PDFs with MHOUs

- MHOU via Scale Varn
- Validation
- PDFs and Predictions

Richard Ball (for NNPDF)

arXiv: 1905.04311
arXiv: 1906.10698

James Stirling Memorial
PDF4LHC Sep 2019
Durham

Uncertainties in PDF fits

- Experimental uncertainties
- Parametric uncertainties
  (α_s, m_q, etc)
- Methodological uncertainties
  (closure testing: small)
- Theoretical uncertainties
  (nuclear, MHOU, HT, etc)

Ultimate aim: 1% uncertainties: need to have all these under control.

Theoretical Uncertainties in PDF fits

- Statistical (Monte Carlo, etc) arXiv: 1704.00428
- Nuclear Corrections arXiv: 1812.09074
- Missing Higher orders (MHOU) arXiv: 1906.10698
- Power corrections (HT)
- Final state corrections

General Strategy:

- compute a theory covariance matrix S_{ij} for each theoretical uncertainty
- add to experimental covariance matrix C_{ij} (exp and th unc independent)
- fit using combined covariance matrix $C_{ij} + S_{ij}$

arXiv: 1801.04842

Increases overall PDF uncertainty, but removes theoretical tensions or biases

(by reducing impact of data sets with significant theoretical uncertainties)

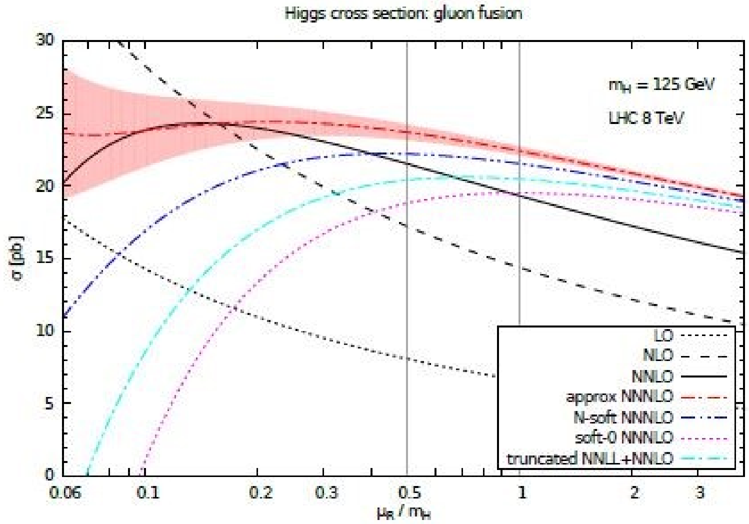
Estimating MHOU by Scale Variation

Ren grp invariance:

$$\mu^2 \frac{d}{d\mu^2}\overline{\sigma}(\alpha_s(\mu^2), \mu^2/Q^2) = 0.$$

- Q^2 is the physical scale
- μ^2 is the ren scale

Estimate MHOU by evaluating xsec at various scales:



Various prescriptions: ren scale, fact scale, used to give envelope estimates

Here want to instead estimate theory covmat by varying parameters and averaging

$$S_{ij} \simeq \langle (T_i(\mu) - T_i)(T_j(\mu) - T_j) \rangle_\mu$$

Scale Variation: Pros and Cons

Pros:

- naturally incorporates ren grp inv: MHOU goes to zero at high orders
- $\alpha_s(\mu^2)$ is universal: same procedure works for any process
- naturally incorporates sum rule constraints
- smooth: kinematic corrlns in e.g. Q^2, x, etc, automatically included
- can also account for corrlns between different processes

Cons:

- how much should we vary the scale? Factor $2, \frac{1}{2}$ usual ...
- can fail for new channels, color structures, kinematic sings…

Validation:

- At NLO, can compare NLO MHOU estimate to NNLO

Scale variation for PDF determination

Factorization (eg DIS):

$$\overline{F}(Q^2, \mu_f^2, \mu_r^2) = \overline{C}\left(\alpha_s(\mu_r^2),\ \mu_r^2/Q^2\right) \otimes \overline{f}\left(\alpha_s(\mu_f^2), \mu_f^2/Q^2\right)$$

For a given factorization (eg $\overline{\mathrm{MS}}$) have *two* sources of MHOU for each observable:

- PDF evolution : 'factorization scale' μ_f : MHOU in splitting functions
- hard coeff fn : 'renormalization scale' μ_r : MHOU in coeff fns / hard xsecs

Variations of μ_f and μ_r must be performed

- independently of each other (two sources of MHOU distinct)
- symmetrically (two sources of MHOU equally important)
- μ_f variations correlated across all processes (PDFs universal)
- μ_r variations correlated within a process, uncorrelated for different processes

In this first study, we assume

- a single μ_f (though singlet/nonsinglet/valence in principle independent)
- five different μ_r (corresponding to DIS NC, DIS CC, DY, jets, top)
- all variations by factor of two either way

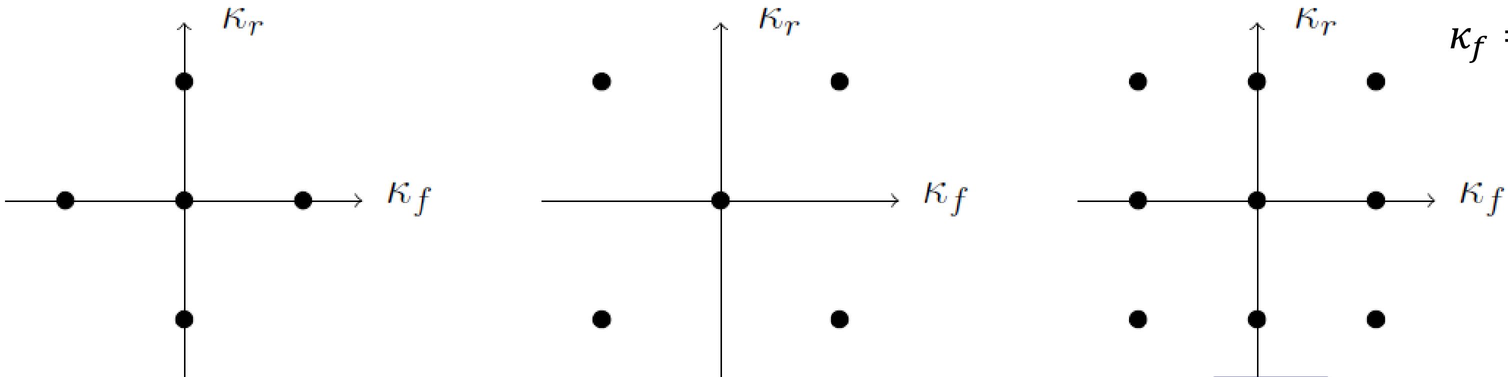
Symmetric Prescriptions

$$S_{ij} = \mathcal{N} \sum \Delta_i(\mu_f, \mu_r)\Delta_j(\mu_f, \mu_r) \qquad \Delta_i(\mu_f, \mu_r) = T_i(\mu_f, \mu_r) - T_i(Q, Q)$$

e.g.

$$\kappa_r = \log\frac{\mu_r}{Q}$$

$$\kappa_f = \log\frac{\mu_f}{Q}$$



5pt

'5bar' pt

9 pt

Same process:

$$S_{ij}^{(9\text{pt})} = \tfrac{1}{4}\{\Delta_i^{+0}\Delta_j^{+0} + \Delta_i^{-0}\Delta_j^{-0} + \Delta_i^{0+}\Delta_j^{0+} + \Delta_i^{0-}\Delta_j^{0-} + \Delta_i^{++}\Delta_j^{++} + \Delta_i^{+-}\Delta_j^{+-} + \Delta_i^{-+}\Delta_j^{-+} + \Delta_i^{--}\Delta_j^{--}\}\,.$$

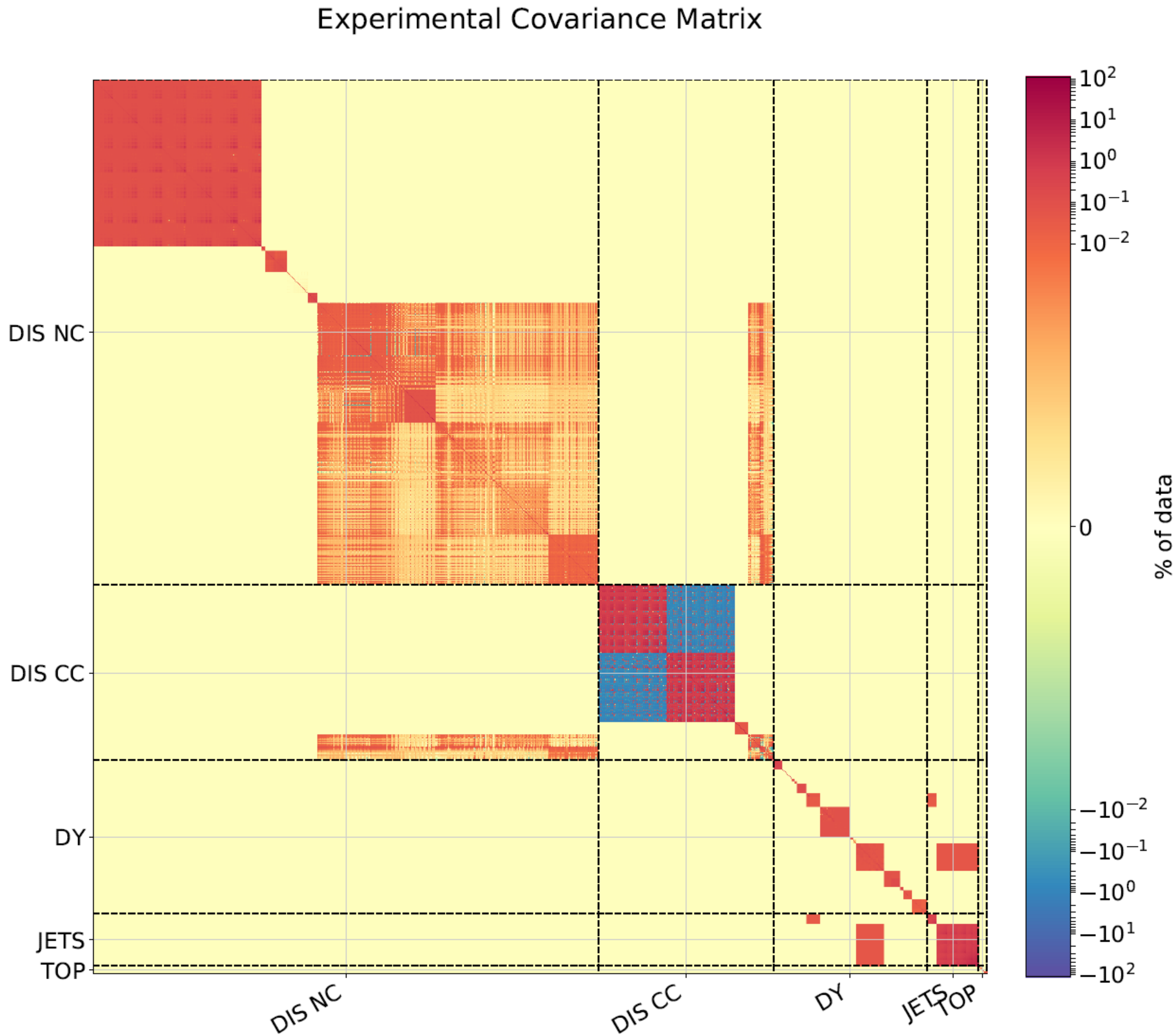
$i, j \in \pi$

Different processes:

$$S_{i_1 j_2}^{(9\text{pt})} = \tfrac{1}{24}\{2(\Delta_{i_1}^{+0} + \Delta_{i_1}^{++} + \Delta_{i_1}^{+-})(\Delta_{j_2}^{+0} + \Delta_{j_2}^{++} + \Delta_{j_2}^{+-}) + 2(\Delta_{i_1}^{-0} + \Delta_{i_1}^{-+} + \Delta_{i_1}^{--})(\Delta_{j_2}^{-0} + \Delta_{j_2}^{-+} + \Delta_{j_2}^{--})\} + 3(\Delta_{i_1}^{0+} + \Delta_{i_1}^{0-})(\Delta_{j_2}^{0+} + \Delta_{j_2}^{0-})\}.$$

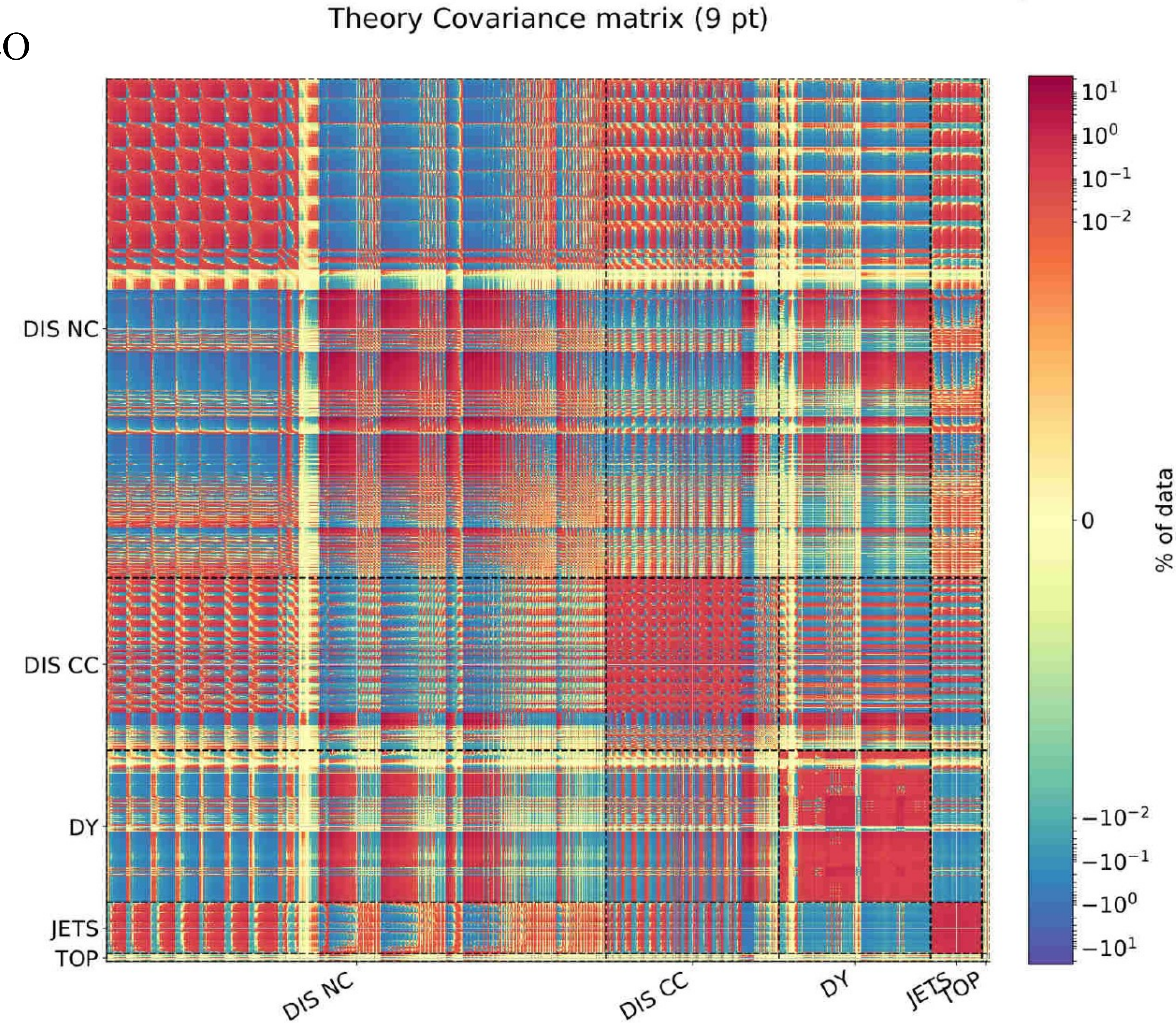
$i_1 \in \pi_1, j_2 \in \pi_2$

$$\mu = \begin{cases} 2Q & + \\ Q & 0 \\ \frac{1}{2}Q & - \end{cases}$$



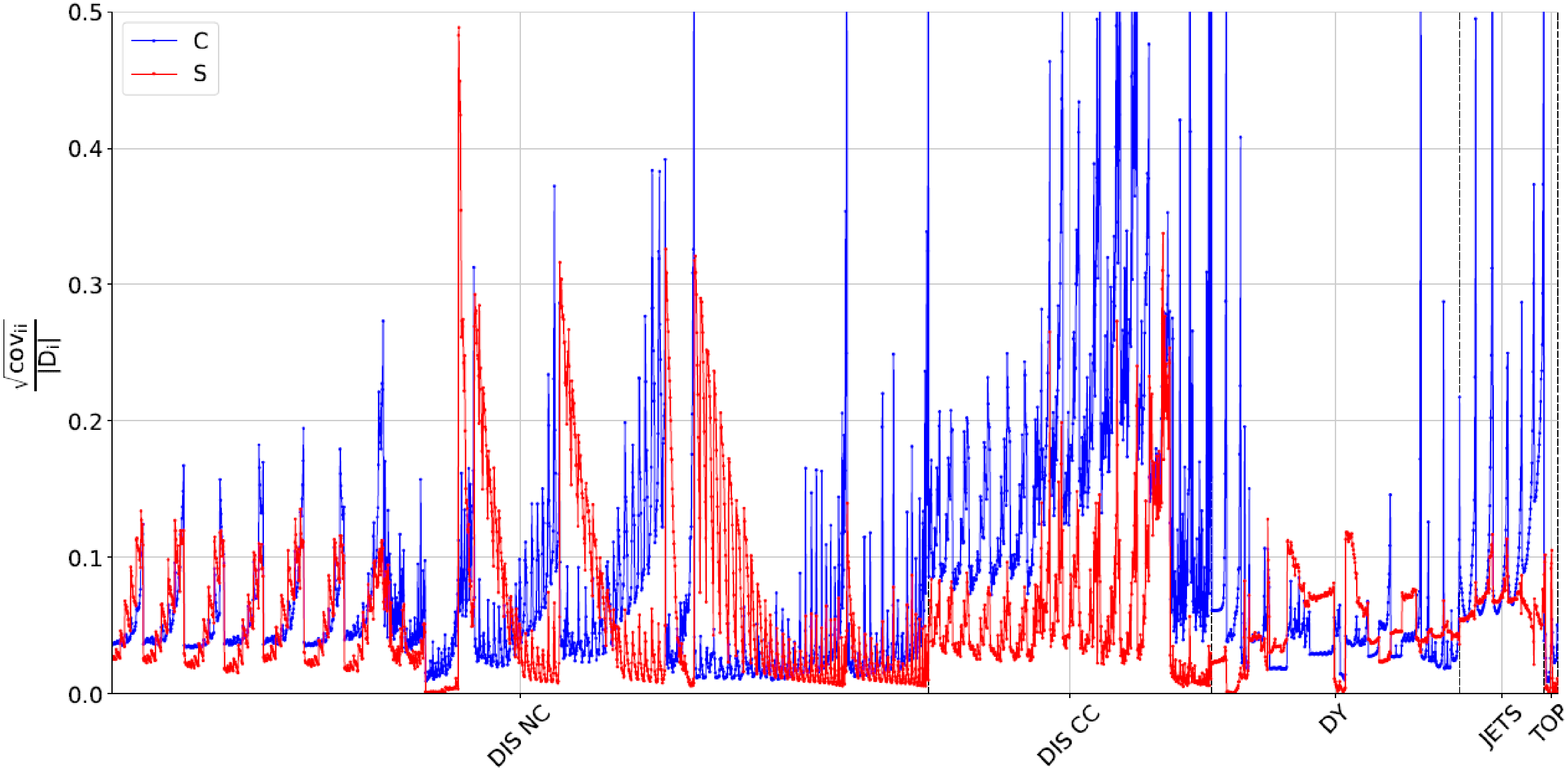
Experimental Covariance Matrix
DIS NC
DIS CC
DY
JETS
TOP
% of data
10^2
10^1
10^0
10^{-1}
10^{-2}
0
-10^{-2}
-10^{-1}
-10^0
-10^1
-10^2

NLO


Theory Covariance matrix (9 pt)
DIS NC
DIS CC
DY
JETS
TOP
% of data
10^1
10^0
10^{-1}
10^{-2}
0
-10^{-2}
-10^{-1}
-10^0
-10^1

NLO

MHOU ($\sqrt{S_{ii}}$) vs Exp Unc ($\sqrt{C_{ii}}$)



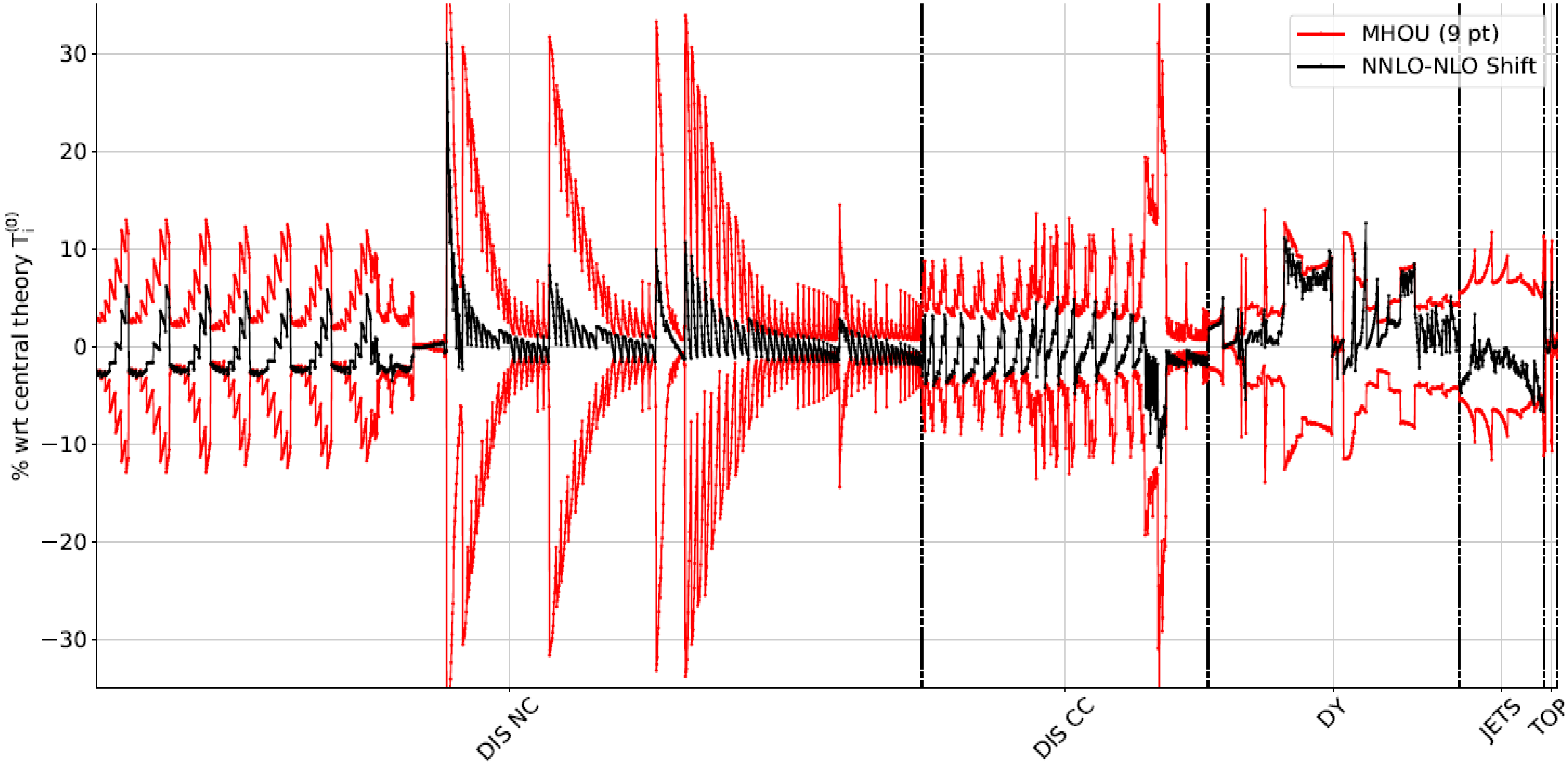
- if $S_{ii} \gg C_{ii}$ data points suppressed in fit
- if $S_{ii} \ll C_{ii}$ MHOU has no effect

NLO

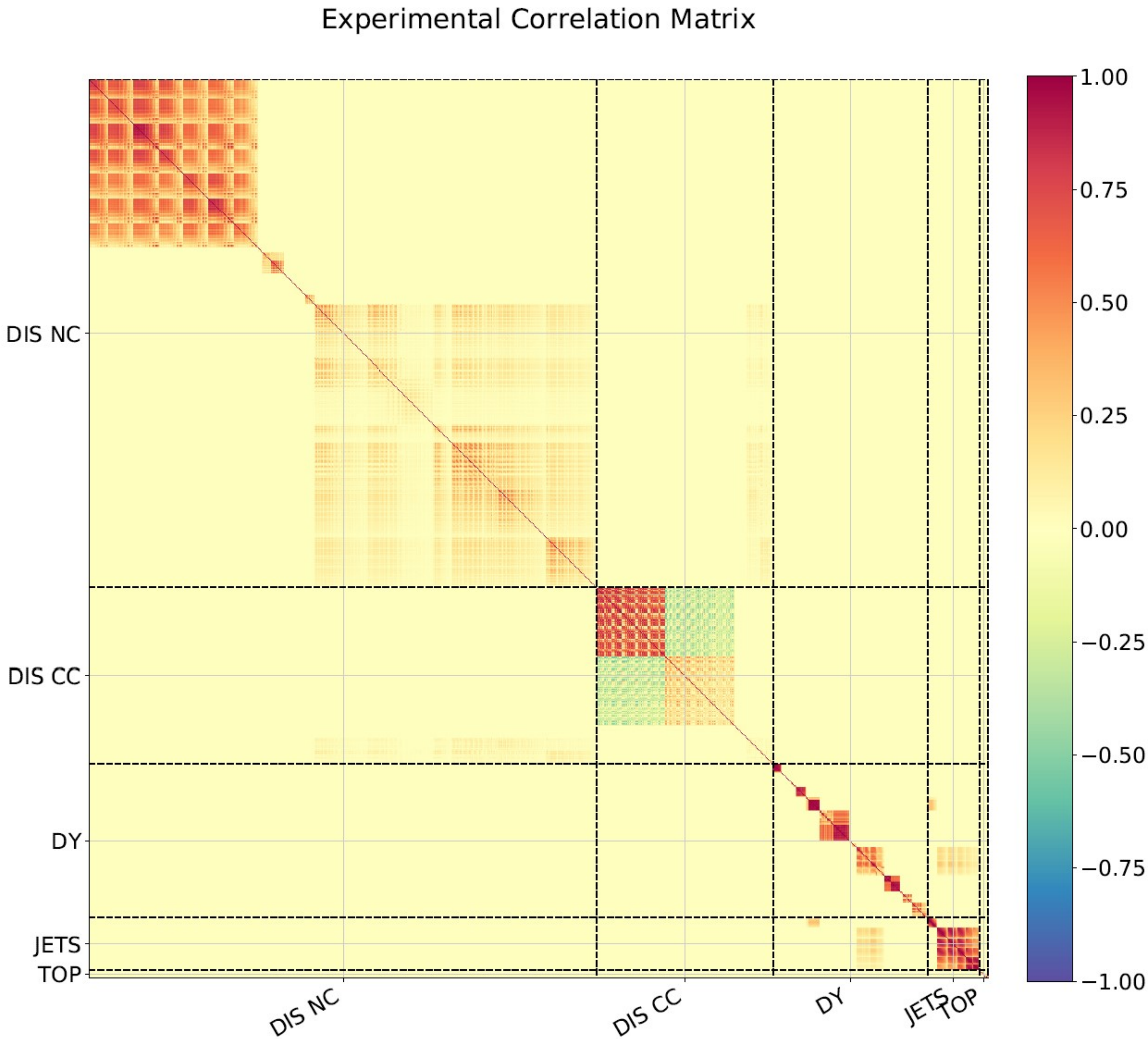
Validation : diagonals

Compare diagonal MHOU ($\sqrt{S_{ii}}$) to 'shift'

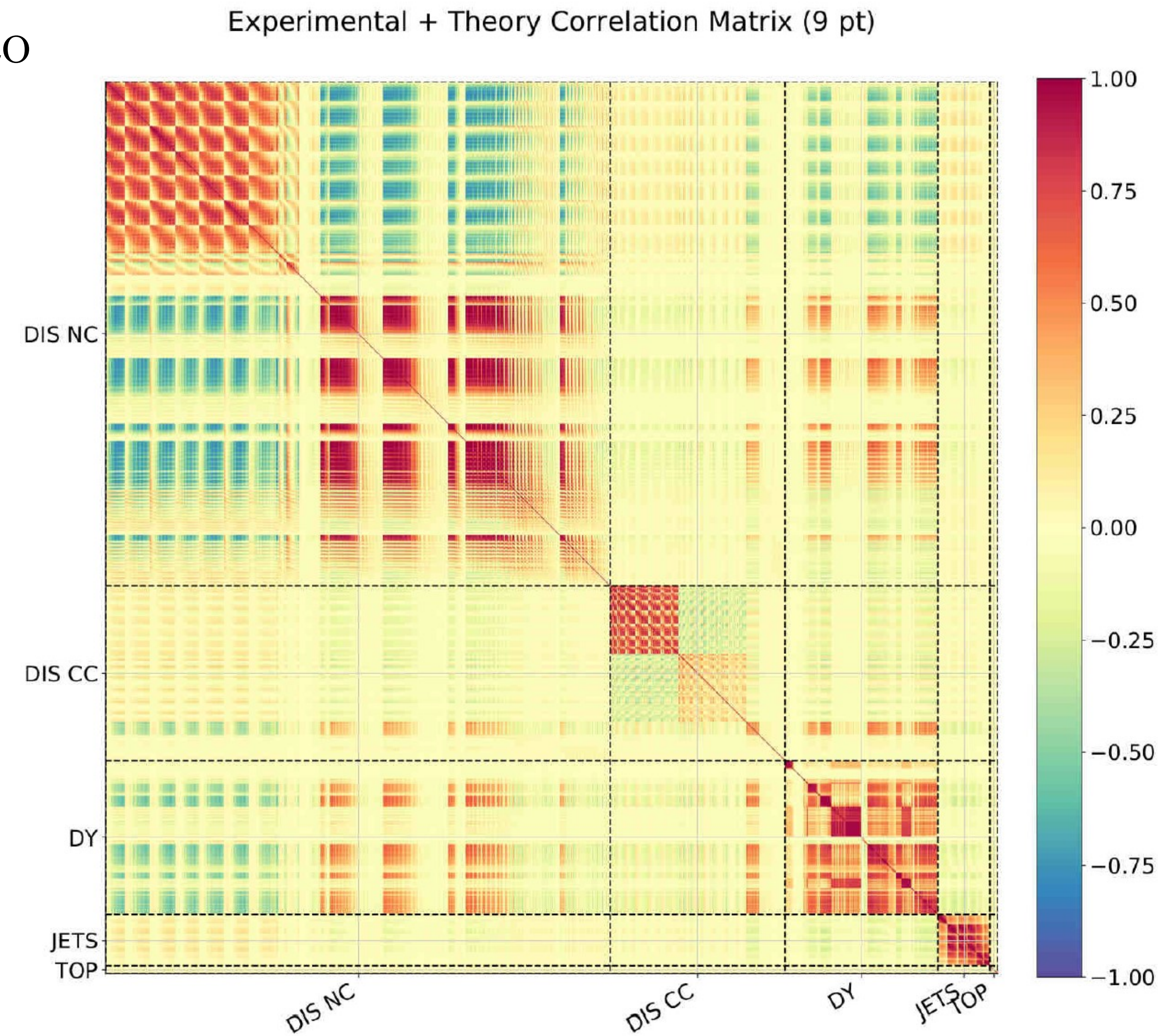
$$\delta_i = (T_i^{\mathrm{NNLO}} - T_i^{\mathrm{NLO}})/T_i^{\mathrm{NLO}}$$



$\delta_i < \sqrt{S_{ii}}$ for all data points : conservative

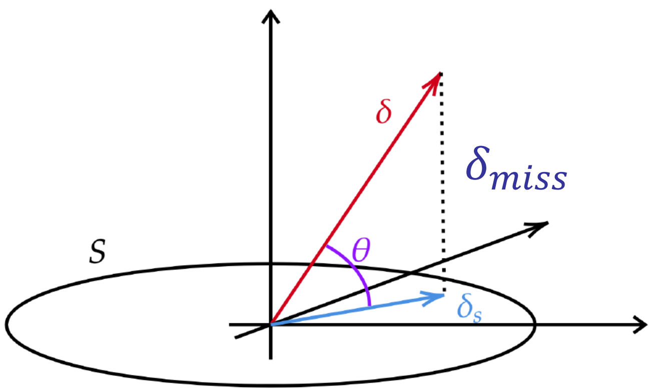

Experimental Correlation Matrix
DIS NC
DIS CC
DY
JETS
TOP
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

NLO


Experimental + Theory Correlation Matrix (9 pt)
DIS NC
DIS CC
DY
JETS
TOP
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

Validation : correlations

- view shift δ_i as a vector in $\sim$ 3000 dimensional space
- diagonalize S_{ij} in this space: gives ellipsoid S in $<$ 30 dim subspace
- project δ_i into S : how much of δ_i lies in S ???

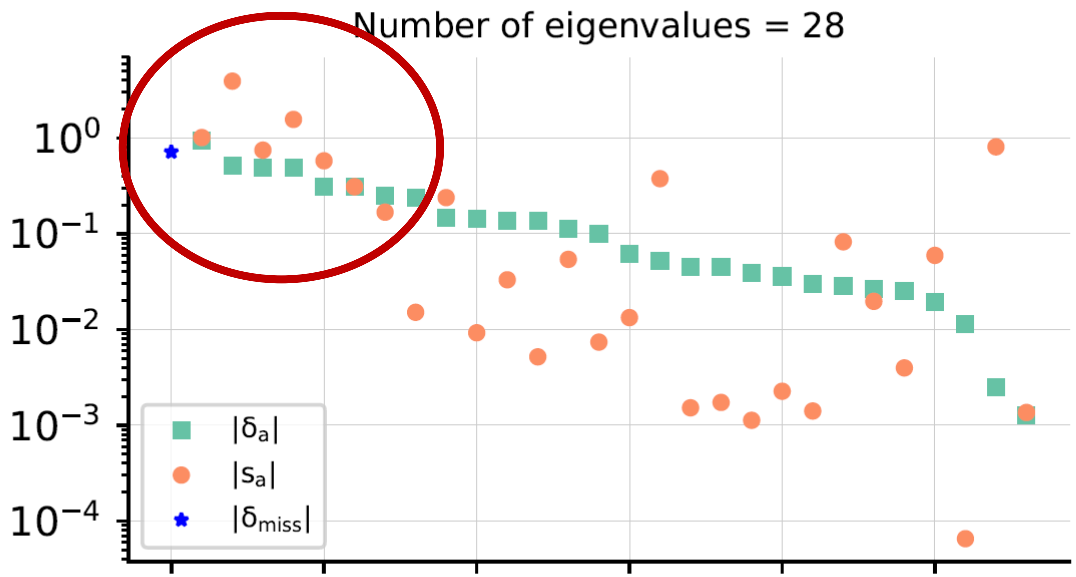


smaller angles θ mean that S_{ij} gives a better estimate of δ_i

Presc.	N_{sub}	Global	DIS NC	DIS CC	DY	JET	TOP
		2819	1593	552	484	164	26
5-pt	8	33°	39°	21°	25°	17°	11°
$\overline{5}$-pt	12	31°	38°	17°	23°	22°	10°
9-pt	28	26°	32°	16°	22°	14°	3°
3-pt	6	52°	54°	36°	39°	24°	12°
7-pt	14	29°	35°	17°	22°	16°	3°

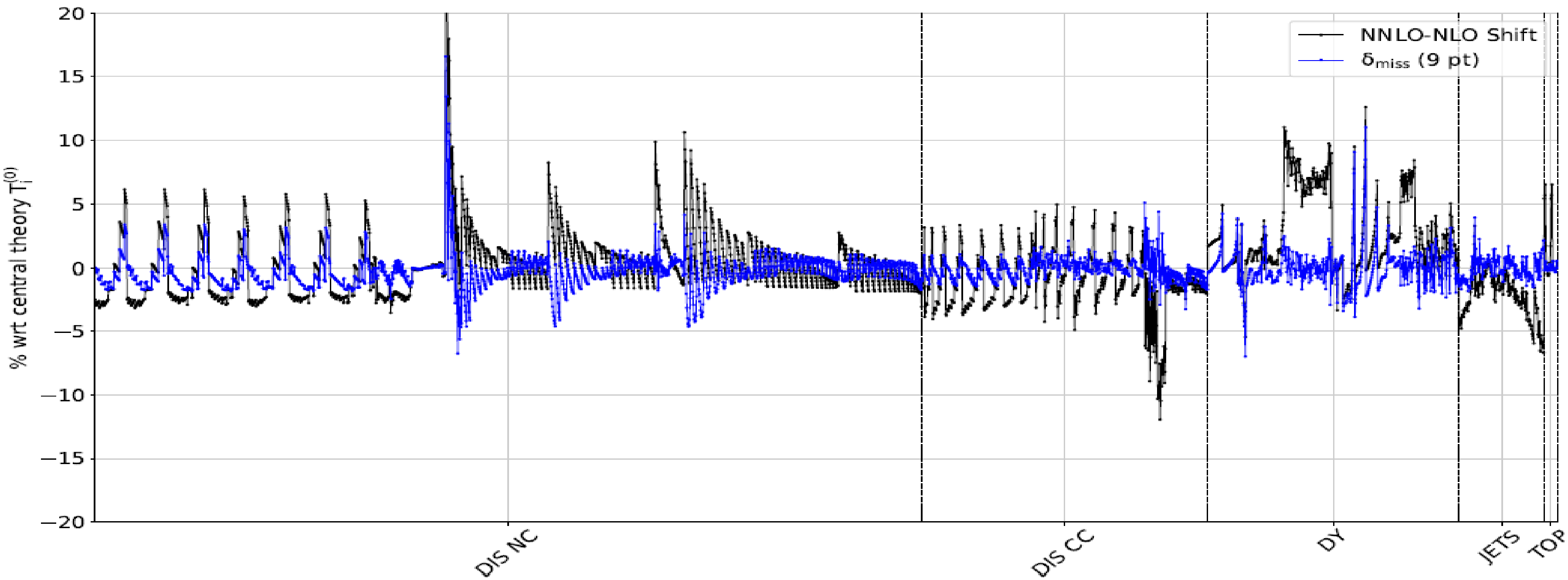
9-pt works best!

NLO, 9pt



For larger projections δ, evals $s > \delta$

$\delta^i_{miss} \ll \delta^i$



NLO global fits with MHOU

- Generate data replicas: $\lim_{N_{\rm rep}\to\infty} \frac{1}{N_{\rm rep}(N_{\rm rep}-1)} \sum_{k=1}^{N_{\rm rep}} \left(D_i^{(k)} - \langle D_i \rangle\right)\left(D_j^{(k)} - \langle D_j \rangle\right) = C_{ij} + S_{ij},$
- Fit PDF replicas: $\chi^2[f^{(k)}] = \frac{1}{N_{\rm dat}} \sum_{i,j=1}^{N_{\rm dat}} (T_i[f^{(k)}] - D_i^{(k)})(C+S)^{-1}_{ij}(T_j[f^{(k)}] - D_j^{(k)})$

Process	$n_{\rm dat}$	$\chi^2/n_{\rm dat}$ in the NNPDF3.1 global fits				
		NLO				NNLO
		C	$C+S^{(9\rm pt)}$	$C+S^{(7\rm pt)}$	$C+S^{(3\rm pt)}$	C
DIS NC	1593	1.088	1.079	1.086	1.095	1.084
DIS CC	552	1.012	0.928	0.933	0.960	1.079
DY	484	1.486	1.447	1.485	1.483	1.231
JETS	164	0.907	0.839	0.858	0.901	0.950
TOP	26	1.260	1.012	1.016	1.077	1.068
Total	2819	1.139	1.109	1.129	1.139	1.105

MHOU improves χ^2:
9pt does best!
($\sim$ NNLO)

NLO global fits with MHOU

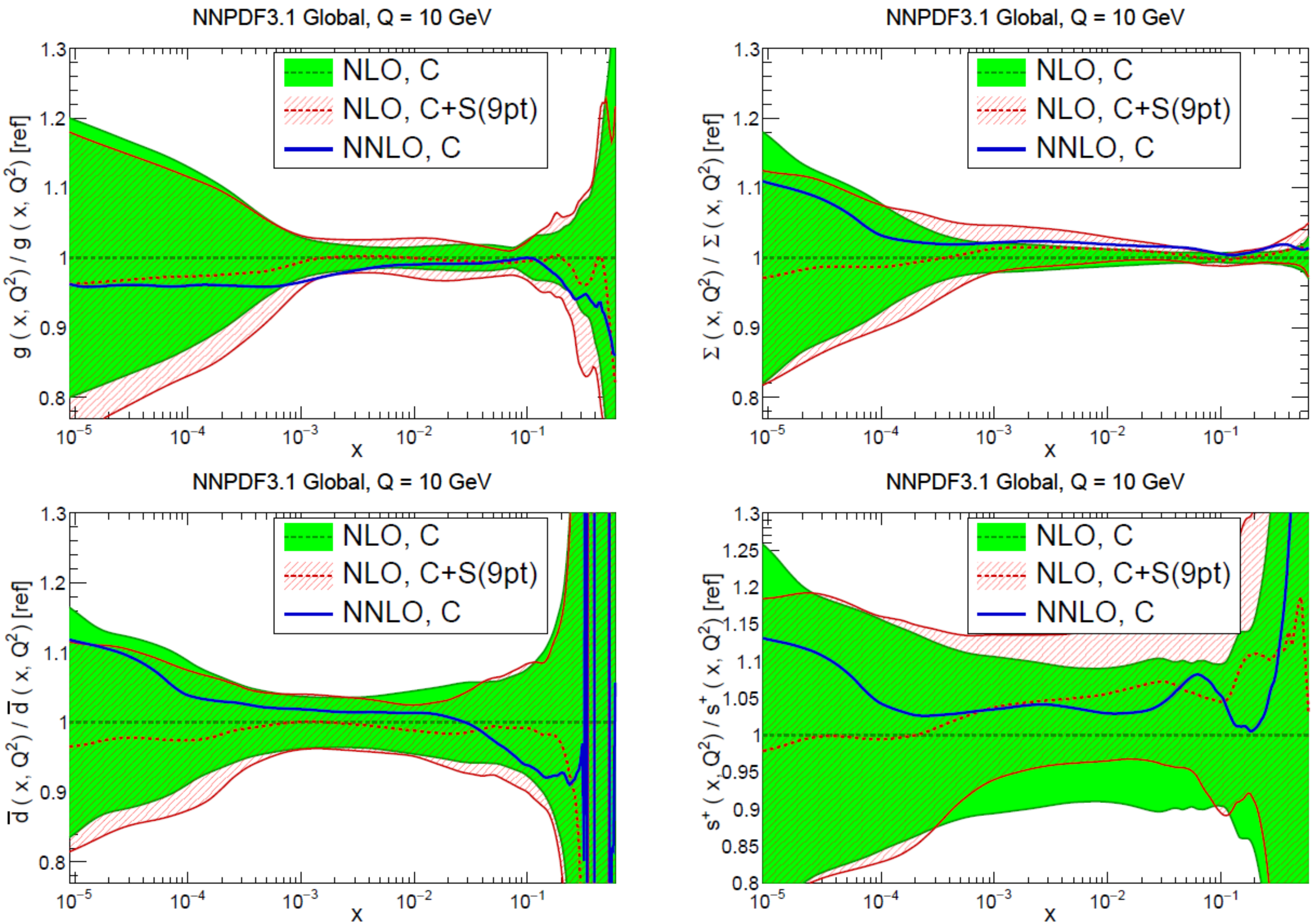
- Generate data replicas: $\lim_{N_{\rm rep}\to\infty} \frac{1}{N_{\rm rep}(N_{\rm rep}-1)} \sum_{k=1}^{N_{\rm rep}} \left(D_i^{(k)} - \langle D_i \rangle\right)\left(D_j^{(k)} - \langle D_j \rangle\right) = C_{ij} + S_{ij},$
- Fit PDF replicas: $\chi^2[f^{(k)}] = \frac{1}{N_{\rm dat}} \sum_{i,j=1}^{N_{\rm dat}} (T_i[f^{(k)}] - D_i^{(k)})(C+S)^{-1}_{ij}(T_j[f^{(k)}] - D_j^{(k)})$

Process	ϕ in the NNPDF3.1 global fits				
	NLO				NNLO
	C	$C+S^{(9\rm pt)}$	$C+S^{(7\rm pt)}$	$C+S^{(3\rm pt)}$	C
DIS NC	0.266	0.412	0.393	0.384	0.305
DIS CC	0.389	0.408	0.427	0.442	0.471
DY	0.361	0.377	0.369	0.379	0.380
JETS	0.295	0.359	0.327	0.333	0.392
TOP	0.375	0.443	0.387	0.405	0.363
Total	0.314	0.405	0.394	0.394	0.362

$$\phi \sim \langle \frac{\sigma_{PDF}}{\sigma_{exp}} \rangle$$

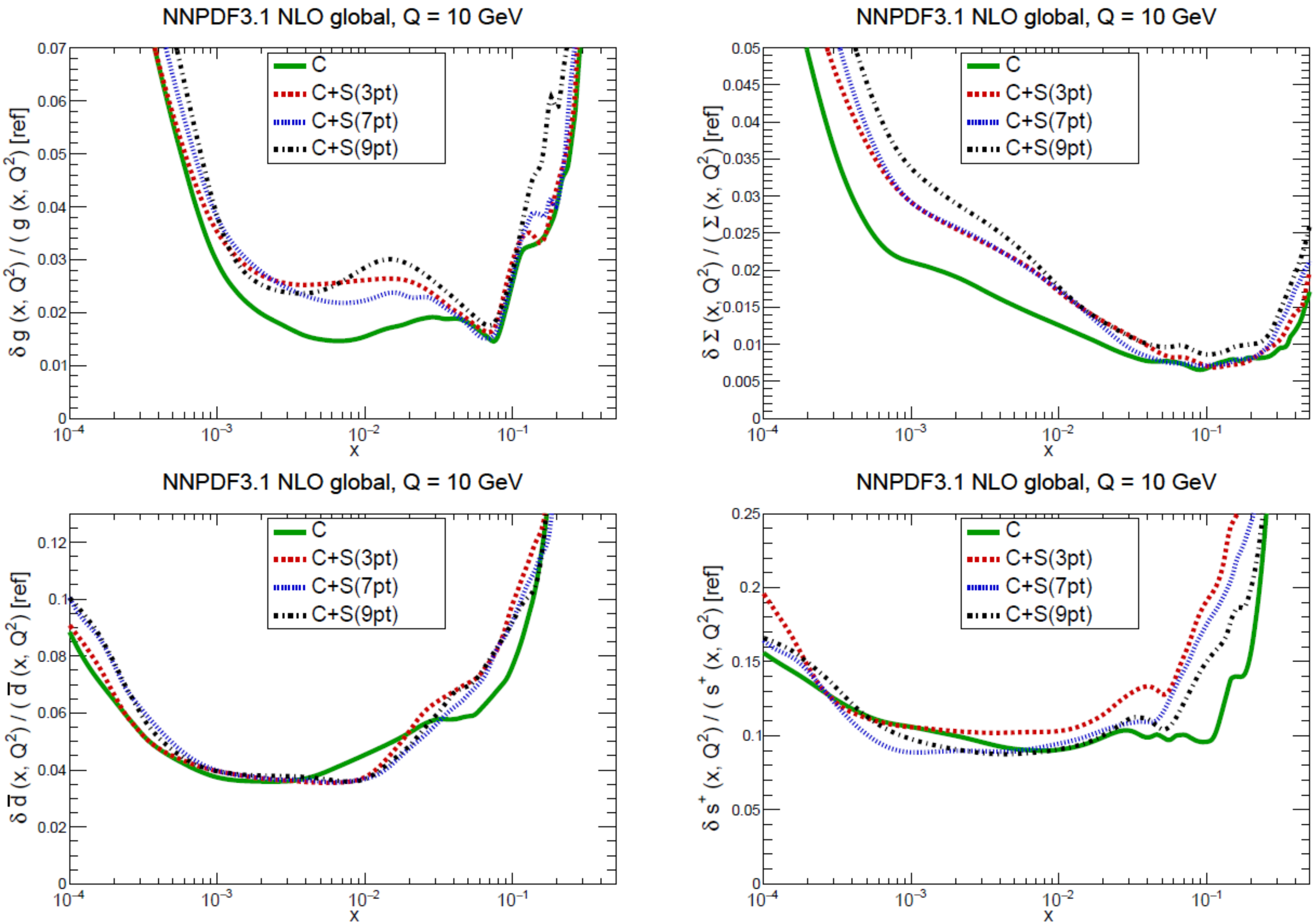
MHOU increase unc:
but only by ~ 30 %
(~ NNLO)

NLO PDFs with and without MHOU



MHOU moves NLO PDF towards NNLO

NLO PDFs with MHOU: uncertainties

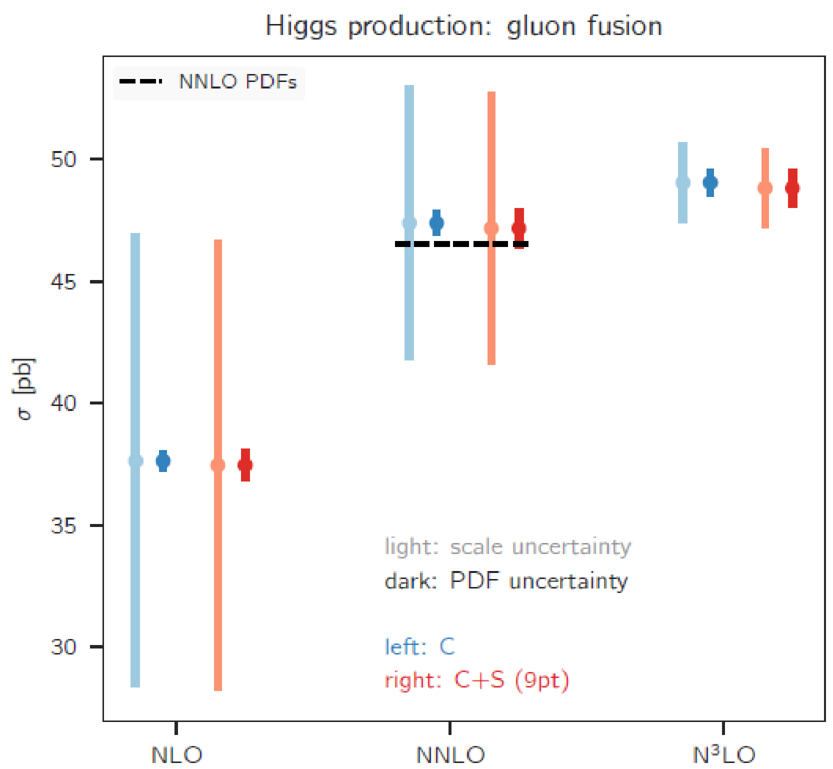


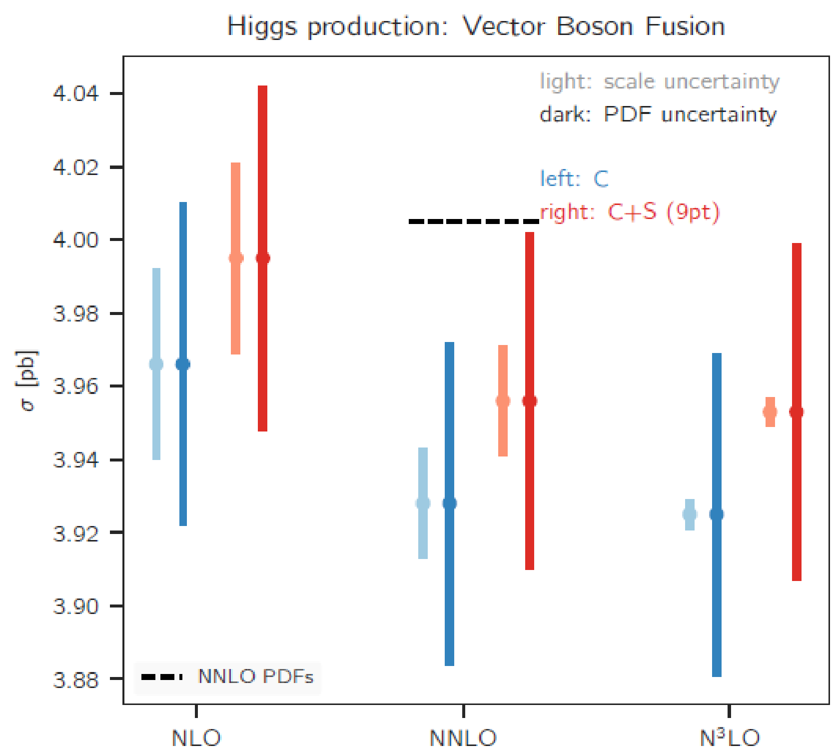
Increase in uncertainties $< 30\%$ in data region

Predictions

$$\sigma_i^0 = \underbrace{\langle \sigma_i[f] \rangle_f}_{\text{Av over reps}} \qquad \mathrm{Var}(\sigma)_{ij} = \underbrace{\langle (\sigma_i[f] - \sigma_i^0)(\sigma_j[f] - \sigma_j^0) \rangle_f}_{\text{PDF unc}} + \underbrace{S_{ij}^{9\mathrm{pt}}}_{\text{MHOU}}$$

Add PDF unc and MHOU in quadrature





MHOU moves NLO prediction towards NNLO result

New PDF4LHC combination?

PDF4LHC 15 = NNPDF3.0 $\oplus$ CT14 $\oplus$ MMHT14

PDF4LHC 20 = NNPDF3.1 $\oplus$ CT18 $\oplus$ 'MHTXXX19' ???

NNPDF3.1: Eur.Phys.J. C77 (2017) 663, on LHAPDF
CT18: (arXiv: 1908.11394 + ?), some PDFs now available
MHTXXX19: (arXiv: 1907.08147 - latest update of MMHT14), no new release

Towards NNPDF4.0

(Juan Cruz-Martinez, next talk)

- new NN architecture, fitted preprocessing, hyperopt
- new faster fitting technology (N3fit) (closure tested)
- new evolution code (replaces Apfel, includes N3LO)
- theory uncertainties at NLO and NNLO
- photon PDF, and electroweak corrections to all datasets
- lots of new datasets (and new processes: prompt photon, dijets, single top)

Summer 2020?

New data for NNPDF4.0

ELECTROWEAK
* ATLAS high-mass Drell-Yan double-differential distributions at 8 TeV
* ATLAS W/Z total xsec at 13 TeV (81pb-1)
* ATLAS triple-differential Z production at 8 TeV (20.2 fb-1)
* ATLAS W+jets differential distributions at 8 TeV
* CMS differential distributions in Z production at 13 TeV
* LHCb W -> e nu rapidity dist, 8 TeV (2 fb-1)
* LHCb Z rapidity distribution, 13 TeV
* CMS W pt distribution, 8 TeV (18.4 fb-1)
* CMS Z+charm at 8 TeV, 19.7 fb-1
* CMS W+charm differential distributions at 13 TeV

JETS and PHOTONS
* ATLAS isolated photon production 8 TeV, 20 fb-1
* ATLAS isolated photon production, 13 TeV, 3.2 fb-1
* ATLAS dijet cross-sections at 7 TeV
* ATLAS inclusive jet cross-sections at 8 TeV from the 2012 dataset
* CMS dijet cross-sections at 7 TeV
* CMS inclusive jet production at 8 TeV, 19.6 fb-1
* CMS triple differential dijet cross-sections at 8 TeV (19.6 fb-1)
* CMS double-differential dijet distributions at 5 TeV
* Inclusive jet and di-jet production in neutral-current DIS from H1 and ZEUS (HERA DIS jets)

prompt photons (at NNLO)

Dijets (at NNLO)

DIS jets (at NNLO)

TOP QUARK
* CMS total xsec of top-pair production at 5.02 TeV, 27.4 pb-1
* CMS double differential distributions top-quark production 8 TeV, 19.7 fb-1
* CMS single differential distributions in top-pair production (lepton+jets) at 13 TeV, L=35.8 fb-1(2016)
* CMS single differential distributions in top-pair production (dilepton) at 13 TeV, 35.8 fb-1(2016)
* CMS single top t-channel total cross section ratio at 7 TeV
* CMS single top t-channel total cross section ratio at 8 TeV
* CMS single top t-channel total cross section ratio at 13 TeV
* ATLAS single top t-channel total cross section ratio and diff. distributions at 7 TeV
* ATLAS single top t-channel total cross section ratio at 8 TeV
* ATLAS single top t-channel total cross section ratio at 13 TeV

single top (at NNLO)

Upgrades

* ATLAS W/Z production, 7 TeV (4.6 fb-1) => added the off-peak and forward Z prod bins
* Final combination of charm and beauty str fns from HERA (Runs I+II): replaces HERA-I charm comb and H1, ZEUS structure functions

Cutoff date for new data: end of 2019

Summary & Outlook

- PDFs with MHOU using scale variation
- Modest increase in PDF unc at NLO
- Increases precision by resolving tensions
- Global fit NNLO + MHOU to follow
- NNPDF4.0: well on its way

Bayesian Theory Uncertainties

RDB + A. Deshpande
arXiv: 1801.04842

data D theory T 'truth' $\mathcal{T}$

- Gaussianity:

$$P(D|\mathcal{T}) \propto \exp\big(-\tfrac{1}{2}(\mathcal{T}_i - D_i)C^{-1}_{ij}(\mathcal{T}_j - D_j)\big),$$

$$P(T|\mathcal{T}) \propto \exp\big(-\tfrac{1}{2}(\mathcal{T}_i - T_i)S^{-1}_{ij}(\mathcal{T}_j - T_j)\big),$$

C_{ij}: exp covmat

S_{ij}: th covmat

- Bayes Thm:

$$P(\mathcal{T}|DT)P(D|T) = P(D|\mathcal{T}T)P(\mathcal{T}|T).$$

- Independence:

$$P(D|\mathcal{T}T) = P(D|\mathcal{T}).$$

'theorists don't bias experiments'

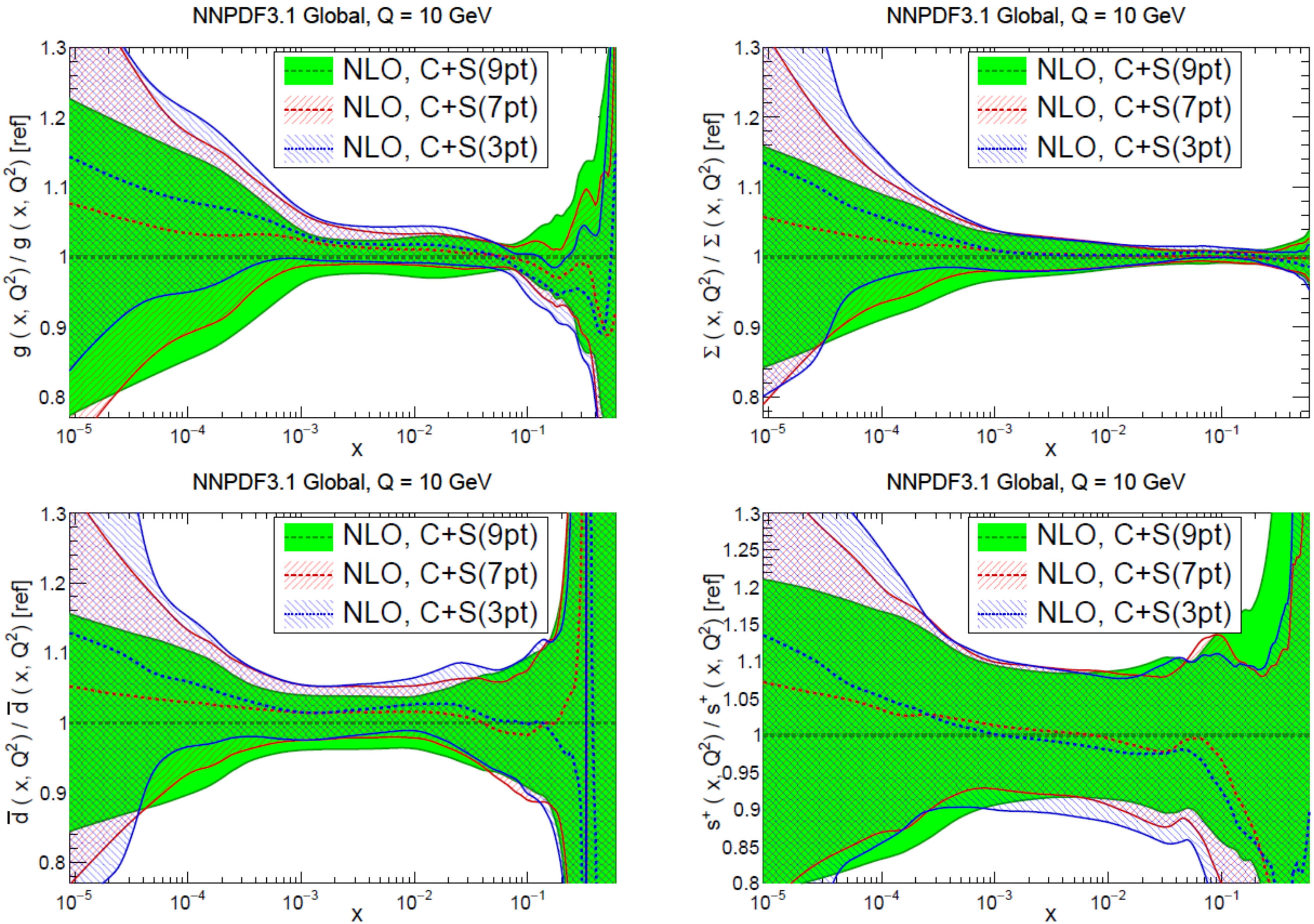
Marginalise on $\mathcal{T}$ (we can never know the 'truth'):

$$P(T|D) \propto \exp\big(-\tfrac{1}{2}(D_i - T_i)(C+S)^{-1}_{ij}(D_j - T_j)\big).$$

Result: $C_{ij} \to C_{ij} + S_{ij}$

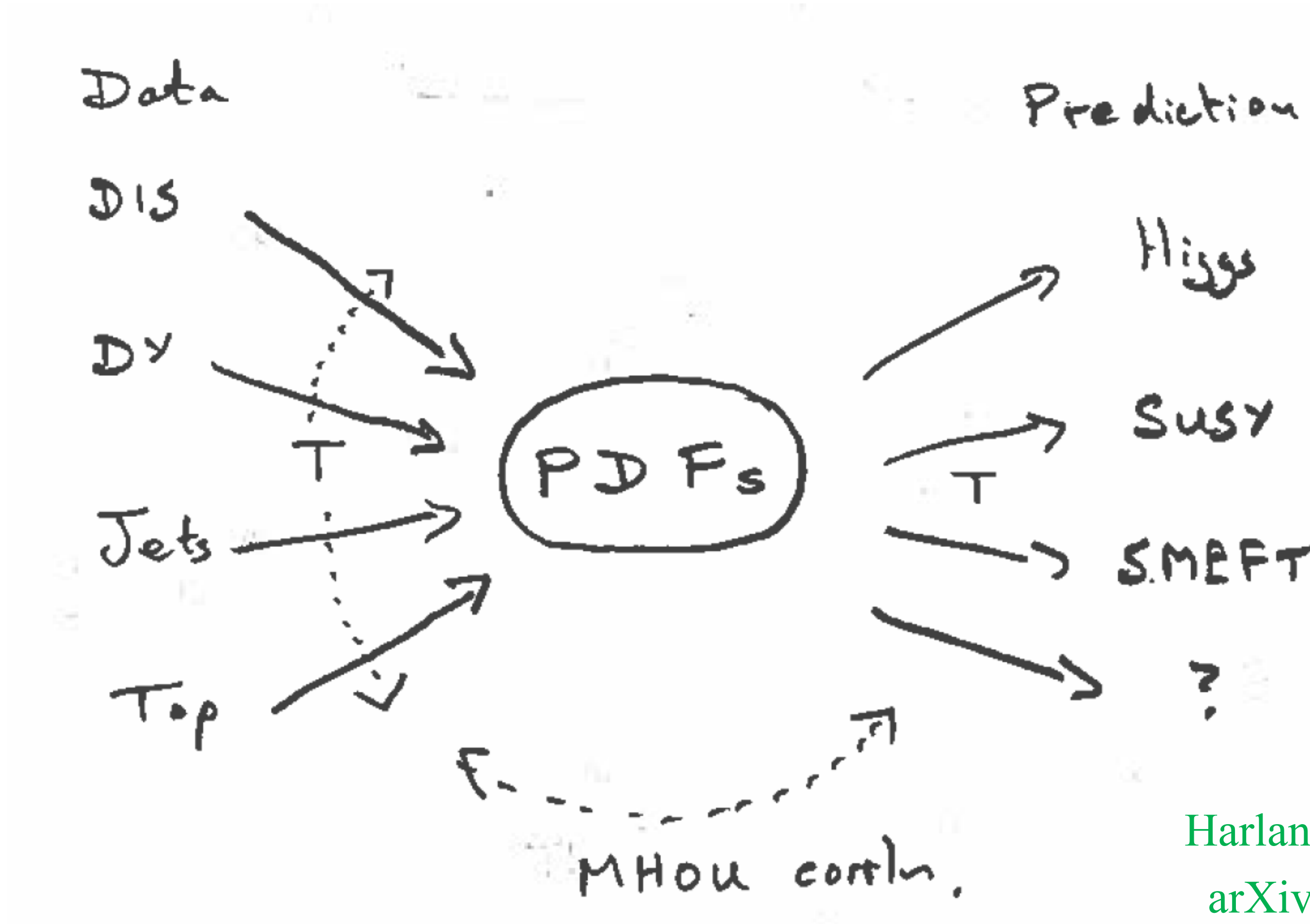
theory uncertainties ↔ exp systematics: add in quadrature because uncorrelated

NLO PDFs with MHOU with various prescriptions



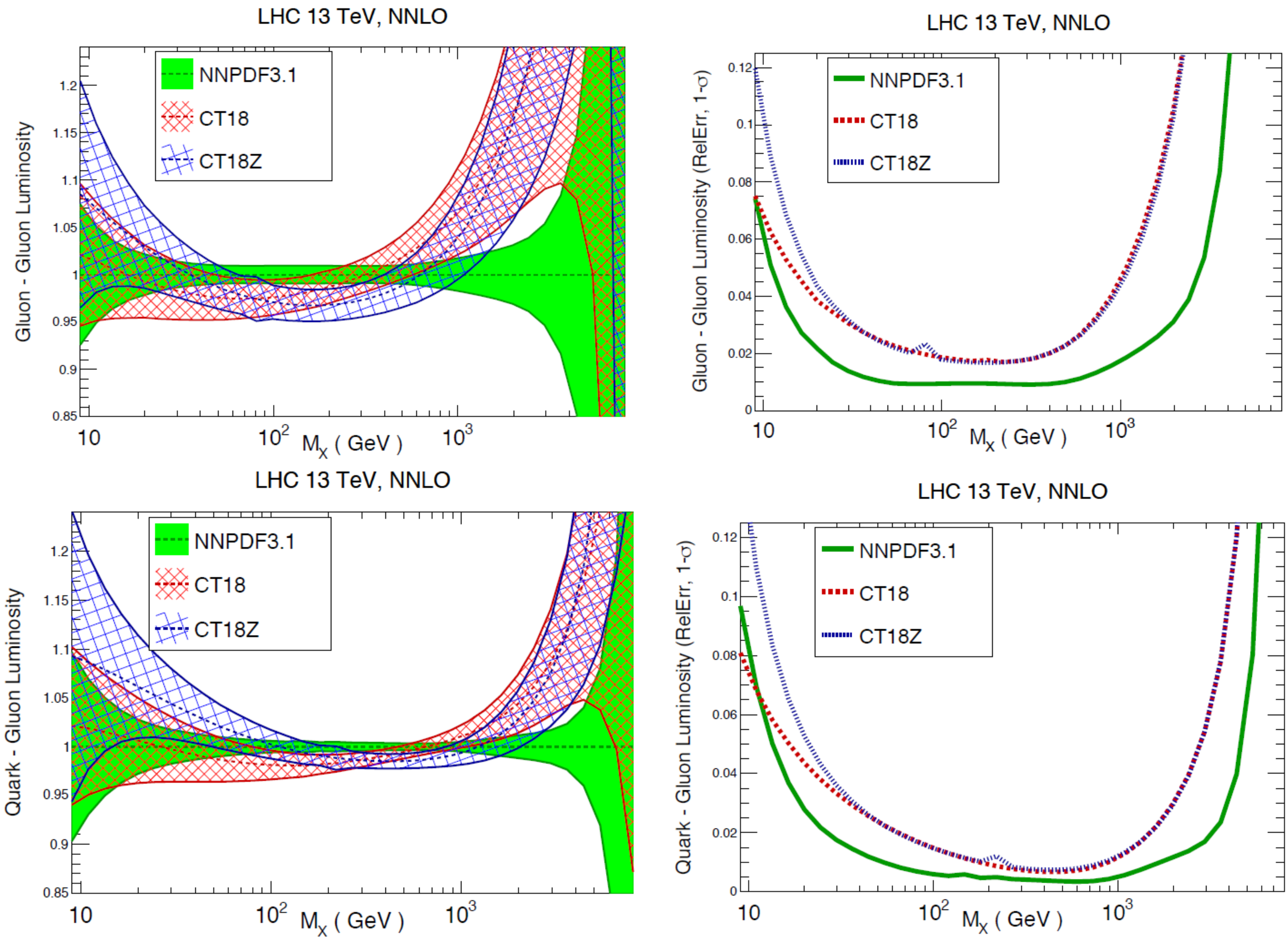
Stable in data region

Missing MHOU Correlations

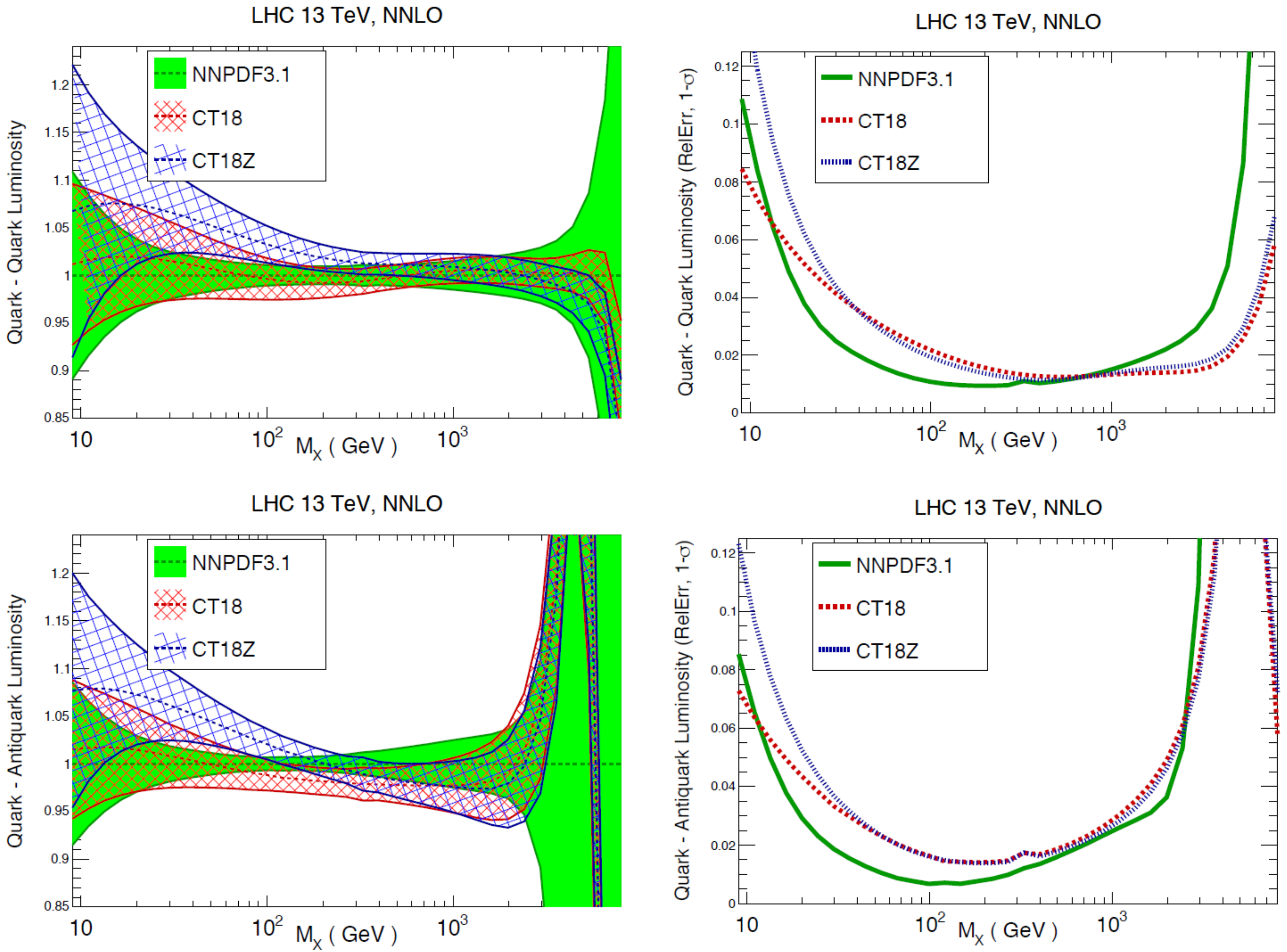


Harland-Lang Thorne
arXiv: 1811.08434

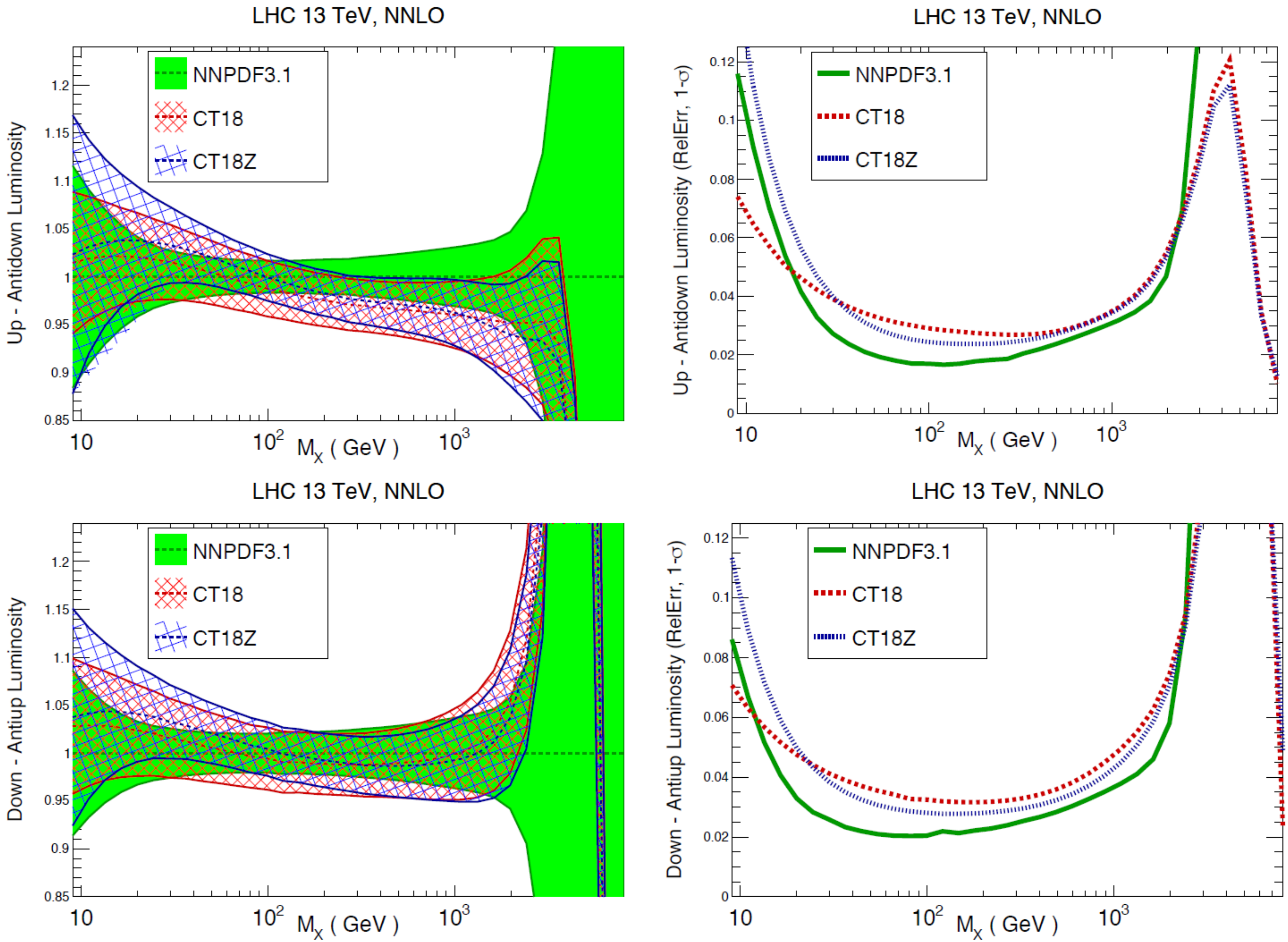
Including correlations between MHOU in PDFs and MHOU in predicted xsec may reduce overall MHOU. But requires extra deliverable beyond PDFs.



LHC 13 TeV, NNLO
Gluon - Gluon Luminosity
NNPDF3.1
CT18
CT18Z
M_X (GeV)
LHC 13 TeV, NNLO
Gluon - Gluon Luminosity (RelErr, 1-σ)
NNPDF3.1
CT18
CT18Z
M_X (GeV)
LHC 13 TeV, NNLO
Quark - Gluon Luminosity
NNPDF3.1
CT18
CT18Z
M_X (GeV)
LHC 13 TeV, NNLO
Quark - Gluon Luminosity (RelErr, 1-σ)
NNPDF3.1
CT18
CT18Z
M_X (GeV)



LHC 13 TeV, NNLO
Quark - Quark Luminosity
NNPDF3.1
CT18
CT18Z
M_X (GeV)
LHC 13 TeV, NNLO
Quark - Quark Luminosity (RelErr, 1-σ)
NNPDF3.1
CT18
CT18Z
M_X (GeV)
LHC 13 TeV, NNLO
Quark - Antiquark Luminosity
NNPDF3.1
CT18
CT18Z
M_X (GeV)
LHC 13 TeV, NNLO
Quark - Antiquark Luminosity (RelErr, 1-σ)
NNPDF3.1
CT18
CT18Z
M_X (GeV)



LHC 13 TeV, NNLO
NNPDF3.1
CT18
CT18Z
Up - Antidown Luminosity
M_X (GeV)
LHC 13 TeV, NNLO
Up - Antidown Luminosity (RelErr, 1-σ)
LHC 13 TeV, NNLO
Down - Antiup Luminosity
LHC 13 TeV, NNLO
Down - Antiup Luminosity (RelErr, 1-σ)