Recent Results and Ongoing Projects within NNPDF

Juan Rojo, VU Amsterdam & Nikhef

PDF4LHC Working Group Meeting, CERN, 2nd December 2024

NNPDF Timeline

NNPDF timescale

☑ Sep 2021: **NNPDF4.0 (paper & code)**

☑ Sept 2022: **PDFs & BSM searches** (A_{FB} high-mass)

☑ Aug 2022: **Intrinsic charm**

☑ Nov 2023: **IC asymmetry** study

☑ Feb 2024: NNPDF4.0 **aN^{3}LO**

☑ Jan 2024: NNPDF4.0 **MHOUs & QED**

☑ June 2024: NNPDF4.0 **aN^{3}LO & QED & MHOU**

☑ June 2024: NNPDF4.0 LO, NLO & NNLO for **Monte Carlo event generators**

What comes next?

NNPDF timescale

- Oct 2024: GPU-based **ML hyperopt**
- Nov 2024: Global PDF fits **confront** precision LHC data
- Nov 2024: Combination of **aN^{3}LO PDFs** for Higgs physics
- WIP: $\alpha_s(m_Z)$ fit based on **aN^{3}LO+QED theory** & closure-tested
- WIP: **Methodological studies** within and beyond NNPDF
- WIP: Closure tests with **built-in inconsistencies**
- WIP: **a new NNPDF release** combining all these developments!

NNPDF timescale

this talk

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NNPDF timescale

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Giacomo's talk

- Nov 2024: Global PDF fits **confront** precision LHC data

- Nov 2024: Combination of **aN^{3}LO PDFs** for Higgs physics

Mark, James, Tommaso, Luigi, ….

Roy's talk

- WIP: $\alpha_s(m_Z)$ fit based on **aN^{3}LO+QED theory** & closure-tested

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- WIP: Closure tests with **built-in inconsistencies**

Stefano's talk

@ DIS 2025!

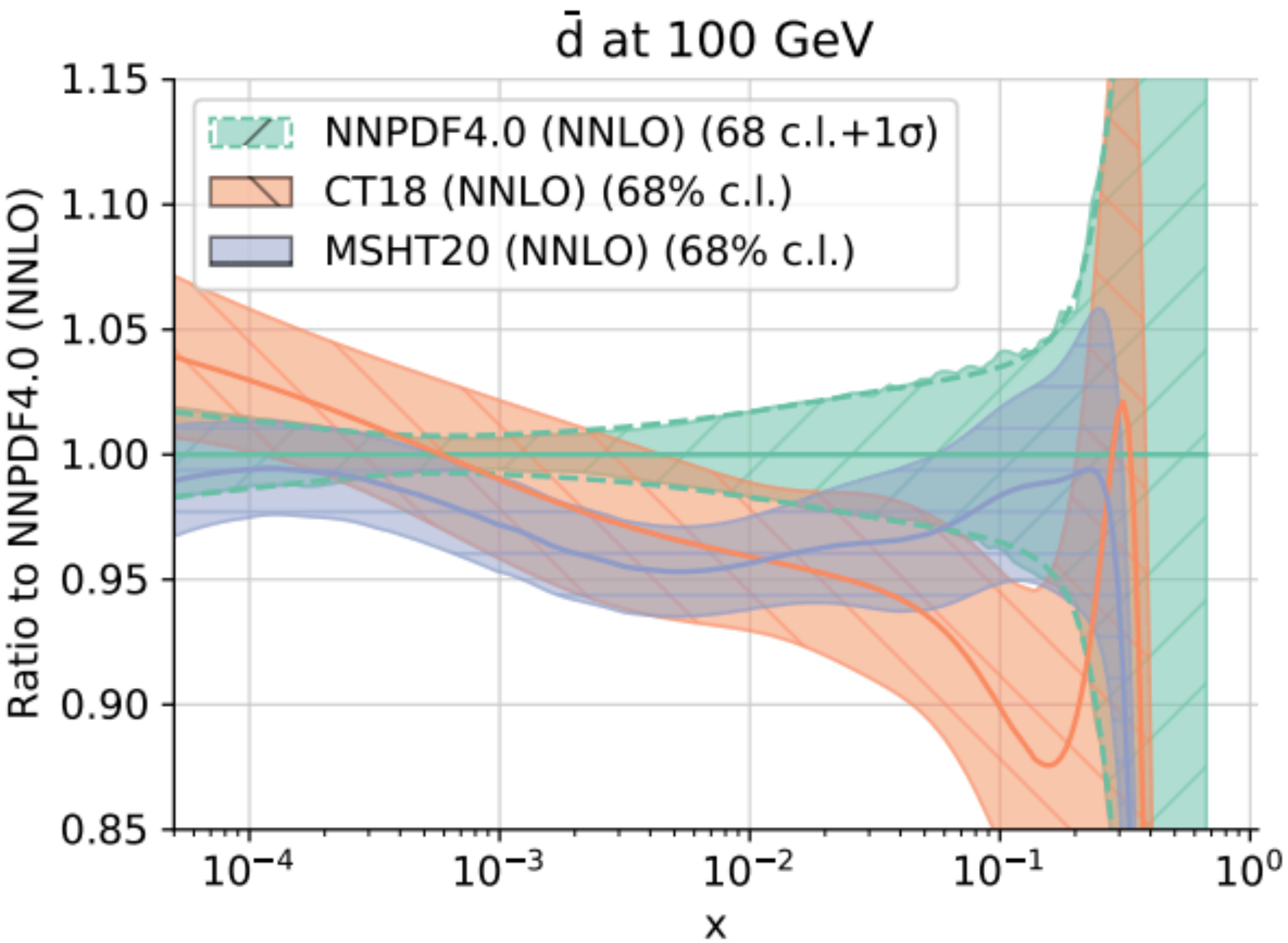
- WIP: **a new NNPDF release** combining all these developments!

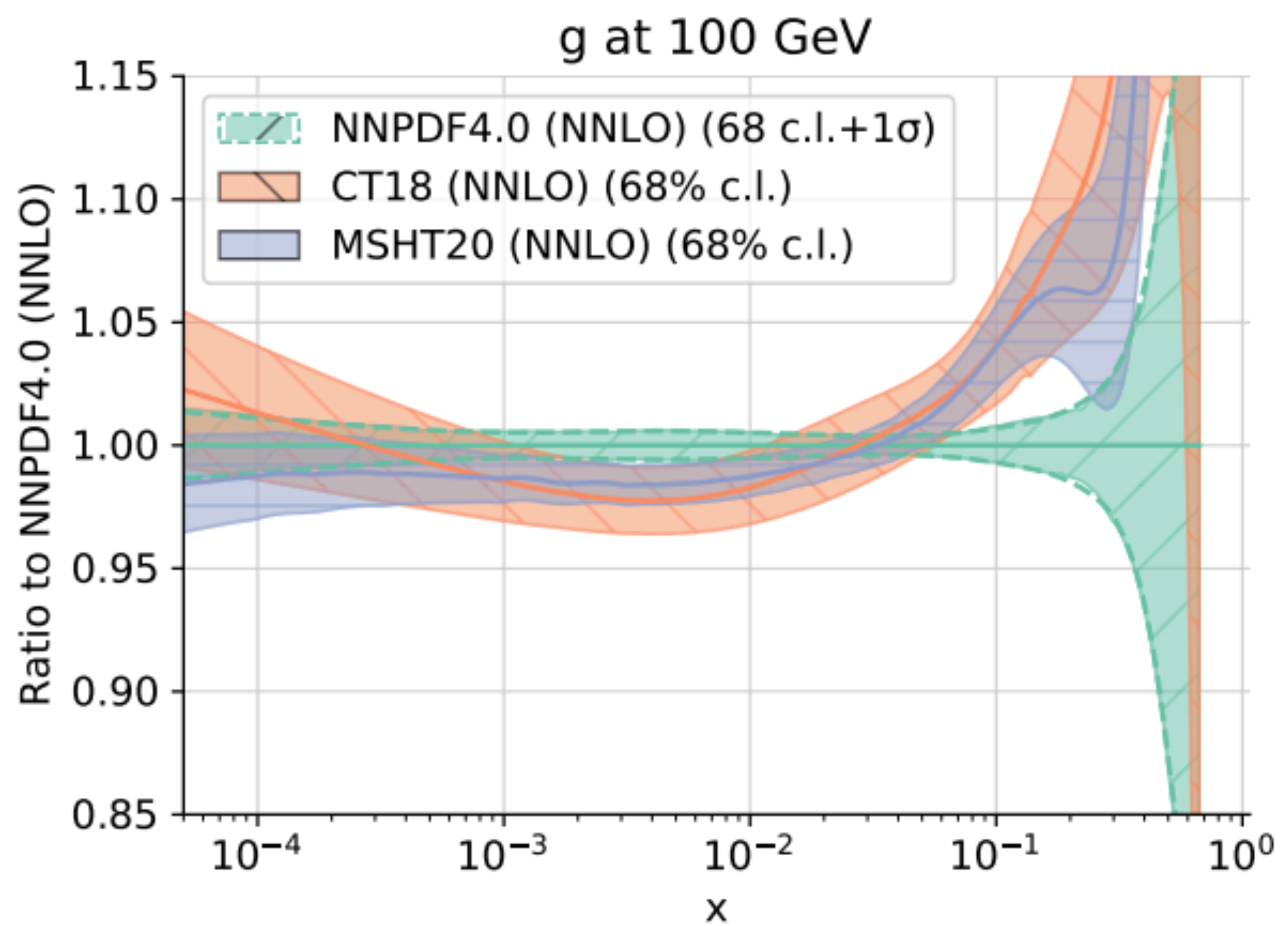
Parton Distributions Confront LHC Data: a Quantitative Appraisal

Chiefa, Costantini, Cruz-Martinez, Nocera, Rabemananjara, Rojo, Sharma, Stegeman, Ubiali, **arXiv:2412.aaaaa**

Motivation

Reducing PDF uncertainties entering LHC predictions requires an **in-depth understanding of the differences and similarities between PDF analysis**





Relevant for Drell-Yan

Relevant for top & jets

Motivation

Reducing PDF uncertainties entering LHC predictions requires an **in-depth understanding of the differences and similarities between PDF analysis**

ATLAS strong coupling extraction from Z p_T data at 8 TeV

	PDF set	$\alpha_s(m_Z)$	PDF uncertainty	g [GeV^2]	q [GeV^4]
baseline	MSHT20 [37]	0.11839	0.00040	0.44	−0.07
	NNPDF4.0 [84]	0.11779	0.00024	0.50	−0.08
	CT18A [29]	0.11982	0.00050	0.36	−0.03
	HERAPDF2.0 [65]	0.11890	0.00027	0.40	−0.04

$$\Delta_{\rm PDF}\left(\text{MSHT20 only}\right) = 0.34\,\%$$

$$\Delta_{\rm PDF}\left(\text{NNPDF4.0} - \text{CT18A}\right) = 1.6\,\%$$

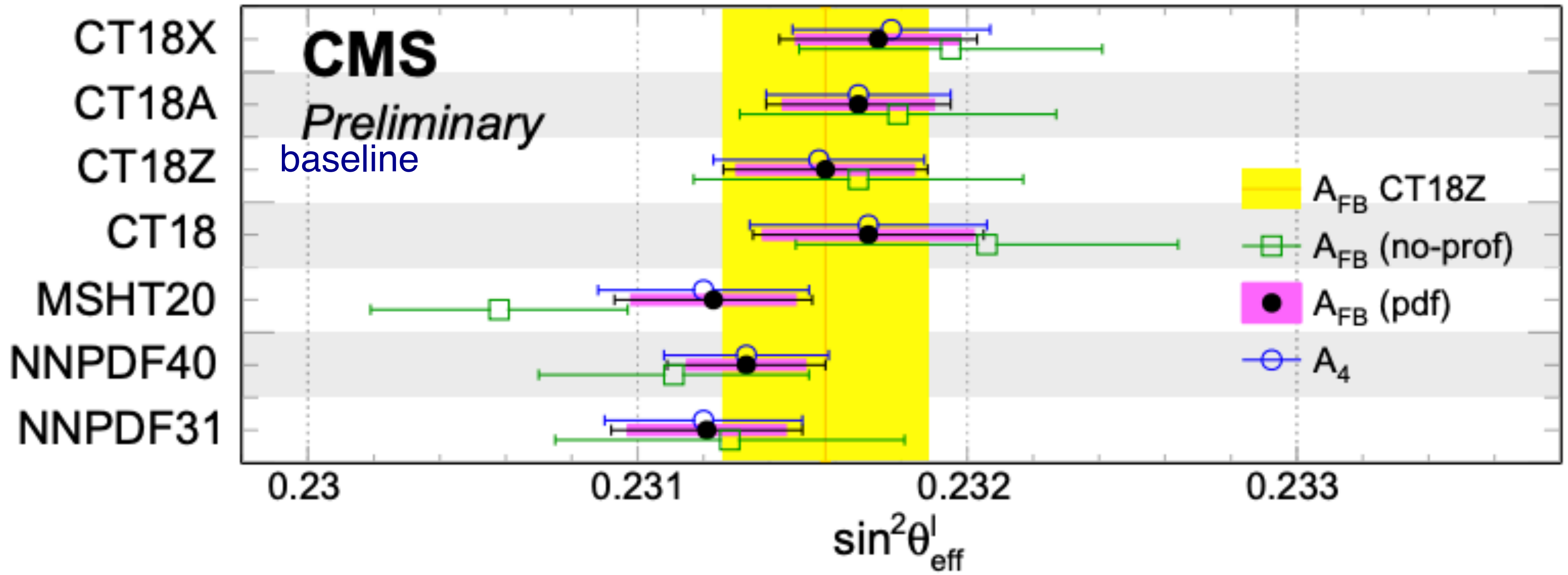
What is the ``true PDF uncertainty'' that should be associated to this measurement?

How to choose ``baseline PDF'' ? Is this an unbiased choice?

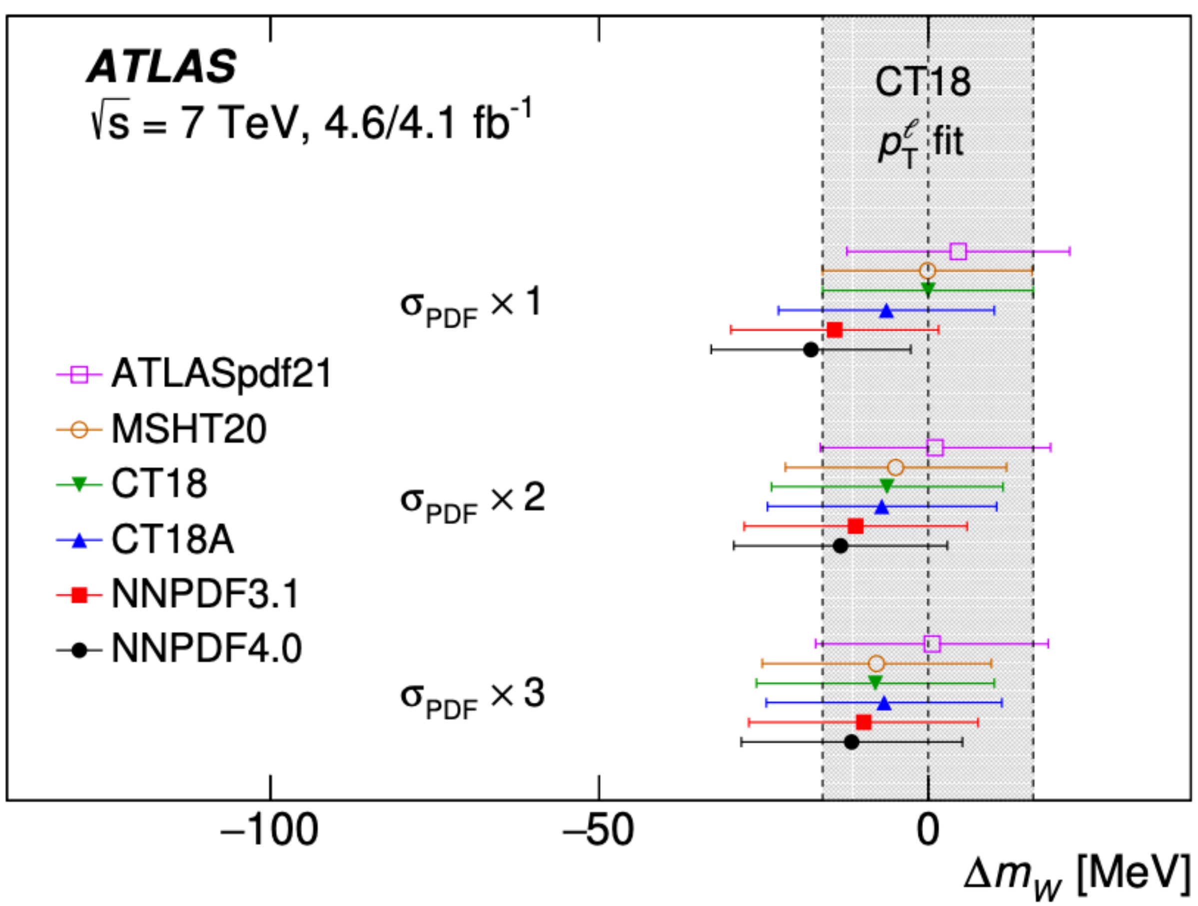
Is **in-situ profiling of PDFs** always justified? Back-reaction to other experiments in global fit?

Motivation

CMS determination of the weak mixing angle at 13 TeV



ATLAS determination of the *W* boson mass



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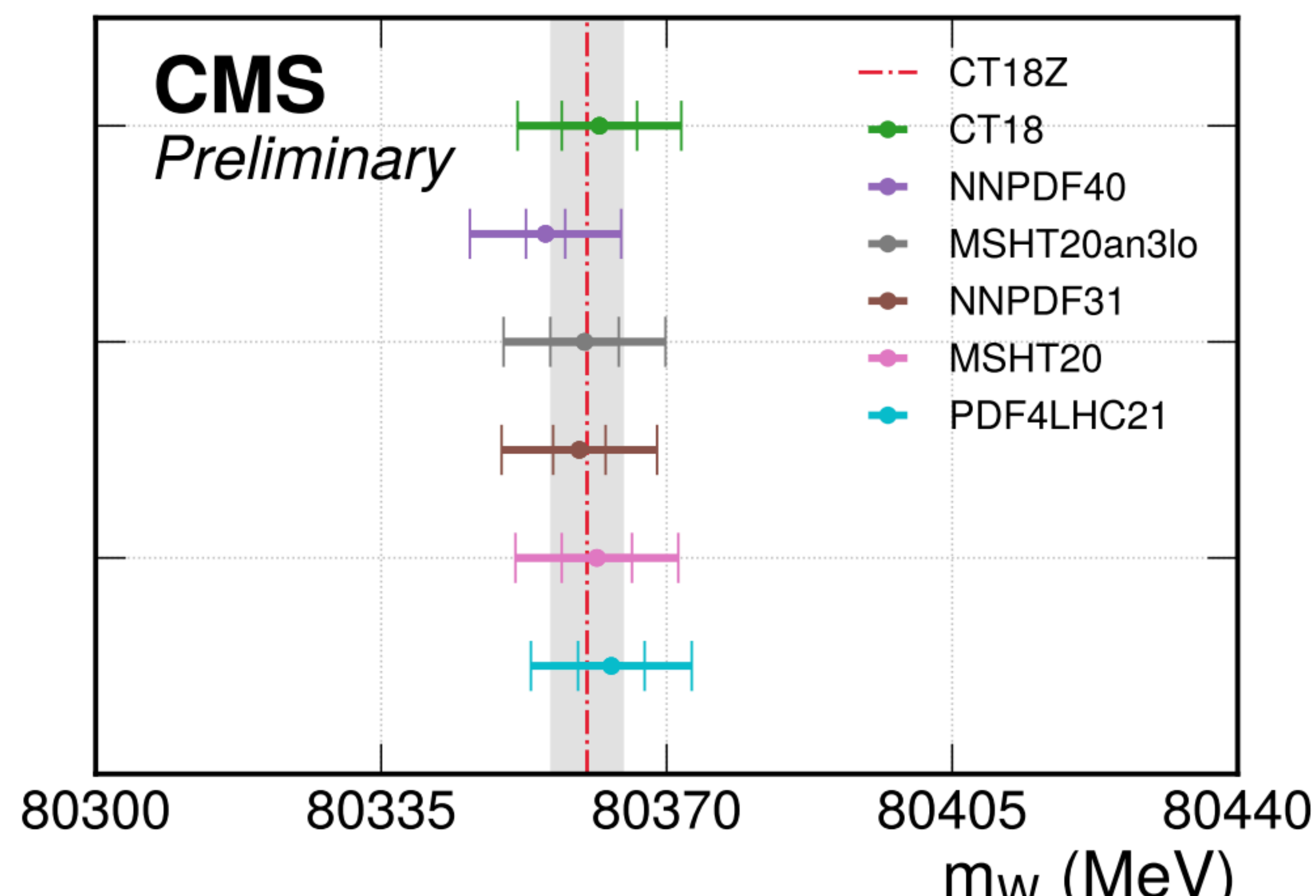


Settings

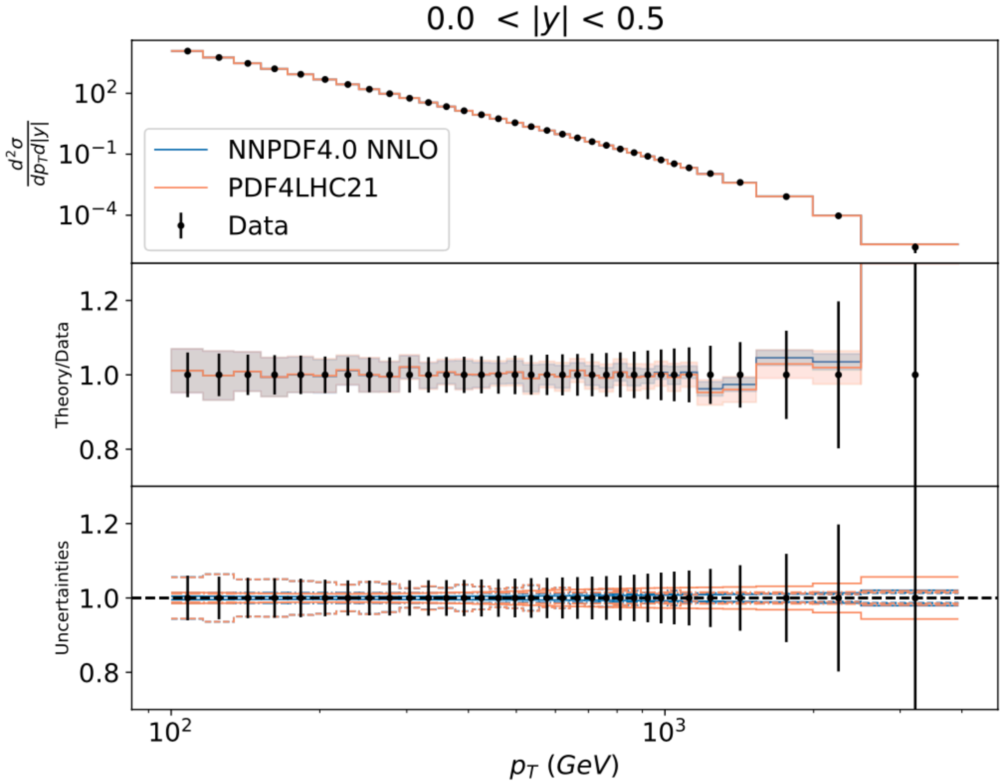
Process	Experiment	Final State	Observable	$\sqrt{s}$ (TeV)	$\mathcal{L}$ (fb^{-1})	$n_{\rm dat}$
W, Z	ATLAS	Z p_T spectrum	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dp_T^{\ell\ell}}$	13	36.1	38
	ATLAS	Z incl. prod.	$\frac{d\sigma}{d\lvert y_{\ell\ell}\rvert}$	8	20.2	7
	CMS	W incl. prod.	$\frac{d\sigma}{d\lvert\eta_\ell\rvert}$	13	35.9	36
	LHCb	Z incl. forward prod.	$\frac{d\sigma}{dy_Z}$	13	5.1	17
LHC jets	ATLAS	incl. jet $R=0.4$ (0.7)	$\frac{d^2\sigma}{dp_T^j d\lvert y_j\rvert}$	13	3.2	177
	ATLAS	di-jets $R=0.4$	$\frac{d^2\sigma}{dm_{jj}d\lvert y^*\rvert}$	13	3.2	136
	CMS	incl. jets $R=0.4$ (0.7)	$\frac{d^2\sigma}{dp_T^j d\lvert y_j\rvert}$	13	36.3 (33.5)	78
DIS-jets	H1	incl. jet (low Q^2)	$\frac{d^2\sigma}{dQ^2dp_T^j}$	0.319	0.29	48
	H1	di-jets (low Q^2)	$\frac{d^2\sigma}{dQ^2d\langle p_T\rangle_2}$	0.319	0.29	48
	H1	incl. jet (high Q^2)	$\frac{d^2\sigma}{dQ^2dp_T^j}$	0.319	0.351	24
	H1	di-jets (high Q^2)	$\frac{d^2\sigma}{dQ^2d\langle p_T\rangle_2}$	0.319	0.351	24
	ZEUS	incl. jet	$\frac{d^2\sigma}{dQ^2dE_T^j}$	0.3	0.038	30
	ZEUS	incl. jet	$\frac{d^2\sigma}{dQ^2dE_T^j}$	0.319	0.082	30
	ZEUS	di-jets	$\frac{d^2\sigma}{dQ^2d\langle E_T\rangle_2}$	0.319	0.374	22
top-pair	ATLAS	hadronic	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dm_{t\bar t}}$	13	36.1	9
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\lvert y_{t\bar t}\rvert}$	13	36.1	12
			$\left(\frac{1}{\sigma}\right)\frac{d^2\sigma}{d\lvert y_{t\bar t}\rvert dm_{t\bar t}}$	13	36.1	11
	ATLAS	ℓ+jets	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dm_{t\bar t}}$	13	36.1	9
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dp_{T,t}}$	13	36.1	8
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\lvert y_t\rvert}$	13	36.1	5
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\lvert y_{t\bar t}\rvert}$	13	36.1	7
	CMS	ℓ+jets	$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dm_{t\bar t}}$	13	137	15
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{dp_{T,t}}$	13	137	16
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\lvert y_{t\bar t}\rvert}$	13	137	10
			$\left(\frac{1}{\sigma}\right)\frac{d\sigma}{d\lvert y_t\rvert}$	13	137	11
			$\left(\frac{1}{\sigma}\right)\frac{d^2\sigma}{d\lvert y_{t\bar t}\rvert dm_{t\bar t}}$	13	137	35

- **NNLO fast grids** for all processes (no *K*-factors)
- Datasets based on **highest lumi**, no overlap with inputs in considered PDF fits
- Include all sources of **experimental & theory uncertainties**
- For datasets with unstable covariance matrix, apply **regularisation prescription**

$$\chi^2_{\rm exp+th} = \sum_{i,j=1}^{n_{\rm dat}} \left(T_i^{(0)} - D_i\right)\left(\left(\mathrm{cov}_{\rm exp} + \mathrm{cov}_{\rm mho} + \mathrm{cov}_{\rm pdf} + \mathrm{cov}_{\rm as}\right)^{-1}\right)_{ij}\left(T_j^{(0)} - D_j\right)$$

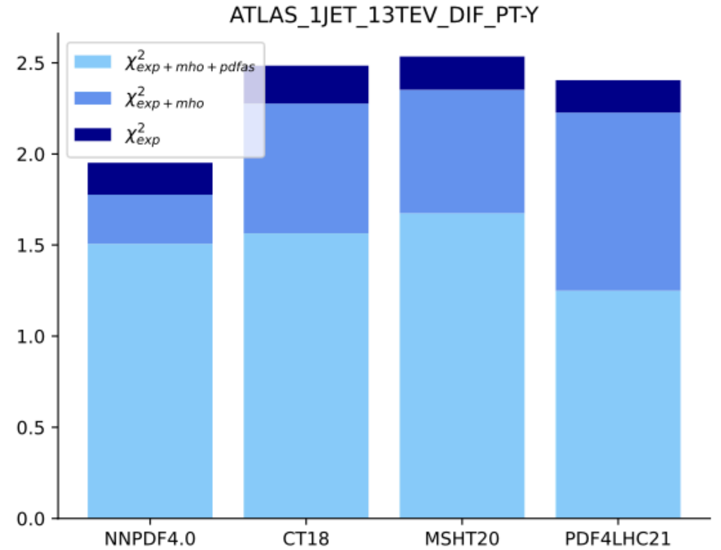
7pt prescription

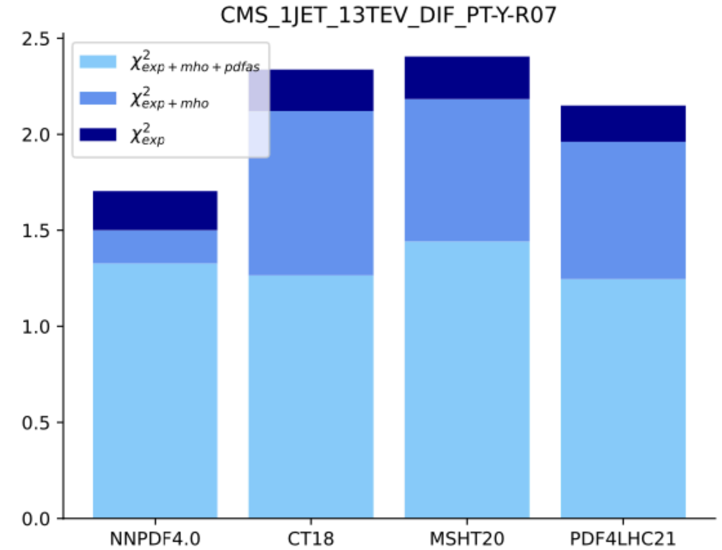
Results

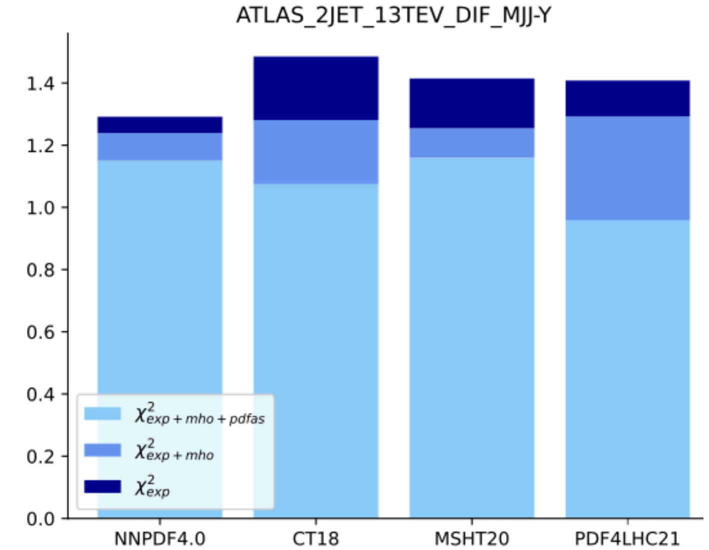


- For each dataset, **evaluate χ^2 breakdown** and data vs theory comparison plots (with shifted systematics)
- **9 different PDF sets considered**, extension to other PDF sets straightforward (fast NNLO QCD grids)
- For ABMP16, set with $\alpha_s(m_Z) = 0.118$ adopted

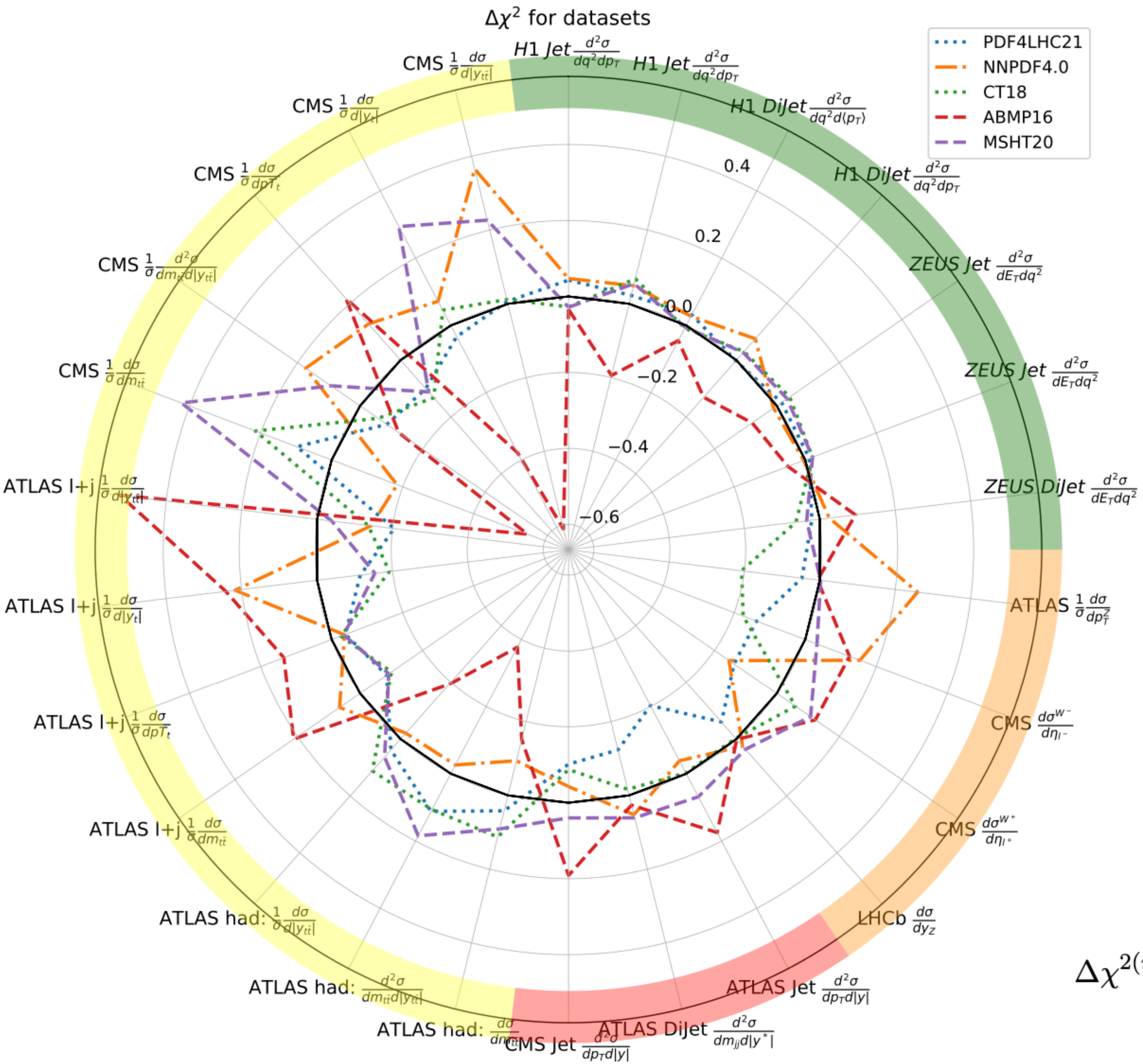
		ABMP16	CT18	CT18A	CT18Z	MSHT20	NN3.1	NN4.0	PLHC15	PLHC21
ATLAS incl. jet	$\chi^2_{\rm exp+th}$	1.84	1.56	1.64	1.38	1.67	1.21	1.51	1.20	1.25
	$\chi^2_{\rm exp}$	2.32	2.48	2.47	2.50	2.53	2.98	1.95	3.02	2.40
CMS incl. jet	$\chi^2_{\rm exp+th}$	1.65	1.26	1.26	1.19	1.44	1.50	1.33	1.25	1.25
	$\chi^2_{\rm exp}$	2.10	2.34	2.31	2.03	2.41	2.28	1.70	2.46	2.15
ATLAS dijet	$\chi^2_{\rm exp+th}$	1.12	1.08	1.09	1.05	1.16	1.09	1.15	1.01	0.96
	$\chi^2_{\rm exp}$	1.35	1.49	1.47	1.48	1.41	1.37	1.29	1.42	1.41







Results

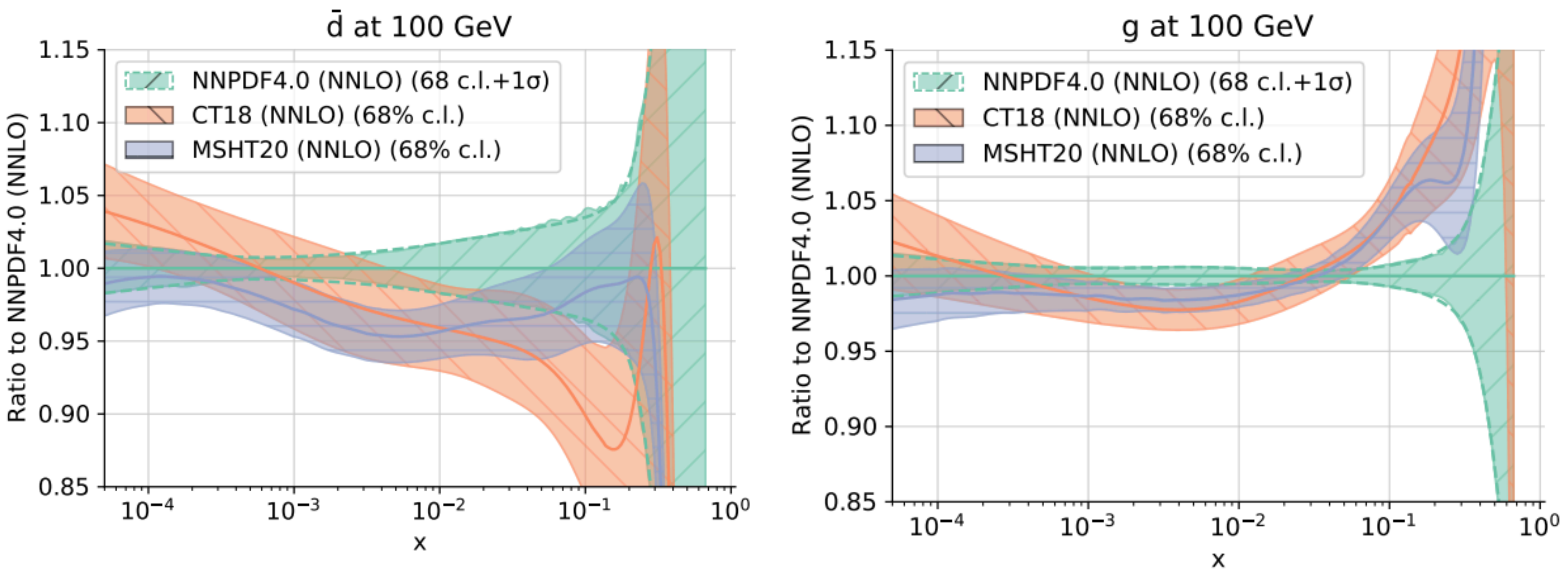


- Despite PDF differences, **no systematic outlier** in dataset description
- Fully accounting for **theory errors** crucial
- PDF4LHC21 represents the **``average" behaviour**
- **Jet data** offers good discrimination power

$$\Delta\chi^{2(i)} = \frac{\chi^{2(i)}_{\text{exp+th}} - \left\langle \chi^2_{\text{exp+th}} \right\rangle_{\text{pdfs}}}{\left\langle \chi^2_{\text{exp+th}} \right\rangle_{\text{pdfs}}}$$

Take-away lesson

Reducing PDF uncertainties entering LHC predictions requires an **in-depth understanding of the differences and similarities between PDF analysis**



Despite NNPDF4.0 displaying **smaller PDF uncertainties as compared to other fits**, its **agreement with Run II data** is of comparable quality (or even better!)

falsifying the claim that NNPDF4.0 errors are somehow ``underestimated"

Ensemble-based hyperoptimization in ML

Cruz-Martinez, Jansen, van Oord, Rabemananjara, Rocha, Rojo, Stegeman, **arXiv:2410.16248**

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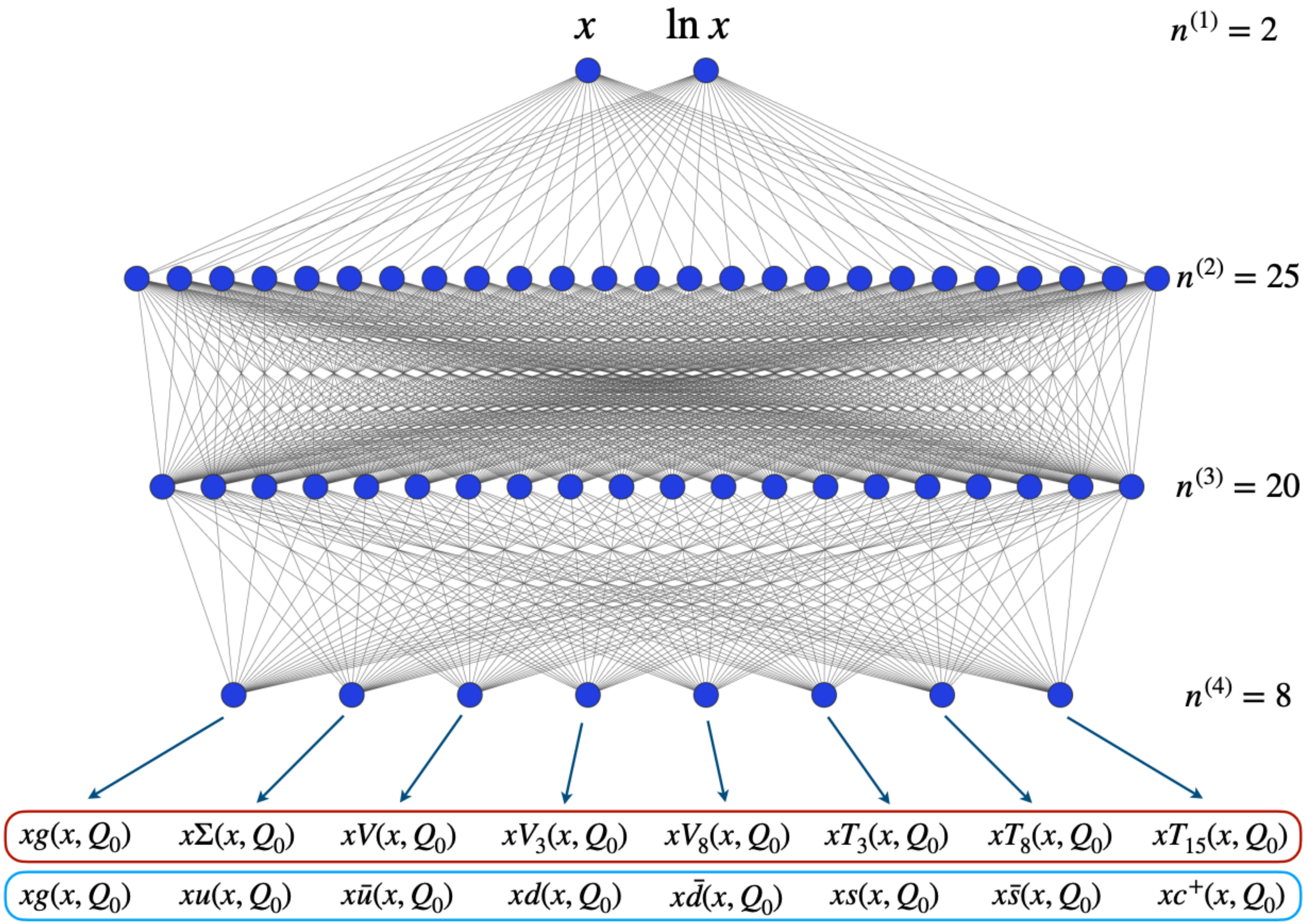
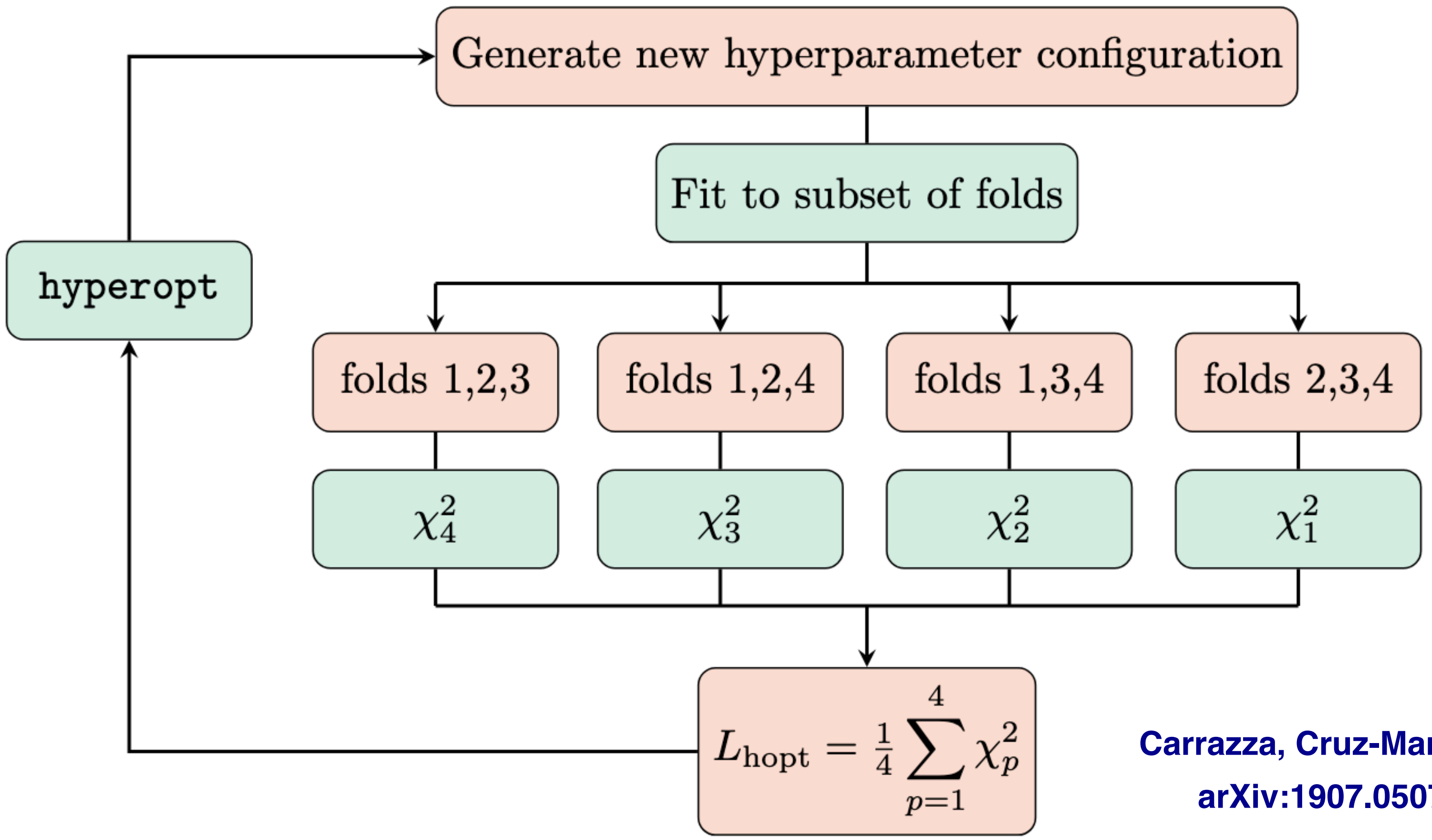
Hyperoptimisation in Machine Learning



- ML applications rely on a **large number of hyperparameters** which are not fixed by the training algorithm: architecture, optimiser, initialisation, stopping, activation functions …
- Choosing hyperparameters is a challenge in many cases. **Bias-free optimisation** is crucial!

Hyperoptimisation in Machine Learning

NNPDF4.0



Carrazza, Cruz-Martinez, arXiv:1907.05075

- Partition global dataset into ***n* folds**
- Exclude one fold at a time, perform *n* fits
- Select hyperparameters leading to **best** χ^2 **to the non-fitted data**

Based on central PDF fit

This work

$$\varphi^2_{\chi^2} \equiv \left\langle \chi^2\left[T, D^{(0)}\right]\right\rangle_{\rm rep} - \chi^2\left[\langle T\rangle_{\rm rep}, D^{(0)}\right]$$

$$\varphi^2_{\chi^2} = \frac{1}{n_{\rm dat}}\sum_{i,j=1}^{n_{\rm dat}} ({\rm cov})^{-1}_{ij}\, T_{ji}$$

$$L^{(\varphi^2)}_{\rm hopt}\left(\hat{\boldsymbol{\theta}}\right) \equiv \left(\frac{1}{n_{\rm fold}}\sum_{p=1}^{n_{\rm fold}}\varphi^2_{\chi^2_p}\left(\hat{\boldsymbol{\theta}}\right)\right)^{-1}$$

- Select hyperparameters leading to **best** χ^2 & **largest PDF errors in non-fitted data**
- **e.g.** models with the **best generalisation power** are selected

Requires major restructure of NNPDF code to be able to train multiple ML models in parallel

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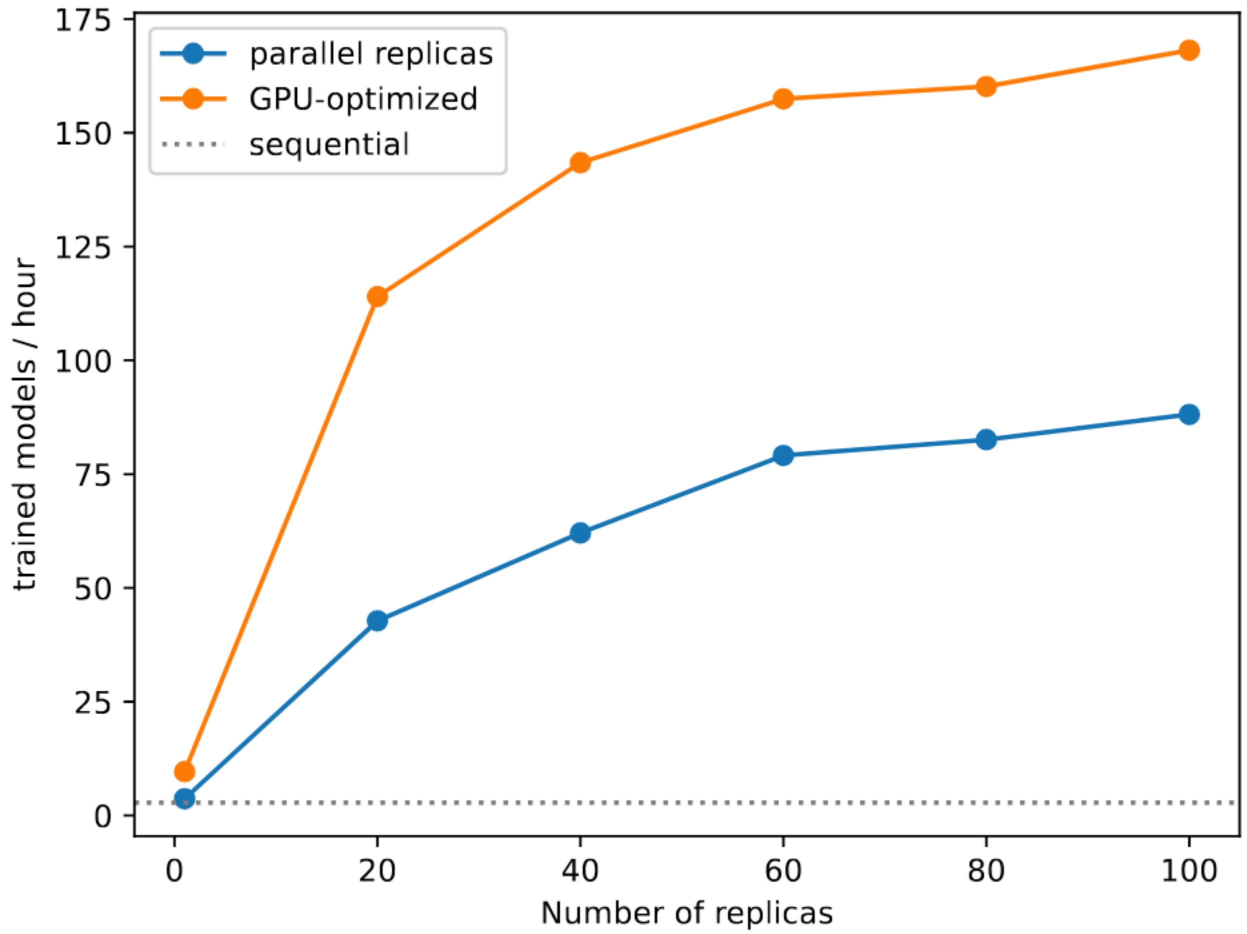
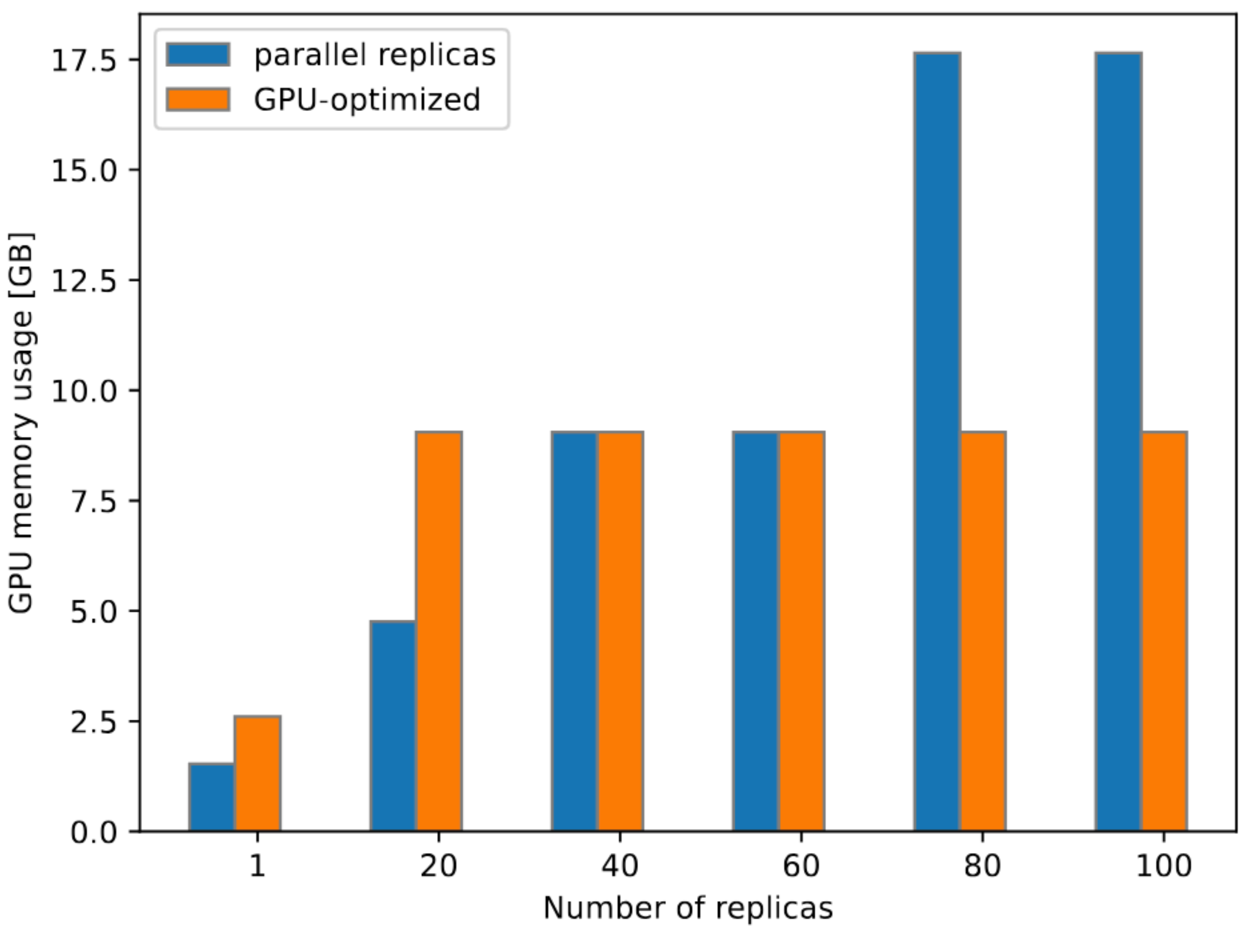
GPU-optimised NNPDF fits

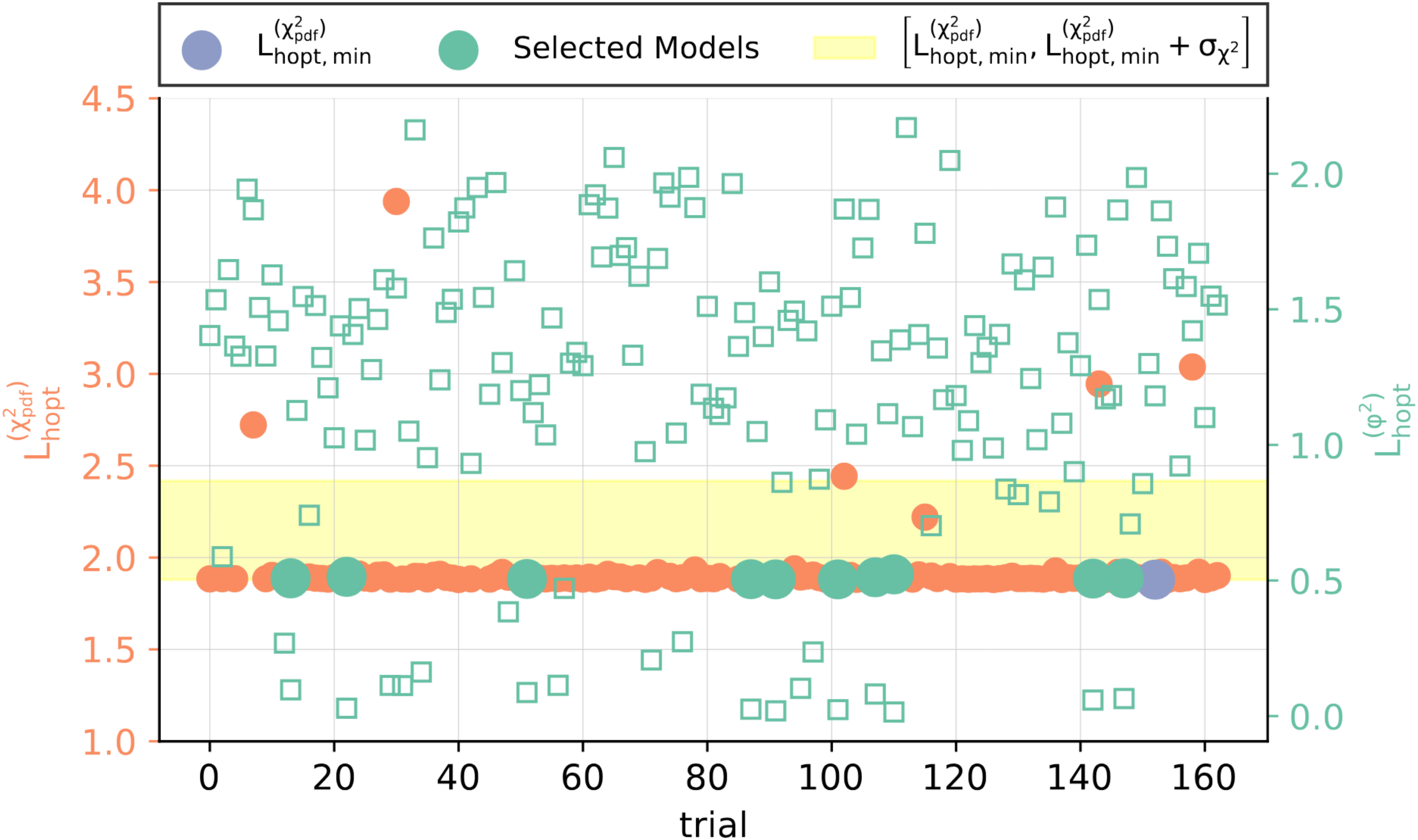




Replicas	10	50	100
Energy reduction	78%	87%	91%
Cost reduction	-45%	47%	55%

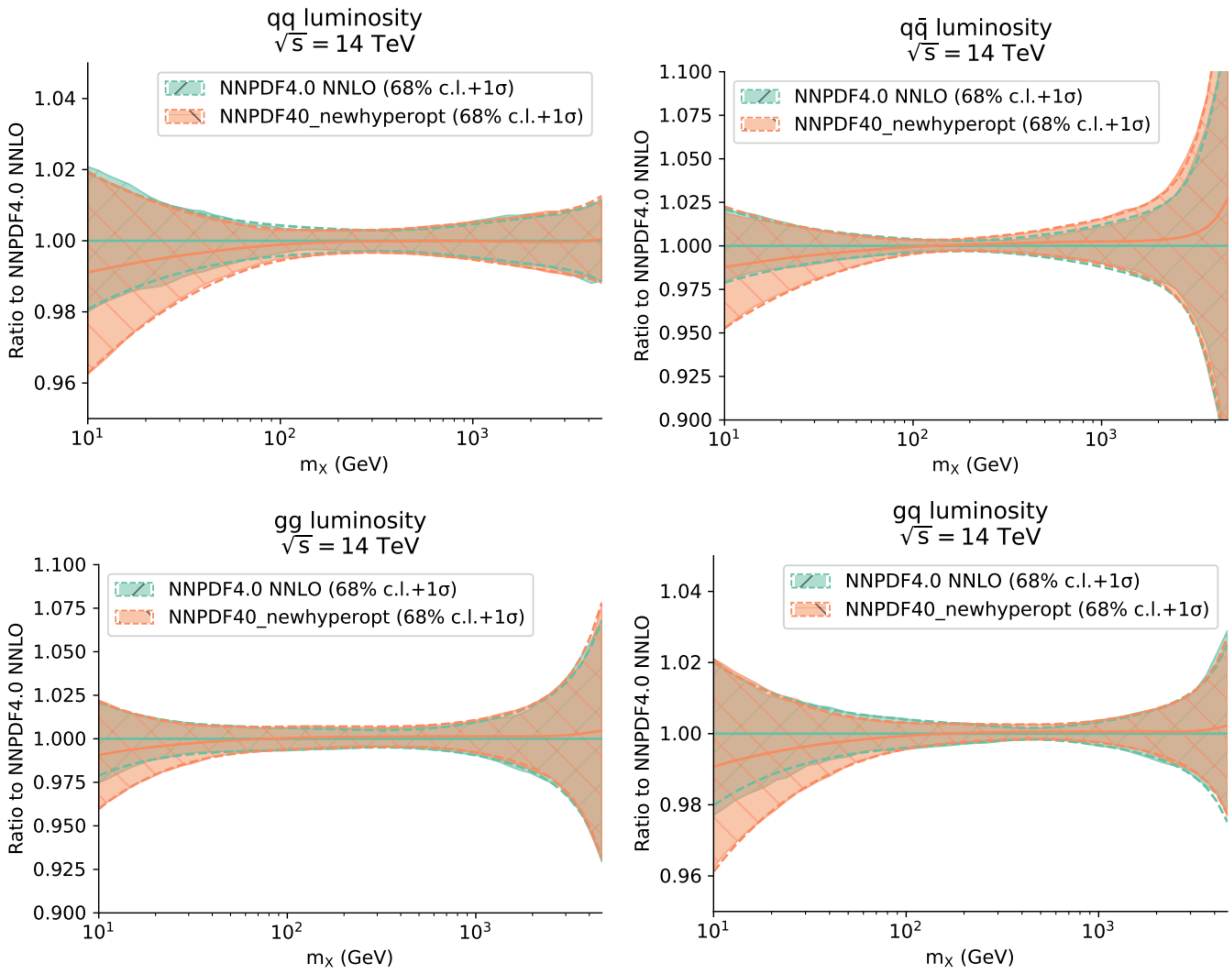
- **Speed up by a factor 200** from new GPU-optimise NNPDF code
- Memory usage kept under control, independent of number of models trained in parallel
- Up to 90% energy reduction: **faster, more affordable, and more sustainable** ML model training!

Results



Select not the best single set of hyperparameters but **instead randomly sample over the complete population of acceptable hyperparameters** displaying comparable performance

Impact on LHC predictions



Despite radical change in hyperparameter determination methodology, **excellent consistency with NNPDF4.0 & moderate increase of PDF errors**: non-trivial validation of NNDF robustness

What’s next?

Towards the next NNPDF release

The developments presented in this talk and in the rest of NNPDF-related talks in the workshop will in the next months be combined **towards a new main NNPDF release**

Theory Calculations

- **NNLO fast interpolation grids** for hadronic processes
- Remove NNLO *K*-factors from fit
- **aN^{3}LO+QED** with **MHOUs** as default theory baseline
- Move to **latest version of Moch et al** $P_{ij}^{(3)}(x)$
- Numerical FONLL as general-mass VFN

Experimental Data

- Most **recent LHC Run-2 datasets,** including some based on full luminosity
- Many of them ready to go from our **PDF appraisal study**
- **HERA DIS+jets** part of the baseline dataset
- **Novel standardised data format** enabling versioning & metadata

Methodology

- New GPU **replica-based hyperopt**, different ML model per replica
- Validation on (inconsistent) **closure tests** and future tests
- **Feature Scaling**, remove large-x pre-processing
- **Updated theory pipeline** based on EKO + YADISM + PineAPPL

Towards the next NNPDF release

INCLUSIVE DIS			
Experiment ID	**Description**	**Publication**	**Hepdata**
JLAB	**Proton, Deuteron and neutron structure function data from JLAB**	Paper	Accardi, tarball here
CHORUSDM	**CHORUS dimuon production measurements**	Paper	Paper
CDHSW	**A measurement of differential cross sections and nucleon structure functions** **in charged current neutrino interactions on iron (F2p, F3p)**	Paper	Hepdata
CCFR/Nutev	**Measurements of F2 and F3 (neutrino) - F3(antineutrino) from CCFR (anti)neutrino-Fe data**	Paper1 Paper2	Hepdata
ZEUS	**Event count at large x**	Paper	

DRELL YAN, V pT, and DIBOSC			
Experiment ID	**Description**	**Publication**	**Hepdata**
ATLAS_WZ_276TEV_RAP	**ATLAS W, Z inclusive production at 2.76 TeV: fiducial xsecs and asymmetries**	Paper	n/a
ATLASWZ5TEV	**ATLAS W and Z production, 5 TeV (25 pb^{-1}) total and differential xsec**	Paper	Paper
ATLASZJETS8TEV	**ATLAS Z+jets at 8 TeV**	Paper	
ATLAStbd8TEV	**ATLAS Z full phase-space, 2D (pTZ,yZ) xsec, 8 TeV, 20 fb^{-1}**	Paper	
ATLASZJET13TEV	**ATLAS Z+jet at 13 TeV**	Paper	Paper HepData
ATLASWW13TEV	**ATLAS WW cross section at 13 TeV, 3.12 fb^{-1}**	Paper	HepData
ATLAS_Zjet_13TEV	**ATLAS Z+jet at 13 TeV**	Paper	

			before the end Jan 2020.
ATLAS_WC_13TEV	**ATLAS W+charm at 13 TeV 140 fb-1**	Paper	
CMSZPHI8TEV	**CMS Z Phi* distributions 8 TeV (19.7 fb-1)**	Paper	CMS page
CMS_WPT_8TEV	**CMS W pt distribution, 8 TeV (18.4 fb^{-1})**	Paper	Hepdata
CMS_WC_8TEV	**CMS W+charm at 8 TeV (18.4 fb^{-1})**	Paper	
CMS_tbd_8TEV	**CMS forward-backward asymmetry in Z production at 8 TeV (18.4 fb^{-1})**	Paper	
CMS_Zjet_13TEV	**CMS Z+jet at 13 TeV**	Paper	
CMS_Zb_13TEV **CMS**_Zc_13TEV **CMS**_Zcbratio_13TEV	**CMS Z+b and Z+c at 13 TeV**	Paper	
CMS_DY_DIFF_13TEV	**CMS differential DY cross sections at 13 TeV, 3 fb-1**	Paper	
CMS_W2D_13TEV	**CMS double differential cross-sections for W production at 13 TeV and 35.9 fb^{-1} double differential in pT^lepton and y_lepton** **Also helicities and charge-asymmetry**	Paper	
CMS_WC_13TEV	**CMS differential distributions (lepton rapidity and pT) in W+c production at 13 TeV and 138 fb^{-1}**	Paper	
CMS_ZC_13TEV	**CMS measurement of Z+charm as a function of Z pT at 13 TeV and 36 fb^{-1}**	Paper	
LHCb_tdb_TEV	**LHCb inclusive Z production and differential distributions at 5 TeV**	Paper	
LHCb_Z_dimuons_13TEV_RunII	**LHCb inclusive Z production at 13 TeV, full Run II luminosity**	Paper	

PHOTON PRODUCTION			
Experiment ID	**Description**	**Publication**	**Hepdata**
CDFINCLPHOT	**CDF inclusive photon cross-section**	Paper	
ATLASPHT11	**ATLAS isolated photon production 7 TeV, 4.6 fb^{-1}**	Paper	HepData
ATLASDIPHOT8TEV	**ATLAS diphoton differential**	Paper	HEPData
ATLAS_PHT_13TEV	**ATLAS isolated photon production 13 TeV, 139 fb^{-1}**	Conf note	
CMSPHT11	**CMS isolated photon production 7 TeV, 36 pb^{-1}**	Paper	
CMSPHT15	**CMS isolated photon production 13 TeV, 2.3 fb^{-1}**	Paper	

INCLUSIVE JET PRODUCT			
Experiment ID	**Description**	**Publication**	**Hepdata**
ATLAS3JET11	**ATLAS three jet production 7 TeV, 5 fb $^{-1}$**	Paper	
ATLASJET13TEV	**ATLAS inclusive jet and dijet cross-sections at 13 TeV 3.2fb^{-1}**	Paper	HepData
ATLASJET13TEV	**ATLAS inclusive jet and dijet cross-sections at 13 TeV 3.2fb^{-1}**	Paper	HepData
ALICE_1JET_5TEV	**ALICE inclusive jet production at 5.02 TeV**	Paper	
CMS_1JET_13TEV	**CMS inclusive jet production at 13 TeV, 36.3 fb^{-1}**	Paper	HepData

TOP PAIR PRODUCTIO			
Experiment ID	**Description**	**Publication**	**Hepdata**
CMS_TTB_DIFF_13TEV	**CMS single and double differential distributions in the lepton+jet channel** **13 TeV 137 fb^{-1}**	Paper	HepData
ATLAS_TTB_DIFF_PT_NORM_13TEV ATLAS_TTB_DIFF_PT_13TEV ATLAS_TTB_DIFF_TRAP_NORM_13TEV ATLAS_TTB_DIFF_TRAP_13TEV ATLAS_TTB_DIFF_TTRAP_NORM_13TEV ATLAS_TTB_DIFF_TTRAP_13TEV ATLAS_TTB_DIFF_TTM_NORM_13TEV ATLAS_TTB_DIFF_TTM_13TEV	**ATLAS single differential distributions of top-pair production in the lepton+jet channel** **13 TeV, 36 fb^{-1}**	Paper	HepData
ATLAS_TTB_DIFF_13TEV_140fb	**ATLAS single and double differential distributions of top-pair production in the di-lepton channel** **(particle level) 13 TeV, 36 fb^{-1}**	Paper	
ATLAS_2D_TTBAR (various distributions)	**ATLAS single and double differential distributions of top-**	Paper	n/a

	13 TeV, 36 fb		
ATLAS_INCL_TOPTOZ_RATIO_7TEV	**ATLAS top-quark pair to Z-boson cross-section ratios, 7 TeV**	Paper	Hepdata
ATLAS_INCL_TOPTOZ_RATIO_8TEV	**ATLAS top-quark pair to Z-boson cross-section ratios, 8 TeV**	Paper	Hepdata
ATLAS_INCL_TOPTOZ_RATIO_13TEV	**ATLAS top-quark pair to Z-boson cross-section ratios, 13 TeV**	Paper	Hepdata
ATLAS_TTBAR_TOT_7TEV_LJET	**ATLAS top-pair production total cross section, lepton+jets, 7 TeV 4.6 fb^{-1}**	Paper	

all datasets studied in the ``appraisal" paper

and many more, NNLO fast grids as baseline

Summary and outlook

- Lots of progress in the NNPDF global analysis framework and related studies: **aN^{3}LO+QED PDFs,** their combinations, and the associated $\alpha_s(m_Z)$ extraction, methodological studies, inclusion of novel datasets with fast NNLO interpolation grids ….

- A quantitative appraisal of PDF fits with precision LHC data **does not indicate better agreement with the data for any specific PDF set**, despite the underlying differences

- **Improved hyperoptimisation** demonstrates the robustness of the NNPDF uncertainty estimate. As a non-trivial bonus, GPU-optimised code displays now major speedups.

- These developments will be combined in the coming months, aiming to for a new release of the NNPDF global fit.

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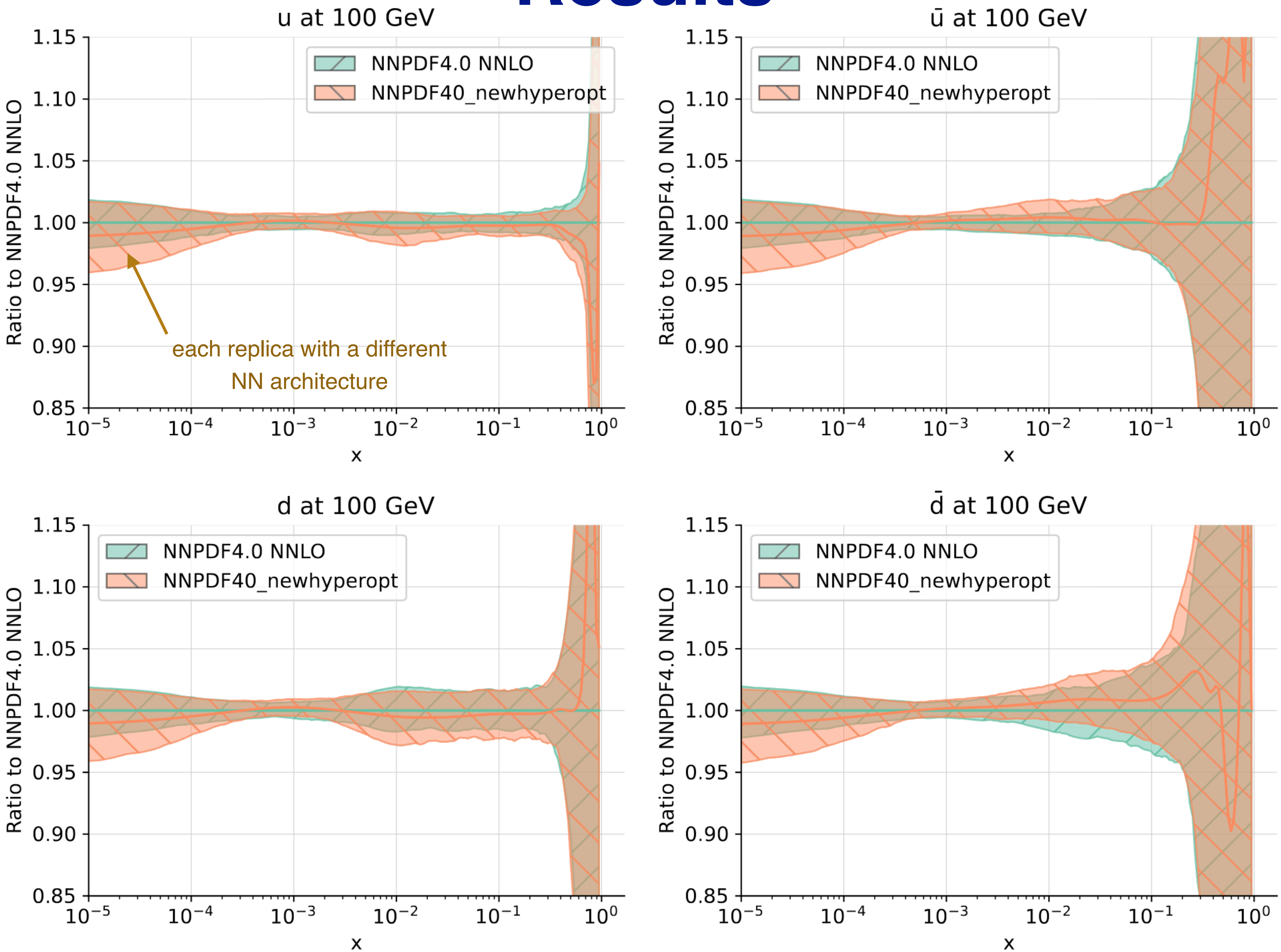
Thanks for your attention

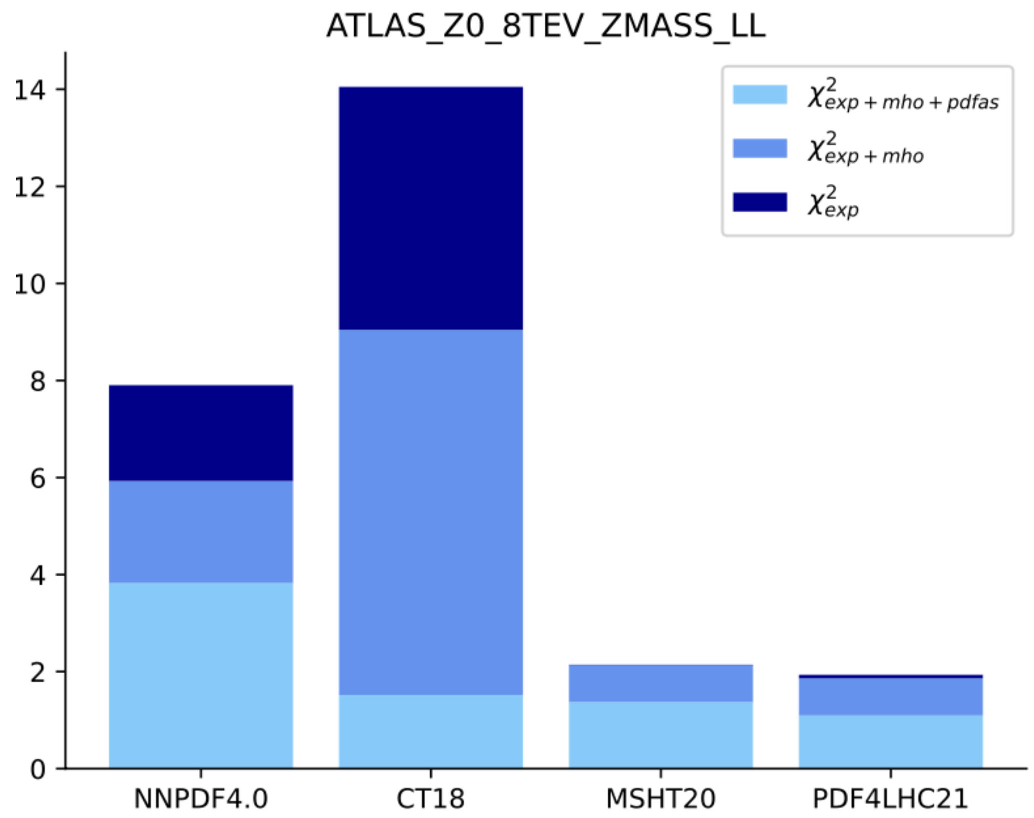
Extra Material

Results



Despite radical change in hyperparameter determination methodology, **excellent consistency with NNPDF4.0 & moderate increase of PDF errors**: non-trivial validation of NNDF robustness

ATLAS 8 TeV Z rapidity distributions



arXiv:2309.09318

- Reanalysis of Z production at 8 TeV (2012 dataset), on **full phase space** (not fiducial) of charged leptons.

(Same dataset as for $\alpha_s(m_Z)$ extraction)

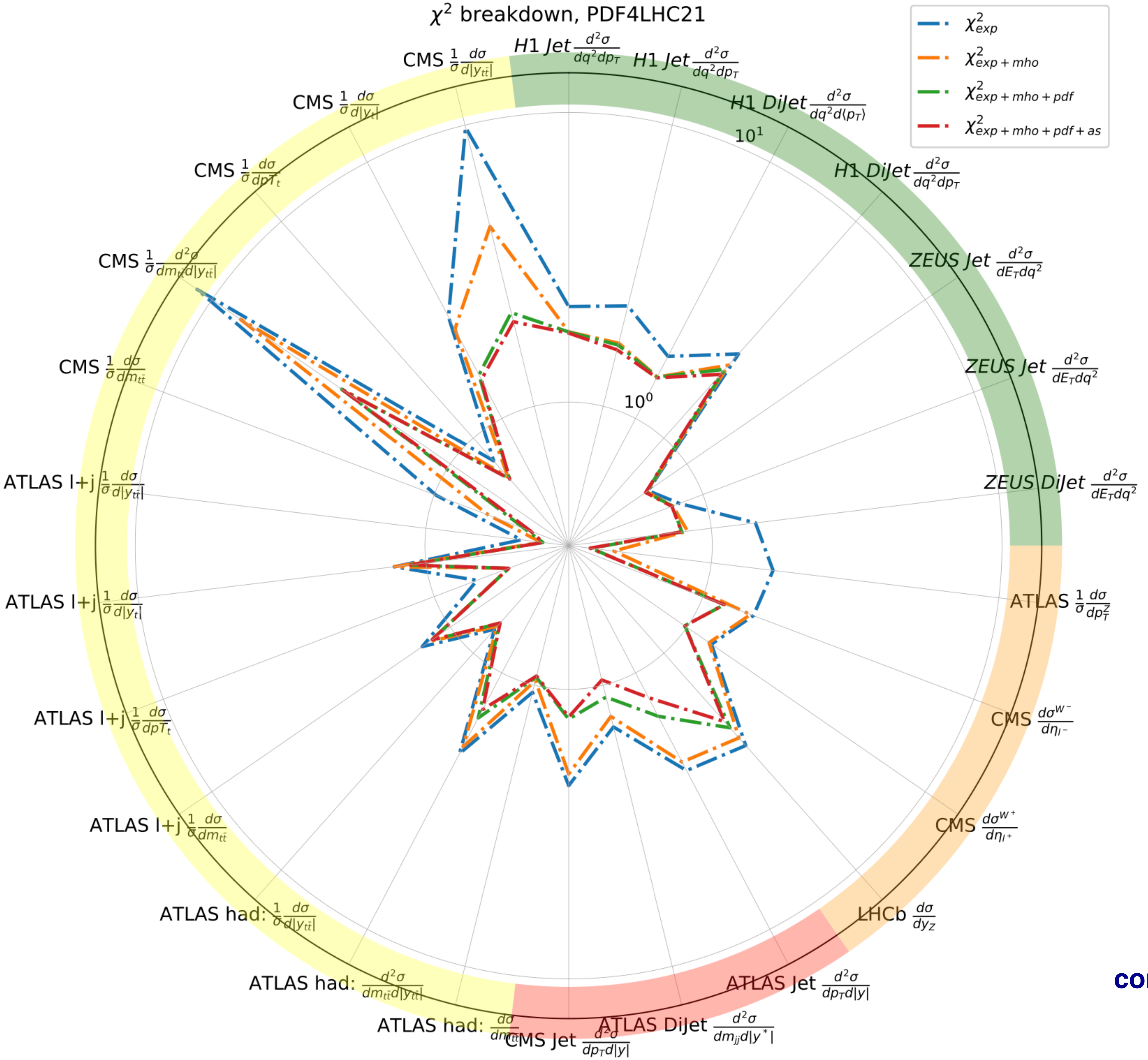
- Overlaps with **arXiv:1710.05167,** included in MSHT20 and NNPDF4.0

- PDF(a): NNPDF4.0 NNLO baseline.
- PDF(b): NNPDF4.0 aN3LO (including MHOUs) [105].
- PDF(c): NNPDF4.0 NNLO including MHOUs [97].
- PDF(d): NNPDF4.0 NNLO including QED corrections [102].
- PDF(e): NNPDF4.0 NNLO excluding the ATLAS 2017 Z production dataset [68].
- PDF(f): Same as PDF(e) now including the ATLAS 2023 Z production dataset [38].
- PDF(g): Same as PDF(f) now with a larger weight applied to the data from [38].
- PDF(h): Same as PDF(f) now including MHOUs.

		NNPDF4.0 NNLO					**in fit**		**in fit with mhou**
Dataset		PDF(a)	PDF(b)	PDF(c)	PDF(d)	PDF(e)	PDF(f)	PDF(g)	PDF(h)
$\|y_{\ell\bar{\ell}}\|$ (2023 paper [38])	$\chi^2_{\rm exp}$	7.902	8.424	8.383	8.774	7.238	3.492	0.175	3.357
	$\chi^2_{\rm exp+th}$	3.825	3.317	3.329	3.932	3.431	2.238	0.168	2.003
$\|y_{\ell\bar{\ell}}\|$ (2017 paper [68])	$\chi^2_{\rm exp}$	1.227	1.179	1.112	1.248	1.244	1.276	1.413	1.168
	$\chi^2_{\rm exp+th}$	1.079	1.048	1.014	1.088	1.085	1.059	1.018	1.008

- Improved $\chi^2_{\rm exp+th}$ once accounting for **MHOU** and **aN³LO corrections**
- Improved $\chi^2_{\rm exp+th}$ once **included with fit**, specially with MHOU $(n_\sigma \sim 2)$
- Weighted fit indicates some **tension** with other DY datasets e.g. LHCb *W,Z*

Results



- Despite PDF differences, **no systematic outlier** in dataset description
- Fully accounting for **theory errors** crucial
- PDF4LHC21 in general represents the **``average" behaviour**
- ABMP16 unfavored by jet data

Breakdown of contributions to $\chi^2_{\rm exp+th}$ for PDF4LHC21