Parton Distributions with MHO uncertainties

Juan Rojo
VU Amsterdam & Nikhef Theory group

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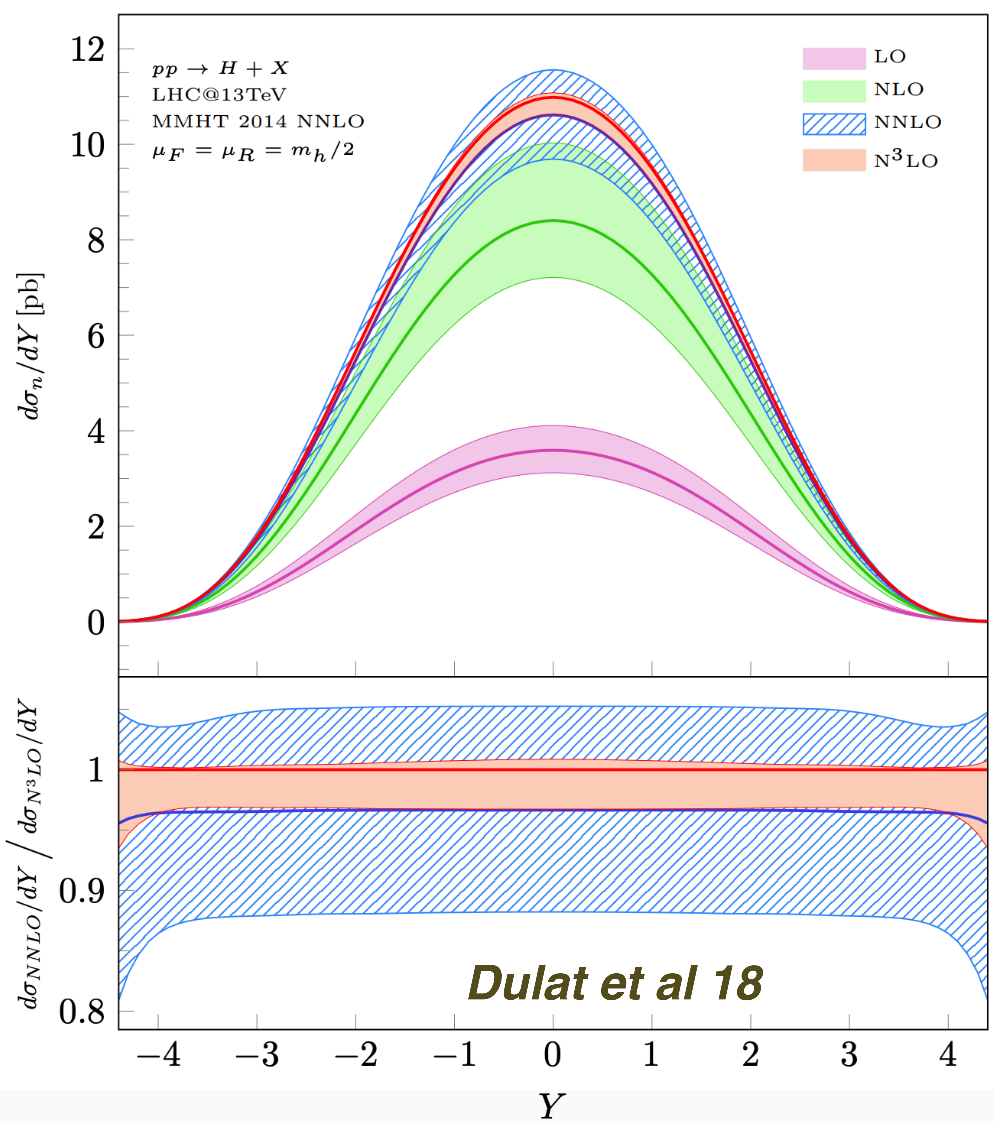
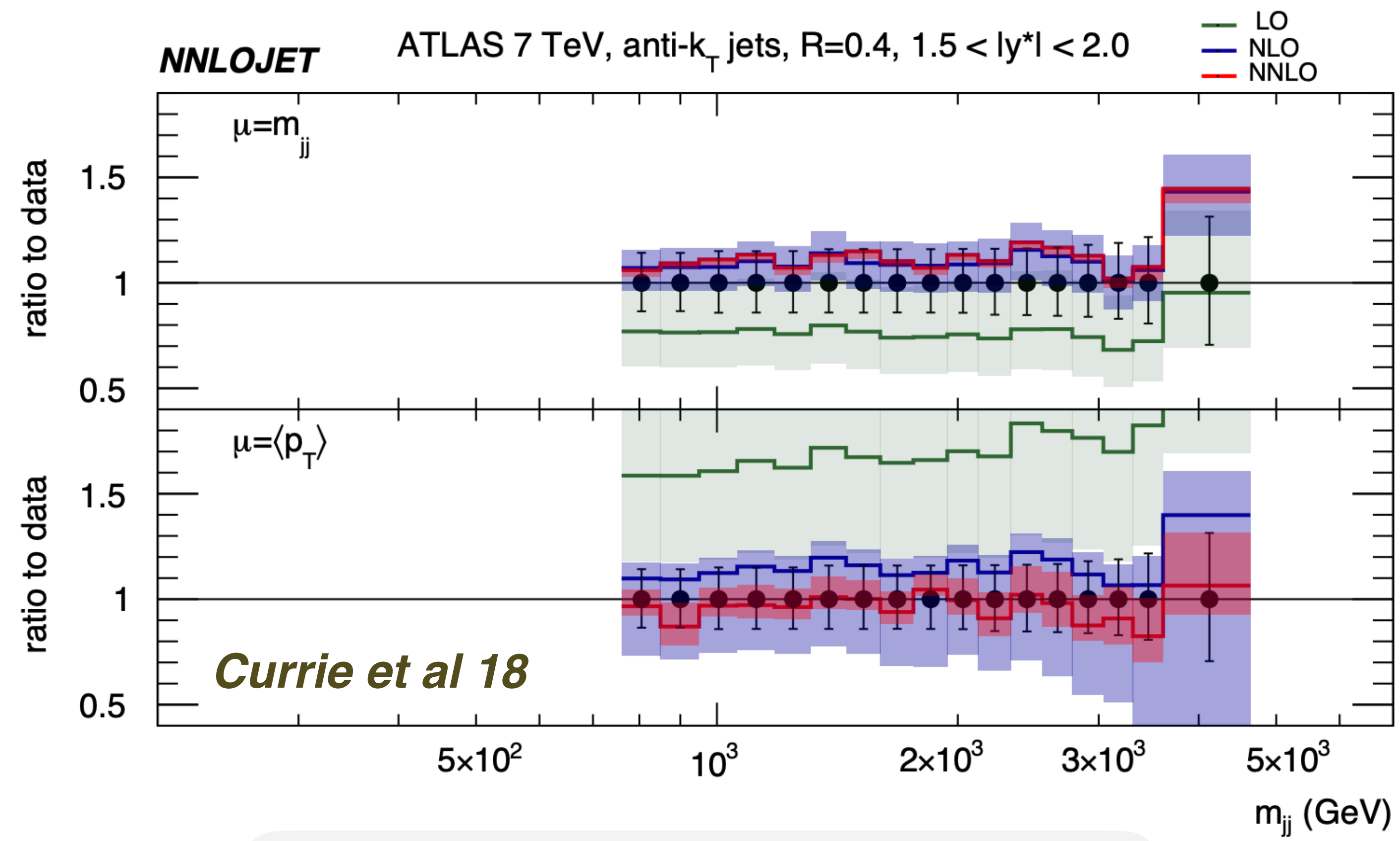
Theory uncertainties from MHOs

Standard global PDF fits are based on **fixed-order QCD calculations**

$$\sigma = \alpha_s^{p}\sigma_0 + \alpha_s^{p+1}\sigma_1 + \alpha_s^{p+2}\sigma_2 + \mathcal{O}(\alpha_s^{p+3})$$

The truncation of the perturbative series has associated a theoretical uncertainty known as **Missing Higher Order (MHO)** uncertainty

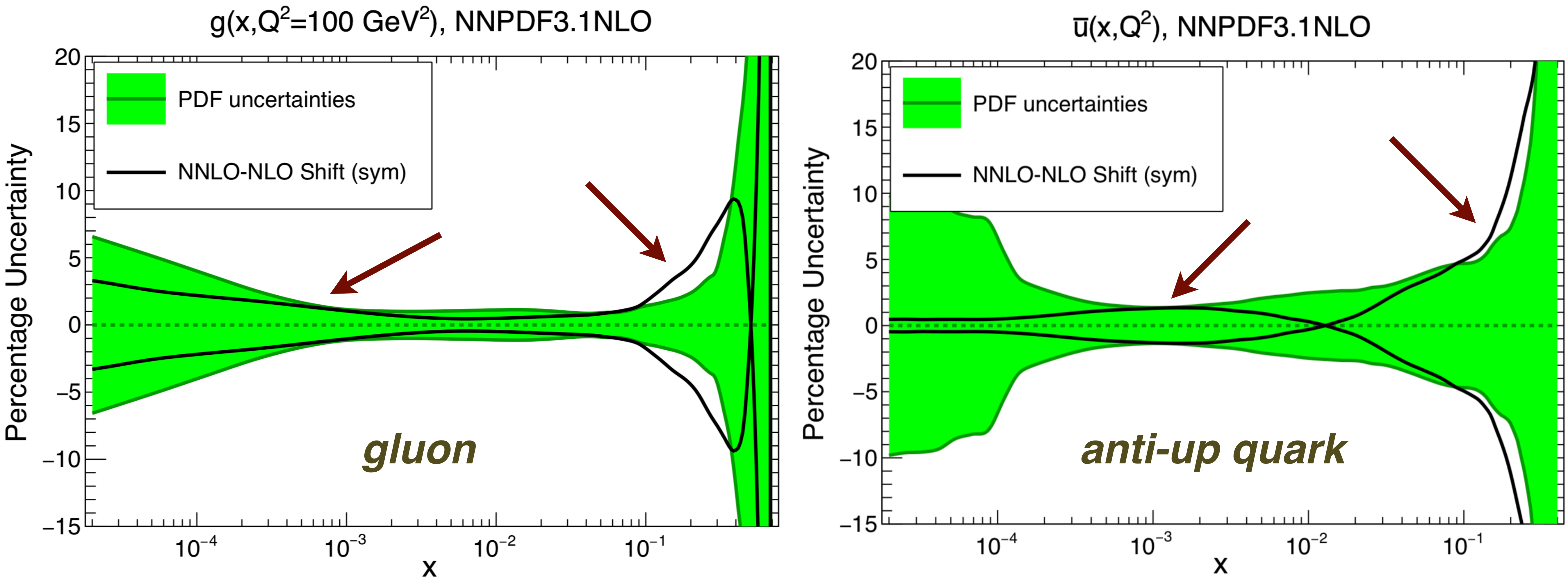




*What is the **impact of MHOUs** in a global PDF fit?*

Theory uncertainties from MHOs

How severe is **ignoring MHOUs** in modern global PDFs fits?



Shift between **NLO and NNLO PDFs** comparable or larger than **PDF errors**

Given the high precision of modern PDF determinations, **accounting for MHOUs** is most urgent!

The strategy

Construct a **theory covariance matrix** from **scale-varied cross-sections** and combine it with the experimental covariance matrix

$$\chi^2 = \frac{1}{N_{\rm dat}} \sum_{i,j=1}^{N_{\rm dat}} \left(D_i - T_i\right) \left({\rm cov}^{({\rm exp})} + {\rm cov}^{({\rm th})}\right)^{-1}_{ij} \left(D_j - T_j\right)$$

In addition, as a **validation tool**, we also:

Perform **multiple PDF fits** for a range of values of μ_R and μ_F
MHOUs on the PDFs estimated as the **envelope of fits** with different scales

This exercise is also useful to understand the impact that varying μ_R and μ_F have on the fitted PDFs (never studied before)

PDF fits with scale variations

Perform **multiple PDF fits** for a range of values of μ_R and μ_F

MHOUs on the PDFs estimated as the **envelope of fits** with different scales

3-points

$$\sigma(\mu_R = Q, \mu_F = Q)$$ central scales

$$\sigma(\mu_R = 2Q, \mu_F = 2Q) \qquad \sigma(\mu_R = Q/2, \mu_F = Q/2)$$

7-points

$$\sigma(\mu_R = 2Q, \mu_F = Q) \qquad \sigma(\mu_R = Q, \mu_F = 2Q)$$

$$\sigma(\mu_R = Q/2, \mu_F = Q) \qquad \sigma(\mu_R = Q, \mu_F = Q/2)$$

9-points

$$\sigma(\mu_R = 2Q, \mu_F = Q/2) \qquad \sigma(\mu_R = Q/2, \mu_F = 2Q)$$

*Require assumptions about the **theory-induced correlations** between different processes, e.g. between DIS and jet production*

PDF fits with scale variations

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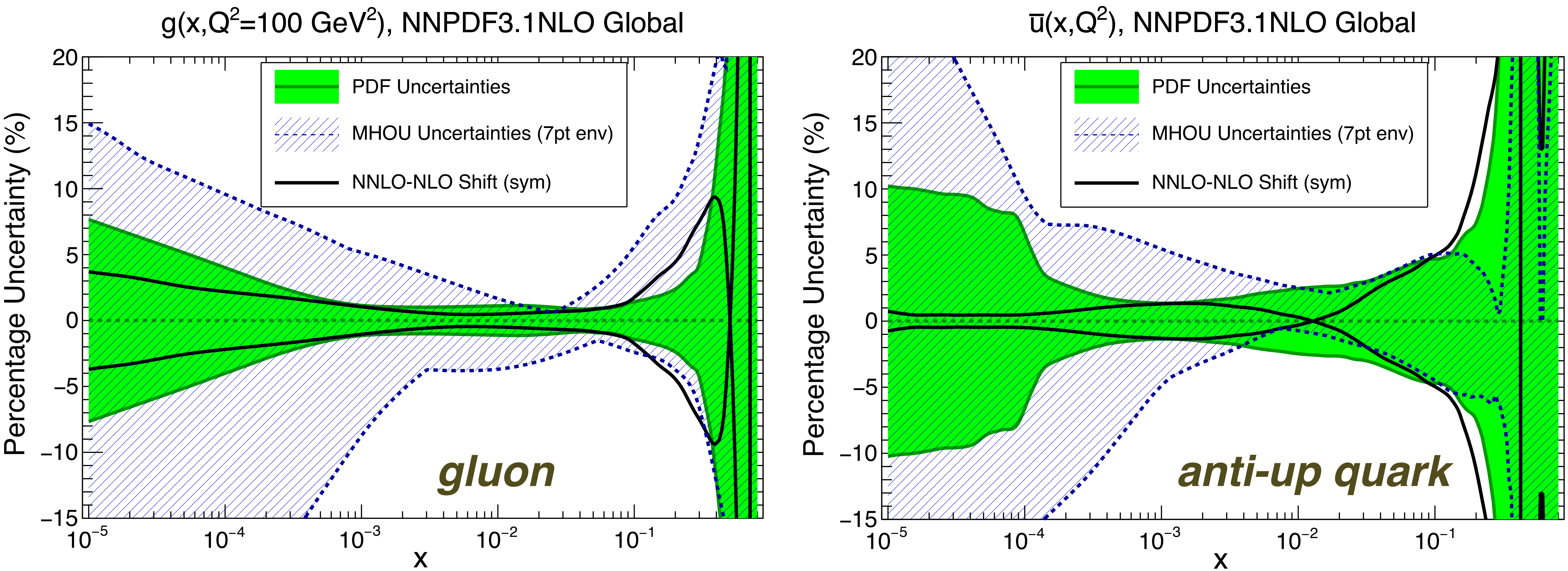

- The scale-variation envelope works fine in most cases (too conservative at small-x?)
- **CPU-intensive** and cumbersome for general LHC applications
- Keep track of scale correlations **between input PDFs** and **produced LHC processes**

PDF fits with scale variations

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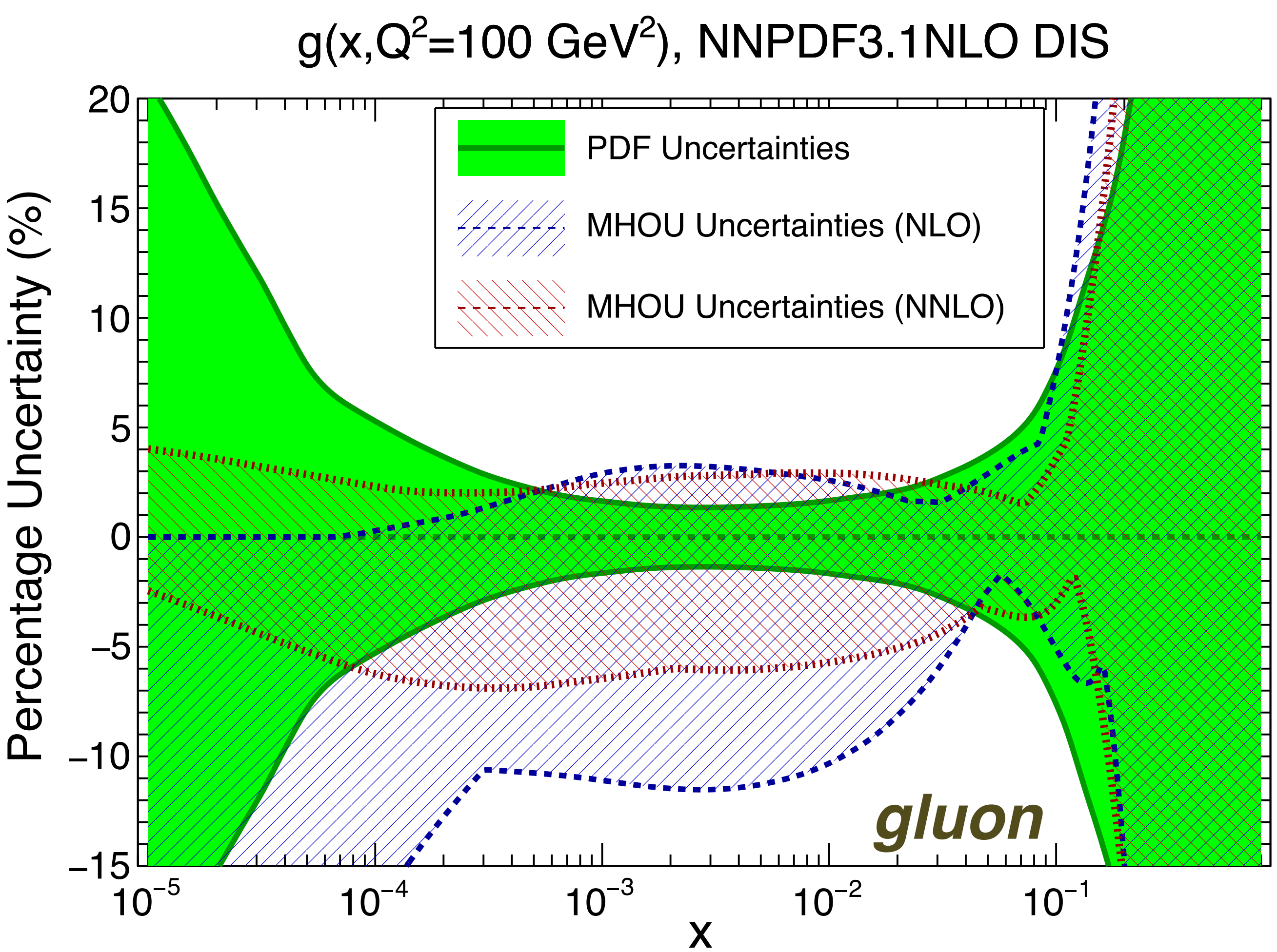
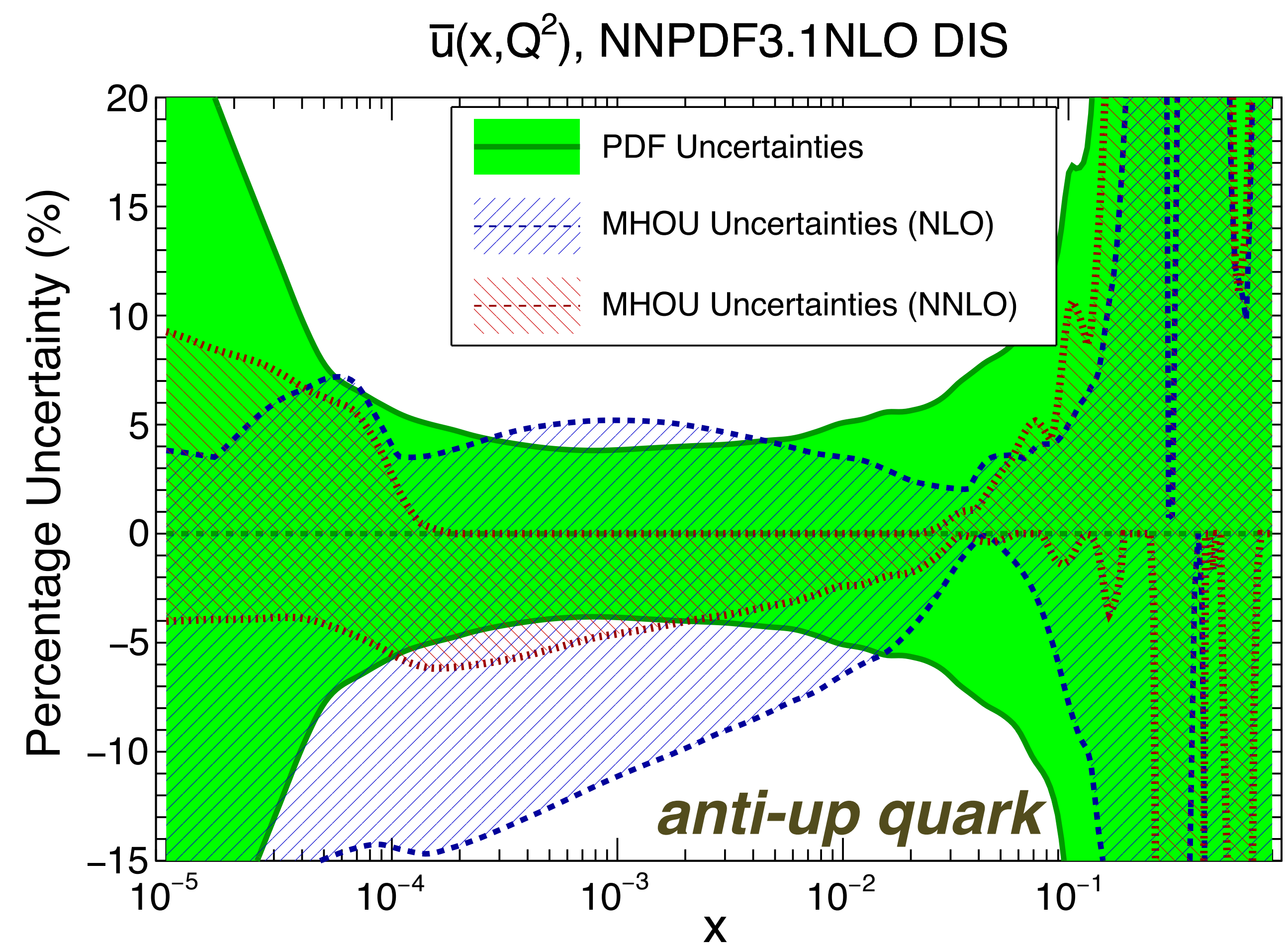
MHOUs on the PDFs estimated as the **envelope of fits** with different scales



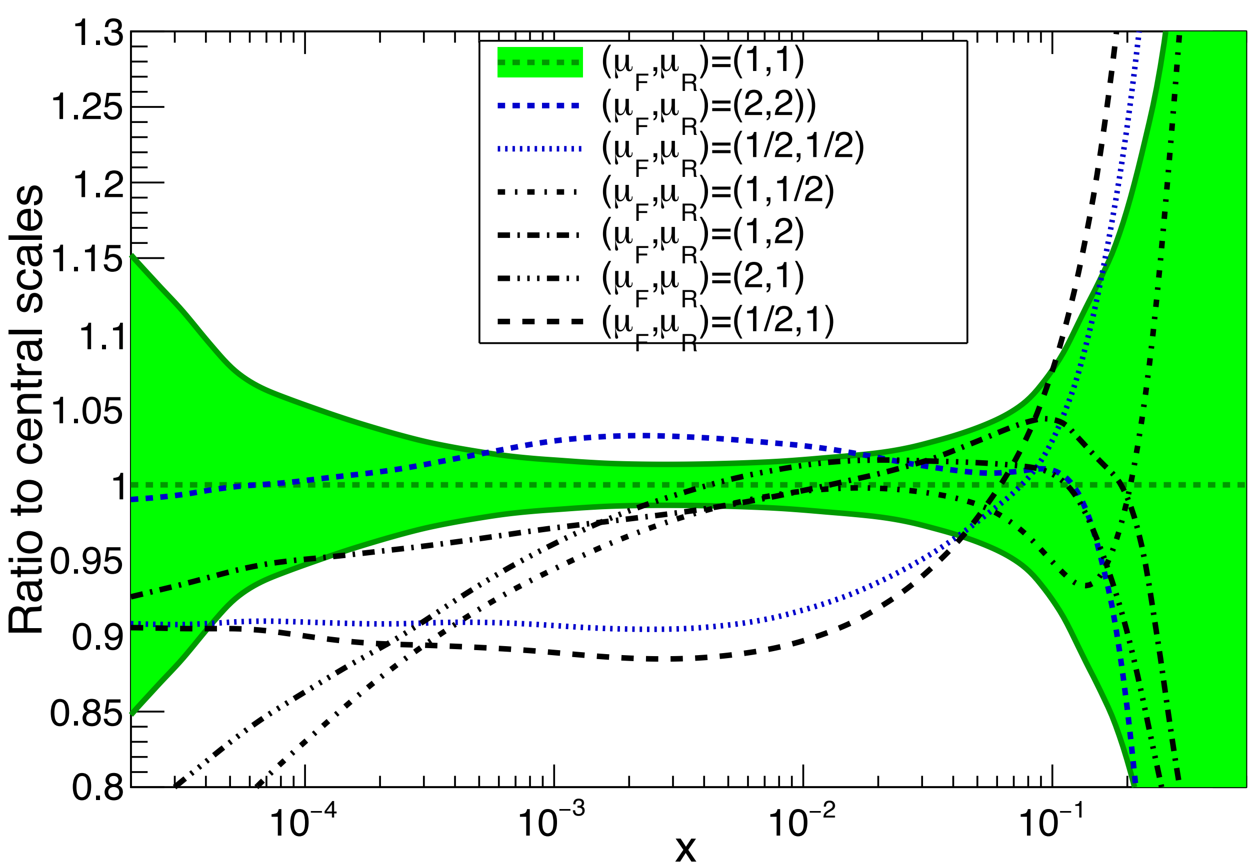


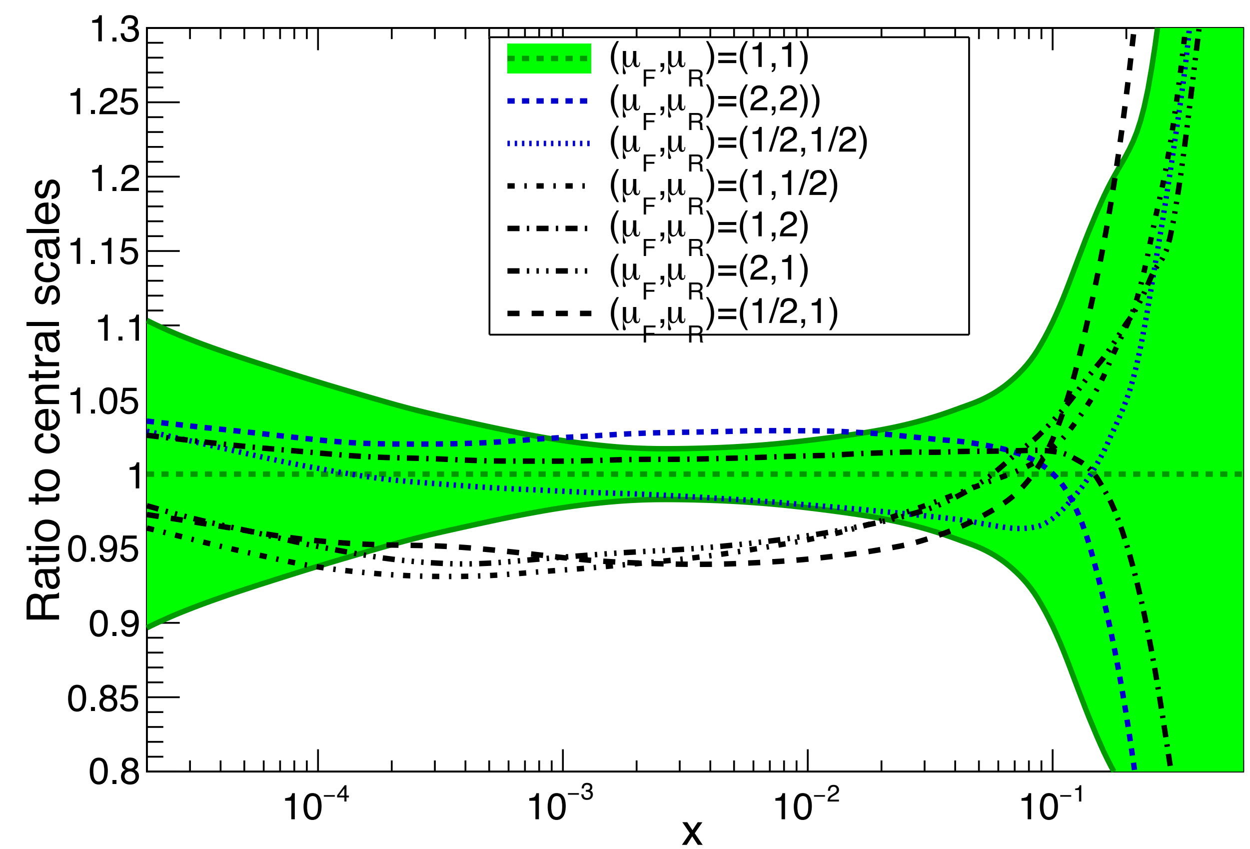
- MHOUs on PDFs decrease when going **from NLO to NNLO theory,** as expected
- MHOUs most relevant when PDF uncertainties are smallest, e.g. at medium-*x*

The role of correlations

MHOUs are **fully correlated uncertainties** (no statistical component):

Can lead to large changes in PDF central values with small changes in χ^2





χ^2	(1,1)	(2,2)	(1/2,1/2))
Global NLO	1.061	1.083	1.103

Self-consistency test: determine ``optimal" values for scales from χ^2 profile

$$\mu_R^{\rm (best)} \simeq 1.4Q\,,\, \mu_R^{\rm (best)} \simeq 1.1Q$$

PDF fits with theory covariance matrix

Construct a **theory covariance matrix** from **scale-varied cross-sections** and combine it with the experimental covariance matrix

- Most global PDF fits are based on the minimisation of a figure of merit of the form:

$$\chi^2 = \frac{1}{N_{\rm dat}} \sum_{i,j=1}^{N_{\rm dat}} (D_i - T_i) \left(\mathrm{cov}^{(\rm exp)}\right)^{-1}_{ij} \left(D_j - T_j\right)$$

- If experimental and theory errors are **independent** and **Gaussian**, one has

$$\chi^2 = \frac{1}{N_{\rm dat}} \sum_{i,j=1}^{N_{\rm dat}} (D_i - T_i) \left(\mathrm{cov}^{(\rm exp)} + \mathrm{cov}^{(\rm th)}\right)^{-1}_{ij} \left(D_j - T_j\right)$$

Ball, Deshpande 18

- The **theory covariance matrix** can be computed in terms of **nuisance parameters**

$$\mathrm{cov}^{(\rm th)}{}_{ij} = \frac{1}{N} \sum_k \Delta_i^{(k)} \Delta_j^{(k)} \qquad \Delta_i^{(k)} \equiv T_i^{(k)} - T_i$$

N: normalisation factor since in general not all nuisance parameters are orthogonal

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Ball, Deshpande 18

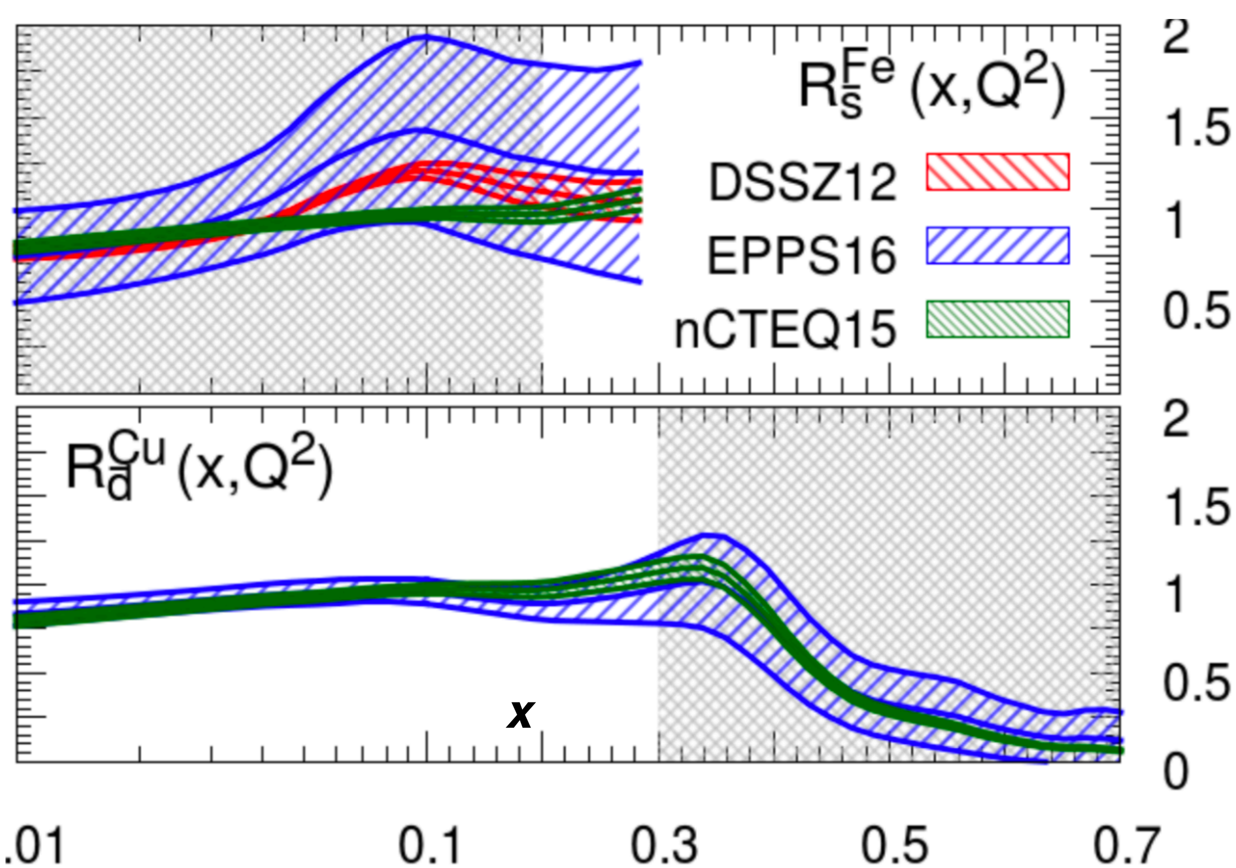
*Accounting for the theory covariance matrix in general will **modify the relative weight** that each of the datasets carries in the global fit: processes with higher MHOUs will be ``**deweighted**''*

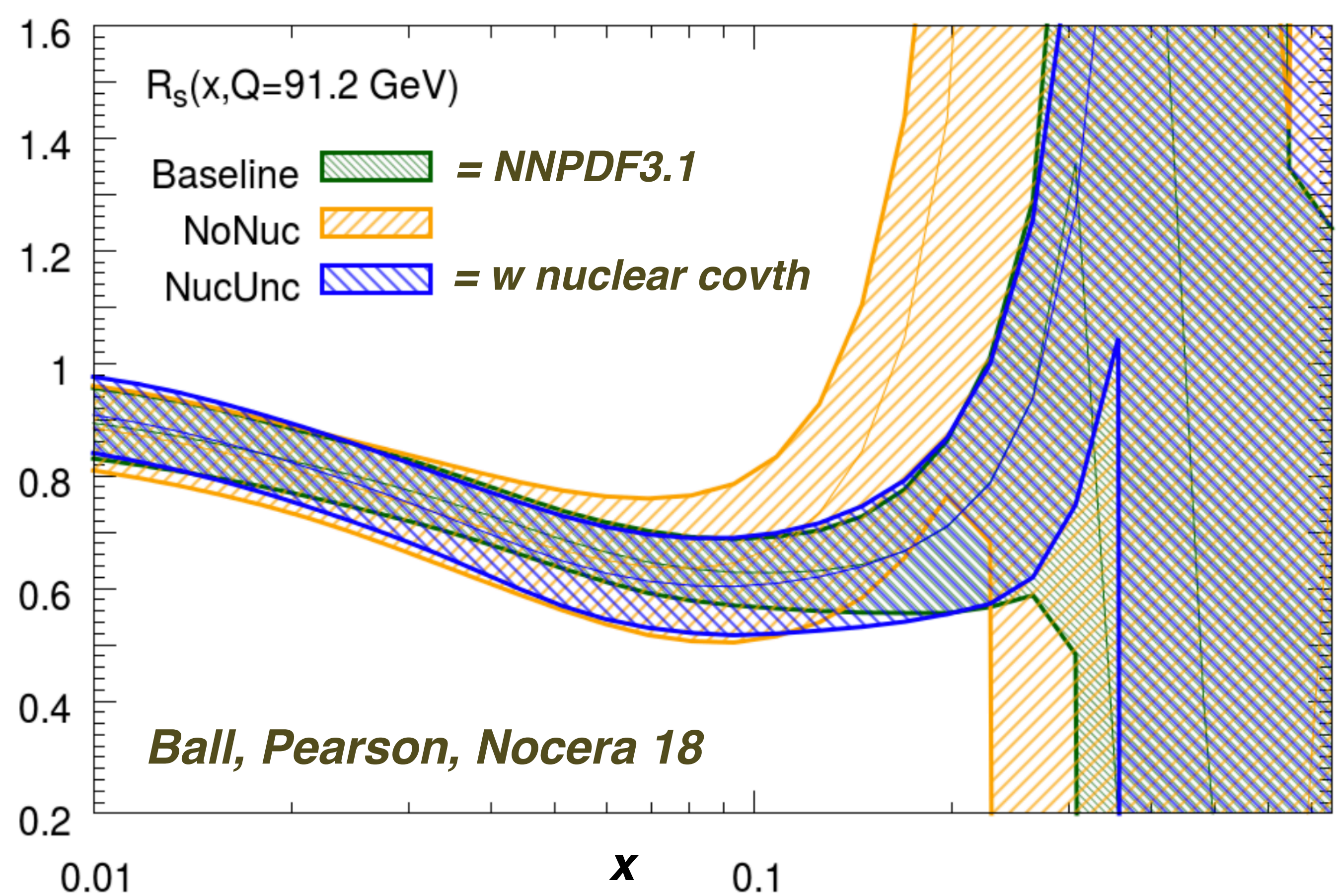
Case study: nuclear uncertainties

Global fits include DIS and DY data involving **heavy nuclear targets:**
assess impact of **theory uncertainties from nuclear effects** in a global PDF fit

$$\mathrm{cov}^{(\mathrm{th})}{}_{ij} = \frac{1}{N}\sum_k \Delta_i^{(k)}\Delta_j^{(k)} \qquad \Delta_i^{(k)} \equiv T_i\left[f_N^{(k)}\right] - T_i\left[f_p\right]$$

where nuisance parameters computed from results of **nuclear PDF fits $\{f_N^{(k)}\}$**





PDF fits with theory covariance matrix

Construct a **theory covariance matrix** from **scale-varied cross-sections** and combine it with the experimental covariance matrix

- Several prescriptions possible. The simplest one is the **3pt prescription,** giving

$$\mathrm{cov}_{ij}^{(\mathrm{th})} = \frac{1}{2}\left(\Delta_i(+,+)\Delta_j(+,+) + \Delta_i(-,-)\Delta_j(-,-)\right)$$

$$\Delta_i(+,+) \equiv \sigma_i(\mu_R = 2Q, \mu_F = 2Q) - \sigma_i(\mu_R = Q, \mu_F = Q)$$

$$\Delta_i(-,-) \equiv \sigma_i(\mu_R = Q/2, \mu_F = Q/2) - \sigma_i(\mu_R = Q, \mu_F = Q)$$

for two points within the same process (say DIS), and for points from different processes:

$$\mathrm{cov}_{ij}^{(\mathrm{th})} = \frac{1}{4}\left[\left(\Delta_i(+,+) + \Delta_i(-,-)\right)\left(\Delta_j(+,+) + \Delta_j(-,-)\right)\right]$$

$\boldsymbol{\mu_F}$ variations correlated among processes, $\boldsymbol{\mu_R}$ variations only within same process

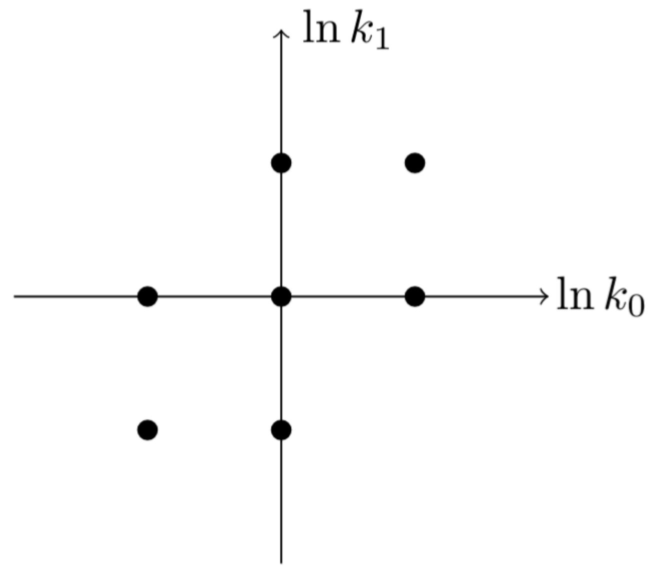
PDF fits with theory covariance matrix

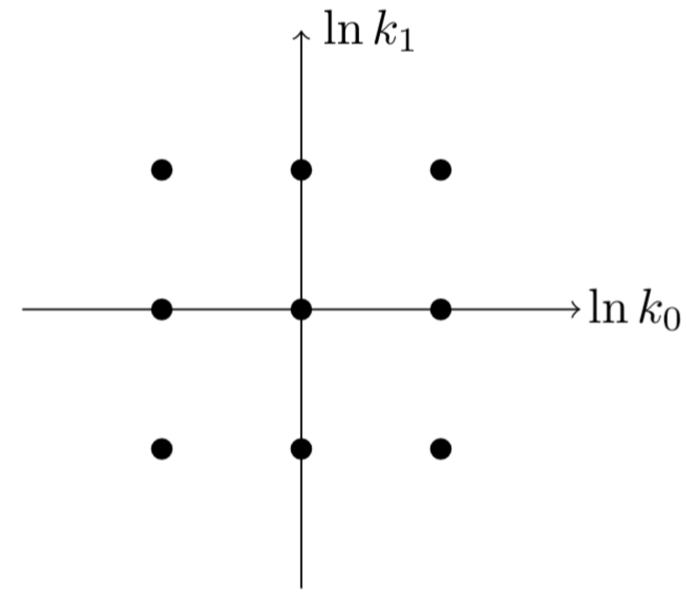
Construct a **theory covariance matrix** from **scale-varied cross-sections** and combine it with the experimental covariance matrix

7pt

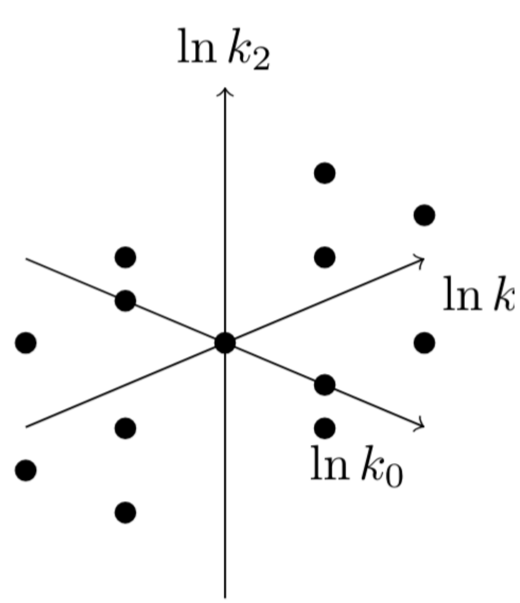
9pt

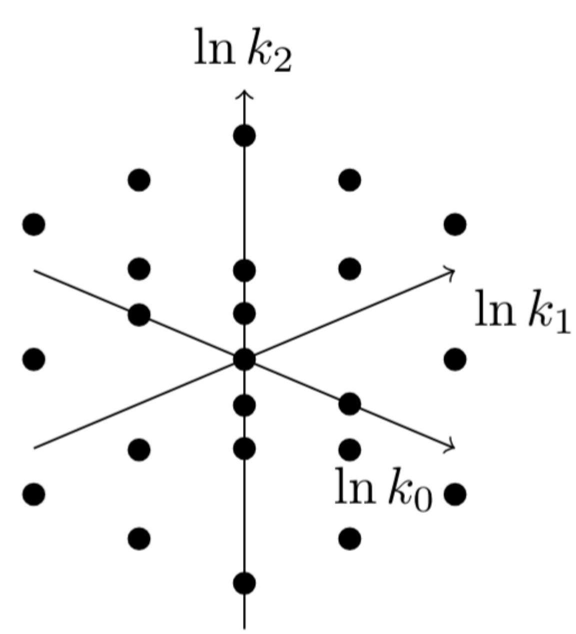
Same process





Different processes



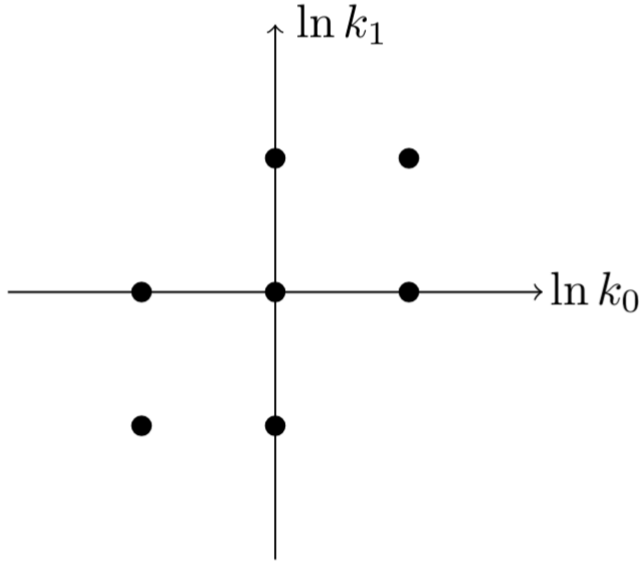


PDF fits with theory covariance matrix

Construct a **theory covariance matrix** from **scale-varied cross-sections** and combine it with the experimental covariance matrix

7pt

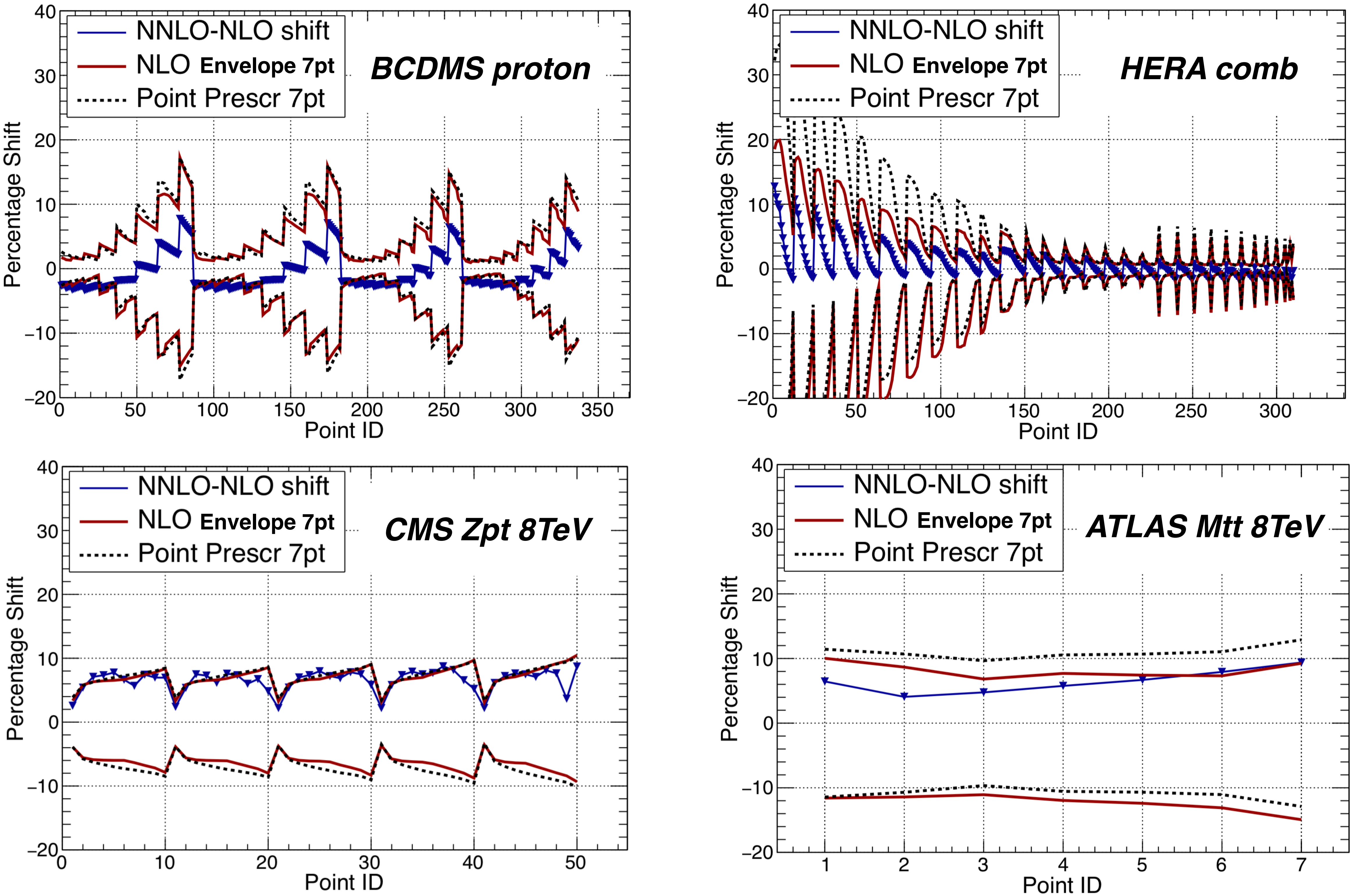
Same process



$$\mathrm{cov}_{ij}^{(\mathrm{th})} = \frac{1}{3}\Big(\Delta_i(+,0)\Delta_j(+,0) + \Delta_i(-,0)\Delta_j(-,0) + \Delta_i(0,+)\Delta_j(0,+)$$
$$+ \Delta_i(0,-)\Delta_j(0,-) + \Delta_i(+,+)\Delta_j(+,+) + \Delta_i(-,-)\Delta_j(-,-)\Big)$$

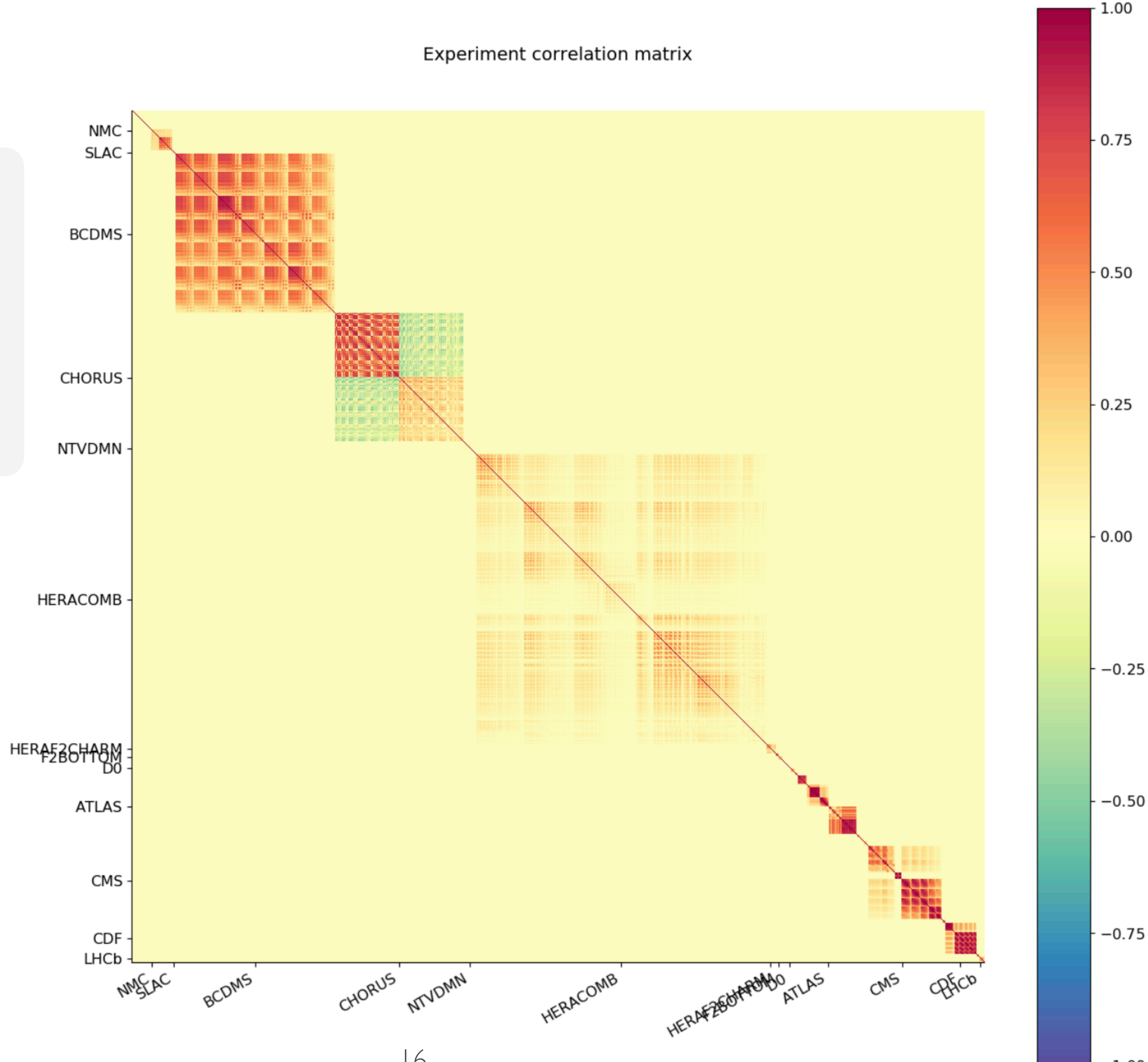
Validating scale variations (I)

Systematic validation of the NLO theory covariance matrix on the `exact' result, the **NNLO-NLO shift**, with the **O(4000) data points** of the global fit



Theory-induced correlations

Theory-induced correlations between different experiments *e.g.* DIS and LHC



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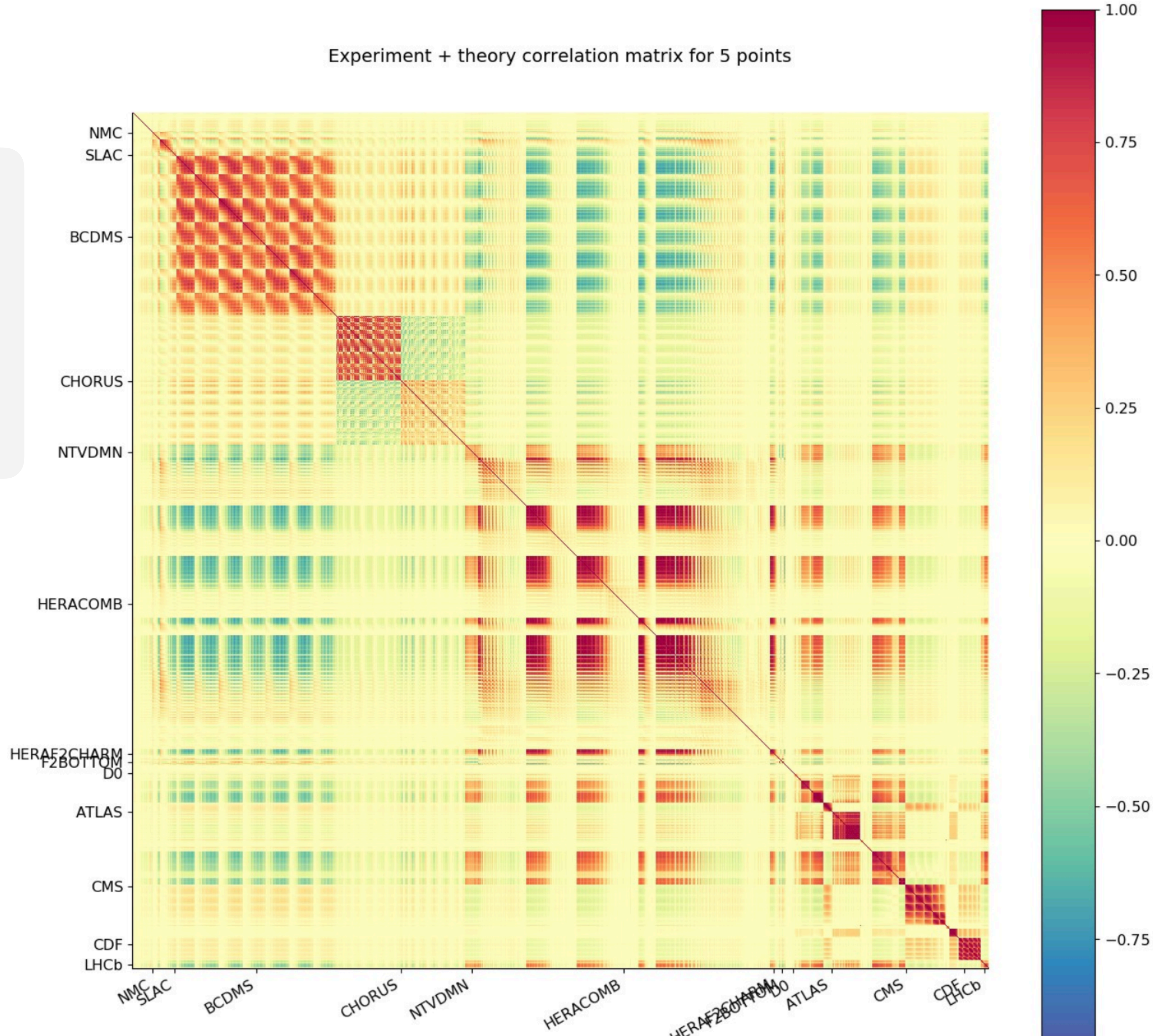

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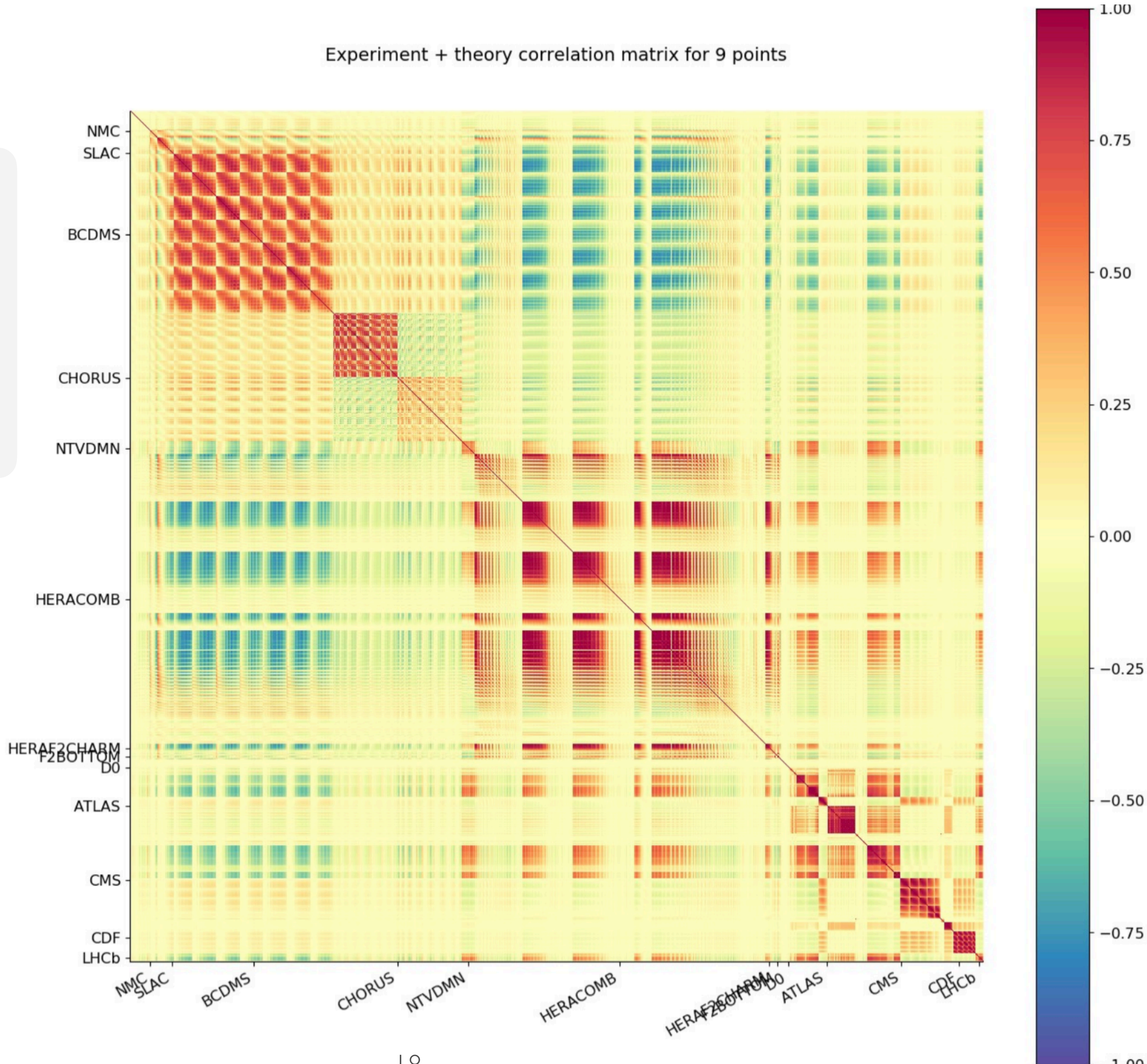

*How we can determine which point prescription reproduces better the **scale-induced correlations?***

Validating scale variations (II)

- The theory covariance matrix is **symmetric, semi-positive definite**: eigenvalues >0 or =0
- We can validate it in terms of the NNLO-NLO shift vector as follows. First diagonalise ***cov$_{th}$*** and determine its ***N_s*** non-zero eigenvalues ***t_a*** and eigenvectors ***v_i^a***
- Then **project the shift vector** onto these eigenvectors

$$\delta_a = \sum_{a=1}^{N_s} \delta_i v_i^a \qquad \delta_i = T_i^{(\mathrm{nnlo})} - T_i^{(\mathrm{nlo})} \ \ (\text{fixed PDF})$$

- A successful prescription for the theory covmat should lead to a **theory χ^2** of ***O(1)***

$$\chi^2_{\mathrm{th}} = \frac{1}{N_s} \sum_{a=1}^{N_s} \frac{\delta_a^2}{t_a^2}$$

- Moreover the *missing* component of the projected shift vector should be small

$$\delta_i^{\mathrm{miss}} \equiv \delta_i - \sum_{a=1}^{N_s} \delta_a v_i^a$$

Validating scale variations (II)

Dataset	cutoff	$\delta_i^{\rm miss}/\delta_i^{\rm max}$		$\chi^2_{\rm th}$
NMCPD	4.74E-08	0.200	4	0.92677
NMC	5.51E-06	0.219	5	3.206
SLACP	4.24E-06	0.078	2	1.2243
SLACD	4.67E-06	0.083	2	1.30069
BCDMSP	1.26E-04	0.272	4	0.83733
BCDMSD	9.90E-05	0.287	4	0.89951
NTVNUDMN	5.18E-05	0.087	4	0.64357
NTVNBDMN	9.25E-05	0.070	3	0.72287
CHORUSNU	4.17E-05	0.180	4	2.5415
CHORUSNB	1.56E-04	0.293	4	0.25108
HERAF2CHARM	2.62E-04	0.132	4	5.65574
HERACOMBNCEM	1.31E-05	0.362	5	1.12059
HERACOMBNCEP460	2.18E-04	0.383	4	0.027879
HERACOMBNCEP575	2.99E-04	0.362	4	0.01798
HERACOMBNCEP820	1.01E-04	0.178	4	0.10718
HERACOMBNCEP920	3.37E-04	0.494	4	0.02354
HERACOMBCCEM	9.68E-07	0.272	4	5.5865
HERACOMBCCEP	5.75E-07	0.346	4	4.84705
ATLASWZRAP36PB	4.61E-06	0.054	3	0.616316
ATLASZHIGHMASS49FB	2.89E-07	0.011	2	0.3839
ATLASLOMASSDY11EXT	8 largest evals	0.000	4	2.435099
ATLASWZRAP11	4.10E-06	0.052	3	0.67529
ATLAS1JET11	1.12E-05	0.020	3	0.38025
ATLASZPT8TEVMDIST	8 largest evals	0.019	8	8.399
ATLASZPT8TEVYDIST	8 largest evals	0.017	8	2.29223
ATLASTTBARTOT	8 largest evals	0.000	3	0.117724
ATLASTOPDIFF8TEVTRAPNORM	1.06E-06	0.036	3	0.137432
CMSWEASY840PB	5.13E-08	0.011	4	10.7403
CMSWMASY47FB	1.47E-08	0.017	4	13.85255
CMSDY2D11	4.17E-05	0.066	3	0.9457
CMSTTBARTOT	8 largest evals	0.000	3	0.118276
CMSTOPDIFF8TEVTTRAPNORM	4.37E-08	0.306	3	0.24383
LHCBZ940PB	1.43E-06	0.014	3	0.2396
LHCBZEE2FB	3.13E-06	0.014	3	0.29634
CDFZRAP	1.86E-06	0.152	3	0.6539
CDFR2KT	5.68E-05	0.070	3	0.3905
D0ZRAP	1.04E-07	0.350	4	4.126
D0WEASY	9.23E-07	0.092	2	0.612
D0MASY	9.76E-07	0.096	2	0.59032

- Correlations within experiments with the **9pt point prescriptions** for ***cov$_{th}$***

- The theory χ^2 should be *O(1)*

$$\chi^2_{\rm th} = \frac{1}{N_s}\sum_{a=1}^{N_s}\frac{\delta_a^2}{t_a^2}$$

- The missing shift vector should be small

$$\delta_i^{\rm miss} \equiv \delta_i - \sum_{a=1}^{N_s}\delta_a v_i^a$$

- Additional validation: able to **reproduce sign** of up to 67% of the entries of the shift matrix $\delta_i\delta_j$

Validating scale variations (II)

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- Correlations within experiments with the **9pt point prescriptions** for ***cov$_{th}$***

- ☑ The theory ***χ²*** should be *O(1)*

$$\chi^2 = \frac{1}{\ldots} \sum^{N_s} \frac{\delta_a^2}{\ldots}$$

$$\delta_i^{\rm miss} \equiv \delta_i - \sum_{a=1}^{N_s} \delta_a v_i^a$$

- ☑ Additional validation: able to **reproduce sign** of up to 67% of the entries of the shift matrix $\boldsymbol{\delta_i \delta_j}$

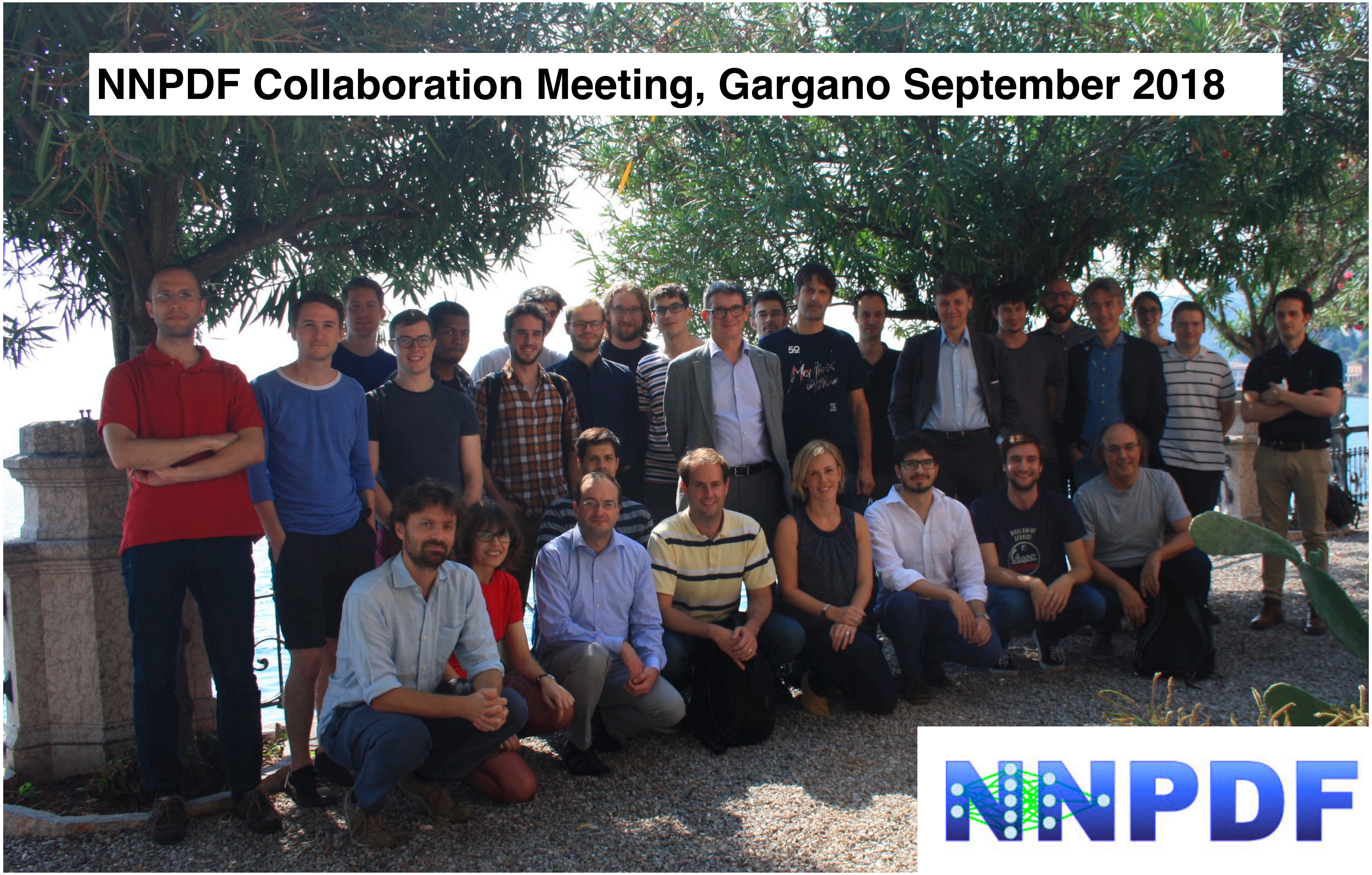
The theory covariance matrix constructed this way **successfully validated** on both the diagonal elements and the correlations of the **NLO=>NNLO shift matrix** (``exact” result)

Summary and outlook

- Systematically quantifying the **impact of MHOUs in global PDF fits** is an important ingredient for the precision phenomenology program at the LHC
- We have developed a novel approach to estimate MHOUs in PDF fits: to carry out **fits with a theory covariance matrix.**
- This approach can be validated both with the **exact NLO=>NNLO shift** and with PDF fits produced with **scale-varied theories**
- Approach can be applied to **other theory uncertainties** e.g. nuclear corrections.
- The theory covariance matrix has been **validated at NLO with the exact result** (the NNLO-NLO shift matrix) both for the diagonal and the off-diagonal elements

NNPDF fits accounting for MHOUs in the global dataset around the corner!

Summary and outlook



Summary and outlook

Extra Material

Theory uncertainties from MHOs

At any finite order, perturbative QCD calculations depend on the unphysical **renormalisation** and **factorisation scales**

$$\sigma(\mu_R, \mu_F) = \sum_{k=0}^{n} \sum_{i,j}^{n_f} \alpha_s^{p+k}(\mu_R)\, \widetilde{\sigma}^{(k)}(\mu_R, \mu_F) \otimes q_i(\mu_F) \otimes q_j(\mu_F) + \mathcal{O}\left(\alpha_s^{p+n+1}\right)$$

In PDF fits, both scales are set to a given fixed value, the typical **momentum transfer of the process *Q*,** and MHOUs are neglected

$$\sigma(\mu_R = Q, \mu_F = Q) = \sum_{k=0}^{n} \sum_{i,j}^{n_f} \alpha_s^{p+k}(Q)\, \widetilde{\sigma}^{(k)}(Q) \otimes q_i(Q) \otimes q_j(Q)$$

At order **N^{k}LO**, the scale dependence of physical cross-sections is expressed in terms the **N^{k-1}LO** splitting functions and partonic cross-sections by imposing:

$$\sigma(\mu_R, \mu_F) = \sigma(Q, Q) + \mathcal{O}\left(\alpha_s^{p+k+1}\right)$$

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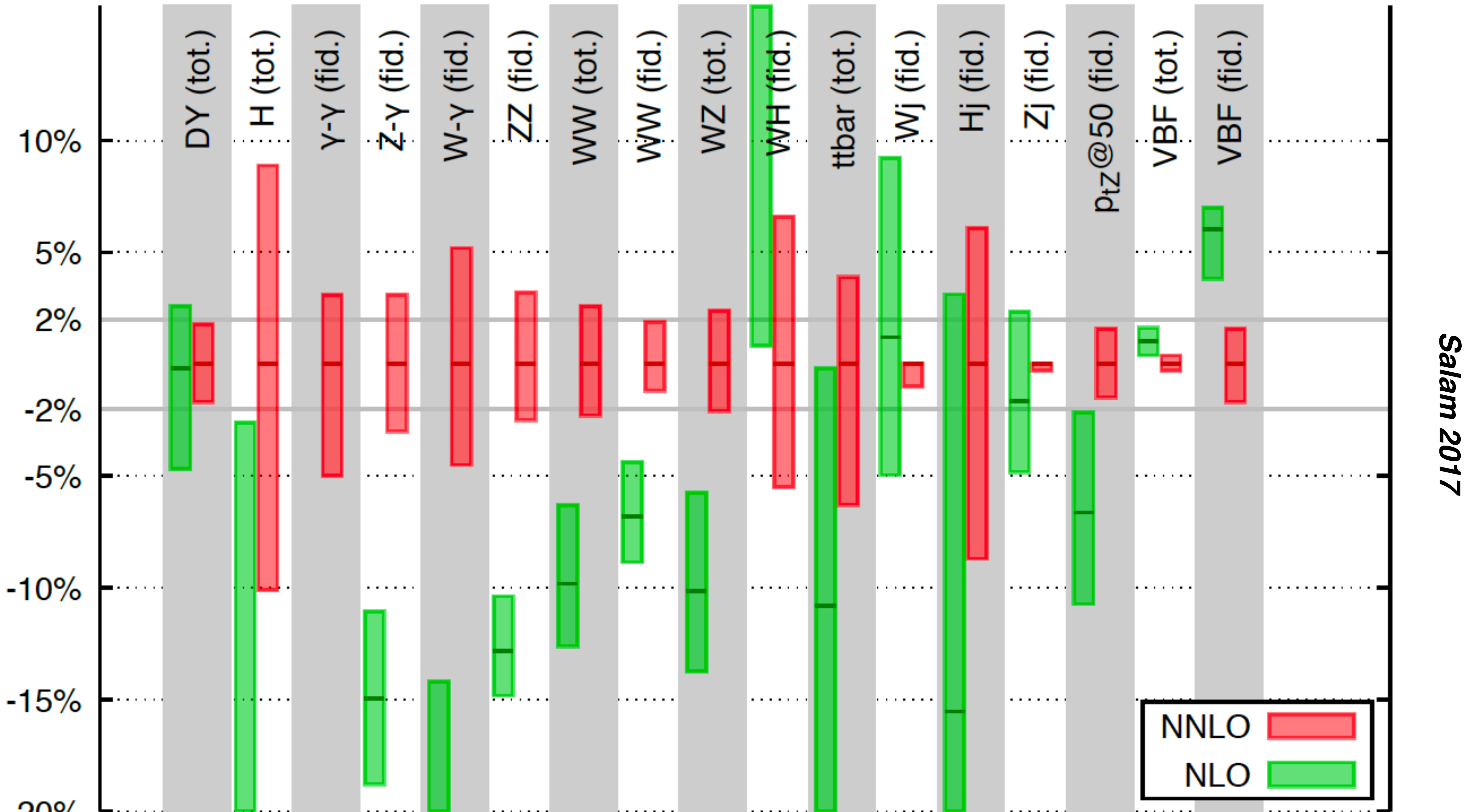
$$\sigma(\mu_R = Q, \mu_F = Q) = \sum_{k=0}^{n} \sum_{i,j}^{n_f} \alpha_s^{p+k}(Q)\, \widetilde{\sigma}^{(k)}(Q) \otimes q_i(Q) \otimes q_j(Q)$$

Scale-dependent terms at **N^{k}LO** predicted from **N^{k-1}LO** results: varying $\boldsymbol{\mu_R}$ and $\boldsymbol{\mu_F}$ within a certain range provides an estimate of MHOUs

$$\Delta_{\rm MHO}^{(\rm max)}\sigma \equiv \max\left((\sigma(\mu_R^{(1)}, \mu_F^{(1)}) - \sigma(Q,Q)), \sigma(\mu_R^{(2)}, \mu_F^{(2)}) - \sigma(Q,Q), \ldots \right)$$

MHOUs from scale variations

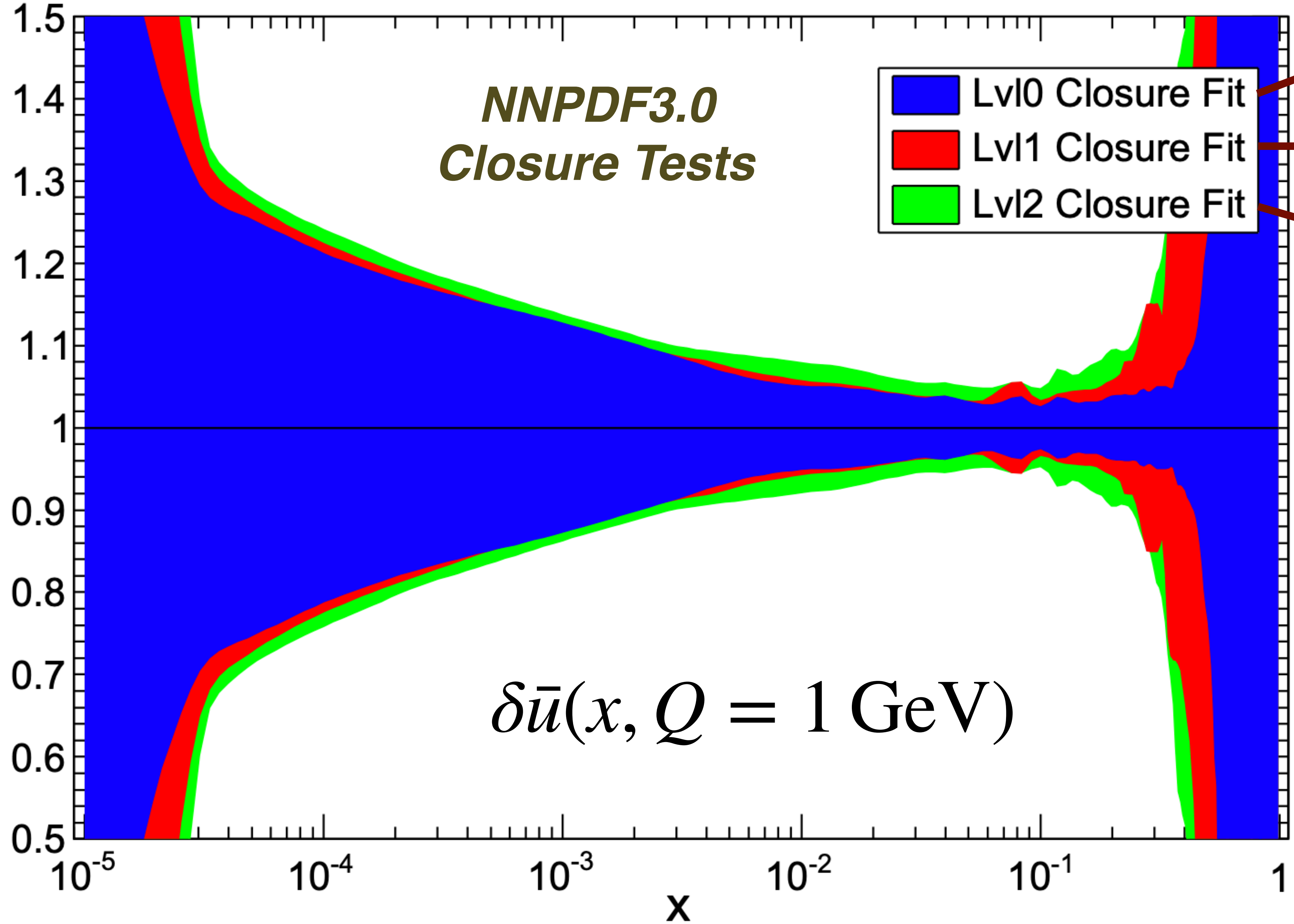


Scale variations not always **best predictor of MHOs**

Is this strategy reliable for the processes **input to the PDF fit?**

PDF uncertainties

PDF uncertainties receive contributions from **different sources**:



extrapolation/ degeneracy

functional form

exp data uncertainties

Parametric theory errors from $\delta\alpha_S$, δm_c are easily accounted for in PDF fits

Theory uncertainties on PDFs from **Missing Higher Orders** never quantified!