HERAFitter

Open Source QCD Fit Project

Version 1.0 (svn -1650)

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Abstract HERAFitter is an open-source package that provides a framework for the determination of the parton distribution functions (PDFs) of the proton and for many different kinds of analyses in Quantum Chromodynamics (QCD). It encodes results from a wide range of experimental measure-

11 number of the existing methods and schemes used for PDF 54 partons. Measurements of inclusive Neutral Current (NC) determination. The data and theoretical predictions are brought⁵ and Charge Current (CC) Deep Inelastic Scattering (DIS) together through numerous methodological options for car- 56 at the lepton-proton (ep) collider HERA provide crucial inrying out PDF fits and plotting tools to help visualise the 57 formation for determining the PDFs. Different processes in results. While primarily based on the approach of collinear proton-proton (pp) and proton-antiproton $(p\bar{p})$ collisions at factorisation, HERAFitter also provides facilities for fits of 59 the LHC and the Tevatron, respectively, provide compledipole models and transverse-momentum dependent PDFs. 60 mentary information to the DIS measurements. The PDFs The package can be used to study the impact of new precise $_{61}$ are determined from χ^2 fits of the theoretical predictions measurements from LHC or elsewhere. This paper describes 62 to the data. The rapid flow of new data from the LHC exthe general structure of HERAFitter and its wide choice of 63 periments and the corresponding theoretical developments, options.

22 **Keywords** PDFs · QCD · Fit · proton structure

1 Introduction

tensive searches for signals of new physics in LHC protonthe validity of the Standard Model (SM) and factorisation in Quantum Chromodynamics (QCD). Using collinear factorisation, inclusive cross sections in hadron collisions may be

$$\sigma(\alpha_{s}(\mu_{R}^{2}), \mu_{R}^{2}, \mu_{F}^{2}) = \sum_{a,b} \int_{0}^{1} dx_{1} dx_{2} f_{a}(x_{1}, \mu_{F}^{2}) f_{b}(x_{2}, \mu_{F}^{2})
\times \hat{\sigma}^{ab}(x_{1}, x_{2}; \alpha_{s}(\mu_{R}^{2}), \mu_{R}^{2}, \mu_{F}^{2})
+ \mathcal{O}\left(\frac{\Lambda_{QCD}^{2}}{Q^{2}}\right)$$
(1)

where the cross section σ is expressed as a convolution of Parton Distribution Functions (PDFs) f_a and f_b with the parton cross section $\hat{\sigma}^{ab}$, involving a momentum transfer qsuch that $Q^2 = |q^2| \gg \Lambda_{QCD}^2$, where Λ_{QCD} is the QCD scale. At Leading-Order (LO) in the perturbative expansion of the strong-coupling constant, the gPDFs represent the probability of finding a specific parton a(b) in the first (second) hadron carrying a fraction x_1 (x_2) of its momentum. The indices a and b in Eq. 1 indicate the various kinds of partons, i.e. gluons, quarks and antiquarks of different flavours that are considered as the constituents of the proton. The PDFs depend on the factorisation scale, $\mu_{\rm F}$, while the parton cross sections depend on the strong coupling constant, 94 The diagram in Fig. 1 gives a schematic overview of the $\alpha_{\rm s}$, and the factorisation and renormalisation scales, $\mu_{\rm F}$ and $\mu_{\rm R}$. The parton cross sections $\hat{\sigma}^{ab}$ are calculable in perturbative QCD (pQCD) whereas PDFs are usually constrained ticles on PDFs can be found in Refs. [8, 9].

 $_{52}$ quires large amounts of experimental data that cover a wide $_{102}$ ture function F_L . These data are the basis of any proton PDF 53 kinematic region and that are sensitive to different kinds of 103 extraction, and are used in all current PDF sets from MSTW

which are providing predictions for more complex processes at increasingly higher orders, has motivated the development of a tool to combine them together in a fast, efficient, opensource framework.

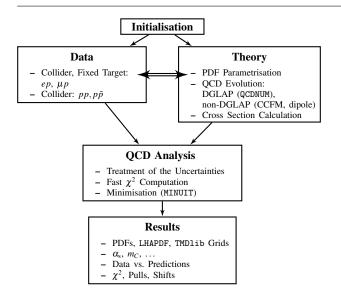
This paper describes the open-source QCD fit frame-69 work HERAFitter [10], which includes a set of tools to fa-The recent discovery of the Higgs boson [1, 2] and the ex- 70 cilitate global QCD analyses of pp, $p\bar{p}$ and ep scattering data. It has been developed for the determination of PDFs proton collisions demand high-precision calculations to test 72 and the extraction of fundamental parameters of QCD such as the heavy quark masses and the strong coupling constant. 14 It also provides a common framework for the comparison of different theoretical approaches. Furthermore, it can be used to test the impact of new experimental data on the PDFs and on the SM parameters.

This paper is organised as follows: The general structure of HERAFitter is presented in Sec. 2. In Sec. 3 the various processes available in HERAFitter and the corresponding theoretical calculations, performed within the framework of collinear factorisation and the DGLAP [11–15] formalism, are discussed. In Sec. 4 tools for fast calculations of the theoretical predictions are presented. In Sec. 5 the methodology to determine PDFs through fits based on various χ^2 86 definitions is described. In particular, different treatments of 87 correlated experimental uncertainties are presented. Alter-88 native approaches to the DGLAP formalism are presented in Sec. 6. The organisation of the HERAFitter code is dis-90 cussed in Sec. 7, specific applications of the package are 91 persented in Sec. 8, which is followed by a summary in

2 The HERAFitter Structure

95 HERAFitter structure and functionality, which can be di-96 vided into four main blocks:

by global fits to a variety of experimental data. The assump- 97 Data: Measurements from various processes are provided tion that PDFs are universal, within a particular factorisation 98 in the HERAFitter package including the information on scheme [3–7], is crucial to this procedure. Recent review ar- 99 their uncorrelated and correlated uncertainties. HERA in-100 clusive scattering data are sensitive to quark and to gluon A precise determination of PDFs as a function of x re- 101 PDFs through scaling violations and the longitudinal struc-



 $\textbf{Fig. 1} \ \ \textbf{Schematic overview of the HERAFitter program}.$

104 [16], CT [17], NNPDF [18], ABM [19], JR [20] and HERA-PDF [21] groups. Measurements of charm and beauty quark production at HERA are sensitive to heavy quark PDFs, jet measurements have direct sensitivity to the gluon PDF. However, the kinematic range of HERA data mostly covers low and medium ranges in x. Measurements from the fixed target experiments, the Tevatron and the LHC provide additional constraints on the gluon and quark distributions at high-x, 138 the distributions of the systematic uncertainties, e.g. Gausbetter understanding of heavy quark distributions and de- 139 sian or LogNormal [32], can also be studied (see Sec. 5.3). composition of the light-quark sea. For these purposes, measurements from fixed-target experiments, the Tevatron and the LHC can be used.

Fitter framework are listed in Tab. 1.

PDFs are evolved to the scale of the measurement \hat{Q}^2 , $Q^2 > 146$ Ref. [21]). Note that following conventions, the PDFs are Q_0^2 . By default, the evolution uses the DGLAP formalism ¹⁴⁷ displayed as parton momentum distributions $xf(x,\mu_F^2)$. [11–15] as implemented in QCDNUM [22]. Alternatively, the CCFM evolution [23–26] as implemented in uPDFevolv [27] can be chosen. The prediction of the cross section for a par- 148 3 Theoretical formalism using DGLAP evolution ticular process is obtained, assuming factorisation, by the convolution of the evolved PDFs with the corresponding 149 In this section the theoretical formalism based on DGLAP parton scattering cross section. Available theory calculations 150 [11–15] equations is described. for each process are listed in Tab. 1. Predictions using dipole 151 models [28-30] can also be obtained.

predictions, is minimised with the MINUIT [31] program. In 156 tions is obtained: HERAFitter various choices are available for the treatment of experimental uncertainties in the χ^2 definition. Correlated experimental uncertainties can be accounted for using a nuisance parameter method or a covariance matrix method as

Experimental Data	Process	Reaction	Theory schemes calculations
HERA, Fixed Target	DIS NC	$\begin{array}{c} ep \rightarrow eX \\ \mu p \rightarrow \mu X \end{array}$	TR', ACOT, ZM (QCDNUM), FFN (OPENQCDRAD, QCDNUM), TMD (uPDFevolv)
HERA	DIS CC	$ep \rightarrow v_e X$	ACOT, ZM (QCDNUM), FFN (OPENQCDRAD)
	DIS jets	$ep \rightarrow e \text{ jets}X$	NLOJet++ (fastNLO)
	DIS heavy quarks	$ep ightarrow ec\bar{c}X, \ ep ightarrow eb\bar{b}X$	TR', ACOT, ZM (QCDNUM), FFN (OPENQCDRAD, QCDNUM)
Tevatron, LHC	Drell-Yan	$pp(\bar{p}) \rightarrow l\bar{l}X, \ pp(\bar{p}) \rightarrow l\nu X$	MCFM (APPLGRID)
	top pair	$pp(\bar{p}) \rightarrow t\bar{t}X$	MCFM (APPLGRID), HATHOR, DiffTop
	single top	$\begin{array}{c} pp(\bar{p}) \rightarrow tlvX, \\ pp(\bar{p}) \rightarrow tX, \\ pp(\bar{p}) \rightarrow tWX \end{array}$	MCFM (APPLGRID)
	jets	$pp(\bar{p}) \rightarrow \mathrm{jets}X$	NLOJet++ (APPLGRID), NLOJet++ (fastNLO)
LHC	DY heavy quarks	$pp \rightarrow VhX$	MCFM (APPLGRID)

Table 1 The list of experimental data and theory calculations implemented in the HERAFitter package. The references for the individual calculations and schemes are given in the text.

described in Sec. 5.2. Different statistical assumptions for

140 Results: The resulting PDFs are provided in a format ready The processes that are currently available within the HERA¹⁴¹ to be used by the LHAPDF library [33, 34] or by TMDlib [35]. HERAFitter drawing tools can be used to display the PDFs with their uncertainties at a chosen scale. As an example, the Theory: The PDFs are parametrised at a starting scale, Q_0^2 , 144 first set of PDFs extracted using HERAFitter from HERA using a functional form and a set of free parameters p. These 145 I data, HERAPDF1.0 [21], is shown in Fig. 2 (taken from

A direct consequence of factorisation (Eq. 1) is that the scale dependence or "evolution" of the PDFs can be predicted by the renormalisation group equations. By requiring QCD Analysis: The PDFs are determined in a least squares physical observables to be independent of μ_F , a representafit: a χ^2 function, which compares the input data and theory 155 tion of the parton evolution in terms of the DGLAP equa-

$$\frac{d f_a(x, \mu_F^2)}{d \log \mu_F^2} = \sum_{b=a\bar{a}, \rho} \int_x^1 \frac{dz}{z} P_{ab} \left(\frac{x}{z}; \mu_F^2\right) f_b(z, \mu_F^2), \qquad (2)$$

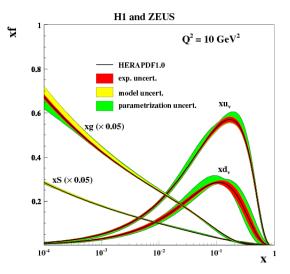


Fig. 2 Distributions of valence (xu_v, xd_v) , sea (xS) and the gluon (g)PDFs in HERAPDF1.0 [21]. The gluon and the sea distributions are scaled down by a factor of 20. The experimental, model and parametrisation uncertainties are shown as coloured bands.

where the functions P_{ab} are the evolution kernels or splitting functions, which represent the probability of finding parton a in parton b. They can be calculated as a perturbative expansion in α_s . Once PDFs are determined at the initial scale $\mu_F^2=Q_0^2$, their evolution to any other scale $Q^2>Q_0^2$ is entirely determined by the DGLAP equations. The PDFs are then used to calculate cross sections for various different processes. Alternative approaches to DGLAP evolution equations, valid in different kinematic regimes, are also implemented in HERAFitter and will be discussed in Sec. 6.

3.1 Deep Inelastic Scattering and Proton Structure

The formalism that relates the DIS measurements to pQCD and the PDFs has been described in detail in many extensive reviews (see e.g. Ref. [36]) and it is only briefly summarised here. DIS is the process where a lepton scatters off 215 Zero-Mass Variable Flavour Number (ZM-VFN): the partons in the proton by a virtual exchanged of a neu- 216 In this scheme [37], the heavy quarks appear as partons in tral (γ/Z) or charged (W^{\pm}) vector boson and, as a result, a 217 the proton at Q^2 values above $\sim m_h^2$ (heavy quark mass) and scattered lepton and a hadronic final state are produced. The 218 they are then treated as massless in both the initial and ficommon DIS kinematic variables are the scale of the pro- 219 nal states of the hard scattering process. The lowest order cess Q^2 , which is the absolute squared four-momentum of 220 process is the scattering of the lepton off the heavy quark the exchange boson, Bjorken x, which can be related in the 221 via electroweak boson exchange. This scheme is expected parton model to the momentum fraction that is carried by $_{222}$ to be reliable in the region where $Q^2\gg m_h^2$. In <code>HERAFitter</code> the struck quark, and the inelasticity y. These are related by 223 this scheme is available for the DIS structure function cal $y = Q^2/sx$, where s is the squared centre-of-mass energy. 224 culation via the interface to the QCDNUM [22] package, thus

alised structure functions:

$$\frac{d^2 \sigma_{NC}^{e^{\pm} p}}{dx dO^2} = \frac{2\pi \alpha^2 Y_+}{x O^4} \sigma_{r,NC}^{e^{\pm} p},\tag{3}$$

$$\sigma_{r,NC}^{e^{\pm}p} = \tilde{F}_2^{\pm} \mp \frac{Y_-}{Y_+} x \tilde{F}_3^{\pm} - \frac{y^2}{Y_+} \tilde{F}_L^{\pm}, \tag{4}$$

where $Y_{\pm} = 1 \pm (1-y)^2$ and α is the electromagnetic coupling constant. The generalised structure functions $\tilde{F}_{2,3}$ can be written as linear combinations of the proton structure functions F_2^{γ} , $F_{2,3}^{\gamma Z}$ and $F_{2,3}^{Z}$, which are associated with pure photon exchange terms, photon-Z interference terms and pure Z exchange terms, respectively. The structure function \tilde{F}_2 is the dominant contribution to the cross section, $x\tilde{F}_3$ becomes important at high Q^2 and \tilde{F}_L is sizable only at high y. In the framework of pQCD, the structure functions are directly related to the PDFs: at LO F_2 is the weighted momentum sum of quark and anti-quark distributions, xF_3 is related to their difference, and F_L vanishes. At higher orders, terms related to the gluon distribution appear, in particular F_L is strongly related to the low-*x* gluon.

The inclusive CC ep cross section, analogous to the NC ep case, can be expressed in terms of another set of structure 199 functions, \tilde{W} :

$$\frac{d^2 \sigma_{CC}^{e^{\pm} p}}{dx dQ^2} = \frac{1 \pm P}{2} \frac{G_F^2}{2\pi x} \left[\frac{m_W^2}{m_W^2 + Q^2} \right] \sigma_{r,CC}^{e^{\pm} p}$$
 (5)

$$\sigma_{r,CC}^{e^{\pm}p} = Y_{+}\tilde{W}_{2}^{\pm} \mp Y_{-}x\tilde{W}_{3}^{\pm} - y^{2}\tilde{W}_{L}^{\pm}, \tag{6}$$

where P represents the lepton beam polarisation. At LO in α_s , the CC e^+p and e^-p cross sections are sensitive to different combinations of the quark flavour densities.

Beyond LO, the OCD predictions for the DIS structure functions are obtained by convoluting the PDFs with appropriate hard-process scattering matrix elements, which are referred to as coefficient functions.

The DIS measurements span a large range of Q^2 from a few GeV² to about 10⁵ GeV², crossing heavy quark mass 209 thresholds, thus the treatment of heavy quark (charm and 210 beauty) production and the chosen values of their masses 211 become important. There are different schemes for the treat-212 ment of heavy quark production. Several variants of these schemes are implemented in HERAFitter and they are briefly 214 discussed below.

The NC cross section can be expressed in terms of gener- 225 it benefits from the fast QCDNUM convolution engine.

Fixed Flavour Number (FFN):

In this rigorous quantum field theory scheme [38–40], only 278 the gluon and the light quarks are considered as partons 279 within the proton and massive quarks are produced pertur- 280 batively in the final state. The lowest order process is the 281 heavy quark-antiquark pair production via boson-gluon fu- 282 sion. In HERAFitter this scheme can be accessed via the 283 QCDNUM implementation or through the interface to the opensource code OPENQCDRAD [41] as implemented by the ABM group. This scheme is reliable for $Q^2 \sim m_h^2$. In QCDNUM, the calculation of the heavy quark contributions to DIS structure functions are available at Next-to-Leading Order (NLO) and only electromagnetic exchange contributions are taken into account. In the OPENQCDRAD implementation the heavy quark contributions to CC structure functions are also available and, for the NC case, the QCD corrections to the coefficient functions in Next-to-Next-to Leading Order (NNLO) are provided in the best currently known approximation [42]. The OPENQCDRAD implementation uses in addition the running heavy quark mass in the \overline{MS} scheme [43].

It is sometimes argued that this scheme reduces the sensitivity of the DIS cross sections to higher order corrections [42]. It is also known to have smaller non-perturbative corrections than the pole mass scheme [44].

General-Mass Variable Flavour Number (GM-VFN):

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In this scheme [45], heavy quark production is treated for $Q^2 \sim m_h^2$ in the FFN scheme and for $Q^2 \gg m_h^2$ in the massless scheme with a suitable interpolation in between. The details of this interpolation differ between implementations. The groups that use GM-VFN schemes in PDFs are MSTW. CT (CTEQ), NNPDF, and HERAPDF. HERAFitter implements different variants of the GM-VFN scheme.

- GM-VFN Thorne-Roberts scheme: The Thorne-Roberts (TR) scheme [46] was designed to provide a smooth transition from the massive FFN scheme at low scales difficult to implement beyond NLO, it was updated to the TR' scheme [47]. There are two variants of the TR' schemes: TR' standard (as used in MSTW PDF sets [16, 47]) and TR' optimal [48], with a smoother transition across the heavy quark threshold region. Both TR' variants are accessible within the HERAFitter package at LO, NLO and NNLO.
- GM-VFN ACOT scheme: The Aivazis-Collins-Olness- 294 3.3 Diffractive PDFs Tung (ACOT) scheme belongs to the group of VFN fac-

of the ACOT scheme are available: ACOT-Full [50], S-ACOT- χ [51, 52], ACOT-ZM [50], $\overline{\text{MS}}$ at LO and NLO. For the longitudinal structure function higher order calculations are also available. A comparison of PDFs extracted from QCD fits to the HERA data with the TR' and ACOT-Full schemes is illustrated in Fig. 3 (taken from [21]).

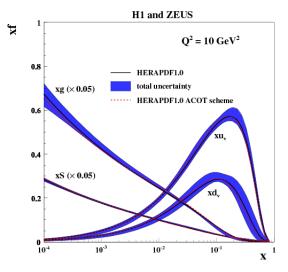


Fig. 3 Distributions of valence (xu_v, xd_v) , sea (xS) and the gluon (g)PDFs in HERAPDF1.0 [21] with their total uncertainties at the scale of $Q^2 = 10 \text{ GeV}^2$ obtained using the TR' scheme and compared to the PDFs obtained with the ACOT-Full scheme using the k-factor technique (red). The gluon and the sea distributions are scaled down by a factor of 20.

3.2 Electroweak Corrections to DIS

Calculations of higher-order electroweak corrections to DIS at HERA are available in HERAFitter in the on-shell scheme $Q^2 \sim m_h^2$ to the massless ZM-VFNS scheme at high scales $Q^2 \gg m_h^2$. Because the original version was technically m_{ZSS} are treated as basic parameters together with the top m_Z are treated as basic parameters together with the top, 289 Higgs and fermion masses. These electroweak corrections ²⁹⁰ are based on the EPRC package [53]. The code calculates the running of the electromagnetic coupling α using the most recent parametrisation of the hadronic contribution [54] as well as an older version from Burkhard [55].

torisation schemes that use the renormalisation method 295 About 10% of deep inelastic interactions at HERA are diffracof Collins-Wilczek-Zee (CWZ) [49]. This scheme uni- 296 tive, such that the interacting proton stays intact $(ep \to eXp)$. fies the low scale $Q^2 \sim m_h^2$ and high scale $Q^2 > m_h^2$ re- 297 The proton is well separated from the rest of the hadronic figions in a coherent framework across the full energy 298 nal state by a large rapidity gap. This is interpreted as the range. Within the ACOT package, the following variants 299 dissociation of the virtual photon into a hadronic system X

with a squared invariant mass much smaller than the photon- 329 sumed to be mediated by the exchange of a hard Pomeron 332 as [60, 61]: or a secondary Reggeon with vacuum quantum numbers. This factorisable Pomeron picture has proved remarkably successful in the description of most of the diffractive data. Diffractive parton distributions (DPDFs) can be determined from QCD fits to diffractive cross sections in a similar way to the determination of the standard PDFs [56].

In addition to the usual DIS variables x, Q^2 , extra kinematic variables are needed to describe the diffractive process. These are the squared four-momentum transfer of the 336 and $\hat{\sigma}^q$ is the parton-parton hard scattering cross section. exchanged Pomeron or Reggeon, t, and the mass m_X of the diffractively produced final state. In practice, the variable 338 The corresponding triple differential CC cross section has m_X is often replaced by the dimensionless quantity $\beta = \frac{Q^2}{m_X^2 + Q^2 - t}$. the form: In models based on a factorisable Pomeron, β may be viewed at LO as the fraction of the Pomeron longitudinal momentum, x_{IP} , which is carried by the struck parton, $x = \beta x_{IP}$, where *P* denotes the momentum of the proton.

$$\frac{d^4\sigma}{d\beta dQ^2 dx_{IP} dt} = \frac{2\pi\alpha^2}{\beta Q^4} \left(1 + (1 - y)^2 \right) \overline{\sigma}^{D(4)} (\beta, Q^2, x_{IP}, t)$$
 (7)

with the "reduced cross section":

$$\overline{\sigma}^{D(4)} = F_2^{D(4)} - \frac{y^2}{1 + (1 - y)^2} F_L^{D(4)}.$$
 (8)

The diffractive structure functions can be expressed as convolutions of calculable coefficient functions with the diffraça matic cuts. tive quark and gluon distribution functions, which in general depend on x_{IP} , Q^2 , β and t.

The diffractive PDFs [57, 58] in HERAFitter are implemented as a sum of two factorised contributions:

$$\Phi_{IP}(x_{IP},t) f_a^{IP}(\beta,Q^2) + \Phi_{IR}(x_{IP},t) f_a^{IR}(\beta,Q^2), \qquad (9)$$

3.4 Drell-Yan Processes in pp or $p\bar{p}$ Collisions

The Drell-Yan (DY) process provides valuable information about PDFs. In pp and $p\bar{p}$ scattering, the Z/γ^* and W production probe bi-linear combinations of quarks. Complementary information on the different quark densities can be obtained from the W^{\pm} asymmetry (d, u and their ratio), the 363 The cross section for production of high p_T hadronic jets ratio of the W and Z cross sections (sensitive to the flavour 364 is sensitive to the high-x gluon PDF (see e.g. Ref. [16]). composition of the quark sea, in particular to the s-quark 365 Therefore this process can be used to improve the determidistribution), and associated W and Z production with heavy 366 nation of the gluon PDF, which is particularly important for quarks (sensitive to c- and b-quark densities). Measurements 367 Higgs production and searches for new physics. Jet producat large boson transverse momentum $p_T \gtrsim m_{WZ}$ are poten- 368 tion cross sections are currently known only to NLO. Calcutially sensitive to the gluon distribution [59].

At LO the DY NC cross section triple differential in inproton centre-of-mass energy $W^2 = ys - Q^2 + m_p^2(1-y)$, 330 variant mass m, boson rapidity y and lepton scattering anwhere m_p is the proton mass. Such a process is often as- 331 gle $\cos \theta$ in the parton centre-of-mass frame can be written

$$\frac{d^3\sigma}{dmdyd\cos\theta} = \frac{\pi\alpha^2}{3ms} \sum_{q} \hat{\sigma}^q(\cos\theta, m)
\times \left[f_q(x_1, m^2) f_{\bar{q}}(x_2, m^2) + (q \leftrightarrow \bar{q}) \right], \quad (10)$$

where s is the squared centre-of-mass beam energy, the parton momentum fractions are given by $x_{1,2} = \frac{m}{\sqrt{s}} \exp(\pm y)$, $f_q(x_1, m^2)$ are the PDFs at the scale of the invariant mass,

$$\frac{d^3\sigma}{dmdyd\cos\theta} = \frac{\pi\alpha^2}{48s\sin^4\theta_W} \frac{m^3(1-\cos\theta)^2}{(m^2-m_W^2) + \Gamma_W^2 m_W^2} \times \sum_{q_1,q_2} V_{q_1q_2}^2 f_{q_1}(x_1, m^2) f_{q_2}(x_2, m^2), \tag{11}$$

For the inclusive case, the diffractive cross section reads as: $_{340}$ where $V_{q_1q_2}$ is the Cabibbo-Kobayashi-Maskawa (CKM) quark $_{341}$ mixing matrix and m_W and $arGamma_W$ are the W boson mass and decay width, respectively.

> The simple LO form of these expressions allows for the analytic calculations of integrated cross sections. In both NC (8) 345 and CC expressions the PDFs depend only on the boson rapidity y and invariant mass m, while the integral in $\cos \theta$ can 347 be evaluated analytically even for the case of realistic kine-

Beyond LO, the calculations are often time-consuming and Monte Carlo generators are often employed. Currently, 351 the predictions for W and Z/γ^* production are available up 352 to NNLO and the predictions for W, Z in association with heavy flavour quarks is available to NLO.

There are several possibilities to obtain the theoretical where $\Phi(x_{I\!P},t)$ are the Reggeon and Pomeron fluxes. The 355 predictions for DY production in HERAFitter. The NLO Reggeon PDFs, f_a^{IR} are fixed as those of the pion, while the 356 and NNLO calculations are time consuming and k-factor or Pomeron PDFs, f_a^{IP} , can be obtained from a fit to the data. 357 fast grid techniques must be employed (see Sec. 4 for details), which are interfaced to programs such as MCFM [62-₃₅₉ 64], available for NLO calculations, or FEWZ [65] and DYNNLO[66] 360 for NLO and NNLO, with electroweak corrections estimated 361 using MCSANC [67, 68].

3.5 Jet Production in ep and pp or $p\bar{p}$ Collisions

 $_{369}$ lations for higher-order contributions to jet production in pp

NLOJet++ program [72, 73] may be used for calculations 418 nique. Both are available in HERAFitter. of jet production. Similarly to the DY case, the calculation is very demanding in terms of computing power. Therefore fast grid techniques are used to facilitate the QCD analyses including jet cross section measurements in ep, pp and $p\bar{p}$ collisions. For details see Sec. 4.

3.6 Top-quark Production in pp or $p\bar{p}$ Collisions

At the LHC, top-quark pairs $(t\bar{t})$ are produced dominantly via gg fusion. Thus, LHC measurements of the $t\bar{t}$ cross section provide additional constraints on the gluon distribution at medium to high values of x, on α_s and on the top-quark mass, m_t [74]. Precise predictions for the total inclusive $t\bar{t}$ cross section are available up to NNLO [75, 76]. Currently, they can be computed within HERAFitter via an interface to the program HATHOR [77].

Fixed-order QCD predictions for the differential $t\bar{t}$ cross section at NLO can be obtained by using the program MCFM [643,4] 78–81] interfaced to HERAFitter with *fast grid* techniques.

Single top quarks are produced by exchanging electroweak bosons and the measurement of their production cross section can be used, for example, to probe the ratio of the u and d distributions in the proton as well as the b-quark PDF. Predictions for single-top production are available at the NLO accuracy by using MCFM.

Approximate predictions up to NNLO in QCD for the differential $t\bar{t}$ cross section in one-particle inclusive kinematics are available in HERAFitter through an interface to the program DiffTop [82, 83]. It uses methods of QCD threshold resummation beyond the leading logarithmic approximation. This allows the users to estimate the impact of the recent $t\bar{t}$ differential cross section measurements on the uncertainty of the gluon density within a QCD PDF fit at NNLO. A fast evaluation of the DiffTop differential cross sections is possible via an interface to fast grid computations [84].

4 Computational Techniques

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Precise measurements require accurate theoretical predic- 455 PDF can be approximated by a set of interpolating funcat higher orders due to the increasing number of relevant 458 and optimised such that the approximation bias is negligibly Feynman diagrams. The direct inclusion of computationally 459 small compared to the experimental and theoretical accudemanding higher-order calculations into iterative fits is thus 460 racy. This method can be used to perform the time consumturbative calculation for small changes in input parameters 462 interpolating functions. Further iterations of the calculation is not necessary at each step of the iteration. Two methods 463 for a particular PDF set are fast, involving only sums over

370 collisions are in progress [69–71]. Within HERAFitter, the 417 the problem: the k-factor technique and the fast grid tech-

4.1 k-factor Technique

The k-factors are defined as the ratio of the prediction of a ⁴²¹ higher-order (slow) pQCD calculation to a lower-order (fast) 422 calculation using the same PDF. Because the k-factors depend on the phase space probed by the measurement, they have to be stored including their dependence on the relevant kinematic variables. Before the start of a fitting procedure, a table of k-factors is computed once for a fixed PDF with the time consuming higher-order code. In subsequent iteration steps the theory prediction is derived from the fast lowerorder calculation by multiplying the pre-tabulated k-factors.

This procedure, however, neglects the fact that the kfactors are PDF dependent, and as a consequence, they have to be re-evaluated for the newly determined PDF at the end of the fit for a consistency check. The fit must be repeated until input and output k-factors have converged. In summary, this technique avoids iteration of the higher-order calculation at each step, but still requires typically a few reevaluations.

In HERAFitter, the *k*-factor technique is also used for the fast computation of the time-consuming GM-VFN schemes 440 for heavy quarks in DIS. "FAST" heavy-flavour schemes are implemented with k-factors defined as the ratio of calcula-442 tions at the same perturbative order but for massive vs. massless quarks, e.g. NLO (massive)/NLO (massless). These k-444 factors are calculated only for the starting PDF and hence, the "FAST" heavy flavour schemes should only be used for quick checks. Full heavy flavour schemes should be used by default. However, for the ACOT scheme, due to exceptionally long computation times, the k-factors are used in the 449 default setup of HERAFitter.

450 4.2 Fast Grid Techniques

451 Fast grid techniques exploit the fact that iterative PDF fit-452 ting procedures do not impose completely arbitrary changes 453 to the types and shapes of the parameterised functions that represent each PDF. Instead, it can be assumed that a generic tions in order to maximise their impact in PDF fits. Perturba- 456 tions with a sufficient number of judiciously chosen suptive calculations become more complex and time-consuming 457 port points. The accuracy of this approximation is checked not possible currently. However, a full repetition of the per- 461 ing higher-order calculations (Eq. 1) only once for the set of have been developed which take advantage of this to solve 464 the set of interpolators multiplied by factors depending on

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the PDF. This approach can be used to calculate the cross 518 sections of processes involving one or two hadrons in the 519 initial state and to assess their renormalisation and factori- 520 sation scale variation.

This technique was pioneered by the fastNLO project [85]22 to facilitate the inclusion of time consuming NLO jet cross 523 section predictions into PDF fits. The APPLGRID [86] project 524 developed an alternative method and, in addition to jets, ex- 525 tended its applicability to other scattering processes, such 526 as DY and heavy quark pair production in association with 527 boson production. The packages differ in their interpolation 528 and optimisation strategies, but both of them construct ta- 529 bles with grids for each bin of an observable in two steps: 530 in the first step, the accessible phase space in the parton mo- 531 mentum fractions x and the renormalisation and factorisa- 532 tion scales μ_R and μ_F is explored in order to optimise the table size. In the second step the grid is filled for the requested observables. Higher-order cross sections can then be obtained very efficiently from the pre-produced grids while varying externally provided PDF sets, μ_R and μ_F , or the strong coupling $\alpha_s(\mu_R)$. This approach can in principle be extended to arbitrary processes. This requires an interface between the higher-order theory programs and the fast interpolation frameworks. Currently available processes for each package are as follows:

The fastNLO project [85] has been interfaced to the NLOJet++ program [72] for the calculation of jet production in DIS [87] as well as 2- and 3-jet production in hadron-hadron collisions at NLO [73, 88]. Threshold corrections at 2-loop order, which approximate the NNLO for the inclusive jet cross section, have also been included into the framework [89] following Ref. [90]. The latest version of the fastNLO convolution program [91] allows for the creation of tables in which renormalisation and factorisation scales can be varied as a function of two pre-defined observables, e.g. jet transverse momentum p_{\perp} and Q for DIS. Recently, the differential calculation of top-pair production in hadron collisions at approximate NNLO [82] has been interfaced to fastNLO [84]. The fastNLO code is available online [92]. Jet cross section grids computed for the kinematics of various experiments can be downloaded from this site.

The fastNLO libraries and tables with theory predictions for comparison to particular cross section measure- 534 When performing a QCD analysis to determine PDFs there PDF evolution from the QCDNUM code.

are generated with the customised versions of the MCFM parton level DY generator [62–64]. Variation of the renormalisation and factorisation scales is possible a posteriori, when calculating theory predictions with the APPL-GRID tables, and independent variation of α_S is also allowed. For higher-order predictions, the k-factors technique can also be applied within the APPLGRID framework.

As an example, the HERAFitter interface to APPLGRID was used by the ATLAS [94] and CMS [95] collaborations to extract the strange quark distribution of the proton. The ATLAS strange PDF extracted employing these techniques is displayed in Fig. 4 together with a comparison to the global PDF sets CT10 [17] and NNPDF2.1 [18] (taken from [94]).

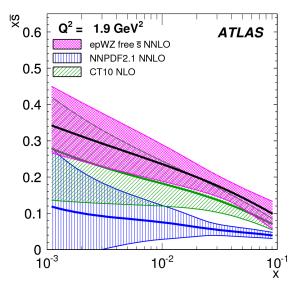


Fig. 4 The strange antiquark distribution versus x for the ATLAS epWZ free \$\bar{s}\$ NNLO fit [94] (magenta band) compared to predictions from NNPDF2.1 (blue hatched) and CT10 (green hatched) at $Q^2 = 1.9 \text{ GeV}^2$. The ATLAS fit was performed using a k-factor approach for NNLO corrections.

533 5 Fit Methodology

ments are included into the HERAFitter package. For 535 are various assumptions and choices to be made concerning, the HERAFitter implementation, the evaluation of the 536 for example, the functional form of the input parametrisastrong coupling constant is done consistently with the 537 tion, the treatment of heavy quarks and their mass values, al-538 ternative theoretical calculations, alternative representations of the fit χ^2 and for different ways of treating correlated sys-In the APPLGRID package [86, 93], in addition to jet 540 tematic uncertainties. It is useful to discriminate or quantify cross sections for $pp(p\bar{p})$ and DIS processes, calcula- 541 the effect of a chosen ansatz within a common framework tions of DY production are also implemented. The grids 542 and HERAFitter is optimally designed for such tests. The

tion of state-of-the-art techniques, either related to the inclu- 576 and sea distributions. Polynomials with argument $\log(x)$ are sion of a new theoretical calculation, or of new approaches 577 considered for better modelling the low-x asymptotic beto treat data and their uncertainties.

fit methodology in HERAFitter. In addition, as an alterna- 580 resulting parametric form reads tive approach to a complete QCD fit, the Bayesian reweighting method, which is also available in HERAFitter, is described.

5.1 Functional Forms for PDF Parametrisation

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tional forms and flavour decompositions:

Standard Polynomials: The standard polynomial form is the most commonly used. A polynomial functional form is used to parametrise the x-dependence of the PDFs, where index jdenotes each parametrised PDF flavour:

$$xf_i(x) = A_i x^{B_i} (1-x)^{C_i} P_i(x).$$
 (12)

The parametrised PDFs are the valence distributions xu_y and xd_v , the gluon distribution xg, and the u-type and d-type sea, $x\bar{U}$, $x\bar{D}$, where $x\bar{U} = x\bar{u}$, $x\bar{D} = x\bar{d} + x\bar{s}$ at the starting scale, which is chosen below the charm mass threshold. The form of polynomials $P_i(x)$ can be varied. The form $(1 + \varepsilon_i \sqrt{x} +$ $D_i x + E_i x^2$) is used for the HERAPDF [21] with additional constraints relating to the flavour decomposition of the light sea. This parametrisation is termed HERAPDF-style. The polynomial can also be parametrised in the CTEQ-style, where $P_i(x)$ takes the form $e^{a_3x}(1+e^{a_4}x+e^{a_5}x^2)$ and, in contrast to the HERAPDF-style, this is positive by construction. QCD number and momentum sum rules are used to determine the normalisations A for the valence and gluon distributions, and the sum-rule integrals are solved analytically.

Bi-Log-Normal Distributions: This parametrisation is motivated by multi-particle statistics and has the following functional form:

$$xf_j(x) = a_j x^{p_j - b_j \log(x)} (1 - x)^{q_j - d_j \log(1 - x)}.$$
 (13)

sum rules.

methodology employed by HERAFitter relies on a flexible 574 Chebyshev Polynomials: A flexible parametrisation based and modular framework that allows for independent integra- 575 on the Chebyshev polynomials can be employed for the gluon 578 haviour of those PDFs. The polynomials are multiplied by In this section we describe the available options for the 579 a factor of (1-x) to ensure that they vanish as $x \to 1$. The

$$xg(x) = A_g(1-x) \sum_{i=0}^{N_g-1} A_{g_i} T_i \left(-\frac{2\log x - \log x_{\min}}{\log x_{\min}} \right), \quad (14)$$

$$xS(x) = (1-x) \sum_{i=0}^{N_S-1} A_{S_i} T_i \left(-\frac{2\log x - \log x_{\min}}{\log x_{\min}} \right), \quad (15)$$

where T_i are first-type Chebyshev polynomials of order i. The normalisation factor A_g is derived from the momentum The PDFs can be parametrised using several predefined func- sum rule analytically. Values of $N_{g,S}$ to 15 are allowed, however the fit quality is already similar to that of the standardpolynomial parametrisation from $N_{g,S} \ge 5$ and has a similar number of free parameters. Fig. 5 (taken from [96]) shows ⁵⁸⁷ a comparison of the gluon distribution obtained with the parametrisation Eqs. 14, 15 to the standard-polynomial one, for $N_{g,S} = 9$.

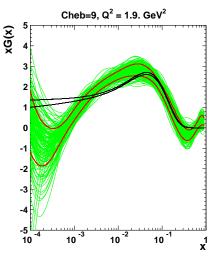
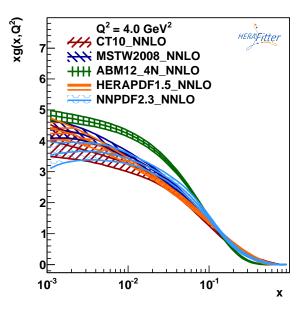


Fig. 5 The gluon density is shown at the starting scale $Q^2 = 1.9 \text{ GeV}^2$. The black lines correspond to the uncertainty band of the gluon distribution using a standard parametrisation and it is compared to the case of the Chebyshev parametrisation [96]. The uncertainty band for the latter case is estimated using the Monte Carlo technique (see Sec. 5.3) with the green lines denoting fits to data replica. Red lines indicate the standard deviation about the mean value of these replicas.

(13) 590 External PDFs: HERAFitter also provides the possibility to access external PDF sets, which can be used to compute 592 theoretical predictions for the cross sections for all the pro-This function can be regarded as a generalisation of the stan- 593 cesses available in HERAFitter. This is possible via an indard polynomial form described above, however, numerical 594 terface to LHAPDF [33, 34] providing access to the global integration of Eq. 13 is required in order to impose the QCD 595 PDF sets. HERAFitter also allows one to evolve PDFs from 596 LHAPDF using QCDNUM. Fig. 6 illustrates a comparison of various gluon PDFs accessed from LHAPDF as produced with the drawing tools available in HERAFitter.



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Fig. 6 The gluon PDF as extracted by various groups at the scale of $Q^2 = 4 \text{ GeV}^2$, plotted using the drawing tools from HERAFitter.

5.2 Representation of χ^2

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The PDF parameters are determined in HERAFitter by minimisation of a χ^2 function taking into account correlated and uncorrelated measurement uncertainties. There are various forms of χ^2 , e.g. using a covariance matrix or providing nuisance parameters to encode the dependence of each correlated systematic uncertainty for each measured data point. The options available in HERAFitter are the following:

Covariance Matrix Representation: For a data point μ_i with a corresponding theory prediction m_i , the χ^2 function can be expressed in the following form:

$$\chi^{2}(m) = \sum_{i,k} (m_{i} - \mu_{i}) C_{ik}^{-1}(m_{k} - \mu_{k}), \tag{16}$$

where the experimental uncertainties are given as a co- $_{650}$ variance matrix C_{ik} for measurements in bins i and k. The covariance matrix C_{ik} is given by a sum of statistical, un- $_{652}$ $_{652}$

$$C_{ik} = C_{ik}^{stat} + C_{ik}^{uncor} + C_{ik}^{sys}. (17)$$

Using this representation one cannot distinguish the effect of each source of systematic uncertainty.

Nuisance Parameter Representation: In this case, the χ^2 is expressed as

$$\chi^{2}(m,b) = \sum_{i} \frac{\left[\mu_{i} - m_{i} \left(1 - \sum_{j} \gamma_{j}^{i} b_{j}\right)\right]^{2}}{\delta_{i,\text{unc}}^{2} m_{i}^{2} + \delta_{i,\text{stat}}^{2} \mu_{i} m_{i} \left(1 - \sum_{j} \gamma_{j}^{i} b_{j}\right)} + \sum_{j} b_{j}^{2},$$
(18)

where, $\delta_{i,\text{stat}}$ and $\delta_{i,\text{unc}}$ are relative statistical and uncorrelated systematic uncertainties of the measurement i. Further, γ^i_j quantifies the sensitivity of the measurement to the correlated systematic source j. The function χ^2 depends on the set of systematic nuisance parameters b_j . This definition of the χ^2 function assumes that systematic uncertainties are proportional to the central prediction values (multiplicative uncertainties, $m_i(1-\sum_j \gamma^i_j b_j)$), whereas the statistical uncertainties scale with the square root of the expected number of events. However, additive treatment of uncertainties is also possible in HERA-Fitter.

During the χ^2 minimisation, the nuisance parameters b_j and the PDFs are determined, such that the effect of different sources of systematic uncertainties can be distinguished.

Mixed Form Representation: In some cases, the statistical and systematic uncertainties of experimental data are provided in different forms. For example, the correlated experimental systematic uncertainties are available as nuisance parameters, but the bin-to-bin statistical correlations are given in the form of a covariance matrix. HERA-Fitter offers the possibility to include such mixed forms of information.

Any source of measured systematic uncertainty can be treated as additive or multiplicative, as described above. The statistical uncertainties can be included as additive or following the Poisson statistics. Minimisation with respect to nuisance parameters is performed analytically, however, for more detailed studies of correlations individual nuisance parameters can be included into the MINUIT minimisation.

5.3 Treatment of the Experimental Uncertainties

Three distinct methods for propagating experimental uncertainties to PDFs are implemented in HERAFitter and reviewed here: the Hessian, Offset, and Monte Carlo method.

Hessian (Eigenvector) method: The PDF uncertainties reflecting the data experimental uncertainties are estimated by examining the shape of the χ^2 function in the neighbourhood of the minimum [97]. Following the approach of Ref. [97], the Hessian matrix is defined by the second derivatives of χ^2 on the fitted PDF parameters. The matrix is diagonalised and the Hessian eigenvectors are

computed. Due to orthogonality these vectors correspond to independent sources of uncertainty in the obtained PDFs.

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Offset method: The Offset method [98] uses the χ^2 function for the central fit, but only uncorrelated uncertainties are taken into account. The goodness of the fit can no longer be judged from the χ^2 since correlated uncertainties are ignored. The correlated uncertainties are propagated into the PDF uncertainties by performing variants of the fit with the experimental data varied by $\pm 1\sigma$ from the central value for each systematic source. The resulting deviations of the PDF parameters from the ones obtained in the central fit are statistically independent, and they can be combined in quadrature to derive a total PDF systematic uncertainty.

The uncertainties estimated by the offset method are generally larger than those from the Hessian method.

Monte Carlo method: The Monte Carlo (MC) technique [99, 100] can also be used to determine PDF uncertainties. The uncertainties are estimated using pseudo-data replicas (typically > 100) randomly generated from the measurement central values and their systematic and statistical uncertainties taking into account all point-to-point correlations. The QCD fit is performed for each replica and the PDF central values and their experimental uncertainties are estimated from the distribution of the PDF parameters obtained in these fits, by taking the mean values and standard deviations over the replicas.

The MC method has been checked against the standard error estimation of the PDF uncertainties obtained by the Hessian method. A good agreement was found between the methods provided that Gaussian distributions of statistical and systematic uncertainties are assumed in the MC approach [32]. A comparison is illustrated in Fig. 7. Similar findings were reported by the MSTW 705 The results of a QCD fit depend not only on the input data global analysis [101].

Since the MC method requires large number of replicas, 707 the eigenvector representation is a more convenient way 708 to store the PDF uncertainties. It is possible to transform $\,^{709}$ bative orders [103].

The nuisance parameter representation of χ^2 in Eq. 18 is derived assuming symmetric experimental errors, however, 715 5.5 Bayesian Reweighting Techniques the published systematic uncertainties are often asymmetric. HERAFitter provides the possibility to use asymmetric 716 As an alternative to performing a full QCD fit, HERAFitter systematic uncertainties. The implementation relies on the 717 allows the user to assess the impact of including new data assumption that asymmetric uncertainties can be described 718 in an existing fit using the Bayesian Reweighting technique.

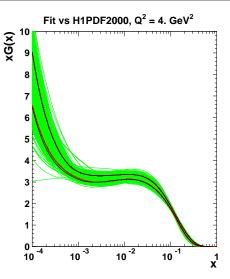


Fig. 7 Comparison between the standard error calculations as employed by the Hessian approach (black lines) and the MC approach (with more than 100 replicas) assuming Gaussian distribution for uncertainty distributions, shown here for each replica (green lines) together with the evaluated standard deviation (red lines) [32]. The black and red lines in the figure are superimposed because agreement of the methods is so good that it is hard to distinguish them.

modified as follows

$$\gamma_i^i \to \omega_i^i b_j + \gamma_i^i,$$
 (19)

where the coefficients ω_i^i , γ_i^i are defined from the maximum and minimum shifts of the cross sections due to a variation of the systematic uncertainty j, S_{ij}^{\pm} ,

$$\omega_{j}^{i} = \frac{1}{2} \left(S_{ij}^{+} + S_{ij}^{-} \right), \qquad \gamma_{j}^{j} = \frac{1}{2} \left(S_{ij}^{+} - S_{ij}^{-} \right).$$
 (20)

⁷⁰⁴ 5.4 Treatment of the Theoretical Input Parameters

but also on the input parameters used in the theoretical calculations. Nowadays, PDF groups address the impact of the choices of theoretical parameters by providing alternative PDFs with different choices of the mass of the charm quarks, MC to eigenvector representation as shown by [102]. 710 m_c , mass of the bottom quarks, m_b , and the value of $\alpha_s(m_Z)$. Tools to perform this transformation are provided with 711 Other important aspects are the choice of the functional form HERAFitter and were recently employed for the repre- 712 for the PDFs at the starting scale and the value of the starting sentation of correlated sets of PDFs at different pertur- 713 scale itself. HERAFitter provides the possibility of different user choices of all these inputs.

by a parabolic function. The nuisance parameter in Eq. 18 is 719 The method provides a fast estimate of the impact of new

PDF sets delivered in the form of MC replicas by [99] and 736 the reweighting/unweighting procedure. No extra informafurther developed by the NNPDF Collaboration [104, 105]. 737 tion is gained by producing a final unweighted set that has a More recently, a method to perform Bayesian Reweighting 738 number of replicas (significantly) larger than N_{eff}. If N_{eff} is studies starting from PDF fits for which uncertainties are 739 much smaller than the original number of replicas the new provided in the eigenvector representation has been also de- 740 data have great impact, however, it is unreliable to use the veloped [101]. The latter is based on generating replica sets 741 new reweighted set. In this case, instead, a full refit should by introducing Gaussian fluctuations on the central PDF set 742 be performed. with a variance determined by the PDF uncertainty given by the eigenvectors. Both reweighting methods are implemented in HERAFitter.

The Bayesian Reweighting technique relies on the fact that MC replicas of a PDF set give a representation of the probability distribution in the space of PDFs. In particular, the PDFs are represented as ensembles of N_{rep} equiprobable (i.e. having weights equal to unity) replicas, $\{f\}$. The central value for a given observable, $\mathcal{O}(\{f\})$, is computed as the average of the predictions obtained from the ensemble as

$$\langle \mathcal{O}(\{f\}) \rangle = \frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} \mathcal{O}(f^k),$$
 (21)

and the uncertainty as the standard deviation of the sample.

Upon inclusion of new data the prior probability distri- 753 6.1 Dipole Models bution, given by theoriginal PDF set, is modified according to Bayes Theorem such that the weight of each replica, w_k , is updated according to

$$w_k = \frac{(\chi_k^2)^{\frac{1}{2}(N_{\text{data}} - 1)} e^{-\frac{1}{2}\chi_k^2}}{\frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} (\chi_k^2)^{\frac{1}{2}(N_{\text{data}} - 1)} e^{-\frac{1}{2}\chi_k^2}},$$
(22)

the χ^2 of the new data obtained using the k-th PDF replica. 762 interaction are embedded in a dipole scattering amplitude. Given a PDF set and a corresponding set of weights, which 763 describes the impact of the inclusion of new data, the pre- 764 of the dipole-proton cross section, are implemented in HERAdiction for a given observable after inclusion of the new data 765 Fitter: the Golec-Biernat-Wüsthoff (GBW) dipole saturacan be computed as the weighted average,

$$\langle \mathcal{O}(\{f\}) \rangle = \frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} w_k \mathcal{O}(f^k). \tag{23}$$

To simplify the use of a reweighted set, an unweighted set (i.e. a set of equiprobable replicas which incorporates the information contained in the weights) is generated according to the unweighting procedure described in [104]. The number of effective replicas of a reweighted set is measured by its Shannon Entropy [105]

$$N_{\text{eff}} \equiv \exp\left\{\frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} w_k \ln(N_{\text{rep}}/w_k)\right\},\tag{24}$$

set containing the same amount of information. This num- 775 called the saturation radius. The cross-section normalisaber of effective replicas, $N_{\rm eff}$, gives an indicative measure of 776 tion σ_0 , x_0 , and λ are parameters of the model fitted to the

720 data on PDFs. Bayesian Reweighting was first proposed for 735 the optimal size of an unweighted replica set produced with

6 Alternatives to DGLAP Formalism

744 QCD calculations based on the DGLAP [11-15] evolution ⁷⁴⁵ equations are very successful in describing all relevant hard scattering data in the perturbative region $Q^2 \gtrsim {
m few} {
m GeV}^2$. At small-x and small- Q^2 DGLAP dynamics may be modi-748 fied by saturation and other (non-perturbative) higher-twist effects. Different approaches alternative to the DGLAP for-750 malism can be used to analyse DIS data in HERAFitter. 751 These include several dipole models and the use of trans-(21) rs2 verse momentum dependent, or unintegrated PDFs (uPDFs).

The dipole picture provides an alternative approach to protonvirtual photon scattering at low x which can be applied to both inclusive and diffractive processes. In this approach, the virtual photon fluctuates into a $q\bar{q}$ (or $q\bar{q}g$) dipole which interacts with the proton [106, 107]. The dipoles can be con-759 sidered as quasi-stable quantum mechanical states, which where $N_{\rm data}$ is the number of new data points, k denotes the 760 have very long life time $\propto 1/m_p x$ and a size which is not specific replica for which the weight is calculated and χ_k^2 is 761 changed by scattering with the proton. The dynamics of the

> Several dipole models, which assume different behaviours 766 tion model [28], a modified GBW model which takes into account the effects of DGLAP evolution, termed the Bartels-768 Golec-Kowalski (BGK) dipole model [30] and the colour glass condensate approach to the high parton density regime, named the Iancu-Itakura-Munier (IIM) dipole model [29].

GBW model: In the GBW model the dipole-proton cross section $\sigma_{\rm dip}$ is given by

$$\sigma_{\text{dip}}(x, r^2) = \sigma_0 \left(1 - \exp\left[-\frac{r^2}{4R_0^2(x)} \right] \right), \tag{25}$$

where r corresponds to the transverse separation between (24) $_{772}^{771}$ the quark and the antiquark, and R_0^2 is an x-dependent scale parameter which represents the spacing of the gluons in the which corresponds to the size of a refitted equiprobable replica₇₄ proton. R_0^2 takes the form, $R_0^2(x) = (x/x_0)^{\lambda} 1/\text{GeV}^2$, and is 777 DIS data. This model gives exact Bjorken scaling when the 816 dipole size r is small.

of the latter. The gluon distribution, parametrised at some 822 14, 15] according to the CCFM evolution equation [23-26]. starting scale by Eq. 12, is evolved to larger scales using 823 DGLAP evolution.

tribution to the total proton momentum is 5% to 15% for xfrom 0.0001 to 0.01 [108]. The inclusive HERA measurements have a precision which is better than 2%. Therefore, 829 CCFM Grid Techniques: The CCFM evolution cannot be contribution of the valence quarks

IIM model: The IIM model assumes an expression for the 833 dipole cross section which is based on the Balitsky-Kovchegov₃₄ 132], the kernel $\tilde{\mathscr{A}}(x'',k_t,p)$ is determined from the MC soequation [109]. The explicit formula for σ_{dip} can be found 835 lution of the CCFM evolution equation, and then folded with in [29]. The alternative scale parameter \tilde{R} , x_0 and λ are fitted 336 a non-perturbative starting distribution $\mathcal{A}_0(x)$ parameters of the model.

6.2 Transverse Momentum Dependent PDFs

QCD calculations of multiple-scale processes and complex 837 final-states can necessitate the use of transverse-momentum 838 dependent (TMD) [7], or unintegrated parton distribution and parton decay functions [110-118]. TMD factorisation cesses, like heavy flavour, vector boson and Higgs production.

123] the DIS cross section can be written as a convolution 847 in both longitudinal and transverse momenta of the TMD 848 parton distribution function $\mathscr{A}\left(x,k_{t},\mu_{F}^{2}\right)$ with the off-shell ⁸⁴⁹ equation is applied: parton scattering matrix elements as follows

$$\sigma_j(x,Q^2) = \int_{-\pi}^1 dz \int d^2k_t \ \hat{\sigma}_j(x,Q^2,z,k_t) \ \mathscr{A}(z,k_t,\mu_F^2),$$
 (26)

where the DIS cross sections $\sigma_i(j=2,L)$ are related to the structure functions F_2 and F_L by $\sigma_i = 4\pi^2 F_i/Q^2$, and the hard-scattering kernels $\hat{\sigma}_i$ of Eq. 26 are k_t -dependent.

The factorisation formula in Eq. 26 allows resummation of logarithmically enhanced small-x contributions to all orders in perturbation theory, both in the hard scattering coefficients and in the parton evolution, fully taking into account torisation scheme [124, 125].

Phenomenological applications of this approach require matching of small-x contributions with finite-x contributions. 818 To this end, the evolution of the transverse momentum de-BGK model: The BGK model is a modification of the GBW 819 pendent gluon density A is obtained by combining the remodel assuming that the spacing R_0 is inverse to the gluon summation of small-x logarithmic corrections [126–128] with distribution and taking into account the DGLAP evolution 821 medium-x and large-x contributions to parton splitting [11,

The cross section σ_i , (j = 2, L) is calculated in a FFN scheme, using the boson-gluon fusion process ($\gamma^* g^* \to q\bar{q}$). The masses of the quarks are explicitly included as param-BGK model with valence quarks: The dipole models are 826 eters of the model. In addition to $\gamma^*g^* o qar q$, the contribuvalid in the low-x region only, where the valence quark con-828 CCFM evolution of valence quarks [129–131].

HERAFitter provides the option of taking into account the 830 written easily in an analytic closed form. For this reason, a MC method is employed, which is, however, time-consuming and thus cannot be used directly in a fit program.

Following the convolution method introduced in [131,

$$x\mathscr{A}(x,k_t,p) = x \int dx' \int dx'' \mathscr{A}_0(x') \widetilde{\mathscr{A}}(x'',k_t,p) \,\delta(x'x''-x)$$
$$= \int dx' \mathscr{A}_0(x') \frac{x}{x'} \,\widetilde{\mathscr{A}}\left(\frac{x}{x'},k_t,p\right), \tag{27}$$

where k_t denotes the transverse momentum of the propagator gluon and p is the evolution variable.

The kernel $\tilde{\mathcal{A}}$ incorporates all of the dynamics of the $_{\text{840}}$ evolution. It is defined on a grid of $50\otimes50\otimes50$ bins in has been proven recently [7] for inclusive DIS. TMD fac- 841 x, k_t, p . The binning in the grid is logarithmic, except for torisation has also been proven in the high-energy (small-x) 842 the longitudinal variable x for which 40 bins in logarithmic limit [119-121] for particular hadron-hadron scattering pro- 843 spacing below 0.1, and 10 bins in linear spacing above 0.1 are used.

Calculation of the cross section according to Eq. 26 in-In the framework of high-energy factorisation [119, 122, 846 volves a time-consuming multidimensional MC integration, which suffers from numerical fluctuations. This cannot be employed directly in a fit procedure. Instead the following

$$\sigma(x,Q^2) = \int_x^1 dx_g \mathscr{A}(x_g, k_t, p) \hat{\sigma}(x, x_g, Q^2)$$
$$= \int_x^1 dx' \mathscr{A}_0(x') \tilde{\sigma}(x/x', Q^2), \tag{28}$$

where first $\tilde{\sigma}(x',Q^2)$ is calculated numerically with a MC integration on a grid in x for the values of Q^2 used in the 852 fit. Then the last step in Eq. 28 is performed with a fast numerical Gauss integration, which can be used directly in the

the dependence on the factorisation scale μ_F and on the fac- 855 Functional Forms for TMD parametrisation: For the starting distribution \mathcal{A}_0 , at the starting scale Q_0^2 , the following form is used:

$$x\mathscr{A}_0(x,k_t) = Nx^{-B}(1-x)^C \left(1 - Dx + E\sqrt{x}\right)$$
$$\times \exp\left[-k_t^2/\sigma^2\right], \tag{29}$$

where $\sigma^2 = Q_0^2/2$ and N, B, C, D, E are free parameters. Valence quarks are treated using the method of Ref. [129] as described in Ref. [131] with a starting distribution taken from any collinear PDF and imposition of the flavour sum rule at every scale p.

The TMD parton densities can be plotted either with HERA-Fitter tools or with TMDplotter [35].

7 HERAFitter Code Organisation

when invoking APPLGRID. Drawing tools built into HERA- 914 the LHC can be found in [143]. Fitter provide a qualitative and quantitative assessment of 915 the measurement, pulls are provided in units of standard de- 922 liders as demonstrated by QCD studies at the LHeC [147]. viations. The pulls are also illustrated in Fig. 8.

In HERAFitter there are also available cache options for fast retrieval, fast evolution kernels, and the OpenMP (Open $_{_{923}}$ 9 Summary Multi-Processing) interface which allows parallel applications of the GM-VFNS theory predictions in DIS.

8 Applications of HERAFitter

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The HERAFitter program has been used in a number of experimental and theoretical analyses. This list includes several LHC analyses of SM processes, namely inclusive Drell-Yan and Wand Z production [94, 95, 133–135], inclusive

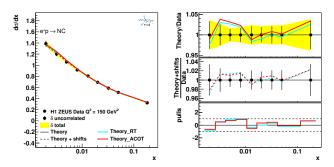


Fig. 8 An illustration of the consistency of HERA measurements [21] and the theory predictions, obtained in HERAFitter with the default drawing tool.

jet production [136], and inclusive photon production [137]. HERAFitter is an open source code under the GNU general 500 The results of QCD analyses using HERAFitter were also public licence. It can be downloaded from a dedicated web- 901 published by HERA experiments for inclusive [21, 138] and page [10] together with its supporting documentation and 902 heavy flavour production measurements [139, 140]. The folfast grid theory files (described in Sec. 4) associated with 903 lowing phenomenological studies have been performed with data files. The source code contains all the relevant infor- 904 HERAFitter: a determination of the transverse momentum mation to perform QCD fits with HERA DIS data as a de- 905 dependent gluon distribution using precision HERA data [131], fault set. The execution time depends on the fitting options 906 an analysis of HERA data within a dipole model [141], the and varies from 10 minutes (using "FAST" techniques as 907 study of the low-x uncertainties in PDFs determined from described in Sec. 4) to several hours when full uncertainties 508 the HERA data using different parametrisations [96] and the are estimated. The HERAFitter code is a combination of 909 impact of QED radiative corrections on PDFs [142]. A re-C++ and Fortran 77 libraries with minimal dependencies, 910 cent study based on a set of PDFs determined with HERAi.e. for the default fitting options no external dependencies 911 Fitter and addressing the correlated uncertainties between are required except the QCDNUM evolution program [22]. The 912 different orders has been published in [103]. An application ROOT libraries are only required for the drawing tools and 913 of the TMDs obtained with HERAFitter W production at

The HERAFitter framework has been used to produce the results. Fig. 8 shows an illustration of a comparison be- 916 PDF grids from QCD analyses performed at HERA [21, tween the inclusive NC data from HERA I with the predic- 917 144] and at the LHC [145], using measurements from ATtions based on HERAPDF1.0 PDFs. The consistency of the 918 LAS [94, 136]. These PDFs can be used to study predictions measurements and the theory can be expressed by pulls, de- 919 for SM or beyond SM processes. Furthermore, HERAFitter fined as the difference between data and theory divided by 920 provides the possibility to perform various benchmarking the uncorrelated error of the data. In each kinematic bin of get exercises [146] and impact studies for possible future col-

924 HERAFitter is the first open-source code designed for stud-925 ies of the structure of the proton. It provides a unique and flexible framework with a wide variety of QCD tools to facilitate analyses of the experimental data and theoretical calculations.

The HERAFitter code, in version 1.1.0, has sufficient options to reproduce the different theoretical choices made in MSTW, CTEQ and ABM fits. This will potentially make 932 it a valuable tool for benchmarking and understanding dif-933 ferences between PDF fits. Such a study would however 934 need to consider a range of further questions, such as the

 $^{^{1}\}mathrm{Default}$ settings in HERAFitter are tuned to reproduce the central HERAPDF1.0 set.

choices of data sets, treatments of uncertainties, input pa- 986 rameter values, χ^2 definitions, etc.

The further progress of HERAFitter is driven by the latest 988 QCD advances in theoretical calculations and in the precision of experimental data.

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