HERAFitter

Open Source QCD Fit Project

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Abstract HERAFitter [1] is an open-source package which 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).

Measurements of lepton-proton deep inelastic scattering in g and of proton-proton (proton-antiproton) collisions at hadron colliders are included in the HERAFitter package, and are used to probe and constrain the partonic content of the proton.

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The PDFs are determined by using the factorisation prop- 66 1 Introduction erties of the hadron cross sections in which short-distance perturbatively calculable parton scattering cross sections and the non-perturbative universal PDFs, are factorised.

ment for QCD analyses using a variety of theoretical calculations and methodological options. A broad range of options for the treatment of the experimental uncertainties is also provided. The general structure of HERAFitter together with the choices of options available within it are described in this paper.

22 Keywords PDFs · QCD · Fit · proton structure

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The recent discovery of the Higgs boson [2, 3] and the ex-68 tensive searches for signals of new physics in LHC proton-The HERAFitter platform provides a common environ- 69 proton collisions demand high-precision calculations and com-70 putations to test the validity of the Standard Model (SM) and 71 factorisation in Quantum Chromodynamics (QCD). Using 72 collinear factorisation, hadron inclusive cross sections may 73 be written as

$$\sigma(\alpha_{\rm s}(\mu_{\rm R}^2), \mu_{\rm R}^2, \mu_{\rm F}^2) = \sum_{a,b} \int_0^1 dx_1 \, dx_2 f_a(x_1, \mu_{\rm F}^2) f_b(x_2, \mu_{\rm F}^2)$$

$$\times \hat{\sigma}^{ab}(x_1, x_2; \alpha_{\rm s}(\mu_{\rm R}^2), \mu_{\rm R}^2, \mu_{\rm F}^2), \tag{1}$$

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 $\hat{\sigma}^{ab}$. At Leading-Order (LO), the PDFs represent the probability of finding a specific parton a(b)in the first (second) proton carrying a fraction x_1 (x_2) of its momentum. The indices a and b in the Eq. 1 indicate the 80 various kinds of partons, i.e. gluons, quarks and antiquarks 81 of different flavours, that are considered as the constituents of the proton. The PDFs depend on factorisation scale, $\mu_{\rm F}$, while the parton cross sections depend on the strong cou- $\alpha_{\rm s}$ pling, $\alpha_{\rm s}$, and the factorisation and renormalisation scales, ₈₅ $\mu_{\rm F}$ and $\mu_{\rm R}$. The parton cross sections $\hat{\sigma}^{ab}$ are calculable in pQCD whereas PDFs are non-perturbative and are thus con-87 strained by global fits to a variety of experimental data. The 88 assumption that PDFs are universal, within a particular fac-89 torisation scheme [4–8], is crucial to this procedure. Recent 90 review articles on PDFs can be found in Refs. [9, 10].

Accurate determination of PDFs as a function of x re-92 quires large amount of hard-process experimental data, cov-93 ering a wide kinematic region with sensitivity to different ya kinds of partons. Measurements of the inclusive Neutral Cur-95 rent (NC) and Charge Current (CC) Deep Inelastic Scatter-96 ing (DIS) at the ep collider HERA provide crucial informay tion for determining the PDFs. Hard processes in pp and $p\bar{p}$ 98 collisions at the LHC and the Tevatron, respectively, provide 99 complementary information to the DIS measurements. The 10 100 PDFs are determined from χ^2 fits of the theoretical predictions to the data [11–15]. The rapid flow of new data from 102 the LHC experiments and the corresponding theoretical developments, which are providing predictions for more com-104 plex processes at increasingly higher orders, has motivated 12 105 the development of a tool to combine them together in a fast, 13 106 efficient, open-source platform.

This paper describes the open-source QCD fit platform 108 HERAFitter which includes a set of tools designed to facilitate comprehensive global QCD analyses of pp, $p\bar{p}$ and epscattering data. It has been developed for the determination $_{14}$ $_{111}$ of PDFs and the extraction of fundamental QCD parameters 14 112 such as the heavy quark masses and the strong coupling con-14 113 stant. It also provides a common platform for comparison of different theoretical approaches. Furthermore, it can be used for direct tests of the impact of new experimental data on the PDFs and on the SM parameters.

This paper is organised as follows. The structure and overview of HERAFitter are presented in section 2. In section 3 the various processes available in HERAFitter and the corresponding theoretical calculations, performed within the framework of collinear factorisation and the DGLAP [16– 20] formalism, are discussed. In section 4 tools for fast calculations of the theoretical predictions used in HERAFitter are presented. In section 5 the methodology of determining PDFs through fits based on various χ^2 definitions is explained. In particular, different treatments of correlated experimental uncertainties are presented. Alternative approaches to the DGLAP formalism are presented in section 6. The HERAFitter code organisation is discussed in section 7, specific applications of the package are given in section 8 and a summary is presented in section 9.

2 The HERAFitter Structure

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In this section the functionality of HERAFitter is described. A block diagram in Fig 1 gives a schematic view of the HERAFitter functionality which can be divided into four main blocks:

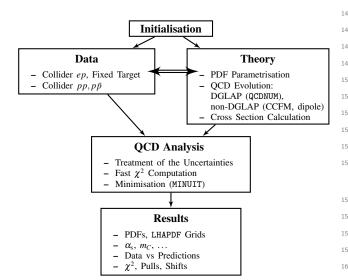


Fig. 1 Schematic structure of the HERAFitter program.

Data: Different measurements from various processes are implemented in the HERAFitter package including the full ties. HERA inclusive scattering data are sensitive to quark PDFs and to gluon PDFs through scaling violations and the longitudinal structure function F_L . These data are the back- 169 QCD Analysis: The PDFs are determined by a least square

Experimental Data	Process	Reaction	Theory calculations, schemes
HERA, Fixed Target	DIS NC	$ep \rightarrow eX$	TR', ACOT, ZM (QCDNUM), FFN (OPENQCDRAD, QCDNUM), TMD (UPDFevolv)
HERA	DIS CC	$ep ightarrow v_e X$	ACOT, ZM (QCDNUM), FFN (OPENQCDRAD)
	DIS jets	$ep \rightarrow e \text{ jets}X$	NLOJet++ (fastNLO)
	DIS heavy quarks	$egin{array}{c} ep ightarrow ecar{c}X, \ ep ightarrow ebar{b}X \end{array}$	ZM (QCDNUM), TR', ACOT, 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
	single top	$pp(\bar{p}) \rightarrow tlvX, \\ pp(\bar{p}) \rightarrow tX, \\ pp(\bar{p}) \rightarrow tWX$	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.

PDF groups [11–15]. They can be supplemented by HERA measurements sensitive to heavy quarks and by HERA jet measurements, which have sensitivity to the gluon PDF. However, the kinematic range of HERA data mostly covers low and medium x ranges. Improvements in precision of PDFs require additional constraints on the gluon and quark distributions at high-x, better understanding of heavy quark distributions and decomposition of the light-quark sea. For these purposes, measurements from the fixed-target experiments, 153 the Tevatron and the LHC can be used. The processes that are currently available in HERAFitter framework are listed 155 in Tab. 1.

156 Theory: The PDFs are parametrised at a starting input scale, Q_0^2 , by a chosen functional form with a set of free parameters **p**. These PDFs are evolved to the scale of the measurement Q^2 , $Q^2 > Q_0^2$. The evolution uses the DGLAP formalism [16-20] (as implemented in QCDNUM [21]) by default, however CCFM evolution [22-25] is also available (as implemented in uPDFevolv [26]). The prediction of the cross section for a particular process is obtained, assuming factorisation, by the convolution of the evolved PDFs and the appropriate hard-process parton scattering cross section. Appropriate theory calculations are listed in Tab. 1. Alternainformation on their uncorrelated and correlated uncertain- 167 tively, predictions using dipole models [27-29] can also be

bone of any proton PDF extraction, and are used by all global 170 fit, minimising a χ^2 function, constructed using the input

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data and theory predictions, with the MINUIT [30] program. In HERAFitter various choices are available to account for the experimental uncertainties. Correlated experimental uncertainties can be accounted for using a nuisance parameter method or a covariance matrix method as described in sec- where the functions P_{ab} are the evolution kernels or splitting tion 5.2. Different statistical assumptions for the distribu- 198 functions, which represent the probability of finding parton tions of the systematic uncertainties, like Gaussian or Log-Normal [31] can also be studied (see section 5.3).

Results: The resulting PDFs are provided in a format ready 202 mined by the DGLAP equations. The PDFs are then used to to be used by the LHAPDF library [32, 33] or by TMDlib [34]. 203 calculate cross sections for various different processes. Al-HERAFitter drawing tools can be used to display the PDFs 204 ternative approaches to DGLAP evolution, valid in different with their uncertainties at a chosen scale. As an example, the 205 kinematic regimes, are also implemented in HERAFitter first set of PDFs extracted using HERAFitter from HERA 206 and will be discussed in section 6. I data, HERAPDF1.0 [35], is shown in Fig. 2 (taken from [35]). Note that the PDFs displayed are parton momentum distributions $xf(x,\mu_F^2)$ since this is how PDFs are conven- 207 3.1 Deep Inelastic Scattering and Proton Structure tionally stored and displayed.

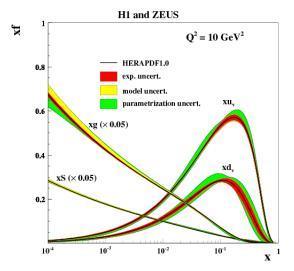


Fig. 2 Distributions of valence (xu_v, xd_v) , sea (xS) and the gluon (g)densities in HERAPDF1.0 [35]. The gluon and the sea distributions are scaled down by a factor of 20. The experimental, model and parametrisation uncertainties are shown as coloured bands.

3 Theoretical formalism using DGLAP evolution

[16–20] evolution is described.

tained:

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

a in parton b. They can be calculated as a perturbative expansion in α_s . Once PDFs are determined at the initial scale Q_0^2 , their evolution to any other scale $Q^2>Q_0^2$ is entirely deter-

208 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 the partons in the proton by a virtual exchange of a NC or CC vector boson and, as a result, a scattered lepton and a multi-hadronic final state are produced. The common DIS kinematic variables are the scale of the process Q^2 , which is the absolute squared four-momentum of the exchange boson, Bjorken x, which can be related in the parton model to the fraction of momentum carried by the struck quark, and the inelasticity y. These are related by $y = Q^2/sx$, where s is the squared centre-of-mass (c.o.m.) energy.

The NC cross section can be expressed in terms of gener-222 alised structure functions:

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

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

where $Y_{\pm} = 1 \pm (1 - y)^2$ and the electromagnetic coupling 224 constant α , the photon propagator and a helicity factor are 225 absorbed in the definition of the reduced cross section σ_r . The generalised structure functions $\tilde{F}_{2,3}$ can be written as linear combinations of the proton structure functions $F_2^{\gamma}, F_{2,3}^{\gamma Z}$ and $F_{2.3}^{Z}$, which are associated to pure photon exchange terms, 229 photon-Z interference terms and pure Z exchange terms, re-In this section the theoretical formalism based on DGLAP 230 spectively. The structure function \tilde{F}_2 is the dominant contribution to the cross section, $x\tilde{F}_3$ becomes important at high A direct consequence of factorisation (Eq. 1) is that scale 232 Q^2 and \tilde{F}_L is sizable only at high y. In the framework of dependence or "evolution" of the PDFs can be predicted by 233 pQCD the structure functions are directly related to the PDFs, the renormalisation group equations. By requiring that phys- 234 i.e. in leading order (LO) F₂ is the weighted momentum sum ical observables are independent of μ_F , a representation of 235 of quark and anti-quark distributions, xF_3 is related to their parton evolution in terms of the DGLAP equations is ob- $\frac{236}{2}$ difference, and F_L vanishes. At higher orders, terms related 237 to the gluon density distribution ($\alpha_s g$) appear, in particular

 F_L is strongly related to the low-x gluon.

case, can be expressed in terms of another set of structure 287 scheme. This scheme has the advantage of reducing the senfunctions, \tilde{W} ::

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

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

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 QCD 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 299 few GeV² to about 10⁵ GeV², crossing heavy-quark mass thresholds, thus the treatment of heavy quark (charm and 301 beauty) production and the chosen values of their masses 302 become important. There are different schemes for the treat- 303 ment of heavy quark production. Several variants of these 304 schemes are implemented in HERAFitter and they are briefly₃₀₅ discussed below.

Zero-Mass Variable Flavour Number (ZM-VFN): In this scheme [37], the heavy quarks appear as partons in the proton at 309 Q^2 values above $\sim m_h^2$ (heavy quark mass) and the heavy 310 quarks are then treated as massless in both the initial and $_{_{311}}$ final states of the hard scattering process. The lowest order 312 process is the scattering of the lepton off the heavy quark via (electroweak) boson exchange. This scheme is expected to be reliable in the region with $Q^2 \gg m_h^2$. In HERAFitter this scheme is available for the DIS structure function calculation via the interface to the QCDNUM [21] package, thus it benefits from the fast QCDNUM convolution engine.

Fixed Flavour Number (FFN): In this rigorous quantum field 320 theory scheme [38–40], only the gluon and the light quarks $_{_{321}}$ are considered as partons within the proton and massive quarks are produced perturbatively in the final state. The lowest order process is the heavy quark-antiquark pair production via boson-gluon fusion. In HERA- Fitter this scheme can be accessed via the QCDNUM implementation or through the in- 324 3.2 Electroweak Corrections to DIS terface to the open-source code OPENQCDRAD [41], as implemented by the ABM group. This scheme is reliable for 325 Calculations of higher-order electroweak corrections to DIS $Q^2 \sim m_h^2$. In QCDNUM, the calculation of the heavy quark con- 326 scattering at HERA are available in HERAFitter in the ontributions to DIS structure functions are available at Next-to- 327 shell scheme. In this scheme the gauge bosons masses M_W Leading-Order (NLO) and only electromagnetic exchange $_{328}$ and M_Z are treated as basic parameters together with the top, contributions are taken into account. In the OPENQCDRAD im- 329 Higgs and fermion masses. These electroweak corrections functions are also available and, for the NC case, the QCD $_{331}$ running of the electromagnetic coupling α using the most corrections to the coefficient functions at Next-to-Next-to 332 recent parametrisation of the hadronic contribution [53], as Leading Order (NNLO) are provided at the best currently 333 well as an older version from Burkhard [54].

285 known approximation [42]. The OPENQCDRAD implementa-The inclusive CC ep cross section, analogous to the NC 286 tion also uses the running heavy-quark mass [43] in the $\overline{\rm MS}$ 288 sitivity of the DIS cross sections to higher order corrections, and improving the theoretical precision of the mass defini-(5) 290 tion.

> (6) 291 General-Mass Variable Flavour Number (GM-VFN): In these schemes [44], 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 inbetween. The details of this 295 interpolation differ between different implementations. The PDF groups that use GM-VFN schemes are MSTW, CT (CTEQ), 297 NNPDF, and HERAPDF. HERAFitter implements different variants of the GM-VFN scheme.

- GM-VFN Thorne-Roberts scheme: The Thorne-Roberts (TR) scheme [45] was designed to provide a smooth transition from the massive FFN scheme at low scales $Q^2 \sim m_h^2$ to the massless ZM-VFNS scheme at high scales $Q^2 \gg m_h^2$. However, the original version was technically difficult to implement beyond NLO, and was updated to the TR' scheme [46]. There are two different variants of the TR' schemes: TR' standard (as used in MSTW PDF sets [11, 46]) and TR' optimal [47], with a smoother transition across the heavy quark threshold region. Both variants are accessible within the HERAFitter package at LO, NLO and NNLO.
- GM-VFN ACOT scheme: The Aivazis-Collins-Olness-Tung (ACOT) scheme belongs to the group of VFN factorisation schemes that use the renormalisation method of Collins-Wilczek-Zee (CWZ) [48]. This scheme unifies the low scale $Q^2 \sim m_h^2$ and high scale $Q^2 > m_h^2$ regions with a smooth interpolation across the full energy range. Within the ACOT package, different variants of the ACOT scheme are available: ACOT-Full [49], S-ACOT- χ [50, 51], ACOT-ZM [49], $\overline{\rm MS}$ at LO and NLO. For the longitudinal structure function higher order calculations are also available. A comparison of PDFs extracted from the QCD fits to the HERA data with the TR' and ACOT-Full schemes is illustrated in Fig. 3 (taken from [35]).

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plementation the heavy quark contributions to CC structure 330 are based on the EPRC package [52]. The code calculates the

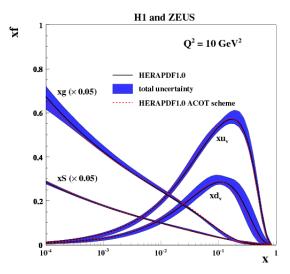


Fig. 3 Overview showing the u- and d-valence, the total sea (scaled), and gluon (scaled) PDFs of the NLO HERAPDF1.0 set [35] with their total uncertainty at the scale of $Q^2 = 10 \text{ GeV}^2$ obtained using the TR' scheme and compared to the PDFs obtained with the ACOT scheme using the k-factor technique (red).

3.3 Diffractive PDFs

the interacting proton stays intact $(ep \rightarrow eXp)$. The proton ³⁶⁸ sity [57]. is well separated from the rest of the hadronic final state 369 by a large rapidity gap. This is interpreted as the dissocia- 370 variant mass M, boson rapidity y and lepton scattering angle tion of the virtual photon into hadronic system X with an $371 \cos \theta$ in the parton c.o.m. frame can be written as [58, 59]: invariant mass much smaller than the photon-proton c.o.m. energy $W = ys - Q^2 + m_p^2(1-y)$, where m_p is proton's mass. Such a process is assumed to be mediated by the exchange of a hard Pomeron 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.

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 exchange Pomeron or Reggeon, t, and the mass M_X of the diffractively produced final state. In practice, the variable M_X is often replaced by dimensionless quantity $\beta = \frac{Q^2}{M_Y^2 + Q^2 - t}$ 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.

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

with the "reduced cross-section":

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

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

The diffractive PDFs in HERAFitter [55, 56] are implemented as a sum of two factorised contributions:

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

where $\Phi(x_{IP},t)$ are the Reggeon and Pomeron fluxes. The Reggeon PDFs, f_a^{IR} are fixed as those of the pion, while the Pomeron PDFs, f_a^{IP} , can be obtained from a fit to the data.

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

358 Drell-Yan process provides further valuable information about PDFs. In pp and $p\bar{p}$ scattering, the Z/γ^* and W production probe bi-linear combinations of quarks. Complementary in-361 formation on the different quark densities can be obtained from the W^{\pm} asymmetry (d, u and their ratio), the ratio of the W and Z cross sections (sensitive to the flavour compo-Diffractive parton distributions (DPDFs) can be determined 364 sition of the quark sea, in particular to the s-quark density), from QCD fits to diffractive cross sections in a similar way 365 and associated W and Z production with heavy quarks (sento the determination of the standard PDFs. About 10% of 366 sitive to c- and b-quark densities). Measurements at large deep inelastic interactions at HERA are diffractive, such that $_{367}$ boson $p_T \gtrsim M_{W,Z}$ are potentially sensitive to the gluon den-

At LO the DY NC triple differential cross section in in-

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

where S is the squared c.o.m. 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, and $\hat{\sigma}^q$ is the parton-parton hard scattering cross section.

The corresponding CC triple differential cross section has 378 the form:

$$\frac{d^{3}\sigma}{dMdyd\cos\theta} = \frac{\pi\alpha^{2}}{48S\sin^{4}\theta_{W}} \frac{M^{3}(1-\cos\theta)^{2}}{(M^{2}-M_{W}^{2}) + \Gamma_{W}^{2}M_{W}^{2}} \times \sum_{q_{1},q_{2}} V_{q_{1}q_{2}}^{2} f_{q_{1}}(x_{1},M^{2}) f_{q_{2}}(x_{2},M^{2}),$$
(11)

where $V_{q_1q_2}$ is the Cabibbo-Kobayashi-Maskawa (CKM) quark For the inclusive case, the diffractive cross-section reads as: 380 mixing matrix and M_W and Γ_W are the W boson mass and 381 decay width, respectively.

> The simple form of these expressions allows analytic (7) 383 calculation of integrated cross sections. In both NC and CC

expressions the PDFs depend only on boson rapidity y and 431 4 Computational Techniques invariant mass M, while the integral in $\cos \theta$ can be solved analytically even for the case of realistic kinematic cuts.

and Monte Carlo generators are often employed. Currently, 434 tive calculations become more complex and time-consuming the predictions for W and Z/γ^* production are available up 435 at higher orders due to the increasing number of relevant to NNLO and the predictions for W, Z in association with $_{436}$ Feynman diagrams. The direct inclusion of computationally heavy flavour quarks is available to NLO.

retical predictions for DY production in HERAFitter. The 439 turbative techniques in combination with modern comput-NLO and NNLO calculations are computing power and time 440 ing hardware do not lead to sufficiently small turn-around consuming and k-factor or fast grid techniques must be em- 441 times. However, a full repetition of the perturbative calculaployed (see section 4 for details), interfaced to programs 442 tion for small changes in input parameters is not necessary such as MCFM [60-62], available for NLO calculations, or 443 at each step of the iteration. Two methods have been de-FEWZ [63] and DYNNLO [64] for NLO and NNLO.

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

The cross section for production of high-transverse-momentum hadronic jets is sensitive to the high-x gluon PDF (see e.g. Ref. [11]) therefore this process can be used to improve the determination of the gluon PDF, which is particularly important for Higgs production and searches for new physics. Jet production cross sections are currently known only to NLO, although calculations for higher-order contributions to jet production in proton-proton collisions are now quite advanced [65-67]. Within HERAFitter, the NLOJet++ program [68, 69] may be used for calculations 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 section 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 sections can provide additional constraints on the gluon den- 464 tion at each step, but still requires typically a few iterations. sity at medium to high values of x, on α_s and on the topsection are available to full NNLO [71]. They can be com- 467 for heavy quarks in DIS. "FAST" heavy-flavour schemes are puted within HERAFitter via an interface to the program $_{468}$ implemented with k-factors defined as the ratio of calcula-HATHOR [72]. Differential tt cross section predictions at NLO 469 tions at the same perturbative order but for massive vs. masscan be obtained using MCFM [62, 73-76] interfaced to HERAFitteless quarks, e.g. NLO (massive)/NLO (massless). These kwith fast grid techniques.

tion are available to NLO accuracy using MCFM.

432 Precise measurements require accurate theoretical predic-Beyond LO, the calculations can no longer be done quickly tions in order to maximise their impact in PDF fits. Perturbademanding higher-order calculations into iterative fits is thus There are several possibilities for obtaining the theo- 438 not possible currently since even the most advanced perveloped which take advantage of this to solve the problem: the k-factor technique and the fast grids technique. Both are 446 available in HERAFitter.

4.1 k-factor Technique

The k-factors are defined as the ratio of the prediction of a higher-order (slow) pQCD calculation to a lower-order (fast) calculation using the same PDF. Because the k-factors depend on the phase space probed by the measurement, they 452 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 k-459 factors 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 calcula-

In HERAFitter the k-factor technique is also used for quark mass, m_t [70]. Precise predictions for the total $t\bar{t}$ cross 466 the fast computation of the time-consuming GM-VFN schemes 471 factors are calculated only for the starting PDF and hence, Single top quarks are produced via electroweak interac- 472 the "FAST" heavy flavour schemes should only be used for tions and single-top cross sections can be used, for example, 473 quick checks. Full heavy flavour schemes should be used to probe the ratio of the u and d densities in the proton as 474 by default. However, for the ACOT scheme, due to excepwell as the b-quark PDF. Predictions for single-top produc- 475 tionally long computation time, the k-factors are used in the 476 default settings in HERAFitter.

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4.2 Fast Grid Techniques

Fast grid techniques exploit the fact that iterative PDF fitting procedures do not impose completely arbitrary changes to the types and shapes of the parameterised functions that 533 represent each PDF. Instead, it can be assumed that a generic 534 PDF can be approximated by a set of interpolating func- 535 tions with a sufficient number of judiciously chosen sup- 536 port points. The accuracy of this approximation is checked 537 and optimised such that the approximation bias is negligibly 538 small compared to the experimental and theoretical accu-539 racy. This method can be used to perform the time consuming higher-order calculations (Eq. 1) only once for the set of 541 interpolating functions. Further iterations of the calculation 542 for a particular PDF set are fast, involving only sums over 543 the set of interpolators multiplied by factors depending on 544 the PDF. This approach can be used to calculate the cross 545 sections of processes involving one or two hadrons in the 546 initial state and to assess their renormalisation and factori- 547 sation scale variation.

This technique was pioneered by the fastNLO project [77] 49 to facilitate the inclusion of time consuming NLO jet cross 550 section predictions into PDF fits. The APPLGRID [78] project 551 developed an alternative method and, in addition to jets, ex- 552 tended its applicability to other scattering processes, such 553 as DY and heavy quark pair production is association with 554 boson production. The packages differ in their interpolation 555 and optimisation strategies, but both packages construct tables with grids for each bin of an observable in two steps: in the first step, the accessible phase space in the parton momentum fractions x and the renormalisation and factorisation 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 obatined 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 [77] has been interfaced to the NLOJet++ program [68] for the calculation of jet production in DIS [79] as well as 2- and 3-jet production in hadron-hadron collisions at NLO [69, 80]. Threshold corrections at 2-loop order, which approximate the NNLO for the inclusive jet cross section, have also been included into the framework [81] following Ref. [82]. The latest version of the fastNLO convolution program [83] 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₊ and Q for DIS. The fastNLO code is avail-

able online [84]. Jet cross-section grids computed for the kinematics of various experiments can be downloaded from this site.

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Dedicated fastNLO libraries and tables with theory predictions for comparison to particular cross section measurements are included into the HERAFitter package. For the HERAFitter implementation, the evaluation of the strong coupling constant is done consistently with the PDF evolution from the QCDNUM code.

In the APPLGRID package [78, 85], in addition to jet cross sections for $pp(\bar{p})$ and DIS processes, calculations of DY production are also implemented. The grids are generated with the customised versions of the MCFM parton level DY generator [60–62]. Variation of the renormalisation and factorisation scales is possible a posteriori, when calculating theory predictions with the APPLGRID tables, and independent variation of the strong coupling constant is also allowed. For NNLO predictions in HERAFitter, the k-factors technique can be also applied within the APPLGRID framework.

As an example, the HERAFitter interface to APPLGRID was used by the ATLAS [86] and CMS [125] collaborations to extract the strange quark density 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 [12] and NNPDF2.1 [13] (taken from [86]).

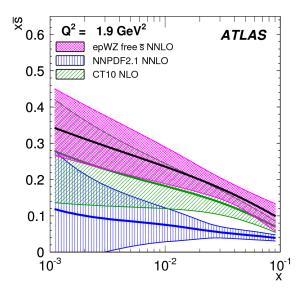


Fig. 4 The strange antiquark density versus x for the ATLAS epWZ free \bar{s} NNLO fit [86] (magenta band) compared to predictions from NNPDF2.1 (blue hatched) and CT10 (green hatched) at $Q^2 = 1.9 \text{ GeV}^2$. The ATLAS fit was performed using a k-factor approach for NNLO corrections.

556 5 Fit Methodology

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are various assumptions and choices to be made concerning, 596 sum rules. for example, the functional form of the input parametrisation, the treatment of heavy quarks and their mass values, al- 597 Chebyshev Polynomials: A flexible parametrisation based tests. The methodology employed by HERAFitter relies on 603 form reads a flexible and modular framework that allows for independent integration of the state-of-the-art techniques, either related to the inclusion of a new theoretical calculation, or of new approaches to treat data and their uncertainties.

In this section we describe the available options for the fit methodology in HERAFitter. In addition, as an alternative 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

The PDFs can be parametrised using several predefined func- 611 tional forms and different 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:

$$xf_j(x) = A_j x^{B_j} (1 - x)^{C_j} P_j(x).$$
(12)

The parametrised PDFs are the valence distributions xu_v 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 [35] 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, $P_i(x)$ 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:

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

This function can be regarded as a generalisation of the standard polynomial form described above, however, numerical When performing a QCD analysis to determine PDFs there 595 integration of Eq. 13 is required in order to satisfy the QCD

ternative theoretical calculations, alternative representations 598 on the Chebyshev polynomials can be employed for the gluon of the fit χ^2 , different ways of treating correlated system- 599 and sea distributions. Polynomials with argument $\log(x)$ are atic uncertainties. It is useful to be able to discriminate or 600 considered for better modelling the low-x asymptotic of those quantify the effect of the chosen ansatz, within a common $_{601}$ PDFs. The polynomials are multiplied by a factor of (1-x)framework, and HERAFitter is optimally designed for such $_{602}$ to ensure that they vanish as $x \to 1$. The resulting parametric

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

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

where T_i are first-type Chebyshev polynomials of order i. The normalisation factor A_g is derived from the momentum 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 [87]) shows a comparison of the gluon density obtained with the parametrisation Eqs. 14, 15 to the standard-polynomial one, for $N_{g,S}$ =

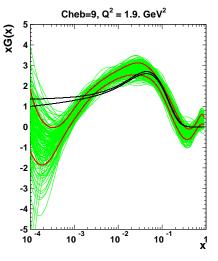
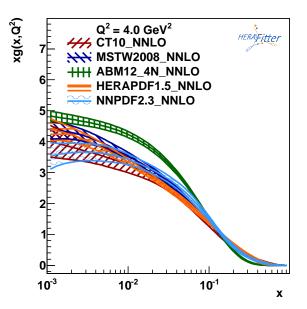


Fig. 5 The gluon density is shown at the starting scale. The black lines correspond to the uncertainty band of the gluon distribution using a standard parametrisation and it is compared to the case of the Chebyshev parametrisation [87]. The uncertainty band for the latter case is estimated using the Monte Carlo technique (see section 5.3) with the green lines denoting fits to data replica. Red lines indicate the standard deviation about the mean value of these replicas.

613 External PDFs: HERAFitter also provides the possibility (13) 614 to access external PDF sets, which can be used to compute

theoretical predictions for the cross sections for all the pro- 639 cesses available in HERAFitter. This is possible via an in- 640 terface to LHAPDF [32, 33] providing access to the global PDF sets. HERAFitter also allows to evolve PDFs from LHAPDF with QCDNUM using the corresponding grids as a starting scale. Fig. 6 illustrates a comparison of various 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 PDF 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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imisation of the χ^2 function taking into account correlated 666 be included as additive or following the Poisson statistics. and uncorrelated measurement uncertainties. There are vari- 667 Minimisation with respect to nuisance parameters is perous forms of the χ^2 e.g. using a covariance matrix or pro- 668 formed analytically, however for more detailed studies of each correlated systematic uncertainty for each measured 670 in the MINUIT minimisation. 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 m_i . Three distinct methods for propagating experimental uncercan 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 covariance matrix $C_{i,k}$ for measurements in bins i and k. The covariance matrix C_{ik} is given by a sum of statistical, uncorrelated and correlated systematic contributions:

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

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

Nuisance Parameters Representation: In this case the χ^2 form 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^i quantifies the sensitivity of the measurement to the correlated systematic source j. The function χ^2 depends in addition on the set of systematic nuisance parameters b_i . This definition of the χ^2 function assumes that systematic uncertainties are proportional to the central prediction values (multiplicative errors), whereas the statistical uncertainties scale with the square root of the expected number of events.

During the χ^2 minimisation, the nuisance parameters b_i 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 covariance matrix. HERAFitter offers the possibility to include such mixed forms of information.

664 Any source of measured systematic uncertainty can be treated The PDF parameters are determined in HERAFitter by \min_{-665} as additive or multiplicative. The statistical uncertainties can viding nuisance parameters to encode the dependence of 669 correlations individual nuisance parameters can be included

5.3 Treatment of the Experimental Uncertainties

673 tainties to PDFs are implemented in HERAFitter and reviewed here: the Hessian, Offset, and Monte Carlo method.

Hessian (Eigenvector) method: The PDF uncertainties reflecting the uncertainties in experimental data are estimated by examining the shape of χ^2 in the neighbourhood of the minimum [88]. Following approach of Ref. [88], 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

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Offset method: The Offset method [89] uses the χ^2 function for the central fit, however 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 arrive at the 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 technique [90, 91] 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 [31]. A comparison is illustrated in Fig. 7. Similar findings were reported by the MSTW global analysis [92].

Since the MC method requires large number of replicas, 730 the eigenvector representation is a more convenient way $\ensuremath{^{731}}$ [94].

The nuisance parameter representation of χ^2 in Eq. 18 is derived assuming symmetric experimental errors, however, 738 5.5 Bayesian Reweighting Techniques the published systematic uncertainties are often asymmetric. HERAFitter provides the possibility to use asymmetric 739 As an alternative to performing a full QCD fit, HERAFitter systematic uncertainties. The implementation relies on the 740 allows the user to assess the impact of including new data assumption that asymmetric uncertainties can be described 741 in an existing fit using the Bayesian Reweighting technique.

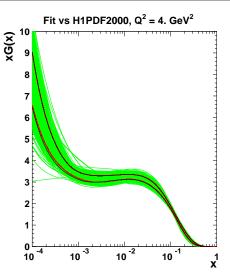


Fig. 7 Comparison between the standard error calculations as employed by the Hessian approach (black lines) and the MC approach (with more than 100 replicas) assuming Gaussian distribution for uncertainty distributions, shown here for each replica (green lines) together with the evaluated standard deviation (red lines) [31]. The black lines in the figure are difficult to see because agreement of the methods is so good that thet are mostly covered by the red lines.

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 variaion of the systematic uncertainty j, S_{ij}^{\pm} ,

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

5.4 Treatment of the Theoretical Input Parameters

728 The results of a QCD fit depend not only on the input data 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 to store the PDF uncertainties. It is possible to transform 732 PDFs with different choices of the mass of the charm quarks, MC to eigenvector representation as shown by [93]. Tools 733 m_c , mass of the bottom quarks, m_b , and the value of $\alpha_s(M_Z)$. to perform this transformation are provided with HERAFitter Other important aspects are the choice of the functional form and were recently employed for the representation of 735 for the PDFs at the starting scale and the value of the starting correlated sets of PDFs at different perturbative order 736 scale itself. HERAFitter provides the possibility of different user choices of all these inputs to the theory.

by a parabolic function. The nuisance parameter in Eq. 18 is 742 The method provides a fast estimate of the impact of new

PDF sets delivered in the form of MC replicas by [90] and 759 reweighting/unweighting procedure. No extra information is further developed by the NNPDF Collaboration [95, 96]. 760 gained by producing a final unweighted set that has a num-More recently, a method to perform Bayesian Reweighting 701 ber of replicas (significantly) larger than N_{eff} . If N_{eff} is much studies starting from PDF fits for which uncertainties are 762 smaller than the original number of replicas the new data provided in the eigenvector representation has been also de- 763 have great impact, however it is unreliable to use the new veloped [92]. The latter is based on generating replica sets 764 reweghted set. Instead a full refit should be performed. by introducing Gaussian fluctuations on the central PDF set with a variance determined by the PDF uncertainty given by the eigenvectors. Both reweighting methods are imple- 765 6 Alternatives to DGLAP Formalism mented in HERAFitter.

the PDFs are represented as ensembles of N_{rep} equiprobable (i.e. having all weight 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- 776 6.1 Dipole Models bution, given by the prior PDF set, is updated according to Bayes Theorem such that the weight of each replica, w_k , is 777 The dipole picture provides an alternative approach to protonupdated 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 chi-square of the new data obtained using the k-th PDF 785 are embedded in a dipole scattering amplitude. replica. Given a PDF set and a corresponding set of weights, 786 data can be computed as the weighted average,

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

To simplify the use of 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 [95]. The number of effective replicas of a reweighted set is measured by its Shannon Entropy [96]

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

which corresponds to the size of a refitted equiprobable replicage proton. R_0^2 takes the form, $R_0^2(x) = (x/x_0)^{\lambda} 1/\text{GeV}^2$, and is set containing the same amount of information. This number 798 called the saturation radius. The cross-section normalisation of effective replicas, $N_{\rm eff}$, gives an indicative measure of the σ_{09} σ_{0} , x_{0} , and λ are parameters of the model commonly fitted to

₇₄₃ data on PDFs. Bayesian Reweighting was first proposed for ₇₅₈ optimal size of an unweighted replica set produced using the

The Bayesian Reweighting technique relies on the fact 766 QCD calculations based on the DGLAP [16-20] evolution that MC replicas of a PDF set give a representation of the 767 equations are very successful in describing all relevant hard probability distribution in the space of PDFs. In particular, 768 scattering data in the perturbative region $Q^2 \gtrsim$ few GeV². 769 At small-x and small- Q^2 DGLAP dynamics may be modi-770 fied by non-perturbative QCD effects like saturation-based 771 dipole models and other higher twist effects. Different approaches that are alternatives to the DGLAP formalism can be used to analyse DIS data in HERAFitter. These include several different dipole models and the use of transverse mo-(21) mentum dependent, or unintegrated PDFs (uPDFs).

virtual 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 (22) interacts with the proton [97]. The dipoles can be considered as quasi-stable quantum mechanical states, which have very where $N_{\rm data}$ is the number of new data points, k denotes the 183 long life time $\propto 1/m_p x$ and a size which is not changed by specific replica for which the weight is calculated and χ^2_k is 784 scattering with the proton. The dynamics of the interaction

Several dipole models which assume different behaviour which describes the impact of the inclusion of new data, the 787 of the dipole-proton cross section are implemented in HERAFitter: prediction for a given observable after inclusion of the new 788 the Golec-Biernat-Wüsthoff (GBW) dipole saturation model [27], a modified GBW model which takes into account the effects of DGLAP evolution, termed the Bartels-Golec-Kowalski 791 (BGK) dipole model [29] and the colour glass condensate approach to the high parton density regime, termed the Iancu-⁷⁹³ Itakura-Munier (IIM) dipole model [28].

> 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) $_{795}^{794}$ the quark and the antiquark, and R_0^2 is an x-dependent scale 796 parameter which represents the spacing of the gluons in the the DIS data. This model gives exact Bjorken scaling when 840 in perturbation theory, both in the hard scattering coeffithe dipole size r is small.

BGK model: The BGK model is a modification of the GBW 843 torisation scheme [120, 121]. model assuming that the spacing R_0 is inverse to the gluon 844 density and taking into account the DGLAP evolution of the $_{845}$ scheme, using the boson-gluon fusion process ($\gamma^*g^* o q\bar{q}$). latter. The gluon density parametrised at some starting scale 846 The masses of the quarks are explicitly included as paramby Eq. 12 is evolved to larger scales using DGLAP evolu- 847 eters of the model. In addition to $\gamma^*g^* \to q\bar{q}$, the contribution.

BGK model with valence quarks: The dipole models are valid in the low-x region only, where the valence quark conx from 0.0001 to 0.01 [98]. The inclusive HERA measurements have a precision which is better than 2%, therefore, in HERAFitter the contribution of the valence quarks can be taken into account [99].

IIM model: The IIM model assumes an expression for the $_{857}$ a non-perturbative starting distribution $\mathcal{A}_0(x)$ dipole cross section which is based on the Balitsky-Kovchegov equation [100]. The explicit formula for σ_{dip} can be found in [28]. The alternative scale parameter \tilde{R} , x_0 and λ are fitted parameters of the model.

6.2 Transverse Momentum Dependent PDFs

QCD calculations of multiple-scale processes and complex $_{861}$ evolution. It is defined on a grid of $50 \otimes 50 \otimes 50$ bins in final-states can necessitate the use of transverse-momentum 862 x, k_t, p . The binning in the grid is logarithmic, except for dependent (TMD) [8], or unintegrated, parton distribution 863 the longitudinal variable x for which 40 bins in logarithmic and parton decay functions [101-109]. TMD factorisation 864 spacing below 0.1, and 10 bins in linear spacing above 0.1 has been proven recently [8] for inclusive DIS. TMD fac- 865 torisation has also been proven in the high-energy (small-x) 866 limit [110–112] for particular hadron-hadron scattering pro- 867 volves a time-consuming multidimensional MC integration cesses, like heavy flavor, vector boson and Higgs produc- 868 tion,

In the framework of high-energy factorisation [110, 113, 870 equation is applied: 114] the DIS cross section can be written as a convolution in both longitudinal and transverse momenta of the TMD parton density function $\mathscr{A}(x, k_t, \mu_F^2)$ with the off-shell parton scattering matrix elements, as follows

$$\sigma_j(x,Q^2) = \int_x^1 dz \int d^2k_t \ \hat{\sigma}_j(x,Q^2,z,k_t) \ \mathscr{A}\left(z,k_t,\mu_F^2\right)$$
 (26) 871 where first $\tilde{\sigma}(x',Q^2)$ is calculated numerically with a MC

Eq. 26, are k_t -dependent and the evolution of the transverse- 875 fit. momentum dependent gluon density \mathcal{A} is obtained by combining the resummation of small-x logarithmic contributions 876 Functional Forms for TMD parametrisation: For the startton splitting [16, 19, 20] according to the CCFM evolution 878 form is used: equation [24, 118, 119].

The factorisation formula (26) allows resummation of logarithmically enhanced small-x contributions to all orders

cients and in the parton evolution, fully taking into account the dependence on the factorisation scale μ_F and on the fac-

The cross section σ_j , (j = 2, L) is calculated in a FFN tion from valence quarks is included via $\gamma^* q \to q$ by using a 849 CCFM evolution of valence quarks [122, 123].

850 CCFM Grid Techniques: The CCFM evolution cannot be tribution to the total proton momentum is 5% to 15% for 851 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 [123, 124], the kernel $\tilde{\mathscr{A}}(x'', k_t, p)$ is determined from the MC so-856 lution of the CCFM evolution equation, and then folded with

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

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

Calculation of the cross section according to Eq. 26 inwhich suffers from numerical fluctuations. This cannot be employed directly in a fit procedure. Instead the following

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

integration on a grid in x for the values of Q^2 used in the with the DIS cross sections σ_j , (j = 2, L) related to the struc- 873 fit. Then the last step in Eq. 28 is performed with a fast nuture functions F_2 and F_L . The hard-scattering kernels $\hat{\sigma}_j$ of $_{874}$ merical gauss integration, which can be used directly in the

[115–117] with medium-x and large-x contributions to par- $_{877}$ ing distribution \mathcal{A}_0 , at the starting scale Q_0^2 , the following

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

where $\sigma^2 = Q_0^2/2$ and N, B, C, D, E are free parameters. Va- 911 from any collinear PDF and imposition of the flavor sum 914 theory predictions in DIS. In addition, the HERAFitter refrule at every scale p.

In HERAFitter there are also available cache options, lence quarks are treated using the method of Ref. [122] as 912 fast evolution kernels, and the OpenMP (Open Multi-Processing) described in Ref. [123] with a starting distribution taken 913 interface which allows parallel applications of the GM-VFNS 915 erences and GNU public licence are provided together with The TMD parton densities can be plotted either with HERAFittethe main source code.

provided tools or with TMDplotter [34].

7 HERAFitter Code Organisation

HERAFitter is an open source code and it can be downloaded from the dedicated webpage [1] together with its supporting documentation and fast grid theory files (described in section 4) associated with data files. The source code contains all the relevant information to perform QCD fits with HERA DIS data as a default set ¹. The performance time depends on the fitting options and varies from 10 minutes (using "FAST" techniques as described in section 4) to several hours when full uncertainties are estimated. The HERAFitter code is a combination of C++ and Fortran 77 libraries with minimal dependencies, i.e. for the default fitting options no external dependencies are required except the QCDNUM evolution program [21] and CERN libraries. The ROOT libraries are only required for the drawing tools and provide a qualitative and quantitative assessment of the results. Fig. 8 shows an illustration of a comparison between the inclusive NC data from HERA I with the predictions based on HERAPDF1.0 PDFs. The consistency of the measurements and the theory can be expressed by pulls, defined as the difference between data and theory divided by the uncorrelated error of the data. In each kinematic bin of the measurement, pulls are provided in units of standard deviation (sigma). The pulls are also illustrated in Fig. 8.

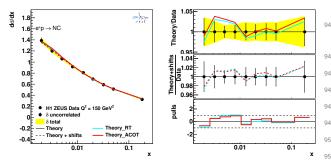


Fig. 8 An illustration of the consistency of HERA measurements [35] and the theory predictions, obtained in HERAFitter with the default drawing tool.

917 8 Applications of HERAFitter

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 [86, 125-128], inclusive jet production [129], and inclusive photon production [130]. The results of QCD analyses using HERAFitter were also published by HERA experiments for inclusive [35, 131] and 925 heavy flavour production measurements [132, 133]. The following phenomenological studies have been performed with HERAFitter: a determination of the transverse momentum dependent gluon density using precision HERA data [123], an analysis of HERA data within a dipole model [99], the 930 study of the low-x uncertainties in PDFs determined from 931 the HERA data using different parametrisations [87] and 932 the impact of QED radiative corrections on PDFs [134]. A when invoking APPLGRID. Drawing tools inbuilt in HERAFitter recent study based on a set of PDFs determined with the 1935 tween different orders has been published in [94].

> The HERAFitter framework has been used to produce 937 PDF grids from QCD analyses performed at HERA [35, 938 135] and at the LHC [136], using measurements from AT-₉₃₉ LAS [86, 129]. These PDFs can be used to study predictions 940 for SM or beyond SM processes. Furthermore, HERAFitter provides the possibility to perform various benchmarking 942 exercises [137] and impact studies for possible future col-943 liders as demonstrated by QCD studies at the LHeC [138].

9 Summary

945 HERAFitter is an open-source platform designed for studies 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. HERAFitter allows for direct comparisons of various theoretical approaches under the same settings. Different methodologies in treating the experimental and model uncertainties and can be used for benchmarking studies. The progress of HERAFitter is driven by the latest QCD advances in theoretical calculations and in the precision of experimental data.

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¹Default settings in HERAFitter are tuned to reproduce the central 956 **Acknowledgements** HERAFitter developers team acknowledges the HERAPDF1.0 set.

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