MSHT20 PDFs Determination of $\alpha_S(M_Z^2)$ at up to Approximate N3LO

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ECT* Trento, Alphas-2024 Workshop

6th February 2024

In collaboration with L.A. Harland-Lang and R.S. Thorne.

Outline

- 1. MSHT PDF Overview
- 2. MSHT α_S Depedence
- 3. MSHT α_S Bounds
- 4. MSHT PDF + α_S dependence
- 5. Conclusions

MSHT20 PDF Overview

- MSHT20 New PDF set from MSHT group for precision LHC era (2012.04684). More data, extended methodology, improved theory.
- Global fit \Rightarrow 61 different datasets, \gtrsim 4500 datapoints 10 Structure Func., 6 neutrinos, 2 fixed target DY, 8 HERA, 8 Tevatron, 27 LHC.
- Many developments since, only relevant ones shown:

alphas-2022 workshop + Snowmass

- Extraction of $\alpha_S(M_Z^2)$ at NLO and NNLO: 2106.10289. \rightarrow^+ Snowmass
- Approximate N3LO (aN3LO) PDFs with theoretical uncertainties: 2207.04739.
- Solution Top mass determination in MSHT at NNLO: 2306.14885. $\rightarrow \alpha_{S}$ -m_t correlation
- Impact of Jet, Dijet and Z p_T data at up to aN3LO in MSHT: 2312.12505.
- Determination of $\alpha_{\mathcal{S}}(M_Z^2)$ at up to aN3LO.
- Upcoming! (preliminary results here)
- Also QED PDFs, PDF experiment sensitivities, EIC study, PDF4LHC21, etc.

New since alphaS 2022 workshop!

MSHT20 PDF $\alpha_{S}(M_{Z}^{2})$ Overview

- MSHT20 NNLO $\alpha_S(M_Z^2)$ extraction went into Snowmass report (2203.08271) following alphaS-2022 workshop.
- Also in most recent PDG 2023 update $\alpha_S(M_Z^2)$ combination (2312.14015): \sim
- $\alpha_S(M_Z^2)$ sensitivity in PDF fit comes from:
 - ► Direct α_S(M²_Z) dependence in coefficient functions.

$$F(x, Q^2) = \sum_{i=q,\bar{q},g} \left[C_i(\alpha_s(Q^2)) \otimes f_i(Q^2) \right](x)$$
$$C(\alpha_5) = \alpha_5^i [C_0 + \alpha_5 C_1 + \alpha_5^2 C_2 + \alpha_5^3 C_3 + \dots]$$

• Indirect $\alpha_S(M_Z^2)$ dependence through PDF evolution.

$$\frac{d\boldsymbol{f}}{d\ln\mu_f^2} \equiv \frac{d}{d\ln\mu_f^2} \left(\begin{array}{c} \Sigma \\ g \end{array} \right) = \left(\begin{array}{c} P_{qq} & n_f P_{qg} \\ P_{gq} & P_{gg} \end{array} \right) \otimes \left(\begin{array}{c} \Sigma \\ g \end{array} \right) \equiv \boldsymbol{P} \otimes \boldsymbol{f}$$
$$\boldsymbol{P}(x, \alpha_t) = \alpha_* \boldsymbol{P}^{(0)}(x) + \alpha^2 \boldsymbol{P}^{(1)}(x) + \alpha^3 \boldsymbol{P}^{(2)}(x) + \alpha^4 \boldsymbol{P}^{(3)}(x) + \dots$$



PDG 2023 Update - 2312.14015.

MSHT20 Approximate N3LO PDF Overview

- As experiments become more precise, need to improve accuracy and precison of theoretical predictions.
- In particular as PDFs become more precise we need:
 - Move to higher orders (N3LO) in QCD.
 - Inclusion of theoretical uncertainties.

 \Rightarrow we can address both in one go! \Rightarrow MSHT20aN3LO PDFs.

- Idea is to include known N3LO effects already into PDFs and to parameterise remaining unknown pieces via nuisance parameters.
- Variation of these remaining unknown N3LO pieces then provides a theoretical uncertainty within an approximate N3LO fit (aN3LO).
- Vary actual unknown higher order pieces to get MHOU uncertainty, rather than rely on scale variations as a proxy for this.



More information J. McGowan, T.C., L.A. Harland-Lang, R.S. Thorne: 2207.04739

What do we already know for N3LO PDFs?

- Full N3LO PDFs need all N3LO pieces for both PDFs and included cross-sections to be known, not yet possible as some pieces missing.
- Still, a lot of information is known already (schematic summary):

Theory	Utility	Order required	What's known?	
1. Splitting functions $P_{ab}^{(3)}(x)$	PDF evolution	4-loop	Mellin moments, leading small-x behaviour, plus some leading large-x in places. <i>Plus new FHMV results</i> .	
2. Transition matrix elements $A^{(3)}_{ab,H}(x)$	Transitions between number of flavours in PDFs at mass thresholds	3-loop	Mellin moments, leading small-x behaviour, plus some leading large-x in places. <i>Plus new Ablinger et al</i> .	
3. DIS Coefficient functions (NC DIS) $C_{H,a}^{VF,(3)}$	Combine with PDFs and Transition Matrix Elements to form Structure Functions (NC DIS)	N3LO	Some approximations to FFNS (low Q^2) coefficient functions at α_S^3 (with exact LL pieces at low x , NLL unknown), ZM-VFNS (high Q^2) N3LO coefficient functions known exactly. Therefore GM-VFNS not completely known.	
4. Hadronic Coefficients (K-factors)	Determine cross-sections at N3LO	N3LO	Very little (none in usable form for PDFs)	

• Knowledge of lower orders can guide us for remaining unknown pieces. References in backup!

More information in articles: T.C., L.A. Harland-Lang, A.D. Martin, R.S. Thorne: 2106.10289, *Eur.Phys.J.C 81 (2021) 8, 744.* T.C., L.A. Harland-Lang, R.S. Thorne: *Upcoming!*

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MSHT $\alpha_S(M_7^2)$ determination

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MSHT α_S dependence - NLO and NNLO (previous)

- Default PDFs provided at standard fixed value of $\alpha_S(M_Z^2) = 0.118$.
- Can also allow α_S to be a free parameter in the fit.
- Global fit nature of PDFs \Rightarrow can provide a precise, accurate determination of α_S .
- Individual datasets have different dependences on α_{S} , but robust determination utilising all datasets. $\alpha_{S,NNLO}(M_Z^2) < \alpha_{S,NLO}(M_Z^2)$ as NNLO corrections +ve, so
- The best fit values <u>were</u> found to be: fitting same data \Rightarrow lower α_s .



MSHT20 α_{S} dependence - NLO and NNLO ${}^{(\rm new)}$

Preliminary!

• New MSHT20 NNLO $\alpha_S(M_Z^2)$ determination - added data (ATLAS 8 TeV jets), updated theory.



 Very close to previous NNLO result of 0.1174, consistent well within uncertainties. Also consistent with World Average.
 T.C., L.A. Harland-Lang, R.S. Thorne (upcoming).

MSHT20 α_5 dependence - NNLO and aN3LO (first ever!)

- First PDF $\alpha_S(M_Z^2)$ determination at aN3LO.
- Consistent with NNLO determination within uncertainties.
- Good perturbative convergence of $\alpha_{\mathcal{S}}$ determination.



• Approximate N3LO as whilst splitting functions, DIS coefficient functions, heavy quark transition matrix elements are largely known (latter - see talk by J. Blümlein), N3LO xsecs still unknown. T.C., L.A. Harland-Lang, R.S. Thorne (upcoming).

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MSHT $\alpha_S(M_z^2)$ determination

MSHT20 dataset α_S dependence - Fixed Target • Perform fits for range $0.112 < \alpha_S(M_Z^2) < 0.122$ in steps of 0.001,

and examine individual dataset α_5 dependence via fit quality.



Preliminary!

Consistent with α_S pulls seen in previous studies, and between orders.

Deuteron datasets often prefer larger α_S .

SLACd prefers higher α_S , unlike SLACp.

Perhaps evidence of Q^2 dependence of deuterium corrections?

- Fixed target (e.g. BCDMS, NMC, SLAC) high x experiments are dominated by non-singlet ⇒ cleaner means of evaluating α_S.
- HERA has more limited α_S sensitivity (not shown) as it is lower $x \Rightarrow$ singlet- α_S correlation. T.C., L.A. Harland-Lang, R.S. Thorne (upcoming).

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MSHT20 dataset α_S dependence - Drell-Yan Preliminary!

• Perform fits for range $0.112 < \alpha_S(M_Z^2) < 0.122$ in steps of 0.001, and examine individual dataset α_S dependence via fit quality.



Consistent with α_S pulls seen in previous studies, and between orders (NNLO and aN3LO).

LHCb 7 and 8 TeV W, Z to muons prefer slightly raised α_S . Different to LHCb electron data.

CMS 8 TeV W also favour higher α_S .

• High precision W, Z data have indirect sensitivity to α_S through their precision (via smaller effects in evolution and cross-sections), often prefer higher α_S values.

T.C., L.A. Harland-Lang, R.S. Thorne (upcoming).

MSHT $\alpha_{S}(M_{z}^{2})$ determination

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MSHT20 dataset α_S dependence - Jets

Preliminary!

• Perform fits for range $0.112 < \alpha_S(M_Z^2) < 0.122$ in steps of 0.001, and examine individual dataset α_S dependence via fit quality.



- Jet datasets have direct sensitivity to α_S , generally prefer lower α_S , also favour lower high x gluon \Rightarrow some correlation.
- Generally weaker sensitivity at aN3LO due to unknown K-factors.

MSHT20 Inclusive Jet or Dijet data?

- Dijets may have some advantages here 3D measurement now possible, non-unitary nature of inclusive jets, etc
- We have also investigated dijets instead:
 - Obtain better fit quality at NNLO and aN3LO than inclusive jets.
 - Moreover, dijet fit quality improves further slightly at aN3LO.

	Ν.	$\chi^2/$	χ^2/N_{pts}		N.	χ^2/N_{pts}	
Inclusive Jets	/vpts	NNLO	aN3LO	Dijets	Wpts	NNLO	aN3LO
Total	472	1.39	1.43	Total	266	1.12	1.04
Total (+ATLAS 8 TeV jets)	643	1.67	1.61	Total	266	1.12	1.04

- Limited effect on PDFs at aN3LO gluon consistent between dijets/inclusive jets. Dijets slightly more constraining on gluon.
- Results here leading colour, full colour effects limited on PDFs.



MSHT20 α_{S} dependence - Jets vs Dijets ^{T.C., L.A. Harland-Lang,} R.S. Thorne: Upcoming!

• LHC 7 and 8 TeV Inclusive Jet and Dijet pulls on $\alpha_S(M_Z^2)$:



- Inclusive jet pulls consistent between orders, differences seen for dijets. Pulls on α_S consistent at aN3LO (but not NNLO).
- Global $\Delta \chi^2$ profiles at NNLO and aN3LO in inclusive jet/dijet fits:



• At NNLO dijets result in larger $\alpha_S(M_Z^2)$, by aN3LO both fits give consistent $\alpha_S(M_Z^2)$ determination, $\alpha_S(M_Z^2) = 0.1170$.

MSHT20 dataset α_S dependence - TopPreliminary!• Perform fits for range $0.112 < \alpha_S(M_Z^2) < 0.122$ in steps of 0.001,
and examine individual dataset α_S dependence via fit quality.



• m_t dependence not included in differential data, only in $\sigma_{t\bar{t}}$ data.

• Top data do not set our strongest bounds on α_S , but do provide slightly weaker bounds \Rightarrow robustness of bounds from global fit.

MSHT20 Top mass α_S Correlation



• Without top data, no m_t sensitivity and no m_t - α_s correlation.

- Total $\sigma_{t\bar{t}}$ data and rapidity differential data show significant m_t - α_S correlation. Reducing m_t and $\alpha_S \Rightarrow$ cross-sections \approx unchanged.
- Data differential in p_T or m_{tt} much less correlated.
- Overall at level of total fit, limited correlation seen (only done at NNLO so far) \Rightarrow can extract m_t at fixed α_s . TC and M.A. Lim: arXiv:2306.14885.

MSHT20 ATLAS 8 TeV Z $p_T \alpha_S$ dependence Preliminary!

- ATLAS 8 TeV Z p_T data with $p_T^Z > 30$ GeV is in the MSHT PDF fit.
- What bounds does it offer within the global PDF fit on $\alpha_S(M_Z^2)$?



- If you do individual dataset extraction you use $\Delta\chi^2 = 1$ for bounds.
- If you do do in a global fit, factoring in tensions with other data you use $\Delta \chi^2 = T^2 = 7.25$ for bounds.
- $p_T^Z > 30$ GeV not very constraining on $\alpha_S(M_Z^2)$ in global PDF fit.
- ATLAS Z $p_T \alpha_S$ result used $p_T^Z < 29 \text{GeV}$ part of spectrum. Used MSHT20 aN3LO PDFs to correspond to accuracy used in resummation.

ATLAS 8 TeV Z $p_T \alpha_S$ dependence (aside): Preliminary!

• Most sensitivity to $\alpha_S(M_Z^2)$ comes from the Sudakov peak region.



• Need fine control ($\mathcal{O}(1\%)$) of effects in small q_T region:

- Missing higher order uncertainties.
- Non-perturbative effects $\mathcal{O}(\Lambda_{NP}/q_T)^2$.
- Flavour thresholds $\mathcal{O}(m_q/q_T)^2$.
- Power corrections $\mathcal{O}(q_T/Q \log^n(q_T/M_Z))^2$.
- Also need to carefully propagate into α_S uncertainty:
 - PDF profiling and tolerance.
 Theory uncertainties.

Results may be very sensitive to theory correlations across spectrum.

Meeting on theory uncertainties in LHC precision measurements, Feb 26th, CERN.

$\mathsf{MSHT}\ \alpha_{\mathcal{S}}\ \mathsf{Bounds}$

More information in articles: T.C., L.A. Harland-Lang, A.D. Martin, R.S. Thorne: 2106.10289, *Eur.Phys.J.C 81 (2021) 8, 744.* T.C., L.A. Harland-Lang, R.S. Thorne: *Upcoming!*

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MSHT $\alpha_S(M_7^2)$ determination

3. MSHT α_S Bounds

 $\alpha_s(M_7^2)$

MSHT20 α_{S} bounds - NNLO

Consistent with α_S bounds seen in previous studies, and between orders (NNLO and aN3LO).

BCDMSp data strongest constraint upwards: $\Delta \alpha_S(M_Z^2)$ = +0.0014.

SLACp and ATLAS 8TeV Zp_T both give upper bound: $\Delta \alpha_S(M_Z^2) = +0.0018.$

CMS/ATLAS (dilepton) $t\bar{t}$ single diff. would give lower/same upper α_S bound, but not used.



nd between orders NNLO and aN3LO).

> ATLAS 8 TeV Z data gives lower bound: $\Delta \alpha_S(M_Z^2)$ = -0.0010.

NMC deuteron, ATLAS 8 TeV High Mass DY give lower bounds of $\Delta \alpha_S(M_Z^2)$ -0.0017, -0.0018.

Preliminary!

• Therefore upper/lower bounds are +0.0014/-0.0010 at NNLO.

 $\alpha_{S,\text{NNLO}}(M_Z^2) = 0.1171 \pm 0.0014 \xrightarrow{\text{Consistent with World Average}}{\text{of } 0.1180 \pm 0.0009}$ T.C., L.A. Harland-Lang, R.S. Thorne: *Upcoming!*Thomas Cridge DESY MSHT $\alpha_S(M_Z^2)$ determination 6th February 2024 21/25

 $\alpha_{\rm e}(M_7^2)$

MSHT20 α_{S} bounds - aN3LO

Preliminary!

Consistent with α_S bounds seen in previous studies, (NNLO and aN3LO).

BCDMSp data strongest constraint upwards: $\Delta \alpha_{S}(M_{7}^{2})$ = +0.0013.

 F_{2}^{c} provides upwards bound of: $\Delta \alpha_S(M_z^2) = +0.0020.$

CMS and ATLAS (dilepton) $t\overline{t}$ single diff. would give slightly higher upper α s bounds, but not used.



and between orders

SLAC deuteron data gives lower bound: $\Delta \alpha_S(M_7^2)$ = -0.0016

NMC deuteron. ATLAS 8 TeV Z both give lower bounds of $\Delta \alpha_{S}(M_{7}^{2})$ = -0.0017

Missing Higher Order Uncertainties now included, in particular causes some LHC bounds to weaken as unknown N3LO K-factors.

• Therefore upper/lower bounds are +0.0013/-0.0016 at aN3LO.

$$M_{S,\mathrm{aN3LO}}(M_Z^2) = 0.1170 \pm 0.0016$$

Consistent with (NNLO) World Average of 0.1180 ± 0.0009 .

T.C., L.A. Harland-Lang, R.S. Thorne: Upcoming!

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MSHT $\alpha_{s}(M_{\pi}^{2})$ determination

MSHT PDF $\alpha_{\mathcal{S}}$ Dependence

More information in articles: T.C., L.A. Harland-Lang, A.D. Martin, R.S. Thorne: 2106.10289, *Eur.Phys.J.C 81 (2021) 8, 744.* T.C., L.A. Harland-Lang, R.S. Thorne: *Upcoming!*

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MSHT $\alpha_S(M_7^2)$ determination

MSHT20 PDF α_S dependence

Forte, Kassabov: 2001.04986

• Correlations between PDFs and $\alpha_S \Rightarrow$ necessity of global fit.



• Changes generally within PDF uncertainties for $\Delta \alpha_S(M_Z) \approx \pm 0.001$.

- Gluon anti-correlated with $\alpha_S(M_Z^2)$ for $x \leq 0.1$ as maintains $dF_2/dQ^2 \sim \alpha_S g$. Implies correlated at high $x \gtrsim 0.1$ by momentum sum rule.
- Larger effect at low Q^2 as less evolution distance.
- Smaller effects on quarks, reduced/increased at high/low x by splitting. s less impacted, at high x may absorb some of change.

MSHT20 aN3LO pieces α_S dependence

- Technical aside we have theory "nuisance" parameters for the few unknown (at time of publication) theoretical ingredients at aN3LO.
 - How do the posteriors change with $\alpha_S(M_Z^2)$?
- Most change very little. Splitting functions show some change:



- Changes within uncertainties, well within for everything except P_{gg} shows most change, as expected it's the most correlated with α_{S} .
- As seen in dataset χ^2 profiles, unknown aN3LO K-factors weaken α_S sensitivity. May obtain stronger bounds as these become known. T.C., L.A. Harland-Lang, R.S. Thorne: *Upcoming!*

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Preliminary!

4. MSHT PDF + α_S dependence

MSHT20 Cross-section PDF + α_S dependence

• Cross-section uncertainties at NNLO/aN3LO (left/right) at the LHC.



- Direct α_S uncertainty through xsec is small for DY. Total α_S sensitivity larger due to change of PDFs with α_S.
- Direct α_S uncertainty of ggF Higgs is larger ($\sim 2 3\%$), reduced by anti-correlation of gluon with α_S .
- Higher energies sample lower x quarks \Rightarrow larger α_S uncertainties.
- Interplay of direct and indirect (through PDFs) effects \Rightarrow importance of treating PDFs+ α_S together.

Summary

More information in articles:

J. McGowan, T.C., L.A. Harland-Lang, R.S. Thorne: 2207.04739, *Eur.Phys.J.C 83 (2023) 3, 185.* T.C., L.A. Harland-Lang, A.D. Martin, R.S. Thorne: 2106.10289, *Eur.Phys.J.C 81 (2021) 8, 744.* T.C., L.A. Harland-Lang, R.S. Thorne: *Upcoming!*

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MSHT $\alpha_S(M_7^2)$ determination

MSHT20 PDF set availability

- All PDFs used, those relevant for $\alpha_S(M_Z^2)$ and many others provided on LHAPDF and http://www.hep.ucl.ac.uk/msht/.
- Small selection (all already available):

PDF set	$\alpha_S(M_Z^2)$ central value	$\alpha_{S}(M_{Z}^{2})$ range	QCD Order
MSHT20an3lo_as118	0.118	-	aN3LO
MSHT20nnlo_as118	0.118	-	NNLO
MSHT20nlo_as118	0.118	-	NLO
MSHT20nlo_as120	0.120	-	NLO
MSHT20an31o_as_smallrange	0.118	0.114 - 0.120	aN3LO
MSHT20nnlo_as_largerange	0.118	0.108 - 0.130	NNLO
MSHT2Onlo_as_largerange	0.120	0.108 - 0.130	NLO
MSHT20qed_an31o	0.118	-	aN3LO (+NLO QED)

- Many more PDF sets online! Please use them.
- We provide the $\Delta \chi^2$ values with $\alpha_S(M_Z^2)$.

Conclusions

T.C., L.A. Harland-Lang, R.S. Thorne: Upcoming!

- Analysed α_S dependence of global PDF fit using MSHT20 NNLO and aN3LO sets.
- Used PDF sensitivity to α_S and global fit nature to extract $\alpha_S(M_Z^2)$ best fit value and uncertainty (via dynamical tolerance procedure) à la PDF uncertainty. Consistent with World Average

• Newly obtained:

Preliminary!

of 0.1180 \pm 0.0009.

 $\alpha_{S,\text{NNLO/aN3LO}}(M_Z^2) = 0.1171 \pm 0.0014 \ / \ 0.1170 \pm 0.0016$

- Consistent central values, slightly larger aN3LO uncertainty due to inclusion of MHOU theory uncertainty.
- Investigated dependence of different datasets on $\alpha_S(M_Z)$ within the global PDF fit and set bounds on $\alpha_S(M_Z^2)$.
- Examined α_S - m_t and PDF- α_S correlations and latter effect on 13/14 TeV LHC cross-section uncertainties.
- All PDF sets made available for use by community!

Backup Slides

MSHT20 α_S bounds - Constraining Datasets Preliminary!

• The most constraining datasets on $\alpha_S(M_Z^2)$ within our global PDF fit are:

Order best fit $\alpha_S(M_Z^2)$	best fit $\alpha_{e}(M^{2})$	Upper/Lower bounds			
	1	2	3		
NNLO 0.1171	+0.0014 (BCDMS proton)	+0.0018 (ATLAS 8 TeV Z p _T)	+0.0018 (SLAC proton)		
	-0.0010 (ATLAS 8 TeV Z)	-0.0017 (NMC deuteron)	-0.0018 (ATLAS High Mass DY)		
aN3LO 0.1170	0 1170	+0.0013 (BCDMS proton)	$+0.0020 (F_2^c)$	+0.0024 (CMS 7 TeV W + c)	
	0.1170	-0.0016 (SLAC deuteron)	-0.0017 (NMC deuteron)	-0.0017 (ATLAS 8 TeV Z)	

- Find similar results between NNLO and aN3LO and as previous results:
 - BCDMS proton data provides tightest upper bound, but other datasets also bound.
 - Deuteron data (SLAC, NMC) provide lower bounds, as do LHC Drell-Yan data.
- Top datasets do not provide strongest bounds, but offer further slightly weaker bounds (though note m_t dependence not incorporated).
 T.C., L.A. Harland-Lang, R.S. Thorne: Upcoming!

MSHT20 α_S bounds - NNLO (with m_t examined)



- $\alpha_S(M_Z^2)$ bounds from <u>NNLO fit</u> where m_t variation examined.
- CMS 8 TeV $y_{t\bar{t}}$ lepton+jet data provides competitive upper bound on α_S (identical to BCDMS proton data), total cross-section $\sigma_{t\bar{t}}$ also provides slightly weaker upper bound. TC and M.A. Lim: arXiv:2306.14885.

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MSHT20 $\alpha_S(M_7^2)$ determination

What do we already know for N3LO PDFs?

- Full N3LO PDFs need all N3LO pieces for both PDFs and included cross-sections to be known, not yet possible as some pieces missing.
- Still, a lot of information is known already (schematic summary):

Theory	Utility	Order required	What's known?	
1. Splitting functions $P_{ab}^{(3)}(x)$	PDF evolution	4-loop	Mellin moments ³⁻⁵ , leading small-x behaviour ^{3,6-11} , plus some leading large-x in places ³ . <i>Plus new</i> $^{12-15}$.	
2. Transition matrix elements $A^{(3)}_{ab,H}(x)$	Transitions between number of flavours in PDFs at mass thresholds	3-loop	Mellin moments ^{16,17} , leading small-x behaviour ^{18–19} , plus some leading large-x in places ^{19,20} . <i>Plus new</i> ^{21–23} .	
3. DIS Coefficient functions (NC DIS) $C_{H,a}^{VF,(3)}$	Combine with PDFs and Transition Matrix Elements to form Structure Functions (NC DIS)	N3LO	Some approximations to FFNS (low Q^2) coefficient functions at α_S^3 (with exact LL pieces at low x, NLL unknown) ²⁴⁻²⁶ , ZM-VFNS (high Q^2) N3LO coefficient functions known exactly ²⁷ . Therefore GM-VFNS not completely known.	
4. Hadronic Coefficients (K-factors)	Determine cross-sections at N3LO	N3LO	Very little (none in usable form for PDFs)	

• Knowledge of lower orders can guide us for remaining unknown pieces.

How do we use this info.? - Splitting Functions Ingredient 1

- We need singlet P_{gg} , P_{gq} , P_{qg} , P_{qq}^{ps} and non-singlet, e.g. $P_{qq}^{ns,+}$.
- What do we know and how do we incorporate this information?:
 - ► Even low-integer *N* Mellin Moments (4-8)(now 5-10 known¹²⁻¹⁵)
 - constrain intermediate and high x via $\int_0^1 dx \, x^{N-1} P(x)$.
 - Parameterise P⁽³⁾_{ab}(x) with functions f_{1,...,k} where k = No. of known moments and vary basis for uncertainty.
 - Exact LL form at low x from resummation included in f_e(x, ρ_{ab}). E.g. for P³_{ag}:

$$f_{e}(x,\rho_{qg}) = \frac{C_{A}^{3}}{3\pi^{4}} (\frac{82}{81} + 2\zeta_{3}) \frac{1}{2} \frac{\ln^{2}(1/x)}{x} + \rho_{qg} \frac{\ln 1/x}{x}$$

- Uncertainty on this through coefficient of leading missing low x log as theory nuisance parameter (TNP) ρ_{ab} .
- Include relevant high x known pieces also in $f_e(x)$.
- So overall: $P_{ab}^{(3)}(x) = \sum_{i=1}^{k} A_i f_i(x) + f_e(x, \rho_{ab}) \qquad \begin{array}{c} 1 \text{ TNP per Splitting} \\ Function = 5 \text{ TNPs.} \end{array}$ Thomas Cridge DESY MSHT20 $\alpha_s(M^2)$ determination 6th February 2024 5/38

Comparison of Splitting Functions

- Now 5 moments for P_{gg} , P_{gq} ^{12,13} and 10 for P_{qq}^{PS} , P_{qg} ^{14,15}.
- Largely good agreement with MSHT determinations in central values.
- Exception is P_{gq} , least well determined (one extra low x log unknown).
- Reduction in P_{qq}^{PS} , P_{qg} uncertainties. Impacts reduced once in PDF fit.



How can we incorporate N3LO knowledge into PDFs?

- Consider usual PDF fit probability: $P(T|D) \propto \exp(-\chi^2) \propto \exp(-\frac{1}{2}(T-D)^T H_0(T-D))$ $\propto \exp(-\frac{1}{2}\sum_{k=1}^{N_{pt}} \frac{1}{s_k^2}(D_k - T_k - \sum_{\alpha=1}^{N_{corr}} \beta_{k,\alpha}\lambda_{\alpha})^2 + \sum_{\alpha=1}^{N_{corr}} \lambda_{\alpha}^2)$ Experimental Nuisance parameters
- Include known N3LO pieces + parameterise remaining unknown pieces \Rightarrow theory nuisance parameters (θ') and allow to vary \rightarrow uncertainty.
 - \blacktriangleright Probes precisely the missing higher order terms. \checkmark
 - ► Allows inclusion of known N3LO information (a lot) without needing to wait for remaining few pieces. ✓ (LA. Harland-Lang, R.S. Thorne 1811.08434 NNPDF 2207.07616
 - ► Avoids scale variations can underestimate MHOU, issue of correlation between PDF fit and use, no need to raise Q² cut on data to enable downwards scale variations. √
 - \blacktriangleright Exactly same data can be included at all orders. \checkmark

(Theoretical Nuisance Parameters more generally \rightarrow F. Tackmann SCET Workshop 2019)

Perform aN3LO fit - PDF impacts:

- Gluon enhanced at small x due to higher power large logs that appear.
- Gluon uncertainty increased at small x due to theory uncertainty, largely on splitting functions.
- Heavy quarks c and b (perturbatively generated) raised due to increase in gluon at lower x and raised A_{Hg} at high







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MSHT20 $\alpha_{S}(M_{\pi}^{2})$ determination

Perform aN3LO fit - PDF impacts:

• Milder effects on other PDFs:



Fit with no N3LO k-factors gives very similar PDFs to full aN3LO fit
 ⇒ Effect of approximate N3LO fitted k-factors on PDFs is very mild.
 Theory uncertainty from MHOUs enlarges PDF uncertainty at small x.

6. Backup Slides

Impact of aN3LO evolution on PDFs:

- <u>aN3LO</u> evolution benchmarking use toy PDFs, no fit, no other complications and check impacts, as in hep-ph/0511119 (NNLO).
- Difference relative to NNLO evolution:



- Agreement between groups down to 10^{-3} , i.e. over data region.
- Up to few percent level effects on PDFs here due to N3LO evolution.
- Differences outside this with larger uncertainties at (very) low x.
- New information provides some additional constraints but still consistent with previous determinations.
- Different groups agree when using the same splitting functions.

Selection of some aN3LO references (others on slides)

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Old Results from here onwards!

MSHT20

- MSHT20 New PDF set from MSTW/MMHT/MSHT group for precision LHC era. arXiv:2012.04684, very extensive paper.
- Significant developments on all three fronts theoretical, experimental, methodological.
 - Theoretical Vast majority of processes included have full NNLO QCD theory, with NLO EW where relevant.
 - Experimental Many new datasets, more precise, more channels, more differential.
 - Methodological Extended parameterisation to allow fitting accuracy to < 1% if data allows, better knowledge of central values (52 PDF parameters) and uncertainties (32 eigenvectors - 64 directions).
- Global fit ⇒ 61 different datasets 10 Structure Function, 6 neutrinos, 2 fixed target DY, 8 HERA, 8 Tevatron, 27 LHC.

6. Backup Slides

MSHT α_S dependence - NLO and NNLO (previous)

- Default PDFs provided at standard fixed value of $\alpha_S(M_Z^2) = 0.118$.
- Can also allow α_S to be a free parameter in the fit.
- Global fit nature of PDFs \Rightarrow can provide a precise, accurate determination of α_S .
- Individual datasets have different dependences on α_{S} , but robust determination utilising all datasets. $\alpha_{S,NNLO}(M_Z^2) < \alpha_{S,NLO}(M_Z^2)$ as NNLO corrections +ve, so
- The best fit values <u>were</u> found to be: fitting same data \Rightarrow lower α_s .



6. Backup Slides

MSHT20 dataset α_S dependence - Fixed Target/DIS • Perform fits for range $0.108 < \alpha_S(M_Z^2) < 0.130$ in steps of 0.001, and examine individual dataset α_S dependence via fit quality.



- BCDMS, SLAC high x experiments, dominated by non-singlet \Rightarrow cleaner means of evaluating α_s .
- HERA is lower x and dominated by α_S and gluon so correlation.

MSHT20 dataset α_S dependence - Jets/ Zp_T

• Perform fits for range $0.108 < \alpha_S(M_Z^2) < 0.130$ in steps of 0.001, and examine individual dataset α_S dependence via fit quality.



• Jets, Zp_T datasets have direct sensitivity to α_S , prefer lower α_S .

MSHT20 dataset α_S dependence - Top

• Perform fits for range $0.108 < \alpha_S(M_Z^2) < 0.130$ in steps of 0.001, and examine individual dataset α_S dependence via fit quality.





- Top data generally prefer lower α_S , but:
 - Total σ poor fit at NLO (+ unrealistic m_t), large NNLO corrections \Rightarrow NLO less relevant.
 - 2 m_t dependence not included in differential data, fixed at 173.3 GeV.

• Top data will not used to set global bounds on $\alpha_S(M_Z^2)$.

6. Backup Slides

MSHT20 dataset α_S dependence - W, Z

• Perform fits for range $0.108 < \alpha_S(M_Z^2) < 0.130$ in steps of 0.001, and examine individual dataset α_S dependence via fit quality.



• High precision W, Z data have indirect sensitivity to α_S through their precision, generally prefer higher α_S values (but not always).

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MSHT20 $\alpha_S(M_7^2)$ determination

6th February 2024

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MSHT20 α_{S} bounds

- Can use these fits at fixed α_S in steps of 0.001 to determine bounds each dataset places on $\alpha_S(M_Z^2)$.
- Apply Dynamical Tolerance Method apply to α_S in same way as to PDF eigenvectors.
- Hypothesis testing criteria determine point at which $\Delta \chi_i^2$ exceeds that set by 68% CL.

- Sets Tolerance $T_i = \sqrt{\chi_i^2}$ which determines bounds from dataset *i*.
- Tightest bounds around best fit α_S then sets overall global fit uncertainty bounds on α_S.

6. Backup Slides

MSHT20 α_S bounds - NNLO



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MSHT20 $\alpha_S(M_7^2)$ determination

oth February 2024

6. Backup Slides



Procedure for combining PDF and α_S dependence

- Within Hessian approach to PDF uncertainties, correct manner to determine combined PDF+ $\alpha_S(M_Z^2)$ uncertainty for any quantity, including correlations between PDFs and α_S is:
 - Take PDFs determined at $\alpha_S(M_Z^2) \pm \Delta \alpha_S(M_Z^2)$ and treat as additional pair of eigenvectors.
 - 2 Determine quantity to obtain $\Delta \sigma_{\alpha_s}$.
 - Sombine uncertainties in quadrature:

Quadrature as whilst central values correlated errors uncorrelated. CT: 1004 4624

$$\Delta \sigma = \sqrt{(\Delta \sigma_{\rm PDF})^2 + (\Delta \sigma_{\alpha_s(M_Z^2)}^2)}$$

- Works provided central PDFs are best fit PDFs with $\alpha_S(M_Z^2)$ free.
- Choice of $\Delta \alpha_S(M_Z^2)$ up to user but recommended to be close to our 1σ bounds, e.g. ± 0.001 for simplicity and near that of world average.

MSHT20 $\sigma \alpha_S$ dependence - W, Z

- Larger PDF uncertainties at Tevatron than LHC as samples larger x.
- Direct α_S uncertainty only fraction of % as NLO correction is ~ 20%.



N.B. "Direct" α_S uncertainty = direct effect of α_S on xsec. "Indirect" α_S uncertainty = effect of α_S on PDFs and through them onto xsec.

- Indirect α_S uncertainty is larger from change in PDFs with α_S quarks increase below $x \lesssim 0.1$ with increasing α_S .
- Higher energies sample lower x quarks \Rightarrow larger α_S uncertainties.
- Conclusion: α_S uncertainty smaller than PDF uncertainty, Total PDF + α_S uncertainty only ~ 20% larger than PDF uncertainty.

MSHT20 $\sigma \alpha_{S}$ dependence - top

- At Tevatron main production is $q\bar{q}$ $\mathcal{O}(\alpha_s^2)$ and samples $x \sim 0.2$.
- Direct α_5 uncertainty ~ 2%. Indirect part small as transition region.



PDF uncertainties reduce with energy as sampling lower x gluon, which is more constrained.

- At LHC have gg fusion, and samples lower x, gluon fixed point of evolution is $x \sim 0.1$ with increasing α_{S} below this decreasing gluon.
- Indirect $\alpha_{\rm S}$ sensitivity cancels across fixed point for 8 TeV, but larger for 13 TeV - increasing α_S increases $\sigma_{t\bar{t}}$ but reduces gluon so anti-correlation and reduced net α_S uncertainty now ~ 1.5%.
- At 100 TeV more anti-correlation therefore α_5 uncertainty $\sim 1.2\%$.

MSHT20 $\sigma \alpha_S$ dependence - Higgs

• gg fusion is $\mathcal{O}(\alpha_5^2)$ with large +ve NLO and NNLO contributions \Rightarrow direct α_5 uncertainty contribution is 2-3%.



PDF uncertainties reduce with energy as sampling lower x gluon, which is more constrained.

- Tevatron, LHC and FCC probe $x \approx 0.06, 0.01 0.02, 0.001$, in all regions gluon anti-correlated with α_5 .
- Also some correlated contribution from high x poorly constrained g.
- Therefore indirect α_S sensitivity reduces σ as gluon reduced, more so at LHC and FCC.
- Net conclusion: Total PDF+ α_S uncertainty is factor of 1.6-1.7x PDF.

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BCDMSp data



Fig. from MRST paper: hep-ph/9803445.

• BCDMSp data spans large Q^2 range, even within itself it needs fall in structure function with Q^2 to be flatter \Rightarrow reduced α_S favoured.

MSHT20 PDF α_S dependence - quarks

• Correlations between PDFs and α_s .

Changes of PDFs generally within PDF uncertainties, certainly at larger scales



- High x quarks reduced with increasing α_S as increases splitting.
- Small x quarks increase with α_S as reinforced by gluon splitting.
- Strange relatively insensitive to α_S , partly due to compensation in BR $B(D \rightarrow \mu)$ which can change normalisation.
- High x strange raised as poorly determined and compensates for reduction in u, d. Low x strange raised by gluon splitting with α_S.

MSHT20 $\alpha_{S}(M_{Z}^{2})$ effects on global fit χ^{2}

$\alpha_S(M_Z^2)$	$\Delta \chi^2_{\rm global}(\rm NLO)$	$\Delta \chi^2_{\rm global}(\rm NNLO)$
0.108	1188.6	909.6
0.109	991.0	715.0
0.110	813.6	553.1
0.111	654.8	405.4
0.112	556.5	290.0
0.113	434.4	192.6
0.114	324.5	118.2
0.115	230.2	61.8
0.116	151.7	21.8
0.117	91.3	2.6
0.1174	-	0
0.118	50.3	2.7
0.119	10.7	22.1
0.120	1.1	61.1
0.1203	0	-
0.121	3.3	119.3
0.122	27.1	197.9
0.123	56.1	296.1
0.124	110.8	414.4
0.125	177.5	553.8
0.126	257.8	715.0
0.127	351.2	902.0
0.128	469.0	1107.8
0.129	602.0	1344.6
0.130	748.6	1596.7

The quality of the global fit versus $\alpha_S(M_Z^2)$ at NLO and NNLO relative to the best fits at $\alpha_S(M_Z^2) = 0.1203, 0.1174$

respectively. The number of data points in the global fit is 4363.

MSHT20 α_S heavy quark mass link

• Correlations between m_c and $\alpha_s(M_Z^2)$.

More information in article: TC et al, arXiv: 2106.10289, *Eur.Phys.J.C* 81 (2021) 8, 744.

m_c (GeV)	$\chi^2_{ m global}$	$\chi^2_{\tilde{\sigma}c\bar{c}}$	$\alpha_S(M_Z^2)$
	4363 pts	79 pts	
1.2	5134	153	0.1172
1.25	5123	143	0.1172
1.3	5118	137	0.1173
1.35	5117	133	0.1173
1.4	5119	132	0.1174
1.45	5125	132	0.1175
1.5	5136	135	0.1175
1.55	5150	140	0.1176
1.6	5168	144	0.1177

The quality of the fit versus the quark mass m_c at NNLO with $\alpha_S(M_7^2)$ left free.

- Preferred value of $\alpha_S(M_Z^2)$ when fit as free parameter at fixed m_c increases as m_c is increased.
- Occurs as large charm mass suppresses charm, increased α_S speeds up evolution and compensates for this to therefore still fit the data.

MSHT20 m_c dependence

- Default charm (pole) mass $m_c = 1.4$ GeV, vary in steps of 0.05GeV in range 1.2GeV $\leq m_c \leq 1.6$ GeV and examine fit qualities.
- Assume all perturbative heavy flavour, i.e. no intrinsic non-perturbative component ⇒ neither fitted nor intrinsic charm.



- Overall global fit dependence (left) centred on $m_c \approx 1.35 \text{GeV}$.
- HERA heavy flavour combined charm and bottom (right) prefer charm mass very close to our default $m_c = 1.4 \text{GeV}$.
- Very low values of m_c clearly disfavoured, in contrast to MMHT14.

MSHT20 m_b dependence

• Default bottom (pole) mass $m_b = 4.75$ GeV, vary in steps of 0.25GeV in range 4.0GeV $\leq m_b \leq 5.5$ GeV and examine fit qualities.



- Overall global fit dependence (left) centred on $m_b \approx 4.5 \text{GeV}$.
- HERA heavy flavour combined charm and bottom (right) prefer bottom mass very close to our default $m_b = 4.75 \text{GeV}$.
- Very low values of m_b clearly disfavoured, in contrast to MMHT14.

6. Backup Slides

MSHT20 PDF m_c dependence



More information in article: TC et al, arXiv:2106.10289, Eur. Phys. J.C 81 (2021) 8, 744.

MSHT20 PDF m_b dependence



More information in article: TC et al, arXiv:2106.10289, Eur. Phys. J.C 81 (2021) 8, 744.

MSHT20 PDFs in 3- and 4- Flavour Number Schemes

- In MSHT20 we use GM-VFNS with maximum of 5 active flavours.
- Could instead keep info. about heavy quark in coefficient functions only, i.e. only generate heavy quarks in final state ⇒ FFNS.
- Can determine 3- and 4- flavour scheme PDFs from our default GM-VFNS but with evolution of b (4-)/ b and c (3-) turned off.
- Turn off also contribution of heavy quark to running coupling as relevant \Rightarrow coupling runs more quickly above $m_{c,b}$.



• Also slower evolution so less quarks at small x and more at high x. More information in article: TC et al, arXiv:2106.10289, *Eur.Phys.J.C* 81 (2021) 8, 744.

Acknowledgments



This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 101002090 COLORFREE).