ATLASpdf21

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Diffraction and Low-x 2022
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On behalf of ATLAS

ATLASpdf21 is a PDF fit to diverse PDF sensitive ATLAS data sets which have full information on correlated systematic uncertainties and for which NNLO QCD +NLO EW predictions are available

Key Features are:

- Experimental systematic correlations are applied not only within data sets but also between data sets with common systematic sources and information is made public
- Scale uncertainties are considered
- Flexible parametrisation achieves good description of data not in the fit such as Tevatron W,Z data and pD/pp Drell-Yan data from E866 and E906– but we have much more control over correlated systematic uncertainties
- An enhanced tolerance is used for realistic PDF uncertainty estimation
- There is fair agreement with modern PDF sets CT, MSHT, NNPDF and a better fit to ATLAS data

ATLASpdf21 is a fit to many different sorts of ATLAS data:

- W,Z boson production
- W,Z boson +jets
- T-tbar data
- Direct photon production
- Inclusive jet production

These are the processes which are known to have PDF sensitivity

It is a fit to NNLO in QCD and NLO in EW achieved either by direct NNLO grids or by NLO grids + k-factor corrections

The HERA data provided the backbone of the fit (as with ALL modern PDF fits) and provide good constraints from ~ $10^{-4} < x < 0.1$-0.4 (depending on which PDF) but they cannot provide:

- Flavour separation in the sea
- High-x gluon

These come from ATLAS- in addition to further constraints on all PDFs x> 0.001

Data set	$\sqrt{s}$ [TeV]	Luminosity [fb^{-1}]	Decay channel	Observables entering the fit
Inclusive $W, Z/\gamma^*$ [9]	7	4.6	e, μ combined	η_l (W), y_Z (Z)
Inclusive Z/γ^* [13]	8	20.2	e, μ combined	$\cos\theta$ in bins of $y_{\ell\ell}, M_{\ell\ell}$
Inclusive W [12]	8	20.2	μ	η_μ
$W^\pm$ + jets [23]	8	20.2	e	p_T^W
Z + jets [24]	8	20.2	e	p_T^{jets} in bins of $\lvert y_{\text{jets}}\rvert$
$t\bar{t}$ [25, 26]	8	20.2	lepton + jets, dilepton	$m_{t\bar{t}}$, p_T^t, $y_{t\bar{t}}$
$t\bar{t}$ [15]	13	36	lepton + jets	$m_{t\bar{t}}$, p_T^t, y_t, $y_{t\bar{t}}$
Inclusive isolated γ [14]	8, 13	20.2, 3.2	-	E_T^γ in bins of η^γ
Inclusive jets [16–18]	7, 8, 13	4.5, 20.2, 3.2	-	p_T in bins of $\lvert y_{\text{jets}}\rvert$

Some features of the analysis are:

- All data sets included have full information on correlated systematic uncertainties
- This allows us to consider experimental correlations between data sets as well as within data sets. This cannot be done by the global PDF fits – but it matters if we are seeking an ultimate O(1%) accuracy on PDFs. ATLAS now makes this information public
- We consider the impact of scale uncertainties for each data set and where they are comparable to the experimental precision (in most cases they are smaller) we include these theoretical uncertainties in the fit. This applies for inclusive W,Z production

- We consider a fit restricted to $Q^2 < (500\text{GeV})^2$, to check we are not 'fitting away' new physics
- We include 13 TeV data- not yet done by CT or MSHT

- We extend our parametrisation from 16 to 21 parameters since the ATLAS data allow us to release some constraint, in particular we allow ubar ≠ dbar as $x \to 0$ and sbar, dbar, ubar can all have differing shapes as $x \to 0$. Note such constraints have only recently been dropped from global fits like MSHT.

- We consider enhanced tolerance for the final estimate of experimental uncertainties. This becomes necessary with many diverse data sets. We consider how far the PDF parameters can change before any data set is pushed outside its 68%CL, this results in $\Delta\chi^2 = T^2$, T=3.

Correlation of systematic sources between data sets

Systematics	8 TeV W + jets	8 TeV Z + jets	8 TeV $t\bar{t}$ lepton + jets	13 TeV $t\bar{t}$ lepton + jets	8 TeV inclusive jets
Jet flavour response	JetScaleFlav2	Flavor Response	flavres-jes	JET29NP JET Flavour Response	syst JES Flavour Response*
Jet flavour composition	JetScaleFlav1Known	Flavor Comp	flavcomp-jes	JET29NP JET Flavour Composition	syst JES Flavour Comp
Jet punchthrough	JetScalepunchT	Punch Through	punch-jes	-	syst JES PunchThrough MC15
Jet scale	JetScalePileup2	PU OffsetMu	pileoffmu-jes	-	sys JES Pileup MuOffset
	-	PU Rho	pileoffrho-jes	JET29NP JET Pileup RhoTopology	sys JES Pileup Rho topology*
	JetScalePileup1	PU OffsetNPV	pileoffnpv-jes	JET29NP JET Pileup OffsetNPV	syst JES Pileup NPVOffset
	-	PU PtTerm	pileoffpt-jes	JET29NP JET Pileup PtTerm	syst JES Pileup Pt term
Jet JVF selection	JetJVFcut	JVF	jetvxfrac	-	syst JES Zjets JVF
B-tagged jet scale	-	btag-jes	JET29NP JET BJES Response	-	-
Jet resolution	-	jeten-res	JET JER SINGLE NP	-	-
Muon scale	-	-	mup-scale	MUON SCALE	-
Muon resolution	-	-	muonms-res	MUON MS	-
Muon identification	-	-	muid-res	MUON ID	-
Diboson cross-section	-	-	dibos-xsec	Diboson xsec	-
Z + jets cross section	-	-	zjet-xsec	Zjets xsec	-
Single-t cross section	-	-	singletop-xsec	st xsec	-

Entries in the same row are considered 100% correlated for the central fit

Cross checks are made of alternative degrees of correlation for inclusive jets since jet radius R=0.6 is used for these, rather than R=0.4 which is used for the other for the other data sets: V+jets and t-tbar in lepton+jets channel.

Note these are mostly the JES correlations, which are the largest, lepton correlations are much smaller

The PDF parametrisation

valence quark distributions (xu_v, xd_v) and the light anti-quark distributions ($x\bar{u}$, xd, $x\bar{s}$).

$$xq_i(x) = A_i x^{B_i}(1-x)^{C_i} P_i(x), \qquad P_i(x) = (1 + D_i x + E_i x^2 + F_i x^3)$$

And for the gluon an extra negative term is added, which gives more flexibility at low-x

$$xg(x) = A_g x^{B_g}(1-x)^{C_g} P_g(x) - A'_g x^{B'_g}(1-x)^{C'_g},$$

(consequences of not adding this extra term have been explored and mostly affect quality of fits to HERA data)

The *A* parameters for the valence quarks and the gluon are set by the sum-rules.
The *A,B,C* parameters of the light quark sea are all free parameters
as are the *B,C* parameters of the valence and the *B,C,A',B'* parameters of the gluon.

D,E,F parameters are added until there is no further significant improvement in χ2

$$P_{u_v}(x) = 1 + D_{u_v} x + E_{u_v} x^2, \quad P_{d_v}(x) = 1 + D_{d_v} x \text{ and } P_g(x) = 1 + D_g x,$$

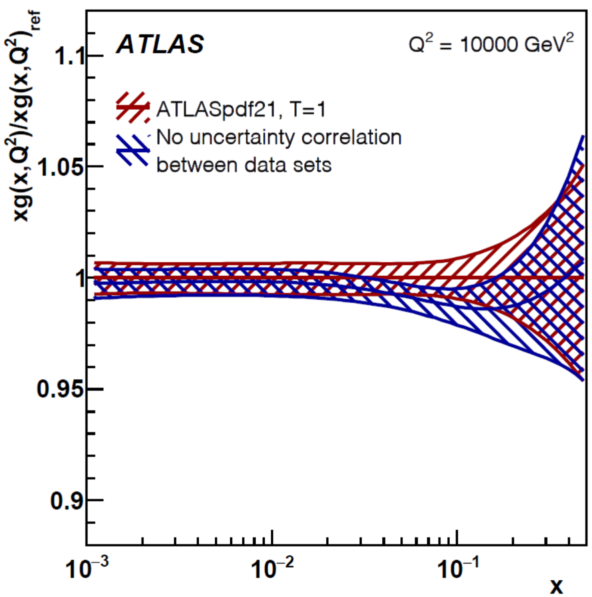
This results in a 21 parameter fit.
In addition further parameters, F_{uv} *and* D_{dbar}, are considered as part of a parametrisation uncertainty. These parameters are the only further *D,E,F* parameters which give a visible (if small) shape change even though χ2 is not significantly improved.

In addition to this a fit using 21 parameters with Chebyshev polynomials was considered, the χ2 of this fit was somewhat worse than our central fit and the PDF shapes are within the uncertainty bands.

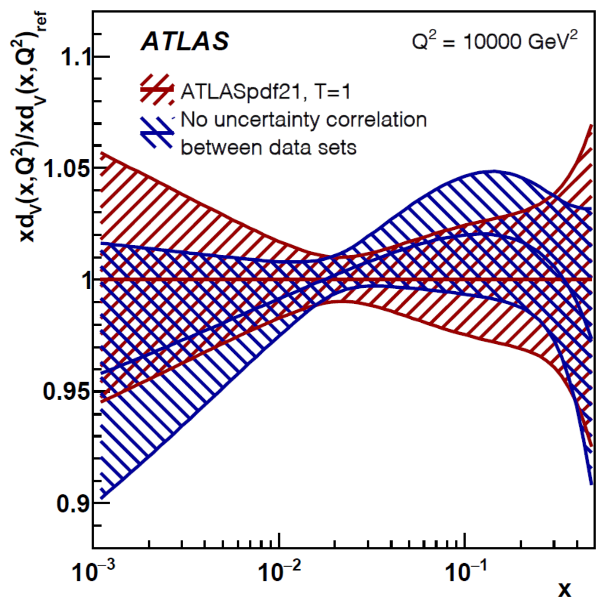
Effect of correlations between data sets

Lets look at a scale relevant for LHC physics and focus on the middling x range where W,Z and Higgs are produced

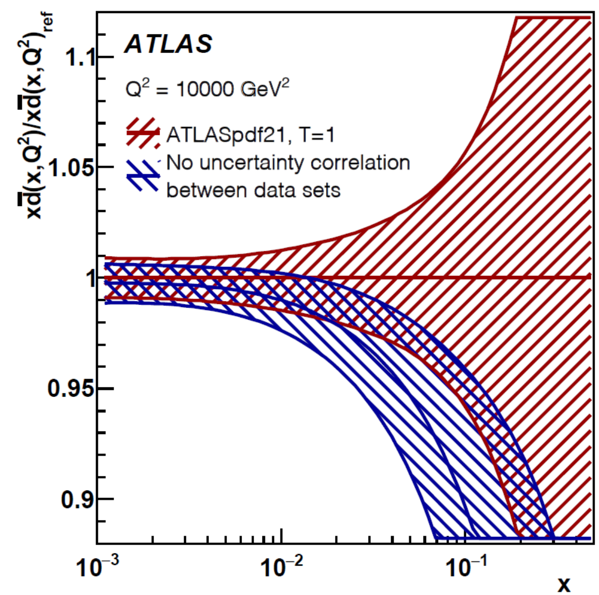
gluon ratio



$d_{valence}$ ratio



$\bar{d}$ ratio



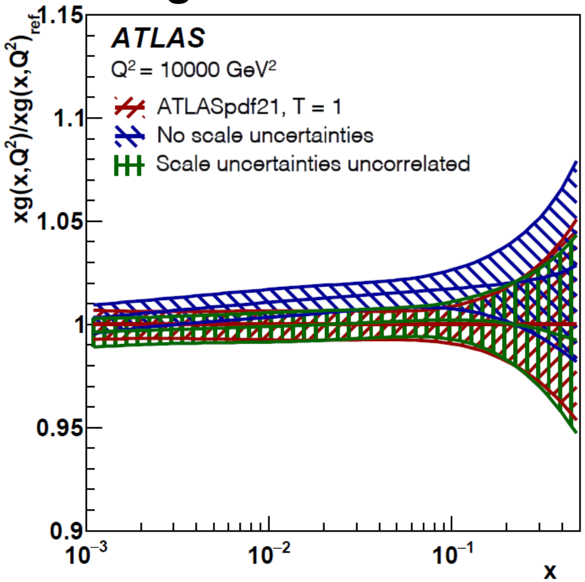
The χ2 of the fit is 30 units better when correlations are included
The difference in PDFs is small for the gluon
But can be large in the d-quark sector
Remember the goal for PDF precision is ~1% for M_W and $\sin^2\theta_W$ measurements if BSM effects are to be seen by the deviations of these parameters from their SM values

Correlations can be important

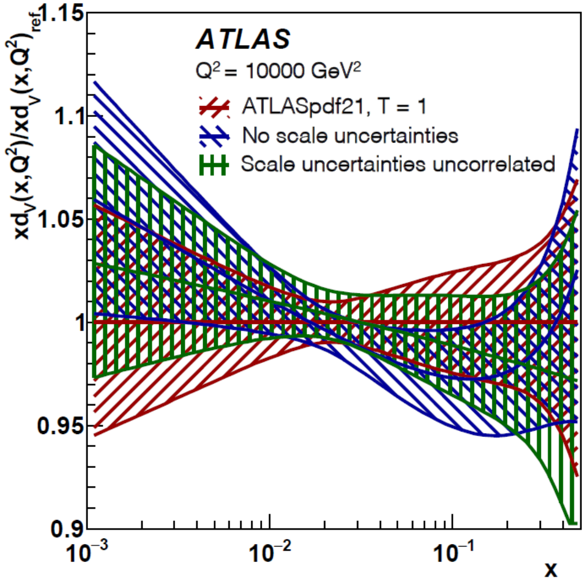
Impact of scale uncertainties

For the inclusive W,Z production at 7 and 8 TeV the experimental uncertainties are comparable to the scale uncertainties and thus the scale uncertainties are included as theoretical uncertainties in the fit. By default they are correlated between the W and Z data and between the 7 and 8 TeV data in the ATLASpdf21 fit.

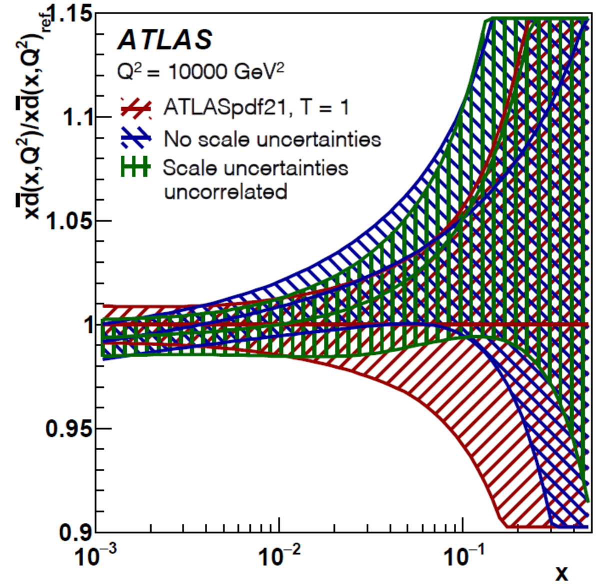
gluon ratio



$d_{valence}$ ratio



$\bar{d}$ ratio



Here we show the ratios of the gluon, d-valence and dbar PDFs with (red) and without (blue) these scale uncertainties included

In green we show the effect of including scale uncertainties but not correlating them between 7 and 8 TeV data

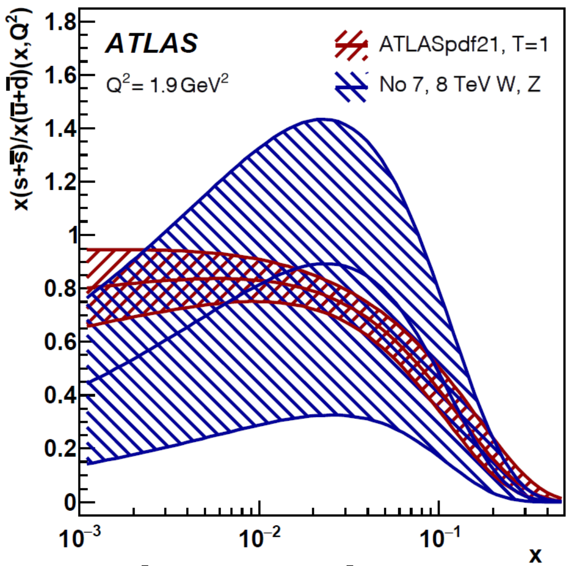
Clearly scale uncertainties can be important if 1% precision is sought

Investigate the impact of each class of data

Impact of inclusive W,Z production data

NOTE: these plots show only experimental uncertainties with $\Delta\chi^2 = 1$

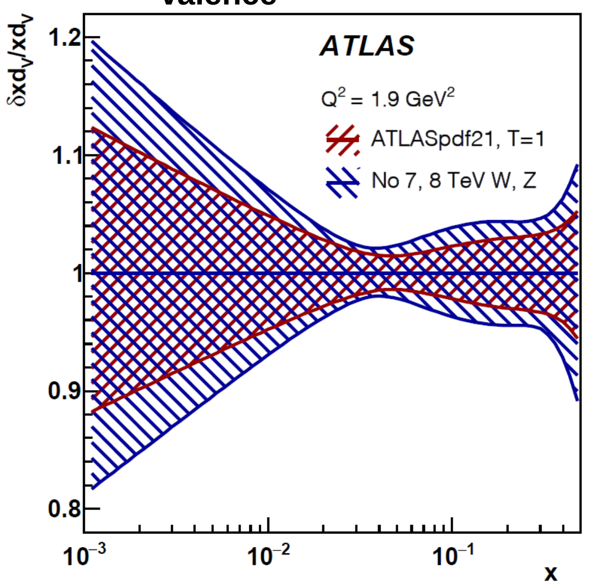
strange/light quarks



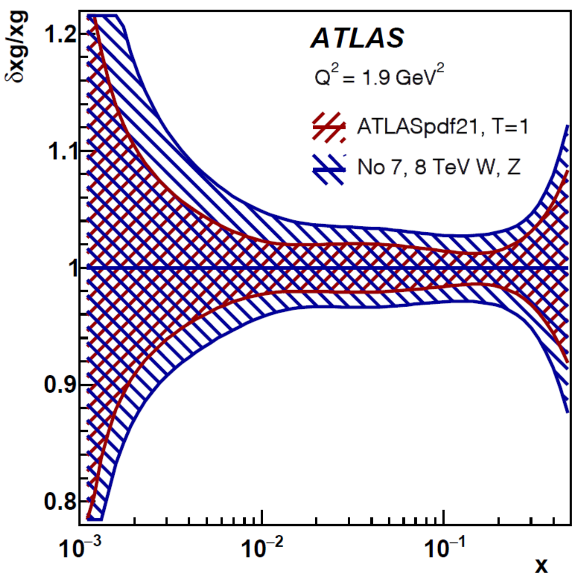
Inclusive W,Z production data at 7 and 8 TeV are removed from the fit
Without these data the ratio of strange to light quarks is very poorly determined

W,Z data also reduce the uncertainties of the valence quarks and the gluon considerably

$d_{valence}$ ratio



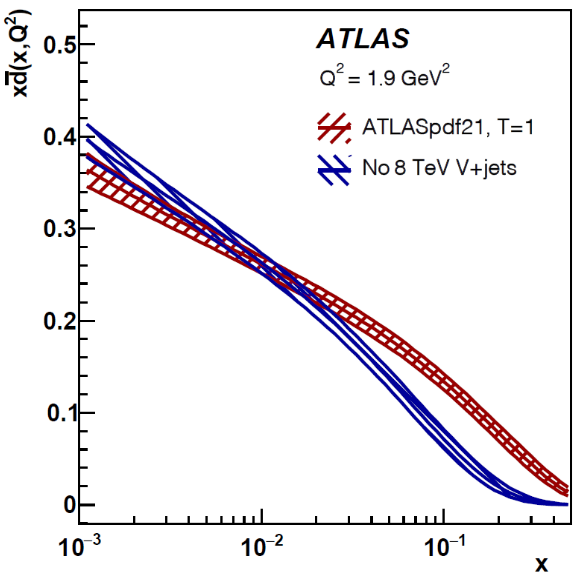
gluon ratio



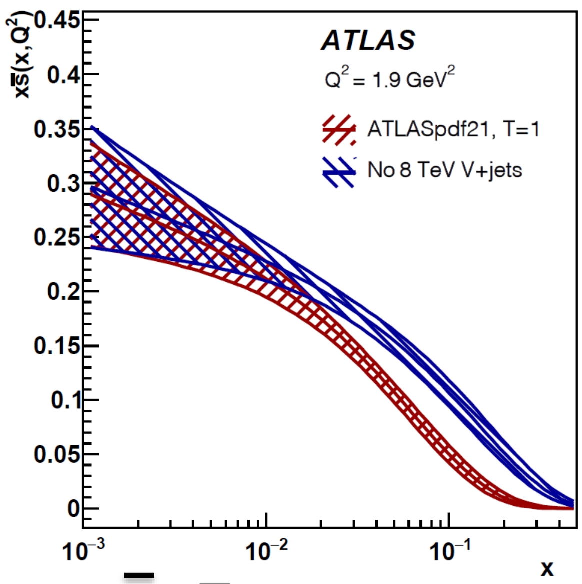
Impact of V + jets data

Is to increase dbar and decrease sbar at high-x

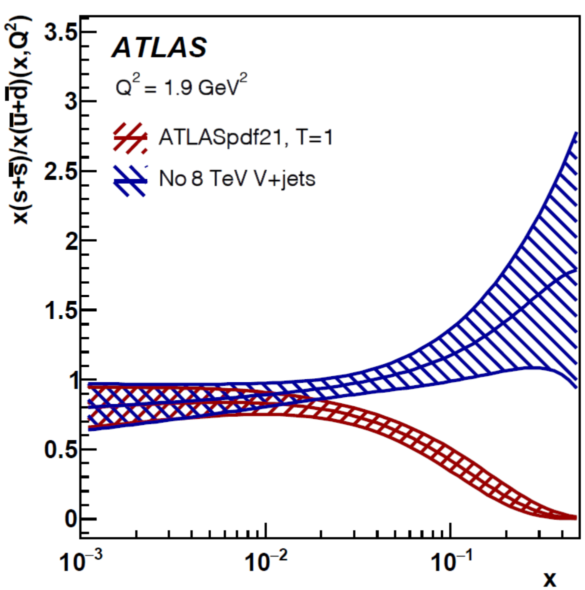
$\bar{d}$



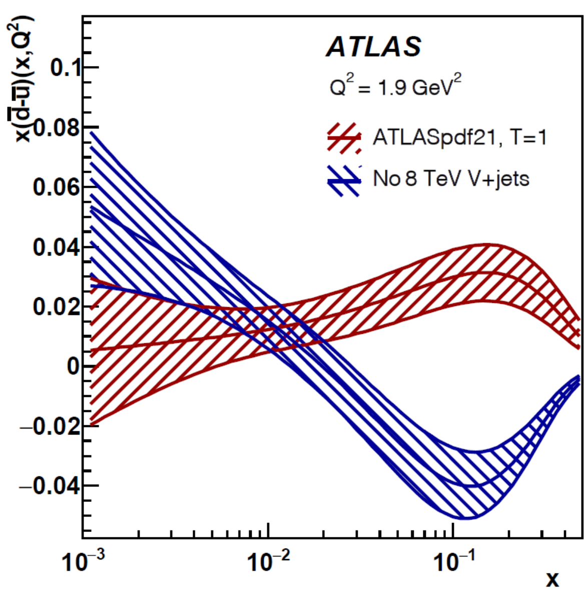
$\bar{s}$



strange/light quarks



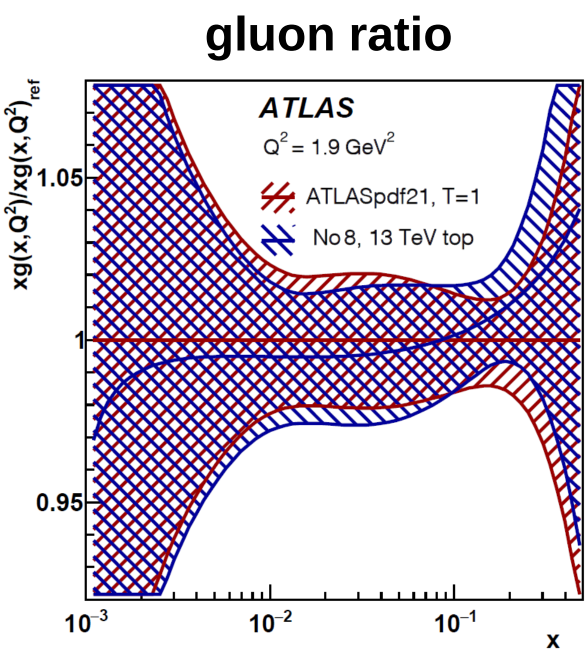
$\bar{d} - \bar{u}$

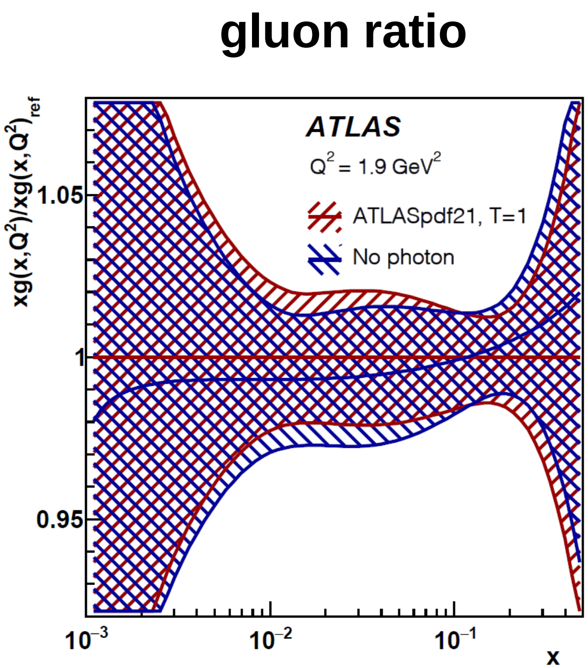


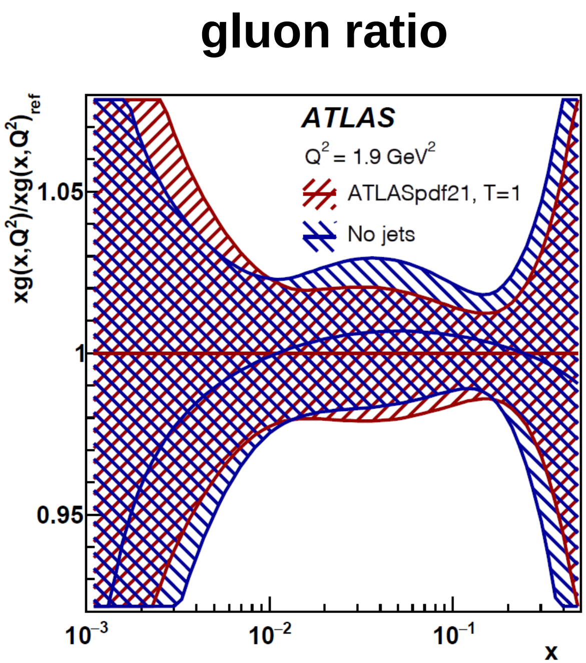
This change looks so dramatic because the V+jets data resolves a double minimum in the rest of the data which are almost equally happy with the blue or red PDFs.

Remember that only experimental uncertainties are shown here. The total uncertainties including model and parametrisation choices are much larger for the blue PDFs, because some of them go to the alternative minimum **See back-up.**

Impact of t-tbar production, direct photon production, and inclusive jet production …………….. Is mostly on the high-x gluon



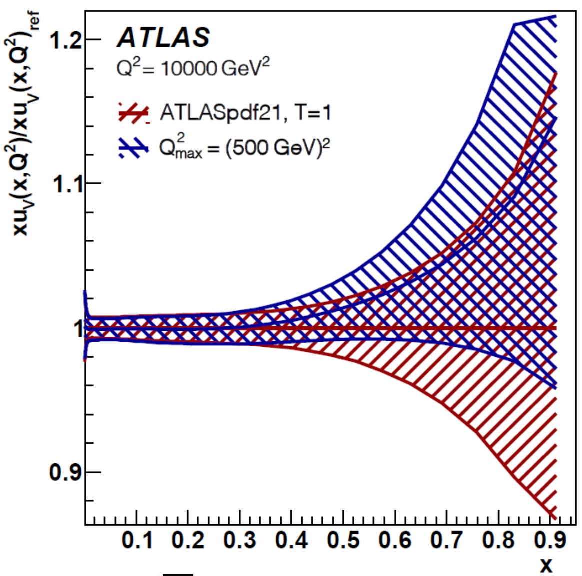




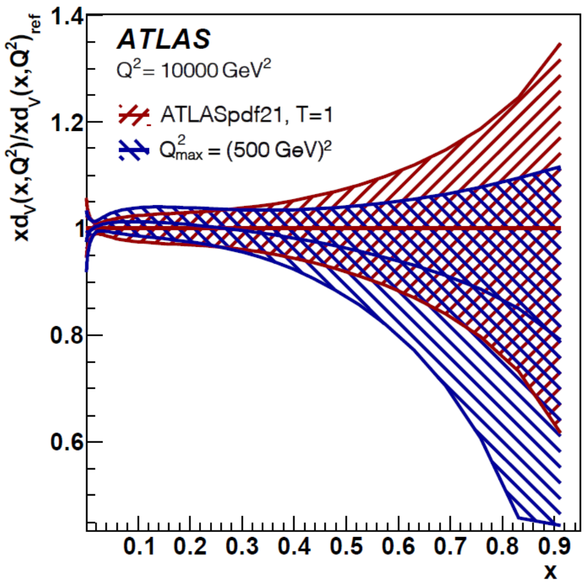
The ratio of the gluon PDF with/without these data is shown to illustrate the slight pulls on the shape and the more significant decrease in uncertainty—mostly from inclusive jets

A fit was made cutting data for which the scale > 500 GeV, to check if the PDFs differ if we cut out possible hidden new physics in the high scale data

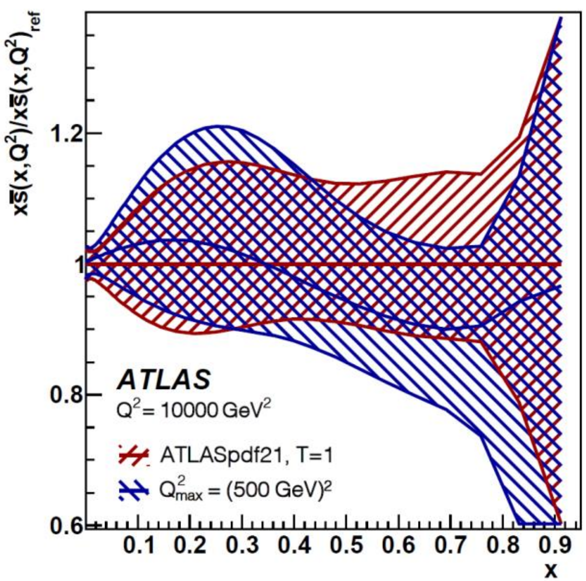
$u_{valence}$ ratio



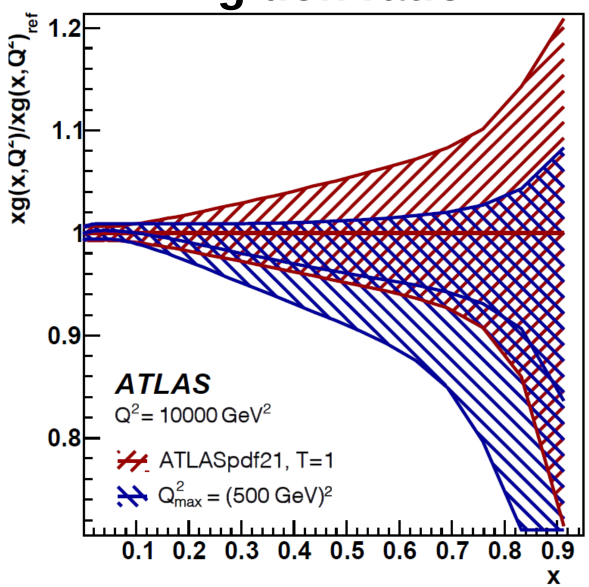
$d_{valence}$ ratio



$\bar{s}$ ratio



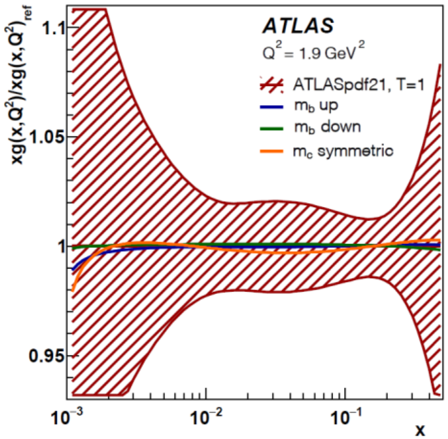
gluon ratio



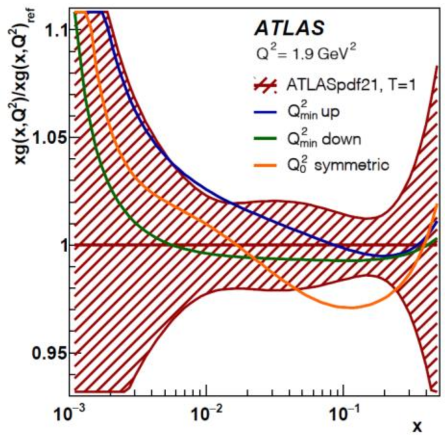
This cut mostly removes inclusive jet production data.
The effect is only seen at high x –note linear x scale- PDFs are not significantly changed
These changes would barely show up on our usual log scale in x

Further uncertainties from model assumptions and parametrisation variation

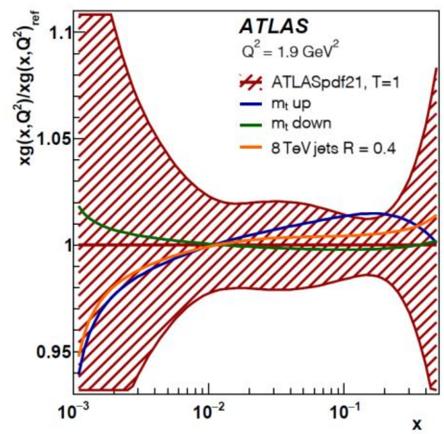
gluon ratio



gluon ratio



gluon ratio



Model uncertainties illustrated in ratio to the central gluon and its experimental uncertainties

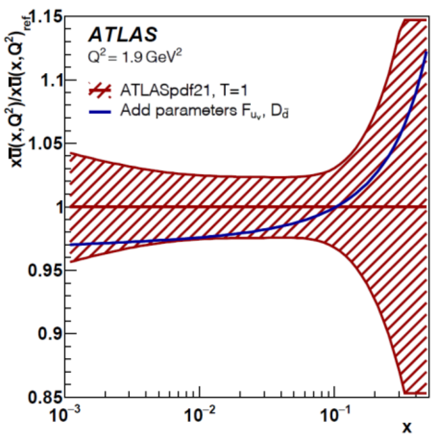
Model uncertainties from the choice of:

- Minimum Q^2 entering the fit
- Heavy quark masses (including top)
- Starting scale for evolution
- Jet radius choice R=0.4 instead of R=0.6 for inclusive jets

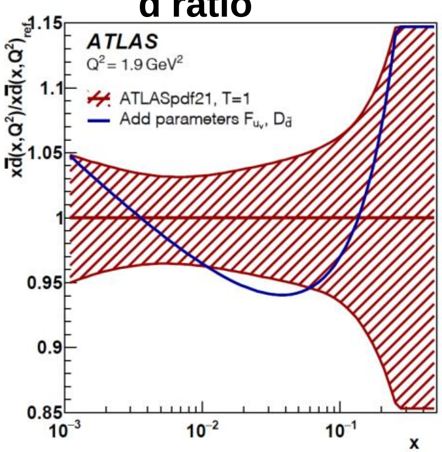
Parametrisation variation including extra F_{uv} and D_{dbar} parameters

Central χ^2/NDF	2010/1620
Model variations	
$Q^2_{\mathrm{min}} = 12.5$ GeV^2	1947/1571
$Q^2_{\mathrm{min}} = 7.5$ GeV^2	2076/1660
$m_c = 1.45$ GeV (sym)	2025/1620
$Q^2_0 = 1.6$ GeV^2 (sym)	2018/1620
$m_b = 4.3$ GeV	2016/1620
$m_b = 4.1$ GeV	2014/1620
$m_t = 175.0$ GeV	2063/1620
$m_t = 172.5$ GeV	2018/1620
$R = 0.4$	2080/1620
Parameter variations	
$F_{u_v}, D_{\bar{d}}$	2007/1620

$\bar{u}$ ratio



$\bar{d}$ ratio



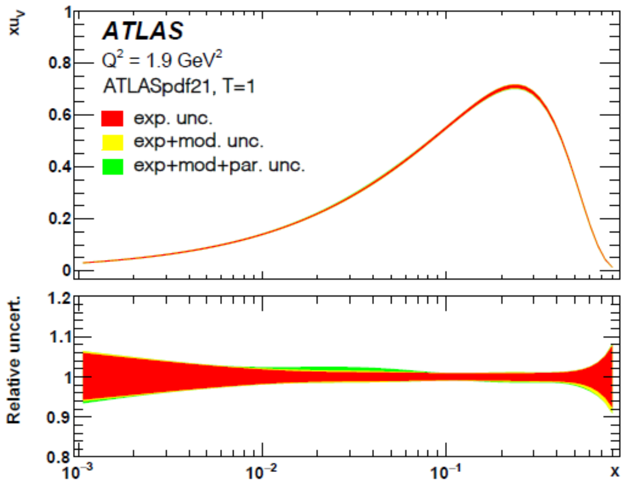
Parametrisation uncertainties illustrated in ratio to the central d-valence and dbar and their experimental uncertainties

Combining uncertainties

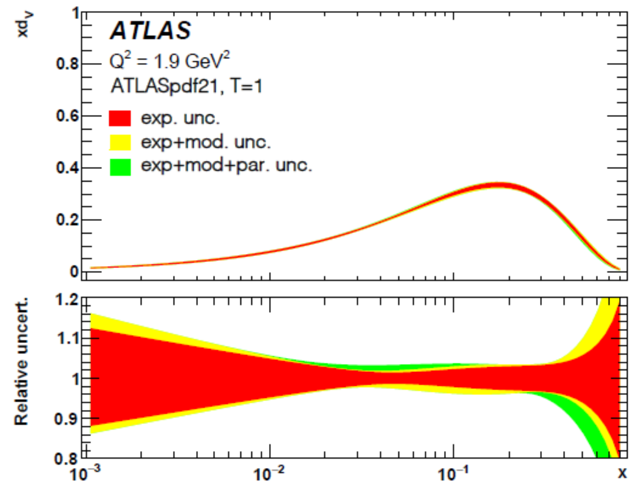
Model uncertainties are added in quadrature, parmetrisation uncertainties are taken as an envelope of the deviation from central fit

These are then added in quadrature on top of the experimental uncertainties

$u_{valence}$

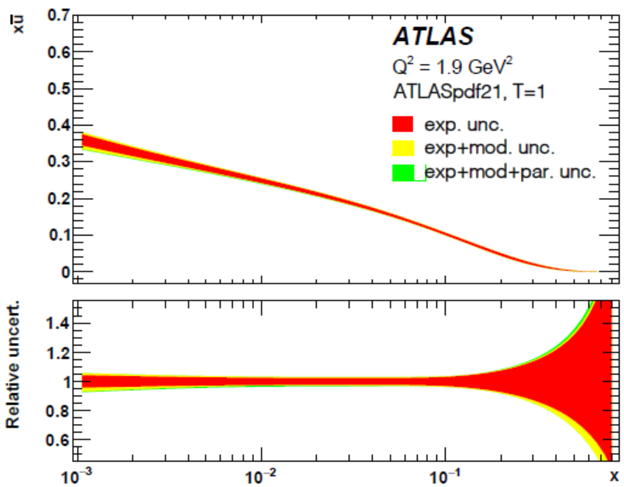


$d_{valence}$

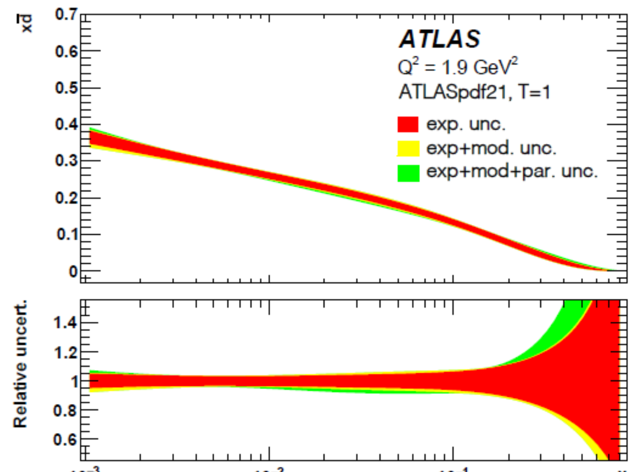


The u-quarks are better determined than the d-quarks for both valence and sea

$\bar{u}$

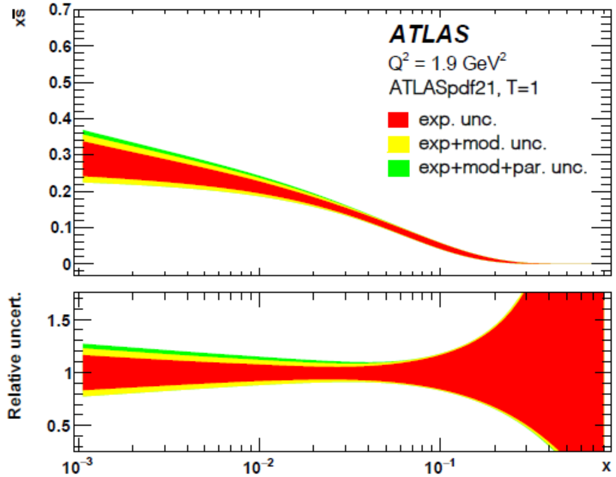


$\bar{d}$

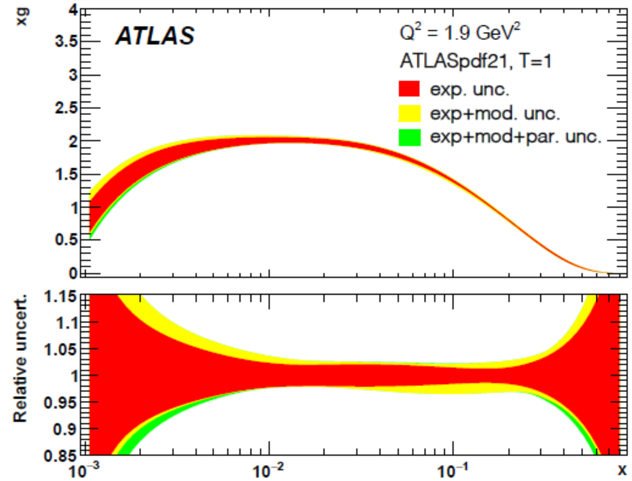


The dbar ~ ubar at low-x even though this is NOT a constraint imposed by the fit

$\bar{s}$

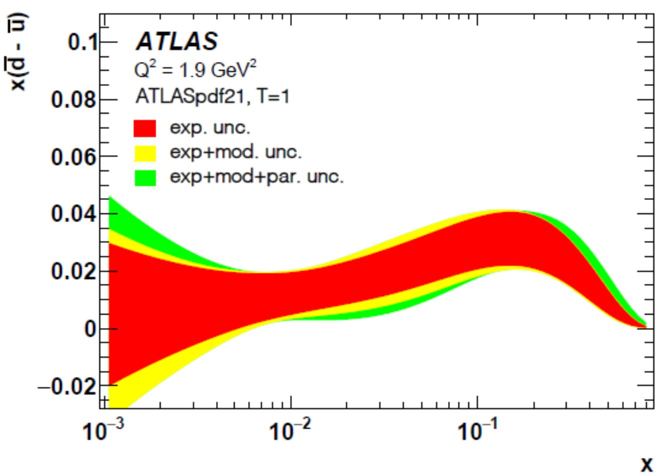


gluon

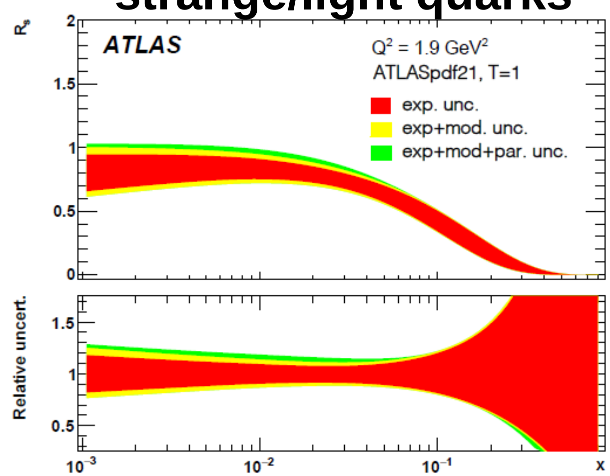


The gluon has the largest contribution from model uncertainty

$\bar{d}$ - $\bar{u}$



strange/light quarks



The strangeness ratio Rs=(s+sbar)/(ubar+dbar) is consistent with unity at low-x and is suppressed at high-x

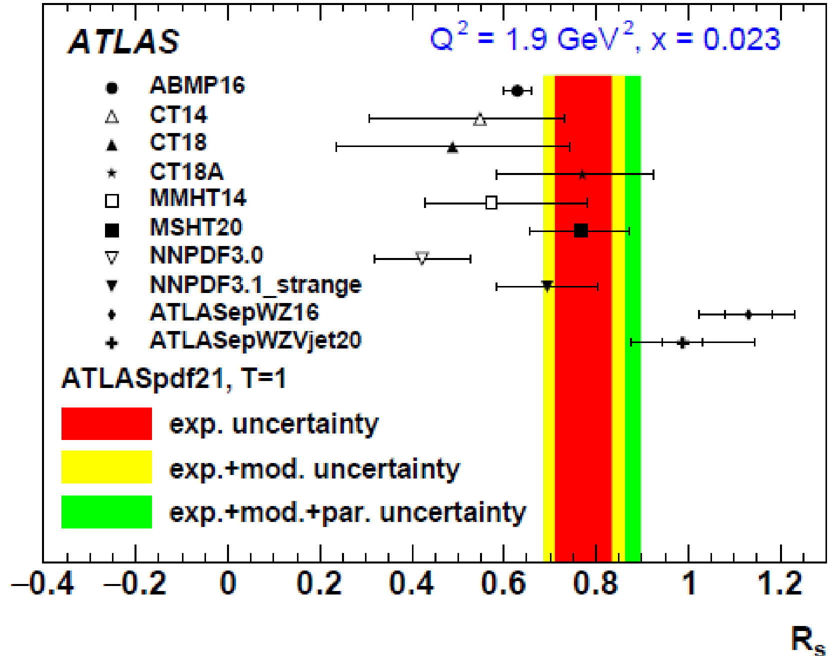
The dbar-ubar is consistent with zero at low-x and is positive at high-x consistent both with E866 data and the new E906 Seaquest data

Strangeness

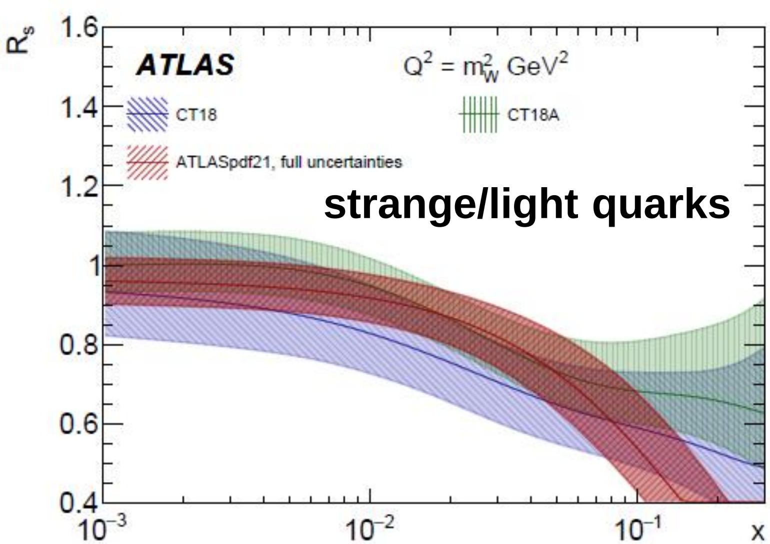
The information on strangeness has often been presented at a single x,Q^2 point and compared to the result of global PDFs

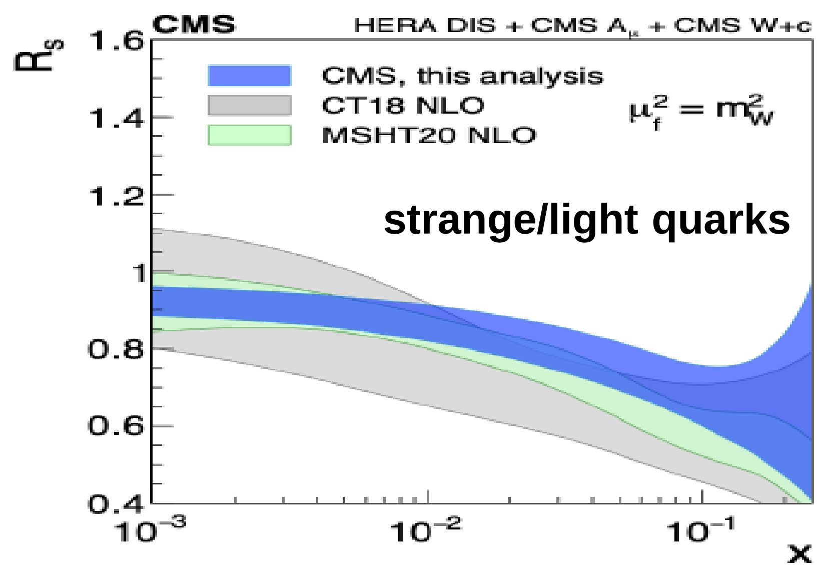
Note that older PDFs CT14, MMHT14,NNPDF3.0 all had Rs~0.5 at low scale (Q^2=1.9GeV^2) **BUT** this has moved up to ~0.8 for CT18A, MSHT20, and NNPDF3.1_strange after ATLAS W,Z 7 TeV data was included (not for CT18 which does not include these data)

ATLAS older fits had Rs~1.0 and have moved down to Rs~0.8 due to input of new data, V+jets and W,Z 8 TeV and greater flexibility of low-x parametrisation



See the more interesting shape of the strangeness ratio at higher scale m_W^2 compared to CT18 and CMS





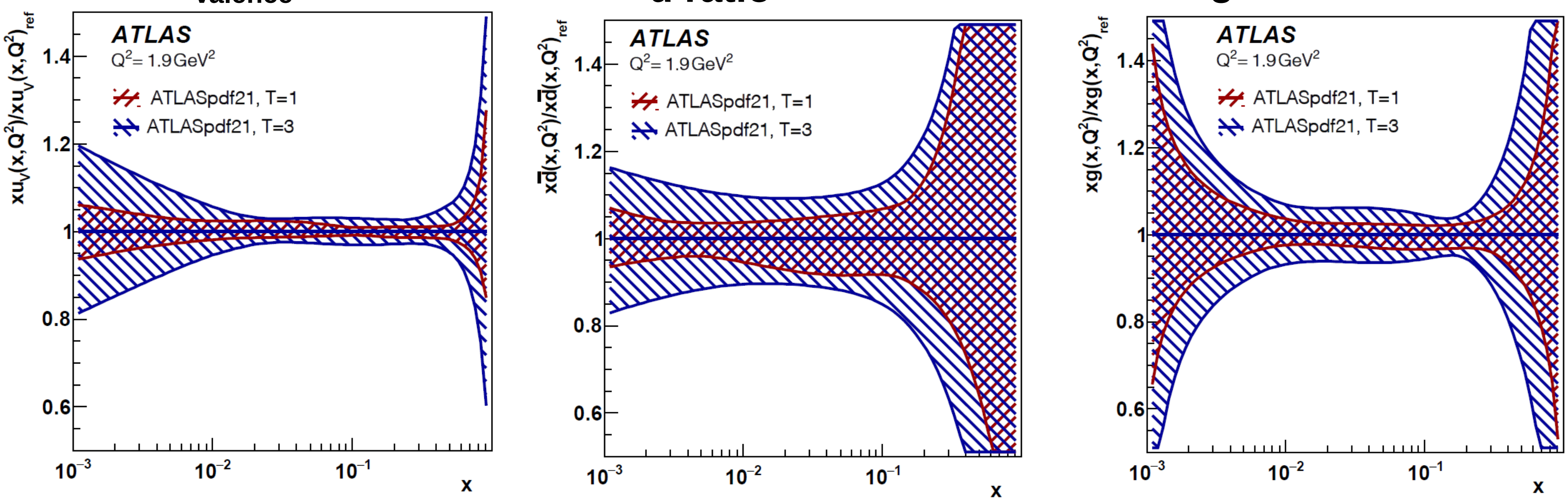
χ2 tolerance,

So far we have applied the conventional $\Delta\chi 2 = T^2 = 1$ for 68%C.L.

When diverse data sets are included global fitters consider $T > 1$. Historically values of T~7- 10 have been considered by MSHT and CT.

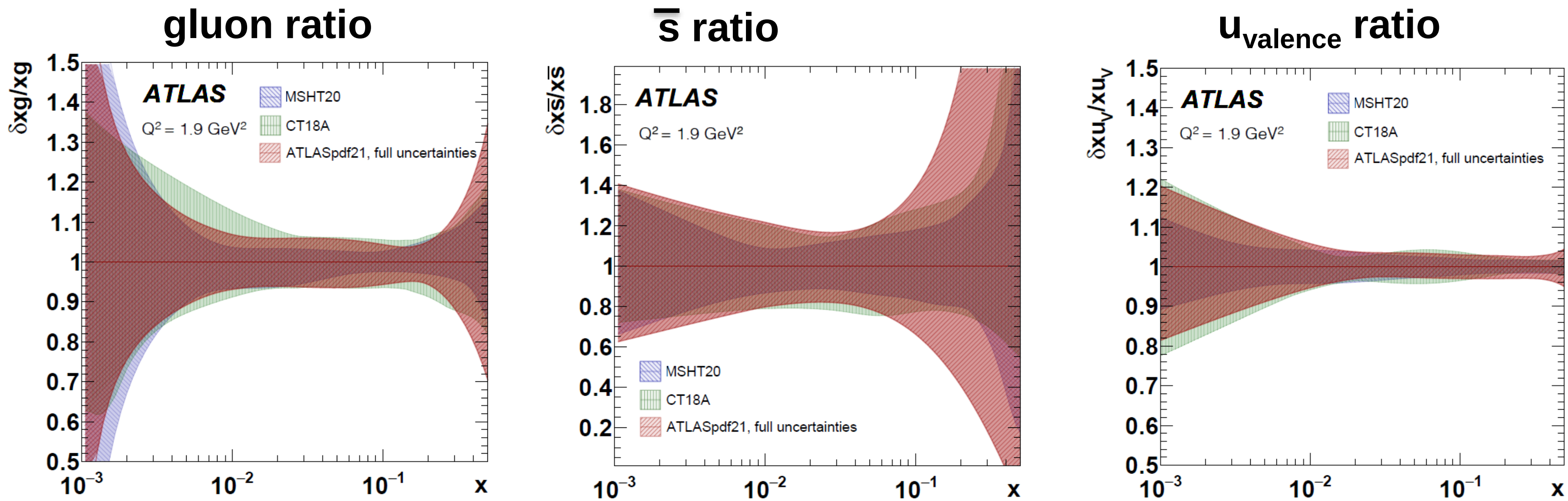
We have followed the MSHT dynamic tolerance procedure (first used for MSTW2008) and obtained an appropriate tolerance for T=3 for the ATLAS data sets included in the fit such that all data sets are fitted within their 68%CL for variations of all eigenvectors.

$u_{valence}$ ratio **$\bar{d}$ ratio** **gluon ratio**



Change from T=1 to T=3 for various PDFs for Full uncertainties including model and parametrisation

Now compare ATLASpdf21 uncertainties to those of modern global PDFs



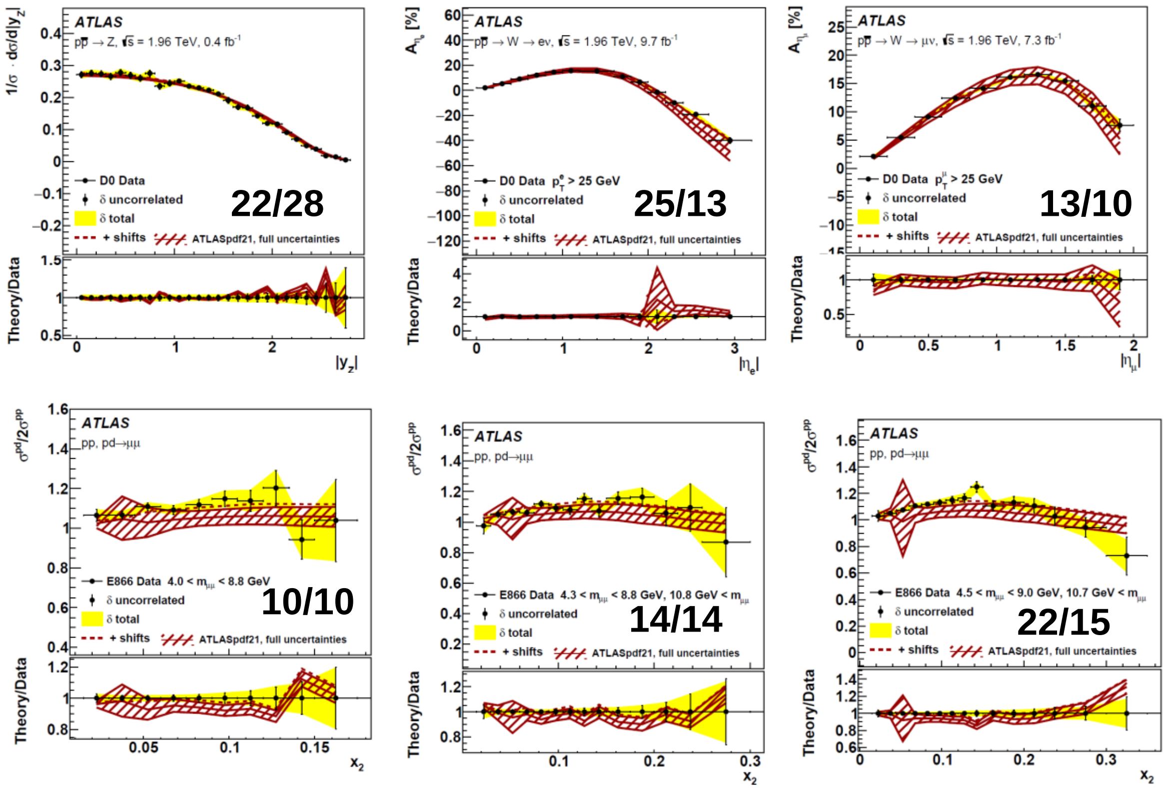
Uncertainties are competitive for x < 0.1 and somewhat larger at high-x depending on the PDF

Note that without enhanced tolerance we would be claiming to do better than global fits for x> 0.1 where we have much less constraining data.

Global fits use older DIS fixed target data and Drell-Yan data as well as Tevatron data, which constrain high-x. However, they are subject to unknown systematic uncertainties and/or unknown correlations of systematic uncertainties on these older data.

ATLASpdf21 is able to describe the most significant of these older data sets well--we no longer need them to set the central values of the PDFs at high-x---
the price we pay for not using them is the larger high-x uncertainties, this should improve with future ATLAS data.

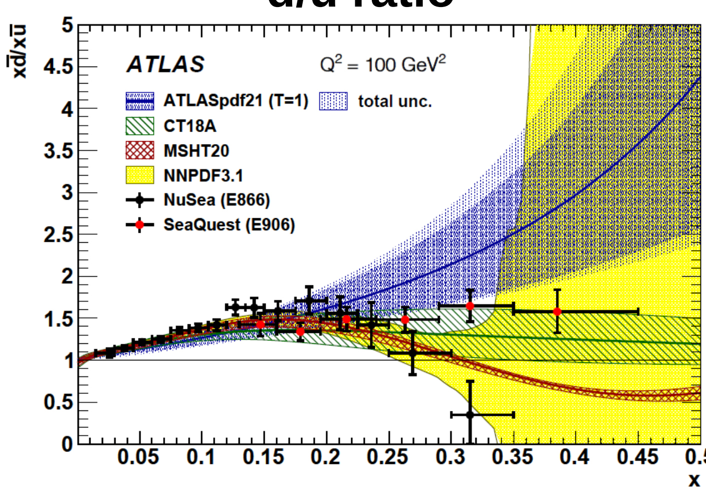
Description on Tevatron W,Z data and E866,E906 Drell-Yan data



The description of Tevatron W,Z data are similar to those of the global fits

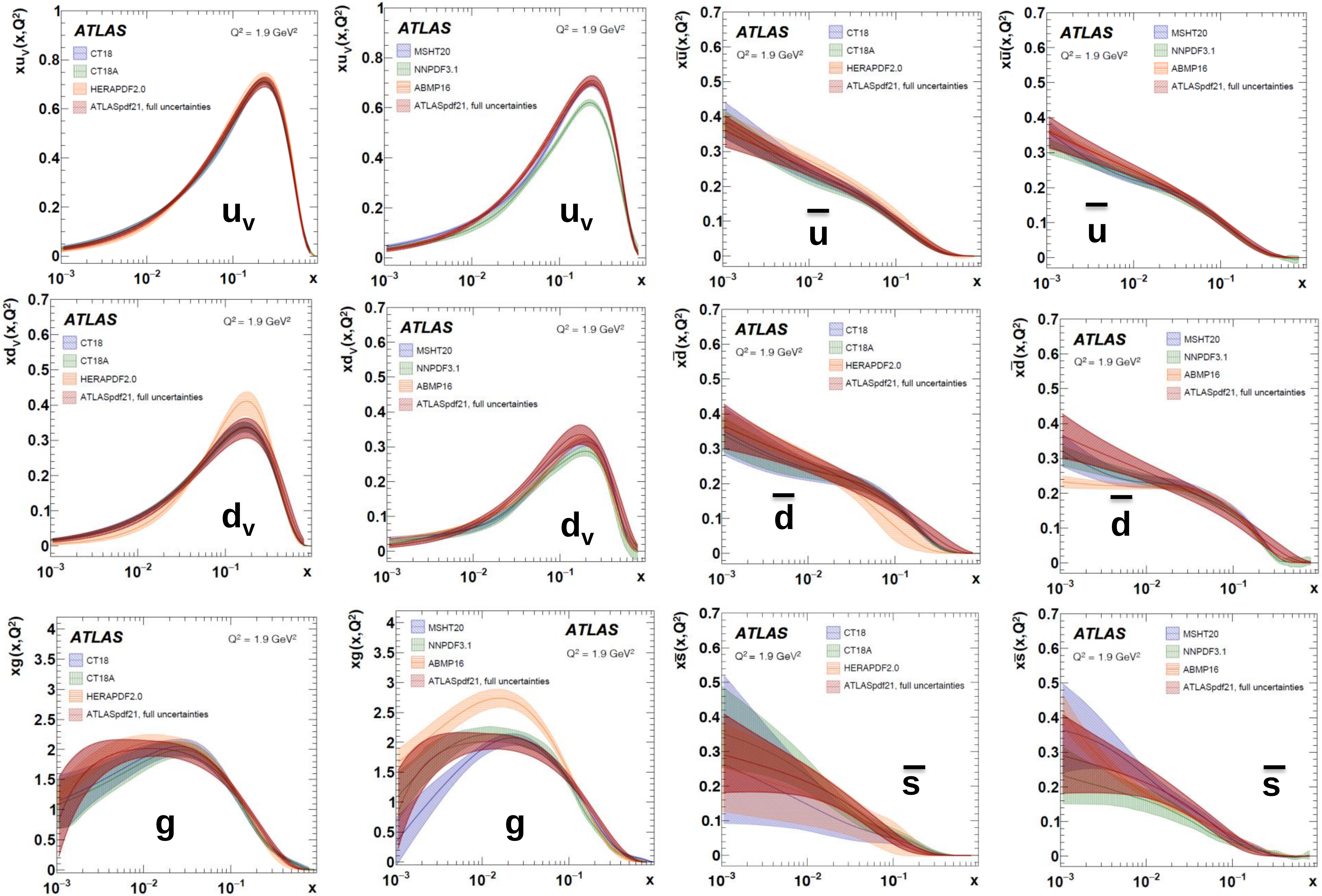
The description of the E866 pD/pp Drell-Yan data are also acceptable BUT..

$\bar{d}/\bar{u}$ ratio



One can see that the highest mass bin is not so well fitted and this is because the ATLASpdf21 is in better agreement with the new E906 SeaQuest data, shown here converted into the dbar/ubar ratio

Now compare ATLASpdf21 PDFs to modern global PDFs



In summary, they agree with the other PDFs as well as the other PDFs agree with each other! (A focus on high-x PDFs in back-up)

Summary/Conclusion

- ATLASpdf21 fits to all PDF sensitive data sets which have information on correlated systematic uncertainties and NNLO QCD +NLO EW predictions

- Correlations between data sets are included and information made public

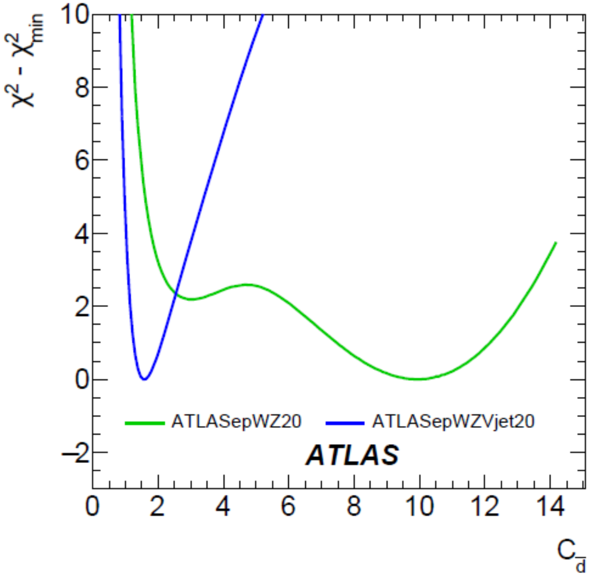
- Scale uncertainties are considered and included when comparable to experimental uncertainties

- Flexible parametrisation achieves good description of data not in the fit such as Tevatron W,Z data and pD/pp Drell-Yan data from E866 and E906– but we have much more control over correlated systematic uncertainties

- An enhanced tolerance is used for realistic PDF uncertainty estimation

- There is fair agreement with modern PDF sets CT, MSHT, NNPDF and a better fit to ATLAS data

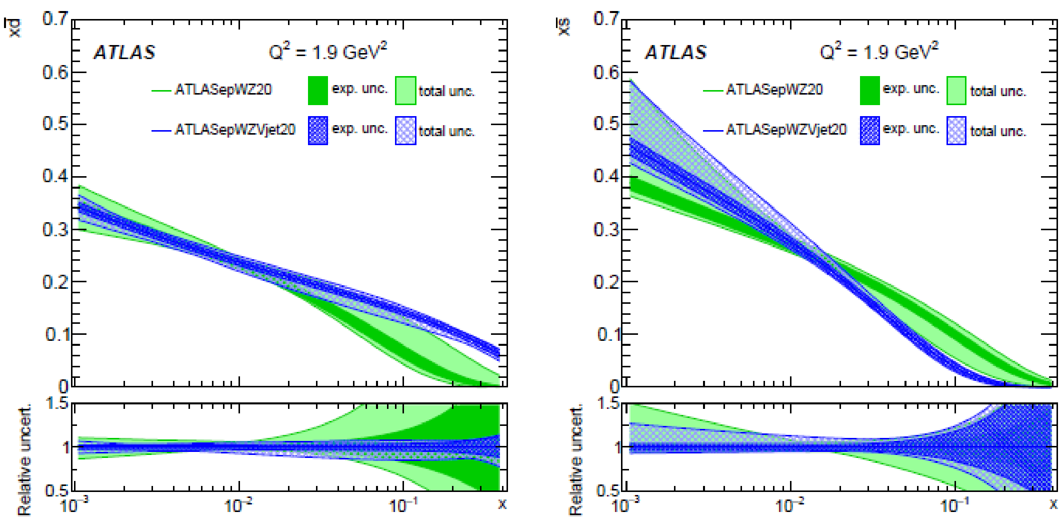
backup



Data apart from V+jets data (HERA and ATLAS W,Z 7 TeV) are happy with wither C_{dbar} low or high, which means high-x dbar hard or soft resp

V+jets data is only happy with C_{dbar} low. So high-x dbar hard.

Plots from ATLAS pdf paper on input of V+jets arXiv:2101.05095



When full uncertainties are evaluated on the green fit, (which does not have V+jets data and thus has C_{dbar} high, dbar soft) some of the model/parametrisation variations fall into the alternative minimum with C_{dbar} much lower and dbar hard, thus uncertainties are large and there is no big tension between the V+jets data and the other data.

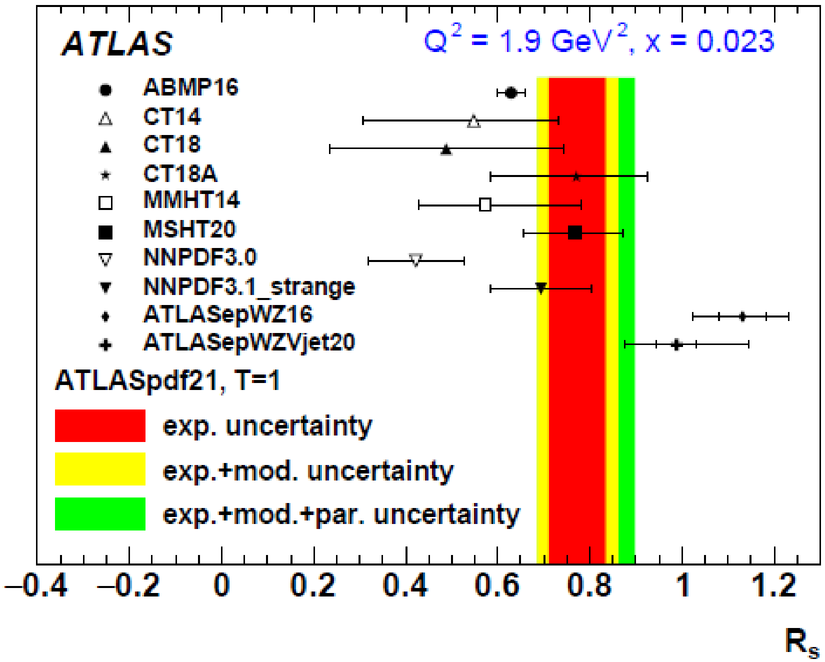
dbar hard goes with sbar soft: (dbar+sbar) act together in most processes

Strangeness

The information on strangeness has often been presented at a single x,Q^2 point and compared to the result of global PDFs

Note that older PDFs CT14, MMHT14,NNPDF3.0 all had Rs~0.5 at low scale (Q^2=1.9GeV^2) **BUT** this has moved up to ~0.8 for CT18A, MSHT20, and NNPDF3.1_strange after ATLAS W,Z 7 TeV data was included (not for CT18 which does not include these data)

ATLAS older fits had Rs~1.0 and have moved down to Rs~0.8 due to input of new data, V+jets and W,Z 8 TeV and greater flexibility of low-x parametrisation



The history of these changes is:

ATLASepWZ16 to ATLASepWZVjets20
Input of V+jets data suppresses Rs at high-x and this has a knock-on effect at x=0.023 so that Rs~ 1.15 →1.0

ATLASepWZVJets20 to ATLASpdf21

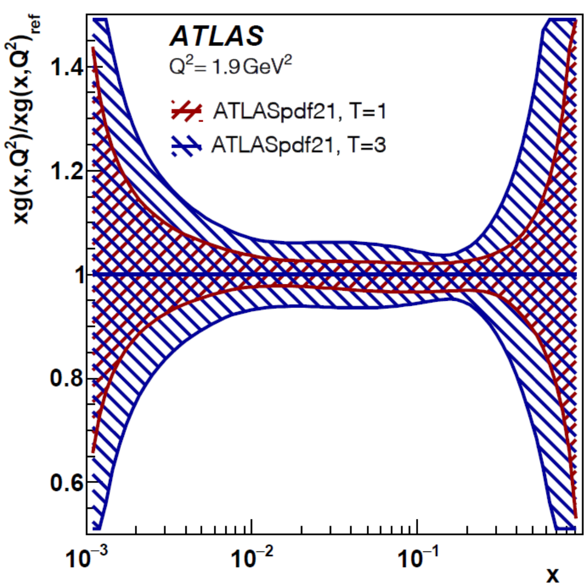
- More flexible low-x parametrisation corresponds to lower edge of Vjets20 error-band Rs~ 1.0 →0.85
- Addition of W,Z 8 TeV data Rs~ 0.85 →0.8

$\chi 2$ tolerance, so far we have applied the conventional $\Delta\chi 2 = T^2 = 1$ for 68%C.L. When diverse data sets are included global fitters consider $T > 1$. Historically values of T~7- 10 have been considered by MSHT and CT.

We have followed the MSHT dynamic tolerance procedure (first used for MSTW2008).

As briefly as possible:

Recognise that the global minimum is a compromise and is not the minimum for each of the data sets. Changing a parameter in one direction can give a better fit to one data set and a worse fit to another. How much change is acceptable is set by considering the eigenvector combinations of the parameters of the fit and treating each eigenvector as a different hypothesis. Then one varies the parameters down each eigenvector to the point where the hypothesis is unacceptable for a particular data set $\chi 2_n > \sim N + \sqrt{(2N)}$. This is done for each data set and each direction down each eigenvector.



In practice this criterion is a little more sophisticated AND it is weighted to account for the fact that the $\chi 2_n$ for each data set at the global minimum $\chi 2_{n,0}$ is usually not N but is larger than this. The resulting tolerable changes in the eigenvectors correspond to T values 2.4-4.2. A value of T=3 is chosen for the overall tolerance.

This increases the experimental component of the uncertainties and thus the total uncertainties.

χ^2 formula

These two form the partial χ2 for each data set

$$\chi^2 = \sum_{ik}\left(D_i - T_i(1-\sum_j \gamma_{ij} b_j)\right) C^{-1}_{\mathrm{stat},ik}(D_i, D_k)\left(D_k - T_k(1-\sum_j \gamma_{kj} b_j)\right)$$

partial

$$+ \sum_i \log \frac{\delta^2_{i,\mathrm{uncor}} T_i^2 + \delta^2_{i,\mathrm{stat}} D_i T_i}{\delta^2_{i,\mathrm{uncor}} D_i^2 + \delta^2_{i,\mathrm{stat}} D_i^2}$$

log penalty term

This is a correlated term between data sets

$$+ \sum_j b_j^2$$

correlated term

- D_i represents the measured data and T_i represents the corresponding data predictions
- $\delta_{i,uncor}$ and $\delta_{i,stat}$ are the uncorrelated systematics and statistical uncertainties on D_i
- Correlated systematics, described by γ_{ij}, are accounted for using the nuisance parameters b_j
- $C_{stat,ik}$ is the statistical (plus uncorrelated) covariance matrix
- The log penalty term is a small bias correction term

The diagonal term of the C matrix $C_{\mathrm{stat,ii}} = \delta^2_{i,\mathrm{uncor}} T_i^2 + \delta^2_{i,\mathrm{stat}} D_i T_i$
this log term adjusts the χ2 to be equivalent to log-likelihood
These are small corrections

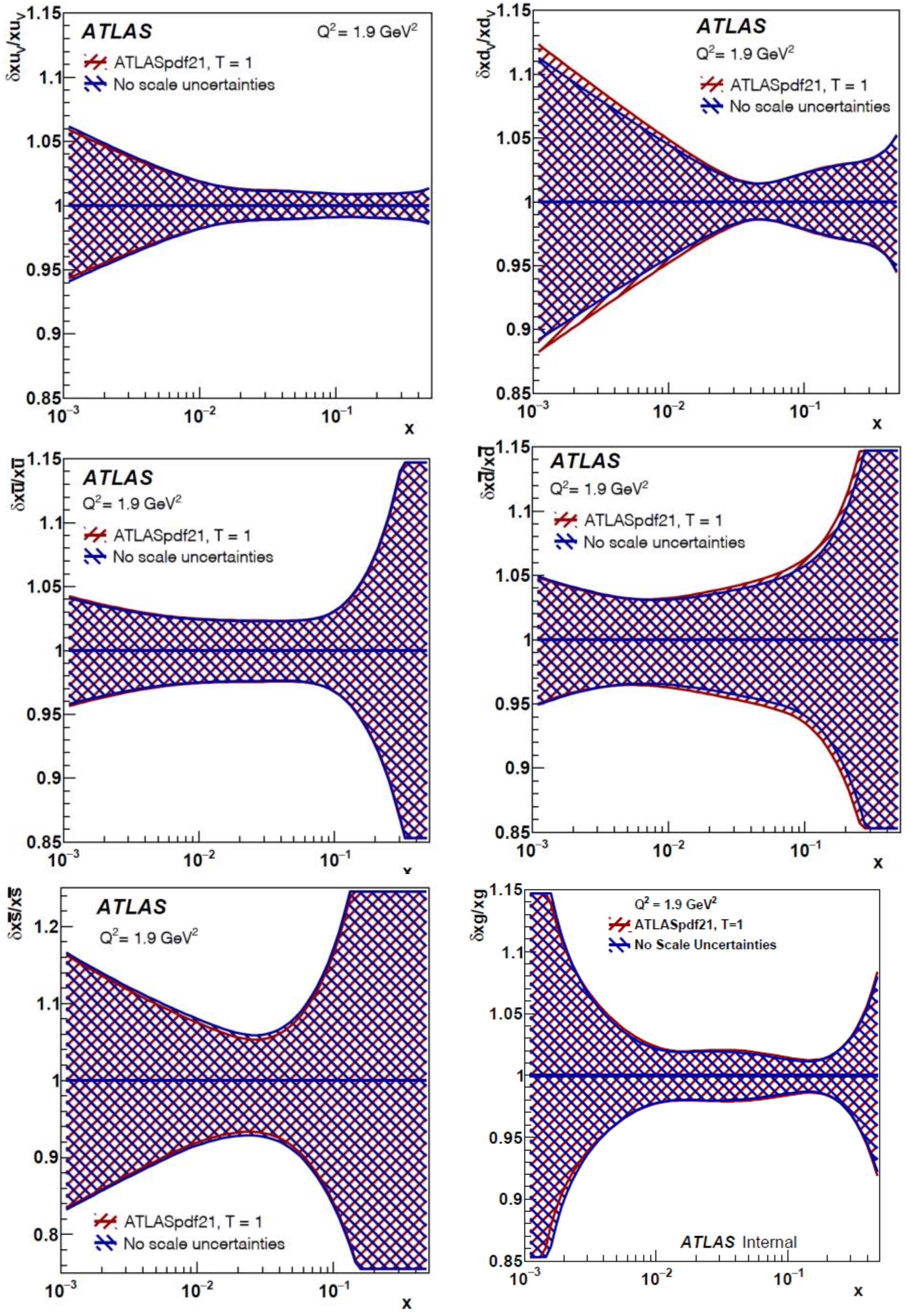
total χ^2/NDF	2010/1620
HERA χ^2/NDP	1112/1016
HERA correlated term	50
ATLAS W, Z 7 TeV χ^2/NDP	68/55
ATLAS Z/γ^* 8 TeV χ^2/NDP	208/184
ATLAS W 8 TeV χ^2/NDP	31/22
ATLAS W and Z/γ^* 7 and 8 TeV correlated term	71=(38+33)
ATLAS direct γ 13/8 TeV χ^2/NDP	27/47
ATLAS direct γ 13/8 TeV correlated term	6
ATLAS V + jets 8 TeV χ^2/NDP	105/93
ATLAS $t\bar{t}$ 8 TeV χ^2/NDP	13/20
ATLAS $t\bar{t}$ 13 TeV χ^2/NDP	25/29
ATLAS inclusive jets 8 TeV χ^2/NDF	207/171
ATLAS V + jets 8 TeV and $t\bar{t}$ + jets 8,13 TeV and $R = 0.6$ inclusive jets 8 TeV correlated term	87=(16+9+21+41)

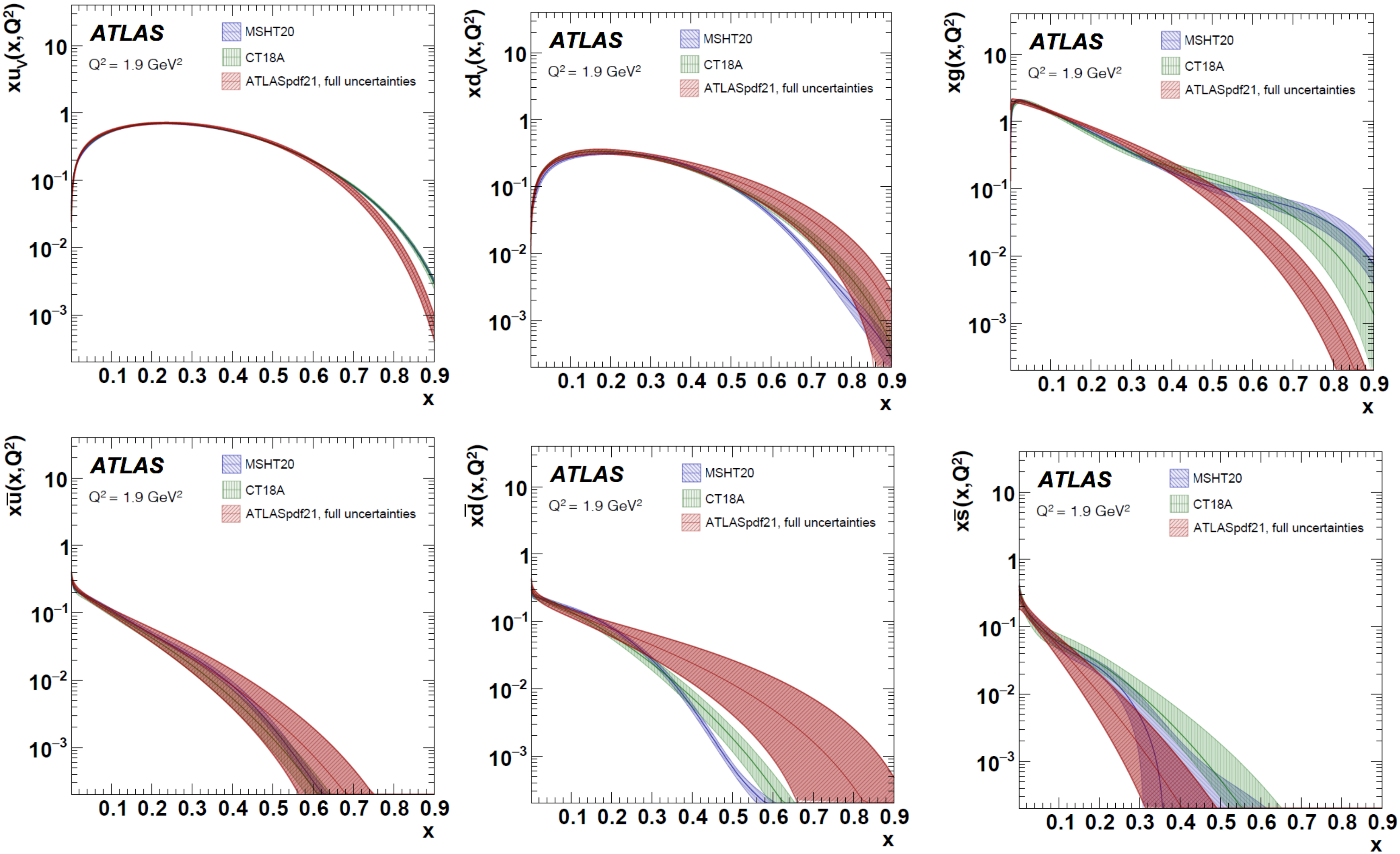
- This is a **better fit than that achieved by global fits to these data**

There is mild tension between the W,Z data at 8 TeV and the W,Z data at 7 TeV. The *partial* χ^2/NDP for the W,Z data at 7 TeV decreases from 68/55 to 50/55 if the W,Z data at 8 TeV are excluded from the fit, whereas the *partial* χ^2/NDP for the W,Z data at 8 TeV decreases from 239/206 to 222/206 if the W,Z data at 7 TeV are excluded from the fit. These increases in χ^2 are most pronounced for the cc data at 7 TeV around the Z mass-peak (66 – 116 GeV) and for the 8 TeV mass bins around the Z peak. As already remarked, theoretical scale uncertainties for both W,Z data at 7 and 8 TeV are added to the fit uncertainties. If these uncertainties are not added the tension between W,Z data at 7 and 8 TeV increases. The *partial* χ^2/NDP for W,Z data at 7 TeV increases to 80/55 and the *partial* χ^2/NDP for W,Z data at 8 TeV increases to 268/206 if both data sets are included in the fit and scale uncertainties are not applied.

Effect of scale uncertainties on mild tension between inclusive W,Z data at 7 and 8 TeV

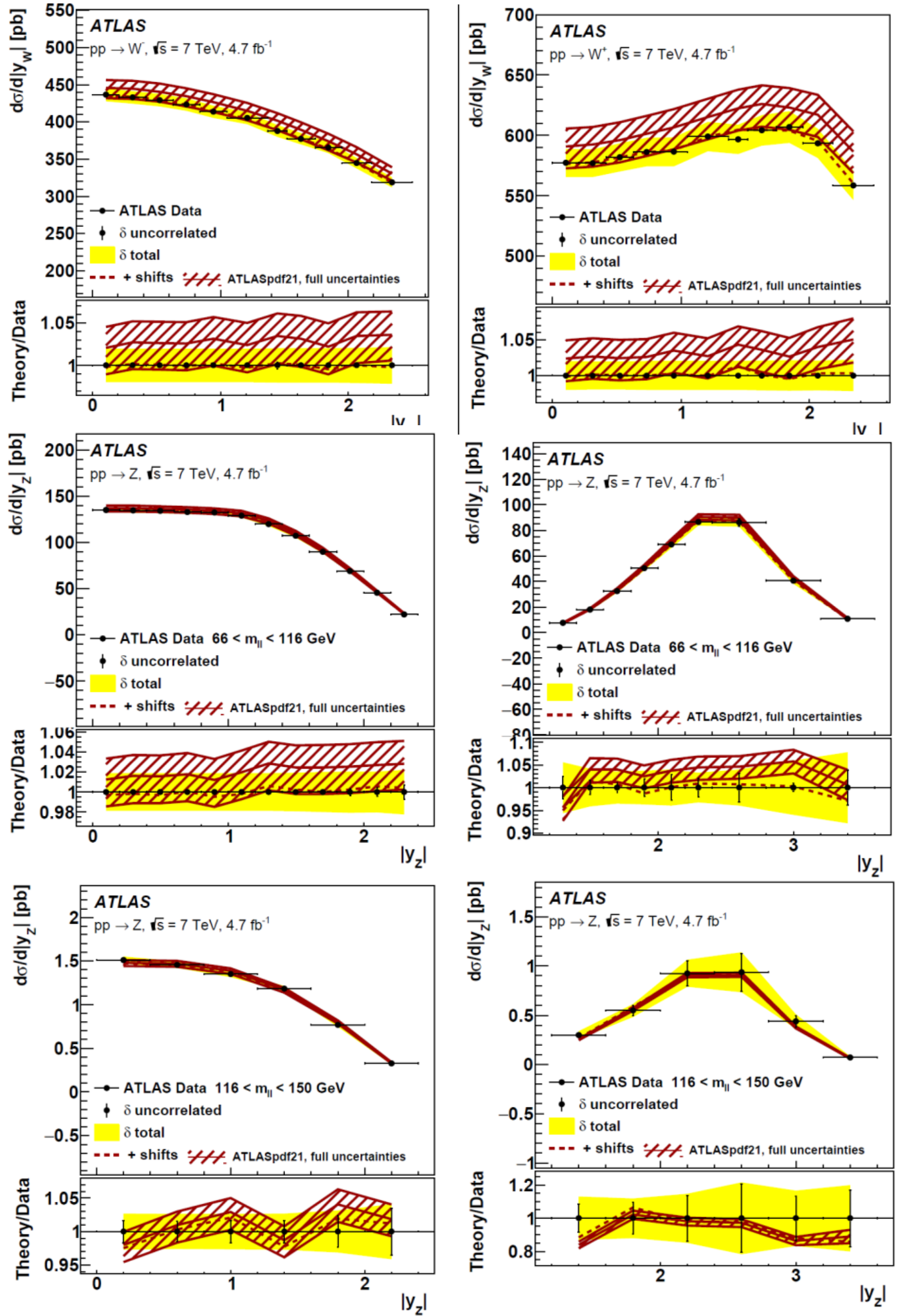
The addition of scale uncertainties has only a minor effect on the overall PDF uncertainty





High- x comparison with other PDFs

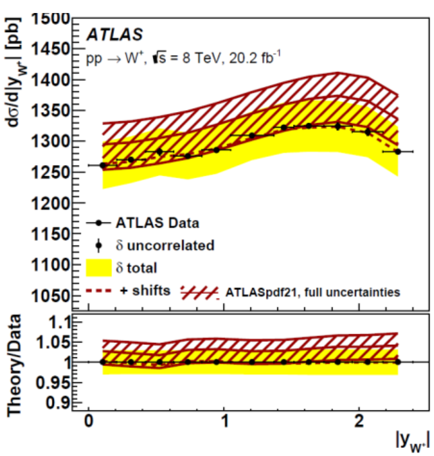
All the data: 7 TeV W,Z production

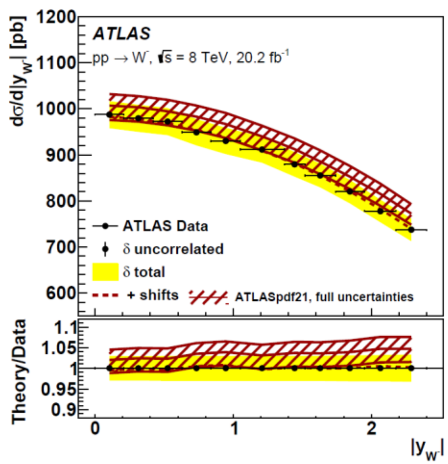


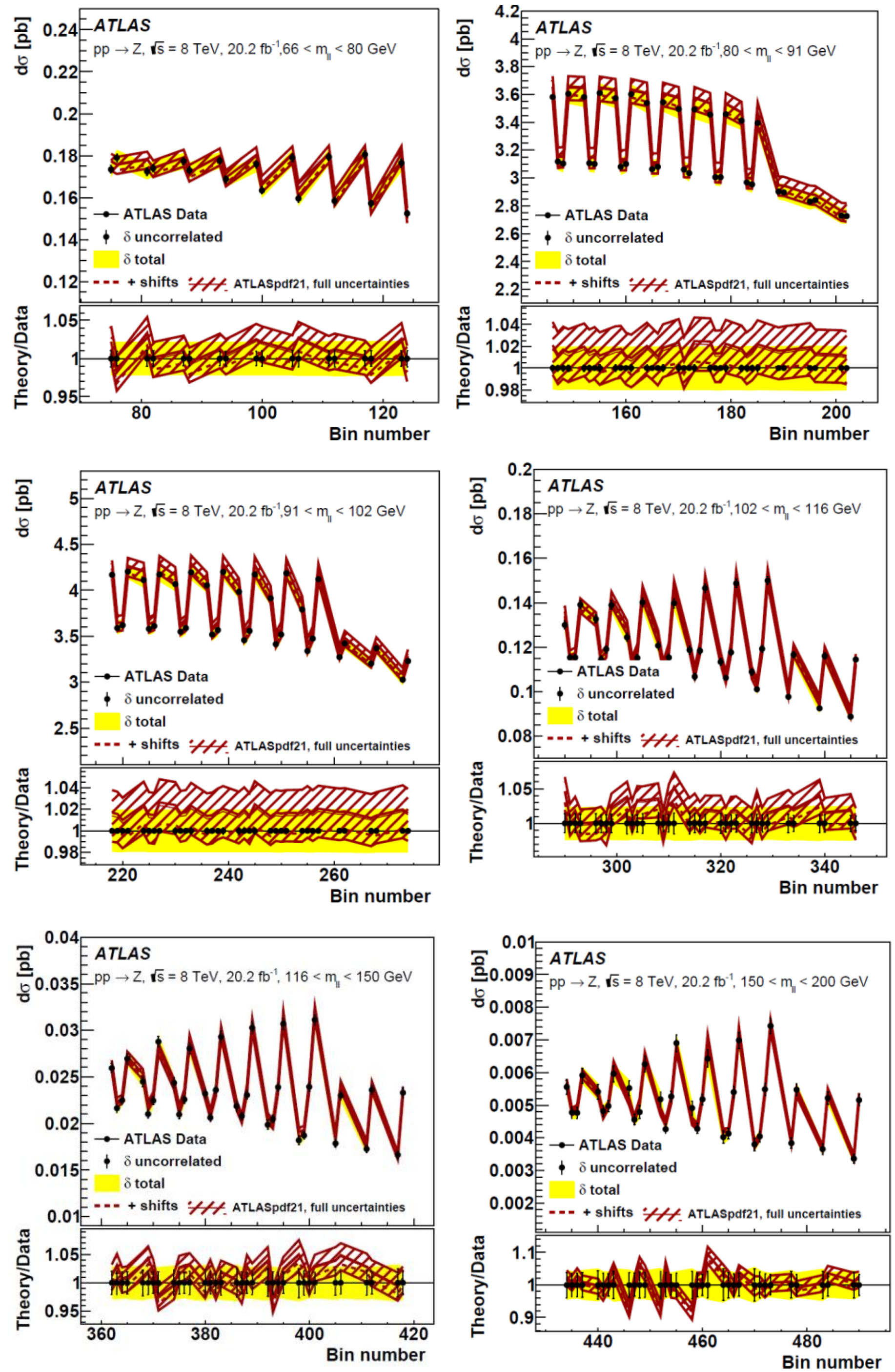
It is interesting to observe that the N3LO cross section for Z bosons is expected to be 2% lower than the NNLO cross section which would bring the data into agreement with the theory without need for shifts of systematic uncertainty

8 TeV W,Z production

It is interesting to observe that the N3LO cross section for Z bosons is expected to be 2% lower than the NNLO cross section which would bring the data into agreement with the theory without need for shifts of systematic uncertainty







dbar-ubar and Rs compared to other PDFs not shown in main body of the talk