CT18 studies (related to flavoured jets at the LHC)

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Family of CT18 PDFs

- CT18: nominal set (NNLO and NLO; work ongoing on N3LO); enhanced precision (denser) grids available
- CT18A: same as above except ATLAS 7 TeV W and Z data included
- CT18As, CT18As_lat: s and sbar not equal, lattice information included
- CT18X: same as CT18, but special scale mimicking low-x resummation used for DIS
- CT18Z: special scale and ATLAS W/Z data both included
- CT18qed: NNLO QCD and NLO QED evolution
- CT18lux
- CT18 neutron photon PDFs
- CT18LO: same data set, LO formalism (not recommended)
- CT18FC: fitted charm series; 4 model series (BHPS (CT18 and CT18X), MBMC, MCME, each with 3 sets with $\Delta\chi^2$ =0, 10, 30
- CT18_NF4: four flavor scheme
- CT18MC: NLO PDFs intended for MC use (within next few weeks)
- See talks at DIS24 by Aurore Courtoy, Marco Guzzi, Pavel Nadolsky
- See also https://cteq-tea.gitlab.io

Prelude: uncertainties

- PDF uncertainties depend first on the experimental uncertainties of the data
- Data from two measurements, or even from within the same measurement, can both be very precise, but the result of adding both to the PDF fit can be an increase in the PDF uncertainty (or more likely) a smaller decrease in uncertainty than expected) if the data are in tension with each other
- The resultant PDF uncertainty relies on the definition of a tolerance, i.e. what is a significant increase from the global minimum χ², i.e. PDF uncertainty can be adjusted by changing the tolerance
- $\Delta \chi^2$ =1 is not applicable for ~4000 data points from different experiments
- NB: CT (Tier 2) and MSHT (dynamic tolerance) have introduced criteria to restrict the pull of data sets that disagree with global fit
- More details in extra slides

PDF uncertainties

CT and MSHT both use a Hessian technique to determine the central PDF. By definition, this is at the best χ^2 . This is not necessarily true for NNPDF.

The plot on the right shows a Lagrange Multiplier scan for the gluon distribution at a Q value of 125 GeV at an x value of 0.01.

The pulls of the individual experiments are in general not Gaussian, but the combined pulls of all of the data sets are.

This is a very time-consuming (and specific) way of studying the PDF uncertainty. The L2 sensitivity T²=10 / provides similar, but more general, useful for information.

The uncertainty is determined by allowing an excursion from that central value. CT18 uses $\Delta\chi^2$ =37 for a 68% CL error.



Towards a new generation of CT202X PDFs

- New LHC Run 2 data added: (di)jet, vector boson, ttbar based on experiment selections recommended in 2305.10733, 2307.11153
- Work on implementation of N3LO contributions
- A number of other areas of development next-generation PDF uncertainty quantification Bezier curves META combination ML stress-testing multi-Gaussian approaches subtracted heavy-quark PDFs in S-ACOT-MPS scheme...

Post CT18 data



The most precise new experiments tend to have an elevated χ^2/N_{pt} , in the same pattern as observed for CT18

 χ^2/N_{pt} increases for experiments 124 and 125 (NuTeV), 126 and 127 (CCFR) and 203 (E866 DY), 266 and 267 (CMS 7TeV Ach), 268 (ATLAS 7TeV W, Ach).

 χ^2/N_{pt} decreases for experiments 249 (CMS 8 TeV Ach), 250 (LHCb 8 TeV W/Z)

2024-04-09

P. Nadolsky, DIS 2024

Impact of new data

Pulls on the gluon PDF by the new data type





After including DY, $t\bar{t}$, and inc. jet data simultaneously, we get a softer gluon. Note that new DY and $t\bar{t}$ data favor a softer gluon, new inc. jet data prefer a harder gluon.

Mild changes in the gluon uncertainty

PRELIMINARY



 $g(x,Q=100.0{
m GeV})~90\%{
m CL}$

1.20

2024-04-09

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2024-04-09

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dijet data tend to have larger uncertainties, leading to smaller χ^2 than inclusive jets, but similar constraints on PDFs

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Impact of new jet data on gluon



Taming PDF uncertainties in CT202X PDFs

Several efforts to refine PDF uncertainty quantification:

- understand conceptual underpinnings of the multivariate inverse problem. Much can be learned from non-HEP statistics applications
- suppress aleatory and perturbative uncertainties (e.g., from higher-order contributions)
- comprehensively estimate epistemic uncertainties (e.g., due to the PDF parametrization forms)



The final Hessian error set (50-60) approximates the total uncertainty due to the above factors.

P. Nadolsky, DIS 2024

GMVN schemes in a nutshell

Heavy-flavor production dynamics is nontrivial due to the interplay of massless and massive schemes which are different ways of organizing the perturbation series

Massive Schemes: final-state HQ with $p_T \le m_Q \Rightarrow p_T$ -spectrum can be obtained in the **fixed-flavor number (FFN) scheme**. - No heavy-quark PDF in the proton. Heavy flavors generated as massive final states. m_Q is an infrared cut-off. - Power terms $\left(p_T^2/m_Q^2\right)^p$ are correctly accounted for in the perturbative series.

Massless schemes: $p_T \gg m_Q \gg m_P \Rightarrow$ appearance of log terms $\alpha_s^m \log^n (p_T^2/m_Q^2)$ that spoil the convergence of the fixed-order expansion. Essentially, a **zero mass (ZM) scheme**.

- Heavy quark is considered essentially massless and enters also the running of α_s .

- Need to resum these logs with DGLAP: initial-state logs resummed into a heavy-quark PDF, final-state logs resumed into a fragmentation function (FF)

Interpolating (GMVFN) schemes: composite schemes that retain key mass dependence and efficiently resum collinear logs, so that they combine the FFN and ZM schemes together. They are crucial for:

- a correct treatment of heavy flavors in DIS and PP,
- accurate predictions of key scattering rates at the LHC,
- global analyses to determine proton PDFs.

M. Guzzi DIS24

QCD cross sections @N3LO



Work in progress

DIS: The CTEQ-TEA code implements complete flavor decompositions of DIS SFs at N3LO using approximate zero-mass Wilson coefficients with a rescaling variable (the **Intermediate-Mass VFN scheme**, cf. the figure)

Boting Wang's and Keping Xie's Theses, SMU

Imminent implementation of massive N3LO heavyquark coefficients to obtain N3LO DIS cross sections in the SACOT-MPS General-Mass VFN scheme

see talk of Marco Guzzi at DIS

	Factorization	Mass dependence	Mass dependence of the	Introduce heavy-quark
	schemes	in the FC terms	FE and subtraction terms	PDFs at large Q
	\mathbf{FFN}	Exact	N/A	no
	ZM	None	None	yes
	IM	Approximate	Approximate	yes
_	GM	Exact	Approximate	yes

- **DGLAP evolution** is performed at N3LO with APFEL/APFEL++.
- Drell-Yan: Ongoing work to include N3LO DY effects using NNLO ApplFast + N3LO/N2LO K-factor tables

2024-04-09

Main idea behind S-ACOT-MPS (massive phase space)

$$\sigma = FC + FE - SB$$

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FC = Flavor creation contributions with full mass dependence FE = Flavor excitation contribution with approximate mass dependence

Mass fully retained in the PS in all terms. Kinematical power corrections under control.

Subtraction well defined at the guark mass threshold

FE and Subtraction is facilitated by introducing residual PDF:

Subtracted and Residual PDFs are provided in the form of LHAPDF grids for phenomenology applications: https://sacotmps.hepforge.org/downloads?f=PDFs

More details in K. Xie PhD Thesis: "Massive elementary particles in the standard model and its supersymmetric triplet higgs extension." https://scholar.smu.edu/hum sci physics etds/7, 2019.

(available from public codes)

 $\delta f_O(x,\mu)$ $_{-q}(x)$ $\langle m_Q \rangle$

at LO

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step
$$(\mu^2)$$

allows us to get (FE-Subtraction) in one
step
$$f^2) = f_Q(x,\mu^2) - rac{lpha_s}{2\pi} \log\left(rac{\mu^2}{m_Q^2}
ight) f_Q(x,\mu^2) \otimes P_{Q\leftarrow 2\pi}$$

Charm and b quark distributions

- Perturbative view is that c and b quarks are not present in the proton at scales lower then their masses
- They can be produced in the initial state at scales higher then their masses through gluon splitting into quark-antiquark pairs (thus primarily at lower x)
 - only things that drive production (besides the gluon distribution) are the heavy quark mass and the value of $\alpha_s(m_z)$
- But the proton can also have an intrinsic charm (and bottom for that matter) component arising from scattering contributions beyond leading twist
 - there are models (BHPS, incorporated by the CTEQ group), and increasingly, predictions from lattice gauge theory, some of which have been incorporated into CT fits
- CT has published PDF sets in which an intrinsic component of charm is modeled. The addition of this intrinsic component leads to a small, but noticeable, reduction in global χ^2



FIG. 5: The change $\Delta \chi^2$ in the goodness of fit to the CT14 (left) and CT14HERA2 (right) data sets as a function of the charm momentum fraction $\langle x \rangle_{\rm IC}$ for the BHPS (blue) and SEA (red) models.



Greatest sensitivity for BHPS models comes from BCDMS and ATLAS 7 TeV W and Z

FIG. 8: Ratio of $c(x,Q)_{IC}/c(x,Q)_{CT14}$ within the CT14 uncertainties at 90% C.L. at the scale Q = 2 GeV (left) and Q = 100 GeV (right).

The L₂ sensitivity

- For data to influence the PDF fit in a particular region of x and Q², two conditions must be met
 - the parton-level dynamics must depend on a particular PDF (say that of the gluon), as manifested in a statistical correlation
 - the data must have sufficient resolving power to contribute to the PDF likelihood analysis
- The L₂ sensitivity incorporates both of these features
- The L₂ sensitivity is a way of viewing the pulls of all of the experiments used in a global PDF fit, for a particular parton flavor, as a function of a kinematic variable, such as parton x
 - or, when plotted for a PDF luminosity, as a function of the mass
- The fit value for a particular PDF(x,Q) is determined by the sum of these pulls

L₂ sensitivity

$$S_{f,L2}^{\rm H}(E) \equiv \frac{\vec{\nabla}\chi_E^2 \cdot \vec{\nabla}f}{\Delta^{\rm H}f} \\ = \left(\Delta^{\rm H}\chi_E^2\right) \ C^{\rm H}(f,\chi_E^2)$$

2nd Lagrangian technique

 C^H represents the cosine of the correlation angle between PDF flavor f (or any defined quantity) and experimental χ²



The importance of an experiment for a particular PDF depends not only on the correlation of the cross section with that PDF, but the degree to which the cross section can determine that PDF.

Can also be defined for the MC PDF approach

A positive value of the L2 sensitivity indicates the data wants to pull the PDF down, while a negative value indicates an upwards pull.

An ATLAS, CTEQ-TEA, and MSHT X.Jing et al.,arXiv:2306.03918 comparative study of NNLO and aN3LO PDF sensitivities



- Comparisons of strengths of constraints from individual data sets in 8 PDF analyses using the common L_2 sensitivity metric. [Definitions in the backup.]
- An interactive website (<u>https://metapdf.hepforge.org/L2/</u>) to plot such comparisons [2070 figures in total; a code L2LHAexplorer to plot L2 sensitivities for LHAPDF grids] 2024-04-09 P. Nadolsky, DIS 2024

What defines the c and b quark distributions in CT18?

- Use the L2 sensitivity to show the most sensitive experiments (in this case the 8 most sensitive)
- Some experiments have positive L2 sensitivity (want to pull charm down), while others have negative (want to pull charm up)
- The sum (at each x value) is approximately zero



CT18 NNLO c(x, 100 GeV)



- Compare sensitivities of charm quark and gluon (at Q=100 GeV)
- Very similar (as might be expected), since this is perturbative charm (so would also be similar for b-quark distributions)



V+HF: inputs for (s),b,c PDFs

• A heavy flavor quark can be present in the initial state or produced through gluon splitting



- The calculation can be performed in a scheme where there are only 4 parton flavours (4FNS) or in which the b-quark is included (5-FNS)
- The kinematics can drive the subprocess for the production, as for example, whether the final state heavy quark (jet) has to pass only some minimum p_T requirement, or whether it has to roughly balance the boson transverse momentum
- If it's the former, then the final state c or b quark is likely to arise through gluon splitting, especially given the additional gluon splittings that may occur in a parton shower (*JHEP* 02 (2018) 059)

this effect is more pronounced if there is a hierarchy of scales, i.e. $p_T^{jet} > p_T^{charm}$ (would be useful to measure differentially in p_T^{jet})

arXiv:1707.00657;JHEP02 (2018) 059



FIG. 19: Transverse momentum distribution of Z bosons produced in association with at least one charm jet at the LHC for $\sqrt{S} = 8$ TeV. Both panels show SHERPA MEPS@LO predictions (obtained by using proper charm tagging) for Z+jets production with a successively increasing number of multileg matrix elements taken into account (i.e. $n_{\rm ME} = 1, 2, 3$ where the $n_{\rm ME} = 1$ curves serve as the reference).

Intrinsic charm

Probing HF content of the proton



ATLAS13 TeV, Z+c-jet, 140 fb^{-1} arXiv:2403.15093

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Z+c jets (arXiv:2109.08084)



Future inputs



Figure 1. Left: Rapidity distributions of prompt charm at the LHC 13 TeV in the very forward region (yc > 8) [11]. The error band represents the CT18NLO induced PDF uncertainty at 68% CL. **Right**: NLO theory predictions for the rapidity distributions obtained with CT18NLO and CT18XNLO PDFs compared to B^{\pm} production data [28] from LHCb 13 TeV.

Summary

- A key aspect of understanding the physics of heavy flavor jets at the LHC is the understanding of heavy flavor quark distributions in the proton
- c and b quarks are produced perturbatively through gluon splitting, but there is the possibility of an intrinsic component, which however has not been firmly established
- From BHPS-type of models for intrinsic charm, expect the effects to be primarily at higher x
 - we are starting to probe this region with LHCb, and will probe even higher x values with forward detectors at the LHC
- A full utilization of this data in PDF fits requires:
 - a proper match/mapping of algorithms used in NNLO theory and in the data, i.e. the reason for this workshop
 - GM-VFN schemes that work at N3LO in the PDF fitting



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CT18QED: Photon PDF in the CTEQ-TEA global analysis



K. Xie, T. Hobbs, et al.

minimum and therefore enabces photon slightly.

The PDF uncertainties for the combination in the PDF4LHC21 exercise is shown below. Same data sets used for all PDF fits.

NNPDF3.1'is the smallest and CT18 is the largest, with MSHT20 in-between.

NB: MSHT20 nominally does not use a fixed tolerance, but instead cuts off an eigenvector direction when a particular experiment is badly fit. Thus, the uncertainty can be notably affected by one experiment.









evaluated at

In a global PDF fit, there are tensions between the input data sets, by definition. These tensions are most easily demonstrated by the use of the L2 sensitivity above. For, example, some data sets pull the gluon up at $x \sim 0.01$, some down.

The end result of the pulling is the central PDF. The PDF uncertainty reflects the size of those pulls/tensions.

Typical χ^2 /dof are of the order of 1.1 for >4000 points, or very unlikely from the pure statistical POV. $\Delta \chi^2 = 1$ does not capture the full uncertainty. CT and MSHT use different criteria to define those tensions/define the uncertainty.



It is difficult to perform a directly similar comparison to NNPDF, as they don't use the Hessian formalism. However, as part of the PDF4LHC exercise, fits were carried out to a reduced data set, using similar theory parameters, in which equivalent results should be obtained, if the uncertainty criteria were the same. The uncertainties are larger than for the full fit.

CT18red and MSHT20red agree for the most part. There are fewer experiments included, so less likely for a particular experiment to truncate the uncertainty from a particular eigenvector.

NNPDF consistently has a consistently smaller uncertainty, **i** especially at low x, partially explained in 2404.10056.



This difference is even more prominent when the PDF luminosities are compared (above). For gg fusion at the Higgs mass, it is a factor of 2.



uncertainties are reduced even further for 4.0



Large inflow of new measurements @LHC

Precise measurements Z + c/b-jets available from the ATLAS, CMS and LHCb collaborations at the LHC



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W+c jets

• Measurement carried out inclusively, and differentially as function of p_T and η of lepton



Differential cross sections

- Require an isolated lepton (e or μ) with p_T>30 GeV and |η|<2.1
- Require a jet with $p_T>25$ GeV with $|\eta_{jet}|<2.5$. Jets not selected if $\Delta R(jet, l)<0.5$
- Data are larger then (NLO+PS) predictions for lepton p_T less then 65 GeV, but compatible within uncertainties
- NNLO corrections for W+c predicted to be on the order of 5% for lepton p_T less then 60 GeV and about 1% for larger p_T values
 - JHEP 06 (2021) 100
- This would improve the level of agreement with the data

arXiv:2112.00895 (submitted to EPJC)



NNLO W+c-jet cross section calculation

- Large reduction in uncertainties from NLO->NNLO
- NNLO scale uncertainties smaller then PDF uncertainties
- NB: the NNLO calculation used flavor tagging for the charm jet; the experimental measurement used the antikT algorithm with later flavor identification; NNLO corrections to subleading CKM-mediated processes not included in this calculation (but are now available)



Photon+charm jets

- Photons measured in central and forward rapidity
- Jets are defined with antikT algorithm, R=0.4; p_T^{jet}>20 GeV

if jet contains a b-hadron with p_T >5 GeV within ΔR =0.3 of jet, then it is assigned as a b-jet; if there is no b-hadron, but there is a charm hadron, it is assigned as a c-jet

- All predictions agree reasonably well with data (relatively large uncertainties)
- There are differences at high E_T when intrinsic charm included in predictions of similar size to uncertainties
- NNLO predictions would be very useful (have to deal with photon isolation) Phys.Lett.B776(2018) 295



Photon+b jets

- 5FNS scheme works better then 4FNS scheme
- Best description of the data provided by Sherpa with up to 3 additional partons included in 5FNS scheme
- Again, NNLO would be useful



Z+b jets

- The b quark is treated as perturbatively produced by all PDF fitting groups; i.e. inside the proton, at higher Q² scales, only things that drive it are the b-quark mass and the value of $\alpha_s(m_Z)$ $b \longrightarrow \mathcal{N} Z$
- Also sensitive to final state gluon splitting



Calculation can be performed either in 4FNS or 5FNS

ATLAS JHEP 07 • Partial run 2 dataset: 3	<u>(2020) 44</u> 5.6 fb⁻¹	CMS- • Full ru	 <u>CMS-SMP-20-015 arxiv:2112.09659</u> Full run 2 dataset: 137 fb⁻¹ 					
 Z + ≥ 1 or ≥ 2 b jets, b b-jet tagger: ≈ 70% eff 	-jet p _T > 20 GeV, y iciency	.5 • Z + ≥ • b-jet t	 Z + ≥ 1 or ≥ 2 b jets, b-jet p_T > 30 GeV η < 2.4 b-jet tagger: ≈ 50% efficiency (tight WP) 					
 Testing several MC predictions with 4 and 5 FNS: 5FNS includes b quark in PDF 								
Kinematic variable	Acceptance cut		Object	Selection				
Lepton $p_{\rm T}$	$p_{\rm T} > 27 \; {\rm GeV}$		Dressed leptons	$p_{\rm T}$ (leading) > 35 GeV, $p_{\rm T}$ (subleading) > 25 GeV, $ \eta < 2.4$				
Lepton η	$ \eta < 2.5$		Particle-level bjet	$1 < M_{\ell\ell} < 111$ bhadron jet, $p_T > 30 \text{ GeV}, \eta < 2.4$				
$m_{\ell\ell}$	$m_{\ell\ell} = 91 \pm 15 \text{ GeV}$,					
<i>b</i> -jet p_{T}	$p_{\rm T} > 20 \text{ GeV}$							
<i>b</i> -jet rapidity	y < 2.5							
<i>b</i> -jet–lepton angular distance	$\Delta R(b\text{-jet}, \ell) > 0.4$			16				

Z+b jet

- The b quark is treated as perturbatively produced by all PDF fitting groups;
 i.e. inside the proton, at higher Q² scales only things that drive the PDF are the b-quark mass and the value of α_s(m_z)
- Also sensitive to gluon splitting (and multiplicative factor of parton shower)



• Calculation can be performed either in 4FNS or 5FNS

4FNS underestimates cross section; better agreement with5FNS



17

ATLAS JHEP 07 (2020) 44

Most important information comes from differential distributions, though

NNPDF3.1 PDF is the most up-to-date of the PDFs shown; would be nice to have comparisons of more modern PDFs as well (CT18, MSHT20, NNPDF4.0 (NNPDF3.1')

ATLAS JHEP 07 (2020) 44



CMS 137 fb⁻¹ (13 TeV) a Sev De Data (pp \rightarrow Z + \geq 1 b jet) Statistical unc. Theoretical syst. unc. 10 $\frac{d\sigma}{d(p_T^{b\,jet})}$ sizeable Total unc. MG5_aMC (NLO, NNPDF 3.1, CP5) MG5_aMC (NLO, NNPDF 3.0, CUETP8M1) MG5_aMC (LO, NNPDF 3.1, CP5) MG5_aMC (LO, NNPDF 3.0, CUETP8M1) ______ difference 10depending on Sherpa whether 10^{-2} massless or 10⁻³ massive NLO+PS 10^{-4} prediction used 1.5 0.5 PDF \oplus scales $\oplus \alpha_s$ PDF ⊕ scales 1.5 <u>Pred.</u> Data 0.5 1.50.5₽ PDF 200 300 400 100 500

arxiv:2112.09659 CMS-SMP-20-015

600

[GeV]

p_^{b jet}

18

Z+b at NNLO prediction

Carried out by combining a massless NNLO and a massive NLO computation at order (α_s^3) (arXiv:2005.03016)

> initial state b-guarks from gluon splitting resummed by PDF evolution; finite b-guark mass effects also incorporated (presumably same could be done for Z+c)

note: massless calculation means IR-safe definition of jet flavour must be used; not consistent with experimental choice

desired to have data unfolded to level of partonic flavour-kT jets or some equivalent



Figure 3: As in Fig. 2, now for the absolute psudorapidity distribution of the leading flavour- $k_{\rm T}$ b-jet. 19

panel, and the ratio to the NLO 5fs prediction in the lower panel. The shown uncertainty of the FONLL distributions are due to scale variations alone.

What is the L₂ sensitivity...continued?

- The L₂ sensitivity provides a visualization of what is happening inside the PDF fit
- It can be considered as a faster version of Lagrange Multiplier scans (but dependent on the Gaussian approximation)
- The L₂ sensitivity streamlines comparisons among independent analyses, using the log-likelihood (χ²) values for the fitted experiments and the error PDFs
- Both the L₂ and LM methods explore the parametric dependence of the χ^2 function in the vicinity of the global minimum
- The L₂ sensitivity has been used internally by CT (in CT18), by the PDF4LHC21 benchmarking group (to determine which data sets should be in the reduced PDF fit used for benchmarking), and now by CT, MSHT and ATLASpdf in this upcoming paper

Strange/charm PDFs

- Consider the strange quark PDF
- There is a large difference between CT18 and CT18A/MSHT20/NNPDF3.1 due almost entirely to the ATLAS 7 TeV W/Z data (see my talk on Monday)
- The difference between the W and Z cross sections requires a larger strange quark (s-sbar->Z)
- All 3 groups fit the ATLAS W/Z data equally poorly
- Because of its fitting criteria, CT18 does not use the 7 TeV W/Z data for its main fit (but it is in CT18A)
- W+c data offer another window on the strange quark distribution
- NNPDF3.1 has a different charm distribution then CT18/MSHT20, due to its fitting the charm distribution as a free parameter, rather then generating perturbatively through gluon splitting; an intrinsic charm component may be present at high x
- CT has published PDF sets in which an intrinsic component of charm is modeled. The addition of this intrinsic component leads to a small, but noticeable, reduction in global χ²
- $Z+c/\gamma+c$ offers another window on the charm quark

PDF4LHC21: arXiv:2203.05506



(W+c) strange quark PDF

- Derived CMS strange quark consistent with that obtained by CT18 and MSHT20 for x<0.01; somewhat larger at higher x
 - NB: MSHT20 includes ATLAS 7 TeV W/Z data



strangeness suppression factor

arXiv:2112.00895 (submitted to EPJC)

(W+c) strange quark PDF



arXiv:2112.00895 (submitted to EPJC)

W+c at NNLO-differential

JHEP 06 (2021) 100





W+c at NNLO



NNLO uncertainties very small; potential for constraining asymmetry