(0,2)}$
- Photon PDF

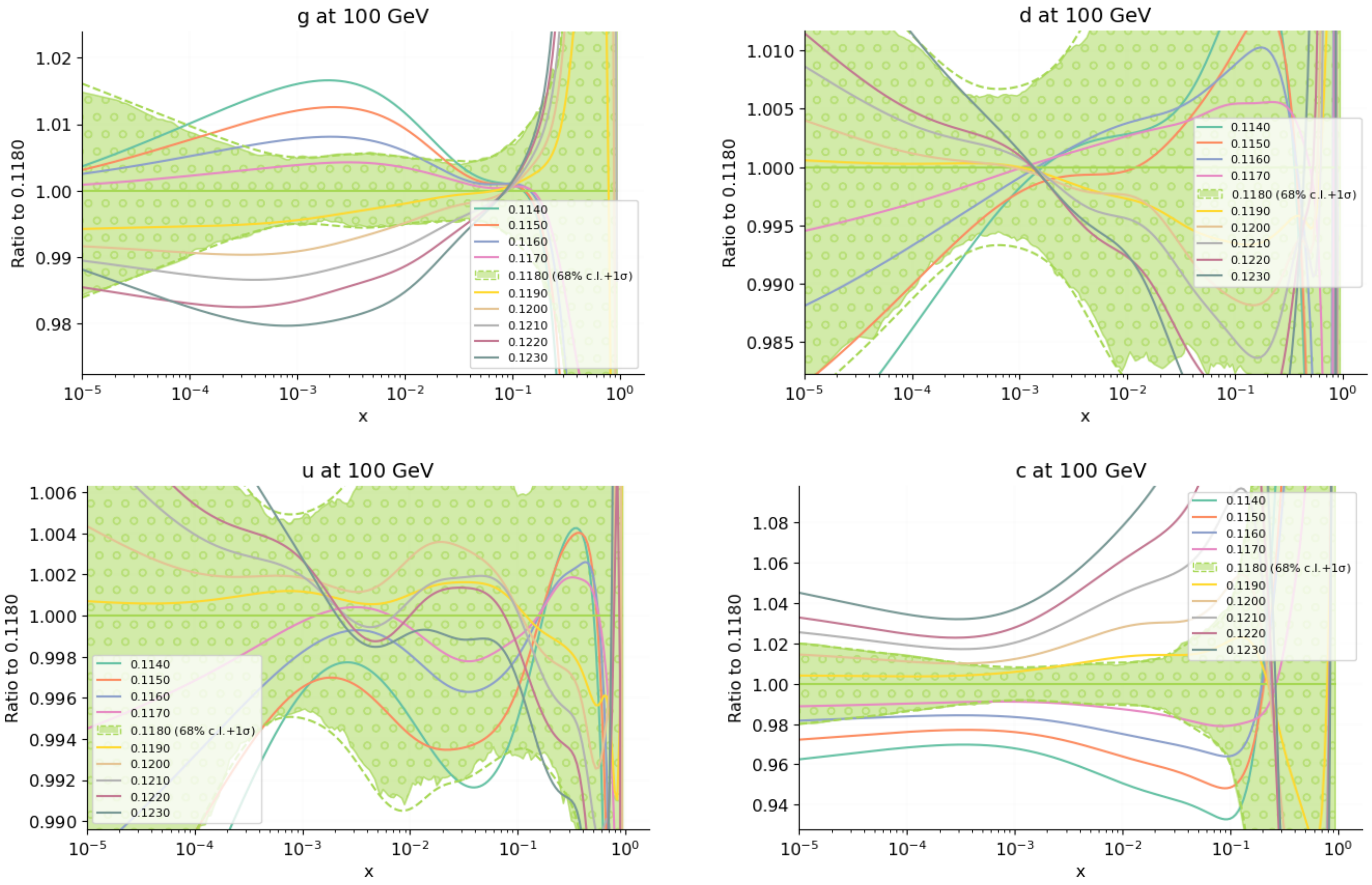
PDFs at $\mathrm{aN^3LO_{QCD}} \otimes \mathrm{NLO_{QED}}$ with photon PDF represents the **most accurate PDFs**



- Photon subtracts momentum from the gluon PDF
- QED effect similar in magnitude to aN3LO corrections

- α_s from PDF fits

PDFs and α_s are correlated



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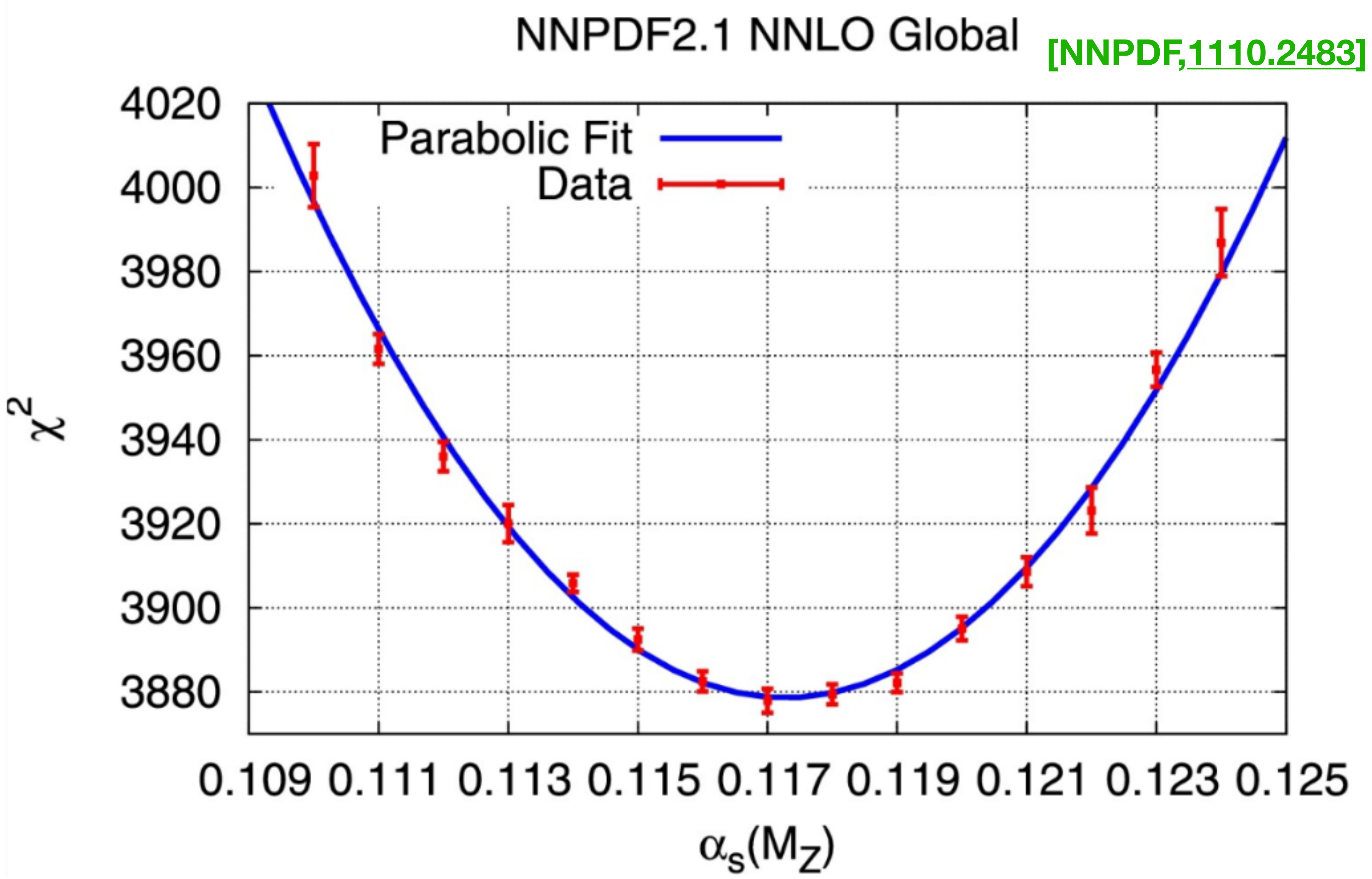
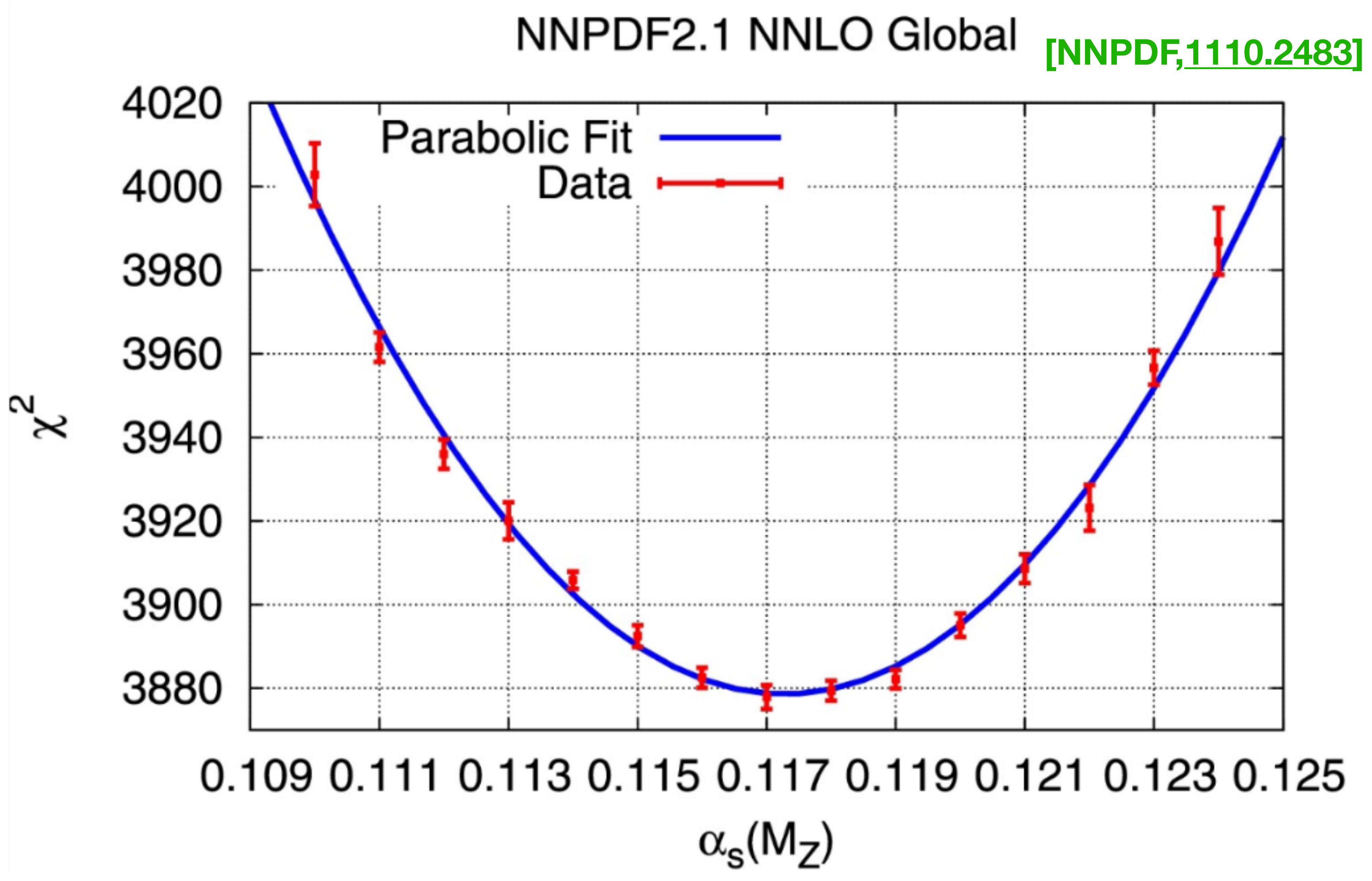


[NNPDF,1110.2483]

In many cases α_s is determined by extracting it from a parabolic fit to the χ^2 profile

PDFs and α_s are correlated



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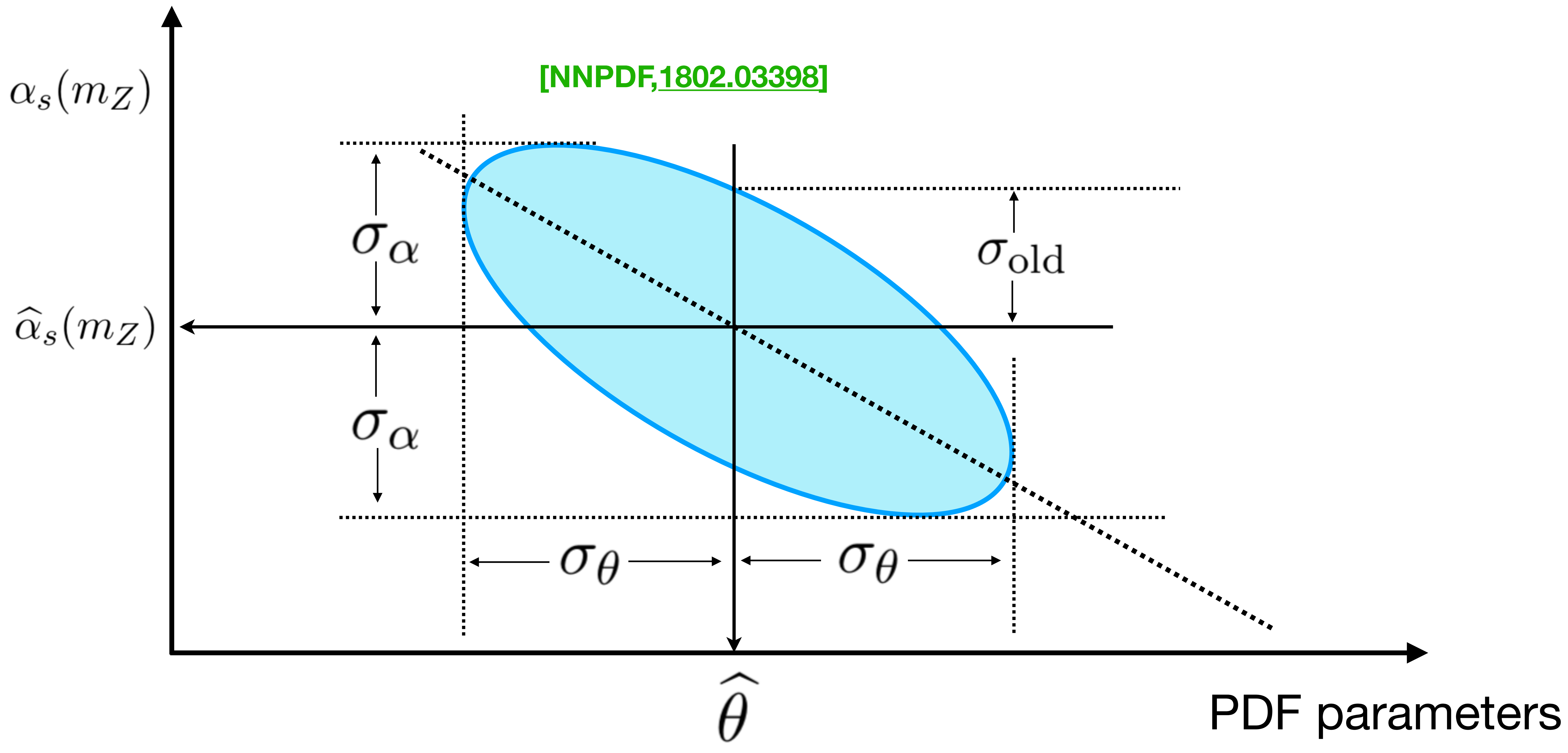

In this way correlations between PDF parameter fluctuations and α_s are not fully taken into account

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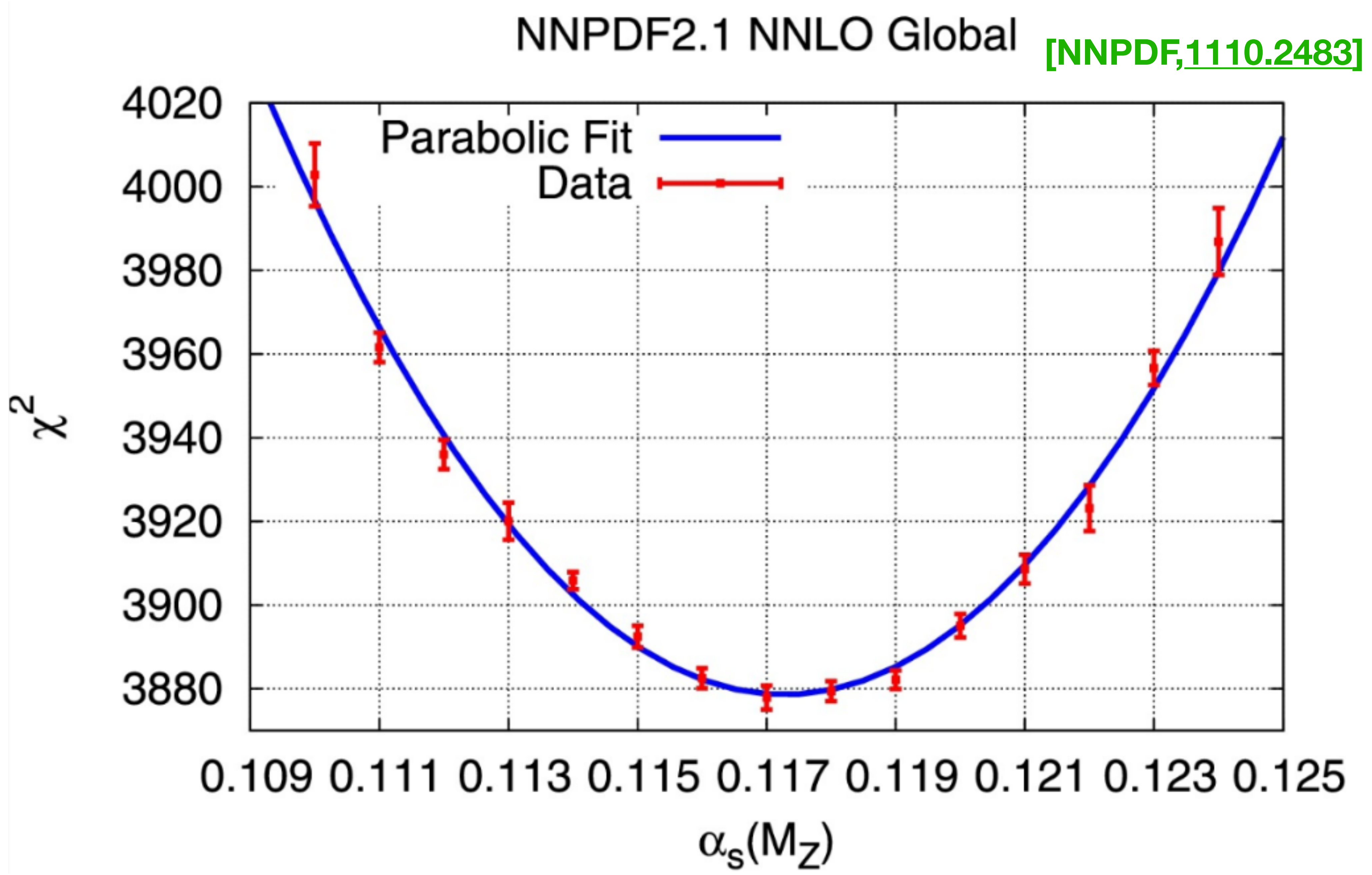

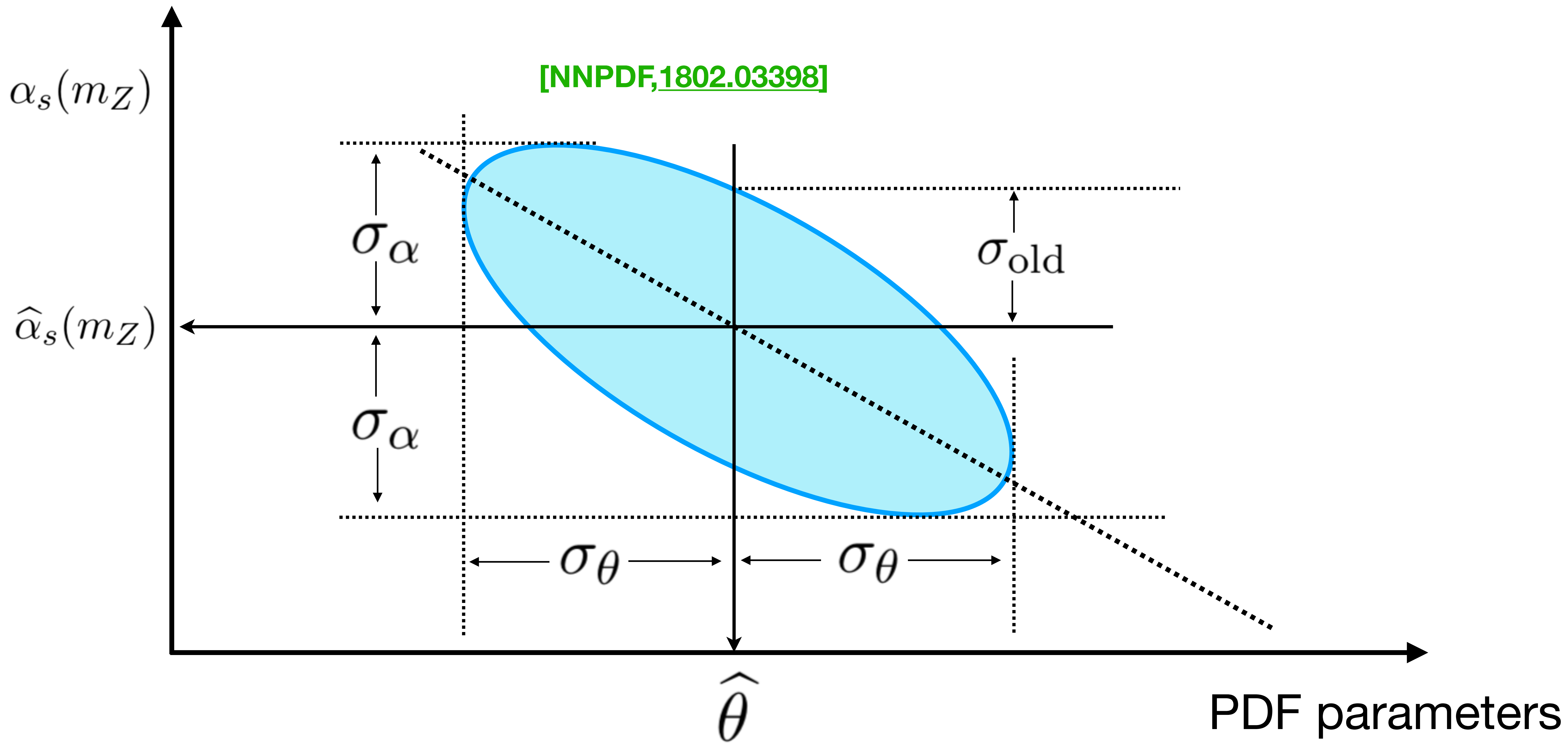

In many cases α_s is determined by extracting it from a parabolic fit to the χ^2 profile

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Ideally minimise α_s and PDF simultaneously

How to account for correlations between PDFs and α_s?

NNPDF can't (easily) treat α_s as another trainable parameter

Rerunning Monte Carlo generators and DGLAP evolution at every training step is not feasible, therefore predictions are stored in precomputed grids

Unlike partonic cross-sections, DGLAP is not a simple expansion in α_s

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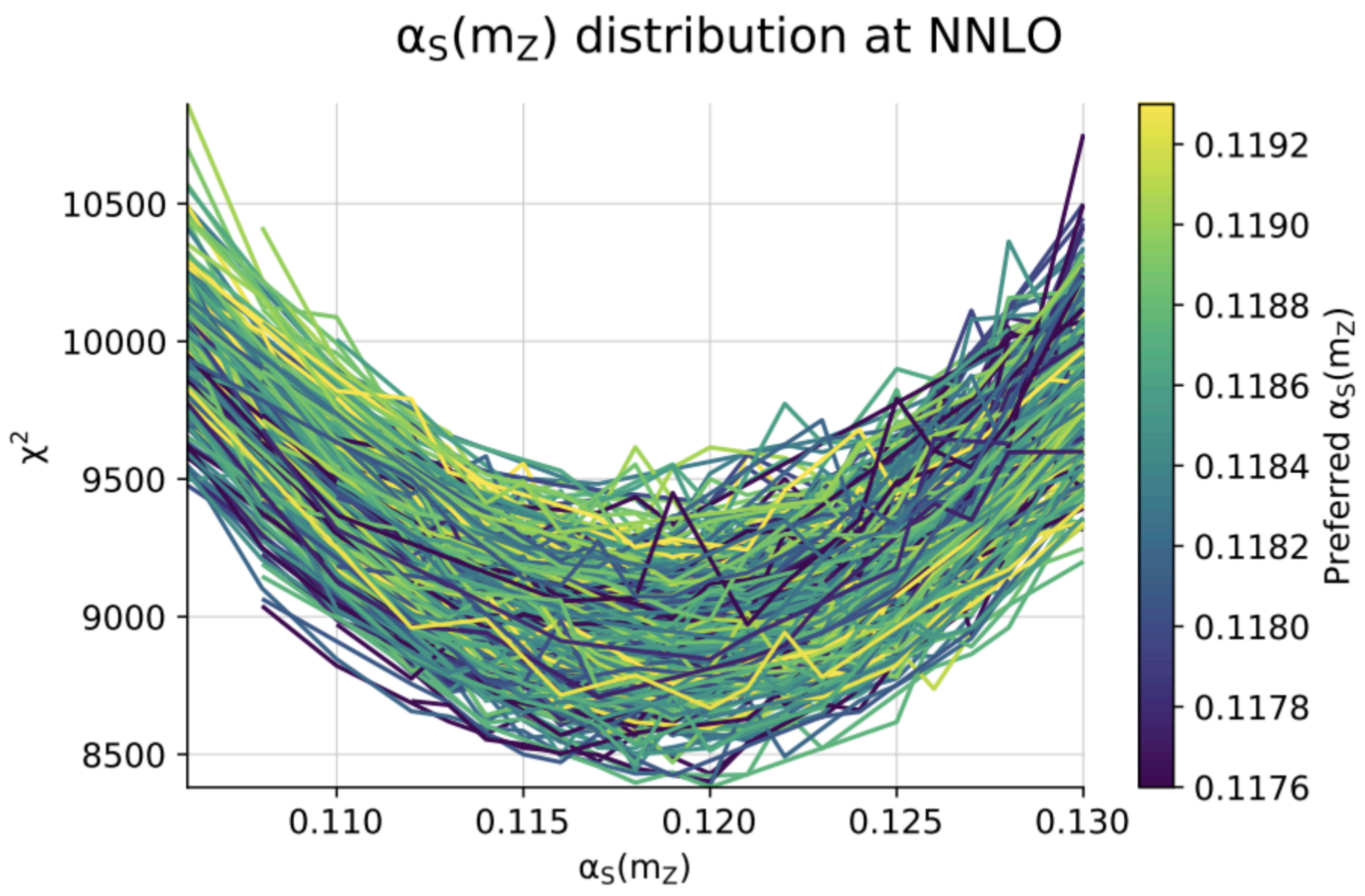
Unlike partonic cross-sections, DGLAP is not a simple expansion in α_s

Two methods have been developed to avoid this limitation:

1) **Multiple fits** of the same data replica, changing only the value of $\alpha_s(m_Z)$, thereby **correlating PDFs** at different $\alpha_s(m_Z)$
   [NNPDF, 1802.03398]
2) Based on **a single fit** with an $\alpha_s(m_Z)$ **theory covmat,** and computing the fit's preferred value for alphas a posteriori in a Bayesian framework
   [Ball, Pearson, 2105.05114]



Correlated replicas fitted to the same data replica at different α_s

- Results

Many effects studied….

Definition of the bias-variance ratio

The bias variance ratio as computed by Andrea was defined as the mean of the ratios. Note that averages are computed as the average over the bootstrap sample, not the exact value o

Is the unc computed correctly? (waiting response from Andrea)

Settings		(as for PDFs)
CRM min		28
CRM min (		08
CRM_min_quartic	0.856241 ± 0.118033	0.863550 ± 0.116322
CRM lin singlebatch	0.934201 ± 0.099931	0.951168 ± 0.099192
CRM mean	0.956343 ± 0.108697	0.958840 ± 0.105729
CMR_mean_alpha	19.50692 ± 4.440705	11.14937 ± 1.992662
CRM_mean_alternative	2.697771 ± 0.304362	2.727734 ± 0.297442
CRM mean (fullsample)	0.894193 ± 0.100804	0.905534 ± 0.099769
PFM	0.896151 ± 0.111656	0.898179 ± 0.111422
TCM	1.137260 ± 0.106517	1.138338 ± 0.109129
CRM LOG min	1.144239 ± 0.184387	1.099132 ± 0.173814
CRM LOG min (cubic)	0.860679 ± 0.121940	0.859844 ± 0.115734
CRM LOG min (quartic)	0.858068 ± 0.120877	0.860889 ± 0.117834

Main results

This table contains the main results. They are all done with EXA evolution and without PDF positivity at small-x.

Settings	TCM	CRM	EXP
NNPDF3.1-like	0.11894 ± 0.00054	0.11889 ± 0.00047	0.11864 ± 0.00043
NNPDF3.1-like, MHOU	0.11900 ± 0.00071		
NNLO	0.12050 ± 0.00035	0.12063 ± 0.00036	0.12045 ± 0.00028
NNLOxQED	0.12092 ± 0.00034	0.12103 ± 0.00037	0.12078 ± 0.00027
NNLO, MHOU	0.11990 ± 0.00071	0.11990 ± 0.00063	0.11991 ± 0.00045
NNLOxQED, MHOU	0.12023 ± 0.00058	0.12014 ± 0.00064	0.12017 ± 0.00044
N3LO, 3pt	0.11867 ± 0.00053	0.11865 ± 0.00052	0.11871 ± 0.00038
N3LOxQED, 3pt	0.11871 ± 0.00053	0.11875 ± 0.00052	0.11862 ± 0.00038
N3LO, MHOU	0.11915 ± 0.00071	0.11913 ± 0.00069	0.11902 ± 0.00050
N3LOxQED, MHOU	0.11943 ± 0.00068	0.11949 ± 0.00067	0.11931 ± 0.00050
N3LOxQED, MHOU, sample t0	0.11932 ± 0.00071	0.11932 ± 0.00070	0.11927 ± 0.00049

	0.12023 ± 0.00035	0.12034 ± 0.00038	0.12018 ± 0.00027	nnlo.pdf
QED	0.12092 ± 0.00034	0.12103 ± 0.00037	0.12078 ± 0.00027	nnlo_qed.pdf
MHOU	0.11936 ± 0.00072	0.11944 ± 0.00071	0.11961 ± 0.00043	nnlo_mhou.pdf
QED, MHOU	0.12023 ± 0.00058	0.12014 ± 0.00064	0.12017 ± 0.00044	nnlo_qed_mhou.pdf

metric pseudodata cuts

CRM is with pseudodata resampling

iteration of 240619-01-rs-nnpdf40-alphas-tcm-mhou

alphas-tcm-mhou-notopjet

alphas closure tests

Created by Roy Stegeman, last modified on Apr 27, 2025

Settings	Rbv	weighted mean	bootstrapped mean
CRM, no pos, no int, 25 L1	0.793875 ± 0.085003	0.118044 ± 0.000078	0.118022 ± 0.000065
CRM, no pos, 25 L1			
CRM, no pos, no int, 25 L1, don't fix t0theoryid (d'Agostini bias)	3.831740 ± 0.160884	0.119450 ± 0.000077	0.119447 ± 0.000056
TCM, baseline, 100 L1	0.803437 ± 0.056767	0.118132 ± 0.000039	0.118136 ± 0.000027
TCM, no pos, no int, 100 L1	0.718230 ± 0.043797	0.117997 ± 0.000040	0.118002 ± 0.000031
TCM, no pos, 100 L1	0.705975 ± 0.047318	0.117984 ± 0.000041	0.117985 ± 0.000029
TCM, no pos, no int, 25 L1, faketheoryid=0.118, prior assumption = 0.119	0.795496 ± 0.076737	0.118105 ± 0.000080	0.118101 ± 0.000059
TCM, no pos, no int, 25 L1,	0.729069 ± 0.070595	0.118014 ± 0.000081	0.118013 ± 0.000061

	weighted mean	bootstrapped mean
3759	0.118138 ± 0.000178	0.118146 ± 0.000092
0307	0.118124 ± 0.000111	0.118124 ± 0.000111
970	0.118116 ± 0.000178	0.118121 ± 0.000098
055	0.118102 ± 0.000176	0.118128 ± 0.000113
3943	0.118054 ± 0.000178	0.118051 ± 0.000097
320	0.118037 ± 0.000181	0.118043 ± 0.000114
0002	0.118042 ± 0.000182	0.118047 ± 0.000090

Top mass dependence

The mtop=172.5 fits below use k-factors to rescale ATLASTTBARTOT7TEV and CMST

NNLO

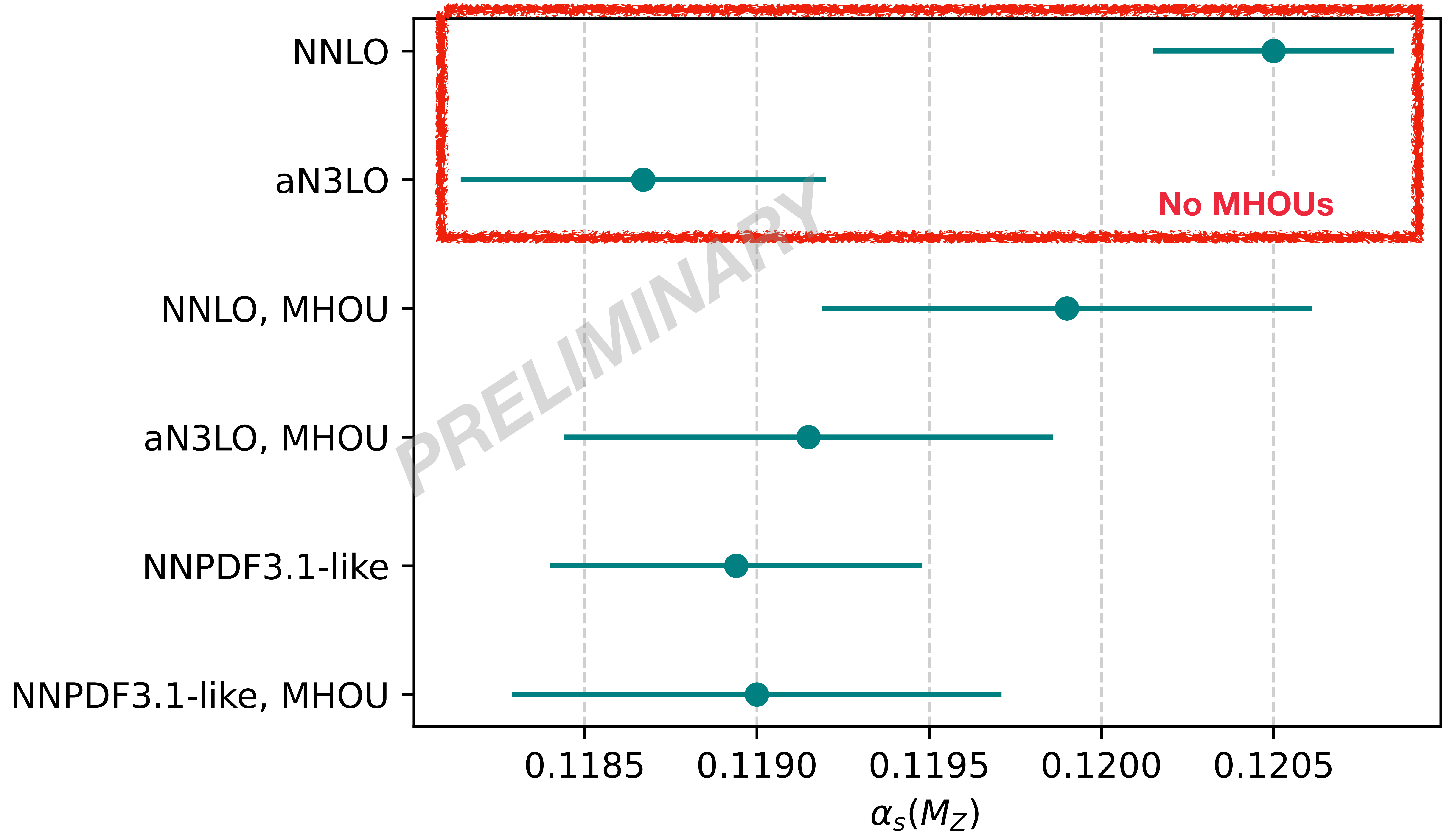
Settings	TCM	CRM	EXP
mtop=175,	0.12077 ± 0.00036	0.12091 ± 0.00031	0.12074 ± 0.00028
mtop=173.2	0.12030 ± 0.00036	0.12058 ± 0.00030	0.12037 ± 0.00028
mtop=172.5	0.12036 ± 0.00037	0.12056 ± 0.00032	0.12040 ± 0.00028
mtop=171.8	0.12022 ± 0.00037	0.12042 ± 0.00040	0.12020 ± 0.00028
mtop=170	0.11992 ± 0.00038	0.12007 ± 0.00040	0.11991 ± 0.00028

Impact of truncated evolution

The results below differ from the table on top only in the evolution, where the first table uses EXA evolution while here we use TR

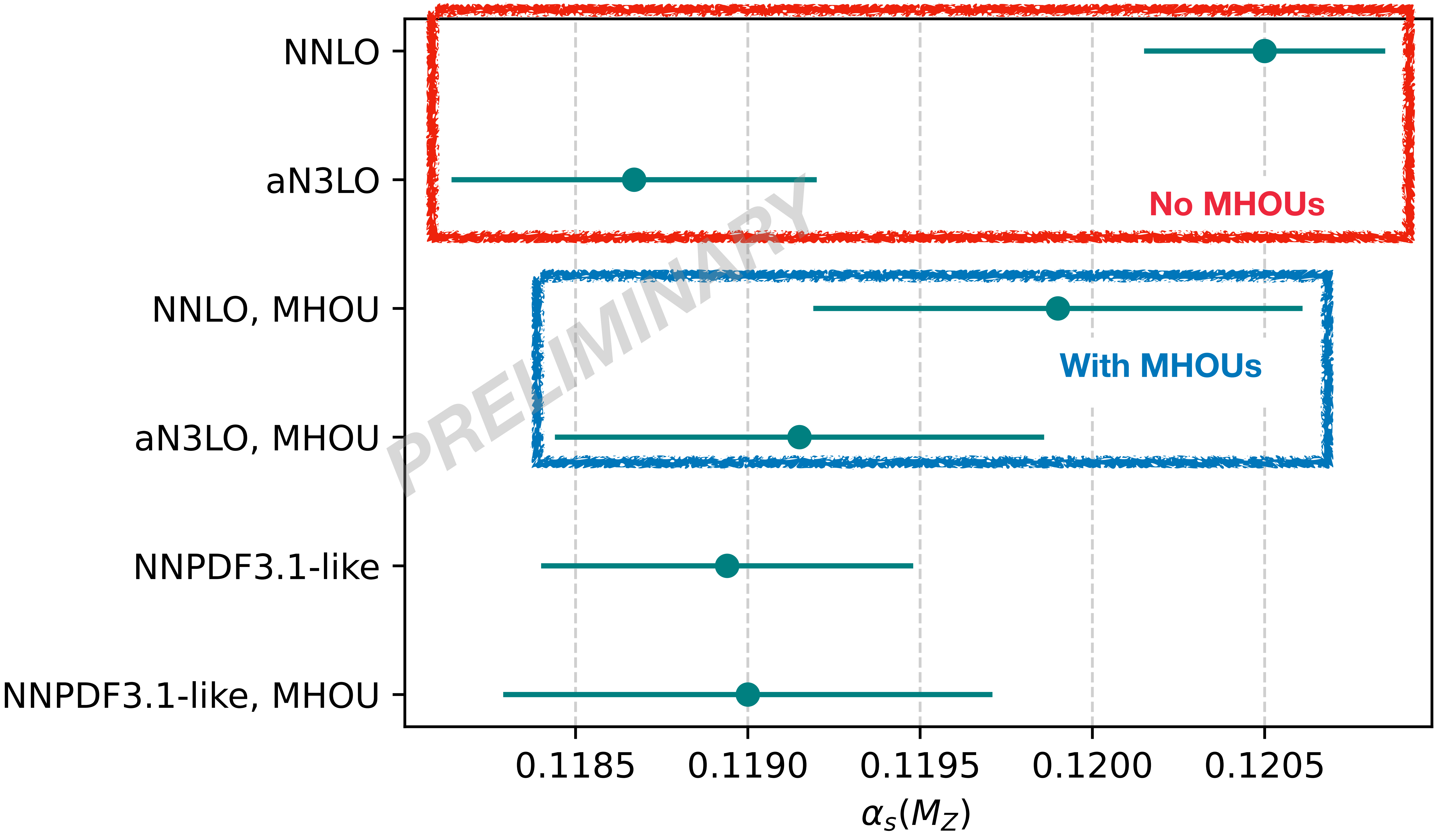
Settings	TCM	CRM	EXP
NNPDF3.1		0.1185 ± 0.0005	
NNPDF3.1-like	0.11876 ± 0.00055	0.11873 ± 0.00053	0.11832 ± 0.00042
NNLO	0.12023 ± 0.00035	0.12036 ± 0.00036	0.12016 ± 0.00027
NNLO, MHOU	0.11946 ± 0.00067	0.11958 ± 0.00063	0.11946 ± 0.00043
N3LO, 3pt	0.11880 ± 0.00054	0.11896 ± 0.00056	0.11899 ± 0.00039
N3LO, MHOU	0.11917 ± 0.00070	0.11942 ± 0.00066	0.11942 ± 0.00050

Impact of missing higher order uncertainties (MHOUs) and aN^{3}LO



These and following results for the NNPDF4.0 dataset

Impact of missing higher order uncertainties (MHOUs) and aN^{3}LO



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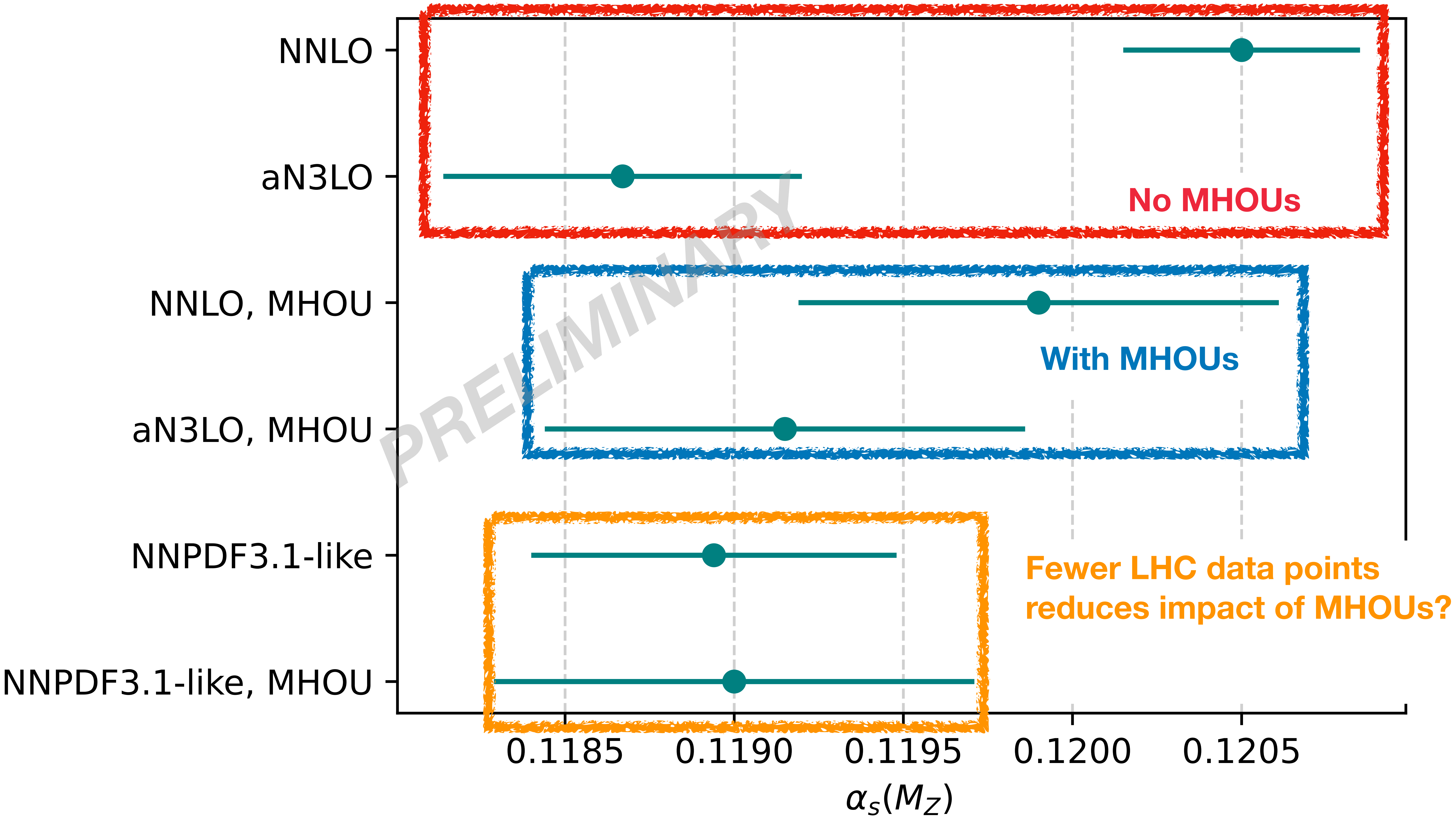
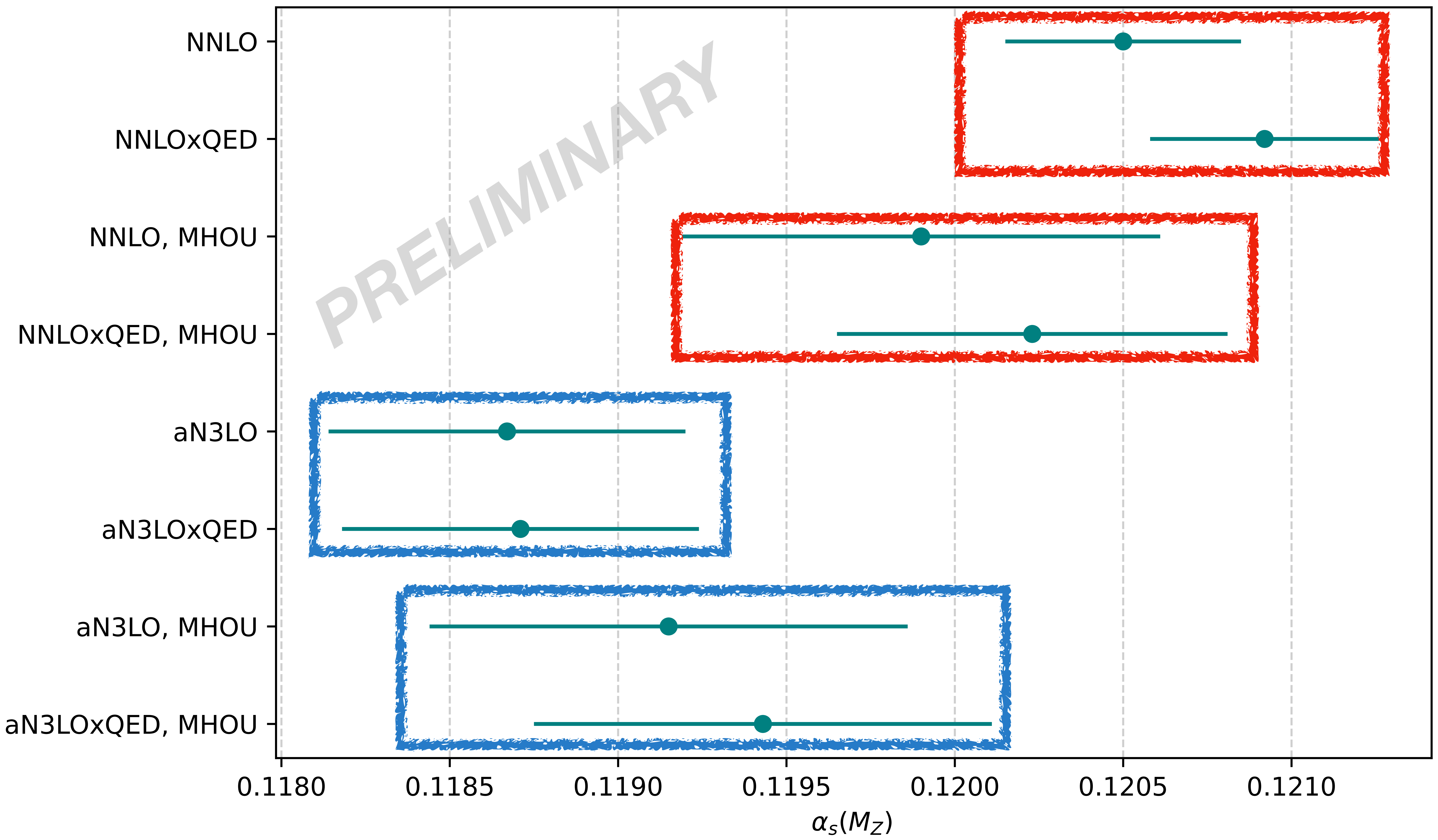


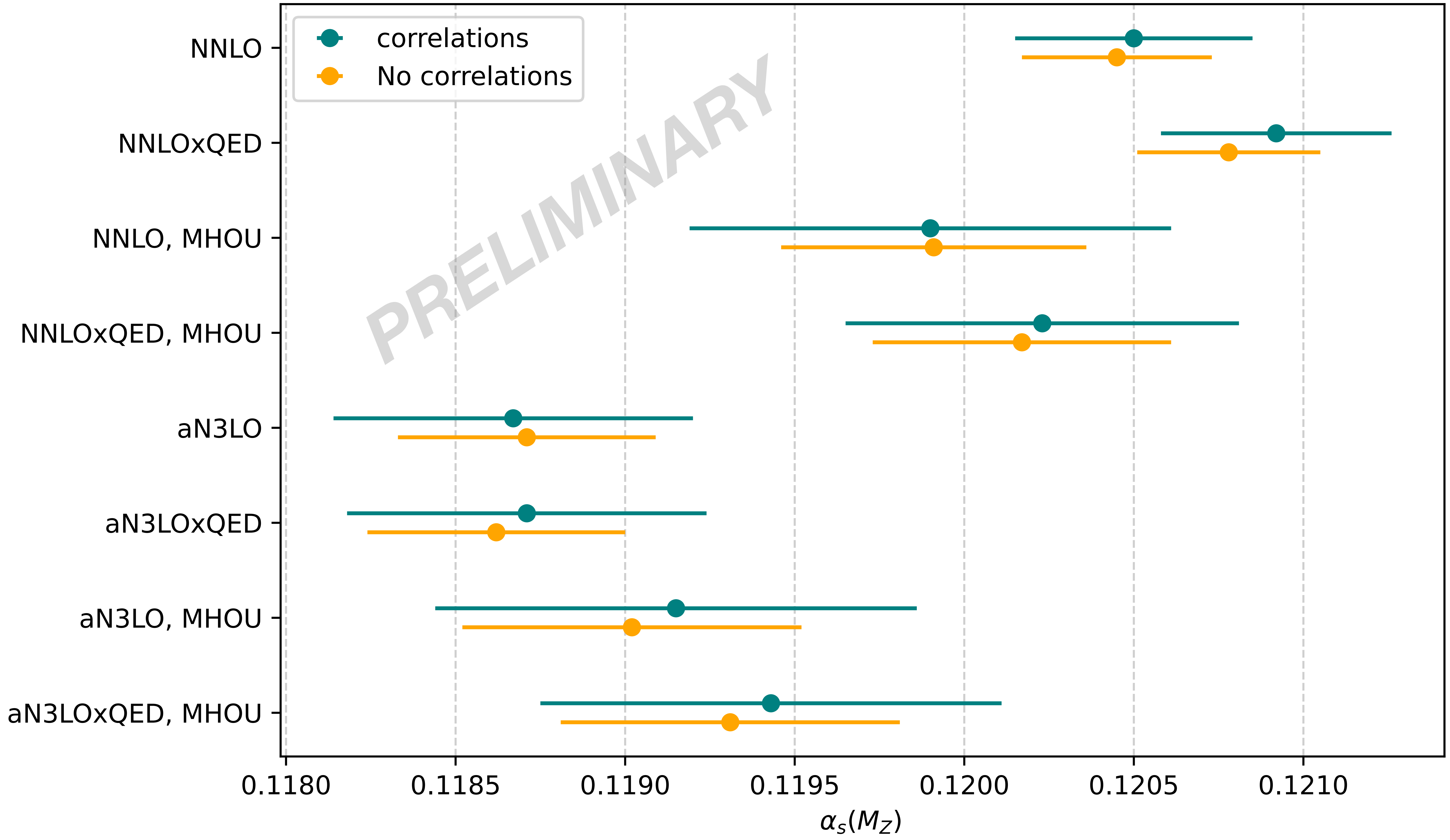
These and following results for the NNPDF4.0 dataset

Impact of QED corrections and the photon PDF



No consistent picture of QED shifts, but clearly QED cannot be neglected

Impact of PDF-α_s correlations



Correlations increase the uncertainty by 25% to 60%

$\alpha_s(m_Z)$ at different values of m_t pole mass

m_t [GeV]	NNLO	NNLO, MHOU
175	0.1208(4)	0.1200(6)
172.5	0.1204(4)	0.1200(7)
170	0.1200(4)	0.1198(6)

PRELIMINARY

- PDG value is $m_t = 172.4(7)$
- Impact is negligible

Q: How to validate the methodologies?

A: Closure tests [Del Debio, Giani, Wilson, 2111.05787]

Basic idea: generate a global pseudo dataset from theory predictions and extract α_s from this

PDFs at input scale Q_0 $\otimes$ **Wilson coefficients + DGLAP depending on α_s** $\rightarrow$ **pseudodata** $\rightarrow$ **methodology** $\rightarrow$ **extracted α_s**

Is α_s the same?*

Q: How to validate the methodologies?

A: Closure tests [Del Debio, Giani, Wilson, 2111.05787]

*

Experimental data is sampled from a distribution, therefore pseudodata = prediction + noise

Basic idea: generate a global pseudo dataset from theory predictions and extract α_s from this

PDFs at input scale Q_0 $\otimes$ **Wilson coefficients + DGLAP depending on α_s** $\rightarrow$ **pseudodata** $\rightarrow$ **methodology** $\rightarrow$ **extracted α_s**

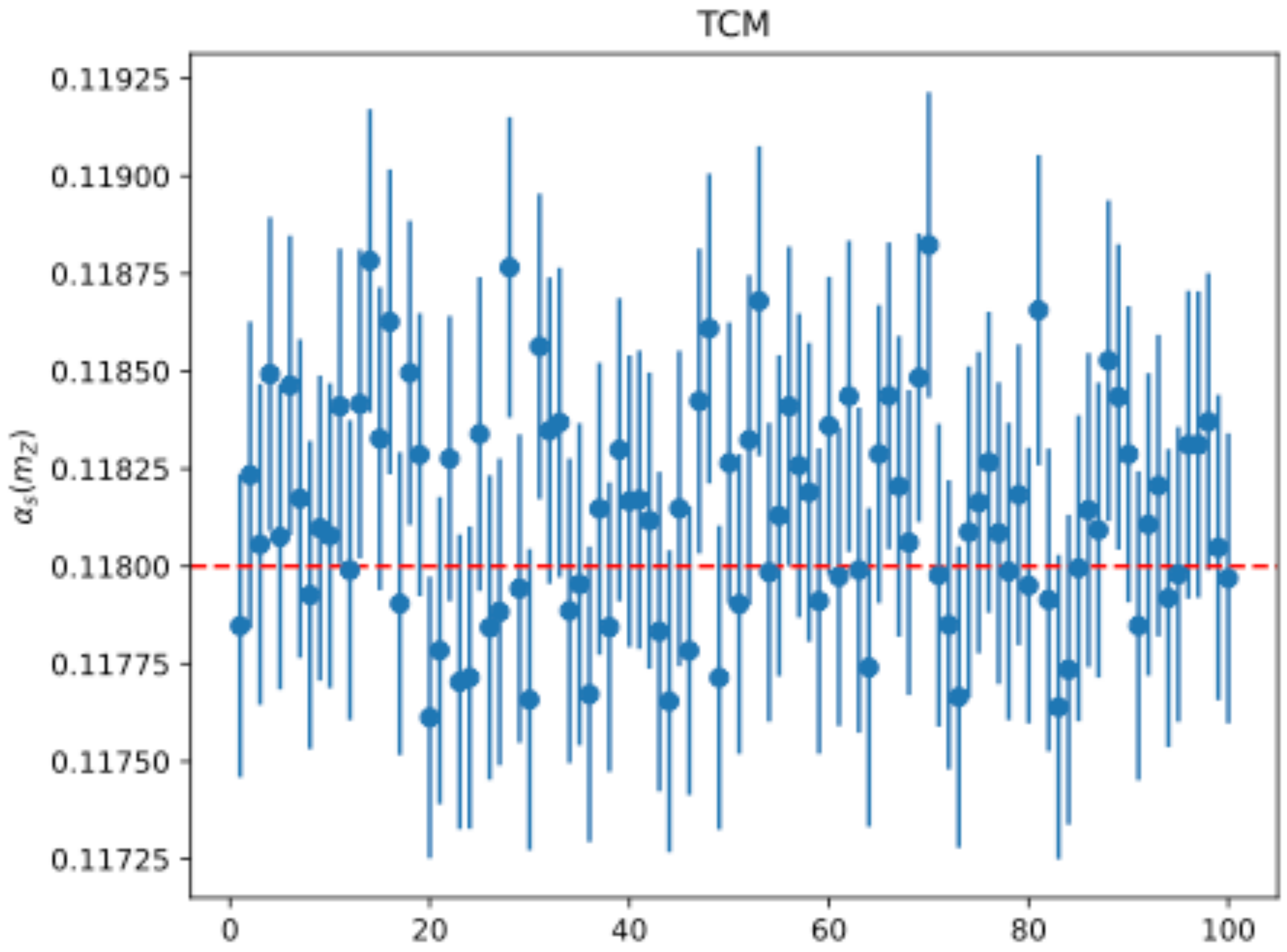
Is α_s the same?*

The closure test suggests a bias…

1) Generate pseudodata samples around $\alpha_s(m_Z) = 0.118$
2) Extract $\alpha_s(m_Z)$ for each pseudodata sample
3) Check if our method returns the correct answer ❌

We find a three-sigma indication for a bias!

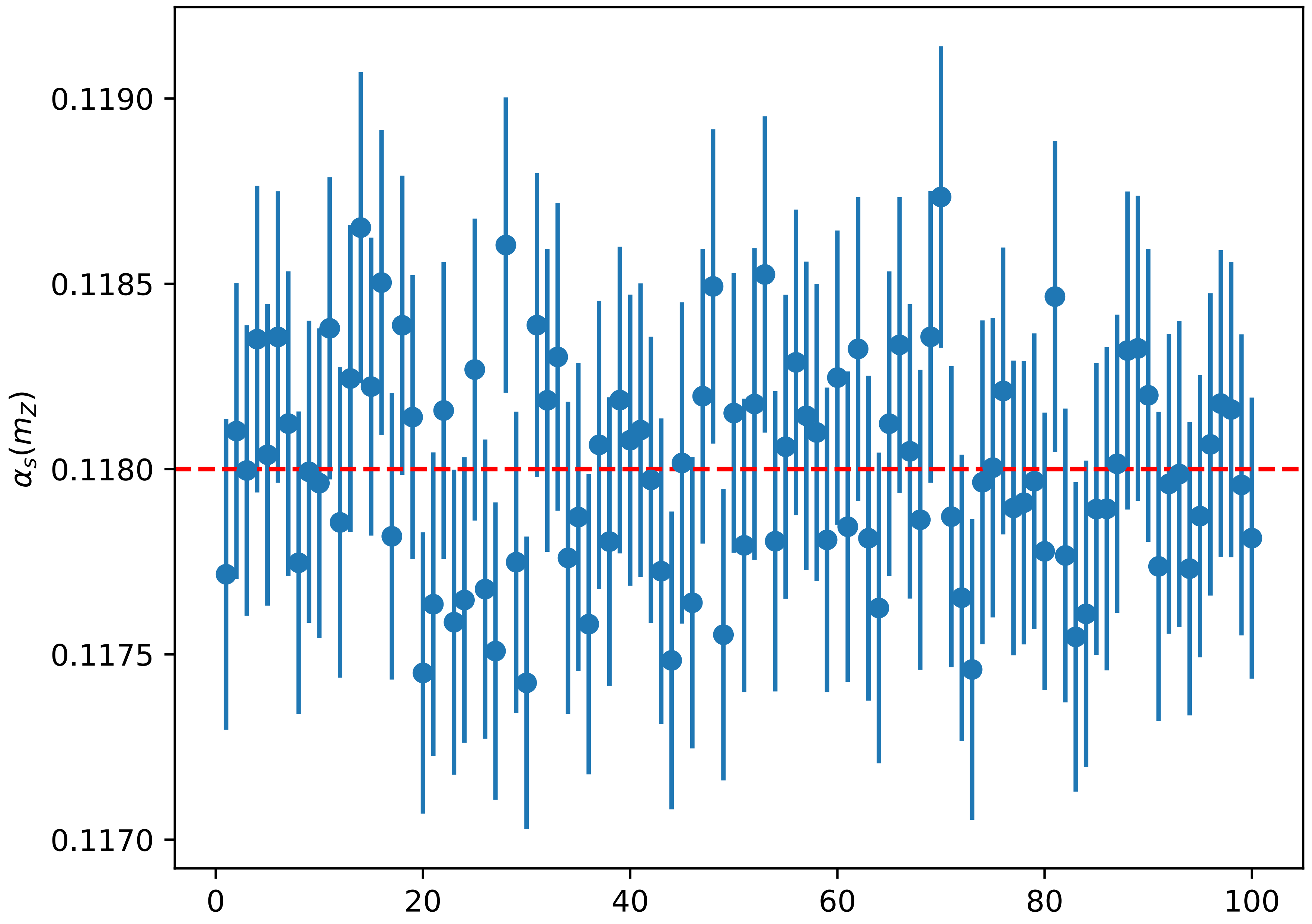
$\alpha_s(m_Z) = 0.11813(4)$



…but we can understand the origin!

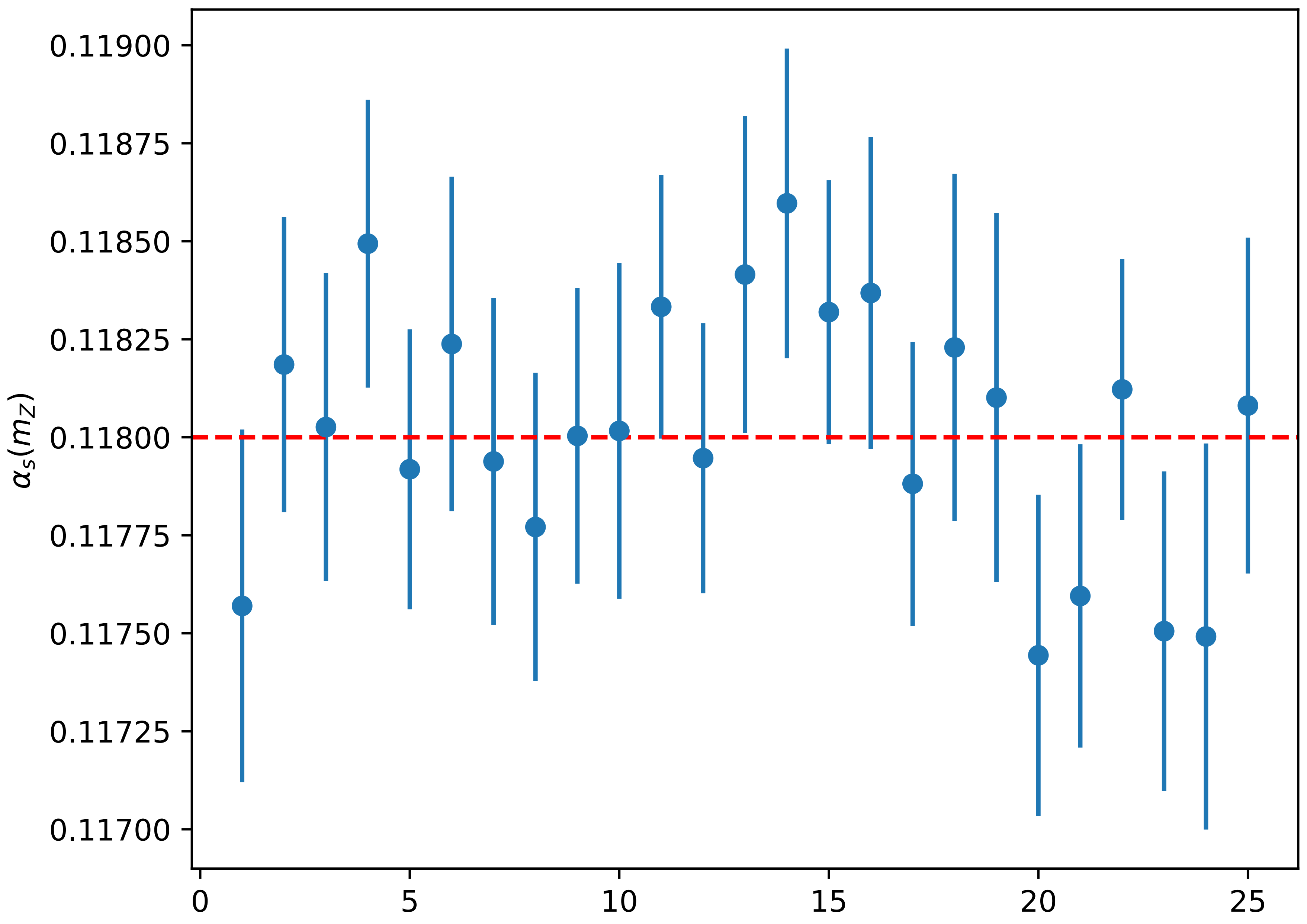
In NNPDF4.0 we enforce positivity of observables not only for the central PDF but for all replicas

Theory covmat method



$\alpha_s(m_Z) = 0.11798(4)$ ✔

Correlated replicas method



$\alpha_s(m_Z) = 0.11804(8)$ ✔

Both methodologies pass the closure test!

But how do we account for this bias?

Accounting for the positivity bias

- Simple solution: remove positivity from the fit

- Actually not so simple: the two methods no longer agree

- Conservative option: add shift due to bias as a linear correction to the uncertainty
  In this case 0.1194-0.1187=0.0007

	Theory covmat	Correlated replicas
with positivity	0.1194(7)	0.1193(7)
W/o positivity	0.1187(9)	0.1191(9)

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	Theory covmat	Correlated replicas
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$$\alpha_s(M_Z)^{\text{aN3LO,QED,MHOU}} = 0.1194^{+0.0007}_{-0.0007}{}^{\text{PDF}}{}_{-0.0007}{}^{\text{positivity}} = 0.1194^{+0.0007}_{-0.0014}$$

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PRELIMINARY

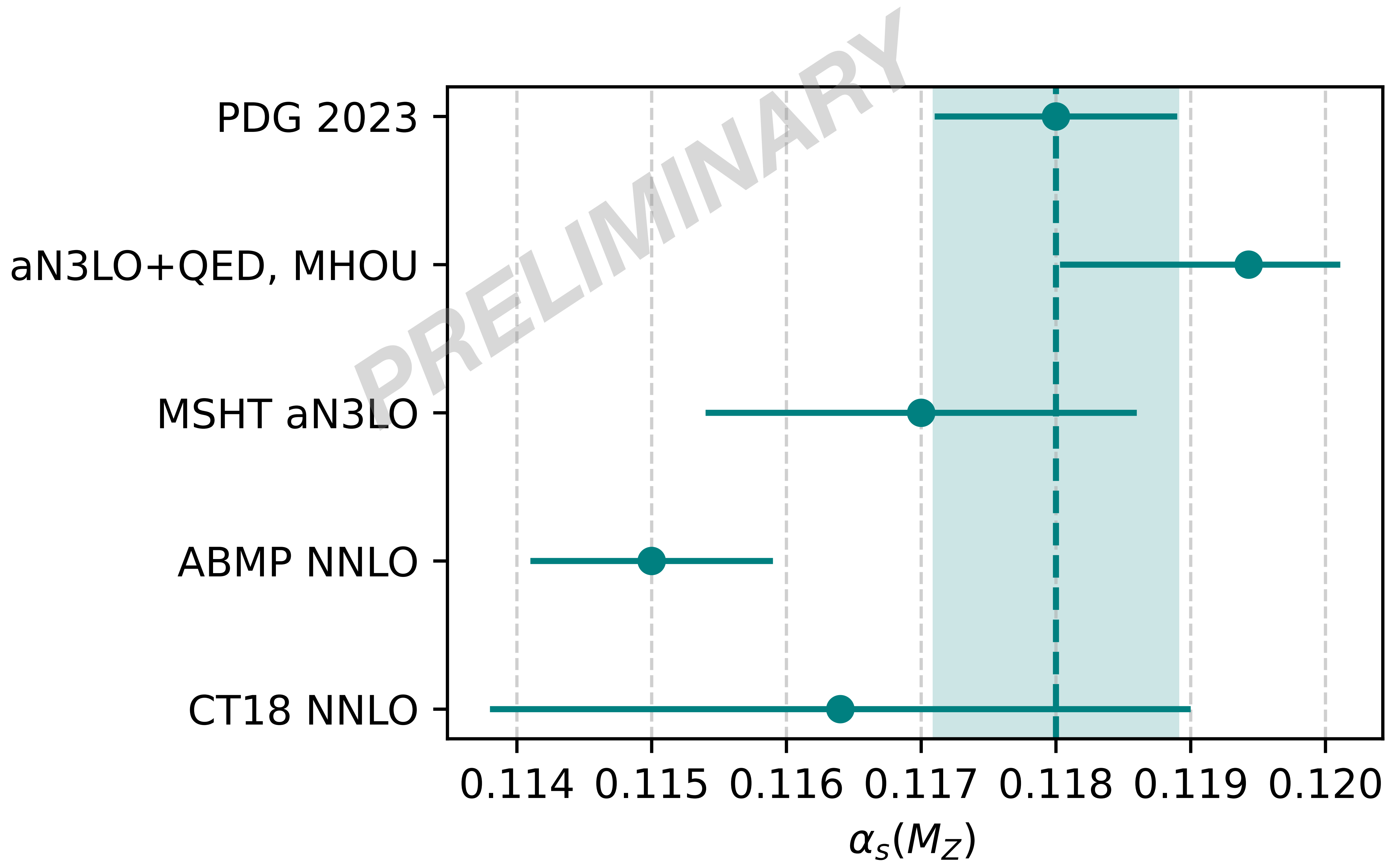
$$\alpha_s(M_Z)^{\mathrm{aN3LO,QED,MHOU}} = 0.1194^{+0.0007}_{-0.0007}{}^{\mathrm{PDF}}{}_{-0.0007}{}^{\mathrm{positivity}} = 0.1194^{+0.0007}_{-0.0014}$$

PRELIMINARY

Note: correction is only to the uncertainty, so previous qualitative conclusions remain

Summary and Outlook

- Strong correlations between the PDFs and α_s means that a simultaneous determination is needed
- aN3LO, MHOU, QED each have a significant impact on the value of $\alpha_s(m_Z)$
- Impact of top mass is negligible
- Our methodologies have been validated by means of closure testing
- Account for bias due to positivity constraint
- $\alpha_s(M_Z)^{\text{aN3LO,QED,MHOU}} = 0.1194^{+0.0007}_{-0.0014}$



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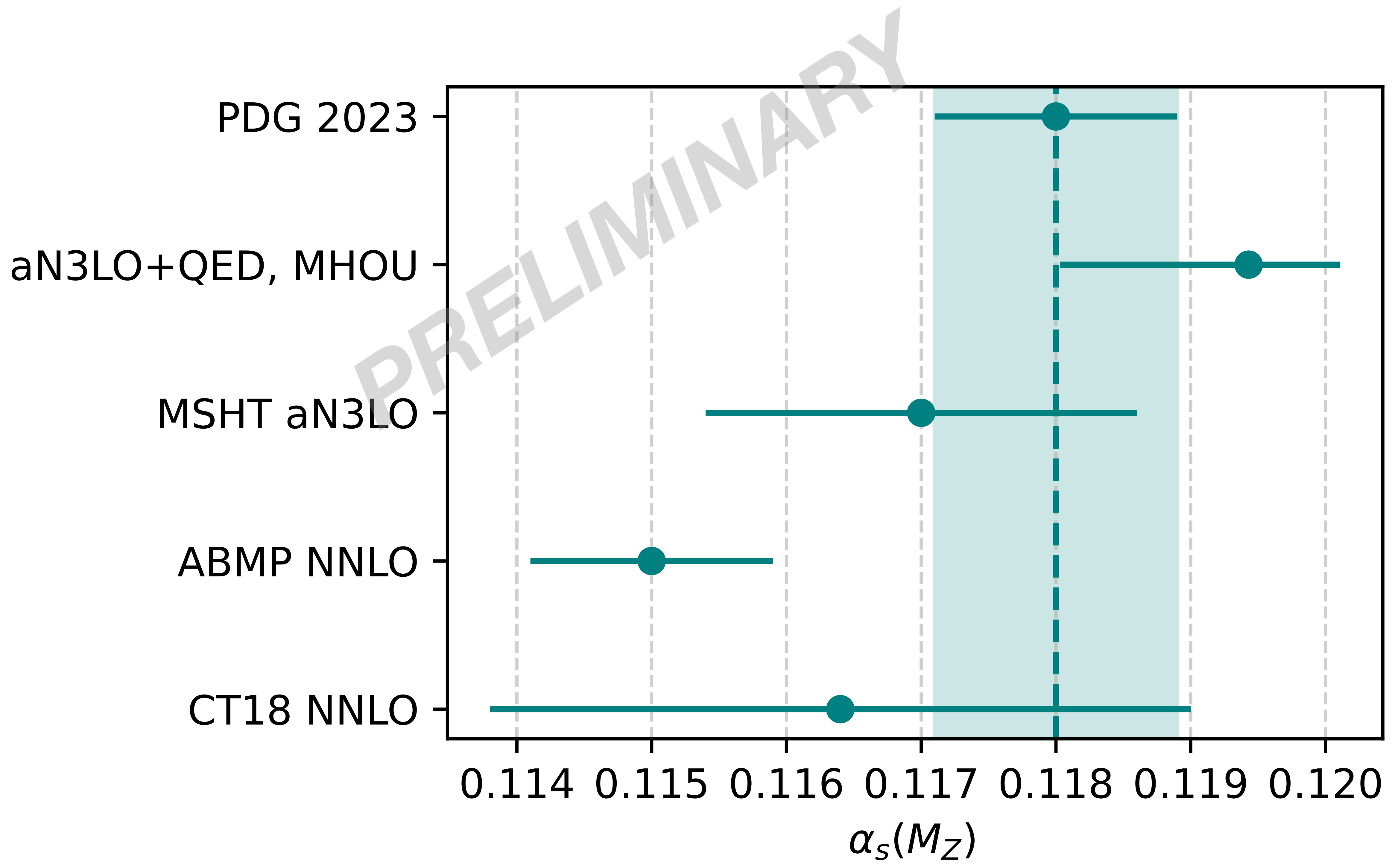


Thank you for your attention!

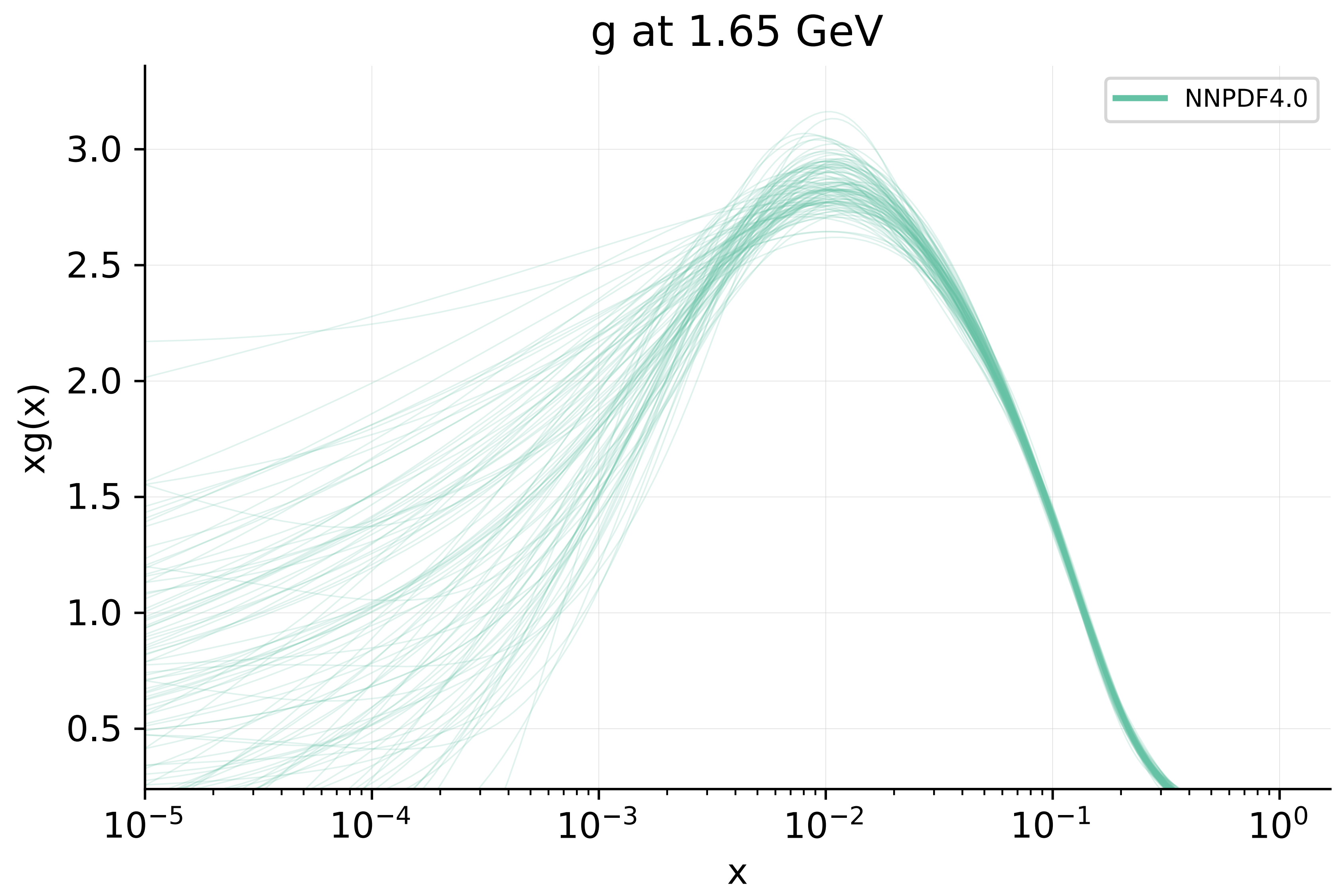
Backup slides

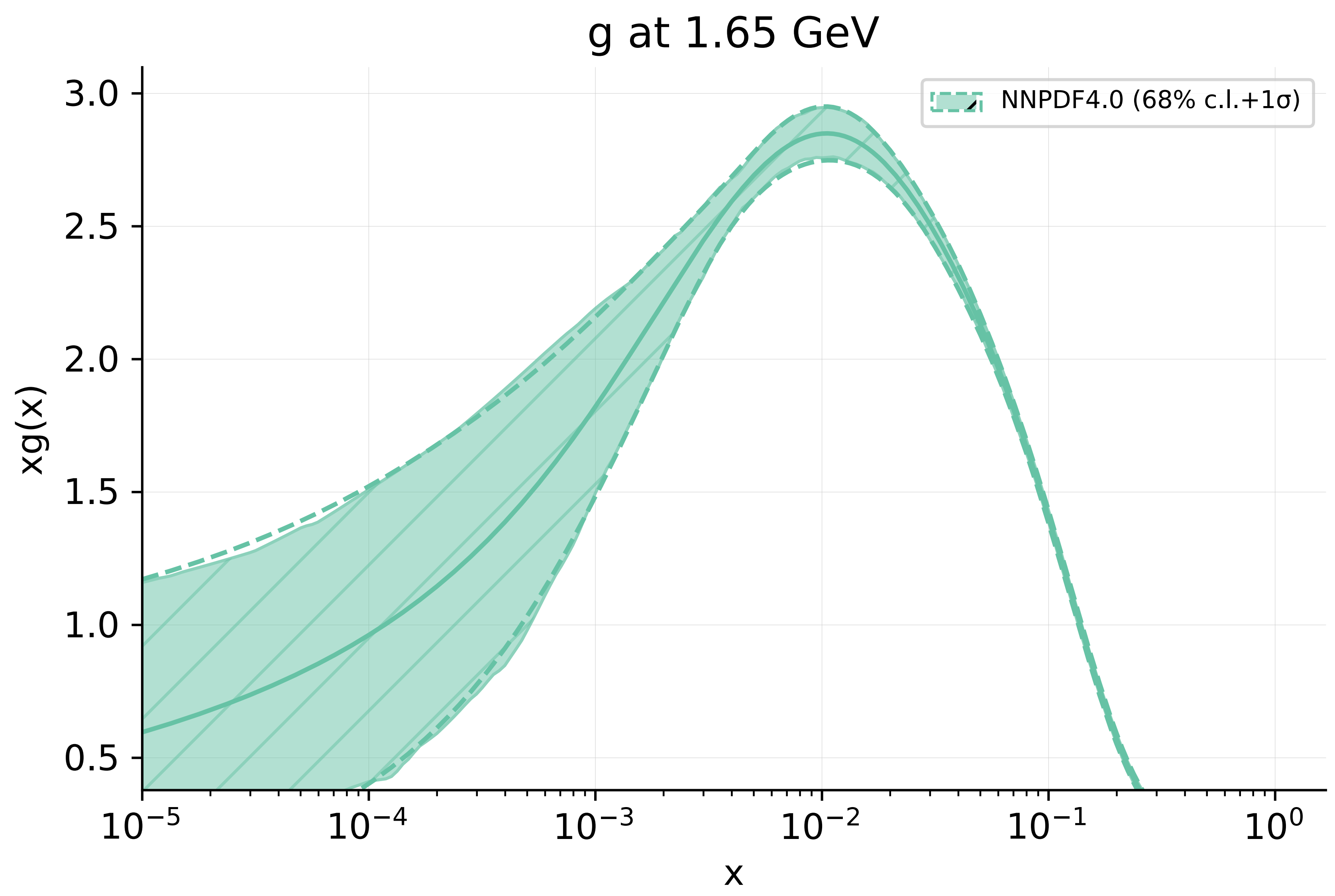
Propagating experimental uncertainty to PDFs

An NNPDF set (usually) consists of 100 PDF replicas produced as follows:

1. Assume experimental data is **defined** by a vector of central values and a covariance matrix
2. Sample this distribution to create 100 Monte Carlo replicas in data space
3. Perform a fit to each of the data replicas

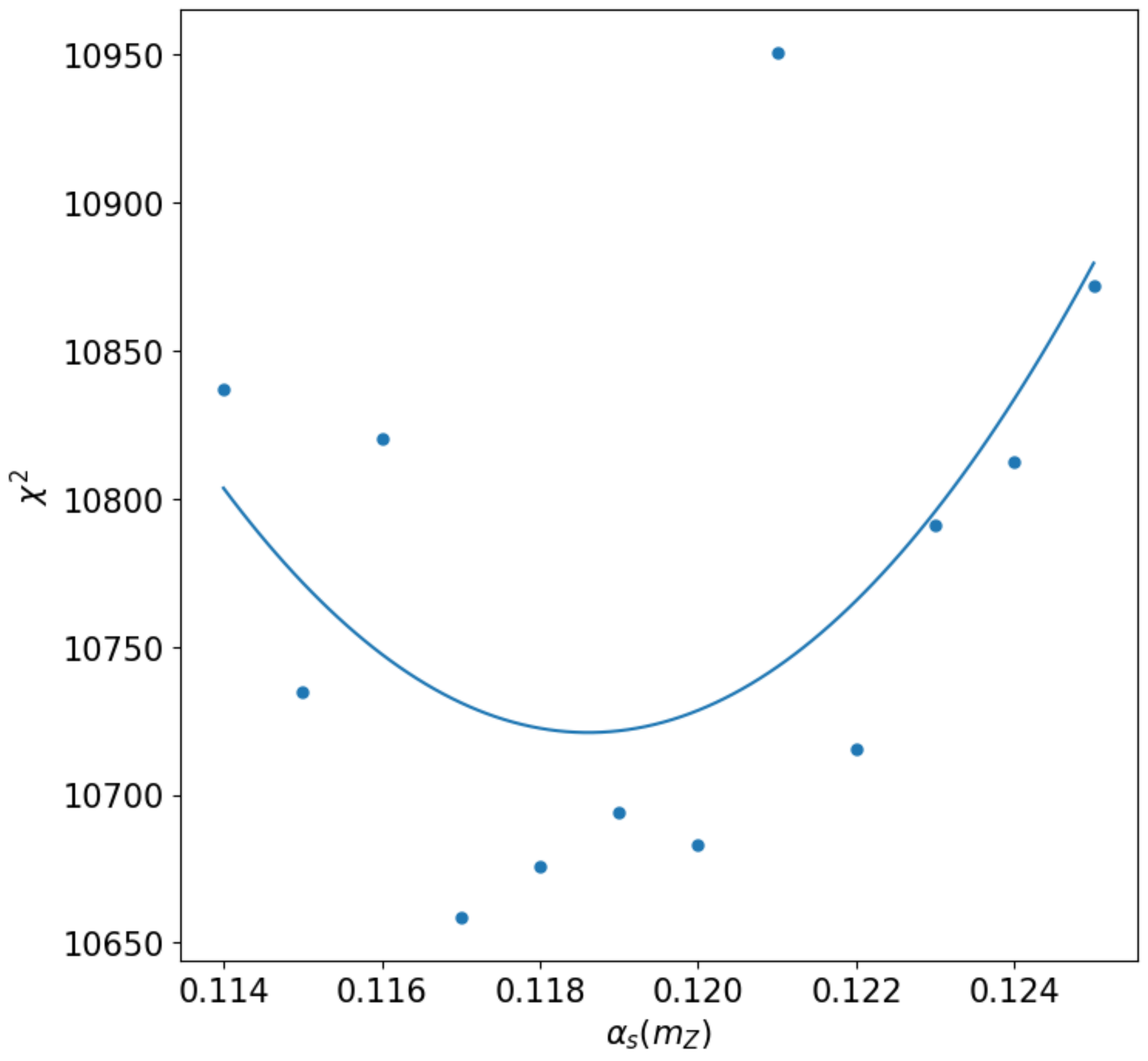
➡A PDF set encoding experimental uncertainties





Simultaneous minimization of PDF and α_s

Correlated replicas method



Simultaneous minimization of PDF and α_s

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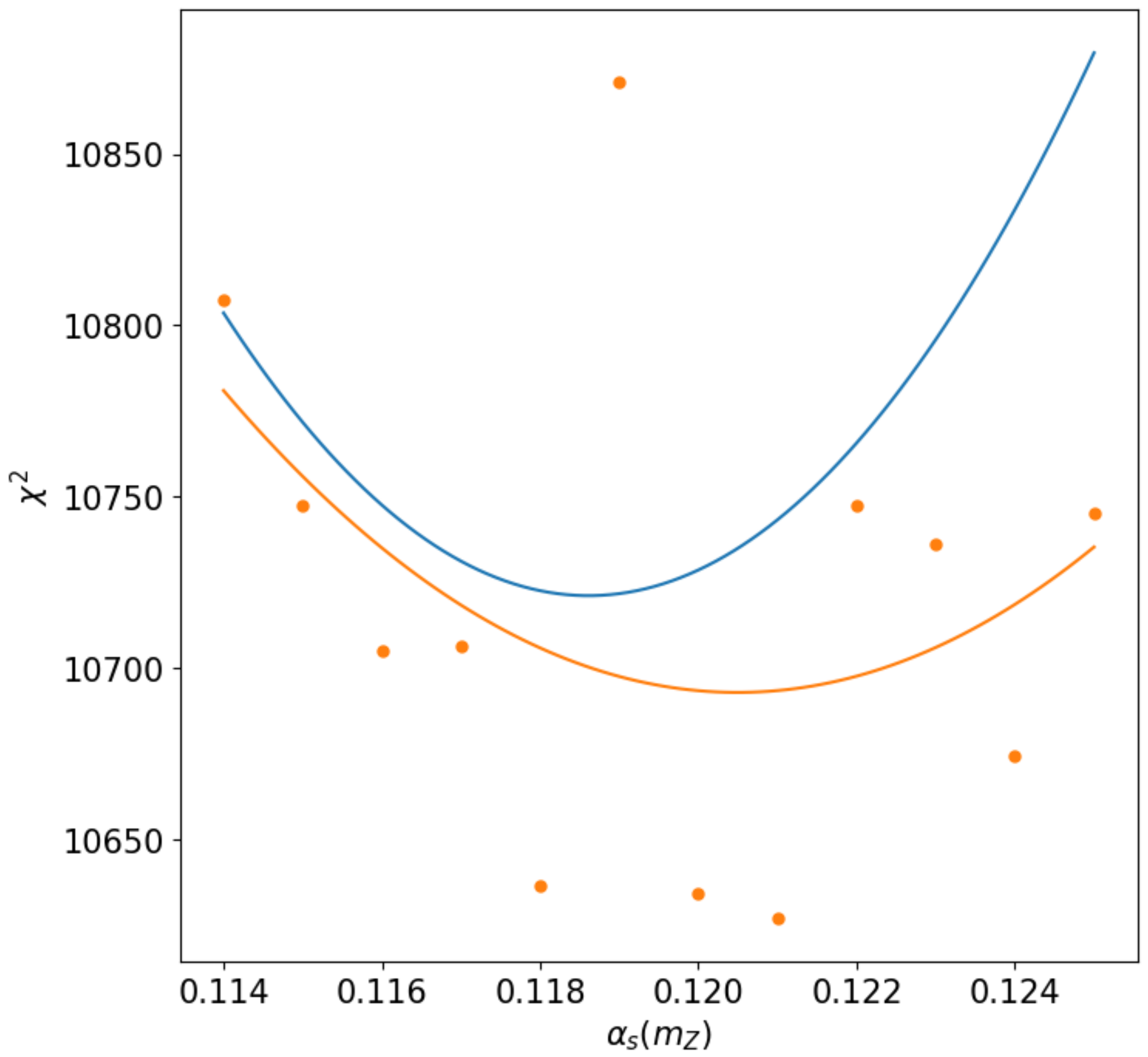
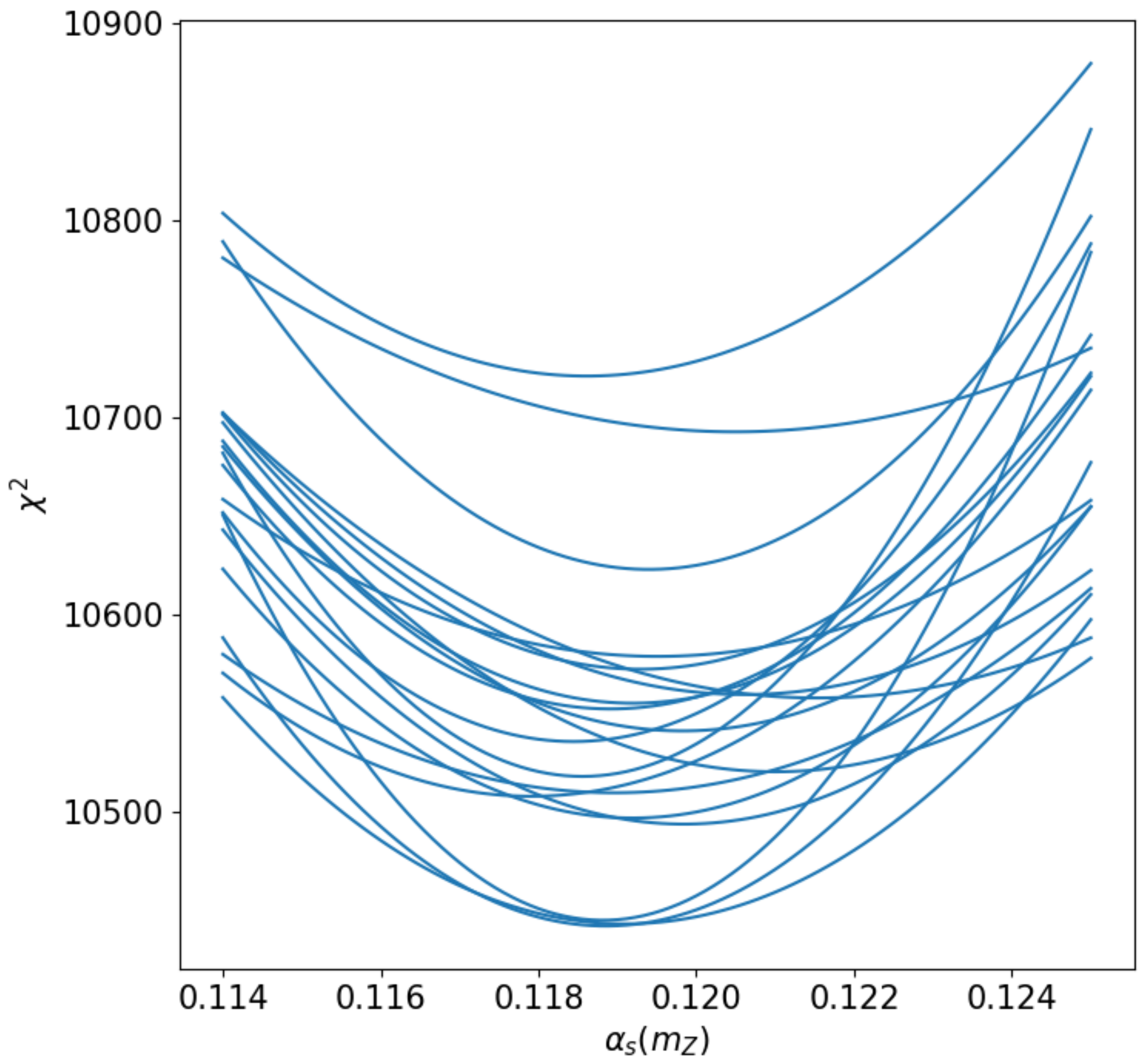


Simultaneous minimization of PDF and α_s

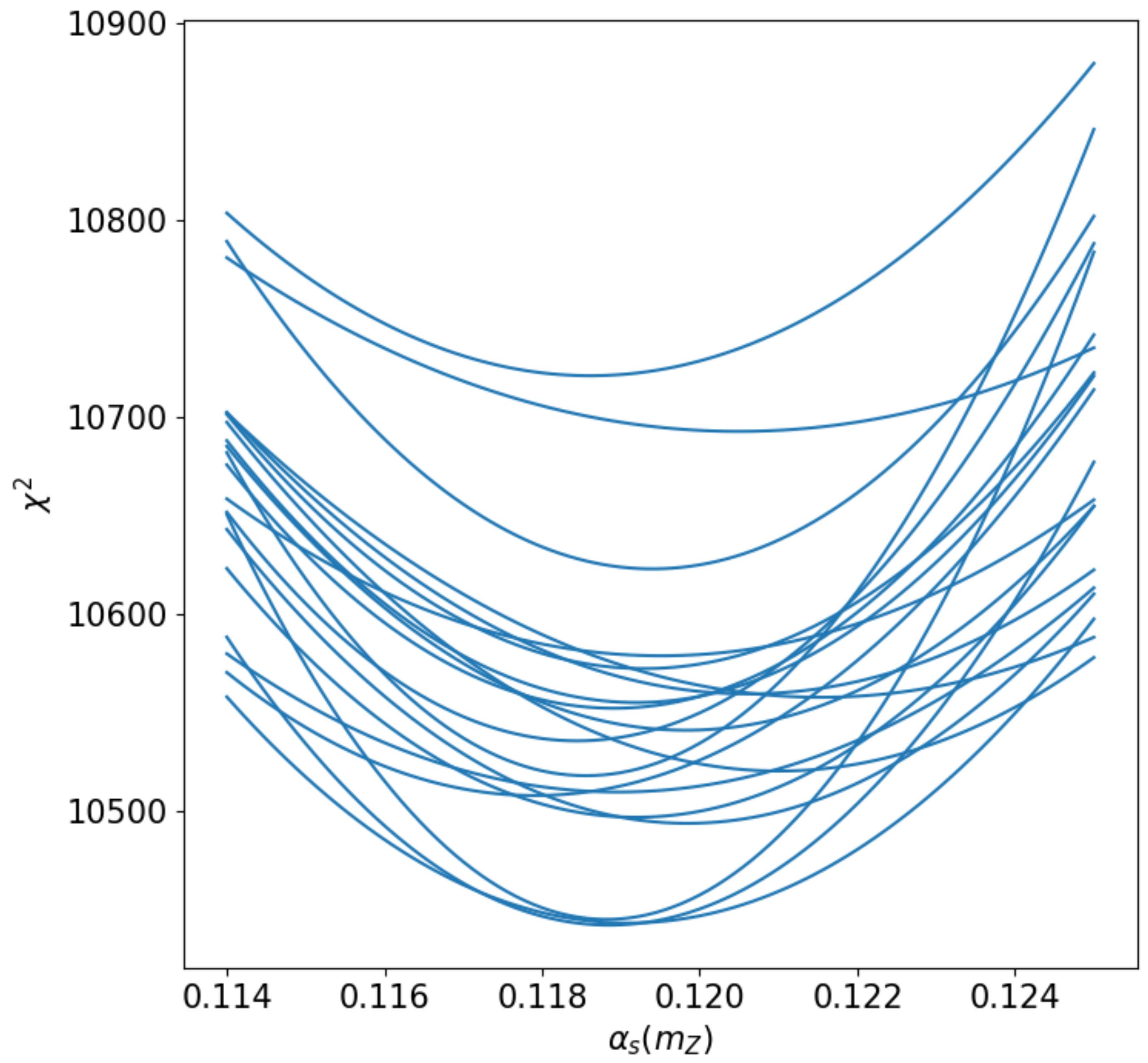
Correlated replicas method

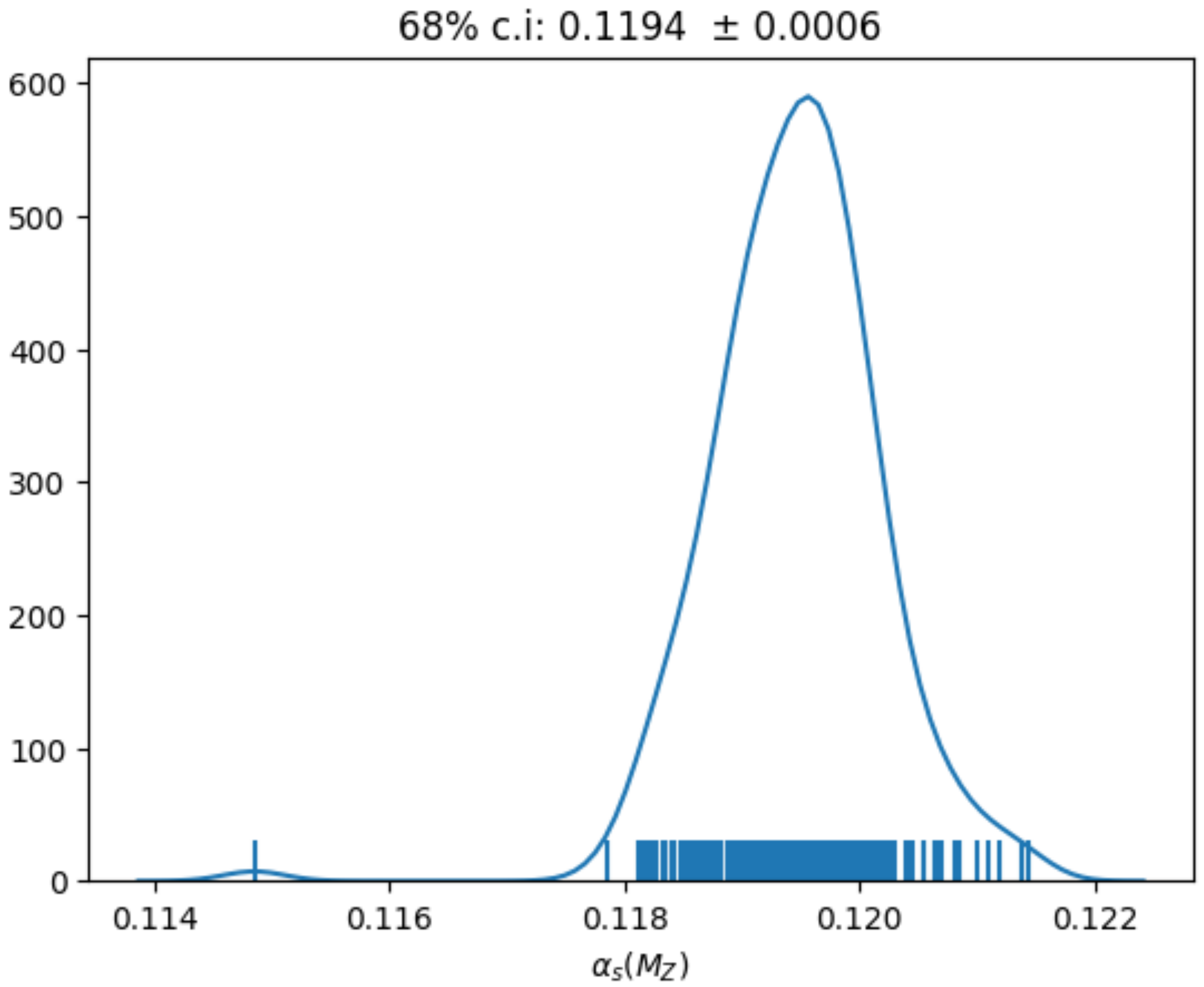


Fit the same data replica at different values of α_s and
fit a parabola for each replica …

Simultaneous minimization of PDF and α_s

Correlated replicas method





Fit the same data replica at different values of α_s and fit a parabola for each replica …

… then look at the distribution of minima of the parabolas

α_s from correlated theory uncertainties
Theory Covariance Method [arXiv:2105.05114]

The "correlated replicas" method is computationally costly because it involves fitting PDFs at many values of α_s

Alternatively, α_s can be determined in a **Bayesian framework** from nuisance parameters:

1. Model the theory uncertainty as a shift correlated for all datapoints
   $T \to T + \lambda \cdot \beta$, for $\beta \equiv T(\alpha_s^+) - T(\alpha_s^-)$
   $$P(T \mid D, \lambda) \propto \exp(\chi^2) = \exp\left(-\frac{1}{2}(T + \lambda \cdot \beta - D)^T C^{-1}(T + \lambda \cdot \beta - D)\right)$$

2. Choose a prior
   $$P(\Delta\alpha_s) \propto \exp\left(-\frac{1}{2}\lambda^2\right)$$

3. Marginalise over λ to get $P\left(T|D\right)$

4. Compute the posterior for λ
   $$P(\lambda \mid T, D) = \frac{P(T \mid D, \lambda)P(\lambda)}{P(T \mid D)} \propto \exp\left[-\frac{1}{2}Z^{-1}(\lambda - \bar{\lambda})\right]$$

$$Z = 1 - \beta^T(C + \beta\beta^T)^{-1}\beta \qquad \bar{\lambda}(T, D) = \beta^T(C + \beta\beta^T)^{-1}(D - T)$$

This idea can be extended to a real PDF fit [arXiv:2105.05114]

1) Perform fit with $C^{exp} \to C^{exp} + C^{\alpha_s}$, $C^{\alpha_s} = \beta\beta^T$

2) Once the fit has completed, compute α_s shift preferred by data as encoded in the fit

Prior dependence in the Theory Covariance Method

For some aspects of the fit we have to assume a value of $\alpha_s(m_Z)$, in reality we don't know the result so what if we choose "wrong"?

Consider the following

Pseudodata at $\alpha_s(m_Z) = 0.118$

Prior assumption is $\alpha_s(M_Z) = 0.117$

Result moves towards the true result. We update assumption and iterate!