A Variable Flavour Number Scheme at NNLO

Robert Thorne

April 29, 2005

University of Cambridge

Royal Society University Research Fellow

Heavy Quarks

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).

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

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

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

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.

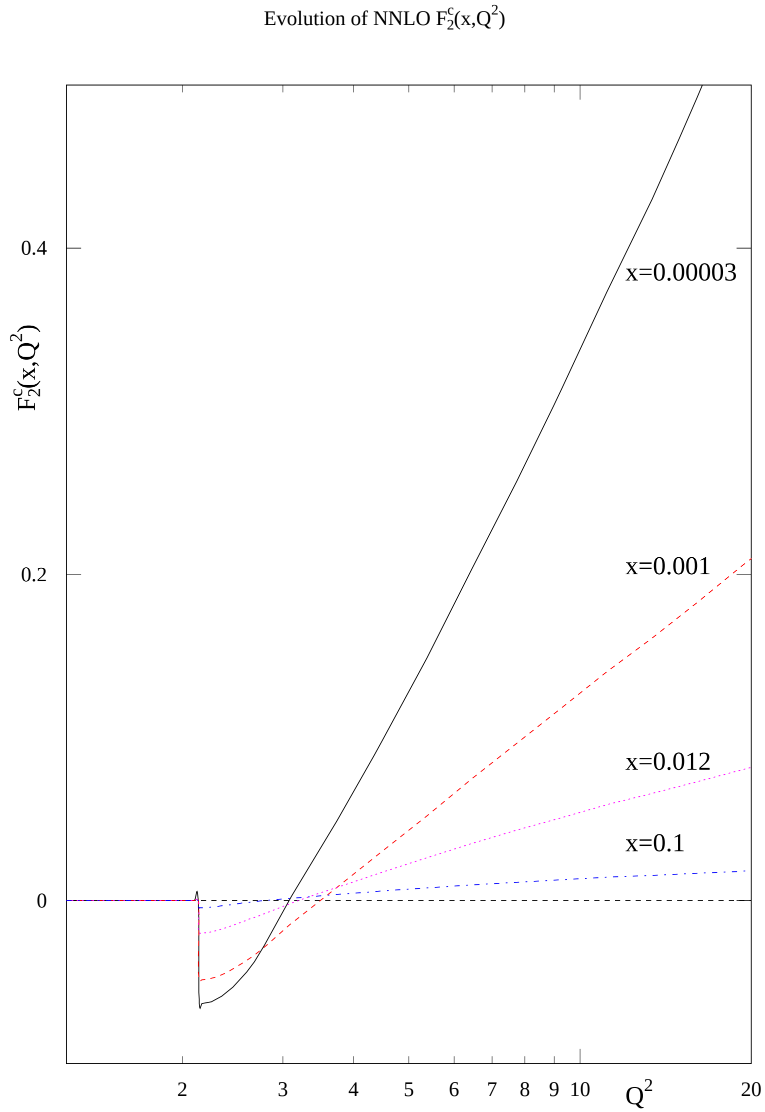
IN ZMVFNS coefficient functions already lead to discontinuity at NLO, i.e.

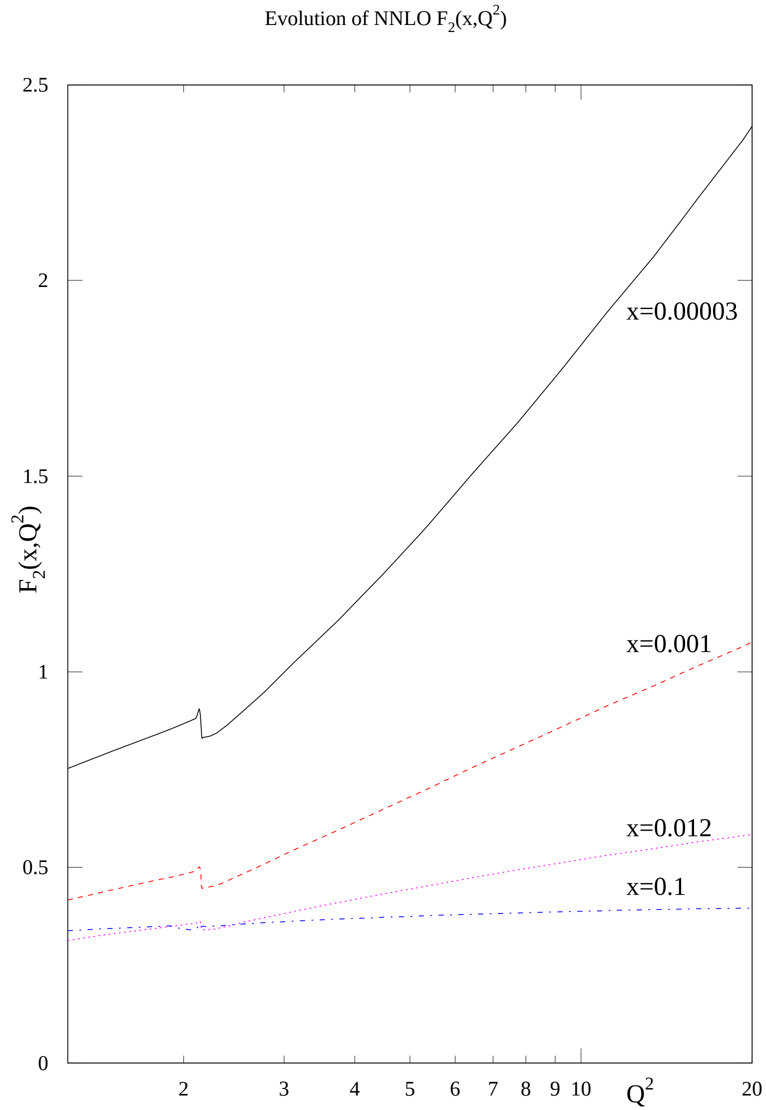
$$F_2^H(x,Q^2) = 0 \quad Q^2 < m_H^2, \qquad\qquad = \frac{\alpha_S}{4\pi} C_{2,g} \otimes g^{n_f+1}(Q^2) \quad Q^2 > m_H^2.$$

However, this is very small at NLO.

Larger effect at NNLO. Also negative at smallish x. ($x \sim 0.001$).

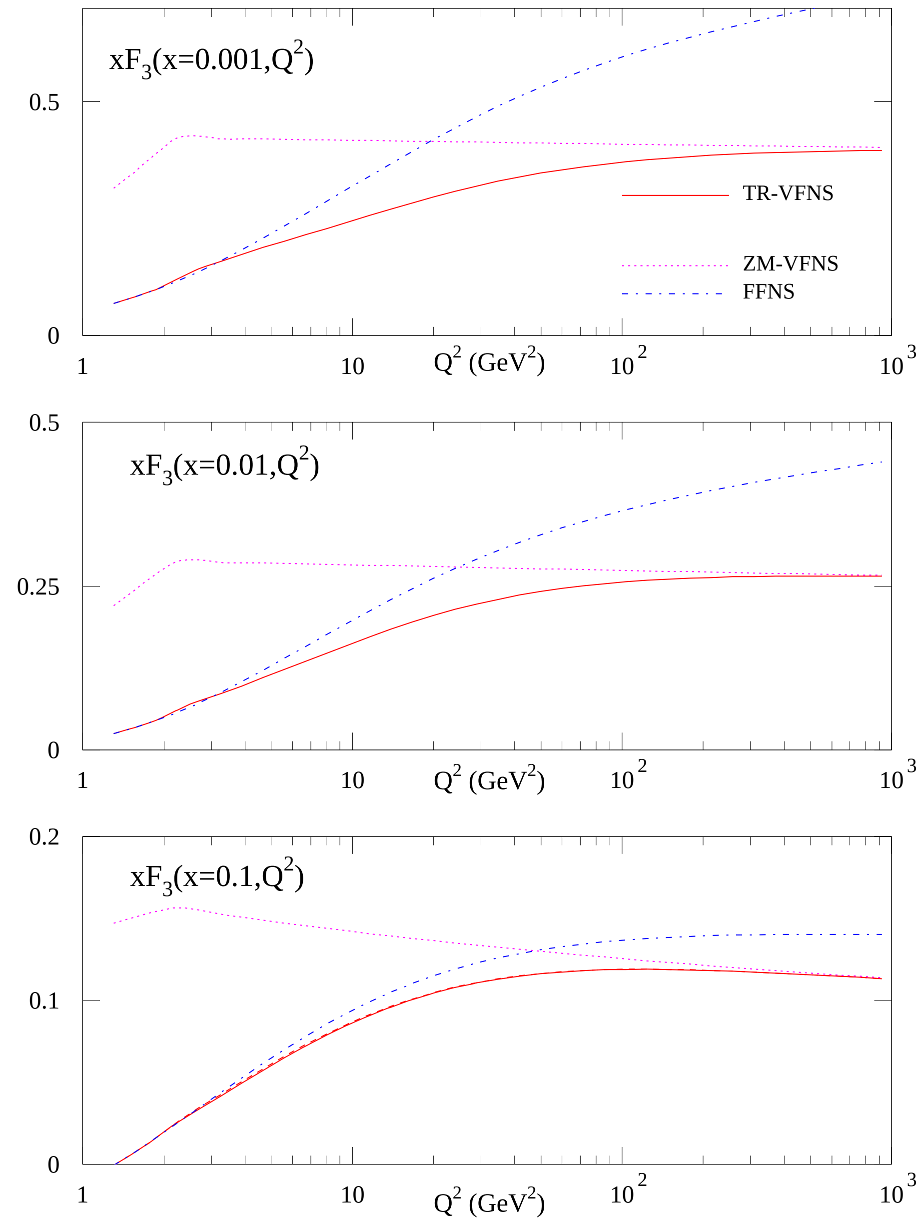
ZMVFNS not really feasible at NNLO. Huge discontinuity in $F_2^c(x,Q^2)$. Significant in $F_2^{Tot}(x,Q^2)$.





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

Conclusion also easily reached by looking at the extrapolation between the two simple kinematic regimes for xF_3, measured using neutrino scattering at NuTeV.



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 $Q^2/m_H^2 \to \infty$, and if we use the zeroth order cross-section for photon-heavy quark scattering, $(1+4m_H^2/Q^2)\delta(z-1/(1+m_H^2/Q^2))$, this is the original ACOT scheme.

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 $C_{2,g}^{VF,1}(Q^2/m_H^2)$.

Alternatively $C_{2,HH}^{VF,0}(Q^2/m_H^2)$ not uniquely defined. True for $C_{2,HH}^{VF,n}(Q^2/m_H^2)$.

Original ACOT prescription violated threshold $W^2 > 4M^2$ 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 $C_{2,HH}^{VF,0}(Q^2/m_H^2)$ 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 – $C_{2,HH}^{VF,0}(Q^2/m_H^2) \propto (P_{qg}^0)^{-1}$, 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

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

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

Tends to standard $C^{ZM,0}_{2,HH}(z) = \delta(1 - z)$ for $Q^2/m_H^2 \rightarrow \infty$ but respects threshold requirement $W^2 = Q^2(1 - x)/x \geq 4m_H^2$ for quark-antiquark production. Moreover it is 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

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

and to impose that $C^{VF,0}_{L,HH}(Q^2/m_H^2, z) \equiv 0$, despite the fact that $C^{0}_{L,HH}(Q^2/m_H^2, x) = 4zm_H^2/Q^2\delta(z - 1/(1 + m_H^2/Q^2))$ for single quark-photon scattering.

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.

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

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 $Q^2 = m_H^2$.

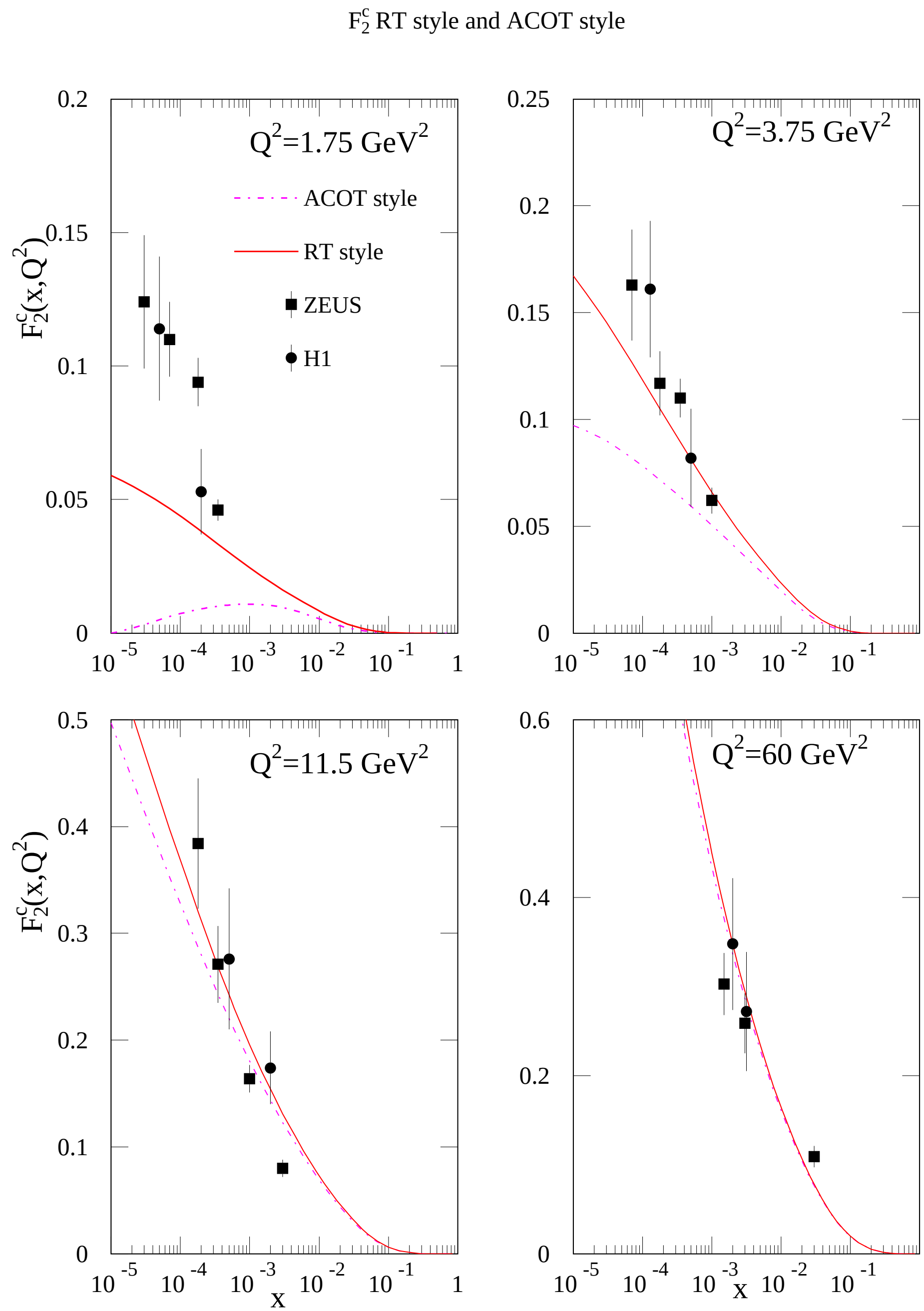
This difference in choice is extremely important at low Q^2 (if using $\mu^2 = Q^2$).

This can be clearly seen in the plot comparing the two at NLO.

$\mathcal{O}(\alpha_S^2)$ part is dominant at for $Q^2 \leq m_c^2$. "Frozen" part very significant for $m_c^2 \leq Q^2 \leq 12\mathrm{GeV}^2$. Clearly improves match to data.

Switching from standard n_f-flavour NLO to standard n_f+1-flavour NLO $\rightarrow$ large discontinuity in $F_2^H(x, Q^2)$.

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 damped as $z \to 1$.

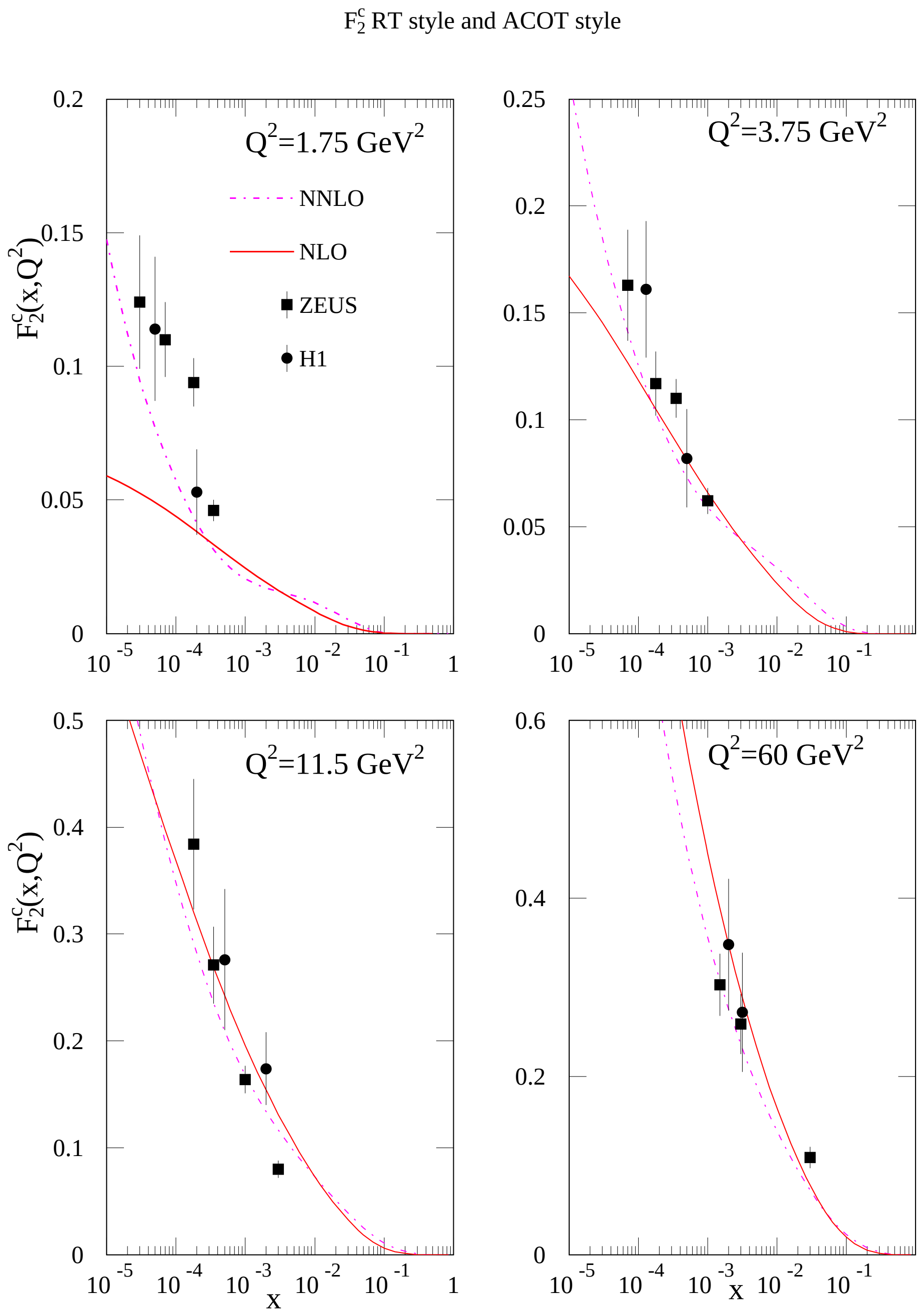
Amount of information similar to previous approximate NNLO splitting functions (van Neerven, Vogt), which were very good.

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

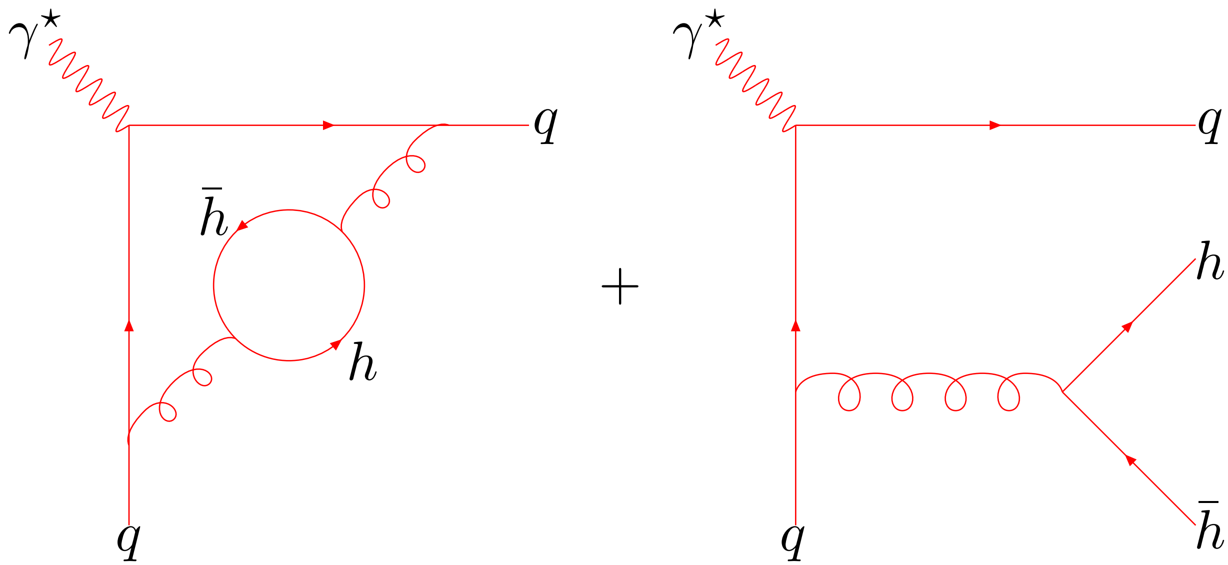
Approximation in $\mathcal{O}(\alpha_S^3)$ heavy flavour coefficient functions for $Q^2 \leq m_H^2$ and frozen for $Q^2 > m_H^2$.

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

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



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 strucure 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. At moment all in light flavours.

Conclusions

Discontinuities in both parton distributions and coefficient functions at NNLO. Makes variable flavour number scheme VFNS more necessary than ever. ZMVFNS badly discontinuous. FFNS only approximate at NNLO.

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, i.e. correct order for n_f flavours, additional constant for $n_f + 1$ flavours. 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 greatly, and not too sensitive to modelling.

Can be used in full NNLO global fits for partons.