Heavy quarks and CTEQ-TEA PDFs at (N)NNLO

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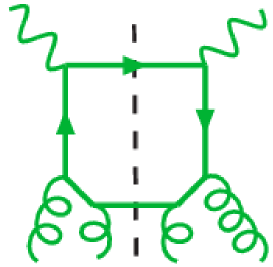
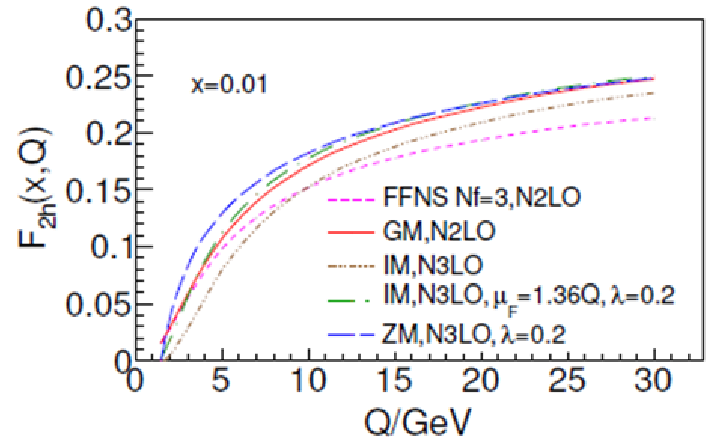
Shanghai Jiao Tong University: J. Gao

Xinjiang University: S. Dulat, I. Sitiwaldi





Massive quark scattering in a global context

Eventually, the exciting ideas discussed at this workshop are applied to answer deep physics questions, for instance, to better determine unpolarized sea PDFs in heavy-flavor (HF) processes

The global QCD analysis by CTEQ-TEA offers a systematic theoretical framework to get such answers

Precision determination of PDFs requires to follow consistent QCD theory to the HF scattering contributions at every step:

- **in the experimental analyses**
- **in the PDFs**
- **in the hard cross sections**

Consistent choices for

- heavy-quark factorization scheme
- heavy-quark masses
- heavy-quark higher-twist terms

Demystifying QCD factorization with massive quarks at NNLO

1. SACOT-MPS factorization scheme for heavy-quark scattering

[Keping Xie, Ph. D. thesis, https://tinyurl.com/XiePhD2019, 2019]

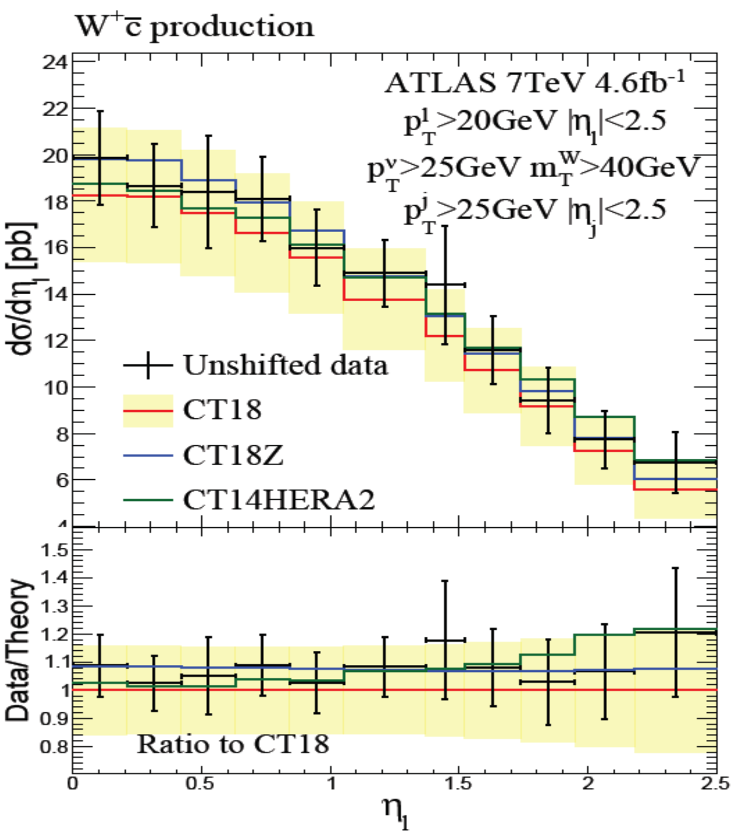
2. Twist-4 contributions with heavy quarks: intrinsic charm, fitted charm, …

[T.-J. Hou et al., arXiv:1707.00657]

Heavy-quark calculations at the NNLO frontier

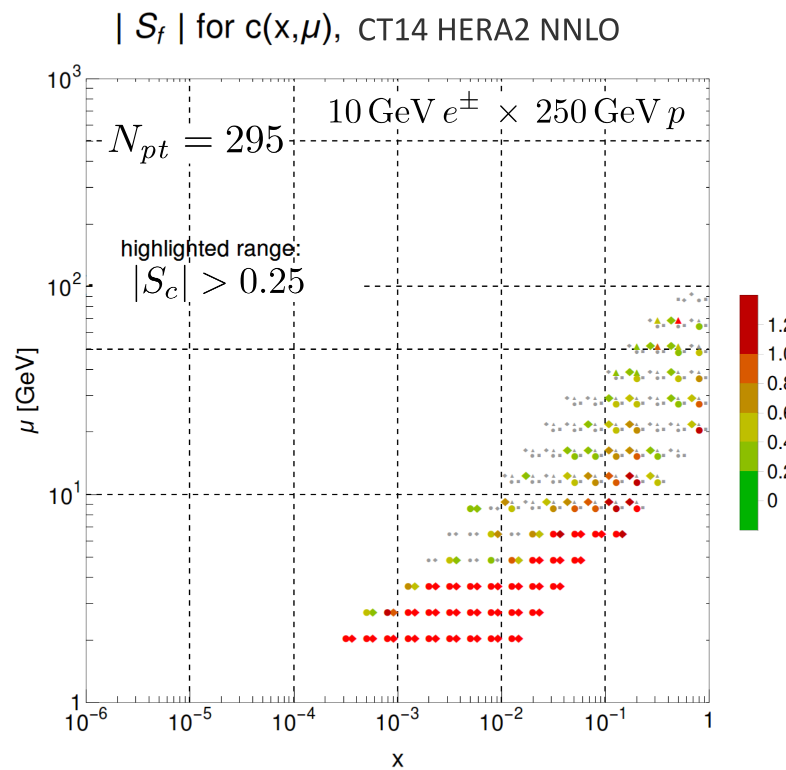
Numerous heavy-flavor measurements are available and become increasingly suitable for precise tests of QCD and nucleon/nuclear PDFs

The LHC: $pp \to VQX$;
$V = W^{\pm}c$; $Q = c, b$ ...



T.-J. Hou et al.,arXiv:1912.10053

HERA, EIC: DIS and semi-inclusive DIS

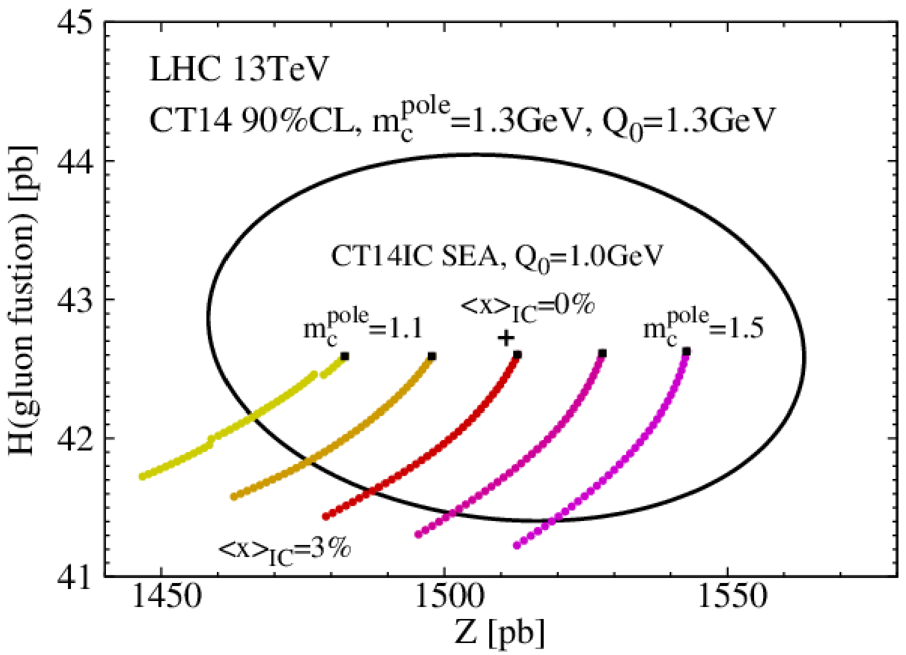


Projected EIC sensitivity to the charm PDF [T. Hobbs, B.T. Wang, P.N., Olness]

Various precision cross sections are sensitive to heavy quarks

Heavy-quark (s, c, b) PDFs are the least constrained distributions;

- their uncertainties affect a variety of electroweak precision measurements and new physics searches



Dependence of the LHC Z and Higgs production on the charm mass and intrinsic charm component [T.-J. Hou et al., arXiv:1707.00657]

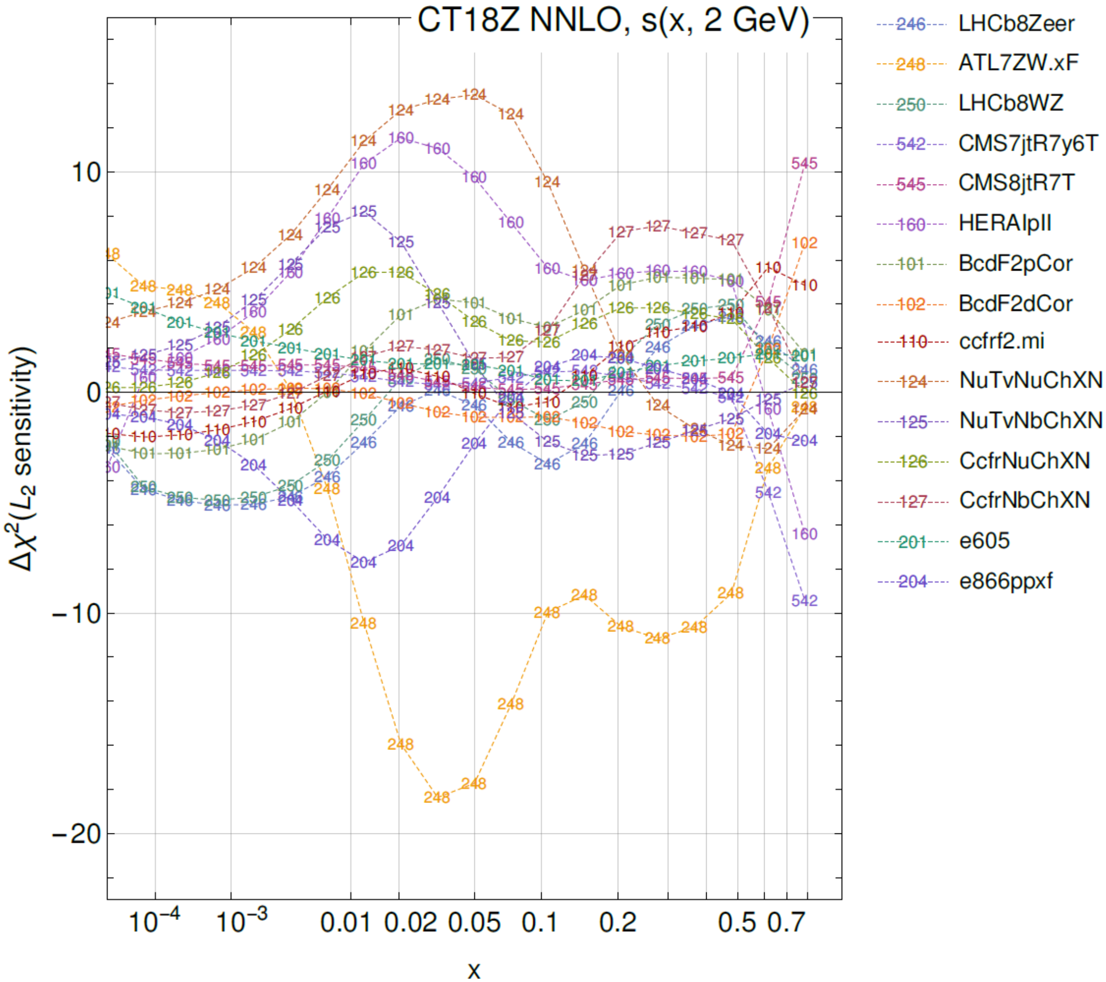
CT18 PDFs with new LHC data

T.-J. Hou et al.,arXiv:1912.10053

Included experiments:

- Combined HERA1+2 DIS
- LHCb 7 TeV Z, W muon rapidity dist.
- LHCb 8 TeV Z rapidity dist.
- ATLAS 7 TeV inclusive jet
- CMS 7 TeV inclusive jet
- ATLAS 7 TeV Z pT dist.
- LHCb 13 TeV Z rapidity dist.
- CMS 8 TeV Z pT and rapidity dist.
- CMS 8 TeV W, muon asymmetry dist.
- ATLAS 7 TeV W/Z, lepton(s) rapidity c
- CMS 7,8 TeV tT differential dist.
- ATLAS 7,8 TeV tT differential dist.

PDF uncertainties in many DIS, vector boson production data sets are sensitive to s, c PDFs



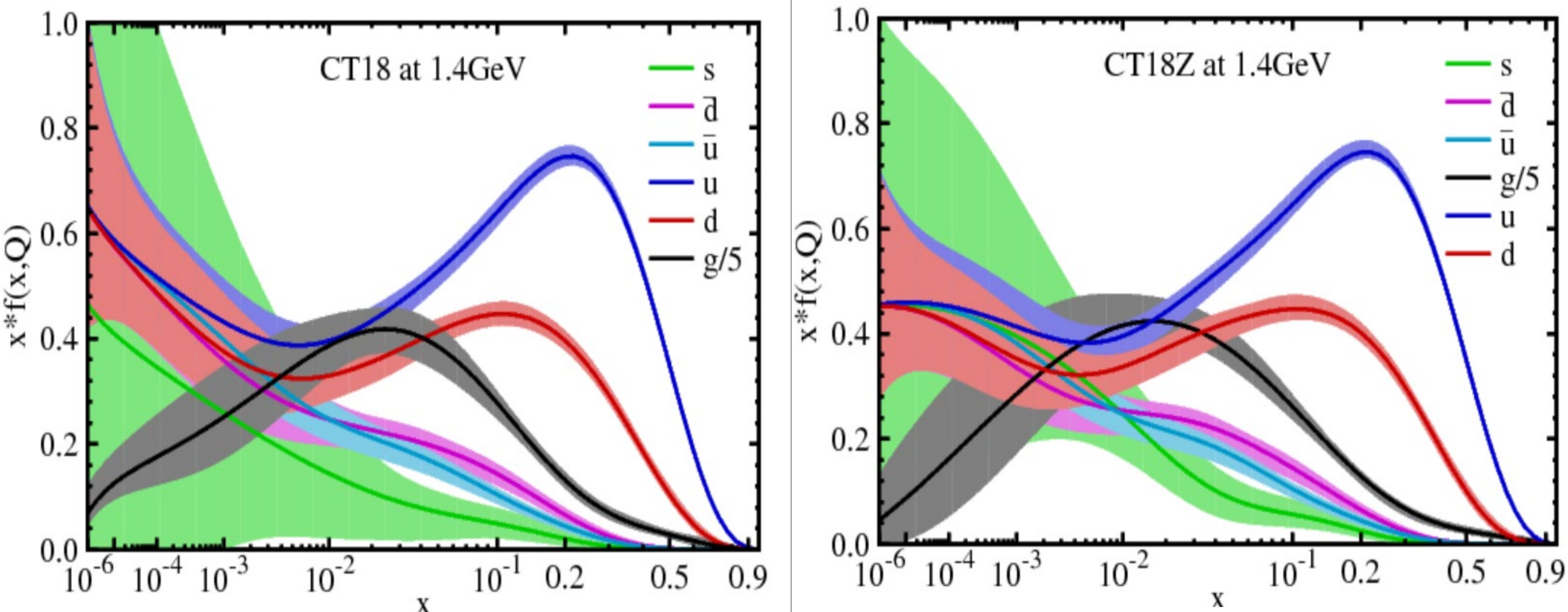
Sensitivity of CT18Z experiments to the strangeness PDF

Note strongly opposing pulls on χ^2 from some experiments

CT18 parton distributions

[T.-J. Hou et al.,arXiv:1912.10053]

Four PDF ensembles: CT18 (default), A, X, and Z



CT18Z has enhanced gluon and strange PDFs at $x \sim 10^{-4}$, and reduced light-quark PDFs at $x < 10^{-2}$. **CT18 PDFs are fitted to HERA-I combined charm cross sections (1211.1182), CCFR and NuTeV dimuon production, as well as inclusive DIS cross sections**

SACOT
= Simplified Aivazis-Collins-Olness-Tung scheme

ACOT, PRD 50 3102 (1994); Collins, PRD 58 (1998) 094002;
Kramer, Olness, Soper, PRD (2000) 096007; Tung, Kretzer, Schmidt, J.Phys. G28 (2002) 983

The default heavy-quark scheme of CTEQ-TEA PDFs
Implementation is based upon, and closely follows, the proof of QCD factorization for DIS with massive quarks *(Collins, 1998)*

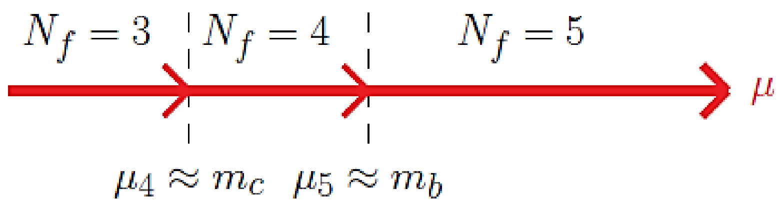
MPS/χ prescription $\equiv$ Kinematic matching based on **m**assive **p**hase **s**pace to improve perturbative convergence near HF production threshold

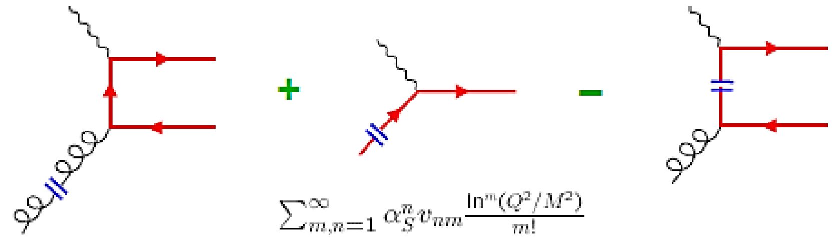
Applied
- to NNLO in NC DIS (Guzzi et al.; arXiv:1108.5112)
- to NLO in heavy-flavor hadroproduction using MCFM

(Xie, Campbell, Nadolsky, 2019-2020)

In CC dimuon DIS, the NNLO correction is relatively small (Berger, Gao, arXiv:1710.04258)

SACOT-MPS scheme: advantages

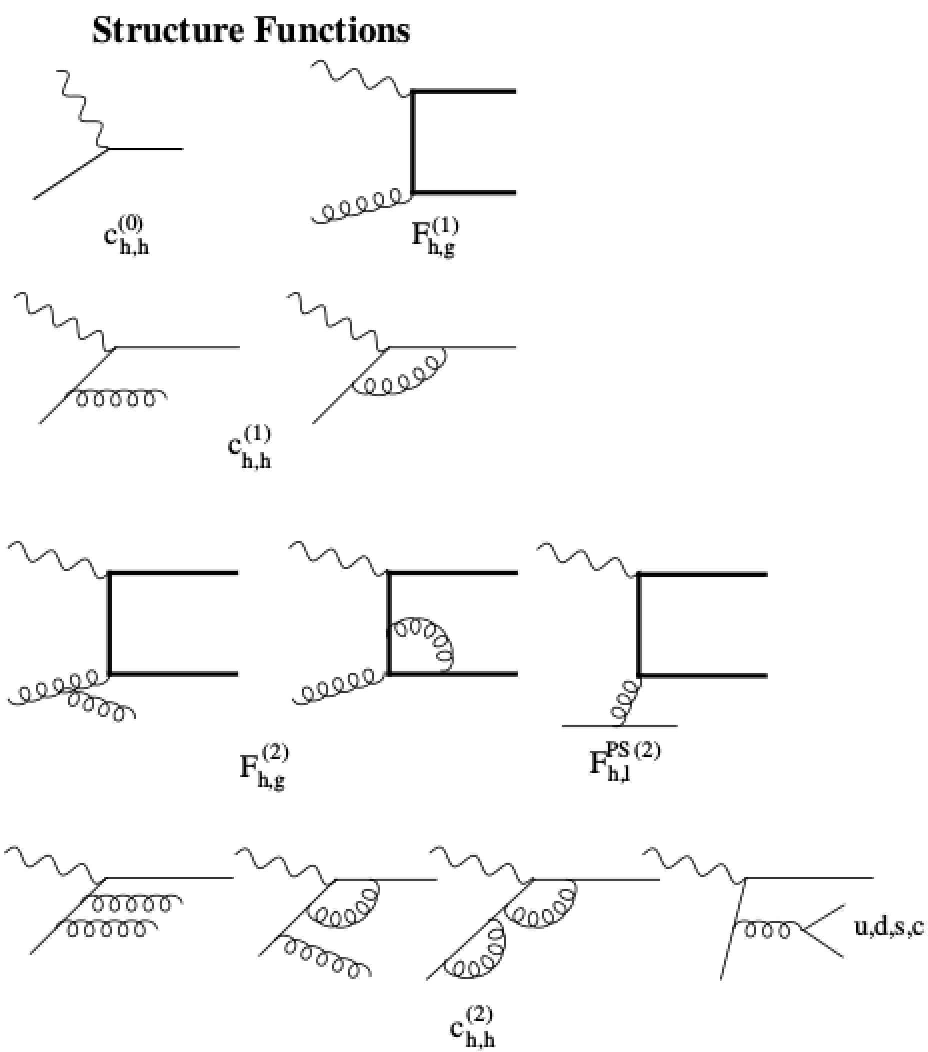


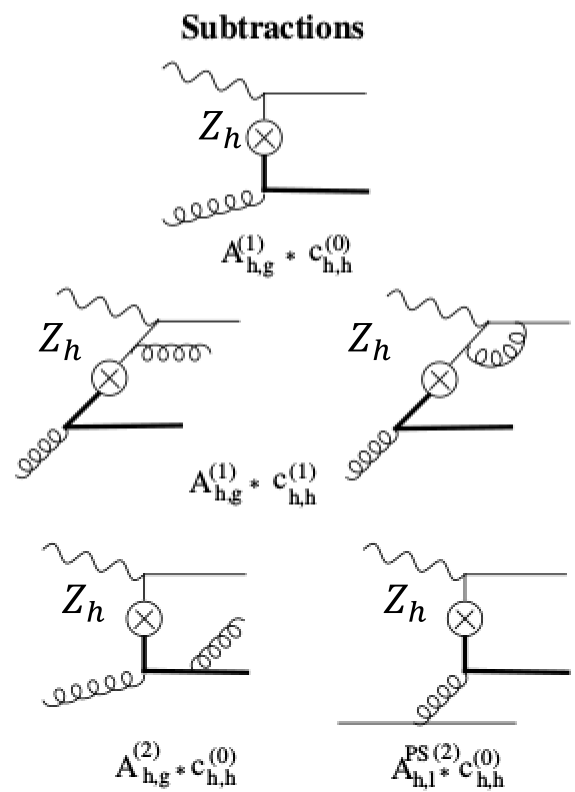


- A general-mass variable-flavor number (GM-VFN) scheme
  - Perturbatively convergent at all factorization scales $Q \gtrsim m_Q$
  - reduces to the zero-mass $\overline{MS}$ scheme at $Q^2 \gg m_Q^2$, without additional renormalization
  - reduces to the fixed-flavor number scheme at $Q^2 \sim m_Q^2$
- Relatively simple
  - One value of N_f (and one PDF set) in each Q range
  - Sets $m_Q = 0$ in $|M|^2$ with incoming c or b
  - Straightforward matching based on kinematical rescaling

Other common heavy-quark schemes: FONLL, TR', SACOT-m_T,...

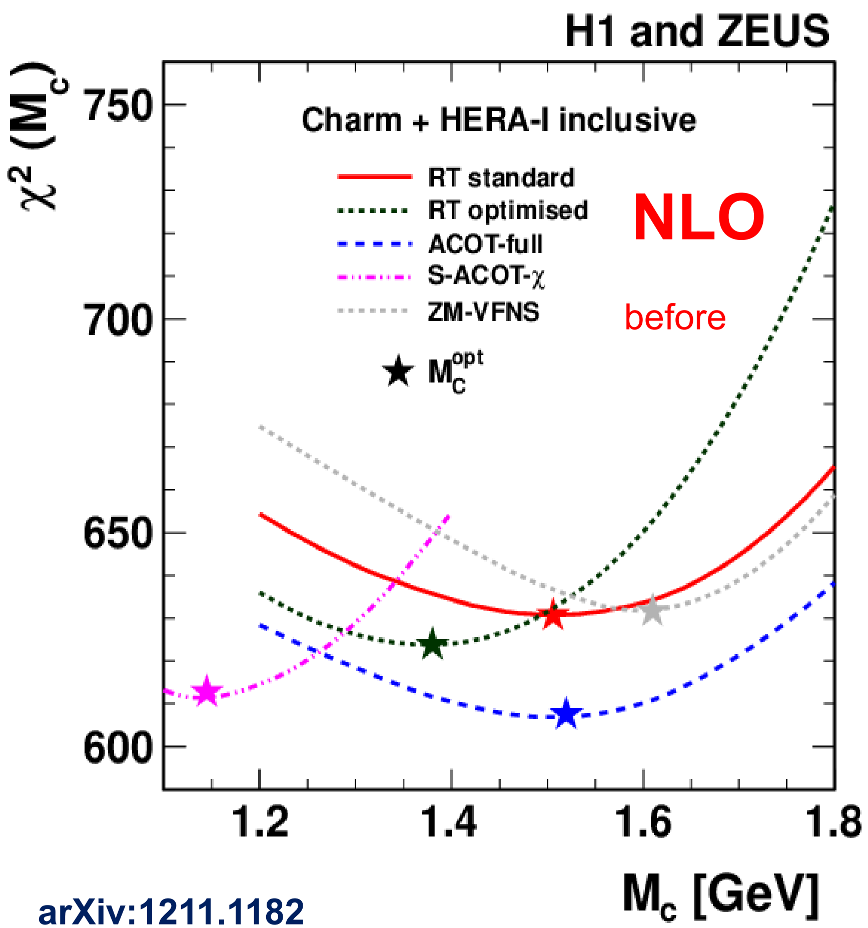
Twist-2: factorization for DIS in S-ACOT-χ scheme up to NNLO



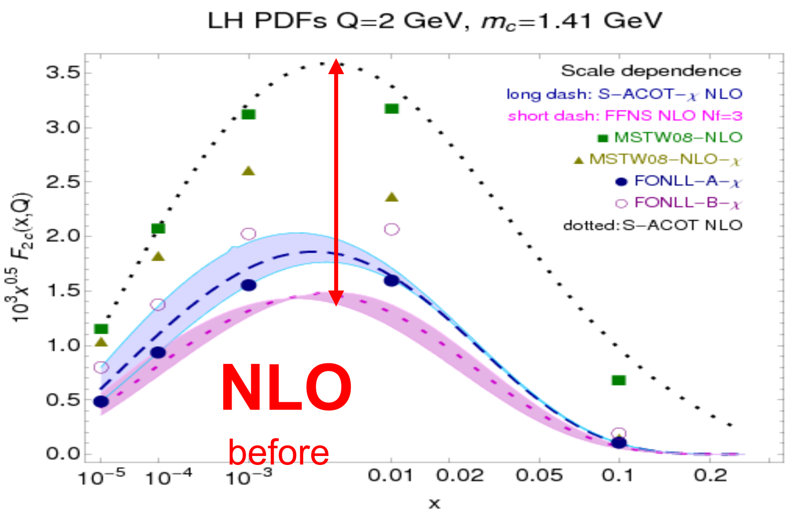


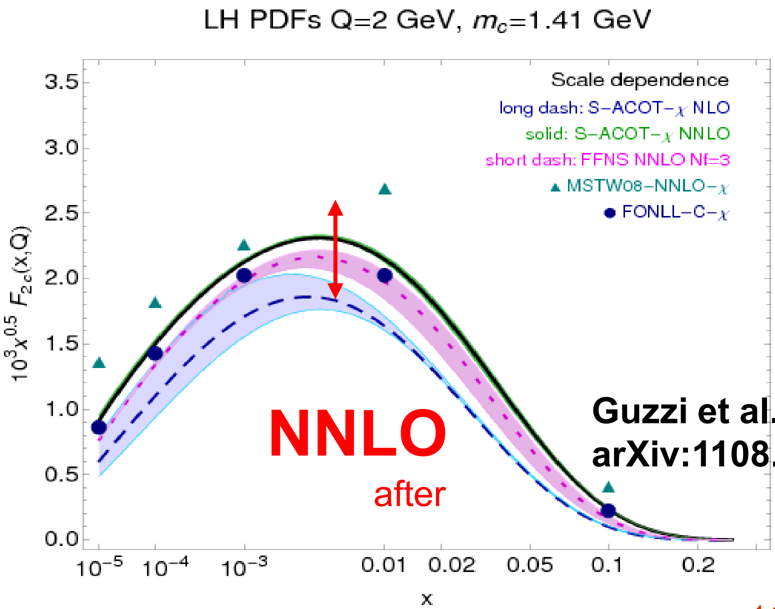
Leading-power radiative contributions to neutral-current DIS charm production in the CTEQ-TEA NNLO analysis

NNLO=$\mathcal{O}(\alpha_s^2)$: dependence on matching parameters is suppressed, GM-VFN schemes are more predictive at NNLO



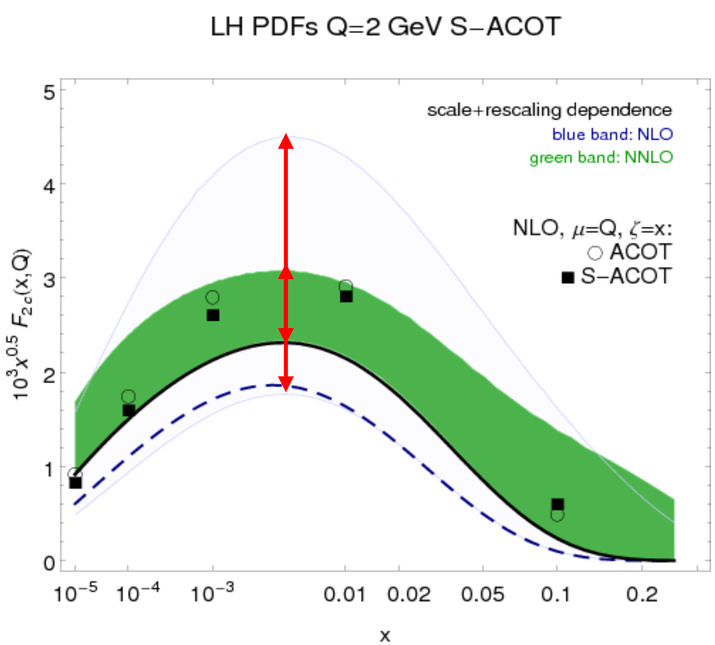
arXiv:1211.1182



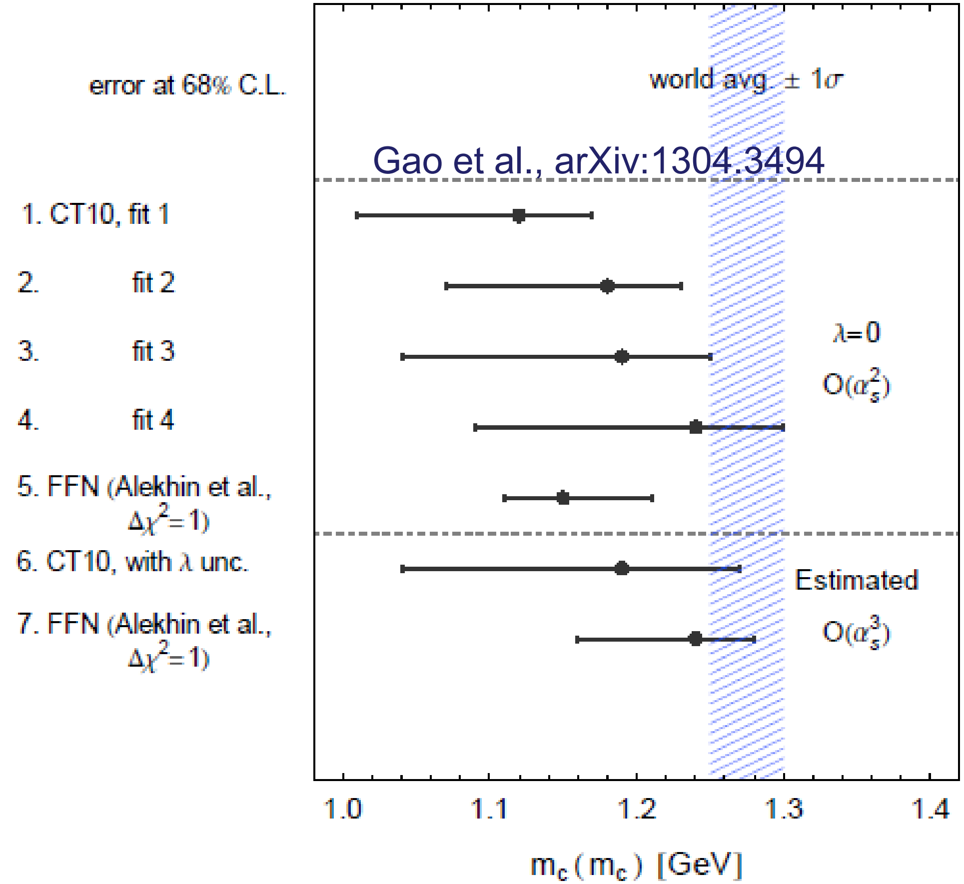


Guzzi et al.; arXiv:1108.5112

GM-VFN schemes are more predictive at NNLO

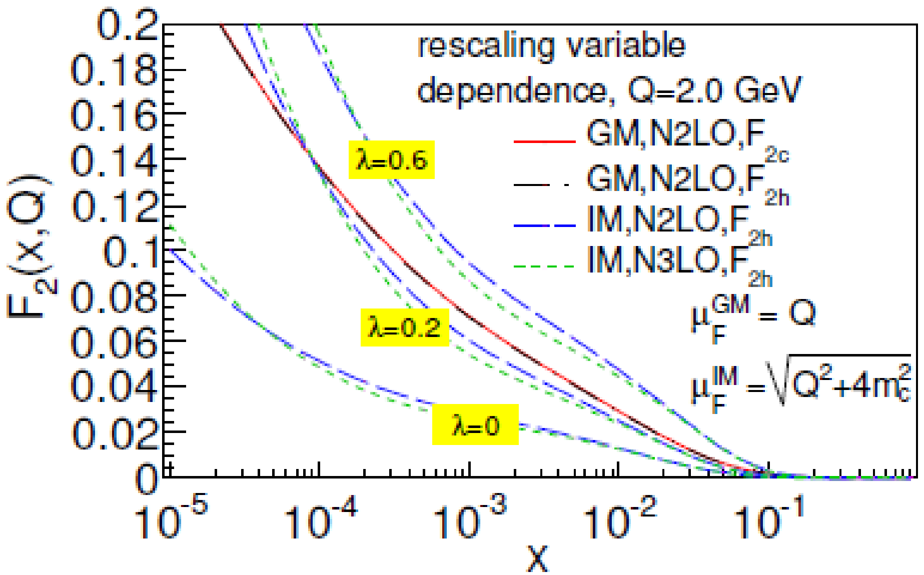


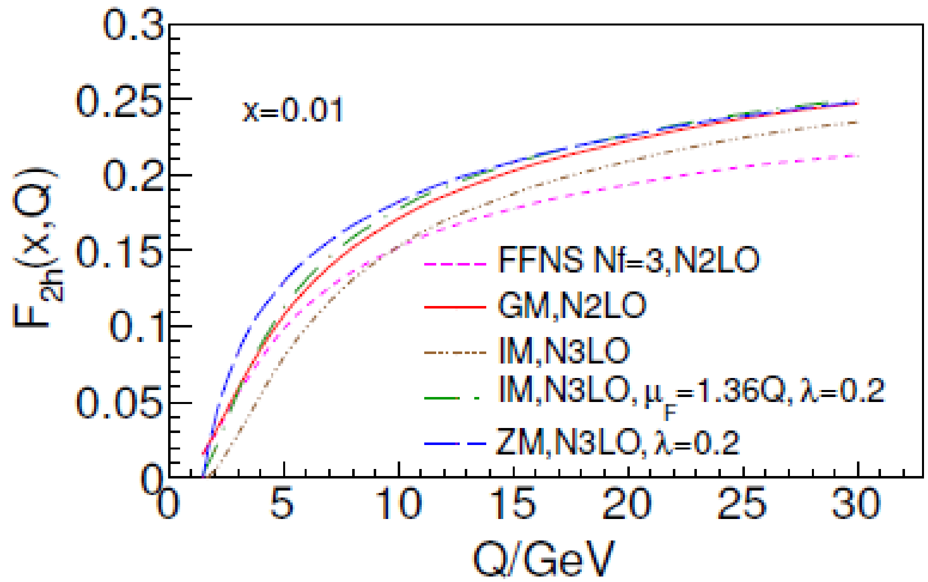
From Guzzi et al.; arXiv:1108.5112;
see also J. Rojo et al., 1003.1241, p. 110



At $O(\alpha_s^2)$ and approximate $O(\alpha_s^3)$, constraints on $m_c(m_c)$ have been first obtained from combined HERA-I data in the FFN scheme [arXiv:1212.2355]. Constraints on both m_c^{pole} or $m_c(m_c)$ in GM-VFNS have been also obtained by CT, MMHT, and NNPDF under varied assumptions. They are comparable with FFNS and the PDG value for $m_c(m_c)$.

The SACOT-MPS scheme can be straightforwardly extended to N3LO DIS



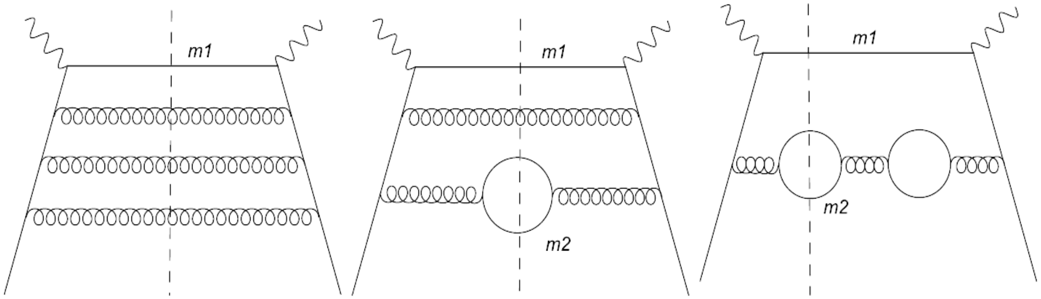


The intermediate-mass (IM) approximation to the SACOT-MPS scheme, using approximate N3LO matrix elements

The exact flavor structure of the GM-VFN scheme at N3LO is readily reproduced

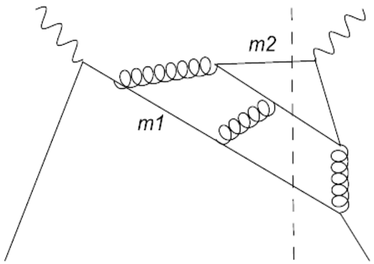
[Bowen Wang, Ph. D. thesis, 2015;
see also Stavreva et al., arXiv:1203.0282]

Flavor classes in the IM scheme at N3LO

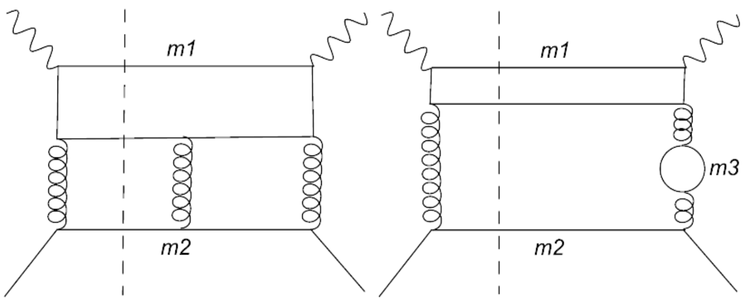


(a) T_1 (b) T_2 (c) T_3

Figure 9.6: Representative diagrams from FC_2 class.

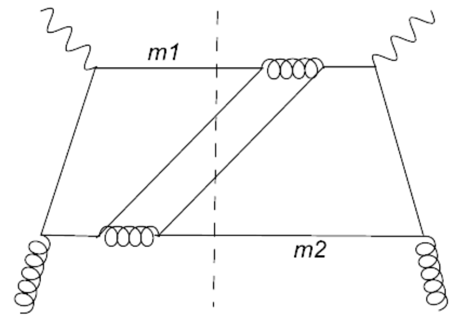


The representative diagram for FC_{11} class.

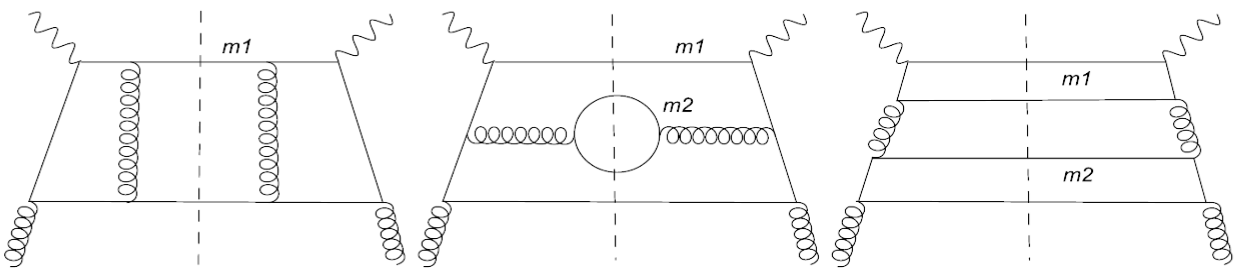


(a) T_1 (b) T_2

Figure 9.8: Representative diagrams from FC_{02} class.



The representative diagram for FC^g_{11} class.



(a) T_1 (b) T_2 (c) T_3

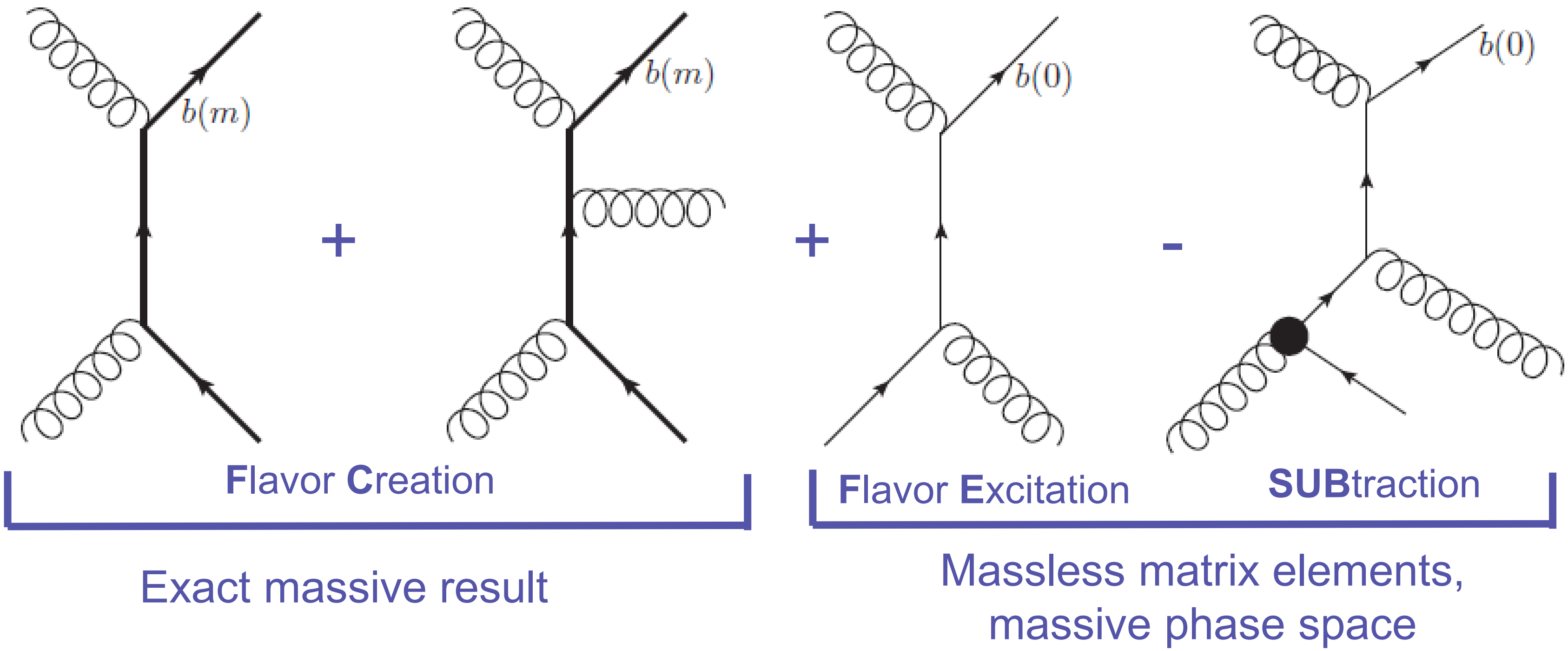
Figure 9.9: Representative diagrams from FC^g_2 class.

SACOT-MPS scheme for heavy-quark production at hadron colliders

NEW

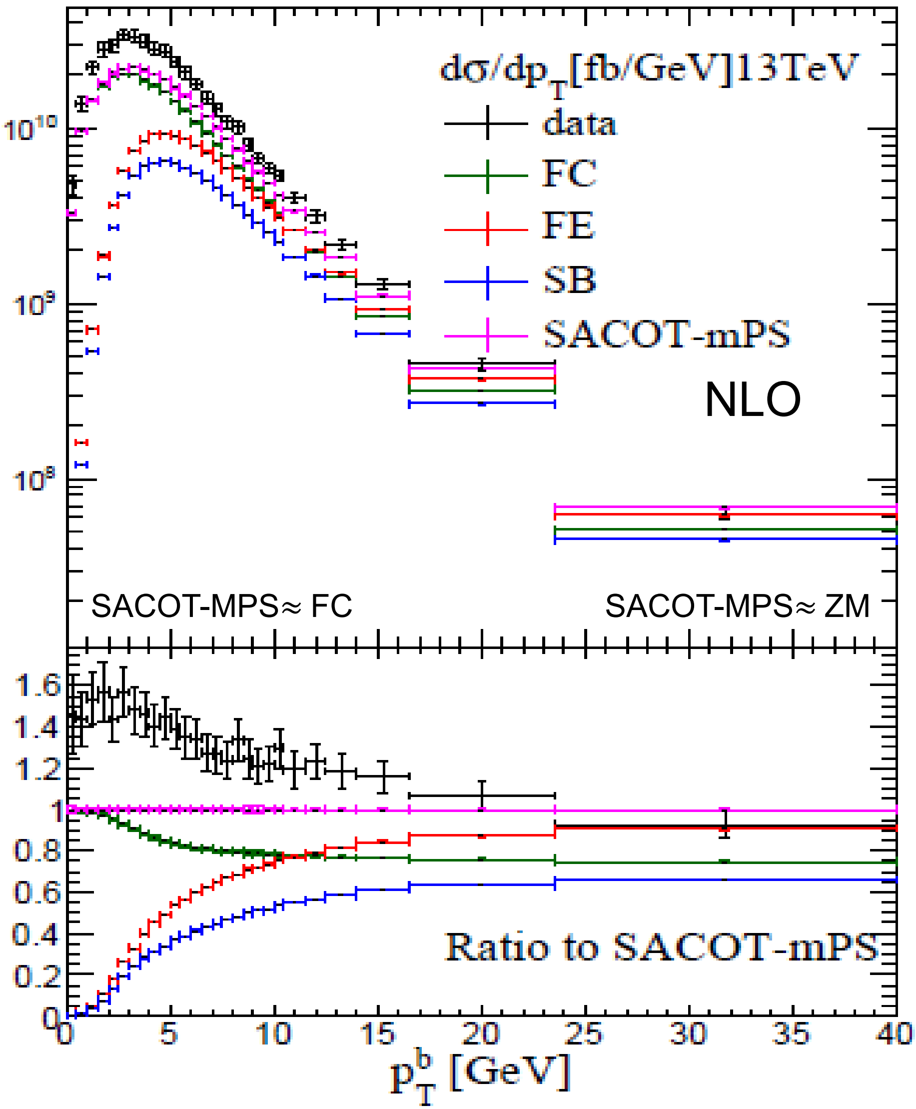
[K. Xie, Ph. D. thesis, https://tinyurl.com/XiePhD2019, 2019]

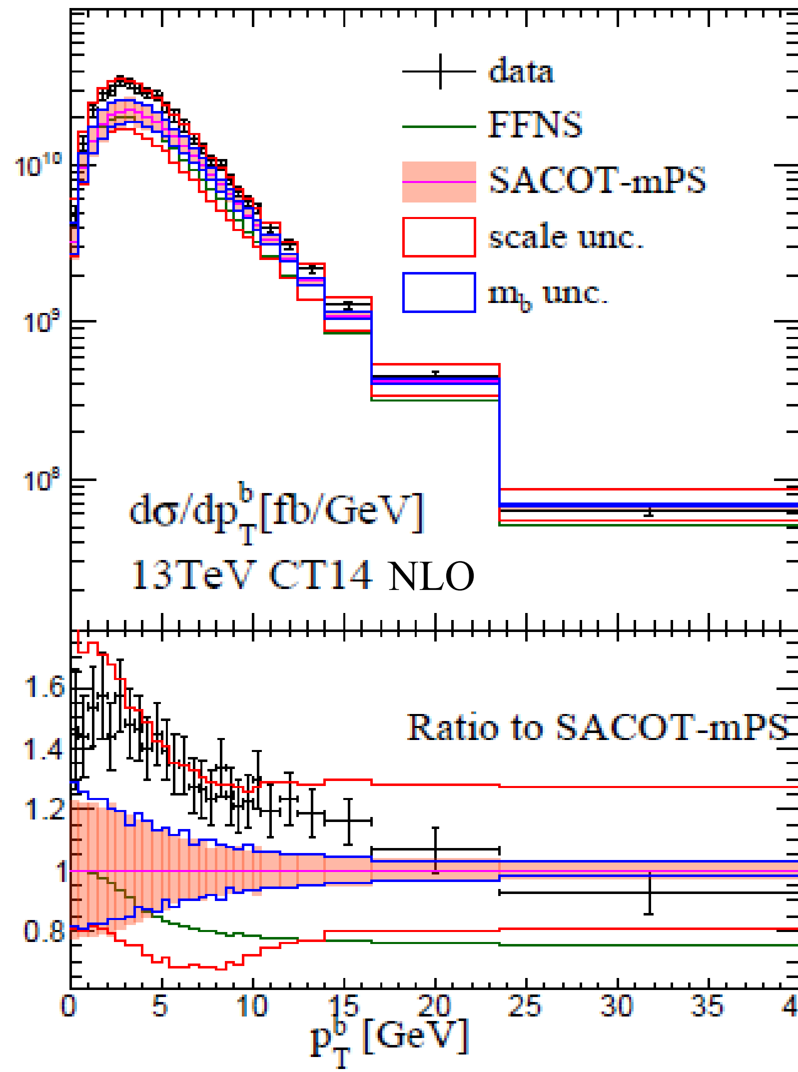
- A straightforward implementation for $pp \to bX$, other processes
- Realized in the MCFM code



α_s and PDFs with $N_f = 5$ in all terms

SACOT-MPS NLO predictions for b-quark production at LHCb 13 TeV





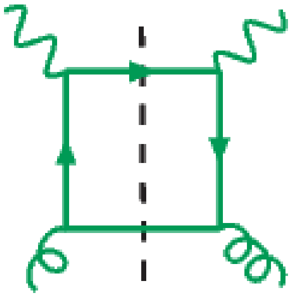
SACOT-MPS is in better agreement with data than either FFN or ZM schemes; readily extendable to other processes and NNLO

Fitted charm, intrinsic charm…

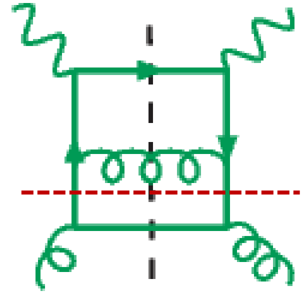
Are twist-2 NNLO contributions sufficient for describing the most precise experiments?

A twist-4 contribution in HERA DIS charm production ($\subset$ "intrinsic charm")

Twist-2
$\gamma^* g \to c\bar{c}$



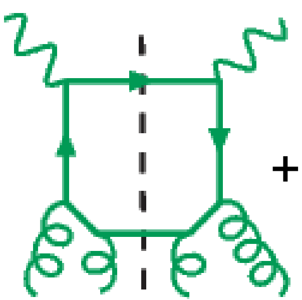
Order $\alpha_s(Q)$



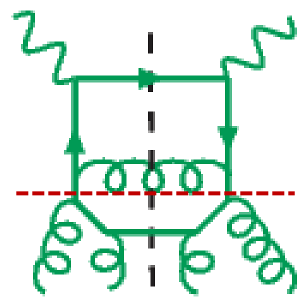
$\alpha_s^2(Q) \cdot \ln(Q^2/m_c^2)$

A ladder; must be resummed in $c(x, Q)$ in the $N_f = 4$ scheme at $Q^2 \gg m_c^2$; e.g., in the ACOT scheme

Twist-4
$\gamma^*(gg) \to c\bar{c}$



+…



$\Lambda \lesssim 1$ GeV

$\alpha_s^2(Q) \cdot (\Lambda^2/Q^2)$
or $\alpha_s^2(Q) \cdot (\Lambda^2/m_c^2)$

$\alpha_s^3(Q) \cdot (\Lambda^2/m_c^2) \ln(Q^2/m_c^2)$

Can be of order ~10% of the twist-2 α_s^2 term

The ladder subgraphs can be resummed as a part of $c(x, Q)$ in the $N_f = 4$ scheme at $Q^2 \gg m_c^2 > \Lambda^2$;

contribute to the boundary condition for $c(x, Q_0)$ at $Q_0 \approx m_c$;

obey twist-2 DGLAP equations.

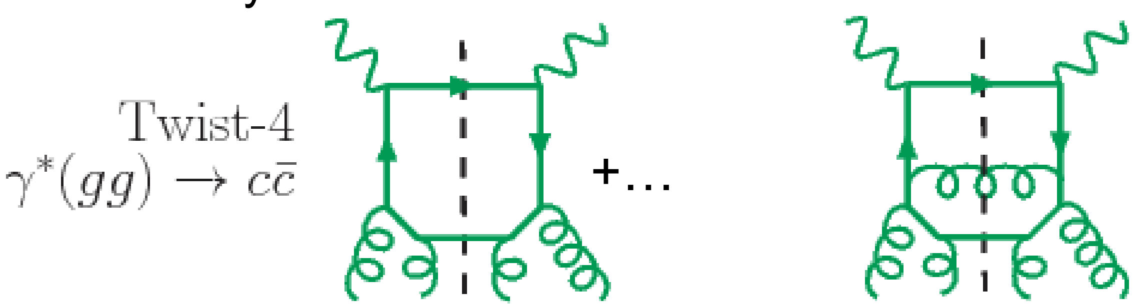
CT14 IC study: answers to important questions

What are phenomenological constraints on the “intrinsic charm” from the global QCD data?

⇒ The CT14 charm PDFs allow a “nonperturbative” component carrying a total momentum fraction of $1-2\%$ in DIS at $Q \approx m_c$.

Can we estimate its impact on the LHC predictions?

Yes, based on the simplest approximation of the “nonperturbative” charm contribution. In most cases, the estimated impact is less than the net CT14 PDF uncertainty.



$\alpha_s^2(Q) \cdot (\Lambda^2/Q^2)$ or $\alpha_s^2(Q) \cdot (\Lambda^2/m_c^2)$

$\alpha_s^3(Q) \cdot (\Lambda^2/m_c^2)\ln(Q^2/m_c^2)$

Note:
“intrinsic charm” ≠ “fitted charm”

PDF fits may include a ``fitted charm'' PDF

``Fitted charm'' = ``higher-twist charm''
+ other (possibly not universal)
higher O(α_s) / higher power terms

QCD factorization theorem for DIS structure function $F(x,Q)$ [Collins, 1998]:

All α_s orders:

$$F(x,Q) = \sum_{a=0}^{N_f} \int_x^1 \frac{d\xi}{\xi} \mathcal{C}_a\left(\frac{x}{\xi}, \frac{Q}{\mu}, \frac{m_c}{\mu}; \alpha(\mu)\right) f_{a/p}(\xi,\mu) + \mathcal{O}(\Lambda^2/m_c^2, \Lambda^2/Q^2).$$

The PDF fits implement this formula up to (N)NLO ($N_{ord} = 1$ or 2):

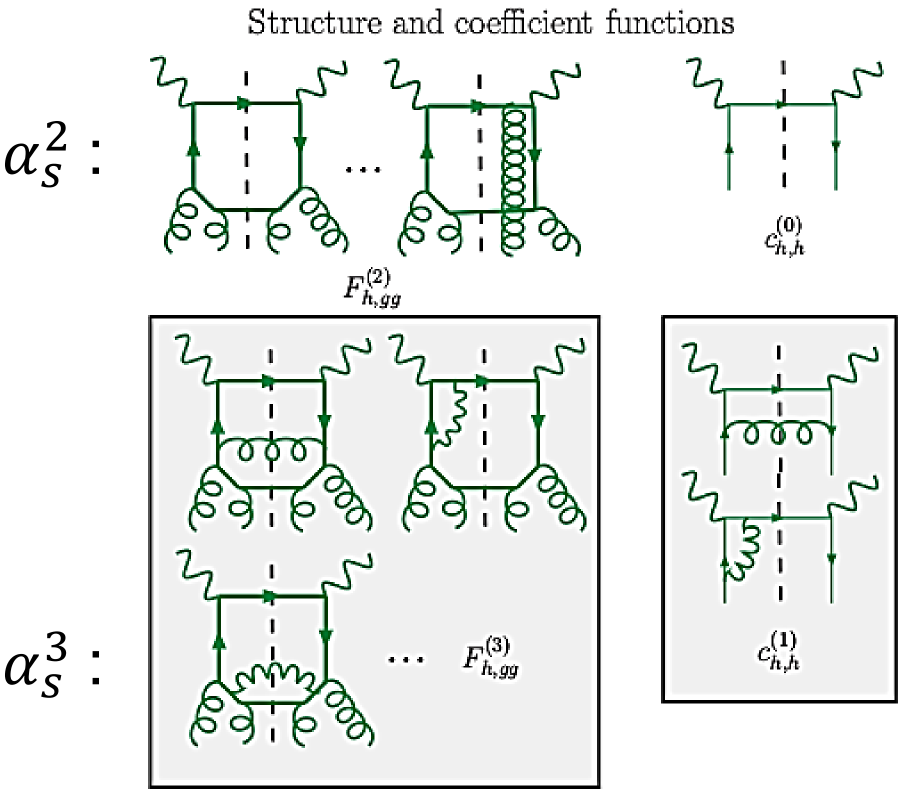
PDF fits:

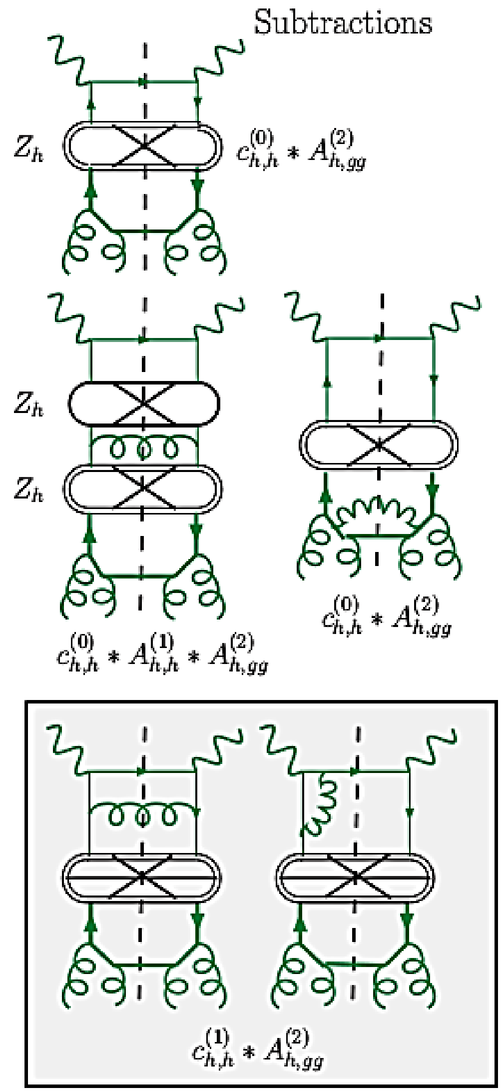
$$F(x,Q) = \sum_{a=0}^{N_f} \int_x^1 \frac{d\xi}{\xi} \mathcal{C}_a^{(N_{ord})}\left(\frac{x}{\xi}, \frac{Q}{\mu}, \frac{m_c}{\mu}; \alpha(\mu)\right) f_{a/p}^{(N_{ord})}(\xi,\mu).$$

The perturbative charm PDF component cancels at $Q \approx m_c$ up to a higher order

The 'fitted charm component' may approximate for missing terms of orders α_s^p with $p > N_{ord}$, or Λ^2/m_c^2, or Λ^2/Q^2

ACOT-like factorization for twist-4 charm contributions (an example)



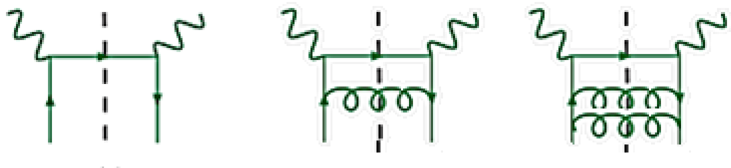


Many novel terms arise, involving
twist-4 nonperturbative functions!

Intrinsic charm contributions, practical implementation

Keep only $c_{h,h} \otimes f_h$:

Discard $C_{h,gg}^{(k)} \otimes f_{gg}$, etc.



In the absence of full computation, we (and other groups) make the simplest approximation:

$$F_{IC}(x, Q_0) = [c_{h,h} \otimes f_{c/p}^{IC}](x, Q_0)$$

$\boldsymbol{c_{h,h}}$ **is the twist-2 charm DIS coefficient function** introduced to factorize the twist-4 ladder terms; defined according to the S-ACOT-χ scheme

IC is compatible with any version of the ACOT scheme (cf. the paper)

$\boldsymbol{f_{c/p}^{IC}(\xi, Q_0)}$ **is a nonperturbative charm parametrization**:
CT14 IC: $f_{c/p}^{IC}(\xi, Q_0)$ is a "**valence-like**" or a "**sea-like**" function, combined with the to the perturbative charm $f_{c/p}^{pert}$ from $g \to c\bar{c}$ splittings

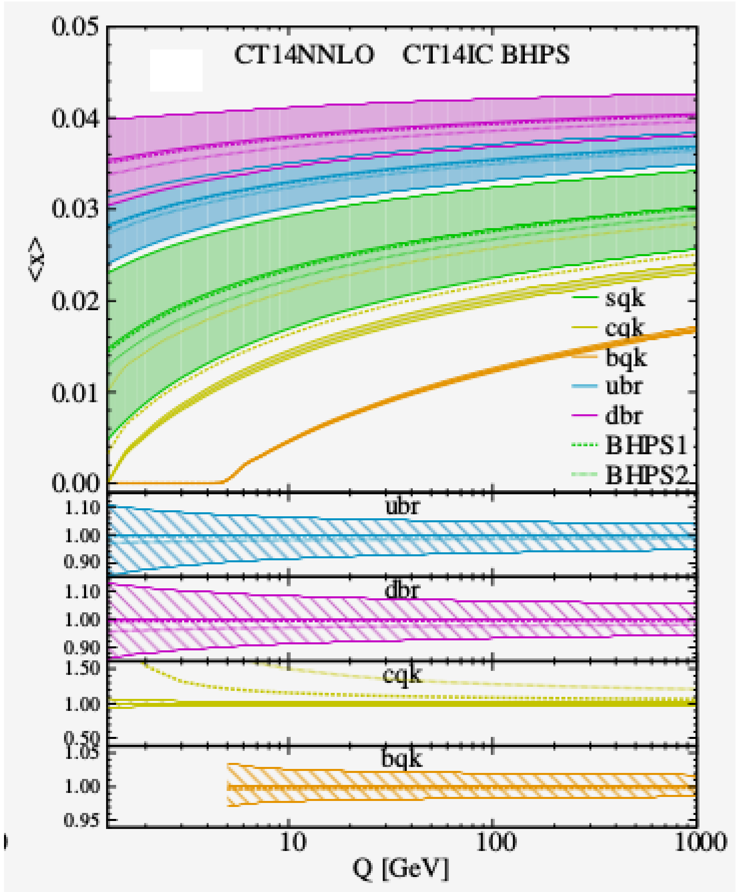
Charm momentum fraction

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

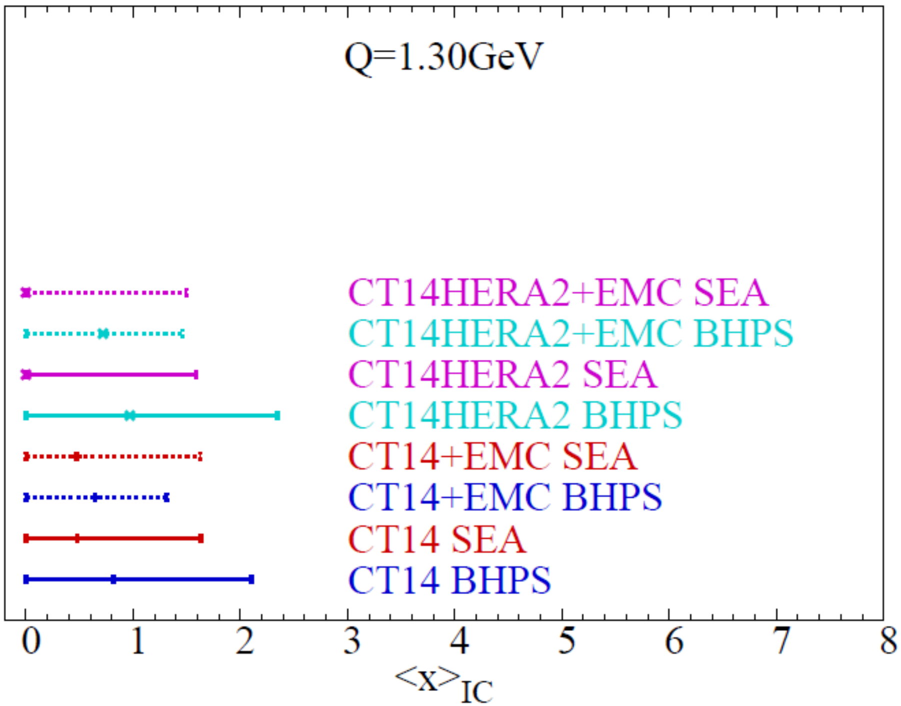
Initial scale $Q_0 \leq m_c$: intrinsic component only

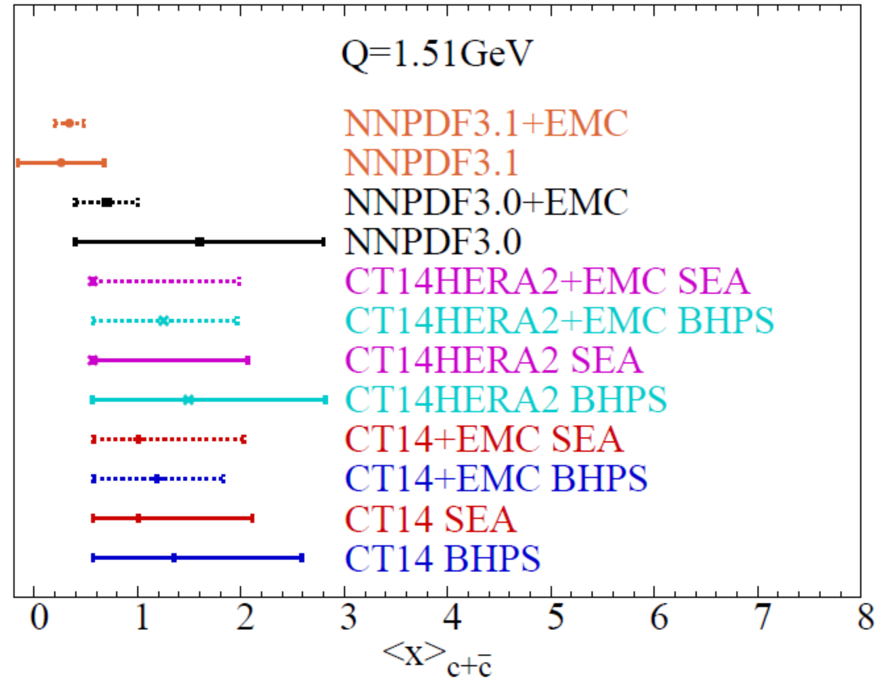
$$\langle x \rangle_{IC} \equiv \langle x \rangle_{c+\bar{c}}(Q_0)$$

At $Q > Q_0$, growth due to perturbative $c(x,Q)$



Allowed $c + \bar{c}$ momentum fractions





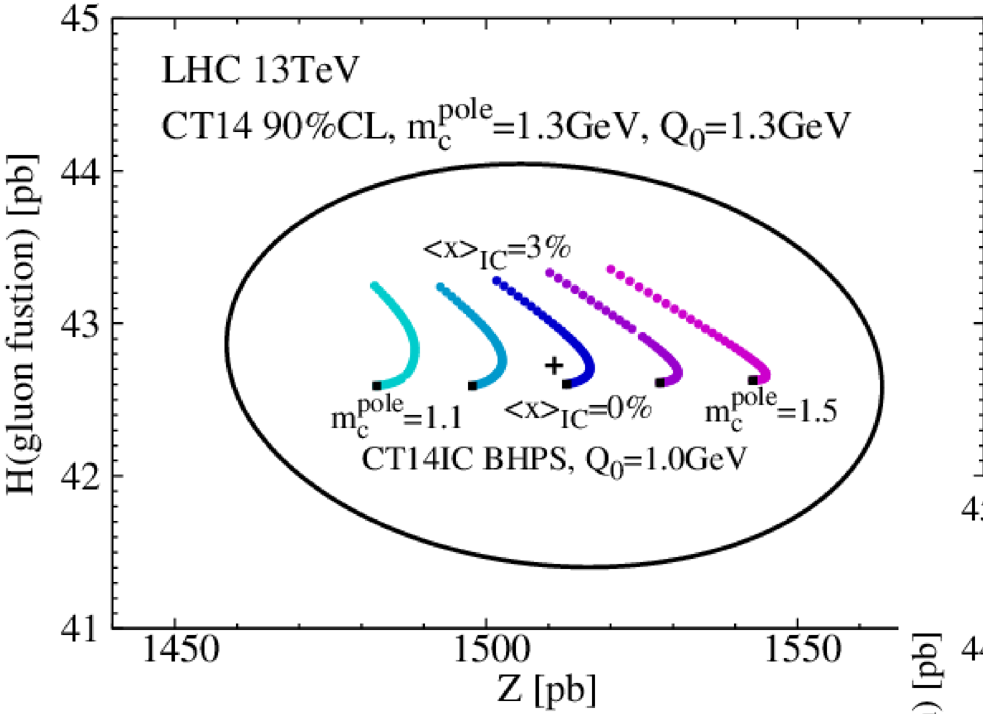
Sources of differences	CT14 IC	NNPDF3.x
α_s order	NNLO only	NLO, NNLO
Settings	90% c.l., $Q_0 = m_c^{pole} = 1.3$ GeV	68% c.l., $Q_0 = m_c^{pole} = 1.51$ GeV
LHC 8 TeV W, Z	Under validation; mild tension with HERA DIS data	Included; strong effect despite a smallish data sample
1983 EMC F_{2c} data included?	Only as a cross check (unknown syst. effects in EMC data)	Optional, strong effect on the PDF error

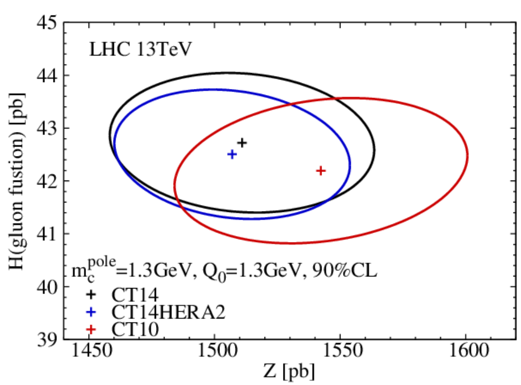
Impact of IC on physical observables

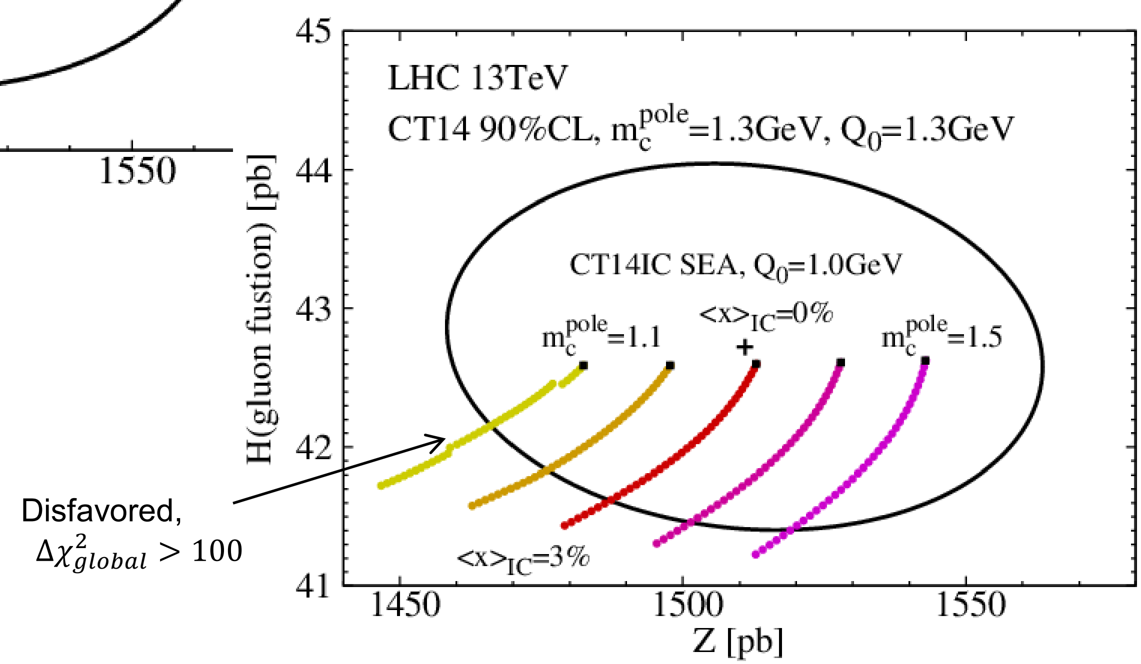
- Mild effects at the LHC
- Smoking gun signatures in SIDIS at the EIC

[Our estimates assume that the IC PDF component does not depend on the hard process.]

LHC: NNLO Total inclusive electroweak boson production cross sections $\sigma_{tot}(pp \to VX)$





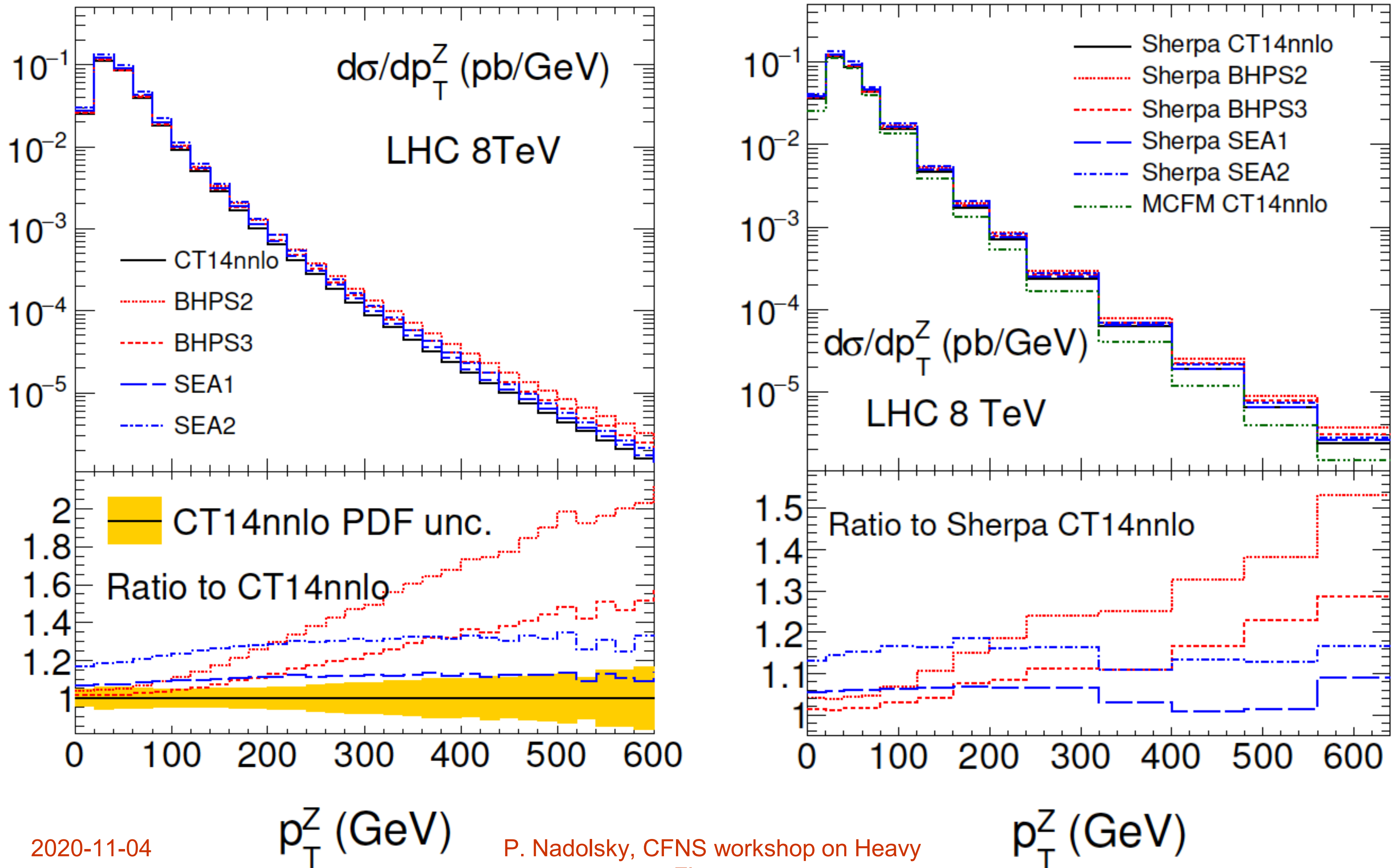


[Hou et al., arXiv:1707.00657]

LHC searches for intrinsic charm

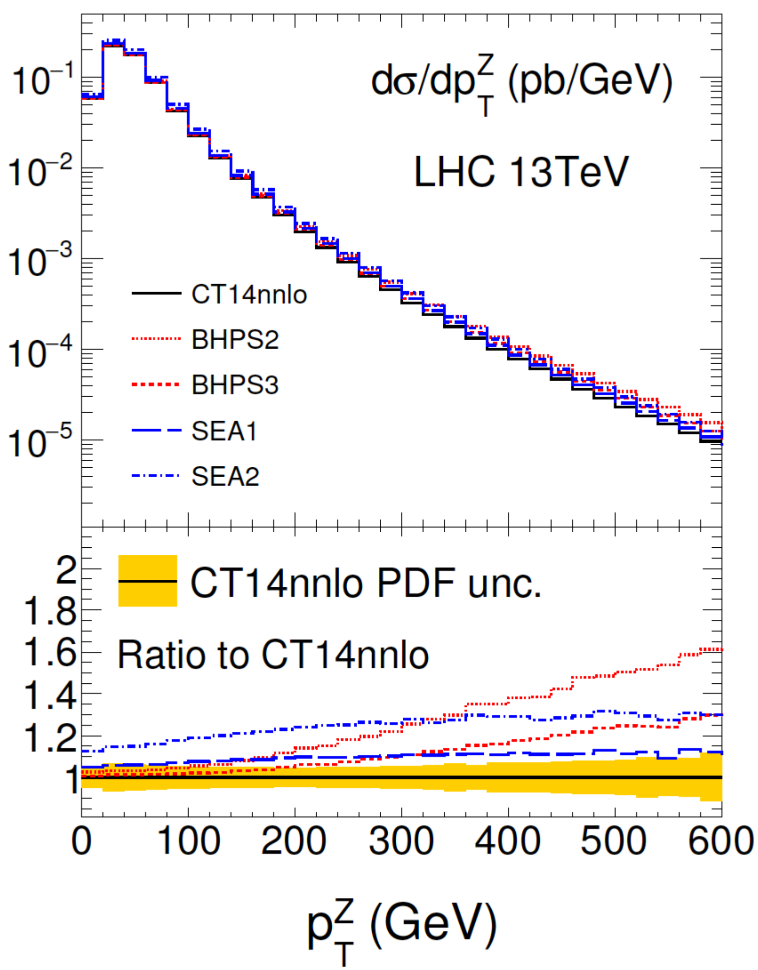
[Hou et al., arXiv:1707.00657]

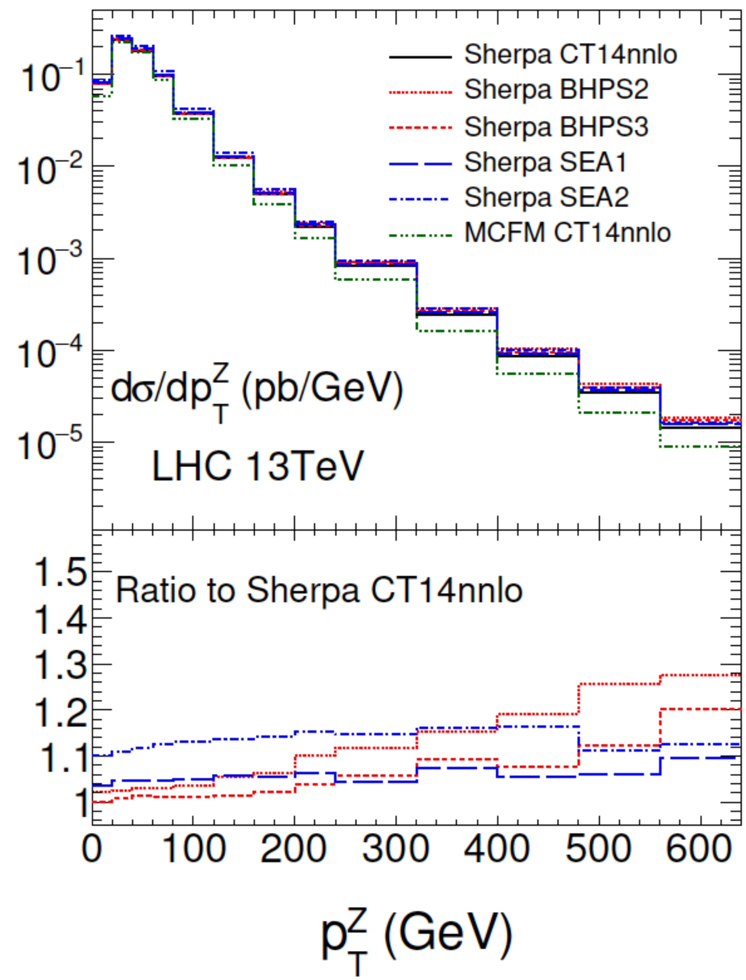
Z+c NLO computation with various models, without (left) and with parton shower (right)



Z+c NLO LHC 13 TeV

[Hou et al., arXiv:1707.00657]





The parton shower has the most significant effect in dampening the hard pT(Z) tail especially for BHPS fits. Sherpa predictions include HO tree-level MEs compared to MCFM and therefore show enhancements in the harder pT(Z) region compared to MCFM. Similarly increasing or decreasing the number of multileg MEs in the merging changes the absolute level of pT.

EIC, charm production

Orders-of-magnitude more events for some IC models

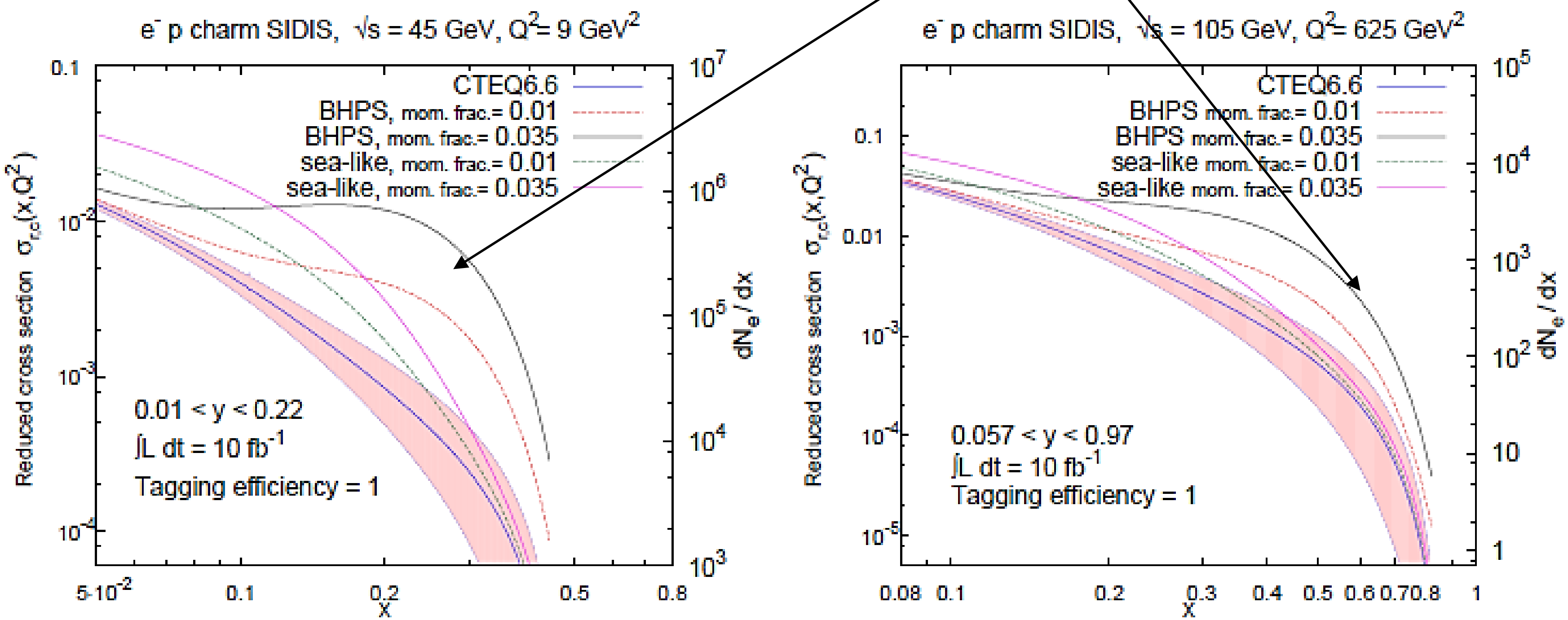


Figure 1.20. Charm contribution to the reduced NC $e^- p$ DIS cross section at $\sqrt{s} = 45$ and 105 GeV. For each IC model, curves for charm momentum fractions of 1% and 3.5% are shown. For comparison we display the number of events dN_e/dx for $10\,\mathrm{fb}^{-1}$, assuming perfect charm tagging efficiency.

[Guzzi, Nadolsky, Olness, in arXiv:1108.1713; T. Hobbs, arXiv:1707.06711; Arratia et al., arXiv:2006.12520]

Summary

1. Heavy-quark processes provide increasingly strong constraints on nucleon/nuclear PDFs

2. SACOT-MPS factorization scheme has been extended to LHC kinematics; provides a streamlined, consistent framework to implement massive HF contributions in a variety of (N)NLO processes

3. Fitted $c(x, Q_0)$ approximates for the twist-4 universal $c(x, Q_0)$ and other missing terms; $\langle x \rangle_{IC} < 2\%$ for BHPS IC and $\langle x \rangle_{IC} < 1.6\%$ for SEA IC at 90% C.L.

   – The twist-4 charm SIDIS cross section consists of ladder diagrams and everything else
   – The **universal** part of ladder contributions can be resummed into $c(x, Q)$ at $Q^2 \gg m_c^2$ in **any version of the ACOT scheme**
   – **the non-universal component is** of order $\boldsymbol{\alpha_s^2\, \Lambda^2/\mathrm{m_c^2}}$; hard to separate from the missing twist-2/N3LO and $O(\Lambda^2/Q^2)$ contributions – unless explicitly computed

Thank you
for your attention

CT18 in a nutshell

- Start with CT14-HERA2 (HERAI+II combined data released after publication of CT14)
- Examine a wide range of PDF parameterizations
- Use as much relevant LHC data as possible using applgrid/fastNLO interfaces to data sets, with NNLO/NLO K-factors, or fastNNLO tables in the case of top pair production. **Benchmark the predictions!**
- Examine **QCD scale dependence** in key processes
- Implement **parallelization** of the global PDF fitting to allow for faster turn-around time
- Validate the results using a **strong set of goodness-of-fit tests** *(Kovarik, PN, Soper,* arXiv:1905.06957*)*
- Use diverse statistical techniques (**PDFSense, ePump, Gaussian variables, Lagrange Multiplier scans**) to examine agreement between experiments

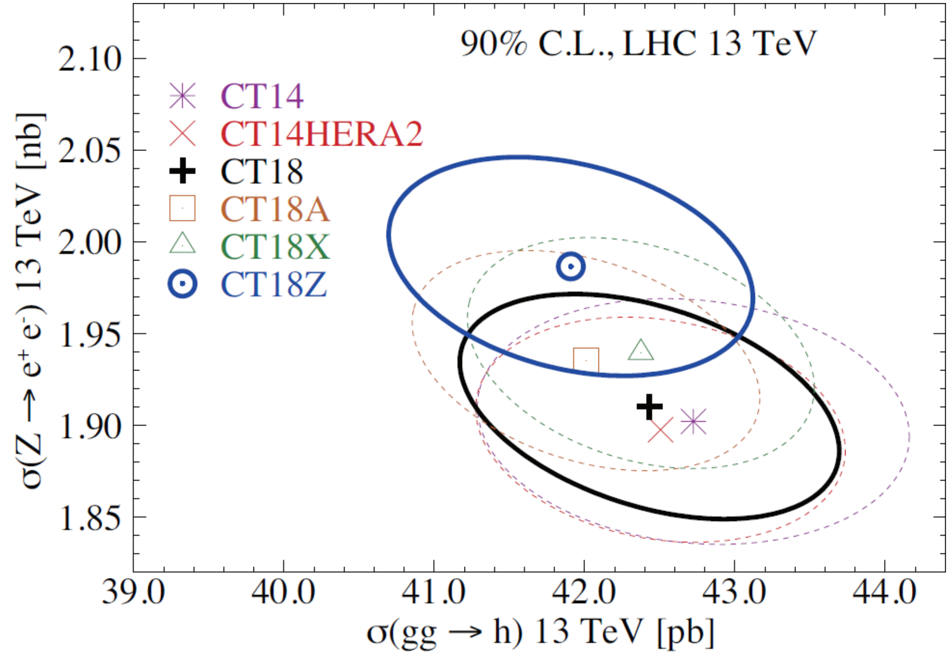
PDF ensemble	Factorization scale in DIS	ATLAS 7 Z/W data included?	CDHSW $F_2^{p,d}$ data included?	Pole charm mass, GeV
CT18	$\mu^2_{F,DIS} = \mathrm{Q}^2$	No	Yes	1.3
CT18A	$\mu^2_{F,DIS} = \mathrm{Q}^2$	Yes	Yes	1.3
CT18X	$\mu^2_{F,DIS} = 0.8^2\left(Q^2 + \frac{0.3\ GeV^2}{x^{0.3}}\right)$	No	Yes	1.3
CT18Z	$\mu^2_{F,DIS} = 0.8^2\left(Q^2 + \frac{0.3\ GeV^2}{x^{0.3}}\right)$	Yes	No	1.4

Sources of differences between NNLO PDFs

There are theoretical and methodological uncertainties that add up to the nominal PDF uncertainty. These include:

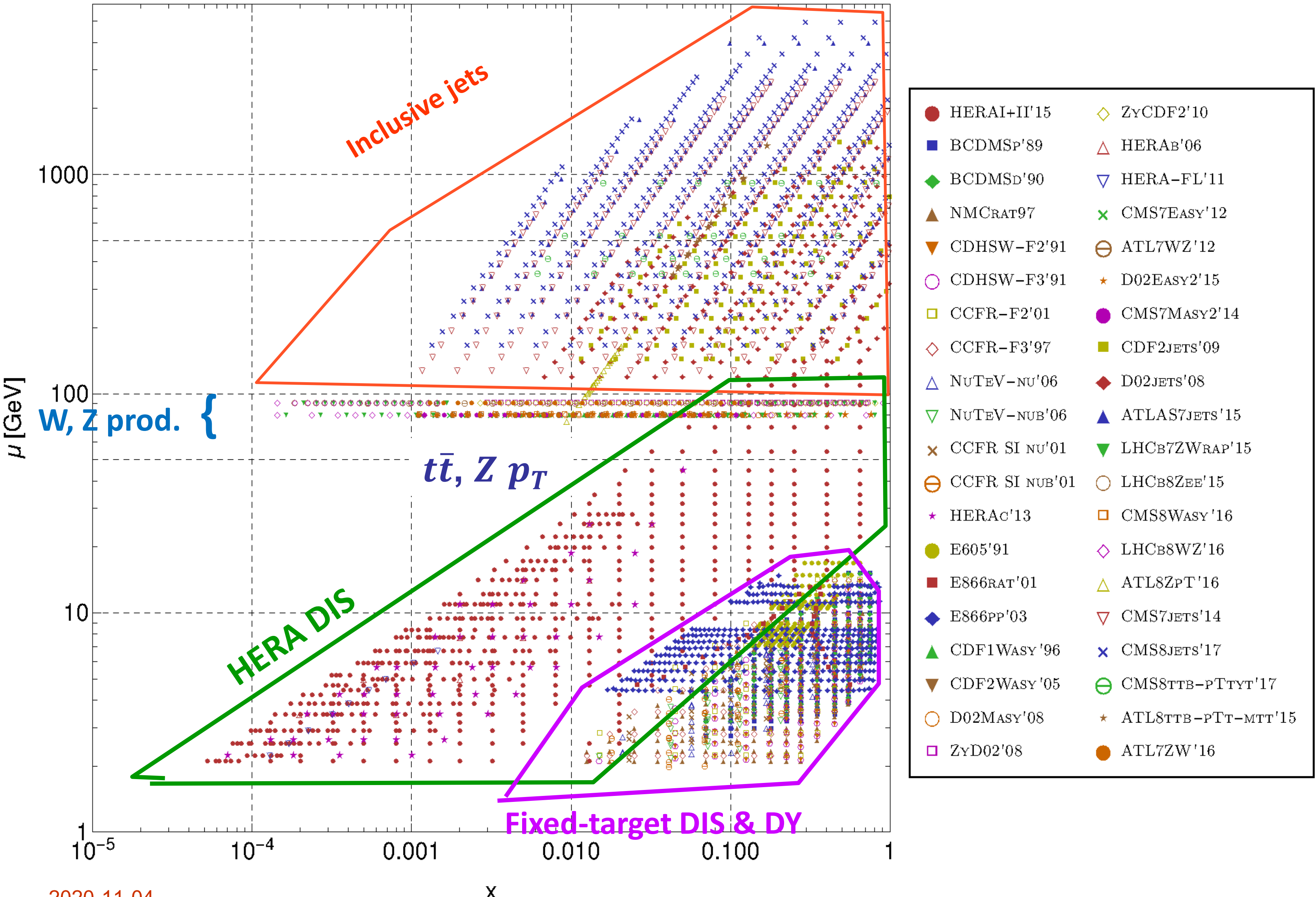
- selecting slightly different data sets
- changing the QCD scales in DIS, etc.
- varying the charm and bottom masses
- **varying parameters of the heavy-quark factorization scheme**
- …

The differences between CT18 and CT18Z reflect some of these factors



CT18Z NNLO cross sections for $gg \to H$ production (Z production) lower by about 1% (higher by 4.9%) compared to CT14HERA2 NNLO

Experimental data in CT18 PDF analysis



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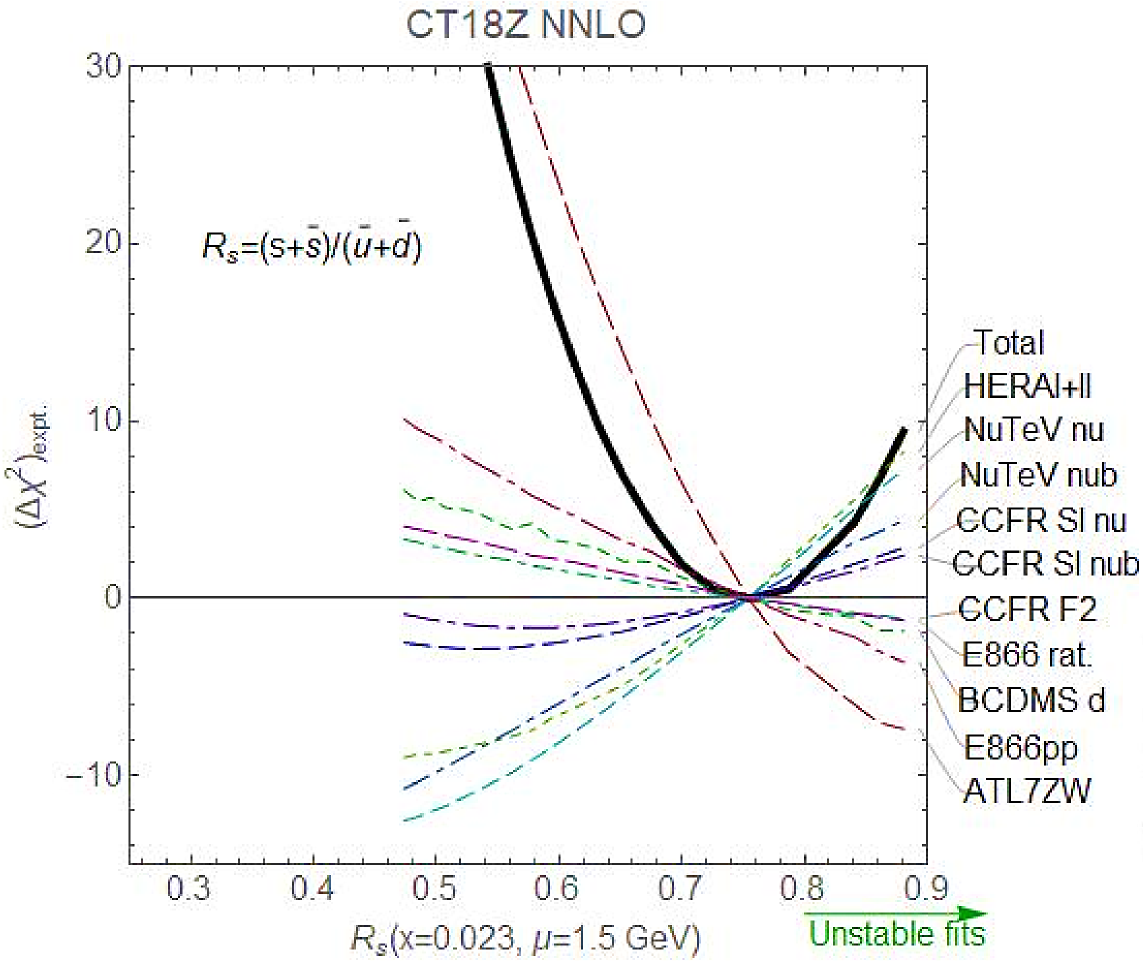
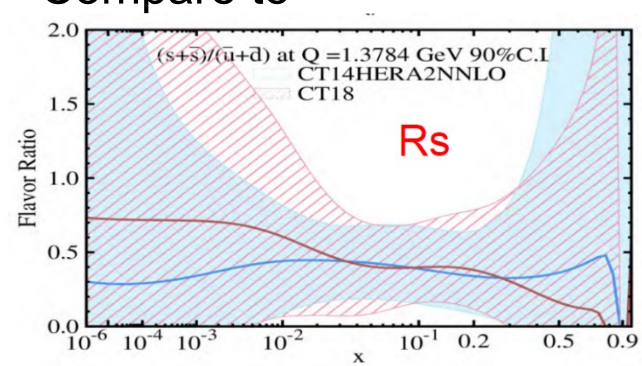
Lagrange Multiplier scan: $R_s(x = 0.023, \mu = 1.5\ GeV)$



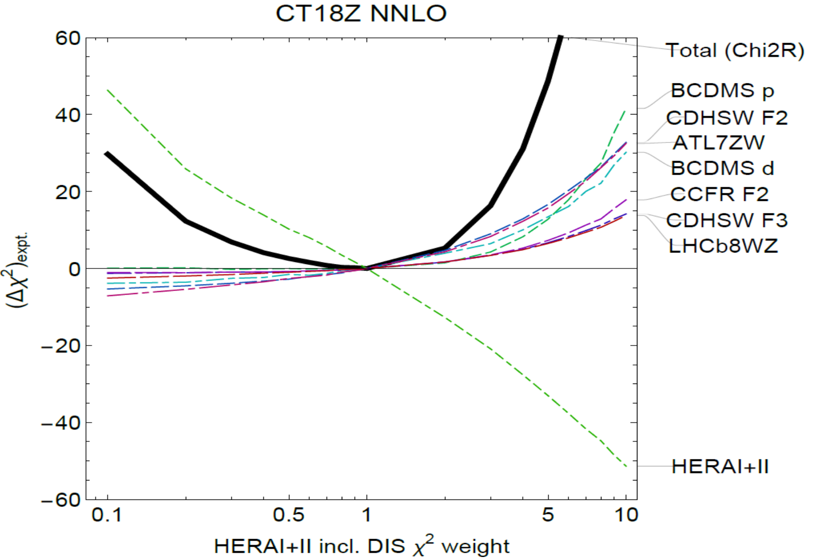
The CT18Z strangeness is increased primarily as a result of including the ATLAS 7 TeV W/Z production data (not in CT18), as well as because of using the DIS saturation scale and $m_c^{pole} = 1.4$ GeV

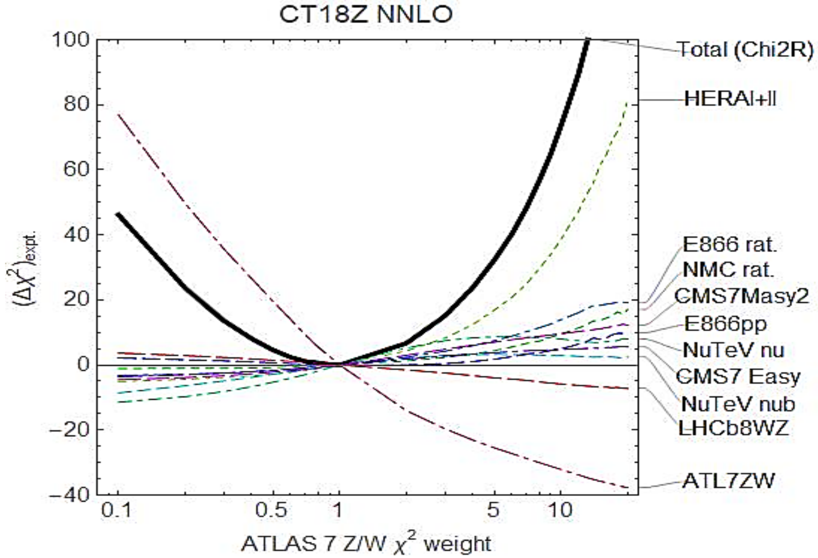
In either CT18 or CT18Z fit, observe instability in the fits for $R_s > 1$ at $x = 0.01 - 0.1$

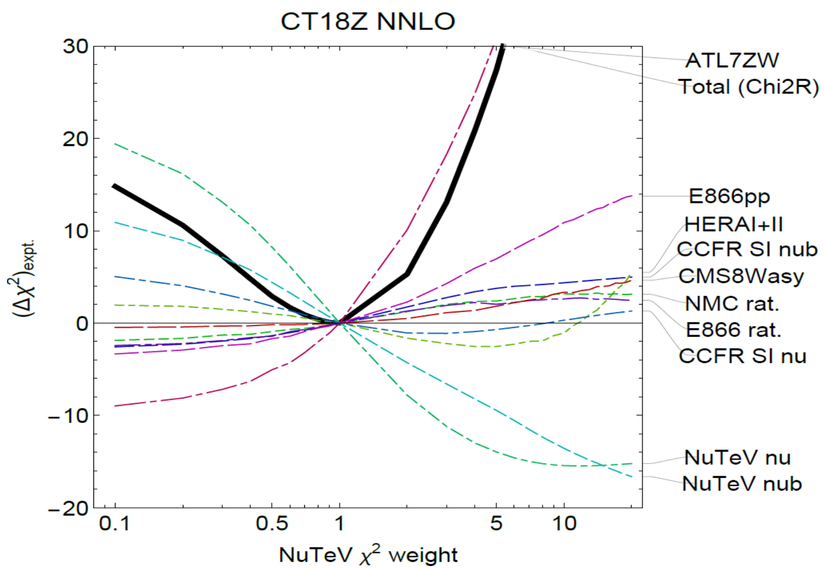
Compare to



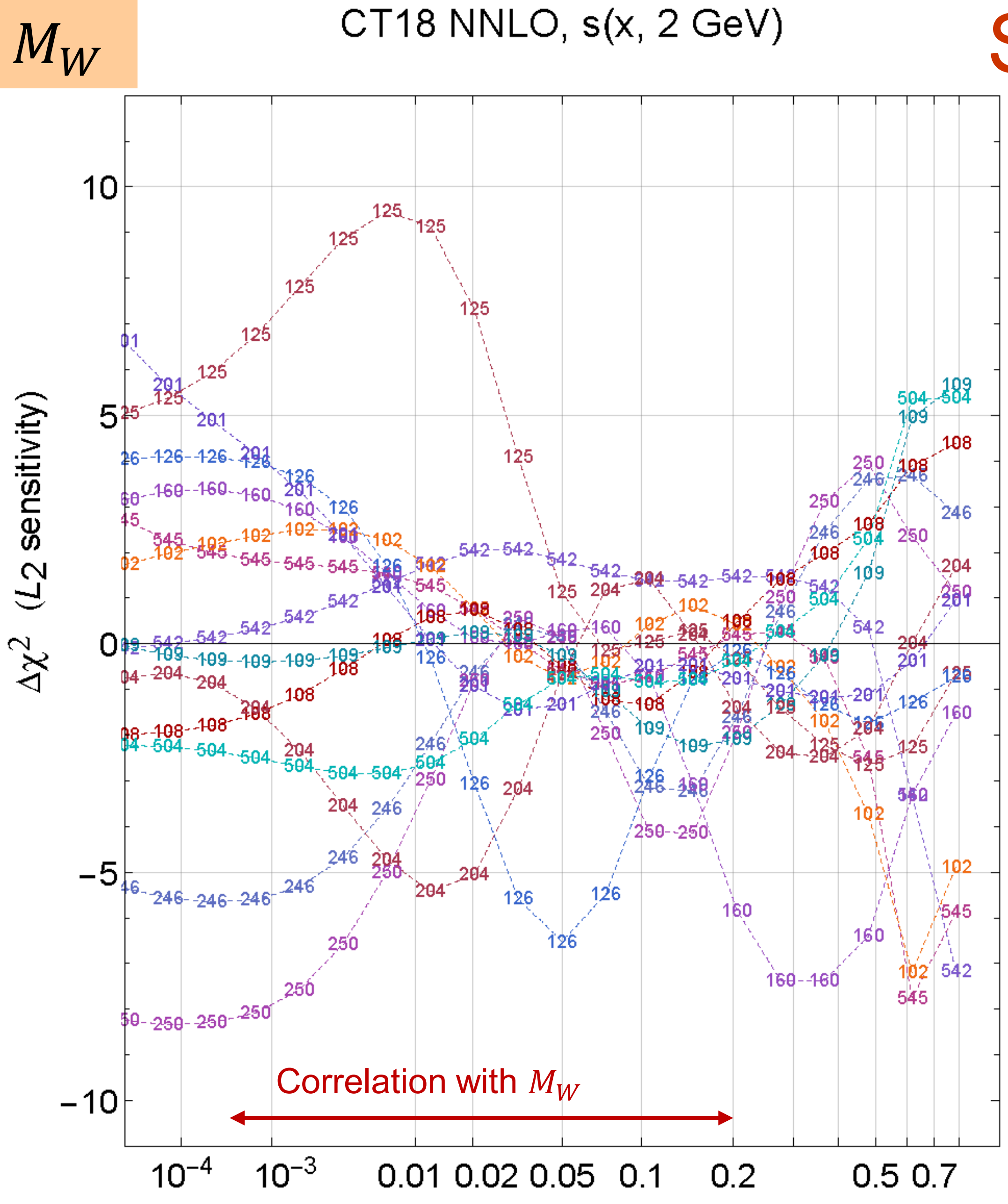
LM scans on χ^2 weights of HERA I+II, ATLAS 7 Z/W, and NuTeV data







Fits with varied weights and LM scans reveal a disagreement between important DIS [primarily HERA, CCFR, NuTeV,…] and DY [primarily ATL7ZW, E866, LHCb8WZ,…] experiments. This is more pronounced for large$-x$ gluon as well as strangeness.



Strangeness, CT18

M_W

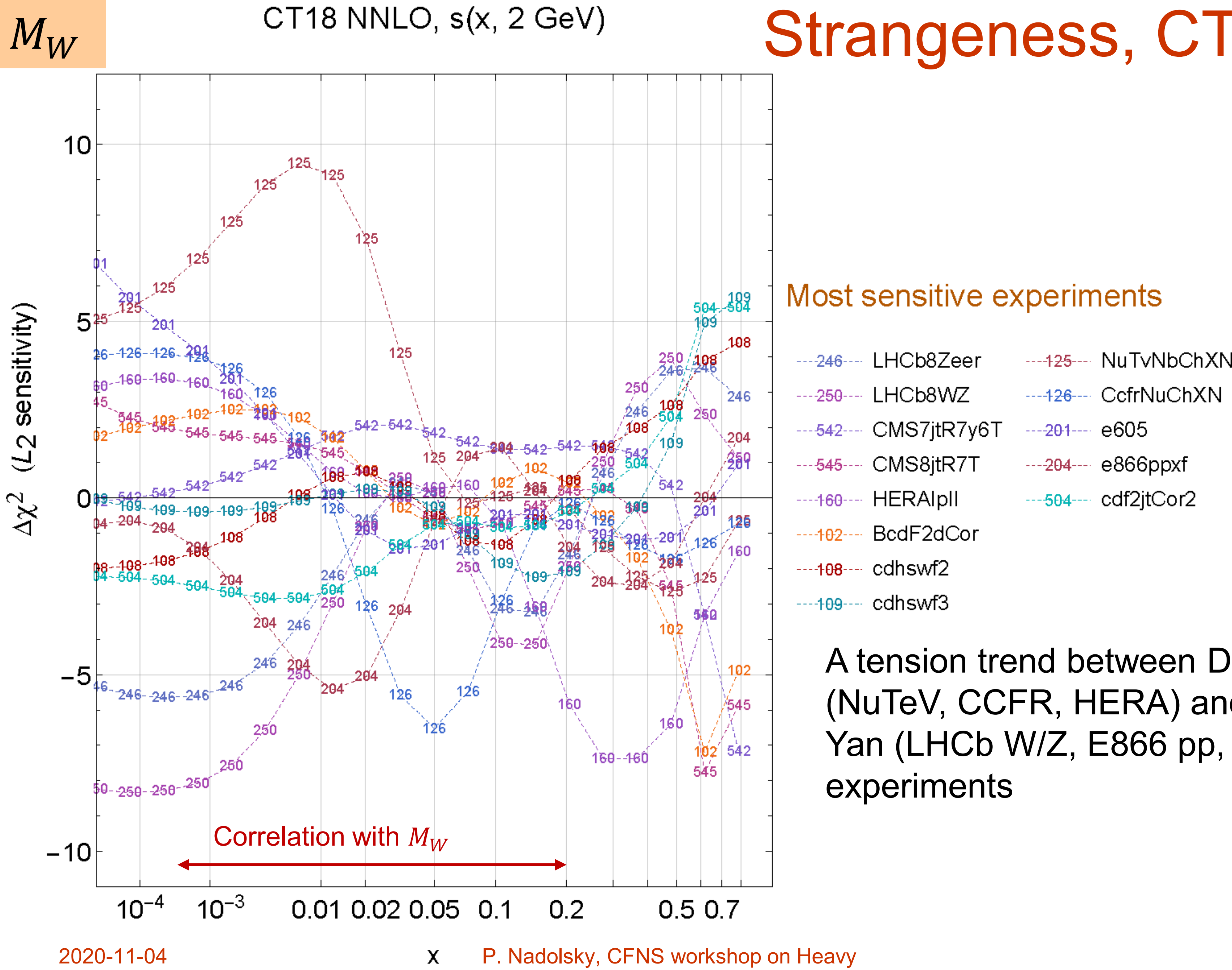
The global view can be obtained using the L_2 sensitivity technique – a Hessian approximation to the LM scan (Hobbs et al., arXiv:1904.00022)

Most sensitive experiments

- 246 LHCb8Zeer
- 250 LHCb8WZ
- 542 CMS7jtR7y6T
- 545 CMS8jtR7T
- 160 HERAIpII
- 102 BcdF2dCor
- 108 cdhswf2
- 109 cdhswf3
- 125 NuTvNbChXN
- 126 CcfrNuChXN
- 201 e605
- 204 e866ppxf
- 504 cdf2jtCor2

Strangeness, CT18

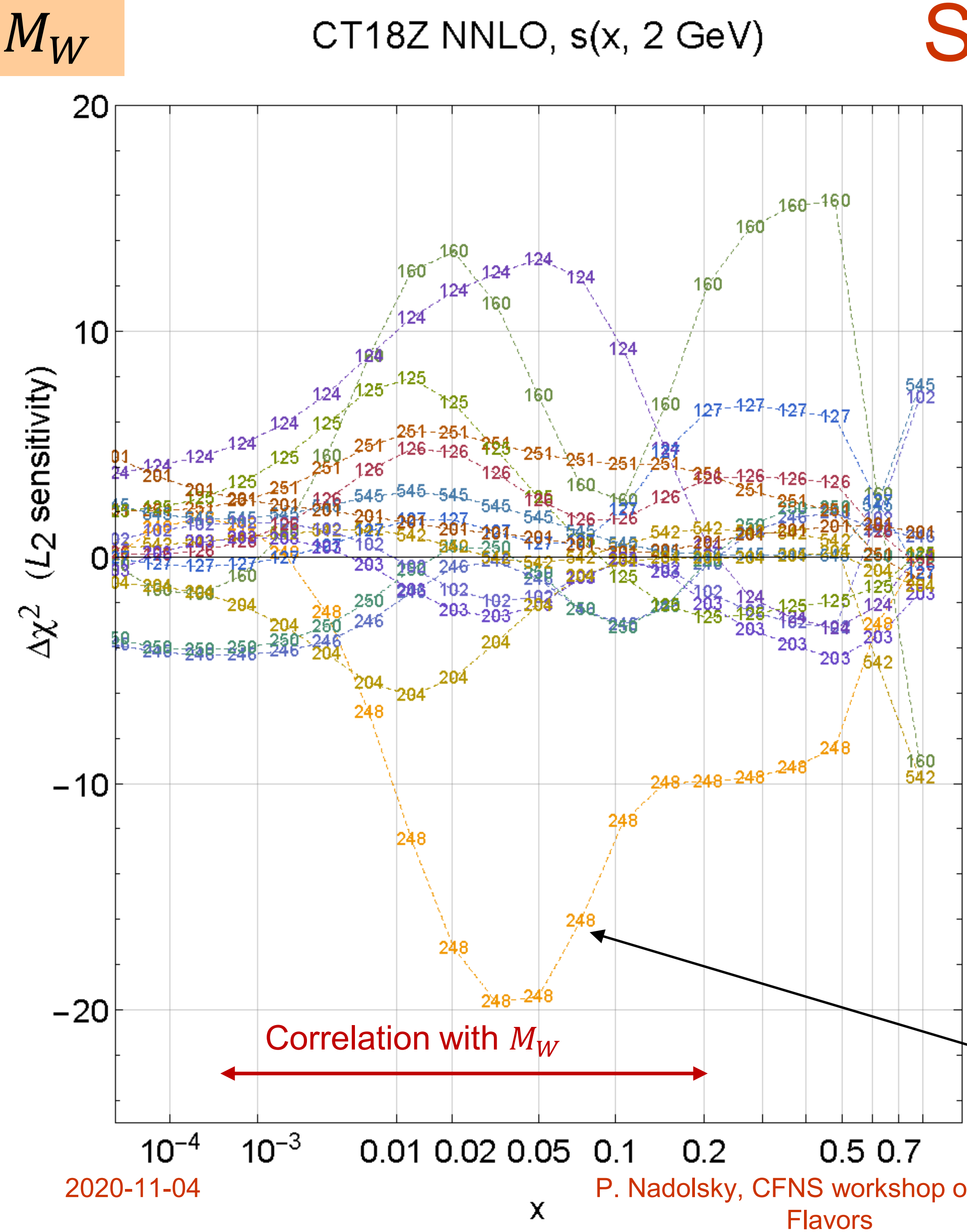
M_W



A tension trend between DIS (NuTeV, CCFR, HERA) and Drell-Yan (LHCb W/Z, E866 pp, …) experiments

M_W

Strangeness, CT18Z



Most sensitive experiments

- 246 LHCb8Zeer
- 248 ATL7ZW.xF
- 250 LHCb8WZ
- 251 ATL8DY
- 542 CMS7jtR7y6T
- 545 CMS8jtR7T
- 160 HERAIpII
- 102 BcdF2dCor
- 124 NuTvNuChXN
- 125 NuTvNbChXN
- 126 CcfrNuChXN
- 127 CcfrNbChXN
- 201 e605
- 203 e866f
- 204 e866ppxf

A tension trend between DIS (HERA I+II, CCFR, NuTeV) and Drell-Yan (ATLAS 7 Z/W, LHCb W/Z, E866 pp, …) experiments

pronounced pull of ATLAS7 Z/W data

Parametrizations of $c(x, Q_0)$

1. "**Valence-like**" $c(x, Q_0)$ according to the BHPS model: BHPS1 and BHPS2

Brodsky et al PLB 1980

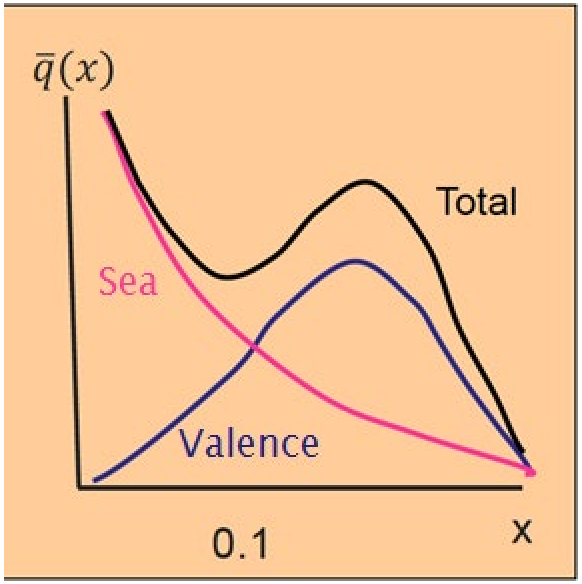
$$c(x) = \bar{c}(x) = \frac{1}{2} A x^2 \left[\frac{1}{3}(1-x)\ (1+10x+x^2) - 2x(1+x)\ln(1/x) \right]$$

2. "BHPS3 model: include intrinsic $u\bar{u}$, $d\bar{d}$, and $c\bar{c}$ with **numerical** solutions for the BHPS model.

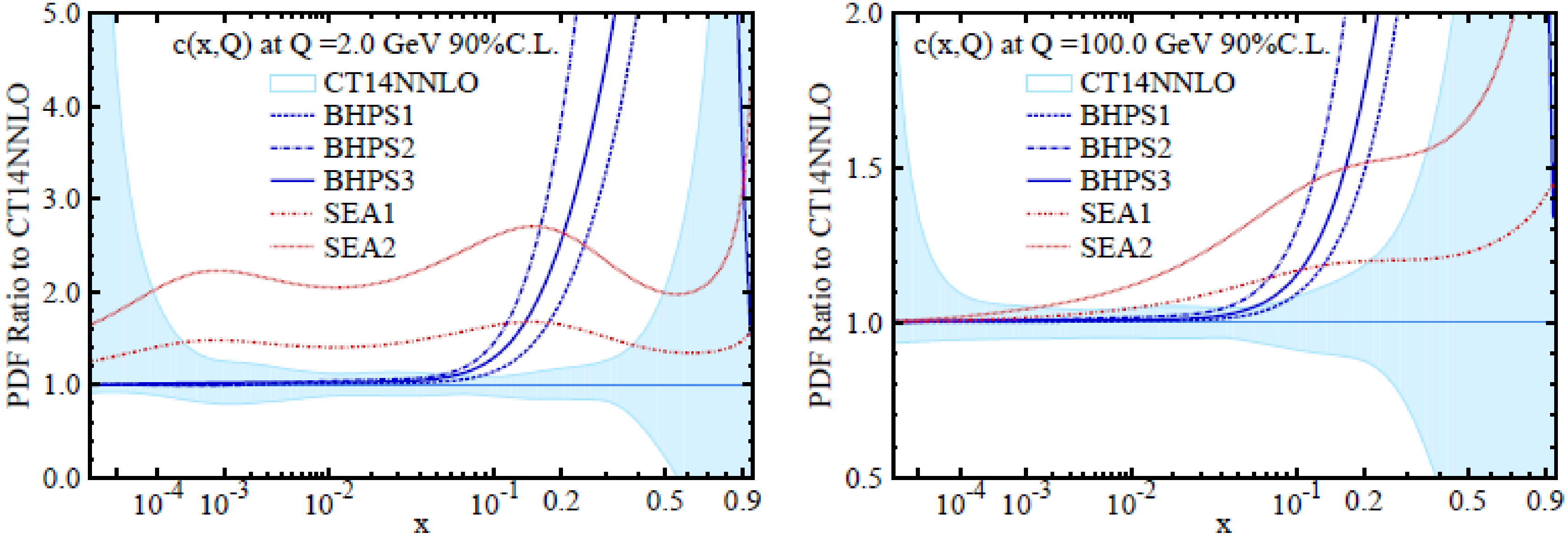
   ⇒ Physical behavior of $c/\bar{u}$, $c/\bar{d}$ ratios

3. ``**Sea-like**" $c(x, Q_0)$: SEA1, SEA2

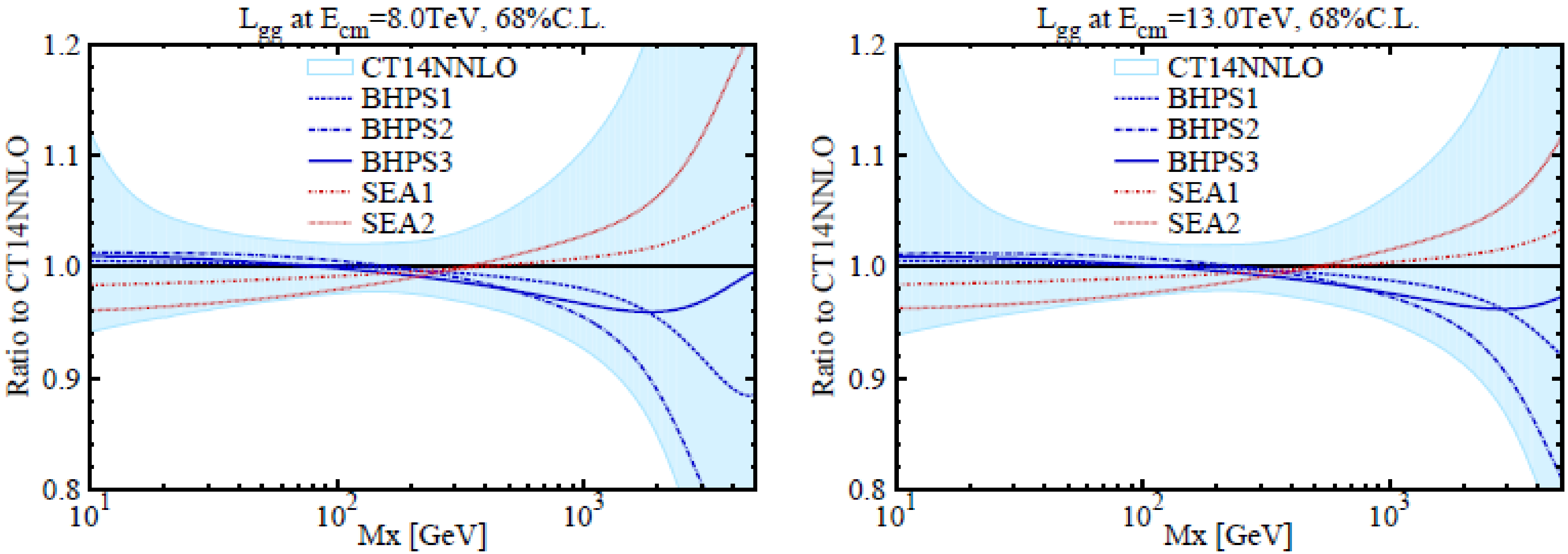
$$c(x) = \bar{c}(x) = A\left[\bar{d}(x, Q_0) + \bar{u}(x, Q_0)\right]$$



Impact of IC on the PDFs and their ratios



Impact of IC on gg luminosities

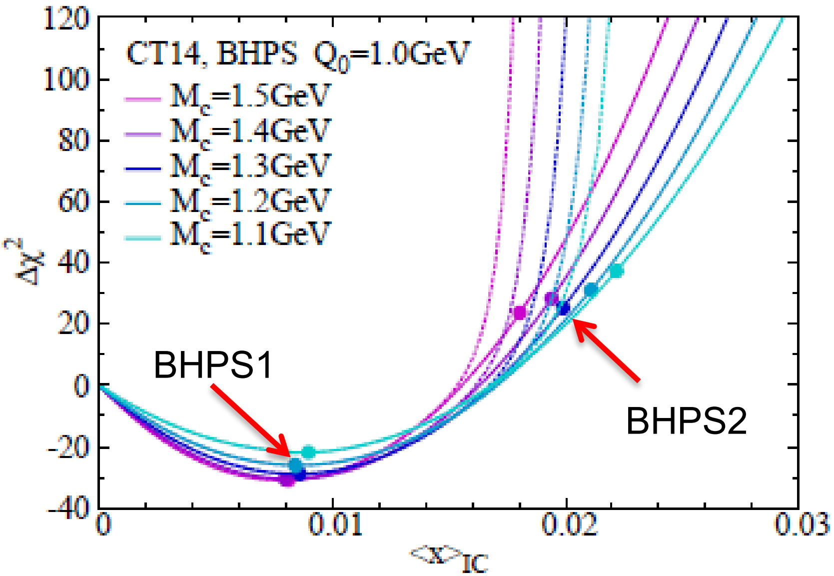


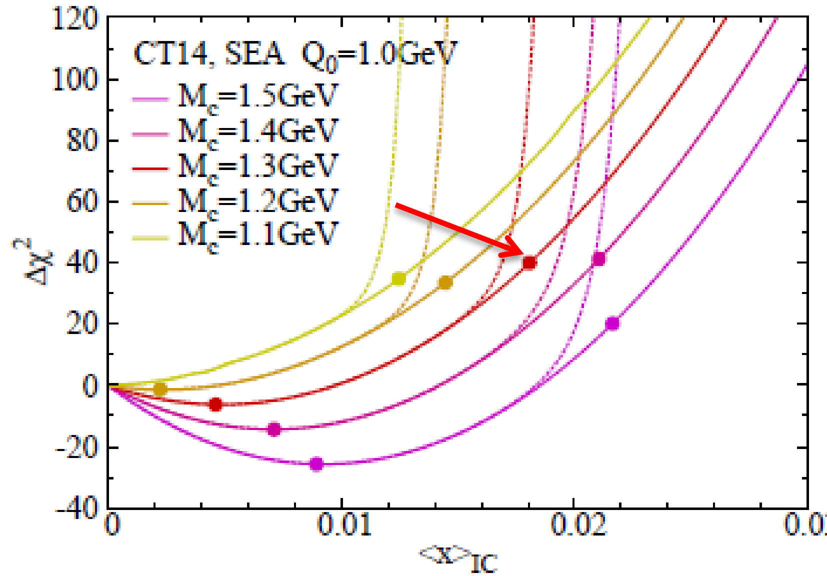
At √s = 8 TeV the most prominent distortions are from the SEA2 model which is suppressed at lower MX and is notably larger than CT14 for MX in the TeV range. The BHPS models are almost coincident with CT14 for MX < 200 GeV: BHPS1 and BHPS2 are suppressed above MX > 300 GeV, while BHPS3 is suppressed for 0.3 <MX < 3 TeV and enhanced above this energy by approximately 3%.

The impact on the Higgs cross section is small, with sizable impacts on the high-mass gg PDF luminosities, but still within uncertainties.

DEPENDENCE OF FIT ON THE CHARM-QUARK MASS

The combined HERA charm production and inclusive DIS data play an important role in the description of the goodness of fit. mc is a key input scale.





BHPS model: the position of the χ^2 minimum is relatively stable as mc is varied, while the upper limit on the amount of IC decreases to 1.7%. BHPS model is not dramatically affected by variations of mc

SEA model: limits on the amount of IC allowable are shifted towards higher values.
ubar and dbar are well constrained by data (vector boson production in pp and pbar p) in the intermediate/small x region, and cannot change too much

Study of $R_c = (c + \bar{c})/(\bar{u} + \bar{d})$ suppression ratio