## Parton Distribution Functions for Discovery at Next Generation Colliders

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## Nuclear, Hadronic and Particle Physics

Nucleons make up all nuclei, hence most of the visible matter in the Universe



## QCD, a theory for nucleon structure



three non-relativistic quarks

ACD (factorisation, evolution)

indefinite number of relativistic quarks and gluons

Nucleons can be prepared in definite spin states

Colliders: past, present, future



## Theoretical framework

Factorisation of physical observables



Perturbative expansion of coefficient functions

$$C_{Ii}(y, \alpha_s) = \sum_{k=0} a_s^k C_{Ii}^{(k)}(y), \qquad a_s = \alpha_s / (4\pi)$$

Perturbative (DGLAP) evolution of PDFs

$$\frac{\partial}{\partial \ln \mu^2} f_i(x,\mu^2) = \sum_{j=1}^{n_f} \int_x^1 \frac{dz}{z} P_{ji}\left(z,\alpha_s(\mu^2)\right) f_j\left(\frac{x}{z},\mu^2\right) \quad P_{ji}(z,\alpha_s) = \sum_{k=0}^{n_f} a_s^{k+1} P_{ji}^{(k)}(z)$$

## Parton Distributions



## A global PDF determination: the underlying strategy



Assume a reasonable PDF parametrisation

Obtain theoretical predictions for various processes and compare predictions to data Determine the best-fit parameters via minimisation of a proper figure of merit (*e.g.*  $\chi^2$ ) Self-validate PDF's accuracy and precision

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PDFs for Discovery at Colliders

## Data, Accuracy and Precision



## Proton PDFs

PDF uncertainty is often the dominant source of uncertainty in LHC cross sections

Higgs boson characterisation

Determination of SM parameters, such as the mass of the W boson Searches for beyond SM physics at large invariant mass of the final state



Plot from the CERN Yellow Report 2016

EPJC 76 (2016) 53

## Nuclear and Polarised PDFs



nuclei do not behave as a simple incoherent superposition of protons and neutrons

nPDFs enter theoretical predictions of signal and background events at high-energy neutrino observatories such as KM3NET and IceCube

search for exotic forms of QCD matter, such as the gluon-dominated Color Glass Condensate

interplay with proton PDFs, given the data used



$$\Delta G(\mu^2) = \int_0^1 dx \Delta g(x,\mu^2)$$

# 1. Some selected NNPDF results

## The NNPDF methodology in a nutshell

Neural network parametrisation of PDFs

- ▶ redundant and flexible parametrisation,  $\mathcal{O}(200)$  parameters
- requires a proper minimisation algorithm and stopping criterion

#### $\Rightarrow$ reduce the theoretical bias due to the parametrisation

#### 2 Monte Carlo propagation of errors

- generate experimental data replicas assuming multi-Gaussian probability distribution
- validate against experimental data to determine the sample size
- $\Rightarrow$  no need to rely on linear error propagation

PDF replicas are equally probable members of a statistical ensemble which samples the probability density  $\mathcal{P}[f_i]$  in the space of PDFs

$$\langle \mathcal{O} 
angle = \int \mathcal{D} f_i \mathcal{P}[f_i] \mathcal{O}[f_i]$$

Expectation values for observables are Monte Carlo integrals

$$\langle \mathcal{O}[f_i(x,Q^2)] \rangle = \frac{1}{N_{\mathsf{rep}}} \sum_{k=1}^{N_{\mathsf{rep}}} \mathcal{O}[f_i^{(k)}(x,Q^2)]$$

and similarly for uncertainties, correlations, etc.

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## Proton PDFs: NNPDF4.0 [2109.02653]

- Refined theoretical framework [EPJ C79 (2019) 282; EPJ C81 (2021) 37; EPJ C80 (2020) 1168]
  - $\rightarrow$  nuclear uncertainties for both deuteron and heavy nuclei included by default
  - $\rightarrow$  NNLO charm-quark massive corrections implemented (a bug in the NLO corrected)
  - ightarrow EW corrections not included to ensure consistency with data, but carefully checked
  - $\rightarrow$  charm PDF parametrised on the same footing as other PDFs
- Improved implementation of PDF properties [JHEP11(2020)129]
   → extended positivity constraints for light quark/antiquark and gluon PDFs
   → extended integrability constraints of non-singlet light quark PDF combinations
- New PDF parametrisation and optimisation [EPJC79(2019)676]
   → single neural network to parametrise eight independent PDF combinations
   → check of the independence of the results from the chosen parametrisation basis
   → new optimisation strategy based on gradient descent rather than genetic algorithms
   → scan of the hyperparameter space to find the optimal minimisation settings
- Complete statistical validation of PDF uncertainties [Acta Phys.Polon. B52 (2021) 243]  $\rightarrow$  (multi-)closure tests to validate PDF uncertainties in the data region  $\rightarrow$  future tests to check the sensibleness of PDF uncertainties in extrapolation regions
- Open source fitting code [EPJC 81 (2021) 958]

https://nnpdf.mi.infn.it/nnpdf-open-source-code/

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## Proton PDFs: NNPDF4.0 [2109.02653]

Data set	$N_{\mathrm{dat}}$	$\chi^2/N_{\rm dat}$
Fixed-target DIS	1881	1.10
HERA	1208	1.21
$\sigma_c$	37	2.11
$\sigma_{b}$	26	1.48
Fixed-target Drell-Yan	189	1.00
CDF	28	1.31
D0	37	1.00
ATLAS	621	1.18
Drell-Yan, 7, 8, 13 TeV	153	1.32
W+jet, 8 TeV	32	1.15
single top, 7, 8, 13 TeV	14	0.36
di-jets, 7 TeV	90	1.93
jets, 8 TeV	171	0.61
top pair, 7, 8, 13 TeV	16	2.30
$Zp_T$ , 8 TeV	92	0.86
direct photon, 13 TeV	53	0.72
CMS	411	1.40
Drell-Yan, 7, 8 TeV	154	1.34
single top, 7, 8, 13 TeV	3	0.43
di-jets, 7 TeV	54	1.67
di-jets, 8 TeV	122	1.50
top pair, 5, 7, 8 TeV	29	0.84
top pair, 13 TeV	21	0.67
$Zp_T$ , 8 TeV	28	1.42
LHCb	116	1.53
Total	4491	1.17



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#### Proton PDFs at the LHC



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## Proton PDFs at the LHC



Satisfactory description of all datasets no evidence for tensions

Sizeable constraint from NOMAD data consistent with collider data

- Moderate suppression of strange PDF
- Good consistency of  $R_s$  across PDF sets

$$R_s(x,Q^2) = \frac{s(x,Q^2) + \bar{s}(x,Q^2)}{\bar{u}(x,Q^2) + \bar{d}(x,Q^2)}$$



 $[c](Q) \equiv \int_0^1 dx \, x[c(x,Q) + \bar{c}(x,Q)]$ 

 $10^{2}$ Q (GeV)

#### Proton PDFs at the LHC





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Impact determined from pseudodata  $e^{\pm}p$  (NC and CC DIS);  $e^{\pm}d$  (NC DIS)  $E_{\ell} \times E_{p}$  [GeV]: 18× 275; 10× 100; 5× 100  $\mathcal{L} = 100 \text{ fb}^{-1}$ ;  $\sigma_u = 1.5/2.3\%$ ;  $\sigma_c = 2.5/4.3\%$ 

## Nuclear PDFs at the LHC



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## Nuclear PDFs at the EIC





#### Polarised PDFs at RHIC and at the EIC



NNPDFpolEIC [PLB 728 (2014) 524]

2 1.5 1 _<(€0)6 ∨ -0.5 -1 -1.5 -2	(         (         (         (	Fpol1.0 Epol1.1 EpolEIC	Q <sup>2</sup> =10 GeV <sup>2</sup>
		< <u>\</u> \(\(\)\(\)\(\)\(\)\(\)\(\)\(\)\(\)\(\)	
$Q^2 =$	$= 10 \text{ GeV}^2$	$\int_{10^{-3}}^{1} dx  \Delta \Sigma$	$\int_{10}^{1} dx  \Delta g$
NNPDF NNPDF NNPDF	pol1.0 pol1.2 polEIC	$+0.23 \pm 0.15 +0.25 \pm 0.10 +0.24 \pm 0.04$	$\begin{array}{c} -0.06 \pm 1.12 \\ +0.49 \pm 0.75 \\ +0.49 \pm 0.25 \end{array}$

quarks and antiquarks  $\sim 20\% - 30\%$ gluons  $\sim 70\%$  OAM  $\sim 0\%$ 

# 2. Methodological challenges

#### Data inconsistency: tensions between data sets

Give more weight to a data set p  $\chi^2 \rightarrow \chi^2 + w \chi_p^2 \qquad w = N_{\rm dat}/N_{\rm set}$ 

Refit: the total  $\chi^2$  will increase Which data sets get worse? How much?

Refit: the data set  $\chi_p^2$  will decrese Self-consistency? Inconsistency?

 $\begin{array}{l} \mbox{ATLAS $W,Z$ 7 TeV; $N_{\rm dat}=46$; $w=102$ \\ \mbox{ATLAS $t\bar{t}$ 8 TeV; $N_{\rm dat}=6$; $w=786$ \\ \end{array}$ 

Can improve the quality of the dataset BUT description of other datasets deteriorates unnatural PDF shapes appear

Fit quality for D0 el. asy. remains poor

Data set	baseline	wgt.	Total
ATLAS $W, Z$ 7 TeV ATLAS $t\bar{t}$ 8 TeV	1.86 1.86	1.23 1.32	1.18 1.47
Total	1.17		





#### Data inconsistency: experimental correlations

Single inclusive jet data from ATLAS 7 TeV default correlations: terrible  $\chi^2$ 

(correlations across rapidity bins)

decorrelation models: improve the fit a lot

$n_{\rm dat}$	default	part. decorr.	full decorr.
140	1.89	1.28	0.83

no significant effect on the extracted gluon similar gluon irrespective of the rapidity bin



[EPJ C78 (2018) 248; EPJ C80 (2020) 797]

Top pair production from ATLAS 8 TeV

default correlations: terrible  $\chi^2$ 

(correlations across different spectra)

decorrelation models: improve the fit a lot

$n_{\rm dat}$	default	stat. uncorr.	p.s. uncorr
25	7.00	3.28	1.80

appreciable effect on the extracted gluon different gluon depending on the top spectrum



[EPJ C80 (2020) 1; Les Houches proceedings, 2019]

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## Fitting the methodology



Compare to a Test Set (new set of data previously not used at all) Who picks the Test Set? Automatic generalisation based on K foldings Divide the data into n representative sets, fit n-1 sets and use n-th set as test set Hyperoptimise on mean and standard deviation of  $\chi^2_{\text{test},i}$ ,  $i = 1 \dots n$ 

#### Hyperoptimisation



SCAN parameter space; OPTIMISE  $\chi^2_{val}$ ; BAYESIAN UPDATING Hyperoptimisation requires to define a reward (or loss) function to grade each model This is different from the cost function (optimised separately for each model)

cost function: 
$$C = E_{\rm tr}$$
 reward function:  $R = \frac{1}{2}(E_{\rm val} + E_{\rm test})$ 

In a hyperparameter scan one compares the performance of hundreds parameter combinations Some parameters are discrete (type of minimiser), other are continuous (learning rate) One should visualise which parameters are relevant and which parameters are immaterial The *violin* plots are the KDE-reconstructed probability distributions for the hyperparameters

Hyperoptimisation successfully validated in closure tests and in future tests

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PDFs for Discovery at Colliders

## Validation of PDF uncertainties

Data region: closure tests

Fit PDFs to pseudodata generated assuming a known underlying law

Define bias and variance bias difference of central prediction and truth variance uncertainty of replica predictions

> If PDF uncertainty faithful, then E[bias] = variance25 fits, 40 replicas each





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## Validation of PDF uncertainties



Extrapolation regions: future test

Test PDF uncertainties on data sets not included in a given PDF fit that cover unseen kinematic regions

Data set	NNPDF4.0	pre-LHC	pre-HERA
pre-HERA	1.09	1.01	0.90
pre-LHC	1.21	1.20	23.1
NNPDF4.0	1.29	3.30	23.1

Only exp. cov. matrix



## Validation of PDF uncertainties



Extrapolation regions: future test

Test PDF uncertainties on data sets not included in a given PDF fit that cover unseen kinematic regions

Data set	NNPDF4.0	pre-LHC	pre-HERA
pre-HERA pre-LHC NNPDF4.0	1.12	1.17 1.30	0.86 1.22 1.38

Exp+PDF cov. matrix





Acta Phys.Polon. B52 (2021) 243

## Benchmarks

Benchmark of the theory



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# 3. Theoretical challenges

Theory uncertainties in PDF determination

NNLO is the precision frontier for (unpolarized) PDF determination

N3LO is the precision frontier for partonic cross sections at the LHC Mismatch between perturbative order of partonic cross sections and accuracy of PDFs

is becoming a significant source of uncertainty

$$\hat{\sigma} = \alpha_s^p \hat{\sigma}_0 + \alpha_s^{p+1} \hat{\sigma}_1 + \alpha_s^{p+2} \hat{\sigma}_2 + \mathcal{O}(\alpha_s^{p+3}) \qquad \delta(\text{PDF} - \text{TH}) = \frac{1}{2} \left| \frac{\sigma_{\text{NNLO-PDFs}}^{(2)} - \sigma_{\text{NLO-PDFs}}^{(2)}}{\sigma_{\text{NNLO-PDFs}}^{(2)}} \right|$$



#### Theory uncertainties in PDF determination

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Perturbative stability and uncertainty of the gluon PDF



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## Fits with varied scales

Standard technique to estimate MHOU:

vary scales by 2 and 1/2, and compute observables for various scale combinations



Useful for estimating MHOUs in PDFs but want to include them in fitting methodology, and in a way that is also applicable to other theoretical uncertainties

[EPJ C79 (2019) 931]

#### Nuisance parameters

Assuming that theory uncertainties are (a) Gaussian and (b) independent from experimental uncertainties, modify the figure of merit to account for theory errors

$$\chi^2 = \sum_{i,j}^{N_{\text{dat}}} (D_i - T_i)(C + S)_{ij}^{-1} (D_j - T_j); \ (\text{cov}_{\text{th}})_{ij} = \frac{1}{N} \sum_{k}^{N} \Delta_i^{(k)} \Delta_j^{(k)}; \ \Delta_i^{(k)} \equiv T_i^{(k)} - T_i$$

Problem reduced to estimate the th. cov. matrix, e.g. in terms of nuisance parameters

$$\Delta_i^{(k)} = T_i(\mu_R, \mu_F) - T_i(\mu_{R,0}, \mu_{F,0}); \text{ vary scales in } \frac{1}{2} \le \frac{\mu_F}{\mu_{F,0}}, \frac{\mu_R}{\mu_{R,0}} \le 2$$



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#### A theory covariance matrix for MHOU





EPJ C79 (2019) 931; ibid. 838

## Impact on Parton Distributions



PDF uncertainty increase encapsulates NLO-NNLO shift

Overall (rather small) increase in uncertainties Increase in PDF uncertainties due to replica generation is counteracted by extra correlations in fitting minimisation

Tensions relieved: improvement in  $\chi^2$ exp only:  $\chi^2/N_{dat} = 1.139$  exp+th:  $\chi^2/N_{dat} = 1.110$ 

Data whose theoretical descrition is affected by large scale uncertainties are deweighted in favour of more perturbatively stable data

EPJ C79 (2019) 931; ibid. 838

## Theory uncertainty in PDF determination

Experimental+Nuclear correlation matrix CHORUS 1.00 0.75 0.50 0.25 0.00 -0.25 -0.50NUTEV -0.75 DYE605 -1 00 1.00 SLAC -075 - 0 50 BCDMS - 0.25 - 0.00 - -0.25 -0.50 NMC -0.75 NuSea -1.00 WSea

Effect of nuclear uncertainties relevant at large xto reconcile FT DIS with LHC DY data  $\chi^2_{tot} = 1.17 \rightarrow \chi^2_{tot} = 1.26$  (no nucl. uncs.)  $\chi^2_{LHCb} = 1.54 \rightarrow \chi^2_{tot} = 1.76$  (no nucl. uncs.) The bulk of the effect is due to nuclear uncertainties for heavy nuclei deuteron uncertainties have a comparatively

smaller effect at intermediate values of x



EPJ C79 (2019) 282; EPJ C81 (2021) 37

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## NLO EW corrections in PDF determination

If we aim to PDF accurate to 1% NLO EW corrections do matter especially as higher invariant mass and transverse momentum regions are accessed

Different approaches taken in general-purpose PDF fits NLO EW K-factors (MSHT20); no NLO EW corrections by default (NNPDF4.0)



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## Input from Lattice QCD



Prog.Part.Nucl.Phys. 100 (2018) 107; ibid. 121 (2021) 103908



#### Moments of Parton Distributions

## $\langle 1 \rangle_f = \int_0^1 dx f \qquad \langle x \rangle_f = \int_0^1 x dx f$

ETMC20 <sup>@</sup> <x>u<sup>+</sup>-d<sup>+</sup></x>		ه <x>d+</x>	<x><sub>S</sub>+</x>	<x>g</x>
PNDME20				
Here ETMC19			N <sub>f</sub> =2+1+1	
Mainz19				
χQCD18	H-			processing and the second
			N <sub>f</sub> =2+1	χQCD18a
@ ETMC19				
RQCD18			N <sub>f</sub> =2	
PDFLattice17	*	*	66	ж
	ж	ж		ж
× JAM19	×	×	ж	× 2.0 ×
				μ=2 Gev
0.1 0.15 0.2 0.25 0.3	0.2 0.3 0.4 0.5 0.6	0.1 0.15 0.2 0.25 0.3 0.35	0 0.03 0.06 0.09 0.12	0.1 0.2 0.3 0.4 0.5 0.6

g <sub>A ETMC19 ⊷®↔</sub>	<1>_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{	<1>	<1>_{_{\Delta S^+}} _{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_{_	<x><sub>Δu</sub> -Δd</x>
CalLat18 🛥				
PNDME18		••• <b>=</b> •••	N <sub>f</sub> =2+1+1	PNDME20
LHPC19				
Mainz19				
PACS19				
χQCD18	·	2- <b></b> -4	N <sub>f</sub> =2+1	
ETMC19 ⊶⊡⊶			N <sub>f</sub> =2	
PDFLattice17 -X	-*-		·····×·····	
				μ=2 06 γ
1 1.1 1.2 1.3	0.7 0.8 0.9 1	-0.5 -0.4 -0.3 -0.2	-0.2 -0.1 0	0.15 0.2 0.25 0.3

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#### Quasi-PDFs and Pseudo-PDFs



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## Can New Physics hide in the Proton?

Replace the SM  $\longrightarrow$  SMEFT Lagrangian  $\mathcal{L}_{\mathrm{SMEFT}} = \mathcal{L}_{\mathrm{SM}} + \sum_{i}^{N_{\mathrm{d6}}} \frac{c_i}{\Lambda^2} \mathcal{O}_i^{(6)} + \sum_{j}^{N_{\mathrm{d8}}} \frac{c_j}{\Lambda^4} \mathcal{O}_j^{(8)}$ assumption: new physic states are heavy
the Lagrangian contains only light SM particles
BSM effects included as a momentum expansion
based on all SM symmetries

number of couplings reduced by symmetries

Can Wilson coefficients be determined from LHC data?

Can BSM effects be reabsorbed into PDFs?  $\sigma_{\rm LHC} = f_i^{\rm SM} \otimes f_j^{\rm SM} \otimes \tilde{\sigma}_{\rm SM}$   $\sigma_{\rm LHC} = f_i^{\rm SMEFT} \otimes f_j^{\rm SMEFT} \otimes \tilde{\sigma}_{\rm SM} \times K$   $K = 1 + \sum_m^{N_{\rm d6}} c_m \frac{\kappa_m}{\Lambda^2} + \sum_{m,n}^{N_{\rm d6}} c_m c_n \frac{\kappa_{mn}}{\Lambda^4}$ 



## Can New Physics hide in the Proton?

Can Wilson coefficients be determined from LHC data?



JHEP 04 (2019) 100; JHEP 11 (2021) 089

Can BSM effects be reabsorbed into PDFs?

PRL 123 (2019) 132001; JHEP 07 (2021) 122; Maria Ubiali's seminar in March 2021

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## 4. To conclude

## Summary

A precise and accurate determination of PDFs is key to do discovery. Collider measurements are reducing PDF uncertainties to few percent. This opens up some challenges. Understand experimental systematic uncertainties and their correlations. Refine the theoretical accuracy of a PDF determination. Represent theory uncertainties into PDF uncertainties. Deploy a robust fitting methodology and good statistical tests of it. Benchmark efforts may benefit from public releases of PDF codes and inputs.

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## Thank you