PQCD Formulations with Heavy Quark Masses and Global Analysis

Robert S Thorne\textsuperscript{1} and W.K. Tung\textsuperscript{2}.
\textsuperscript{1} University College London, \textsuperscript{2} Michigan State University and University of Washington

Abstract
We critically review heavy quark mass effects in DIS and their impact on global analyses. We lay out all elements of a properly defined general mass variable flavor number scheme (GM VFNS) that are shared by all modern formulations of the problem. We then explain the freedom in choosing specific implementations and spell out, in particular, the current formulations of the CTEQ and MSTW groups. We clarify the approximations in the still widely-used zero mass variable flavor scheme (ZM VFNS), mention the inherent flaws in its conventional implementation, and consider the possibility of mending some of these flaws. We discuss practical issues concerning the use of parton distributions in various physical applications, in view of the different schemes. And we comment on the possible presence of intrinsic heavy flavors.

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1 Introduction

The proper treatment of heavy flavours in global QCD analysis of parton distribution functions (PDFs) is essential for precision measurements at hadron colliders. Recent studies [1–4] show that the standard-candle cross sections for \( W = Z \) production at the LHC are sensitive to detailed features of PDFs that depend on heavy quark mass effects; and certain standard model as well as beyond standard model processes depend crucially on better knowledge of the c-quark parton density, in addition to the light parton flavors. These studies also make it clear that the consistent treatment of heavy flavours in perturbative QCD (PQCD) require theoretical considerations that go beyond the familiar textbook parton picture based on massless quarks and gluons. There are various choices, explicit and implicit, which need to be made in various stages of a proper calculation in generalised PQCD including heavy quark mass effects. In the global analysis of PDFs, these choices can affect the resulting parton distributions. Consistent choices are imperative; mistakes may result in differences that are similar to, or even greater than, the quoted uncertainties due to other sources (such as the propagation of input experimental errors). In this report, we will provide a brief, but full, review of issues related to the treatment of heavy quark masses in PQCD, embodied in the general mass variable flavor scheme (GM VFNS).

In Sec. 2, we describe the basic features of the modern PQCD formalism incorporating heavy quark masses. In Sec. 3, we first delineate the common features of GM VFNS, then identify the different (but self-consistent) choices that have been made in recent global analysis work, and compare their results. For readers interested in practical issues relating to the use (or choice) of PDFs in various physics applications, we present a series of comments in Sec. 4 intended as guidelines. In Sec. 5, we discuss the possibility of intrinsic heavy flavors.

We note that, this review on GM VFNS and global analysis is not intended to address the specific issues pertinent to heavy flavor production (especially the final state distributions). For this particular process, somewhat different considerations may favor the adoption of appropriate fixed flavor number schemes (FFNS). We shall not go into details of these considerations; but will mention the FFNS along the way, since the GM VFNS is built on a series of FFNS’s. We will comment on this intimate relationship whenever appropriate.

2 General Considerations on PQCD with Heavy Flavor Quarks

The quark-parton picture is based on the factorization theorem of PQCD. The conventional proof of the factorization theorem proceeds from the zero-mass limit for all the partons—a good approximation at energy scales (generically designated by \( Q \)) far above all quark mass thresholds (designated by \( m \)). This clearly does not hold when \( Q = m \) is of order 1. It has been recognised since the mid-1980’s that a consistent treatment of heavy quarks in PQCD over the full energy range from \( Q \) to \( m \) can be formulated [5]. In 1998, Collins gave a general proof of the factorization theorem (order-by-order to all orders of perturbation theory) that is valid for non-zero quark masses [6]. The resulting general theoretical framework is conceptually simple: it represents a straightforward generalisation of the conventional zero-mass (ZM) modified minimal subtraction (\( \overline{\text{MS}} \)) formalism and it contains the conventional approaches as special cases in their respective regions of applicability; thus, it provides a good basis for our discussions.

The implementation of any PQCD calculation on physical cross sections requires attention to a number of details, both kinematical and dynamical, that can affect both the reliability of the predictions. Physical considerations are important to ensure that the right choices are made between perturbatively equivalent alternatives that may produce noticeable differences in practical applications. It is important to make these considerations explicit, in order to make sense of the comparison between different calculations in the literature. This is what we shall do in this section. In subsequent sections, we shall point out the different choices that have been made in recent global analysis efforts.

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\(^1\)Heavy quarks, by definition, have \( m \text{ QCD} \). Hence we always assume \( Q \gg m \text{ QCD} \). In practice, \( i = c, b, t \).
Heavy quark physics at HERA involve mostly charm (c) and bottom (b) production; at LHC, top (t) production, in addition, is of interest. For simplicity, we often focus the discussion of the theoretical issues on the production of a single heavy quark flavor, which we shall denote generically as \( H \), with mass \( m_H \). The considerations apply to all three cases, \( H = c; b; t \). For global analysis, the most important process that requires precision calculation is DIS; hence, for physical predictions, we will explicitly discuss the total inclusive and semi-inclusive structure functions, generically referred to as \( F(x; Q^2) \), where \( x \) represents either the conventional label \( (1;2;3) \) or the alternative \( (T;L;3) \) where \( T=L \) stands for transverse/longitudinal respectively.

### 2.1 The Factorization Formula

The PQCD factorization theorem for the DIS structure functions has the general form

\[
F(x; Q^2) = \sum_k f_k(x; Q^2) C_k = \sum_k f_k(x; Q^2) C_k = \int_0^1 \frac{dz}{z} C_k \frac{Q}{m_H} \frac{m_H}{s} \tag{1}
\]

Here, the summation is over the active parton flavor label \( k \), \( f_k(x; Q^2) \) are the parton distributions at the factorization scale \( Q \), \( C_k \) are the Wilson coefficients (or hard-scattering amplitudes) that can be calculated order-by-order in perturbation theory. The lower limit of the convolution integral is determined by final-state phase-space constraints: in the conventional ZM parton formalism it is simply \( x = Q^2/2p \) — the Bjorken \( x \) — but this is no longer true when heavy flavor particles are produced in the final state, cf. Sec. 2.4 below. The renormalization and factorization scales are jointly represented by \( \mu \); in most applications, it is convenient to choose \( \mu = Q \); but there are circumstances in which a different choice becomes useful.

### 2.2 Partons and Schemes for General Mass PQCD

In PQCD, the summation \( F_k \) over “parton flavor” label \( k \) in the factorization formula, Eq. (1), is determined by the factorization scheme chosen to define the parton distributions \( f_k(x; Q^2) \).

If mass effects of a heavy quark \( H \) are to be taken into account, the simplest scheme to adopt is the fixed flavor number scheme (FFNS) in which all quark flavors below \( H \) are treated as zero-mass and one sums over \( k = u; d; s; \ldots; \) up to \( n_f \) flavors of light (massless) quarks. The mass of \( H, m_H \), appears explicitly in the Wilson coefficients \( f_{C_k g} \), as indicated in Eq. (1). For \( H = u; d; s; t, n_f = 3; 4; 5g \) respectively. Historically, higher-order \( (O(\alpha_s^2)) \) calculations of the heavy quark production \( [7] \) were all done first in the FFNS. These calculations provide much improved results when \( n_f (Q) \) is of the order of \( m_H \) (both above and below), over those of the conventional ZM ones (corresponding to setting \( m_H = 0 \)).

Unfortunately, at any finite order in perturbative calculation, the \( n_f \)-FFNS results become increasingly unreliable as \( Q \) becomes large compared to \( m_H \): the Wilson coefficients contain logarithm terms of the form \( \frac{1}{m_H} \ln^m (Q/m_H) \), where \( m = 1; \ldots; n \) at order \( n \) of the perturbative expansion, implying they are not infrared safe — higher-order terms do not diminish in size compared to lower order ones—the perturbative expansion eventually breaks down. Thus, even if all \( n_f \)-flavor FFNS are mathematically equivalent, in practice, the 3-flavor scheme yields the most reliable results in the region \( Q < m_c, \) the 4-flavor scheme in \( m_c < Q < m_b, \) the 5-flavor scheme in \( m_b < Q < m_b, \) and, if needed, the 6-flavor scheme in \( m_b < Q \). (Cf. related discussions later in this section.)

This leads naturally to the definition of the more general variable flavor number scheme (VFNS): it is a composite scheme consists of the sequence of \( n_f \)-flavor FFNS, each in its region of validity, for \( n_f = 3; 4; \ldots; \) as described above; and the various \( n_f \)-flavor schemes are related to each other by perturbatively calculable transformation (finite-renormalization) matrices among the (running) coupling \( \alpha_s \), the running masses \( f_{m_H g} \), the parton distribution functions \( f_{f_k g} \), and the Wilson coefficients \( f_{C_k g} \). These relations ensure that there are only one set of independent renormalization constants, hence make the definition of the composite scheme precise for all energy scale \( (Q) \); and they ensure that physical
predictions are well-defined and continuous as the energy scale traverses each of the overlapping regions \( Q = m_H \) where both the \( n_f \)-flavor and the \((n_f + 1)\)-flavor schemes are applicable. The theoretical foundation for this intuitively obvious scheme can be found in [5, 6], and it was first applied in detail for structure functions in [8]. Most recent work on heavy quark physics adopt this general picture, in one form or another. We shall mention some common features of this general-mass (GM) VFNS in the next few paragraphs; and defer the specifics on the implementation of this scheme, as well as the variations in the implementation allowed by the general framework until Sec. 3.

As mentioned above, the \( n_f \)-flavor and the \((n_f + 1)\)-flavor schemes within the GM VFNS should be matched at some match point \( M \) that is of the order of \( m_H \). In practice, the matching is commonly chosen to be exactly \( M = m_H \), since it has been known that, in the calculational scheme appropriate for GM VFNS, the transformation matrices vanish at this particular scale at NLO in the perturbative expansion [5]; thus discontinuities of the renormalized quantities are always of higher order, making practical calculations simpler in general.

Strictly speaking, once the component \( n_f \)-flavor schemes are unambiguously matched, one can still choose an independent transition scale, \( M \), at which to switch from the \( n_f \) -flavor scheme to the \((n_f + 1)\)-flavor scheme in the calculation of physical quantities in defining the GM VFNS. This scale must again be within the overlapping region, but can be different from \( M = m_H \). In fact, it is commonly known that, from the physics point of view, in the region above the \( m_H \) threshold, up to \( m_H \) with a reasonable-sized constant factor \( \kappa \), the most natural parton picture is that of \( n_f \)-flavor, rather than \((n_f + 1)\)-flavor one. For instance, the 3-flavor scheme calculation has been favored by most HERA work on charm and bottom quark production, even if the HERA DIS kinematic region mostly involves \( Q > m_c \); and it is also used in the dynamically generated parton approach to global analysis [14].

In practice, almost all implementations of the GM VFNS simply choose \( M = m_H \) (often not explicitly mentioning the conceptual distinction between \( M \) and \( m_H \)). The self-consistency of the GM VFNS guarantees that physical predictions are rather insensitive to the choice of the transition point as long as it is within the overlapping region of validity of the \( n_f \)- and \((n_f + 1)\)-flavor ones. The simple choice of \( M = m_H \) corresponds to opting for the lower end of this region for the convenience in implementation. In the following, we shall use the terms matching point and transition point interchangeably. As with all definition ambiguities in perturbative theory, the sensitivity to the choice of matching and transition points diminishes at higher orders.

### 2.3 Treatment of Final-state Flavors

For total inclusive structure functions, the factorization formula, Eq. (1), contains an implicit summation over all possible quark flavors in the final state. One can write,

\[
C_k = \sum_j C_{k}^{j}
\]

where “\( j \)” denotes final state flavors, and \( C_{k}^{j} \) represent the Wilson coefficients (hard cross sections) for an incoming parton “\( k \)” to produce a final state containing flavor “\( j \)” calculable perturbatively from the relevant Feynman diagrams. It is important to emphasize that “\( j \)” labels quark flavors that can be produced physically in the final state; it is not a parton label in the sense of initial-state parton flavors described in the previous subsection. The latter (labeled \( k \)) is a theoretical construct and scheme-dependent.

\[2\text{Technically, this means employing the CWZ subtraction scheme [9] in calculating the higher-order Feynman diagrams. CWZ subtraction is an elegant extension of the R \& S subtraction scheme that ensures the decoupling of heavy quarks at high energy scales order-by-order. This is essential for factorization to be valid at each order of perturbation theory. (In the original R \& S subtraction scheme, decoupling is satisfied only for the full perturbation series—to infinite orders.)}

\[3\text{Specifically, the \( n_f \)-flavor scheme should fail when } x \ln ( m_H / x ) = x \ln ( ) \text{ ceases to be a small parameter for the effective perturbation expansion. However, no theory can tell us precisely how small is acceptably "small"—hence how large } \] is permitted. Ardent FFNS advocates believe even the range of the 3-flavor scheme extends to all currently available energies, including HERA [14]. For GM VFNS, see the next paragraph.\]
(e.g. it is fixed at three for the 3-flavor scheme); whereas the final-state sum (over \( j \)) is over all flavors that can be physically produced. Furthermore, the initial state parton “\( k \)” does not have to be on the mass-shell, and is commonly treated as massless; whereas the final state particles “\( j \)” should certainly be on-mass-shell in order to satisfy the correct kinematic constraints for the final state phase space and yield physically meaningful results.\(^4\) Thus, in implementing the summation over final states, the most relevant physical scale is \( W \)—the CM energy of the virtual Compton process—in contrast to the scale \( Q \) that controls the initial state summation over parton flavors.

The distinction between the two summations is absent in the simplest implementation of the conventional (i.e., textbook) zero-mass parton formalism: if all quark masses are set to zero to begin with, then all flavors can be produced in the final state. This distinction becomes blurred in the commonly used zero-mass (ZM) VFNS, where the heavy quark masses \( f_m \) implicitly enter because the number of effective parton flavors is incremented as the scale parameter crosses each heavy quark threshold. This creates apparent paradoxes in the implementation of the ZM VFNS, such as: for \( Q = m_b < m_c \), \( b \) is not counted as a parton, the partonic process \( + g \rightarrow b \) would not be included in DIS calculations, yet physically this can be significant if \( W^2 = 2m_b \) (small \( x \)); whereas for \( Q > m_b \), \( b \) is counted as a massless parton, the contribution of \( + g \rightarrow b \) to DIS would be the same as that of \( + g \rightarrow c \), but physically this is wrong for moderate values of \( W^2 \), and furthermore, it should be zero if \( W < 2m_b \) (corresponding to large \( x \)). (We shall return to this topic in Sec. 3.1.)

These problems were certainly overlooked in conventional global analyses from its inception until the time when issues on mass-effects in PQCD were brought to the fore after the mid 1990’s \([8, 10–13]\). Since then, despite its shortcomings the standard ZM VFNS continues to be used widely because of its simplicity and because NLO Wilson coefficients for most physical processes are still only available in the ZM VFNS. Most groups produce the standard ZM VFNS as either their default set or as one of the options, and they form the most common basis for comparison between groups, e.g. the “benchmark study” in \([15]\).

It is obvious that, in a proper implementation of PQCD with mass (in any scheme), the distinction between the initial-state and final-state summation must be unambiguously, and correctly, observed. For instance, even in the 3-flavor regime (when \( c \) and \( b \) quarks are not counted as partons), the charm and bottom flavors still need to be counted in the final state—at tree-level via \( W^+ + g \rightarrow c \rightarrow s \rightarrow c \) or \( + g \rightarrow b \) or \( + g \rightarrow c \), provided there is enough CM energy to produce these particles.

### 2.4 Phase-space Constraints and Rescaling

The above discussion points to the importance of the proper treatment of final state phase space in heavy quark calculations. Once mass effects are taken into account, kinematic constraints have a significant impact on the numerical results of the calculation; in fact, they represent the dominant factor in the threshold regions of the phase space. In DIS, with heavy flavor produced in the final state, the simplest kinematic constraint that comes to mind is

\[
W > \frac{M_N}{x_f} \quad (3)
\]

where \( W \) is the CM energy of the vector-boson–nucleon scattering process, \( M_N \) is the nucleon mass, and the right-hand side is the sum of all masses in the final state. \( W \) is related to the familiar kinematic variables \((x; Q)\) by \( W^2 = M_N^2 + Q^2(1 - x) = x \), and this constraint should ideally be imposed on the right-hand side of Eq. (1). Any approach achieving this represents an improvement over the conventional ZM scheme calculations, that ignores the kinematic constraint Eq. (3) (resulting in a gross over-estimate.

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\(^4\)Strict kinematics would require putting the produced heavy flavor mesons or baryons on the mass shell. In the PQCD formalism, we adopt the approximation of using on-shell final state heavy quarks in the underlying partonic process.
of the corresponding cross sections). The implementation of the constraint in the most usual case of NC processes, say \( Z + c! \) (or any other heavy quark) is not automatic (and is absent in some earlier definitions of a GM VFNS) because in this partonic process one must account for the existence of a hidden heavy particle—the \( c! \)—in the target fragment. The key observation is, heavy objects buried in the target fragment are still a part of the final state, and should be included in the phase space constraint, Eq. (3).

Early attempts to address this issue were either approximate or rather cumbersome, and could not be naturally extended to high orders\(^5\). A much better physically motivated approach is based on the idea of rescaling. The simplest example is given by charm production in the LO CC process \( W + s! c \). It is well-known that, when the final state charm quark is put on the mass shell, kinematics requires the momentum fraction variable for the incoming strange parton, in Eq. (1) to be \( x(1 + m_c^2/Q^2) \) [16], rather than the Bjorken \( x \). This is commonly called the rescaling variable. The generalization of this idea to the more prevalent case of NC processes took a long time to emerge [17, 18] which extended the simple rescaling to the more general case of \( Z + c! c + X \), where \( X \) contains only light particles, it was proposed that the convolution integral in Eq. (1) should be over the momentum fraction range \( c < x < 1 \), where

\[
  c = x \left( 1 + \frac{4m_c^2}{Q^2} \right) \quad : 
\]

In the most general case where there are any number of heavy particles in the final state, the corresponding variable is (cf. Eq. (3))

\[
  = x \left( 1 + \frac{(\tau M \tau)^2}{Q^2} \right) : 
\]

This rescaling prescription has been referred to as ACOT in the recent literature [17–19].

Rescaling shifts the momentum variable in the parton distribution function \( f^k(\tau Q) \) in Eq. (1) to a higher value than in the zero-mass case. For instance, at LO, the structure functions \( F(x,Q^2) \) are given by some linear combination of \( f^k(\tau Q) \) in the ZM formalism; but, with ACOT rescaling, this becomes \( f^k(c\tau Q) \). In the region where \( (\tau M \tau)^2/Q^2 \) is not too small, especially when \( f(\tau) \) is a steep function of \( \tau \), this rescaling can substantially change the numerical result of the calculation. It is straightforward to show that, when one approaches a given threshold \( (M_N + \tau M \tau) \) from above, the corresponding rescaling variable \( c! \). Since generally \( f^k(\tau) \to 0 \) as \( \tau \to 1 \), rescaling ensures a smoothly vanishing threshold behavior for the contribution of the heavy quark production term to all structure functions. This results in a universal and intuitively physical, realization of the threshold kinematic constraint for all heavy flavor production processes that is applicable to all orders of perturbation theory. For this reason, most recent global analysis efforts choose this method.

2.5 Difference between \( f_F^{tot, g} \) and \( f_F^{H, g} \) Structure Functions

In PQCD, the most reliable calculations are those involving infra-red safe quantities—these are free from logarithmic factors that can become large (thereby spoiling the perturbative expansion). The total inclusive structure functions \( f_F^{tot, g} \) defined in the GM VFNS are infrared safe, as suggested by the discussion of Sec. 2.2 and proven in Ref. [6].

Experimentally, the semi-inclusive DIS structure functions for producing a heavy flavor particle in the final state is also of interest. Theoretically, it is useful to note that the structure functions \( f_F^{H, g} \) for

\(^5\) In [8], the threshold violation was minimized by an artificial choice of the factorization scale \( m_H^2/Q \). In [12, 13] the kinematic limit was enforced exactly by requiring continuity of the slope of structure functions across the matching point, resulting in a rather complicated expression for the coefficient functions in Eq. (1).

\(^6\) Since it is imposed on the (universal) parton distribution function part of the factorization formula.
producing heavy flavor $H$ are not as well defined as $F_{\text{light}}$. To see this, consider the relation between the two,

$$F_{\text{tot}} = F_{\text{light}} + F_{\text{H}};$$

where $F_{\text{light}}$ denotes the sum of terms with only light quarks in the final state, and $F_{\text{H}}$ consist of terms with at least one heavy quark $H$ in the final state. Unfortunately, $F_{\text{H}}(x; Q, m_H)$ is, strictly speaking, not infrared safe beyond order $s$ (1-loop); they contain residual $\lambda_{H}(Q = m_H)$ terms at higher orders (2-loop and up). The same terms occur in $F_{\text{light}}$ due to contributions from virtual $H$ loops, with the opposite sign. Only the sum of the two, i.e. the total inclusive quantities $F_{\text{tot}}$ are infra-red safe. This problem could be addressed properly by adopting a physically motivated, infrared-safe cut-off on the invariant mass of the heavy quark pair, corresponding to some experimental threshold [20] in the definition of $F_{\text{H}}$ (drawing on similar practise in jet physics). In practice, up to order $s^2$, the result is numerically rather insensitive to this, and different groups adopt a variety of less sophisticated procedures, e.g. including contributions with virtual $H$ loops within the definition of $F_{\text{H}}$. Nonetheless, it is prudent to be aware that the theoretical predictions on $F_{\text{H}}$ are intrinsically less robust than those for $F_{\text{tot}}$ when comparing experimental results with theory calculations.

2.6 Conventions for “LO”, “NLO”, ... Calculations

It is also useful to point out that, in PQCD, the use of familiar terms such as LO, NLO, ... is often ambiguous, depending on which type of physical quantities are under consideration, and on the convention used by the authors. This can be a source of considerable confusion when one compares the calculations of $F_{\text{tot}}$ and $F_{\text{H}}$ by different groups (cf. next section).

One common convention is to refer LO results as those derived from tree diagrams; NLO those from 1-loop calculations, ... and so on. This convention is widely used; and it is also the one used in the CTEQ papers. Another possible convention is to refer to LO results as the first non-zero term in the perturbative expansion; NLO as one order higher in $s$, ... and so on. This convention originated in FFNS calculations of heavy quark production; and it is also used by the MRST/MSTW authors. It is a process-dependent convention, and it depends a priori on the knowledge of results of the calculation to the first couple of orders in $s$.

Whereas the two conventions coincide for quantities such as $F_{\text{tot}}$, they lead to different designations for the longitudinal structure function $F_{\text{L}}^{\text{tot}}$ and the $n_f$-flavor $F_{\text{H}}^{n_f}$, since the tree-level results are zero for these quantities. These designations, by themselves, are only a matter of terminology. However, mixing the two distinct terminologies in comparing results of different groups can be truly confusing. This will become obvious later.

3 Implementations of VFNS: Common Features and Differences

In this section, we provide some details of the PQCD basis for the GM VFNS, and comment on the different choices that have been made in the various versions of this general framework, implemented by two of the major groups performing global QCD analysis.

3.1 Alternative Formulations of the ZM VFNS

As pointed out in Sec. 2.3, the ZM VFNS, as commonly implemented, represents an unreliable approximation to the correct PQCD in some kinematic regions because of inappropriate handling of the final-state counting and phase-space treatment, in addition to the neglect of heavy-quark mass terms in the

\[\text{In the following discussion, we shall overlook logarithmic factors normally associated with fragmentation functions for simplicity. These are similar to those associated with parton distributions, but are less understood from the theoretical point of view—e.g. the general proof of factorization theorem (with mass) [6] has not yet been extended to cover fragmentation.}\]
Wilson coefficients. Whereas the latter is unavoidable to some extent, because the massive Wilson coefficients have not yet been calculated even at 1-loop level for most physical processes (except for DIS), the former (which can be more significant numerically in certain parts of phase space) can potentially be remedied by properly counting the final states and using the rescaling variables, as discussed in Secs. 2.3 and 2.4 under general considerations. Thus, alternative formulations of the ZM VFNS are possible that only involve the zero-mass approximation in the Wilson coefficient. This possibility has not yet been explicitly explored.

3.2 Parton Distribution Functions in VFNS (ZM and GM)

In PQCD, the factorization scheme is determined by the choices made in defining the parton distribution functions (as renormalized Green functions). In a GM VFNS based on the generalized mass subtraction (cf. footnote 3) the evolution kernel of the DGLAP equation is mass-independent; thus the PDFs, so defined, apply to GM VFNS calculations as they do for the ZM VFNS.

In the VFNS, the PDFs switch from the $n_f$-flavor FFNS ones to the $(n_f + 1)$-flavor FFNS ones at the matching point $\mu = m_H$ (cf. Sec. 2.2); the PDFs above/below the matching point are related, order-by-order in $\alpha_s$, by:

$$f_{j}^{\nu F}(\mu^+ \frac{m_H}{\mu}) \; f_{j}^{(n_f+1)FF} = A_{jk} \; f_{k}^{n_fFF} \; A_{jk} \; f_{j}^{\nu F}(\mu^+ \frac{m_H}{\mu});$$

(7)

where $m_H^+$ indicate that the $\mu = m_H$ limit is taken from above/below, and we have used the shorthand $VF/FF$ for VFNS/FFNS in the superscripts. The transition matrix elements $A_{jk} (=m_H)$, representing a finite-renormalization between the two overlapping FFNS schemes, can be calculated order by order in $\alpha_s$; they are known to NNLO, i.e. $\circ \; \mathcal{O} \; (\frac{\alpha_s}{\pi^2})$ [10, 11]. (Note that $A_{jk}$ is not a square matrix.) It turns out, at NLO, $A_{jk} (=m_H) = 0$ [6]; thus $f_{j}^{\nu F}$ are continuous with this choice of matching point. There is a rather significant discontinuity in heavy quark distributions and the gluon distribution at NNLO.

With the matching conditions, Eq. (7) $f_{j}^{\nu F}(\mu^+ \frac{m_H}{\mu})$ are uniquely defined for all values of $\mu_H$. We shall omit the superscript VF in the following. Moreover, when there is a need to focus on $f_{j}^{\nu}$ in the vicinity of $\mu = m_H$, where there may be a discontinuity, we use $f_{j}^{\nu} (\mu^+ \frac{m_H}{\mu})$ to distinguish the above/below branch of the function. As indicated in Eq. (7), $f_{j}^{\nu}$ correspond to the $n_f$-flavor PDFs, and $f_{j}^{\nu}$ to the $(n_f + 1)$-flavor ones.

3.3 The Structure of a GM VFNS, Minimal Prescription and Additional Freedom

Physical quantities should be independent of the choice of scheme; hence, in a GM VFNS, we must require the theoretical expressions for the structure functions to be continuous across the matching point $Q = m_H$ to each order of perturbative theory:

$$F(x; \mu_Q) = C_{k} (m_H = Q); \quad f_{k} (\mu^+ \frac{m_H}{\mu}) = C_{j}^{+} (m_H = Q); \quad f_{j}^{+} (\mu_Q);$$

(8)

$$C_{j}^{+} (m_H = Q); \quad A_{jk} (m_H = Q); \quad f_{k} (\mu_Q);$$

(9)

where we have suppressed the structure function label ( ) on $F$’s and $C$’s, and used the notation $C_{k}^{\pm}$ to denote the Wilson coefficient function $C_{k}$ ($m_H = Q$) above/below the matching point respectively. Hence, the GM VFNS coefficient functions are also, in general, discontinuous, and must satisfy the transformation formula:

$$C_{k} (m_H = Q) = C_{j}^{+} (m_H = Q); \quad A_{jk} (m_H = Q);$$

(10)

order-by-order in $\alpha_s$. For example, at $O (\frac{\alpha_s}{\pi^2})$, $A_{H; Q} = a_{F_{qg}}^{0} \ln (Q = m_H)$, this constraint implies:

$$C_{H_{\mu}}^{\pm} (m_H = Q) = a_{C_{H_{\mu}}^{\pm}} (m_H = Q); \quad a_{F_{qg}}^{0} \ln (Q = m_H) = C_{H_{\mu}}^{\pm} (m_H = Q);$$

(11)
where the numeral superscript (0,1) refers to the order of calculation in $s$ (for $P_{jk}$, the order is by standard convention one higher than indicated), and the suppressed second parton index on the Wilson coefficients (cf. Eq. 2) has been restored to make the content of this equation explicit. Eq. (11) was implicitly used in defining the original ACOT scheme [8]. The first term on the RHS of Eq. (11) when moved to the LHS, becomes the subtraction term of Ref. [8] that serves to define the Wilson coefficient $C_{H,j}^+(m_H=Q)$ (hence the scheme) at order $s$, as well as to eliminate the potentially infra-red unsafe logarithm in the gluon fusion term $(C_{H,j}^+(m_H=Q))$ at high energies.

The GM VFNS as described above, consisting of the general framework of [5, 6], along with transformation matrices $fA_{jk,g}$ calculated to order $z_2$ by [10, 11], is accepted in principle by all recent work on PQCD with mass. Together, they can be regarded as the minimal GM VFNS.

The definition in Eq. (11) was applied to find the asymptotic limits $(Q^2=M^2_H!^n1)$ of coefficient functions in [10, 11], but it is important to observe that it does not completely define all Wilson coefficients across the matching point, hence, there are additional flexibilities in defining a specific scheme [6, 12, 13, 22]. This is because, as mentioned earlier, the transition matrix $fA_{jk,g}$ is not a square matrix—it is $n_f(n_f+1)$. It is possible to swap $O(m_H=Q)$ terms between Wilson coefficients on the right-hand-side of Eq. (11) (hence redefining the scheme) without violating the general principles of a GM VFNS. For instance, one can swap $O(m_H=Q)$ terms between $C_{H,j}^+(m_H=Q)$ and $C_{g,j}^+(m_H=Q)$ while keeping intact the relation (11) that guarantees the continuity of $F(x;Q)$ according to Eq. 8. This general feature, applies to (11) to all orders. It means, in particular, that there is no need to calculate the coefficient function $C_{H,j}^+(m_H=Q)$, for any $i$—it can be chosen as a part of the definition of the scheme. Also, it is perfectly possible to define coefficient functions which do not individually satisfy the constraint in Eq. 3, since Eq. 10 guarantees ultimate cancellation of any violations between terms. However, this will not occur perfectly at any finite order so modern definitions do include the constraint explicitly, as outlined in Sec. 2.4.

The additional flexibility discussed above has been exploited to simply the calculation, as well as to achieve some desirable features of the prediction of the theory by different groups. Of particular interest and usefulness is the general observation that, given a GM VFNS calculation of $fC_{j,g}$, one can always switch to a simpler scheme with constant $fC_{j,g}^+$

$$C_{H,j}^+(m_H=Q)=C_{H,j}^+(0)$$

This is because the shift $(C_{H,j}^+(m_H=Q)C_{g,j}^+(0))$ vanishes in the $m_H=Q!0$ limit, and can be absorbed into a redefinition of the GM scheme as mentioned above. The detailed proof are given in [6, 22]. By choosing the heavy-quark-initiated contributions to coincide with the ZM formulae, the GM VFNS calculation becomes much simplified: given the better known ZM results, we only need to know the full $m_H$-dependent contributions from the light-parton-initiated subprocesses; and these are exactly what is provided by the $n_f$-flavor FFNS calculations available in the literature. This scheme is known as the Simplified ACOT scheme, or SACOT [6, 22].

Further uses of the freedom to reshuffle $O(m_H=Q)$ terms between Wilson coefficients, as well as adding terms of higher order in the matching condition (without upsetting the accuracy at the given order) have been employed extensively by the MRST/MSTW group, as will be discussed in Sec. 3.5.

### 3.4 CTEQ Implementation of the GM VFNS

The CTEQ group has always followed the general PQCD framework as formulated in [5, 6]. Up to CTEQ6.1, the default CTEQ PDF sets were obtained using the more familiar ZM Wilson coefficients, because, the vast majority of HEP applications carried out by both theorists and experimentalists use this calculational scheme. For those applications that emphasized heavy quarks, special GM VFNS PDF sets were also provided; these were named as CTEQnHQ, where $n=4,5,6$. 


The earlier CTEQ PDFs are now superseded by CTEQ6.5 [1] and CTEQ6.6 [3] PDFs; these are based on a new implementation of the general framework described in previous sections, plus using the simplifying SACOT choice of heavy quark Wilson coefficients [8, 21] specified by Eq. 12 above. There are no additional modification of the formulae of the minimal GM VFNS, as described in previous sections. CTEQ uses the convention of designating tree-level, 1-loop, 2-loop calculations as LO, NLO, and NNLO, for all physical quantities, F \text{tot}, F^H, \ldots \text{etc., cf. Sec. 2.6.}

With these minimal choices, this implementation is extremely simple. Continuity of physical predictions across matching points in the scale variable \( \mu = Q \) is guaranteed by Eqs. 8 and 10, and continuity across physical thresholds in the physical variable \( \bar{W} \), for producing heavy flavor final states, are guaranteed by the use of ACOT- rescaling variables [5] as described in Sec. 2.4.

For example, to examine the continuity of physical predictions to NLO in this approach, we have, for the below/above matching point calculations:

\[
\begin{align*}
F^H_2 (x; Q^2) & = s C_2^H (\bar{n} q) - s C_2^+ (\bar{n} g) \ln (Q = m_H), \\
F^H_2^\pm (x; Q^2) & = s C_2^{\pm} (\bar{n} q) - s C_2^\mp (\bar{n} g) \ln (Q = m_H),
\end{align*}
\]

where non-essential numerical factors have been absorbed into the convolution. The continuity of \( F^H_2 (x; Q^2) \) in the scaling variable \( \mu = Q \) is satisfied by construction (Eq. 9) because the relation between the PDFs given by Eq. 7 and that between the Wilson coefficients given by Eq. 8 involve the same transformation matrix \( fA_{\bar{n}q} \) (calculated in [10, 11, 20]). In fact, to this order, \( A_{\bar{n}q} = s F^0_{\bar{n}q} \ln (Q = m_H) \), hence

\[
\begin{align*}
h (h) & = 0 \\
\bar{g}^{\bar{n}q} & = \bar{g}^{\bar{n}q} \\
C_2^{\pm} & = C_2^{\pm}
\end{align*}
\]

at the matching point \( \mu = Q = m_H \). Thus, the two lines in Eq. 13 give the same result, and \( F^H_2 (x; Q^2) \) is continuous. The separate issue of continuity of \( F^H_2 (x; Q^2) \) in the physical variable \( \bar{W} \) across the production threshold of \( \bar{W} = 2m_H \) is satisfied automatically by each individual term (using the ACOT-prescription for the quark terms and straightforward kinematics for the gluon term).

In the CTEQ approach, all processes are treated in a uniform way; there is no need to distinguish between neutral current (NC) and charged current (CC) processes in DIS, (among others, as in MRST/MSTW). All CTEQ global analyses so far are carried out up to NLO. This is quite adequate for current phenomenology, given existing experimental and other theoretical uncertainties. Because NNLO results has been known to show signs of unstable behavior of the perturbative expansion, particularly at small-\( x \), they are being studied along with resummation effects that can stabilize the predictions. This study is still underway.

### 3.5 MRST/MSTW Implementation of the GM VFNS

#### 3.5.1 Prescription

In the TR heavy flavour prescriptions, described in [12, 13] the ambiguity in the definition of \( C_{\bar{n}q}^{V,F,p} (Q^2 = m_H^2) \) was exploited by applying the constraint that \( (d F_{\bar{n}q}^H = c \ln Q^2) \) was continuous at the transition point (in the gluon sector). However, this becomes technically difficult at higher orders. Hence, in [19] the choice of heavy-flavour coefficient functions for \( F_{\bar{n}q}^H \) was altered to be the same as the SACOT(\( \bar{n}q \)) scheme described above. This choice of heavy-flavour coefficient functions has been used in the most recent MRST/MSTW analysis, in the first instance in [2]. To be precise the choice is

\[
C_{\bar{n}q}^{V,F,p} (Q^2 = m_H^2; z) = C_{\bar{n}q}^{V,F,p} (z = x_m a_x)
\]

This is applied up to NNLO in [19] and in subsequent analyses. For the first time at this order satisfying the requirements in Eq. 10 leads to discontinuities in coefficient functions, which up to NNLO...
cancel those in the parton distributions. This particular choice of coefficient functions removes one of the sources of ambiguity in defining a GM VFNS. However, there are additional ambiguities in the MRST/MSTW convention for counting LO, NLO, ... calculations (cf. Sec.2.6), coming about because the ordering in $s$ for $F_2^H (x,Q^2)$ is different above and below matching points in Eqs. [9,11]. (These complications do not arise in the minimal GM VFNS adopted by CTEQ, as already mentioned in the previous subsection.)

For the neutral current DIS $F_2$ structure function, the above-mentioned ambiguities can be see as follows:

$$
\begin{align*}
\text{LO} & : \quad \frac{s}{4} \left( C_{2g}^\mu + C_{2q}^\mu \right) g^{\mu \nu} (n_\nu) \quad C_{2g}^\mu (h + h) \\
\text{NLO} & : \quad \frac{s}{4} \left( C_{2g}^\mu + C_{2q}^\mu \right) g^{\mu \nu} (n_\nu) \quad \frac{s}{4} \left( C_{2g}^\mu (h + h) + C_{2q}^\mu g^{\mu \nu} \right) f^{\mu \nu + 1} \\
\text{NNLO} & : \quad \frac{s}{4} \left( C_{2g}^\mu + C_{2q}^\mu \right) g^{\mu \nu} (n_\nu) \quad \frac{s}{4} \left( C_{2g}^\mu + C_{2q}^\mu g^{\mu \nu} \right) f^{\mu \nu + 1} \\
\end{align*}
$$

with obvious generalization to even higher orders. This means that switching directly from a fixed order with $n_\nu$ active quarks to fixed order with $n_\nu + 1$ active quarks leads to a discontinuity in $F_2^H (x,Q^2)$. As with the discontinuities in the ZM-VFNS already discussed this is not just a problem in principle – the discontinuity is comparable to the errors on data, particularly at small $x$. The TR scheme, defined in [12,13], and all subsequent variations, try to maintain the particular ordering in each region as closely as possible. For example at LO the definition is

$$
F_2^H (x,Q^2) = \frac{s}{4} \left( C_{2g}^\mu (Q^2 = m_H^2) + C_{2g}^\mu (Q^2 = m_H^2) \right) g^{\mu \nu} (Q^2) 
$$

The $O (\frac{s}{4})$ term is frozen when going upwards through $Q^2 = m_H^2$. This generalizes to higher orders by freezing the term with the highest power of $s$ in the definition for $Q^2 < m_H^2$ when moving upwards above $m_H^2$. Hence, the definition of the ordering is consistent within each region, except for the addition of a constant term (which does not affect evolution) above $Q^2 = m_H^2$, which becomes progressively less important at higher $Q^2$, and whose power of $s$ increases as the order of the perturbative expansion increases.

This definition of the ordering means that in order to define a GM VFNS at NNLO [19] one needs to use the $O (\frac{s}{4})$ heavy-flavour coefficient functions for $Q^2 < m_H^2$ (and that the contribution will be frozen for $Q^2 > m_H^2$). This would not be needed in a ACOT-type scheme. As mentioned above, these coefficient functions are not yet calculated. However, as explained in [19], one can model this contribution using the known leading threshold logarithms [23] and leading $\ln (1-x)$ terms derived from the $k_T$-dependent impact factors [24]. This results in a significant contribution at small $Q^2$ and $x$ with some model dependence. However, variation in the free parameters does not lead to a large change.

The above discussions focused on $F_2^H$; but they mostly apply to $F_L$ as well. We only need to mention that, with the adoption of the SACOT prescription for heavy-quark initiated contributions (i.e. using the ZM version of the Wilson coefficient), $F_L^H$ vanishes at order $O (\frac{s}{4})$ as it does in the TR prescriptions. (This zeroth order coefficient function does appear in some older GM VFNS definitions.) According to the MRST/MSTW convention, the order $\frac{1}{s}$ term of $F_L$ (both light and heavy flavour) counts as LO, and so on, whereas In the CTEQ convention each relative order is a power of $s$ lower.

---

8It should be stressed that this model is only valid for the region $Q^2 < m_H^2$, and would not be useful for a NNLO FFNS at all $Q^2$ since it contains no information on the large $Q^2 = m_H^2$ limits of the coefficient functions. A more general approximation to the $O (\frac{s}{4})$ coefficient functions could be attempted, but full details would require first the calculation of the $O (\frac{s}{4})$ matrix elements $A_{g,q}$. This more tractable project is being investigated at present [25].
The general procedure for the GM VFNS for charged-current deep inelastic scattering can work on the same principles as for neutral currents, but one can produce a single charm quark from a strange quark so \( x(1 + m_\text{c}^2/Q^2) \). However, there is a complication compared to the neutral current case because the massive FFNS coefficient functions are not known at \( O \left( \frac{Q^2}{m_\text{c}^2} \right) \) (only asymptotic limits [26] have been calculated). These coefficient functions are needed in a TR-type scheme at low \( Q^2 \) at NLO, and for any GM VFNS at all \( Q^2 \) at NNLO. This implies that we can only define the TR scheme to LO and the ACOT scheme to NLO. However, known information can be used to model the higher order coefficient functions similarly to the TR scheme definition to NNLO for neutral currents. A full explanation of the subtleties can be found in [27].

3.5.2 Scheme variations

The inclusion of the complete GM VFNS in a global fit at NNLO first appeared in [2], and led to some important changes compared to a previous NNLO analysis, which had a much more approximate inclusion of heavy flavours (which was explained clearly in the Appendix of [28]). There is a general result that \( F_{g}(x; Q^2) \) is flatter in \( Q^2 \) at NNLO than at NLO, as shown in Fig. 4 of [2], and also flatter than in earlier (approximate) NNLO analyses. This had an important effect on the gluon distribution. As seen in Fig. 5 of [2], it led to a larger gluon for \( x < 0.001 \) and \( x > 0.01 \), as well as a larger value of \( s \) (\( m_\text{c}^2 \)), both compensating for the naturally flatter evolution, and consequently leading to more evolution of the light quark sea. Both the gluon and the light quark sea were \( 6\% \) greater than in the MRST2004 set [29] for \( Q^2 = 10^{10} \text{GeV}^2 \), the increase maximising at \( x = 0.0001 \) and \( x = 0.01 \). As a result there was a \( 6\% \) increase in the predictions for \( W \) and \( Z \) at the LHC. This would hold for all LHC processes sensitive to PDFs in this \( x \) range, but would be rather less for processes such as \( \pm \) pair production sensitive to \( x < 0.01 \). This surprisingly large change is a correction rather than a reflection of the uncertainty due to the freedom in choosing heavy flavour schemes and demonstrates that the MRST2004 NNLO distributions should now be considered to be obsolete.

To accompany the MRST 2006 NNLO parton update there is an unofficial “MRST2006 NLO” set, which is fit to exactly the same data as the MRST2006 NNLO set. By comparing to the 2004 MRST set one can check the effect on the distributions due to the change in the prescription for the GM VFNS at NLO without complicating the issue by also changing many other things in the analysis. The comparison of the up quark and gluon distributions for the “MRST2006 NLO” set and the MRST2004 NLO set, i.e. the comparable plot to Fig. 5 of [2] for NNLO, is shown in Fig. 1. As can be seen it leads to the same trend for the partons as at NNLO, i.e. an increase in the small-\( x \) gluon and light quarks, but the effect is much smaller – a maximum of a \( 2\% \) change. Also, the value of the coupling constant increases by \( 0.01 \) from the 2004 value of \( s \) (\( m_\text{c}^2 \)) = 0.20. From momentum conservation there must be a fixed point and this is at \( x = 0.05 \). Hence, \( W \) and \( Z \) and lighter particle production could be affected by up to \( 2\% \), and very high mass states by a similar amount, but final states similar in invariant mass to \( \pm \) will be largely unaffected. Hence, we can conclude that the change in our choice of the heavy-flavour coefficient function alone leads to changes in the distributions of up to \( 2\% \), and since the change is simply a freedom we have in making a definition, this is a theoretical uncertainty on the partons, much like the frequently invoked scale uncertainty. Like the latter, it should decrease as we go to higher orders.

3.6 Comparisons

We have tried to make clear that both the CTEQ and the MRST/MSTW approaches are consistent with the PQCD formalism with non-zero heavy quark masses \( m_\text{c} \). In this sense, they are both “valid”. In addition, they both adopt certain practises, such as the numerically significant rescaling-variable approach to correctly treat final-state kinematics (ACOT-), and the calculationally simplifying SACOT prescription for the quark-parton initiated subprocesses. These common features ensure broad agreement in their predictions. This is borne out by the fact that global QCD analyses carried out by both groups show very good agreement with all available hard scattering data, including the high-precision
Fig. 1: A comparison of the unpublished “MRST2006 NLO” parton distributions to the MRST2004 NLO distributions. In order to illustrate the significance of the size of the differences, the uncertainty on the MRST2001 distributions is used for the 2004 distributions.
DIS total inclusive cross sections and semi-inclusive heavy flavor production cross sections; and that
the predictions for higher energy cross sections at LHC for the important W/Z production process agree
rather well in the most recent versions of these analyses [2, 3]. Comparisons of experiment for the
abundant data on total inclusive cross sections (and the associated structure functions) with theory are
well documented in the CTEQ and MRST/MSTW papers. Here we only show the comparison of the
recent H1 data sets on cross sections for charm and bottom production [30] to the latest CTEQ and
MSTW calculations. This figure illustrates the general close agreement between the two calculations.
(Also, see below.)

![H1 Charm Cross Section in DIS](image1)

![H1 Beauty Cross Section in DIS](image2)

Fig. 2: Comparison of the predictions for $\sim c\bar{c}(x; Q^2)$ and $\sim b\bar{b}(x; Q^2)$ compared to preliminary data from H1.

Because the main source of the differences between the two implementations arise from the dif-
f erent conventions adopted for organizing the perturbative calculation, it is impossible to make a direct
(or clear-cut) comparison between the two calculations. By staying with the conventional order-by-order
formulation, the CTEQ approach has all the simplicities of the minimal GM VFNS. With the alternative
LO/NLO/NNLO organization, the MRST/MSTW approach includes specifically chosen higher-order
terms at each stage of the calculation for different physical quantities (e.g. $F^2_{tot}; F^L_{tot}; F^H_{tot}$, in Secs. 3.5.1)
with their associated Wilson coefficients (e.g. Eqs. 15,16). The choices are a matter of taste because, with
the same Wilson coefficients (with heavy quark mass) available in the literature (such as [10, 11]), both
analyses can be extended to the appropriate order, and they should contain the same information. So far,
MRST/MSTW has carried out their analyses to one order higher than CTEQ. In practice, we have seen
one comparison of the “NLO” predictions of the two approaches in Fig. 2 that shows remarkable general
agreement with each other, and with experimental data. Some expected differences at small-$x$, due to the
higher order term included in the MRST/MSTW calculation are present. Compared to experimental data,
the CTEQ curves seem to give a slightly better description of data in this region of difference; but this
should not be taken seriously in view of the above discussions. We intend to make a more quantitative

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9 Some apparent worrying discrepancies in the predictions for the W/Z cross-sections at LHC between [1] and [29] have
been superseded by the recent analyses.
study of the differences between the alternative formulations of a GM VFNS and ZM VFNS in a future publication.

4 Use of Parton Distribution Functions

Some commonly asked questions in the user community for PDFs are along the lines of: (i) Which available PDF set is most appropriate for my particular calculation? and (ii) If PDF set A was obtained using scheme A (say, ZMVFNSTMSTW/GMVFNSTMCTEQ) do I have to use the same scheme A for my Wilson coefficients (otherwise my calculation would be inconsistent)? Whereas it is impossible to answer all such questions at once, the following observations should provide useful guidelines toward the appropriate answers. Foremost, it is important to bear in mind that in the perturbative approach, all calculations are approximate; hence the goodness of the approximation is the most (or only) relevant consideration. Any fast, or absolute, rules or prescriptions would be misguided.

* For applications at very high energy scales, e.g. most LHC processes, it is perfectly fine to use the ZM formulae for the hard-scattering coefficient irrespective of the choice of PDF sets (see below), since the ZM Wilson coefficients are good approximations to the GM ones (valid to $O(M^2/Q^2)$ where $M$ represents the typical mass in the relevant parton subprocess—heavy quarks or other produced particles), and the ZM coefficients are much simpler and much more readily available.

On the other hand, for applications involving physical scales $Q \lesssim (M)$, such as comparison to precision DIS data at HERA, it is important both to use GM Wilson coefficients, and to ensure that these are consistent with those adopted in generating the PDF set to be used in the calculation.

* For the global analyses that yield the PDF sets, it matters whether the ZM VFNS or GM VFNS scheme is used in the calculation, since a substantial fraction of the input DIS data are in the region where $Q$ is not very large compared to the heavy quark masses $m_{c, b}$ (the top quark does not play a significant role in these analysis). Thus, the ZM-VFNS and GM VFNS PDFs can differ in some $x$-range, even if they agree quite well in general (cf. [1]). For example, the widely used CTEQ6.1 (ZM-VFNS) and the most recent CTEQ6.5/CTEQ6.6 (GM VFNS) PDF sets both give excellent fits to the available data, yet the differences (mainly around $x \approx 10^{-3}$) are enough to lead to a 6% shift in the predictions for cross sections for $W$ and similar mass states at the LHC. Higher mass final states are much less affected.

The above differences arise from two sources: (i) the treatment of final-state counting (Sec. 2.3) and phase space (Sec. 2.4); and (ii) mass effects in the Wilson coefficients. The first is numerically significant for reasons explained in those sections, and it can potentially be removed to produce an improved ZM VFNS (Sec. 3.1).

* The differences between PDFs obtained using different GM VFNS implementations, such as those by CTEQ and MSTW groups discussed in the main part of this review, are much smaller than those between the ZM and GM VFNS. This is because the treatments of final states are similar, and the differences in the Wilson coefficients are much reduced also. The current NLO predictions on $W$ and similar mass states at the LHC by the CTEQ and MSTW groups, for instance, are within 2% [4].

* What about single-flavor (say, $n_f$) FFNS PDFs that are commonly believed to be needed for FFNS calculations, such as for heavy flavor production processes? We would like to point out, perhaps surprisingly to many readers, that: (i) with the advent of GM VFNS PDFs, the FFNS PDFs are not in principle needed for consistency; and (ii) the use of $n_f$-flavor FFNS PDFs in a $n_f$-flavor calculation is much less reliable than using the GM VFNS (if the latter is available). The reasons for these assertions are fairly easy to see, as we now explain.

First of all, as we emphasized in Sec. 2.2 the GM VFNS is, by definition, a composite scheme that is the $n_f$-FFNS within the region of validity of the latter. In principle one can use the GM VFNS PDFs in the FFNS calculations within the region where the FFNS is reliable. (In practice this range of
validity (in energy scale ) extends up to several times $m_H$, cf. second to last paragraph of Sec. 2.2. Secondly, since any given $n_f$-FFNS has only a limited range of validity (Sec. 2.2), the global analysis used to determine any $n_f$-FFNS PDF set is inherently a compromise. This compromise is likely to be a fairly bad one for two reasons. Firstly, the limited range of validity implies that only a fraction of the data used in the global analysis can be legitimately applied. If one excludes all the data outside of the region of validity of the theory (not an easily-defined region), the constraining power of the analysis would greatly suffer. If, instead, one includes all the points in the analysis anyway, the PDFs will compensate, much like the case of the fit using the basic ZM VFNS. This can result in a good comparison to data (as in the ZM VFNS [31]), but this is potentially misleading since the compensation is caused by the wrong physics. In either of the cases, the PDFs resulting from a fit using the FFNS will be unreliable. Secondly, Wilson coefficients in the FFNS only exist for the DIS process beyond LO, hence the ZM approximation to $n_f$-FFNS must be used. We note, although this second point is shared by current GM VFNS analyses, the ZM VFNS approximation to GM VFNS is a much better approximation than that of ZM FFNS to $n_f$-FFNS. (For instance, for collider jet data sets, the ZM 3- or 4-flavor calculation would be way-off the correct one. This is not a problem for the GM VFNS case.) These inherent problems motivated an alternative approach to FFNS PDFs in [33]: rather than performing a (imperfect) FFNS global fit, one simply generates them by fixed $n_f$-flavor QCD evolution from a set of initial PDFs obtained in an existing (bona fide) GM VFNS global analysis! Because of the different QCD evolution, however, the PDFs will be different from the original GM VFNS ones crossing heavy flavor thresholds; and the fits to the global data will correspondingly deteriorate, particularly for the high precision HERA data sets at higher $Q^2$. Thus, these PDFs deviate from truth in a different way. The relative merit between this approach and the conventional FFNS global fits is difficult to gauge because there are no objective criteria for making the assessment.

Returning to the original question that started this bullet item, we can summarize the options available to match PDFs with a FFNS calculation such as HQVDIS [32] for heavy quark production: (i) conventional FFNS PDFs (CTEQ, GRV), suitably updated if necessary [34]; (ii) PDFs generated by FFNS evolution from GM VFNS PDFs at some initial scale $Q_0$ (MSTW [33], but also can easily be done with CTEQ); or, (iii) simply use the most up-to-date GM VFNS PDFs (MSTW, CTEQ) for all $Q$. For reasons discussed in the previous paragraphs, each option has its advantages and disadvantages. (i) and even (ii) are theoretically self-consistent, while (iii) is not, e.g. it opens up the awkward question of how many flavours to use in the definition of $S$. However, the PDFs in (iii) are intrinsically much more accurately and precisely determined. Hence, in practical terms it is not obvious which would be most “correct” 10 The choice reduces to a matter of taste, and for some, of conviction. The differences in results, obtained using these options, should not be too large, since they are mostly of one order higher in $S$; and, in an approximate manner, they define the existing theoretical uncertainty. In principle, an approach that combines the advantages of all three, hence could work the best, would be to use PDFs obtained in the GM VFNS, but with the transition scale $T$ (Sec. 2.3) set at a much higher value than $m_H$ for each heavy flavor threshold. But this option is rather cumbersome to implement (as has been hinted in Sec. 2.3), hence has not been done.

10 Although it is certainly better to use a current GM VFNS set of PDFs than an out-of-date FFNS set.
some of the anxieties expressed in the literature).

All in all, for general applications, taking into account all the considerations above, the modern GM VFNS PDF sets are clearly the PDFs of choice.

5 Intrinsic Heavy Flavour

Throughout the above discussions we have made the assumption that all heavy quark flavour is generated from the gluon and lighter flavours through the perturbative QCD evolution, starting from the respective scale \( \mu_H \). This is usually referred to as the radiatively generated heavy flavor scenario. From the theoretical point of view, this is reasonable for heavy flavors with mass scale \( \mu_H \) very much higher than the onset of the perturbative regime, say \( 1 \) GeV. Thus, while this assumption is usually not questioned for bottom and top, the case for charm is less obvious. In fact, the possibility for a non-negligible intrinsic charm (IC) component of the nucleon at \( Q^2 = m_c \) was raised a long time ago [38]; and interests in this possibility have persisted over the years. Whereas the dynamical origin of such a component can be the subject of much debate, the phenomenological question of its existence can be answered by global QCD analysis: do current data support the IC idea, and if so, what is its size and shape? This problem has been studied recently by a CTEQ group [39], under two possible scenarios: IC is enhanced at high values of \( x \) (suggested by dynamical models such as [38]), or it is similar in shape to the light-flavor sea quarks (similar to, say, strange). They found that current data do not tightly constrain the charm distribution, but they can place meaningful bounds on its size. Thus, while the conventional radiatively generated charm is consistent with data, IC is allowed in both scenarios. For the model-inspired (large-\( x \)) case, the size of IC can be as large as \( 3 \) times that of the crude model estimates, though comparison to the EMC \( F_2^c \) data [40] imply contributions somewhat smaller [41]. If such an IC component does exist, it would have significant impact on LHC phenomenology for certain beyond SM processes. For the sea-like IC case, the bound on its size is looser (because it can be easily interchanged with the other sea quarks in the global fits); its phenomenological consequences are likewise harder to pin-point.

From a theoretical point of view, intrinsic heavy flavour and GM VFNS definitions were discussed in [42]. Allowing an intrinsic heavy quark distribution actually removes the redundancy in the definition of the coefficient functions in the GM VFNS, and two different definitions of a GM VFNS will no longer be identical if formally summed to all orders, though they will only differ by contributions depending on the intrinsic flavour. Consider using identical parton distributions, including the intrinsic heavy quarks, in two different flavour schemes. The heavy-quark coefficient functions at each order are different by \( \mathcal{O} \left( \frac{\mu_H^2}{Q^2} \right) \). This difference has been constructed to disappear at all orders when combining the parton distributions other than the intrinsic heavy quarks, but will persist for the intrinsic contribution. The intrinsic heavy-flavour distributions are of \( \mathcal{O} \left( \frac{Q^2_{CD}}{\mu_H^2} \right) \), and when combined with the difference in coefficient functions the mass-dependence cancels leading to a difference in structure functions of \( \mathcal{O} \left( \frac{Q^2_{CD}}{Q^2} \right) \). It has been shown [6] that for a given GM VFNS the calculation of the structure functions is limited in accuracy to \( \mathcal{O} \left( \frac{Q^2_{CD}}{Q^2} \right) \). Hence, when including intrinsic charm, the scheme ambiguity is of the same order as the best possible accuracy one can obtain in leading twist QCD, which is admittedly better than that obtained from ignoring the intrinsic heavy flavour (if it exists) as \( Q^2 \) increases above \( \mu_H^2 \). It is intuitively obvious that best accuracy will be obtained from a definition of a GM VFNS where all coefficient functions respect particle kinematics. In fact, the most recent CTEQ and MSTW prescriptions would provide identical contributions to the structure functions from the same intrinsic charm parton distribution.

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