MSTW and Heavy Flavour Issues

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Heavy Quark issues

Will discuss Charm $\sim 1.4 \text{GeV}$, bottom $\sim 4.75 \text{GeV}$ as heavy flavours.

Quick reminder.

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).

$$F(x,Q^{2}) = C_{k}^{FF,n_{f}}(Q^{2}/m_{H}^{2}) \otimes f_{k}^{n_{f}}(Q^{2})$$

Note that n_f is effective number of light quarks.

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.

Additional problem FFNS known up to NLO (Laenen *et al*), but are not defined at NNLO – $\alpha_S^3 C_{2,Hg}^{FF,3}$ not fully known.

Recent progress by Blümlein *et al* for high Q^2

Variable Flavour

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

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

Partons in different number regions related to each other perturbatively.

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

Perturbative matrix elements $A_{jk}(Q^2/m_H^2)$ (Buza *et al* $\mathcal{O}(\alpha_S^2)$, Blümlein *et al* $\mathcal{O}(\alpha_S^3)$) containing $\ln(Q^2/m_H^2)$ terms relate $f_i^{n_f}(Q^2)$ and $f_i^{n_f+1}(Q^2) \rightarrow$ correct evolution for both.

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

Particular definition. More on this later.

Dependence on m_c at NLO in 2008 fits.

m_c (GeV)	χ^2_{global}	$\chi^2_{F^c_2}$	$\alpha_s(M_Z^2)$
	2699 pts	83 pts	
1.1	2728	263	0.1182
1.2	2625	188	0.1188
1.3	2563	134	0.1195
1.4	2543	107	0.1202
1.45	2541	100	0.1205
1.5	2545	97	0.1209
1.6	2574	104	0.1216
1.7	2627	128	0.1223

Clear correlation between m_c and $\alpha_S(M_Z^2)$.

For low m_c overshoot low Q^2 medium x data badly.

Preference for $m_c = 1.45 \text{GeV}$. Towards lower end of pole mass determinations.

BCDMS and NMC data prefer lower m_c , lower α_S and quicker threshold evolution respectively.

Dependence on m_c at NNLO in 2008 fits.

m_c (GeV)	χ^2_{global}	$\chi^2_{F^c_2}$	$\alpha_s(M_Z^2)$
	2615 pts	83 pts	
1.1	2499	114	0.1158
1.2	2463	88	0.1162
1.26	2546	82	0.1165
1.3	2457	82	0.1166
1.4	2480	95	0.1171
1.5	2527	125	0.1175
1.6	2589	167	0.1180
1.7	2666	217	0.1184

Less correlation between m_c and $\alpha_S(M_Z^2)$.

For high m_c undershoot moderate Q^2 data badly.

Preference for low value of $m_c = 1.26 \text{GeV}$.

Newer data seem to prefer higher mass.

Dependence on m_b at NLO in 2008 fits.

Vary m_b in steps of 0.25 GeV.

m_b (GeV)	χ^2_{global} 2699 pts	$\alpha_s(M_Z^2)$
	<u>-</u>	
4.00	2537	0.1201
4.25	2539	0.1202
4.50	2541	0.1202
4.75	2543	0.1202
5.00	2544	0.1201
5.25	2547	0.1201
5.50	2549	0.1200

Stays fairly flat all the way down to $m_b = 3 \text{GeV}$.

For lower m_b slightly better fit to HERA data, including $F_2^c(x, Q^2)$. Similar at NNLO, but with about half the change in χ^2 .

NLO comparisons to Beauty data (not in global fit) for varying m_b

F₂^b at NLO



Distinct preference for $m_b \approx 4.75 - 5 \text{GeV}$.

Overall global fit, even including current beauty data, would prefer fairly near current default = 4.75GeV.

Variation in cross sections.

$m_c \; [\text{GeV}]$	$\delta\sigma_W(Tev)$	$\delta\sigma_Z(Tev)$	$\delta\sigma_W(LHC)$	$\delta\sigma_Z(LHC)$	$\delta\sigma_H(LHC)$
1.25	-1.0	-1.1	-2.2	-2.4	-1.8
1.30	-0.7	-0.7	-1.4	-1.6	-1.2
1.35	-0.3	-0.4	-0.7	-0.8	-0.6
1.40	0.0	0.0	0.0	0.0	0.0
1.45	0.3	0.3	0.7	0.8	0.6
1.50	0.6	0.7	1.3	1.5	1.2
1.55	0.8	0.9	2.0	2.3	1.8

Fine-tuning of final numbers still ongoing - maybe 0.1 - 0.2% effects.

$m_b \; [{\rm GeV}]$	$\delta\sigma_W({\sf Tev})$	$\delta\sigma_Z(Tev)$	$\delta\sigma_W(LHC)$	$\delta\sigma_Z(LHC)$	$\delta\sigma_H(LHC)$
4.25	-0.1	-0.0	-0.3	0.0	-0.3
4.75	0.0	0.0	0.0	0.0	0.0
5.25	0.1	0.0	0.2	-0.1	0.2

Variation in cross sections at NNLO. About 15 - 20% bigger at NLO in general.

Bigger when probing lower x. 0.1GeV change in m_c can give 1.5% changes. Similar to PDF uncertainty.

3- and 4 Flavour Sets

Will be providing both 3- and 4-flavour sets for a wide variety of charm and bottom quark masses.

As argued in previous MRT paper on subject (2006) and in RT, Tung summary article for HERA-LHC workshop will be basing these on input for GM-VFNS fit.

Full global fit not possible while keeping number of flavours fixed at 3 or 4 due to lack of coefficient functions for many processes.

Argued in previous article that lack of accuracy from this procedure is questionable.

Use appropriate number of flavour in coupling for standard definition of FFNS coefficient functions (depends on renormalisation scheme one defines), i.e. same number as in PDFs at all times.

Doing this decrease in coupling compared to variable flavour, larger β -function.

Also increase in gluon compared to variable flavour, no splitting to heavy quarks.

To lowest order good compensation between two. Leads to invariance of quantities $\propto \alpha_S g(x,Q^2)$, e.g. light flavour evolution, Higgs cross-section.



Considerations of the GM-VFNS - Our Definition

The GM-VFNS can be defined by demanding equivalence of the n_f light flavour and $n_f + 1$ light flavour descriptions at all orders – above transition point $n_f \rightarrow n_f + 1$

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

Hence, the VFNS coefficient functions satisfy

$$C_k^{FF,n_f}(Q^2/m_H^2) = C_j^{VF,n_f+1}(Q^2/m_H^2) \otimes A_{jk}(Q^2/m_H^2),$$

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

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

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 this limit. Can swap $\mathcal{O}(m_H^2/Q^2)$ terms between $C_{2,HH}^{VF,0}(Q^2/m_H^2)$ and $C_{2,g}^{VF,1}(Q^2/m_H^2)$. Various prescriptions (ACOT, TR, Chuvakin-Smith).

Some earlier versions violated threshold $W^2 > 4m_H^2$ in individual terms.

(TR-VFNS) highlighted freedom in choice and enforced kinematics in each term by making $(d F_2/d \ln Q^2)$ continuous at transition (in gluon sector). Complicated to extend.

(S)ACOT(χ) (Tung, *et al*) prescription says make simple choice

 $C_{2,HH}^{VF,0}(Q^2/m_H^2,z) \propto \delta(z-Q^2/(Q^2+4m_H^2)).$ $\to F_2^{H,0}(x,Q^2) = e_h^2 x/x_{\max}(h+\bar{h})(x/x_{\max},Q^2), \qquad x_{\max} = Q^2/(Q^2+4m_H^2)$

 $\to C_{2,HH}^{ZM,0}(z) = \delta(1-z) \text{ for } Q^2/m_H^2 \to \infty. \text{ Also } W^2 = Q^2(1-x)/x \ge 4m_H^2.$

Have adopted this and obvious extensions to higher orders (and now simple modifications). Turns out use different multiplicative factor of $Q^2/(Q^2 + 4m_H^2)$.

Still another difference.

ACOT type schemes have used e.g.

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

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

But LO FFNS and evolution below and NLO definition and evolution above.

TR have used e.g.

$$\begin{aligned} \mathsf{LO} & \quad \frac{\alpha_S(Q^2)}{4\pi} C_{2,Hg}^{FF,n_f,(1)}(Q^2/m_H^2) \otimes g^{n_f}(Q^2) \to \frac{\alpha_S(M^2)}{4\pi} C_{2,Hg}^{FF,n_f,(1)}(1) \otimes g^{n_f}(M^2) \\ & \quad + C_{2,HH}^{VF,n_f+1,(0)}(Q^2/m_H^2) \otimes (h+\bar{h})(Q^2), \end{aligned}$$

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

This difference in choice can be phenomenologically important.

In order to define our 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. Needs modelling. More later.

Different type of Definition

Both the BMSN (Buza *et al*) and FONLL (Nason *et al*) applied the same type of reasoning in initially different contexts. In general terms (for structure functions)

 $F^{\text{GMVFNS}}(x,Q^2) = F_2^{\text{FFNS}}(x,Q^2) - F_2^{\text{asymp}}(x,Q^2) + F_2^{\text{ZMVFNS}}(x,Q^2)$

where the second (subtraction) term is the asymptotic version of the first, i.e., all terms $\mathcal{O}(m_H^2/Q^2)$ omitted. Now use for structure functions in FONLL Forte *et al*.

Differences in exactly how the second and third terms are defined in detail (e.g. Blümlein *et al* do not resum $\ln Q^2/m_H^2$ terms from PDF evolution in F_2^{ZMVFNS}).

Question of whether one only uses above some transition point, else not exactly $F_2^{\rm FFNS}(x,Q^2)$ below $Q^2=m_H^2$.

Realised from the beginning in FONLL approach that each term in the combination $(F_2^{\text{ZMVFNS}} - F_2^{\text{asymp}})$ can be modified by corrections which fall like m_H^2/Q^2 .

In simplest application α_S order of $F^{\text{FFNS}}(x, Q^2)$ at low Q^2 same as that of $F^{\text{ZMVFNS}}(x, Q^2)$ as $Q^2 \to \infty$, like ACOT. Verified Forte *et al*.

Modification in FONLL can avoid this, but leads to extra (higher order) term as $Q^2 \rightarrow \infty$ – not exact cancellation in first two terms.

Ordering tricky problem. Would like any GMVFNS to reduce to exactly correct order FFNS at low Q^2 and exactly correct order ZMVFNS as $Q^2 \rightarrow \infty$. At present none do.

Return to particular TR version of the GMVFNS. Reason for violation of the above is frozen term $\alpha_S^n(m_H^2) \sum_i C_{2,i}^{\text{FFNS}}(m_H^2) \otimes f_i(m_H^2)$ which still persists as $Q^2 \to \infty$ at order Nⁿ⁻¹LO.

Depends on size of PDFs at low scales, so rather small effect at large Q^2 .

However, not strictly necessary. Frozen in original TR prescription from exact condition on derivative of $d F_2/d$, $\ln Q^2$. Could have instead

$$\left(\frac{m_H^2}{Q^2}\right)^a \alpha_S^n(m_H^2) \sum_i C_{2,i}^{\rm FF}(m_H^2) \otimes f_i(m_H^2) \text{ or } \left(\frac{m_H^2}{Q^2}\right)^a \alpha_S^n(Q^2) \sum_i C_{2,i}^{\rm FF}(Q^2) \otimes f_i(Q^2),$$

Any a > 0 provides both exactly correct asymptotic limits, though strictly should have $(m_H^2/Q^2)k(\ln(Q^2/m_H^2))$ from factorization theorem.

Also have the freedom to modify the heavy quark coefficient function, by default

$$C_{2,HH}^{VF,0}(Q^2/m_H^2,z) = \delta(z-x_{\max}).$$

Appears in convolutions for higher order subtraction terms, so do not want complicated x dependence. Simple choice.

$$C_{2,HH}^{VF,0}(Q^2/m_H^2,z) \to (1+b(m_H^2/Q^2)^c)\delta(z-x_{\max})),$$

where again c really encompasses (m_H^2/Q^2) with logarithmic corrections.

Can also modify argument of δ -function, as in Intermediate Mass (IM) scheme of Nadolsky, Tung. Let argument of heavy quark contribution change like

 $\xi = x/x_{\text{max}} \to x \left(1 + \left(x(1 + 4m_H^2/Q^2) \right)^d 4m_H^2/Q^2 \right),$

so kinematic limit stays the same, but if d > 0 small x less suppressed, or if d < 0 (must be > -1) small x more suppressed.

Default a, b, c, d all zero. Limit either by fit quality or *sensible* choices.

 $6~\mbox{extreme}$ variations tried, along with $\mbox{ZM-VFNS}$

GMVFNS1 - b = -1, c = 1.

GMVFNS2 - b = -1, c = 0.5.

 $\mathsf{GMVFNS3} - a = 1.$

- GMVFNS4 b = +0.3, c = 1 fit.
- $\mathsf{GMVFNS5} d = 0.1 \mathsf{fit}.$
- $\mathsf{GMVFNS6} d = -0.2 \mathsf{fit}.$

Variations in $F_2^c(x,Q^2)$ near the transition point at NLO due to different choices of GM-VFNS.

Optimal, a = 1, b = -2/3, c = 1, smooth behaviour.



Variations in $F_2^c(x,Q^2)$ near the transition point due to different choices of GM-VFNS at NNLO.

Very much reduced, almost zero variation until very small x.

Shows that NNLO evolution effects most important in this regime.



Variations in partons extracted from global fit due to different choices of GM-VFNS at NLO. Default at low end.

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Initial \chi^2 can change by 250.
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Converges to within 20 of original.

Better fit for GMVFNS1, GMVFNS3 and GMVFNS6. Best for optimal scheme.

Some changes in PDFs large compared to one-sigma *uncertainty*.

 $\alpha_S(M_Z^2)$ changes by < 0.0004 except for GMVFNS2 - + 0.0007 and ZMVFNS - - 0.0015.





Also implement similar variations in GMVFNS for charged current processes.

HERA data completely insensitive due to large Q^2 .

Some effect on fixed target (anti)neutrino data. χ^2 changes by at most 4 and almost no change in this, or PDFs with refit.

Also make changes in cross-sections for dimuon data. In this case definition of separation into observable cross-section dependent on GMVFNS.

In practice χ^2 changes by at most 1 unit. Essentially no change in PDFs.



Variations in partons extracted from global fit due to different choices of GM-VFNS at NNLO.

Initial changes in $\chi^2 < 20$.

Converge to about 10. None a marked improvement.

At worst changes approach *uncertainty*.

Biggest variation in high-x gluon, which has large uncertainty.

Variations in $\alpha_S(M_Z^2) \sim 0.0003$.

ZMVFNS nonsense in this case.



Model $\mathcal{O}(\alpha_S^3)$ at low Q^2 using known leading threshold logarithms (Laenen and Moch) and leading $\ln(1/x)$ term from k_T -dependent impact factors Catani, *et al.*

Include latter in form

 $\propto (1 - z/x_{\text{max}})^a (\ln(1/z) - b)/z,$

where default a = 20, b = 4.

Variations in a make little difference. Maximum *sensible* variation of b = 2leads to effect in PDFs shown.

Major effect at smallest x.

Moderated significantly if $\mathcal{O}(\alpha_S^3)$ falls away rather than frozen.



The values of the predicted cross-sections at NLO for Z and a 120 GeV Higgs boson at the Tevatron and the LHC (latter for 14 TeV centre of mass energy).

PDF set	$B_{l^+l^-} \cdot \sigma_Z(nb) \; TeV$	$\sigma_{H}(pb)TeV$	$B_{l^+l^-} \cdot \sigma_Z(nb)$ LHC	$\sigma_H(pb) \ LHC$
MSTW08	0.2426	0.7462	2.001	40.69
GMvar1	0.2433	0.7428	2.023	40.76
GMvar2	0.2444	0.7383	2.061	41.29
GMvar3	0.2429	0.7438	2.024	41.03
GMvar4	0.2425	0.7457	1.993	40.60
GMvar5	0.2423	0.7454	1.991	40.56
GMvar6	0.2434	0.7431	2.032	41.00
GMvaropt	0.2434	0.7353	2.041	40.84
ZMVFNS	0.2410	0.7373	1.940	39.45
GMvarcc	0.2427	0.7451	2.001	40.65

At most 1.5% variation at Tevatron in σ_Z .

Up to +3% and -0.5% variation in σ_Z at the LHC. About half as much in σ_H due to higher average x sampled.

ZMVFNS clear outlier at LHC, but not the 8% from ZMVFNS to GMVFNS in CTEQ6.

The values of the predicted cross-sections at NNLO. σ_H calculated using Harlander, Kilgore code.

PDF set	$B_{l^+l^-} \cdot \sigma_Z(nb) \text{ TeV}$	$\sigma_H(pb)TeV$	$B_{l^+l^-} \cdot \sigma_Z(nb)$ LHC	$\sigma_H(pb)$ LHC
MSTW08	0.2507	0.9550	2.051	50.51
GMvar1	0.2509	0.9505	2.054	50.39
GMvar2	0.2514	0.9478	2.061	50.55
GMvar3	0.2516	0.9539	2.062	50.88
GMvar4	0.2507	0.9534	2.050	50.45
GMvar5	0.2509	0.9519	2.046	50.37
GMvar6	0.2509	0.9462	2.057	50.38
GMvaropt	0.2518	0.9530	2.064	50.90
GMvarmod	0.2501	0.9511	2.022	50.03
GMvarmod'	0.2508	0.9482	2.052	50.57

Other than from model dependence maximum variations of order 0.5% at LHC. High-x gluon leads to 1% on σ_H at Tevatron.

Model uncertainties can be > 1% from region at very small x and low Q^2 . Can perhaps input more small-x knowledge here. Effect far smaller when $\mathcal{O}(\alpha_S^3)$ term falls with Q^2 as now suggested.

Conclusions

Using our current default GM-VFNS MSTW have looked at the results of varying both the charm and bottom quark masses in the context of the MSTW2008 global fit. m_c determined with good precision, but rather lower at NNLO than NLO. Global fit without F_2^b data weakly prefers low m_b , but new direct $F_2^b(x,Q^2)$ data prefers $m_b \sim 4.75 - 5$ GeV. Constraint certainly possible in future.

We are providing 3- and 4-flavour sets for the variety of masses.

Discussed variations in definition of GMVFNS, and introduced options for exact reduction to correctly ordered high and low Q^2/m_H^2 limits. New optimal version the smoothest near threshold and best fit at NLO. Little variation in smoothness or fit quality at NNLO.

Examined limits of variation in definitions and looked at variations in PDFs and cross-sections. At NLO PDFs can vary significantly outside experimental uncertainties at small x and cross-sections change by 3%. Default near extreme of variations. ZMVFNS consistently outside range of variation.

At NNLO PDFs usually (well) within uncertainties, and cross-sections rarely change more than 1%. GMVFNS variation significant source of uncertainty at NLO but much less significant at NNLO.

NNLO consequences.

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.



Also illustrated as in the figure below.



Can look at more details

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Preference of each data set.

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changes in m_c





