PDFs and SM parameter measurements in ATLAS and beyond

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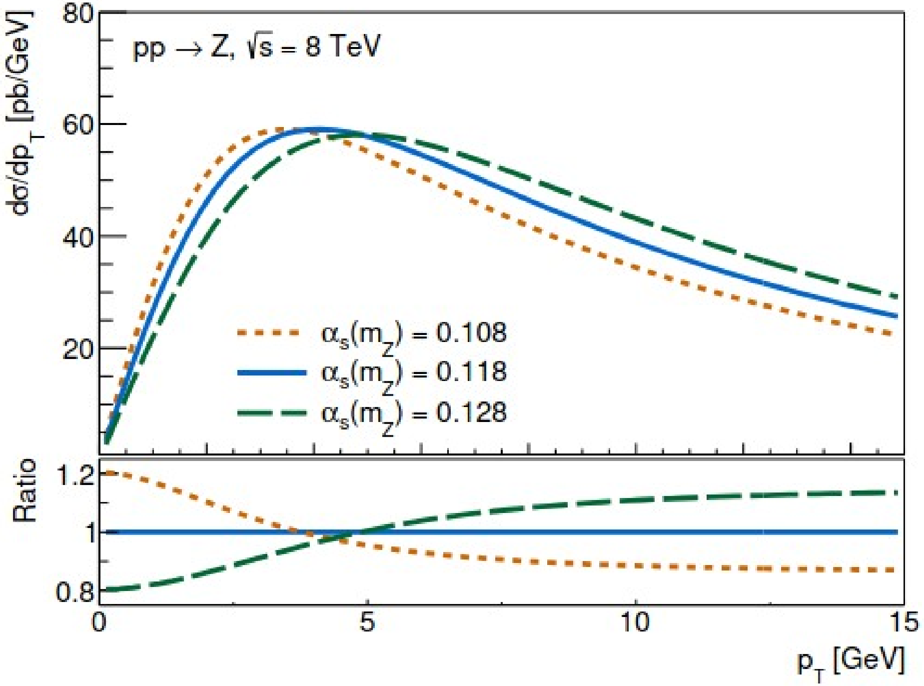
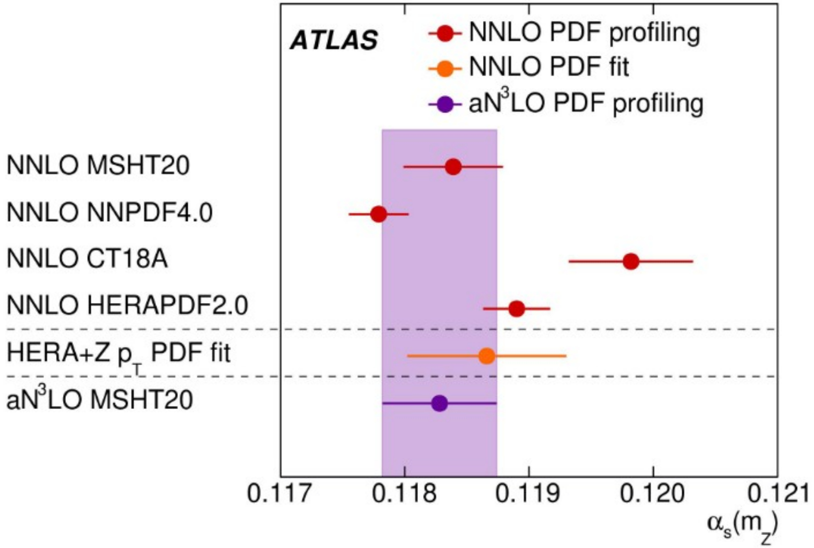
PDF4LHC meeting, December 2^{nd} 2024

Outline

- examples of precision measurements affected by PDF choices
- PDF uncertainty estimates and their impact
- requests and proposals to the PDF community

Examples – α_S from Z boson $d\sigma/dp_T$ peak (ATLAS)





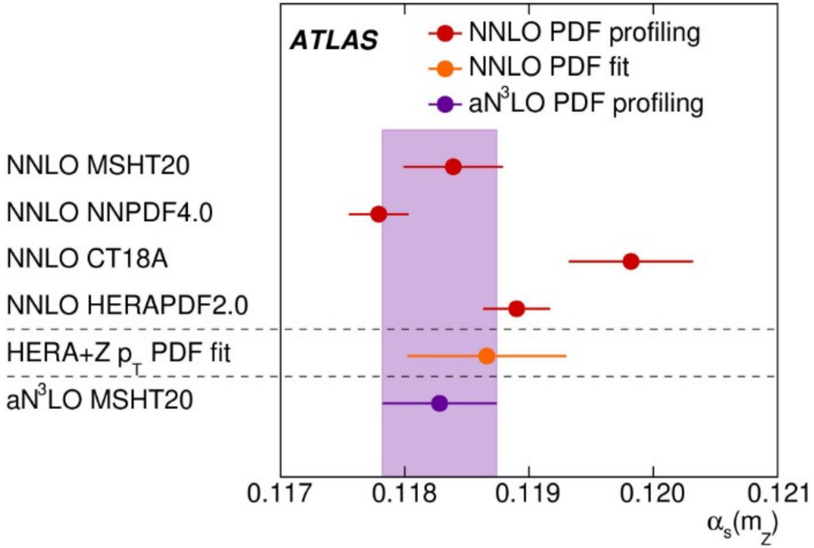
PDF set	$\alpha_s(m_Z)$	PDF uncertainty
MSHT20 [37]	0.11839	0.00040
NNPDF4.0 [84]	0.11779	0.00024
CT18A [29]	0.11982	0.00050
HERAPDF2.0 [65]	0.11890	0.00027

Examples – α_S from Z boson $d\sigma/dp_T$ peak (ATLAS)

Different NNLO PDF sets have a spread of ±0.00102, driven by the NNPDF4.0-CT18A difference (with CT14 the spread would be a factor of 2 smaller). CT18 is not compatible with the rest of PDFs within PDF uncertainties

Adding HERA data to the fit (counted twice), the spread is reduced to ±0.00016, around a central value of 0.11804

Would be interesting/possible to compare the nominal CT18 with a CT18 fit to only HERA data?



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TEEC and ATEEC – Data / theory comparison

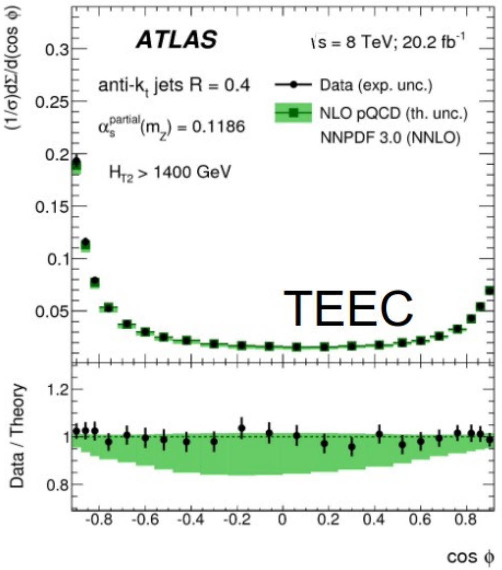
$$\frac{1}{\sigma}\frac{d\Sigma}{d(\cos\phi)} = \frac{1}{\sigma}\sum_{ij}\int \frac{d\sigma}{dx_{Ti}dx_{Tj}d(\cos\phi)} x_{Ti}x_{Tj}dx_{Ti}dx_{Tj}$$

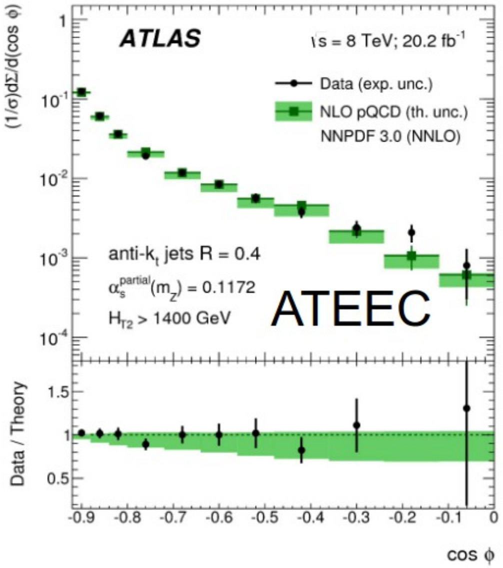
$$\frac{1}{\sigma}\frac{d\Sigma^{\mathrm{asym}}}{d(\cos\phi)} \equiv \frac{1}{\sigma}\frac{d\Sigma}{d(\cos\phi)}\bigg|_{\phi} - \frac{1}{\sigma}\frac{d\Sigma}{d(\cos\phi)}\bigg|_{\pi-\phi}$$

→ Energy-weighted angular distributions:

$$w_{ij} = x_{Ti}x_{Tj} = \frac{E_{Ti}E_{Tj}}{\left(\sum_k E_{Tk}\right)^2}$$

arXiv:1707.02562





→ Theory prediction: NLOJet++ & NP corrections (PYTHIA6 & HERWIG++)

$$\frac{1}{\sigma}\frac{d\Sigma}{d(\cos\phi)} = \frac{\Sigma_{a_i,b_i} f_{a_1}(x_1) f_{a_2}(x_2) \otimes \hat{\Sigma}^{a_1 a_2 \to b_1 b_2 b_3}}{\Sigma_{a_i,b_i} f_{a_1}(x_1) f_{a_2}(x_2) \otimes \hat{\sigma}^{a_1 a_2 \to b_1 b_2}} \qquad \mu_R = \frac{p_{T1}+p_{T2}}{2}; \quad \mu_F = \frac{p_{T1}+p_{T2}}{4}$$

TEEC and ATEEC – α_s results

TEEC

PDF	$\alpha_s(m_Z)$ value	χ^2/N_{dof}
MMHT 2014	0.1151 ± 0.0008 (exp.) $^{+0.0064}_{-0.0047}$ (scale) ± 0.0012 (PDF) ± 0.0002 (NP)	173 / 131
CT14	0.1165 ± 0.0010 (exp.) $^{+0.0067}_{-0.0061}$ (scale) ± 0.0016 (PDF) ± 0.0003 (NP)	161 / 131
NNPDF 3.0	0.1162 ± 0.0011 (exp.) $^{+0.0076}_{-0.0061}$ (scale) ± 0.0018 (PDF) ± 0.0003 (NP)	174 / 131
HERAPDF 2.0	0.1177 ± 0.0008 (exp.) $^{+0.0064}_{-0.0040}$ (scale) ± 0.0005 (PDF) ± 0.0002 (NP) $^{+0.0008}_{-0.0007}$ (mod)	169 / 131

ATEEC

PDF	$\alpha_s(m_Z)$ value	χ^2/N_{dof}
MMHT 2014	0.1185 ± 0.0012 (exp.) $^{+0.0047}_{-0.0010}$ (scale) ± 0.0010 (PDF) ± 0.0004 (NP)	57.0 / 65
CT14	0.1203 ± 0.0013 (exp.) $^{+0.0053}_{-0.0014}$ (scale) ± 0.0015 (PDF) ± 0.0004 (NP)	55.4 / 65
NNPDF 3.0	0.1196 ± 0.0013 (exp.) $^{+0.0061}_{-0.0013}$ (scale) ± 0.0017 (PDF) ± 0.0004 (NP)	60.3 / 65
HERAPDF 2.0	0.1206 ± 0.0012 (exp.) $^{+0.0050}_{-0.0014}$ (scale) ± 0.0005 (PDF) ± 0.0002 (NP) ± 0.0007 (mod)	54.2 / 65

→ Scale and PDF uncertainties > Experimental uncertainty

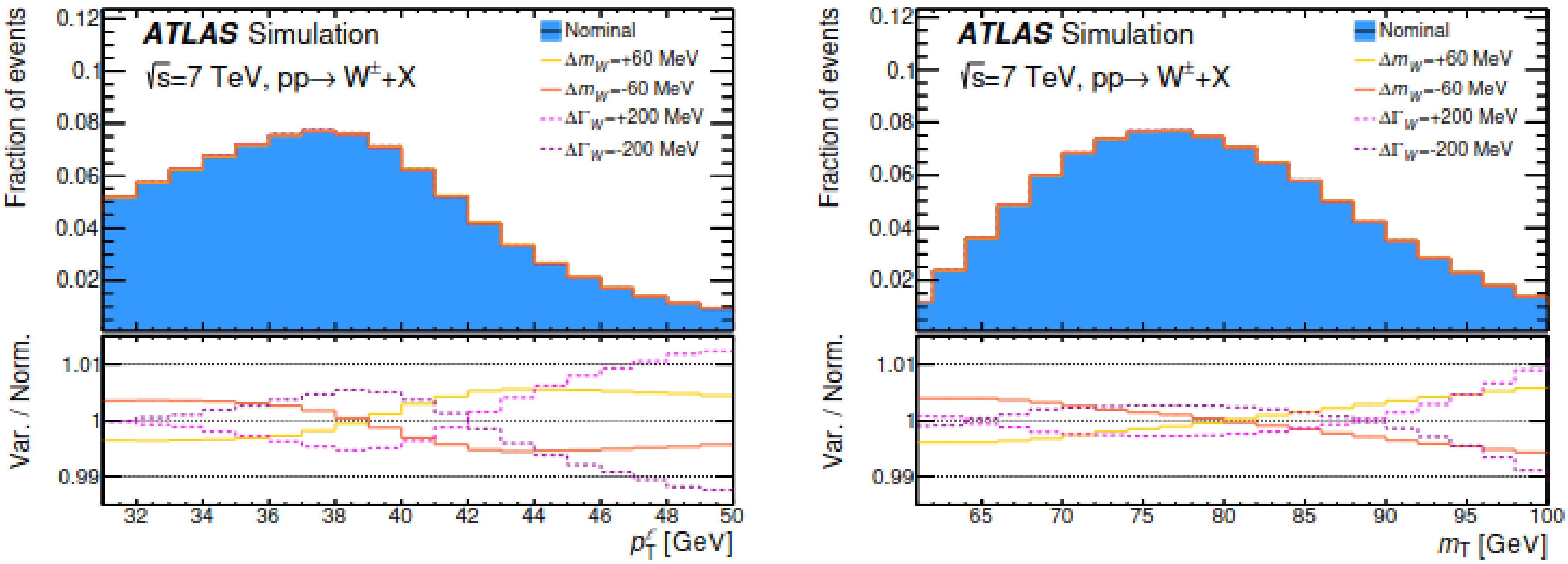
→ PDF uncertainty (eigenvectors) comparable to / smaller than PDF variations for global / all PDF sets

How significant are these differences between various PDF sets?

What fraction of the spread should be added as extra uncertainty?

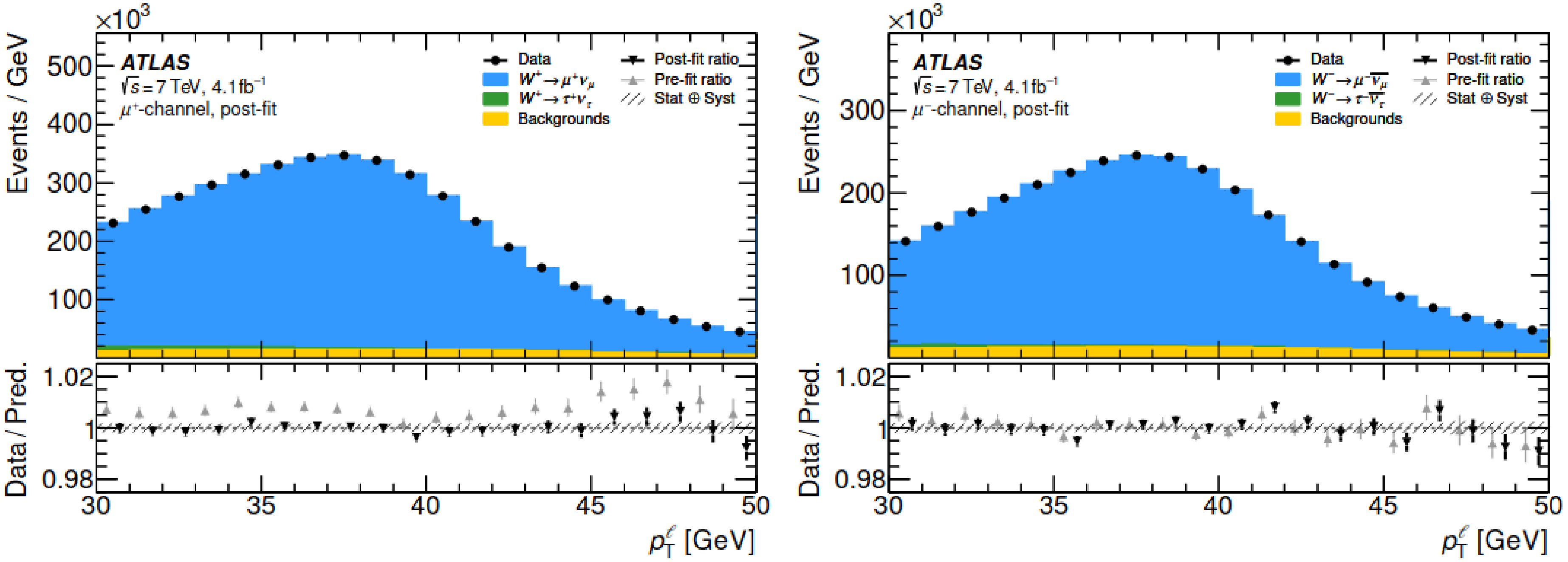
W-boson mass and width in ATLAS

- Lepton p_T and W m_T sensitive to m_W and Γ_W



W-boson mass and width in ATLAS

- Lepton p_T and W m_T sensitive to m_W and Γ_W
- Fits to these parameters and O(200) nuisance experimental and modelling nuisance parameters



Results for different PDF sets

- Mass

Span ~18 MeV
~8 MeV exc. NNPDF

PDF set	Correlation	weight (p_T^ℓ)	weight (m_T)	Combined m_W [MeV]
CT14	52.2%	88%	12%	80363.6 ± 15.9
CT18	50.4%	86%	14%	80366.5 ± 15.9
CT18A	53.4%	88%	12%	80357.2 ± 15.6
MMHT2014	56.0%	88%	12%	80366.2 ± 15.8
MSHT20	57.6%	97%	3%	80359.3 ± 14.6
ATLASpdf21	42.8%	87%	13%	80367.6 ± 16.6
NNPDF3.1	56.8%	89%	11%	80349.6 ± 15.3
NNPDF4.0	59.5%	90%	10%	80345.6 ± 14.9

- Width

Span ~23 MeV
~10 MeV exc. CT14/18

PDF set	Correlation	weight (m_T)	weight (p_T^ℓ)	Combined Γ_W [MeV]
CT14	50.3%	88%	12%	2204 ± 47
CT18	51.5%	87%	13%	2202 ± 47
CT18A	50.0%	86%	14%	2184 ± 47
MMHT2014	50.8%	88%	13%	2182 ± 47
MSHT20	53.6%	89%	11%	2181 ± 47
ATLASpdf21	49.5%	84%	16%	2193 ± 46
NNPDF31	49.9%	86%	14%	2182 ± 46
NNPDF40	51.4%	85%	15%	2184 ± 46

Results for different PDF sets

- Mass

Span ~18 MeV
~8 MeV exc. NNPDF

PDF set	p_T^ℓ fit m_W	p_T^ℓ fit σ_{tot}	p_T^ℓ fit σ_{PDF}	p_T^ℓ fit χ^2/n.d.f.	m_T fit m_W	m_T fit σ_{tot}	m_T fit σ_{PDF}	m_T fit χ^2/n.d.f.
CT14	80358.3	$^{+16.1}_{-16.2}$	4.6	543.3/558	80401.3	$^{+24.3}_{-24.5}$	11.6	557.4/558
CT18	80362.0	$^{+16.2}_{-16.2}$	4.9	529.7/558	80394.9	$^{+24.3}_{-24.5}$	11.7	549.2/558
CT18A	80353.2	$^{+15.9}_{-15.8}$	4.8	525.3/558	80384.8	$^{+23.5}_{-23.8}$	10.9	548.4/558
MMHT2014	80361.6	$^{+16.0}_{-16.0}$	4.5	539.8/558	80399.1	$^{+23.2}_{-23.5}$	10.0	561.5/558
MSHT20	80359.0	$^{+13.8}_{-15.4}$	4.3	550.2/558	80391.4	$^{+23.6}_{-24.1}$	10.0	557.3/558
ATLASpdf21	80362.1	$^{+16.9}_{-16.9}$	4.2	526.9/558	80405.5	$^{+28.2}_{-27.7}$	13.2	544.9/558
NNPDF3.1	80347.5	$^{+15.2}_{-15.7}$	4.8	523.1/558	80368.9	$^{+22.7}_{-22.9}$	9.7	556.6/558
NNPDF4.0	80343.7	$^{+15.0}_{-15.0}$	4.2	539.2/558	80363.1	$^{+21.4}_{-22.1}$	7.7	558.8/558

- Width

Span ~23 MeV
~10 MeV exc. CT14/18

PDF set	p_T^ℓ fit Γ_W	p_T^ℓ fit σ_{tot}	p_T^ℓ fit σ_{PDF}	p_T^ℓ fit χ^2/n.d.f.	m_T fit Γ_W	m_T fit σ_{tot}	m_T fit σ_{PDF}	m_T fit χ^2/n.d.f.
CT14	2228	$^{+67}_{-83}$	24	550.0/558	2202	$^{+48}_{-48}$	5	556.8/558
CT18	2221	$^{+68}_{-76}$	21	534.5/558	2200	$^{+47}_{-48}$	5	548.8/558
CT18A	2207	$^{+68}_{-75}$	18	533.0/558	2181	$^{+47}_{-48}$	5	550.6/558
MMHT2014	2155	$^{+71}_{-78}$	19	546.0/558	2186	$^{+48}_{-48}$	5	562.2/558
MSHT20	2206	$^{+66}_{-79}$	15	556.5/558	2179	$^{+47}_{-48}$	4	559.4/558
ATLASpdf21	2213	$^{+67}_{-73}$	18	531.3/558	2190	$^{+47}_{-48}$	6	545.6/558
NNPDF31	2203	$^{+65}_{-78}$	20	531.7/558	2180	$^{+47}_{-47}$	6	560.4/558
NNPDF40	2182	$^{+69}_{-68}$	12	550.5/558	2184	$^{+47}_{-47}$	4	564.0/558

PDF dependence, PDF uncertainty and their impact

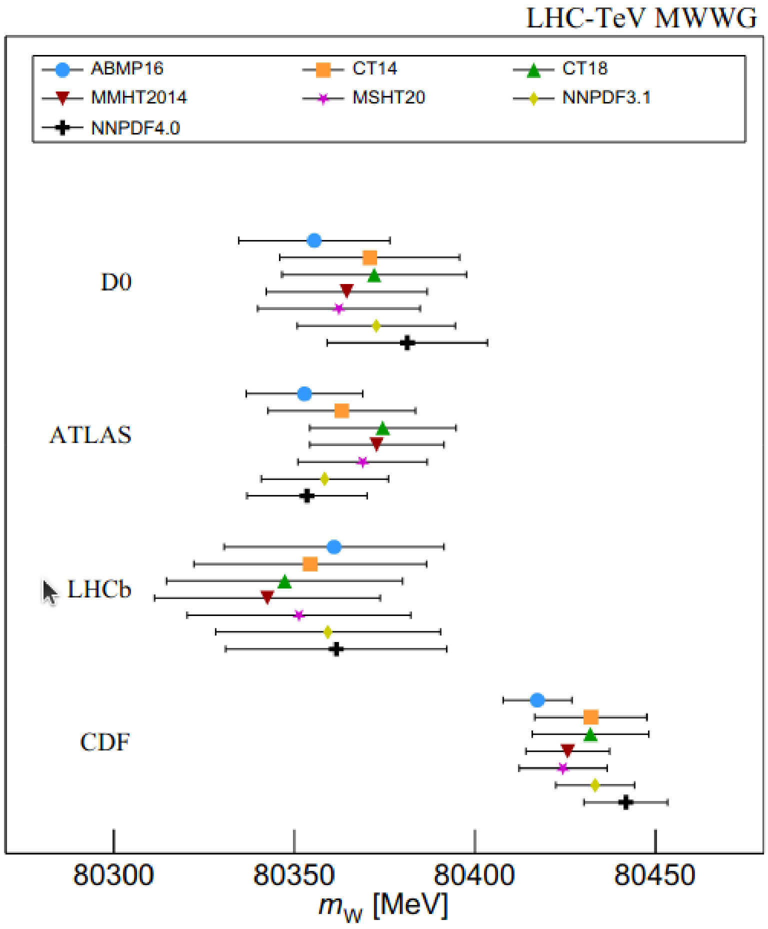
Several, related issues:

- the PDF dependence of measurement results is too large, which points to underestimated uncertainties and “hidden” model dependence
- the significance of the PDF dependence of measurement results can not be calculated
- no well-defined prescription regarding the additional uncertainty to account for such effects

In summary, the error propagation is broken (or almost) at this point, with impact on our uncertainty estimates, averages, interpretation fits, etc

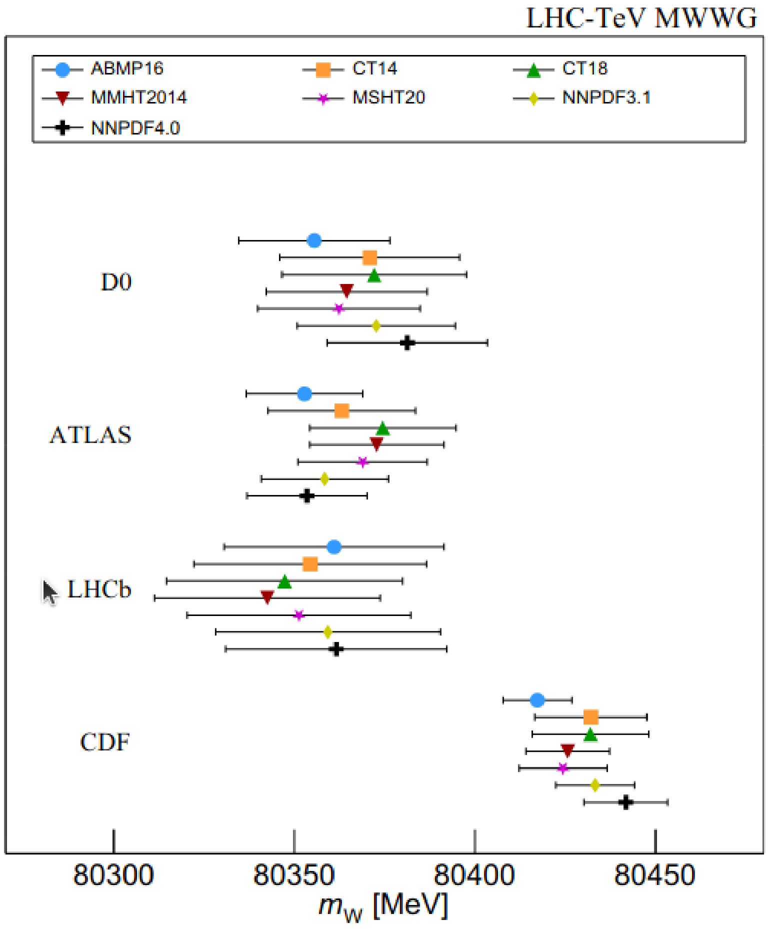
M_W combination

- First rigourous combination of hadron-collider mW measurements, accounting for different QCD accuracy and PDF models
  - D0, 2013, Resbos1, CTEQ6.6
  - ATLAS, 2017, DYNNLO/Pythia, CT10
  - LHCb, 2022, Dyturbo/Powheg/Pythia, <NNPDF31/CT18/MSHT20>
  - CDF, 2023, Resbos2, NNPDF3.1



M_W combination

- First rigourous combination of hadron-collider mW measurements, accounting for different QCD accuracy and PDF models
- Proceeds by extrapolating published measurements to newer PDF sets, using parameterised detector response
- For all measurements, results vary by ~15-20 MeV depending on the PDF set assumed for the measurement



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- Proceeds by extrapolating published measurements to newer PDF sets, using parameterised detector response
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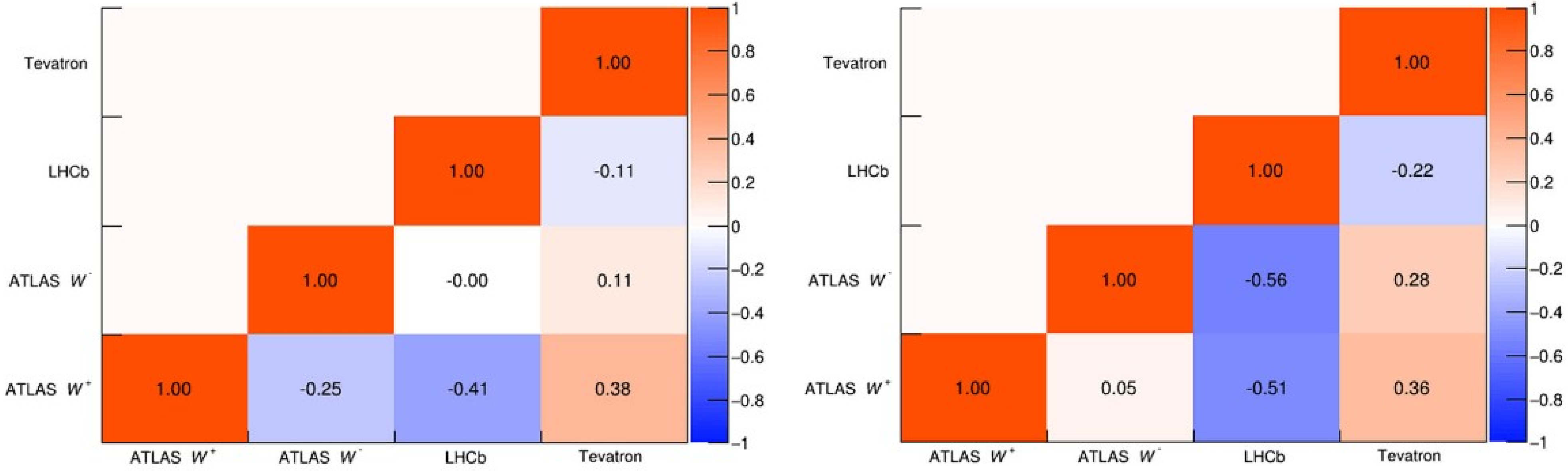
PDF set	D0	CDF	ATLAS	LHCb
CTEQ6	–	14.1	–	–
CTEQ6.6	15.1	–	–	–
CT10	–	–	9.2	–
CT14	13.8	12.4	11.4	10.8
CT18	14.9	13.4	10.0	12.2
ABMP16	4.5	3.9	4.0	3.0
MMHT2014	8.8	7.7	8.8	8.0
MSHT20	9.4	8.5	7.8	6.8
NNPDF3.1	7.7	6.6	7.4	7.0
NNPDF4.0	8.6	7.7	5.3	4.1

Note : none of these measurements profile PDF uncertainties

M_W combination

- Combinations help reducing the model-dependence through partial/negative correlations. But correlations themselves are model dependent:



Discussion

- PDF incompatibility already present in measurements using traditional error propagation
- Profile-likelihood fits aim at reducing PDF dependence by adjusting model parameters to the data
  - Experimentalist's objective : make model dependence "significantly smaller" than model uncertainty
- Likelihood used so far (using Pavel Nadolsky's notation):

$$\chi^{2\prime}(\vec{\lambda}_{\exp}, \vec{\lambda}_{\mathrm{th}}) = \sum_{i=1}^{N_{pt}} \frac{\left[D_i + \sum_\alpha \beta_{i,\alpha}^{\exp} \lambda_{\alpha,\exp} - T_i - \sum_\alpha \beta_{i,\alpha}^{\mathrm{th}} \lambda_{\alpha,\mathrm{th}}\right]^2}{s_i^2} + \sum_\alpha \lambda_{\alpha,\exp}^2 + \sum_\alpha \lambda_{\alpha,\mathrm{th}}^2.$$

with $\Delta\chi^2 = 1$.

- Criticised for not treating PDF NP's consistently with PDF sets using tolerances
  - CT, MSHT

Discussion

- Issue first raised by CT
- Recommendation: consistently use

$$\chi^2(\vec{\lambda}_{\rm exp}, \vec{\lambda}_{\rm th}) = \sum_{i=1}^{N_{pt}} \frac{\left[D_i + \sum_\alpha \beta_{i,\alpha}^{\rm exp} \lambda_{\alpha,\rm exp} - T_i - \sum_\alpha \beta_{i,\alpha}^{\rm th} \lambda_{\alpha,\rm th}\right]^2}{s_i^2} + \sum_\alpha \lambda_{\alpha,\rm exp}^2 + \sum_\alpha T^2 \lambda_{\alpha,\rm th}^2.$$

  with $\Delta\chi^2 = T^2$.

- This is however equivalent to scaling the data uncertainties, hence the total measurement uncertainty, by a factor ~T
  - the final result is worse than when treating PDF uncertainties using offsets
  - Introduces strong uncertainty hierarchy between fits with sets using / not using tolerances

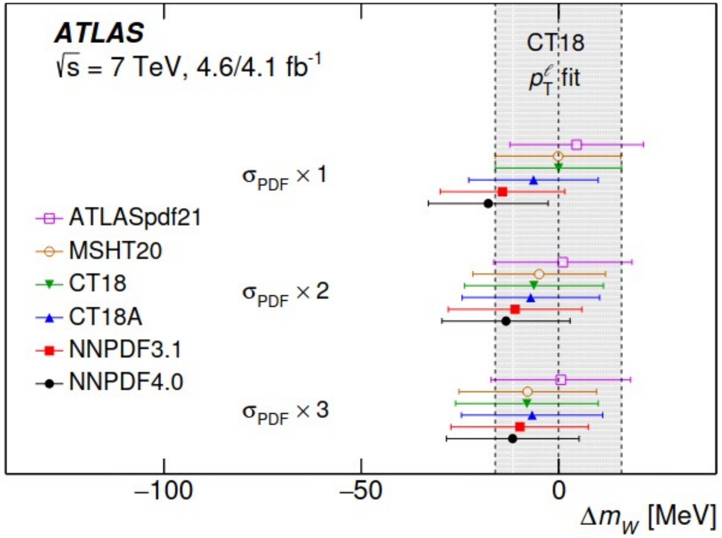
Discussion

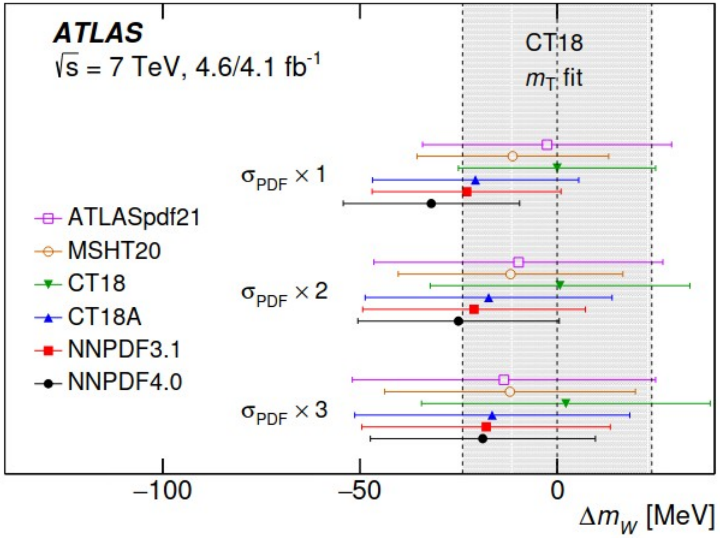
- Second proposal (Tom Cridge/MHST):
  - For fixed value of the POI, marginize PDF NP's accounting for tolerance consistently
  - In a second step, minimize over parameter of interest (ie m_W, $\sin^2\theta_W$..) using criterion of choice, typically $\Delta\chi^2 = 1$.

- This is a more suitable version:
  - in the limit of large T, PDF uncertainties reproduce traditional offset results
  - Experimental uncertainties not penalized
  - Exercises being performed
- Method however also fails to address the question of PDF model dependence
  - With large tolerance factors, PDF NPs "freeze", ie discrepancies between measured central values stay unchanged

Discussion

- 3rd attempt, used in ATLAS, CMS : scale pre-fit PDF uncertainties





  - Larger pre-fit uncertainties → more flexible PDFs that better adapt to the data
  - Different PDF sets still reflect their own choices of parametrisation, datasets, etc
  - Amounts to profile assuming T<1 (!), but starting from enlarged uncertainties
    - Measurement precision degrades overall, but data become more compatible

Discussion

- 3rd attempt, used in ATLAS, CMS : scale pre-fit PDF uncertainties

- However still not satisfactory : how to define a suitable error scaling factor?
  - Natural criterion : scale until model dependence significantly smaller than model uncertainty
  - But how to evaluate the significance of $m_W^{PDF\,A} - m_W^{PDF\,B}$?

- Bottom line : an estimate of the correlations between PDF sets is needed, eg through synchronized CT, MSHT, NNPDF fits to common toy datasets
  - PDF benchmarking proposal by B.Malaescu et al : see early presentation here
  - Related exercises by NNPDF and MSHT
  - Such results would be extremely powerful if provided in a systematic way

Discussion

- Last remark : most of the issues above ultimately originate from the use of a generic, dataset-independent tolerance factor
- Downweighting *any* old or new dataset by a unique factor T is suboptimal:
  - Risk of absorbing theory effects into enlarged data uncertainties
    - cf. presentation last year, including proposals to better separate theory from data uncertainties in PDF fits – any follow up?
  - Many datasets come with cross-checks providing a quantitative estimate of their internal consistency (eg H1 vs ZEUS in the HERA dataset; electrons vs muons in DY cross sections at the LHC; …)
  - Others can be directly compared (W asymmetry in CDF and D0; …)
- A complementary attempt to mitigate these questions would consist of tolerance factors defined per dataset. Not an easy task, but would allow a better discussion of experimental vs. theory uncertainties, an avoid considering penalizing new datasets without specific justification.

Summary

- The PDF dependence of measurement results is an issue as much as last year, regardless of the statistical method being used in a given measurement.
- Our common objective should be to make this dependence smaller if possible, or at least well quantified.
- A rigourous treatment of this question requires knowing the uncertainty correlations between PDF sets. Ideas and proposals exist. How to proceed?
- Several proposals exist to treat the profiling of PDF nuisance parameters with the needed conservatism.
  - A consistent usage of tolerance avoids over-constraining PDF NPs, but doesn't improve the model-dependence. Error scaling helps, but amounts to considering $T<1$ (with however enlarged initial uncertainties)
  - Per-dataset tolerances seem an interesting possibility; feedback welcome.