Heavy Flavour Physics – MRST (MSTW) Approach

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Fixed Flavour

Charm $\sim 1.5\mathrm{GeV}$, bottom $\sim 4.3\mathrm{GeV}$, top $\sim 175\mathrm{GeV}$. Essential to treat first two correctly in global fits for parton distributions. Two distinct regimes:

Near threshold $Q^2 \sim m_H^2$ massive quarks not partons. Created in final state. Described using **Fixed Flavour Number Scheme** (FFNS).

$$F(x, Q^2) = C_k^{FF}(Q^2/m_H^2) \otimes f_k^{n_f}(Q^2)$$

Does not sum $\alpha_S^n \ln^n Q^2/m_H^2$ terms in perturbative expansion. Usually achieved by definition of heavy flavour parton distributions and solution of evolution equations.

Should reall have GVFNS covering whole regime properly.

However FFNS partons sometimes needed because hard cross-sections only calculated with all heavy flavour generated in the final state.

HQVDIS for differential heavy flavour production in DIS, MC@NLO for heavy flavours, HERWIG for heavy flavour production (strictly needs LO partons), *etc.*

However, FFNS must be done properly.

The NLO ($\mathcal{O}(\alpha_S^2)$) coefficient functions for heavy flavour in DIS calculated in scheme where the coupling α_S is fixed at **3** flavours. Partons have to be defined in same way. e.g. at leading order the gluon contribution to F_L is

$$F_L \;=\; \alpha_S \, C^1_{Lg} \otimes g,$$

$$\rightarrow \frac{\partial F_L}{\partial \ln Q^2} \;=\; -\beta_0 \, \alpha_S^2 \, C^1_{Lg} \otimes g \;+\; \alpha_S^2 \, C^1_{Lg} \otimes P^{(0)}_{gg} \otimes g \;\; + \; \text{quark term}.$$

$\beta_0 = (11 - \frac{2}{3} n_f)/4\pi$ and $P^{(0)}_{gg}$ contains a term $-(\frac{2}{3} n_f/4\pi)\delta(1-z)$.

Hence in going from $n_f = 3$ renormalization scheme to the $n_f = 4$ renormalization scheme, the change in these two terms cancels out.

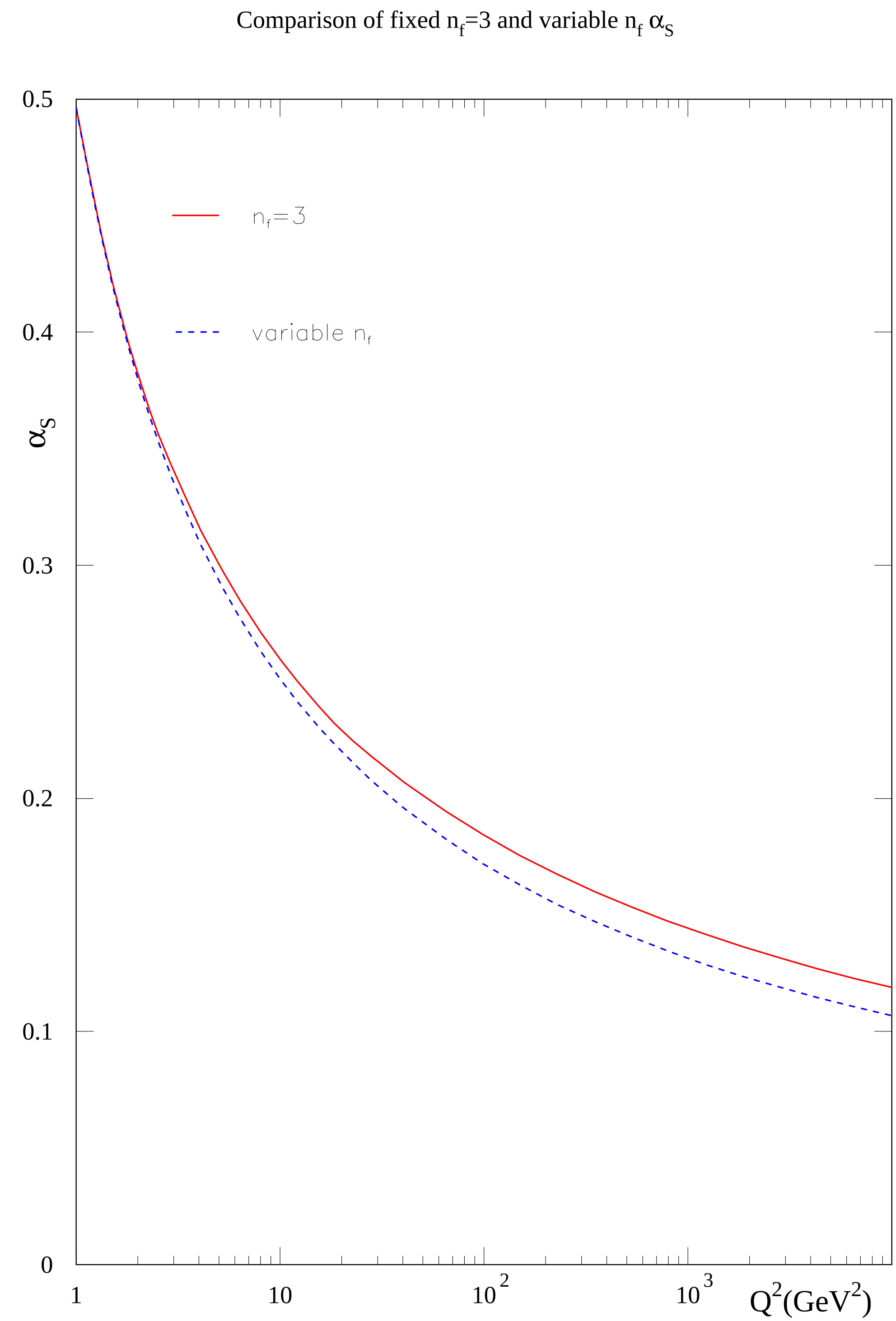
Very often (being frank, usually) done incorrectly.

Thanks to Paul Thompson for drawing this to attention.

Compared to variable-flavour α_S the $n_f = 3$ version is either $\sim 12\%$ smaller at $\mu^2 = M_Z^2$ or if identical at this high scale, hugely bigger at low μ^2.

Cannot really determine $\alpha_S(M_Z^2)$ from a FFNS fit.

It is a $n_f = 3$ definition of $\alpha_S(M_Z^2)$ – simply not the same quantity as usual $n_f = 5$ definition of $\alpha_S(M_Z^2)$.



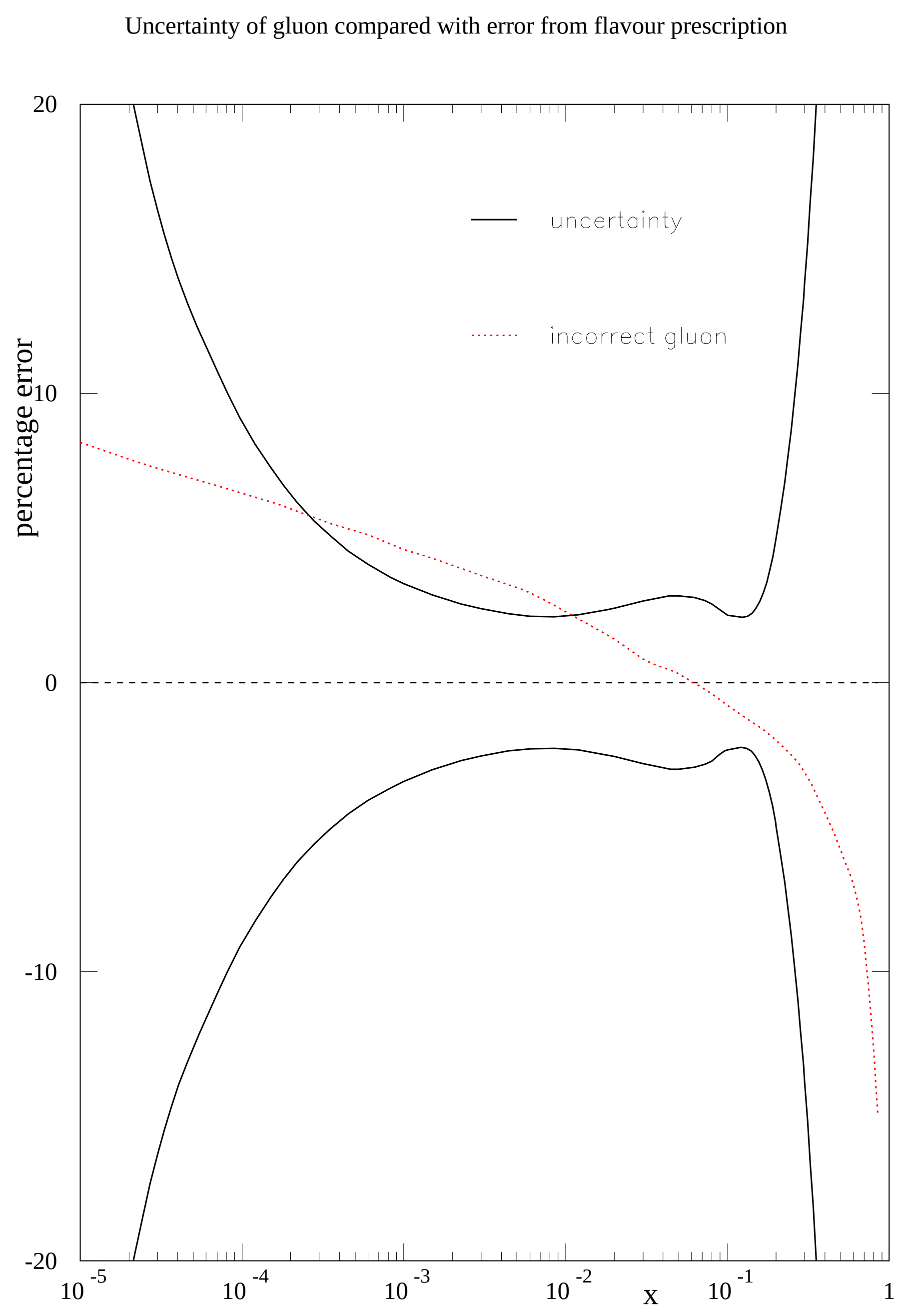
The error made in using the wrong coupling is quite significant.

Coupling too big $\longrightarrow$ evolution too quick.

Compare incorrect and correct gluons at $Q^2 = 100 \mathrm{GeV}^2$. Error can be bigger than uncertainty.

Difference between gluons if fits made using correct and correct coupling treatment is similarly of the order of the size of the uncertainty.

Not enormous. Certainly not insignificant.



MRST generate **FFNS** partons by evolving from usual (MRST04) partons at $Q_0^2 = 1\mathrm{GeV}^2$ but keeping $n_f = 3$ in everything.

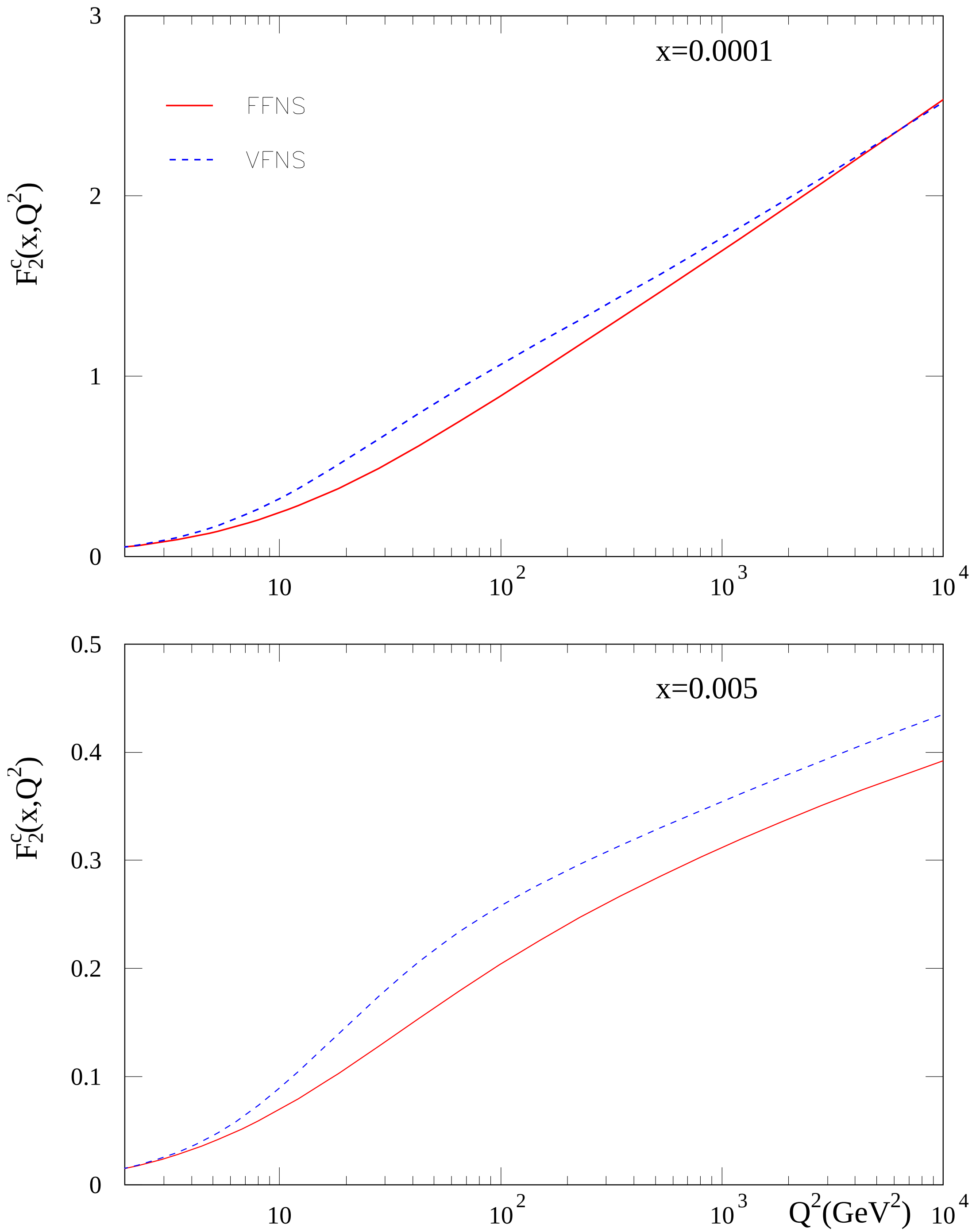
Difficult to do a global fit in FFNS since practically nothing other than neutral current DIS calculated in this scheme.

Charm contribution rather smaller than in VFNS due to lack of summation of logs.

Correct α_S procedure $\rightarrow$ much smaller $F_2^c(x,Q^2)$ than incorrect procedure – α_S in cross-section smaller and small-x gluon smaller.

Attempted global fit still bad for HERA $F_2(x,Q^2)$ – $\chi^2 = 80$ worse.

Evolution of NLO $F_2^c(x,Q^2)$ in FFNS and VFNS



FFNS not defined at NNLO – $\alpha_S^3 C_{2,Hg}^{FF,3}$ unknown. Ordering given by

LO $\quad \frac{\alpha_S}{4\pi} C_{2,Hg}^{FF,1} \otimes g^{n_f}$

NLO $\quad \left(\frac{\alpha_S}{4\pi}\right)^2 (C_{2,Hg}^{FF,2} \otimes g^{n_f} + C_{2,Hq}^{FF,2} \otimes \Sigma^{n_f})$

i.e. $F_2^H(x,Q^2) \neq 0$ at LO, and at LO

$$\frac{d\,F_2^H(x,Q^2)}{d\,\ln Q^2} \to \alpha_S/(2\pi) P_{qg}^0 \otimes g(x,Q^2)$$

and at NLO

$$\frac{d\,F_2^H(x,Q^2)}{d\,\ln Q^2} \to (\alpha_S/(2\pi))^2 P_{qg}^1 \otimes g(x,Q^2).$$

$C_{2,Hg}^{FF,2}$ contains no information on P_{qg}^2 and so $\alpha_S^2 C_{2,Hg}^{FF,2} \otimes g^{n_f}$ cannot represent the NNLO evolution of $F_2(x,Q^2)$.

This is important because unknown $\alpha_S^3 C_{2,Hg}^{FF,3}$ is not just $\mathcal{O}(\alpha_S^3)$, it is $\mathcal{O}(\alpha_S^3 \ln^3(Q^2/m_H^2))$.

Approximations could be made and the correct $Q^2/m_H^2 \to \infty$ limit found.

Variable Flavour

High scales $Q^2 \gg m_H^2$ massless partons. Behave like up, down, strange. Sum $\ln(Q^2/m_H^2)$ terms via evolution. **Zero Mass Variable Flavour Number Scheme** (ZMVFNS). Ignores $\mathcal{O}(m_H^2/Q^2)$ corrections.

$$F(x,Q^2) = C_j^{ZMVF} \otimes f_j^{n_f+1}(Q^2).$$

Partons in different number regions related to each other perturbatively.

$$f_k^{n_f+1}(Q^2) = A_{jk}(Q^2/m_H^2) \otimes f_k^{n_f}(Q^2),$$

Perturbative matrix elements $A_{jk}(Q^2/m_H^2)$ containing $\ln(Q^2/m_H^2)$ terms relate $f_k^{n_f}(Q^2)$ and $f_k^{n_f+1}(Q^2)$ $\rightarrow$ correct evolution for both.

At LO, i.e. zeroth order in α_S, relationship trivial,

$$q(g)_k^{n_f+1}(Q^2) \equiv q(g)_k^{n_f+1}(Q^2).$$

At NLO, i.e. first order in α_S

$$(h+\bar{h})(Q^2) = \frac{\alpha_S}{4\pi} P_{qg}^0 \otimes g^{n_f}(Q^2) \ln\left(\frac{Q^2}{m_H^2}\right), \quad g^{n_f+1}(Q^2) = \left(1+\frac{\alpha_S}{6\pi} \ln\left(\frac{Q^2}{m_H^2}\right)\right) g^{n_f}(Q^2),$$

i.e. the heavy flavour evolves from zero at $Q^2 = m_H^2$ according to standard quark evolution, gluon loses corresponding momentum. Natural to choose $Q^2 = m_H^2$ as transition point.

At NNLO, i.e. second order in α_S, much more complication

$$f_i^{n_f+1}(Q^2) = \left(\frac{\alpha_S}{(4\pi)}\right)^2 \sum_{ij} (A_{ij}^{2,0} + A_{ij}^{2,1} \ln(Q^2/m_H^2) + A_{ij}^{2,2} \ln^2(Q^2/m_H^2)) \otimes f_j^{n_f}(Q^2),$$

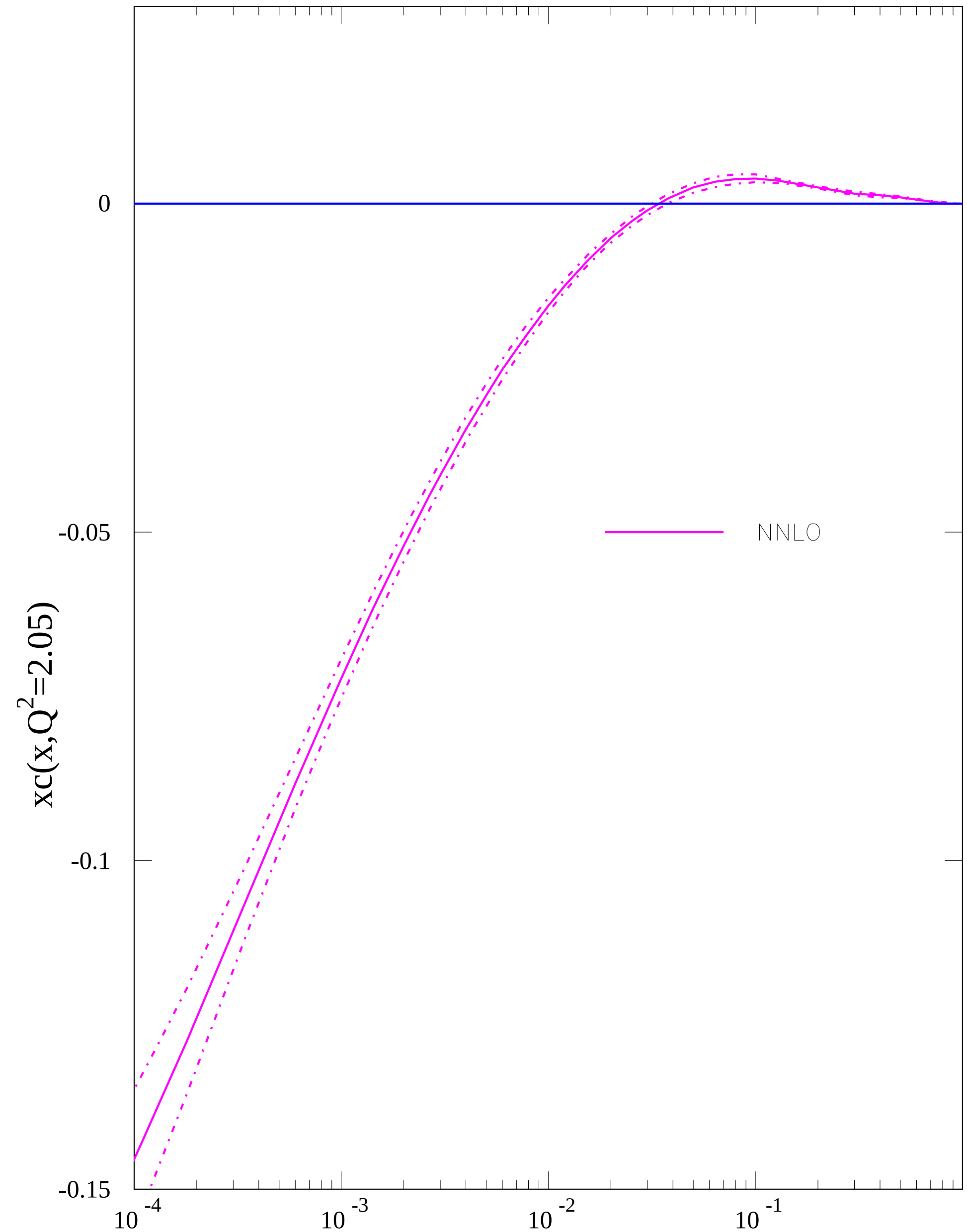
where $A_{ij}^{2,0}$ is generally nonzero. No longer any possibility of a smooth transition. In fact $A_{Hg}^{2,0}$ negative at small x.

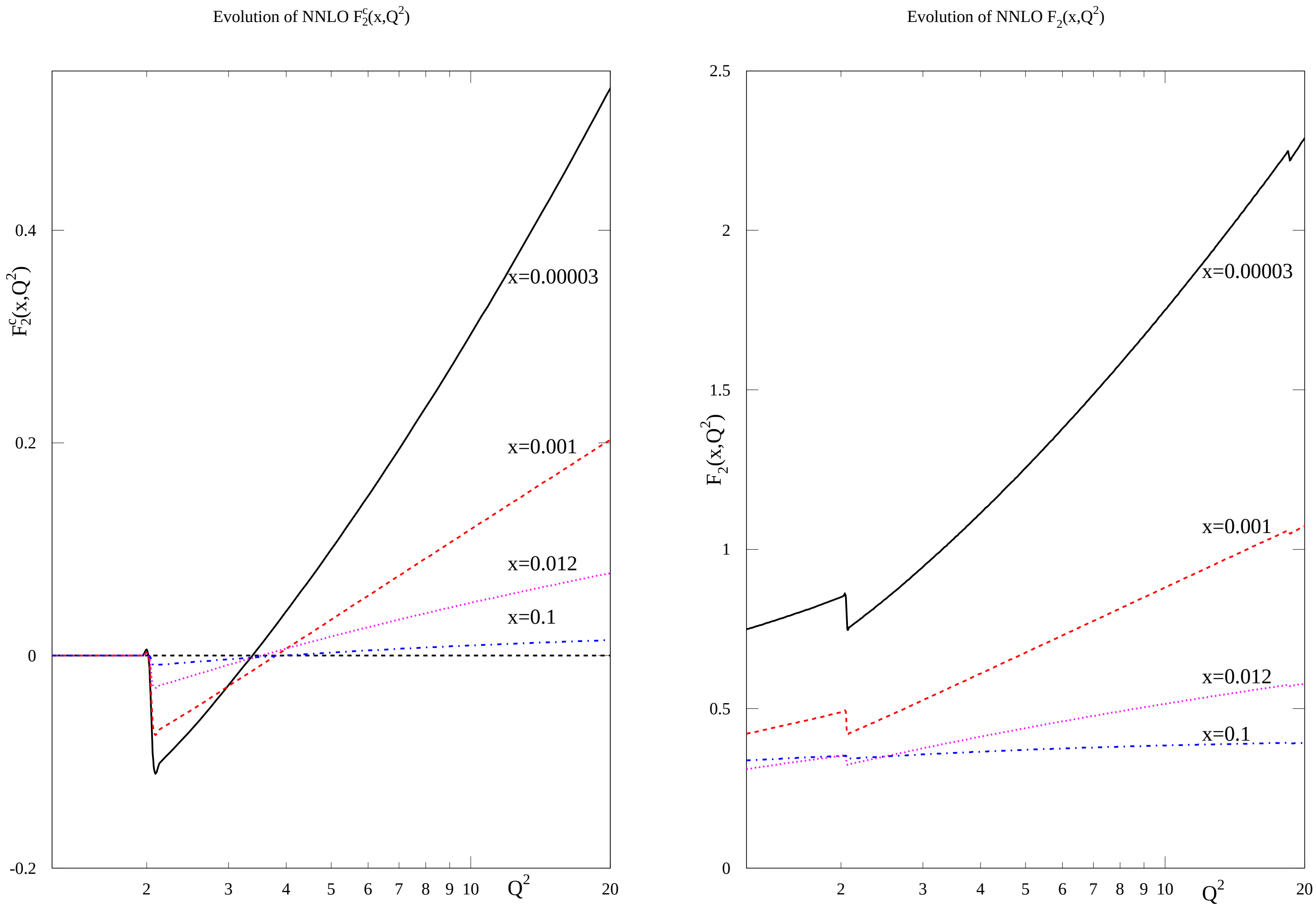
ZMVFNS not really feasible at NNLO. Huge discontinuity in $(c+\bar{c})(x,\mu^2)$ and $F_2^c(x,Q^2)$. Significant in $F_2^{Tot}(x,Q^2)$.

Heavy flavour no longer turns on from zero at $\mu^2 = m_c^2$

$$(c + \bar{c})(x, m_c^2) = A_{Hg}^2(m_c^2) \otimes g(m_c^2)$$

In practice turns on from negative value, (for general gluon).





Could turn on heavy flavour at $\sim 2m_H^2$. Distribution small there. However, $F_2^H(x,Q^2) = 0$ $Q^2 < 2m_H^2$

Need a general **Variable Flavour Number Scheme** (VFNS) taking one from the two well-defined limits of $Q^2 \leq m_H^2$ and $Q^2 \gg m_H^2$.

The VFNS can be defined by demanding equivalence of the n_f (FFNS) and n_f+1-flavour descriptions at all orders,

$$F^H(x,Q^2) = C_k^{FF}(Q^2/m_H^2) \otimes f_k^{n_f}(Q^2) = C_j^{VF}(Q^2/m_H^2) \otimes f_j^{n_f+1}(Q^2)$$
$$\equiv C_j^{VF}(Q^2/m_H^2) \otimes A_{jk}(Q^2/m_H^2) \otimes f_k^{n_f}(Q^2).$$

Hence, the VFNS coefficient functions satisfy

$$C_k^{FF}(Q^2/m_H^2) = C_j^{VF}(Q^2/m_H^2) \otimes A_{jk}(Q^2/m_H^2),$$

which at $\mathcal{O}(\alpha_S)$ gives

$$C_{2,g}^{FF,1}(Q^2/m_H^2) = C_{2,HH}^{VF,0}(Q^2/m_H^2) \otimes P_{qg}^0 \ln(Q^2/m_H^2) + C_{2,g}^{VF,1}(Q^2/m_H^2),$$

The VFNS coefficient functions tend to the massless limits as $Q^2/m_H^2 \to \infty$.

However, $C_j^{VF}(Q^2/m_H^2)$ only uniquely defined in massless limit $Q^2/m_H^2 \to \infty$.

Can swap $\mathcal{O}(m_H^2/Q^2)$ terms between $C_{2,HH}^{VF,0}(Q^2/m_H^2)$ and $C_{2,g}^{VF,1}(Q^2/m_H^2)$.

Original ACOT prescription violated threshold $W^2 > 4m_H^2$ since only needed one quark in final state rather than quark-antiquark pair. Not smooth transition at $Q^2 = m_H^2$ as $n_f \to n_f + 1$.

TR variable flavour number scheme (**TR-VFNS**) recognized ambiguity in definition of $C^{VF,0}_{2,HH}(Q^2/m_H^2)$ for first time and removed it by imposition of physically motivated constraints of $(d\,F_2/d\,\ln Q^2)$ continuous at transition (in gluon sector).

Smoothness guaranteed at $Q^2 = m_H^2$, but approach to $Q^2/m_H^2 \to \infty$ a little odd.

More of a problem, complicated – $C^{VF,0}_{2,HH}(Q^2/m_H^2) \propto (P^0_{qg})^{-1}$, not a simple function.

Various other alternatives since this. Most recently Tung, Kretzer, Schmidt have come up with the ACOT(χ) prescription which I interpret as

$$C^{VF,0}_{2,HH}(Q^2/m_H^2, z) = \delta(z - Q^2/(Q^2 + 4m_H^2)).$$

$$\to F_2^{H,0}(x, Q^2) = (h + \bar{h})(x/x_{max}, Q^2), \qquad x_{max} = Q^2/(Q^2 + 4m_H^2)$$

$\to C^{ZM,0}_{2,HH}(z) = \delta(1-z)$ for $Q^2/m_H^2 \to \infty$. Also $W^2 = Q^2(1-x)/x \geq 4m_H^2$. Moreover – very simple.

For VFNS to remain simple (and physical) at all orders is necessary to choose

$$C^{VF,n}_{2,HH}(Q^2/m_H^2, z) = C^{ZM,n}_{2,HH}(z/x_{max}).$$

It is also important to choose

$$C^{VF,n}_{L,HH}(Q^2/m_H^2, z) \propto C^{ZM,n}_{L,HH}(z/x_{max}),$$

and to impose that $C^{VF,0}_{L,HH}(Q^2/m_H^2, z) \equiv 0$, despite the fact that $C^{0}_{L,HH}(Q^2/m_H^2, x) \neq 0$ for single quark-photon scattering.

$F_L^H(x, Q^2)$ suppressed by v^3 (v is velocity of heavy quark) near threshold. For smoothness have

$$C^{VF,n}_{L,HH}(Q^2/m_H^2, z) = \frac{5}{4}\left(\frac{1}{1+4m_H^2/Q^2} - \frac{1}{5}\right) C^{ZM,n}_{L,HH}(z/x_{max}).$$

Prefactor independent of x, so no problem in convolutions.

Adopting this convention then at NNLO we have, for example,

$$C^{VF,2}_{2,Hg}(Q^2/m_H^2, z) = C^{FF,2}_{2,Hg}(Q^2/m_H^2, z) - C^{ZM,1}_{2,HH}(z/x_{max}) \otimes A^1_{Hg}(Q^2/m_H^2)$$

$$-C^{ZM,0}_{2,HH}(z/x_{max}) \otimes A^2_{Hg}(Q^2/m_H^2).$$

Since $A^2_{Hg}(1, z) \neq 0$, $C^2_{2,Hg}(Q^2/m_H^2, z)$ is discontinuous as we go across $Q^2 = m_H^2$. Compensates exactly for discontinuity in the heavy flavour parton distribution, i.e. $F_2^H(x, Q^2)$ completely continuous.

In practice requires use of $C^{FF,2}_{2,Hg}(Q^2/m_H^2, z)$. Exists as semi-analytic code by Smith and Riemersma. High W^2 and $W^2 \to 4m_H^2$ parts analytic, rest numerical.

I have produced much faster analytic expressions. Exact for $Q^2/m_H^2 \to \infty$, fits to analytic functions for (m_H^2/Q^2) remainders. Slightly approximate, but error in $F_2^H(x, Q^2)$ only $1 - 2\%$ even in most extreme cases.

Useful for FFNS analyses also.

One more problem in defining VFNS. Ordering for $F_2^H(x,Q^2)$ different for n_f and n_f+1 regions.

	n_f-flavour	n_f+1-flavour
LO	$\frac{\alpha_S}{4\pi} C^{FF,1}_{2,Hg} \otimes g^{n_f}$	$C^{VF,0}_{2,HH} \otimes (h+\bar{h})$
NLO	$\left(\frac{\alpha_S}{4\pi}\right)^2 (C^{FF,2}_{2,Hg} \otimes g^{n_f} + C^{FF,2}_{2,Hq} \otimes \Sigma^{n_f})$	$\frac{\alpha_S}{4\pi}(C^{VF,1}_{2,HH} \otimes (h+\bar{h}) + C^{FF,1}_{2,Hg} \otimes g^{n_f+1})$
NNLO	$\left(\frac{\alpha_S}{4\pi}\right)^3 \sum_i C^{FF,3}_{2,Hi} \otimes f_i^{n_f}$	$\left(\frac{\alpha_S}{4\pi}\right)^2 \sum_j C^{VF,2}_{2,Hj} \otimes f_j^{n_f+1}$.

Switching direct from fixed order to same order when going from n_f to $nf+1$ flavours $\longrightarrow$ discontinuity.

Must make some decision how to deal with this.

Up to now ACOT have used e.g.

NLO $\frac{\alpha_S}{4\pi}C^{FF,1}_{2,Hg} \otimes g^{n_f} \rightarrow \frac{\alpha_S}{4\pi}(C^{VF,1}_{2,HH} \otimes (h+\bar{h}) + C^{FF,1}_{2,Hg} \otimes g^{n_f+1})$,

i.e., same order of α_S above and below.

But LO evolution below and NLO evolution above. Slope discontinuous.

TR have used e.g.

LO $$\frac{\alpha_S(Q^2)}{4\pi}C^{FF,1}_{2,Hg}(Q^2/m_H^2) \otimes g^{n_f}(Q^2) \rightarrow \frac{\alpha_S(M^2)}{4\pi}C^{FF,1}_{2,Hg}(1) \otimes g^{n_f}(M^2)$$
$$+C^{VF,0}_{2,HH}(Q^2/m_H^2) \otimes (h+\bar{h})(Q^2),$$

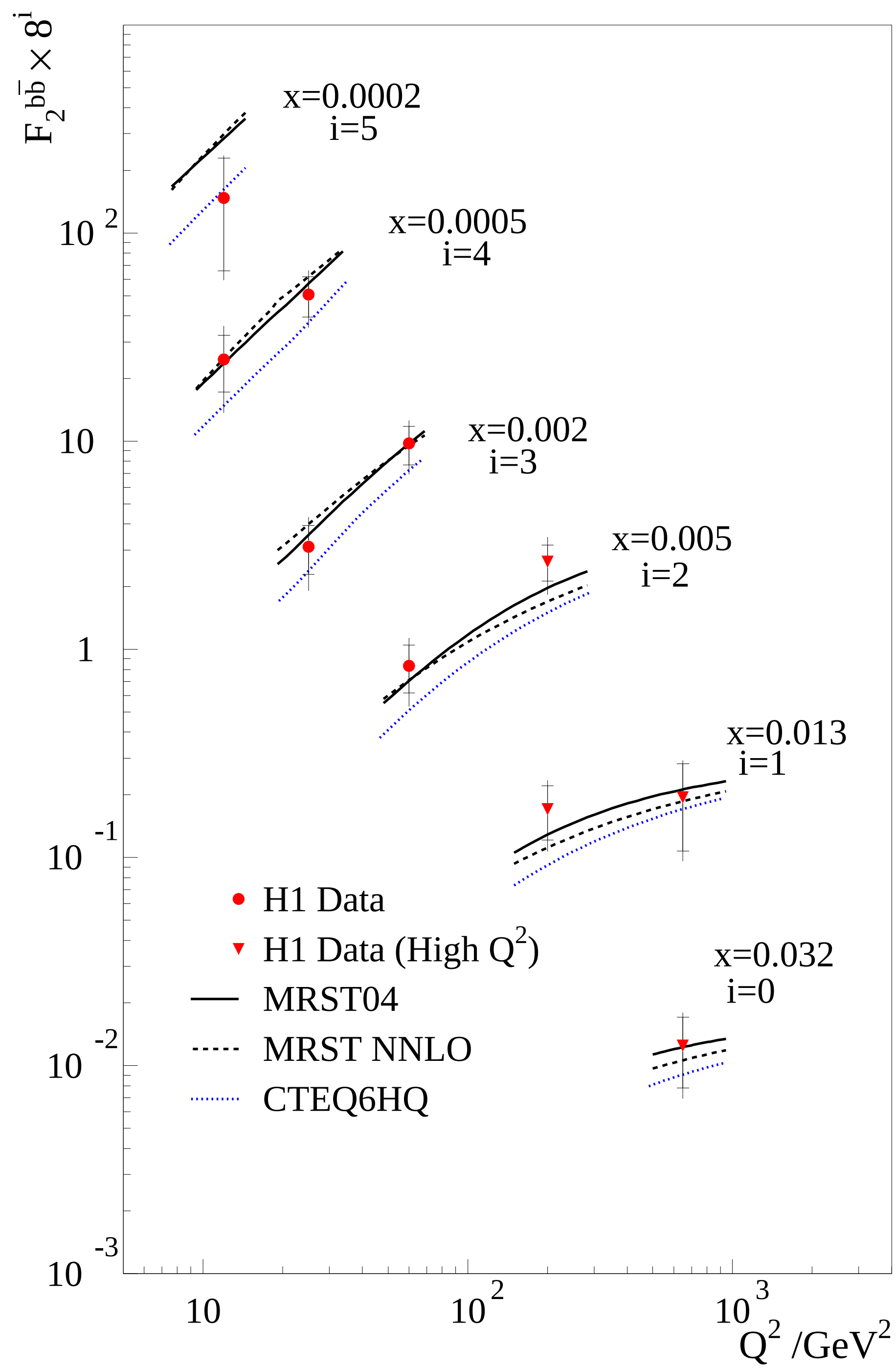
i.e. freeze higher order α_S term when going upwards through $Q^2 = m_H^2$.

This difference in choice is extremely important.

This is the main difference in the NLO predictions from MRST and CTEQ in the comparison to H1 data on $F_2^b(x,Q^2)$.

$\mathcal{O}(\alpha_S^2)$ part is dominant at for $Q^2 \leq m_c^2$. "Frozen" part remains significant. Clearly improves match to data.

Choose TR approach.



In order to define my VFNS at NNLO, need $\mathcal{O}(\alpha_S^3)$ heavy flavour coefficient functions for $Q^2 \leq m_H^2$ and to be frozen for $Q^2 > m_H^2$. However, not calculated.

Know leading threshold logarithms (Laenen and Moch). Leading contribution for W^2 not much above $4m_H^2$.

$$C_{2,Hg}^{FF,3,thresh}(Q^2/m_H^2, z) \sim \frac{1}{1+\eta}\frac{Q^2}{Q^2+4m_H^2}f(\eta), \qquad \eta = \frac{Q^2(1-z)}{z4m_H^2} - 1,$$

i.e. $\eta \to 0$ at threshold and $\eta \to \infty$ as $W^2 \to \infty$.

These occur in gluon sector.

Can also derive leading $ln(1/x)$ term from k_T-dependent impact factors derived by Catani, Ciafaloni and Hautmann.

$$C^{FF,3,lowx}_{2,Hg}(Q^2/m_H^2, z) = 96\frac{\ln(1/z)}{z}f(Q^2/m_H^2), \qquad f(1) \approx 4,$$

and $C^{FF,3,lowx}_{2,Hq}(Q^2/m_H^2, z) = 4/9 C^{FF,3,lowx}_{2,Hg}(Q^2/m_H^2, z)$.

By analogy with known NNLO coefficient functions and splitting functions hypothesize

$$C^{FF,3,lowx}_{2,Hg}(Q^2/m_H^2, z) = \frac{96}{z}(\ln(1/z) - 4)(1 - z/x_{max})^{20} f(Q^2/m_H^2),$$

i.e. $\ln(1/z)$ always accompanied by ~ -4, and effect of small z term heavily damped for $z > 0.1$.

Amount of information similar to previous approximate NNLO splitting functions (van Neerven, Vogt), which were very good.

Can produce full NNLO predictions for charm with discontinuous partons, but continuous $F^H(x,Q^2)$.

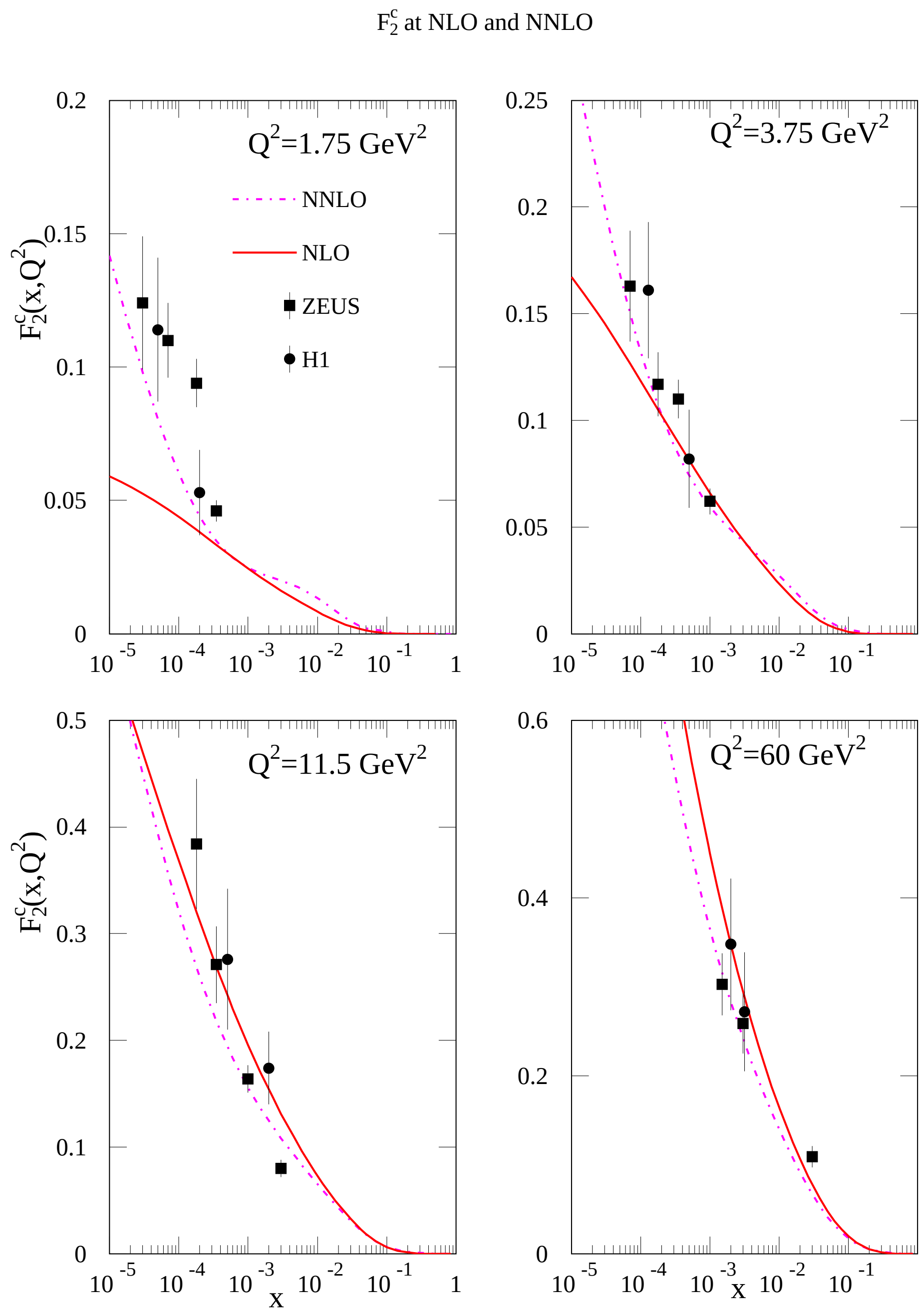
Approximation in $\mathcal{O}(\alpha_S^3)$ heavy flavour coefficient functions for $Q^2 \leq m_H^2$ and frozen for $Q^2 > m_H^2$.

Results not very sensitive to choices in this, within sensible range.

Clearly improves match to lowest Q^2 data, where NLO always too low.

Have $\chi^2 = 97/78$ at NLO for all HERA data with $Q^2 \geq 2\mathrm{GeV}^2$.

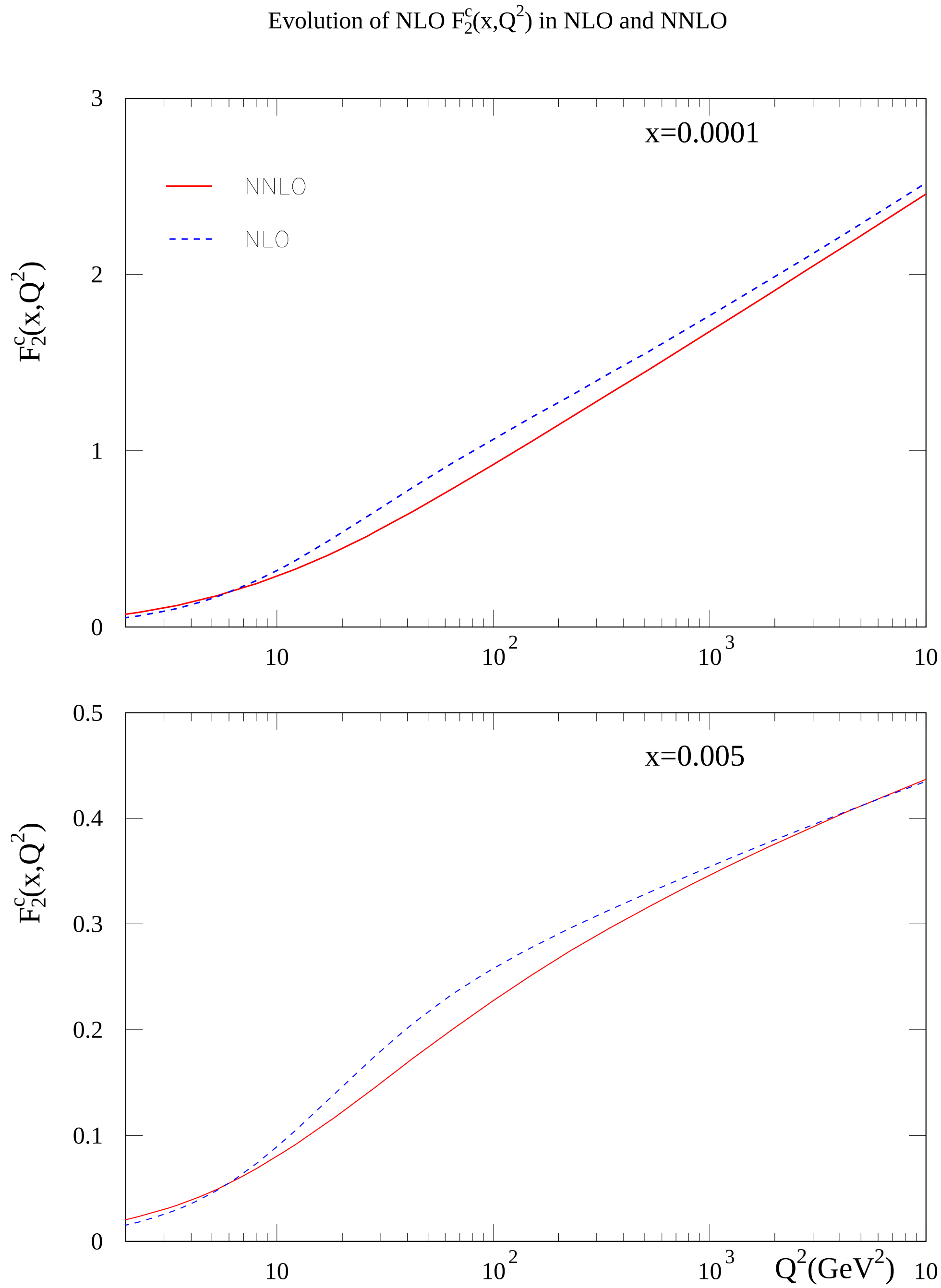
$\rightarrow \chi^2 = 90/78$ at NNLO. Improvement at lowest Q^2, but generally changed shape.



NNLO $F_2^c(x,Q^2)$ starts from higher value at low Q^2.

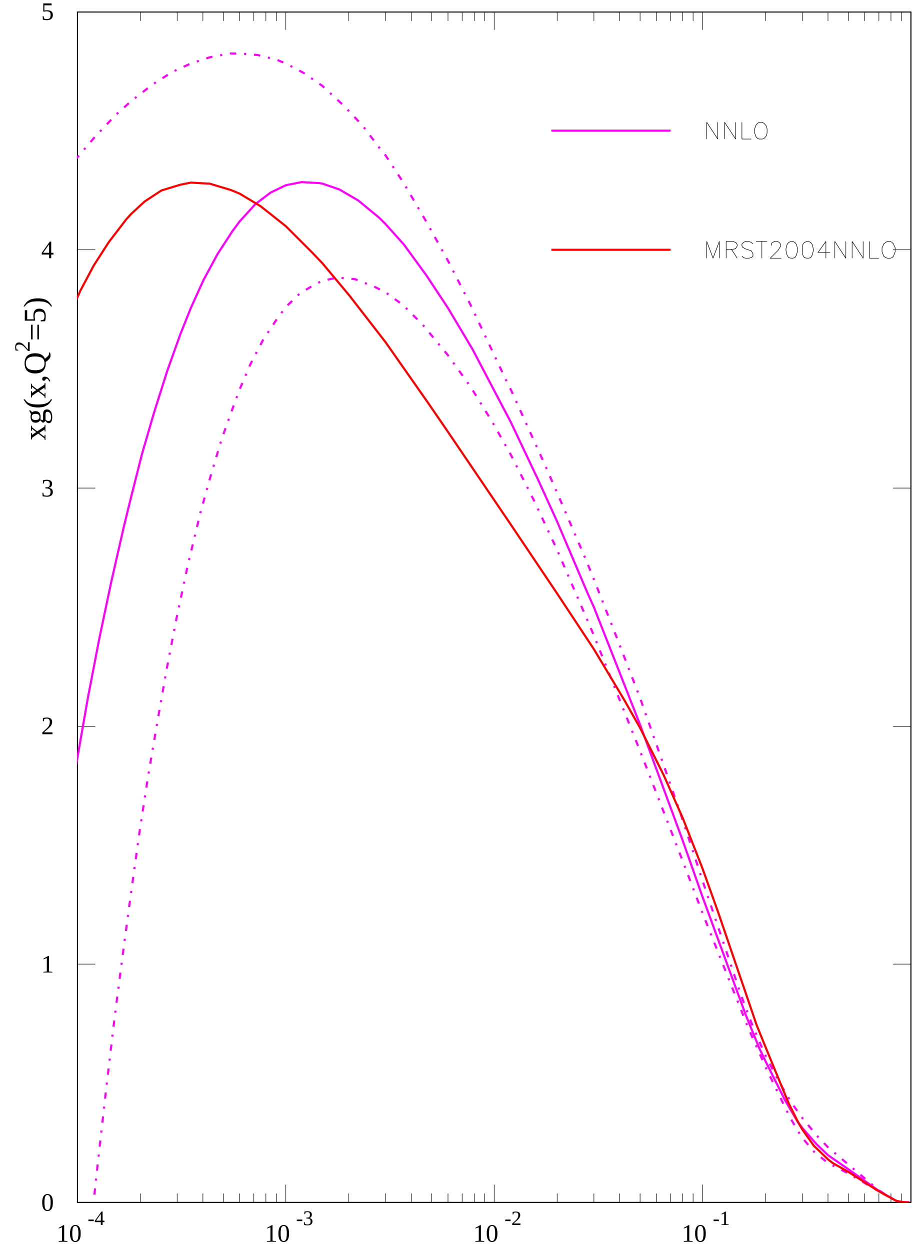
At high Q^2 dominated by $(c+\bar{c})(x,Q^2)$. This has started evolving from negative value at $Q^2 = m_c^2$. Remains lower than at NLO for similar evolution.

General trend – $F_2^c(x,Q^2)$ flatter in Q^2 at NNLO than at NLO. Important effect on gluon distribution going from one to other.

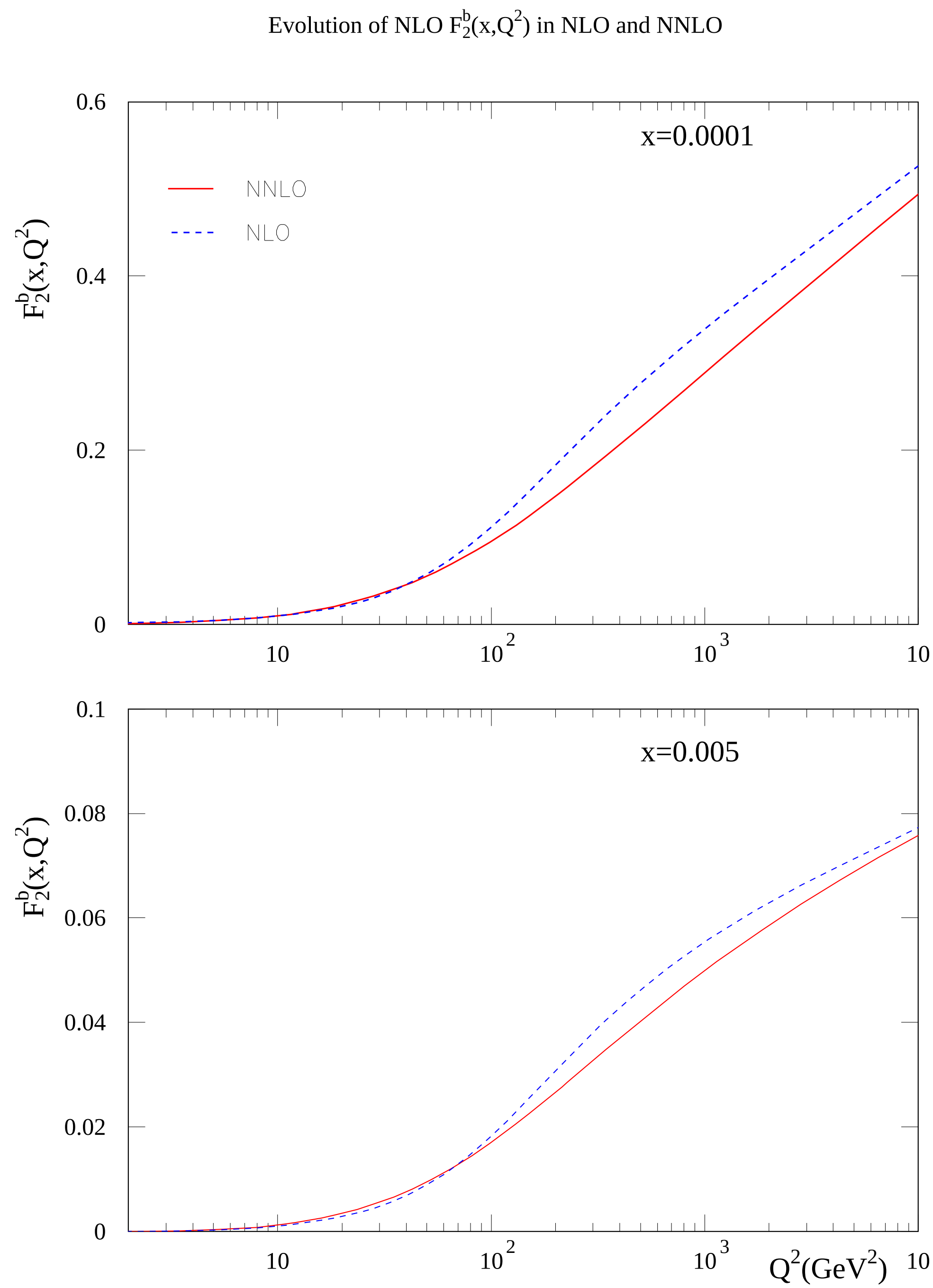


Difference in charm procedure affects gluon compared to approx MRST2004 NNLO fit.

Change greater than uncertainty in some places. Correct heavy flavour treatment vital.



Exactly same consideration for $F_2^b(x, Q^2)$ comparing NNLO and NLO.



Conclusions

Defined a set of MRST FFNS partons at NLO (and at LO) by evolving from standard MRST04 partons at $Q_0^2 = 1\text{GeV}^2$, and keeping $n_f = 3$. FFNS only approximate at NNLO.

Important to use consistent definition of α_S in all quantities, i.e. fix $n_f = 3$. Doing so makes gluon and $F_2^H(x, Q^2)$ smaller than incorrect treatment. Makes fitting data harder. Illustrates need for VFNS.

Discontinuities in both parton distributions and coefficient functions at NNLO. Makes ZMVFNS badly discontinuous.

Generalization of ACOT(χ) prescription leads to physically sensible and simple VFNS.

Must still be careful about matching when going across transition point of $Q^2 = m_H^2$. If done properly guarantees continuity of structure functions. Choose TR method of matching above and below transition. Choice significant – matches data much better.

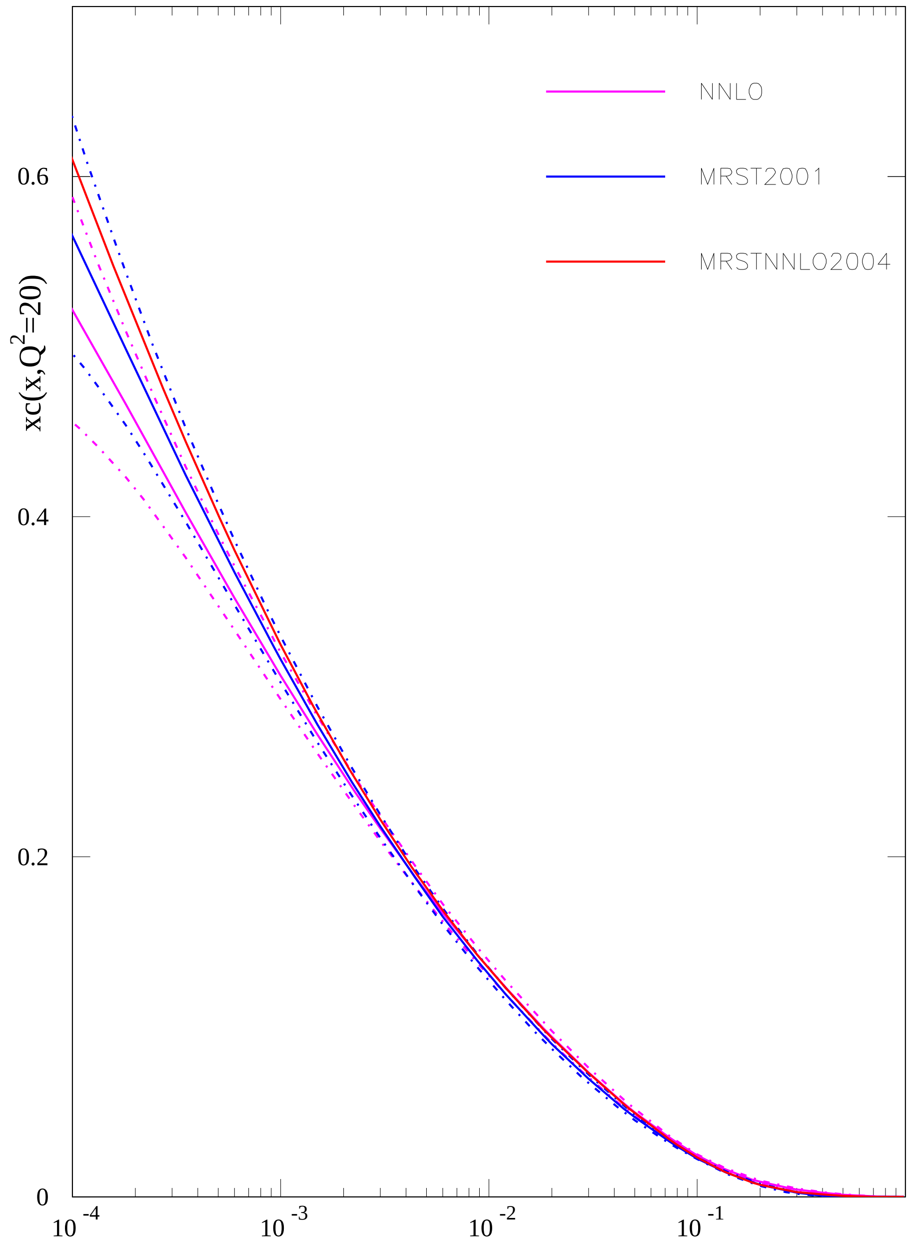
Devised full NNLO VFNS, with small amount of necessary modelling. Seems to improve fit to lowest x and Q^2 data.

Being used in full NNLO global fits for partons. Important impact on gluon.

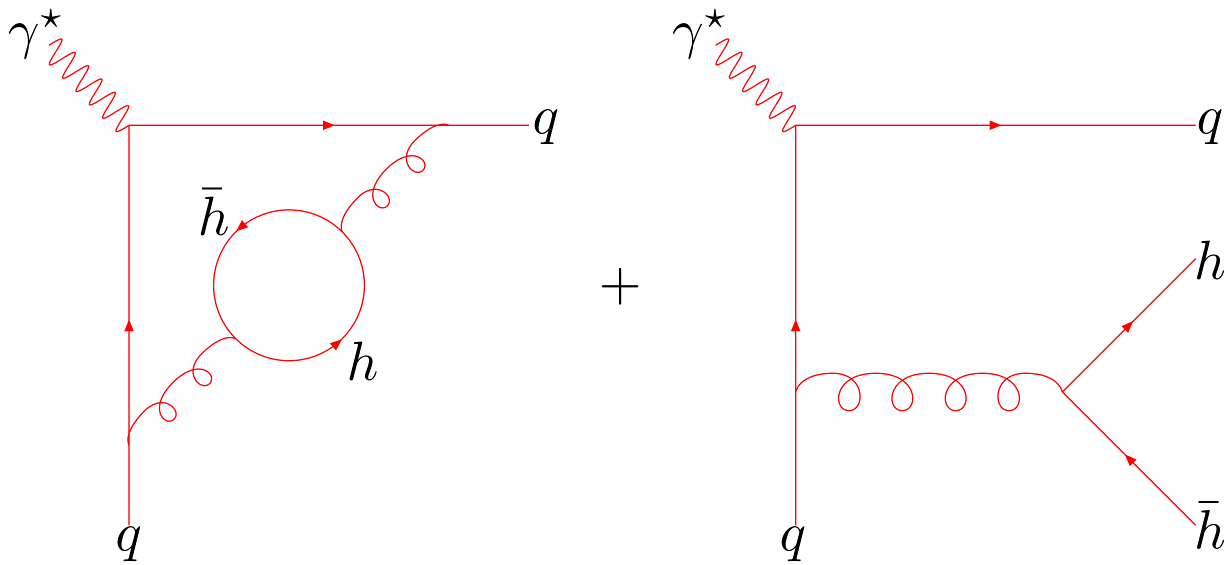
At small x increased evolution from NNLO splitting function allows charm to catch up a bit with NLO which starts from zero at m_c^2.

Always lags a little at higher Q^2

Significantly lags old approx MRST2004 distribution which turned on from zero.



At NNLO also get contribution due to heavy flavours away from photon vertex.



VFNS is defined as before, but complications due to $(\ln^m(1-z)/(1-z))_+$ terms at threshold. This also leads to a discontinuity in the coefficient functions which cancels that in the light quark distributions.

Strictly, left-hand type diagram and soft parts of right-hand type diagram should be light flavour structure function, and hard part of right-hand type diagram contributes to $F_2^H(x, Q^2)$ (Chuvakin, Smith, van Neerven).

Can be implemented (depends on separation parameter), but each contribution tiny, i.e. handful of percent of heavy flavour at high Q^2. At moment all in light flavours.