# **HERAFitter**

# **Open Source QCD Fit Project**

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Abstract The paper presents the HERAFitter project which	23 2	2.3 Jet production in <i>ep</i> and <i>pp</i> collisions	5
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# 17 Keywords PDFs · QCD · Fit

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# 39 1 Introduction

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In the era of the Higgs discovery [1, 2] and extensive searches for signals of new physics at the LHC it is crucial to have accurate Standard Model (SM) predictions for hard scattering processes in hadron-hadron collisions. The most common approach to calculate the SM cross sections for such reactions is to use collinear factorisation in perturbative QCD

collisions . . . . . . . . . .

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(pQCD) [3]:

$$\sigma(\alpha_{s}, \mu_{r}, \mu_{f}) = \sum_{a,b} \int_{0}^{1} dx_{1} dx_{2} f_{a}(x_{1}, \alpha_{s}, \mu_{F}) f_{b}(x_{2}, \alpha_{s}, \mu_{F}) \times \hat{\sigma}^{ab}(x_{1}, x_{2}; \alpha_{s}, \mu_{R}, \mu_{F}).$$
(1)

40 Here the cross section  $\sigma$  for any hard-scattering inclusive process  $ab \rightarrow X + all$  is expressed as a convolution of Parton Distribution Functions (PDFs)  $f_a$  and  $f_b$  with the partonic cross section  $\hat{\sigma}^{ab}$ . The PDFs describe 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 sum over indices a and b in Eq. 1 indicates the various kinds of partons, i.e. gluons, quarks and antiquarks of different flavours, that are considered as the constituents of the proton. Both the PDFs and the partonic cross section depend on the strong coupling  $\alpha_s$ , and the factorisation and renormalisation scales,  $\mu_F$  and  $\mu_R$ , respectively. The partonic cross sections are calculable in pQCD, but the PDFs cannot yet be predicted in QCD they must rather be determined from measurement. PDFs are assumed to be universal such that different scattering reactions can be used to constrain them [4, 5].

Measurements of the inclusive Neutral Current (NC) and Charged Current (CC) Deep-Inelastic-Scattering (DIS) at the ep collider HERA provide crucial information for determining the PDFs. For instance, the gluon density relevant for calculating the dominant gluon-gluon fusion contribution to Higgs production at the LHC can be accurately determined at low and medium x from the HERA data alone. Many processes in pp and  $p\bar{p}$  collisions at LHC and Tevatron, respectively, probe PDFs in the kinematic ranges, inaccessible by DIS measurements. Therefore inclusion of the LHC and Tevatron data in the QCD analysis of the proton structure provide additional constraints on the PDFs, improving either their precision, or providing important information of the correlations of PDF with the fundamental OCD parameters like strong coupling or quark masses. In this context, the processes of interest at hadron colliders are Drell Yan (DY) production, W and Z asymmetries, associated production of W or Z bosons and heavy quarks, top quark, jet and prompt photon production.

Open-source QCD platform HERAFitter encloses the set of tools necessary for a comprehensive global QCD analysis of hadron-induced processes even on the early stage of the experimental measurement. It has been developed for determination of PDFs and extraction of fundamental QCD parameters like heavy quark masses or the strong coupling constant. This tool provides also the basis for comparisons of different theoretical approaches and can be used for direct tests of the impact of new experimental data in the QCD analyses. The processes that are currently included in HERAFitter framework are listed in Tab. 1. The functionality of HERAFitter is schematically illustrated in Fig. 1 and can be represented by the four main blocks:

Data	Process	Reaction	Theory calculations, schemes
HERA	DIS NC	$ep \rightarrow eX$	TR', ACOT ZM (QCDNUM) FFN (OPENQCDRAD, QCDNUM)
	DIS CC	$ep \rightarrow v_e X$	ACOT, ZM (QCDNUM) FFN (OPENQCDRAD)
	DIS jets	$ep \rightarrow e$ jets	NLOJet++ (FastNLO)
	DIS heavy quarks	$egin{aligned} ep & ightarrow ecar{c}X, \ ep & ightarrow ebar{b}X \end{aligned}$	ZM (QCDNUM), TR', ACOT, FFN (OPENQCDRAD, QCDNUM)
Fixed Target	DIS NC	$ep \rightarrow eX$	ZM (QCDNUM), TR', ACOT
Tevatron, LHC	Drell Yan	$ \begin{array}{ c } pp(\bar{p}) \rightarrow l\bar{l}X, \\ pp(\bar{p}) \rightarrow l\nu X \end{array}$	MCFM (APPLGRID)
	top pair	$pp(\bar{p}) \rightarrow t\bar{t}X$	MCFM (APPLGRID), HATHOR
	single top	$ \begin{array}{ c c 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 processes available in the HERAFitter package. The references for the individual calculations and their implementations are given in the text.

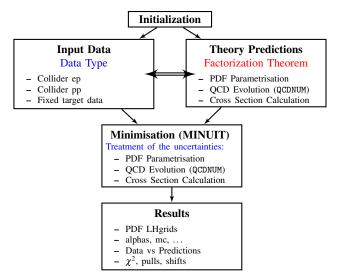


Fig. 1 Schematic structure of the HERAFitter program.

Input data: All relevant cross section measurements from the various reactions are stored internally in HERAFitter with the full information on their uncorrelated and correlated uncertainties. HERA I data sets are the basis of any proton PDF extraction, and they are used by all global PDF groups [6–10]. Additional measurements provide constraints to the sea flavour decomposition (such as the new results from the LHC), as well as constraints to PDFs in the kinematic phase-space regions not covered precisely by HERA I data, such as the high *x* region for the gluon and valence quark distributions.

Theory predictions: Predictions for cross section of different processes are obtained using the factorisation approach (Eq. 1). PDFs are parametrised at a starting scale  $Q_0^2$  by a chosen functional form with a set of free parameters **p**. These PDFs are then evolved from  $Q_0^2$  to the scale of the measurement using the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) [11–15] evolution equations as implemented in QCDNUM [16], and then convoluted with the hard parton cross sections calculated using a relevant theory program (as listed in Tab. 1).

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**PDF fit:** PDFs are extracted from a least square fit by constructing a  $\chi^2$  from the input data and the theory prediction. The  $\chi^2$  is minimized iteratively with respect to the PDF parameters using the MINUIT[17] program. Various choices of accounting for the experimental uncertainties are employed in HERAFitter, either using nuisance parameter method for the correlated systematic uncertainties, or covariance matrix method (see details in section 5.2). In addition, HERAFitter allows to study different statistics assumptions for the distributions of the systematic uncertainties (i.e. Gauss or log-normal) [18]. In the  $\chi^2$  minimization, the fitted parameters **p** and their estimated uncertainties are produced.

**Results:** The resulting PDFs are provided in a format ready to be used by the LHAPDF library [19, 20]. HERAFitter drawing tools can be used to display the PDFs with the uncertainty at a chosen scale. A first set of PDFs extracted by HERAFitter is HERAPDF1.0 [21] (Fig. 2) which is based on HERA I data. Since then several other PDFs sets were produced within the HERA and LHC collaborations. In addition to PDF display, the figures comparing the data used in the fit and the relevant theory predictions are produced. In Fig. 3, a comparison of inclusive NC data from the HERA I running period with predictions based on HERAPDF1.0. It also illuspull information, defined as the difference between data 157 plications of the package are given in section 7. and prediction divided by the uncorrelated uncertaintly of the data, is displayed in units of sigma shifts for each given data bin.

The HERAFitter project provides a versatile environ- 159 In this section the theoretical formalism for various proment for benchmarking studies and a flexible platform for  $_{160}$  cesses available in HERAFitter are described. the QCD interpretation of analyses within the LHC experiments, as already demonstrated by several publicly available results using the HERAFitter framework [22–28].

The outline of this paper is as follows. Section 2 discusses the various processes and corresponding theoretical 162 Deep Inelastic Scattering (DIS) data provide the backbone calculations performed in the DGLAP [11-15] formalism 163 of any PDF fit. The formalism that relates the DIS measure-

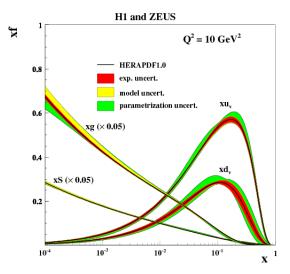


Fig. 2 Summary plots of valence, total sea (scaled) and gluon densities (scaled) with their experimental, model and parametrisation uncertainties at the scale of  $Q^2 = 10 \text{ GeV}^2$  of the HERAPDF1.0 PDF set at NLO [21].

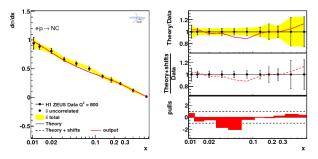


Fig. 3 An illustration of the HERAFitter drawing tools comparing the measurements (in this case HERA I) to the predictions of the fit. In addition, ratio plots are also provided together with the pull distribution (right panel).

trates the comparison to the theory predictions which are 152 the DGLAP formalism are presented in section 6. Section 4 adjusted by the systematic uncertainty shifts when using 153 presents various technique employed by the theory calculathe nuisance parameter method that accounts for cor- 154 tions used in HERAFitter. Section 5 elucidates the methodrelated systematic uncertainties. As an additional con- 155 ology of determining PDFs through fits based on various  $\chi^2$ sistency check between data and the theory predictions, 156 definitions used in the minimisation procedure. Specific ap-

## 158 2 Theoretical Input

### 2.1 Deep Inelastic Scattering Formalism and Schemes

that are available in HERAFitter. Alternative approaches to 164 ments to pQCD and the PDFs has been described in detail

in many extensive reviews (see e.g. [29]) and will only be 212 briefly recapped here. DIS is a lepton scattering off the con-213 stituents of the proton by a virtual exchange of a NC or 214 CC vector boson and, as a result, a scattered lepton and a 215 multihadronic final state are produced. The DIS kinematic 216 variables are the negative squared four-momentum of the 217 exchange boson,  $Q^2$ , the Bjorken x, and the inelasticity y, 218 where  $y = Q^2/sx$  and s is the centre-of-mass energy. 219 The NC cross section can be expressed in terms of generalised structure functions: 221

$$\frac{d^2 \sigma_{NC}^{e^{\pm} p}}{dx dO^2} = \frac{2\pi \alpha^2}{x O^4} \left[ Y_+ \tilde{F}_2^{\pm} \mp Y_- x \tilde{F}_3^{\pm} - y^2 \tilde{F}_L^{\pm} \right], \tag{2}$$

where  $Y_{\pm}=1\pm(1-y)^2$ . The generalised structure functions  $\tilde{F}_{2,3}$  can be written as linear combinations of the proton structure functions  $F_2, F_{2,3}^{\gamma Z}$  and  $F_{2,3}^{Z}$  associated to pure photon exchange terms, photon-Z interference terms and pure zero exchange terms respectively. Structure function  $\tilde{F}_2$  is the dominant contribution to the cross section,  $x\tilde{F}_3$  is 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, i.e. in leading order (LO)  $F_2$  is the weighted momentum sum of quark and anti-quark distributions,  $F_2 \approx x\sum e_q^2(q+\overline{q})$ , and  $xF_3$  is related to their difference,  $xF_3 \approx x\sum 2e_q^2(q-\overline{q})$  (where  $a_q$  is the axial-vecor quark coupling and  $e_q$  the quark electric charge). At higher orders, terms related to the gluon density distribution ( $\alpha_s g$ ) appear, in particular  $F_L$  is strongly related to the low-x gluon.

The inclusive CC ep cross section can be expressed in terms of another set of structure functions and in LO the  $e^+p$  and  $e^-p$  cross sections are sensitive to different quark flavour densities:

$$e^{+}: \ \tilde{\sigma}_{CC}^{e^{+}p} = x\overline{U} + (1-y)^{2}xD$$

$$e^{-}: \ \tilde{\sigma}_{CC}^{e^{-}p} = xU + (1-y)^{2}x\overline{D}.$$
(3)

Here *U* and *D* denote the sum over up- and down-type quarks; 246 the latter include also strange and beauty quarks and the former charm quarks. Beyond LO, the QCD predictions for the DIS structure functions are obtained by convoluting the PDFs with the respective coefficient functions (hard process matrix elements). The treatment of heavy charm and beauty quark production is a crucial point in these calculations and several schemes exist:

- In the Fixed Flavour Number (FFN) scheme [30–32]  $^{254}$  only the gluon and the light quarks are considered as partons within the proton and massive quarks (with mass  $^{256}$   $m_h$ ) are produced perturbatively in the final state. The  $^{257}$  lowest order process is the fusion of a gluon in the proton with a boson from the lepton to produce a heavy quark  $^{259}$  and an antiquark. The modern series of PDFs that use  $^{260}$  this scheme as default are ABM and JR PDF groups.
- In the Zero-Mass Variable Flavour Number (ZM-VFN) 262
   scheme [33] the heavy quark densities are included in 263

the proton for  $Q^2$  values above a threshold  $\sim m_h^2$  and are treated as massless in both the initial and final states. The lowest order process is the scattering of a heavy quark in the proton with the lepton via (electroweak) boson exchange. This scheme is expected to be reliable only in the region  $Q^2 \gg m_h^2$ . This is the scheme that was used in the past by PDF groups.

- In the General-Mass Variable-Flavour Number (GM-VFN) scheme [34] heavy quark production is treated for  $Q^2 \le m_h^2$  in the FFN scheme and for  $Q^2 \gg m_h^2$  in a fully massive scheme. The modern series of PDF groups that use this scheme are MSTW, CT(CTEQ), NNPDF, and HERAPDF.

All three schemes are available in HERAFitter. In the following the implemented variants are briefly discussed.

FFN scheme: In HERAFitter this scheme can be accessed via the QCDNUM implementation or through the interface to the open-source code OPENQCDRAD (as implemented by the ABM group) [35]. The latter implementation also includes the running mass definition of the heavy quark mass [36]. The running mass scheme has the advantage of reducing the sensitivity of the DIS cross sections to higher order corrections, and improving the theoretical precision of the mass definition. 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 ABM implementation the heavy quark contributions to CC structure functions are available and, for the NC case, the QCD corrections to the massive Wilson coefficients at Next-to-Next-to Leading Order (NNLO) are provided at the best currently known approximation [37].

**ZM-VFN** scheme: The scheme is available for the DIS structure function calculation via interface to the QCDNUM package.

**GM-VFN Thorne-Roberts scheme:** The Thorne-Roberts (TR) scheme [38] was designed to provide a smooth transition from the massive FFN scheme at low scales  $Q^2 < m_h^2$  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 [39] which is simpler (and closer to the ACOT-scheme, see below). There are two different variants of the TR' schemes: TR' standard (as used in MSTW PDF sets [6, 39]) and TR' optimal [40], with a smoother transition across the heavy quark threshold region. Both of these variants are accessible within the HERAFitter package at NLO and NNLO.

**GM-VFN ACOT scheme:** The Aivazis-Collins-Olness-Tung scheme belongs to the group of VFN factorisation schemes that use the renormalization method of Collins-Wilczek-Zee (CWZ) [41]. This scheme unifies the low scale  $Q^2$  <

 $m_h^2$  and high scale  $Q^2 > m_h^2$  regions; thus, it provides a smooth interpolation across the full energy regime. It is built upon the massive factorization theorem by Collins [41] to incorporate the heavy quark masses for  $Q^2 > m_h^2$ ; hence, it can be consistently applied order by order in the perturbation theory. Within the ACOT package, different variants of the ACOT scheme are available: ACOT-Full, S-ACOT- $\chi$ , ACOT-ZM,  $\overline{\rm MS}$  at LO and NLO. For the longitudinal structure function higher order calculations are also available. The ACOT-Full implementation takes into account the quark masses and it reduces to ZM  $\overline{\text{MS}}$ scheme in the limit of masses going to zero, but it has the disadvantage that it is computationally intensive (addressed in section 4).

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DIS scattering at HERA are available in HERAFitter, performed in the on-shell scheme where the gauge bosons masses<sup>12</sup>  $M_W$  and  $M_Z$  are treated symmetrically as basic parameters 313 in terms of the computing power and time, and k-factor or together with the top, Higgs and fermion masses. These elec- 314 fast grid techniques must be employed (see section 4 for detroweak corrections are based on the EPRC package [42]. 315 tails), interfaced to programms such as MCFM [47-49], avail-The code provides the running of  $\alpha$  using the most recent 316 able for NLO calculations, or FEWZ [50] and DYNNLO [51] parametrisation of the hadronic contribution to  $\Delta_{\alpha}$  [43], as <sup>317</sup> for NLO and NNLO. well as an older version from Burkhard [44].

## 2.2 Drell Yan processes in pp or $p\bar{p}$ collisions

The Drell Yan (DY) process provides further valuable information about PDFs. In pp and  $p\bar{p}$  scattering, the  $Z/\gamma$  and W production probe bi-linear combinations of quarks. Complementary information on the different quark densities can be obtained from W asymmetry (d, u) and their ratio, the ratio of the W and Z cross sections (sensitive to the flavor composition of the quark sea, in particular to the s density), associated W and Z production with heavy quarks (sensitive to s and c quark densities).

Presently, the predictions for Drell-Yan and W and Z production are known NNLO and W, Z in association with heavy flavour quarks are known to NLO. There are several possibilities for obtaining the theoretical predictions for DY production in HERAFitter. At LO an analytic calculation is available within the package and described below:

The LO DY triple differential cross section in invariant mass M, boson rapidity y and Centre of Mass lepton Scattering (CMS) angle  $\cos \theta$ , for NC, can be written as [45, 46]:

$$\frac{d^3\sigma}{dMdyd\cos\theta} = \frac{\pi\alpha^2}{3MS} \sum_q P_q \left[ f_q(x_1, Q^2) f_{\bar{q}}(x_2, Q^2) + (q \leftrightarrow \bar{q}) \right], \tag{4}$$

 $f_q(x_1,Q^2)$  is the parton number density, and  $P_q$  is a partonic 341 in the proton as well as the b-quark PDF. Precise predictions cross section.

The expression for CC scattering has a simpler form:

$$\frac{d^{3}\sigma}{dMdyd\cos\theta} = \frac{\pi\alpha^{2}}{48S\sin^{4}\theta_{W}} \frac{M^{3}(1-\cos\theta)^{2}}{(M^{2}-M_{W}^{2}) + \Gamma_{W}^{2}M_{W}^{2}}$$

$$\sum_{q_{1},q_{2}} V_{q_{1}q_{2}}^{2} f_{q_{1}}(x_{1},Q^{2}) f_{q_{2}}(x_{2},Q^{2}), \tag{5}$$

where  $V_{q_1q_2}$  is the CKM quark mixing matrix and  $M_W$  and  $\Gamma_W$  are W boson mass and decay width.

The simple form of these expressions allows the calculation of integrated cross sections without the use of Monte-Carlo (MC) techniques which often introduce statistical fluctuations. In both NC and CC expressions PDFs factorise as  $_{309}$  functions dependent only on boson rapidity y and invariant Calculations of higher-order electroweak corrections to  $^{310}$  mass M, while the integral in  $\cos \theta$  can be computed analyt-

The NLO and NNLO calculations are highly demanding

### 2.3 Jet production in *ep* and *pp* collisions

Jet production at high transverse momentum is sensitive to  $_{320}$  the high-x gluon PDF (see e.g. [6]) and can thus increase the precision of the gluon PDF determination, which is particularly important for the Higgs production and searches for new physics. Jet production cross sections are only currently 324 known to NLO, although NNLO calculations are now quite advanced [52, 53]. Within HERAFitter the programms such MCFM and NLOJET++ [54, 55] may be used for the calculation of jet production. Similarly to DY case, the calculation is very demanding in terms of computing power. Therefore, to allow the possibility to include ep, pp or  $p\bar{p}$  jet cross sec-330 tion measurements in QCD fits to extract PDF and  $\alpha_s$  fits fast grid techniques are used (see section 4).

# 332 3 Cross sections for top-quark production in pp and $p\bar{p}$ 333 collisions

Top-quark pairs  $(t\bar{t})$  are produced at hadron colliders dominantly via gg fusion and  $q\bar{q}$  annihilation. Measured  $t\bar{t}$  cross sections provide additional constraints in particular on the gluon density at medium to high values of x, on  $\alpha_s$  and on (4) the top-quark mass,  $m_t$ . Single top quarks are produced via electroweak interactions and single-top cross sections can be where S is the squared CMS beam energy,  $x_{1,2} = \frac{M}{\sqrt{S}} \exp(\pm y)$ , used, for example, to probe the ratio of the u and d densities for the total  $t\bar{t}$  cross section have become available to full NNLO recently [56]. They can be used within HERAFitter via an interface to the program HATHOR [57]. Differential  $t\bar{t}$  cross sections and predictions for single-top production can be used with HERAFitter at NLO accuracy from MCFM [48, 58–61] in combination with fast grid techniques.

## 8 4 Computational Techniques

With increased precision of data, the calculations must also progress to higher accuracy, involving an increased number of diagrams with each additional order, and this translates into computationally demanding calculations even for the DIS processes. Such calculations are too slow to be used iteratively in a fit. There are several methods available which allow fast PDF extractions. Two such techniques are implemented into HERAFitter: the k-factor approximation from lower to higher order in theoretical precision and the fast grid techniques using interfaces to the packages fastNLO and APPLGRID. These techniques are briefly described below.

### k-factor technique:

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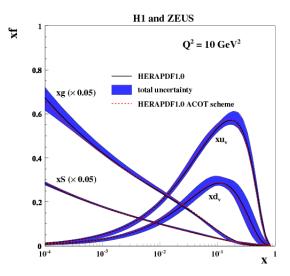
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A k-factor is a ratio of the prediction between a highorder (slow) pQCD calculation and the lowest-order (fast)<sub>394</sub> calculation. These "k-factors" are evaluated as a function of the kinematic variables relevant to the measurement for a fixed PDF (for example the first iteration of the fit) and stored in tables. They can then be applied 'on the fly' to each subsequent fit iteration which will use the fast prediction multiplied by this "k-factor". Having determined a PDF this way the output PDF fit should then be used to recalculate the k-factors and the fit repeated until input and output k-factors have converged.

- For the DIS process, the heavy flavour schemes provide accurate but computationally slow calculations. 404
   In HERAFitter "FAST" schemes were implemented 405
   such that the "k-factors" used can be the ratio between same order calculations but massless vs massive (i.e. NLO (ZM-VFNS)/NLO (ACOT), or the ratio between LO (massless)/NLO (massive). The k 409
   factors are only calculated for the PDF parameters at the first fit iteration and hence, the FAST heavy flavour schemes should only be used for quick checks and the full scheme is recommended. The method 413
   was employed in the QCD fits to the HERA data 414
   when ACOT scheme was used as a cross check of 415
   the central results [21], as shown in Fig. 4.
- In the case of the DY processes the LO calculation 417 described in section 2.2 is such that the PDFs can 418 be factorised, allowing high speed calculations when 419 performing QCD fits over lepton rapidity data. In 420 this case the factorised part of the expression which 421 is independent of PDFs can be calculated only once 422



**Fig. 4** Summary plots of valence, total sea (scaled) and gluon (scaled)densities with their total model uncertainties at the scale of  $Q^2 = 10 \text{ Gev}^2$  obatined using ACOT scheme with k-factor method (red) compared to the HERAPDF1.0 PDF set at NLO using RT scheme

for all minimisation iterations. The leading order code in HERAFitter package implements this optimisation and uses fast convolution routines provided by QCDNUM. Currently the full width LO calculations are optimised for lepton pseudorapidity and boson rapidity distributions with the possibility to apply lepton  $p_{\perp}$  cuts. This flexibility allows the calculations to be performed within the phase space corresponding to the available measurement. The calculated LO cross sections are multiplied by k-factors to obtain predictions at NLO.

## **Fast Grid Techniques:**

- The APPLGRID [62] package allows the fast computation of NLO cross sections for particular processes for arbitrary sets of proton parton distribution functions. The package implements calculations of DY production as well as jet production in  $pp(\bar{p})$  collisions and DIS processes.

The approach is based on storing the perturbative coefficients of NLO QCD calculations of final-state observables measured in hadron colliders in look-up tables. The PDFs and the strong couplings are included during the final calculations, e.g. during PDF fitting. The method allows variation of factorisation and renormalisation scales in calculations.

The look-up tables (grids) can be generated with modified versions of the MCFM parton level generator for DY [47–49] or NLOjet++ [54, 55] code for NLO jet production. The model input parameters are pre-set as usual for MCFM, while binning and definitions of

the cross section observables are set in the APPLGRID 451 code. The grid parameters,  $Q^2$  binning and interpolation orders are also defined in the code.

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APPLGRID constructs the grid tables in two steps: (i) 454 exploration of the phase space in order to optimize 455 the memory storage and (ii) actual grid construction 456 in the phase space corresponding to the requested 457 observables. The NLO cross sections are restored 458 from the grids using externally provided PDFs,  $\alpha_S$ , 459 factorization and renormalization scales. For NNLO 460 predictions k - factors can be applied.

This method was used by the ATLAS collaboration 462 in determining the strange quark density of the pro- 463 ton from W and Z cross sections [22]. An illustration 464 of ATLAS PDFs extracted using k - factor method 465 is shown in Fig. 5 together with the comparison to 466 global PDF sets CT10 [7] and NNPDF2.1 [8].

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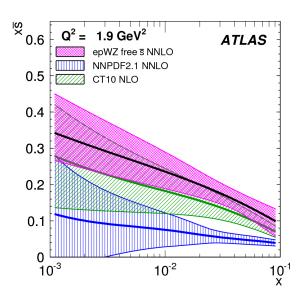


Fig. 5 The strange anti-quark density versus x for the ATLAS epWZ free sbar NNLO fit (magenta band) compared to predictions from NNPDF2.1 (blue hatched) and CT10 (green hatched) at  $Q^2 = 1.9$  $GeV^2$ .

 The fastNLO project [63–65] uses multi-dimensional 471 interpolation techniques to convert the convolutions of perturbative coefficients with parton distribution functions and the strong coupling into simple prod- 472 5 Fit Methodology ucts. The perturbative coefficients are calculated by at  $\mathcal{O}(NNLO)$  for inclusive jet cross sections [68].

The fastNLO libraries are included in the HERAFitter package. In order to include a new measurement into the PDF fit, the fastNLO tables have to be specified. These tables include all necessary information about the perturbative coefficients and the calculated process for all bins of a certain dataset. The fastNLO tables were originally calculated for multiple factors of the factorization scale, and a renormalization scale factor could be chosen freely. More recently, some of the fastNLO tables allow for the free choice [65] of the renormalization and the factorization scale as a function of two pre-defined observables. The evaluation of the strong coupling constant, which enters the cross section calculation, is taken consistently from the QCDNUM evolution code.

The fastNLO methodology were used in the recent CMS analysis with HERAFitter where the impact on the extraction of the PDFs from the inclusive jet cross section is investigated [26]. The impact of the gluon density of CMS inclusive jet data is illustrated in Fig. 6.

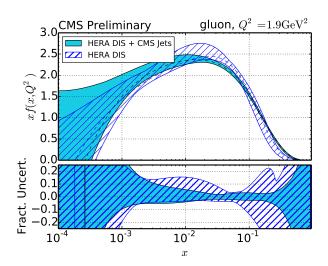


Fig. 6 The gluon density as a function of x as derived from HERA inclusive DIS data alone (cyan) and in combination with CMS inclusive jet data from 2011 (blue hatched) where bands represent the total uncertainty of the PDFs. The PDFs are shown at the starting scale  $Q^2 = 1.9 \text{ GeV}^2$ .

the NLOJET++ program [55] where, in addition to 473 There are considerable number of choices available when the jet production processes available in MCFM, cal- 474 performing a QCD fit analysis which require careful invesculations for jet-production in DIS [66] are avail- 475 tigation (i.e. functional parametrisation form, heavy quarks able as well as calculations for hadron-hadron col- 476 masses, alternative theoretical calculations, method of minlisions [54, 67] which include threshold-corrections 477 imisation, interpretation of uncertaintes etc.). It is desirable to be able to discriminate or quantify the effect of the chosen

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ansatz, ideally within a common framework and HERAFitter<sub>514</sub> is optimally designed for such tests. The methodology em-<sub>515</sub> ployed by HERAFitter relies on a flexible and modular frame<sub>716</sub> work that allows for independent integration of the state-of-<sub>517</sub> the-art techniques, either related to the inclusion of a new <sub>518</sub> theoretical calculation, or to new approaches to treat uncer-<sub>519</sub> tainties

In this section we briefly describe the available options  $^{521}$  in HERAFitter ranging from the functional form used to parametrise PDFs and the choice of the form of the  $\chi^2$  function, to different methods to assess the experimental uncertainties on extracted PDFs.

In addition, as an alternative approach to a complete QCD fit, the reweighting method, which is also available in the  $_{522}$  HERAFitter, is described in this section.

### 5.1 Functional Forms for PDF parametrisation

The PDFs are parametrised at a starting scale which is chosen by the user. Various functional forms can be tested using free parameters to be extracted from the fit:

**Standard Polynomials:** The term standard is understood to refer to a simple polynomial that interpolates between the low and high *x* regions:

$$x f(x) = Ax^{B} (1-x)^{C} P_{i}(x),$$
 (6)

Standard forms are commonly used by PDF groups. The parametrised PDFs at HERA 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  $x\bar{U}=x\bar{u}$ ,  $x\bar{D}=x\bar{d}+x\bar{s}$ . The  $P_i(x)$  for the HERAPDF [21] style takes the simple Regge-inpsired form  $(1+\varepsilon\sqrt{x}+Dx+Ex^2)$  with additional constraints relating to the flavour decomposition of the light sea. For the CTEQ style,  $P_i(x)$  takes the form  $e^{a_3x}(1+e^{a_4}x+e^{a_5}x^2)$ . QCD number and momentum sum-rules are used to determine the normalisations A for the valence and gluon distributions. The sum-rules can be evaluated analytically.

**Log-Normal Distributions:** A bi-log-normal distribution to parametrise the *x* dependence of the PDFs is also available in HERAFitter. This parametrisation is motivated by multiparticle statistics [18]. The following functional form can be used:

$$xf(x) = x^{p-b\log(x)}(1-x)^{q-\log(1-x)}$$
. (7) 539

This function can be regarded as a generalisation of the 541 standard functional form described above. In order to 542 satisfy the QCD sum rules this parametric form requires 543 numerical integration. 544

## **Chebyshev Polynomials:**

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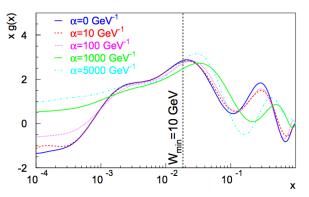
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A flexible Chebyshev polynomial based parametrisation can be used for the gluon and sea densities. The polynomials use  $\log x$  as an argument to emphasize the low x behavior. The parametrisation is valid for  $x>x_{min}=1.7\times 10^{-5}$ . The PDFs are multiplied by (1-x) term to ensure that they vanish as  $x\to 1$ . The resulting parametric form is

$$xg(x) = A_g (1-x) \sum_{i=0}^{N_g-1} A_{g_i} T_i \left( -\frac{2\log x - \log x_{min}}{\log x_{min}} \right), (8)$$

$$xS(x) = (1-x)\sum_{i=0}^{N_S-1} A_{S_i} T_i \left( -\frac{2\log x - \log x_{min}}{\log x_{min}} \right).$$
 (9)

Here the sum over i runs up to  $N_{g,S}=15$  order Chebyshev polynomials of the first type  $T_i$  for the gluon, g, and sea-quark, S, density, respectively. The normalisation  $A_g$  is given by the momentum sum rule. The advantages of this parametrisation are that the momentum sum rule can be evaluated analytically and that for  $N \geq 5$  the fit quality is already similar to the standard Regge-inspired parametrisation with a similar number of parameters. Such study of the parametrisasion uncertainty at low Bjorken  $x \leq 0.1$  for PDFs was presented in [69]. Figure 7 shows that the accuracy of the HERA data allows to determine the gluon density in the kinematic range of  $0.0005 \leq x \leq 0.05$  with a reduced parametrisation uncertainty. An additional regularisation prior leads to a significantly reduced uncertainty for  $x \leq 0.0005$ .



**Fig. 7** Gluon PDF at the scale of  $Q^2 = 1.9 \text{ GeV}^2$  for various values of the length-prior weight using the Chebyshev parametrisation expanded to the 15th order.

External PDFs: HERAFitter also provides the possibility to access external PDF sets, which can be used to construct theoretical predictions for the various processes implemented in HERAFitter. This is possible via an interface to LHAPDF [19, 20] which provides access to the global PDF sets available at LO, NLO or NNLO evolved either locally through the HERAFitter or taken as provided by the LHAPDF grids. Figure 8 is produced

with the drawing tools available in HERAFitter and il- 505 Nuisance Parameters Representation: lustrates the PDFs accessed from LHAPDF.

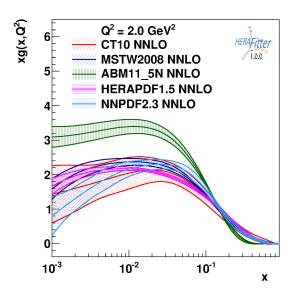


Fig. 8 Gluon density as extracted by various PDF groups at the scale of  $Q^2 = 2 \text{ GeV}^2$ , plotted using the drawing tools from HERAFitter.

# 5.2 $\chi^2$ representation

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The PDF parameters are extracted from a  $\chi^2$  minimization process. For experimental uncertainties there are various forms to represent the  $\chi^2$  function, e.g. using a covariance matrix or representing them by nuisance parameters. In addition, there are various methods to deal with correlated systematic (or statistical) uncertainties (e.g. different scaling options, etc.). Here we summarise the options available in HERAFitter.

Covariance Matrix Representation: For a data point  $\mu_i$ with a corresponding theory prediction  $m_i$ , the  $\chi^2$  function for the case when experimental uncertainties are given as a covariance matrix  $C_{i,j}$  over data bins i and j, can be expressed in the following form:

$$\chi^{2}(m) = \sum_{i,j} (m_{i} - \mu_{i}) C_{ij}^{-1}(m_{j} - \mu_{j}).$$
 (10)

The covariance matrix can be decomposed in statistical, uncorrelated and correlated systematic contributions:

$$C_{ij} = C_{ij}^{stat} + C_{ij}^{uncor} + C_{ij}^{sys}. \tag{11}$$

This representation can not single out the effect of a particular source of systematic uncertainty.

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$$\chi^{2}(m,b) = \sum_{i} \frac{\left[m^{i} - \sum_{j} \gamma_{j}^{i} m^{i} b_{j} - \mu^{i}\right]^{2}}{\delta_{i,\text{stat}}^{2} \mu^{i} \left(m^{i} - \sum_{j} \gamma_{j}^{i} m^{i} b_{j}\right) + \left(\delta_{i,\text{uncor}} m^{i}\right)^{2}} + \sum_{j} b_{j}^{2}.$$
(12)

Here  $\mu^i$  is the measured central value at a point i with relative statistical  $\delta_{i,stat}$  and relative uncorrelated systematic uncertainty  $\delta_{i,unc}$ . Further,  $\gamma_i^i$  quantifies the sensitivity of the measurement  $\mu^i$  at the point i to the correlated systematic source j. The function  $\chi^2$  depends in addition on the set of systematic nuisance parameters  $b_i$ . This definition of the  $\chi^2$  function assumes that systematic uncertainties are proportional to the central prediction values (multiplicative errors), whereas the statistical errors scale with the square root of the expected number

Mixed Form: It can happen that various parts of the systematic and statistical uncertainties are stored in different forms. A situation can be envisaged when the correlated systematic experimental uncertainties are provided as nuisance parameters, but the statistical bin-to-bin correlations are given in the form of a covariance matrix. HERAFitter offers the possibility to include such information, when provided, as well as any other mixed form of treating statistical, uncorrelated and correlated systematic uncertainties.

# 5.3 Treatment of the Experimental Uncertainties

The usage of the nuisance parameters for the experimental uncertainty treatment in QCD fits are quite common and bas an advantage of the flexibile assessment of such uncer-591 tainties on PDFs. Three distinct cases are implemented in 592 HERAFitter and reviewed here: the Hessian, Offset, and Monte Carlo method. Figure 9 illustrates the difference between the Hessian and Monte-Carlo methods both of which can be applied and plotted with HERAFitter.

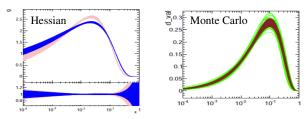


Fig. 9 Differences in the experimental uncertainties on the gluon (left) and d-valence quark (right) densities extracted through different methods in HERAFitter: Hessian(left) versus Monte Carlo (right).

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Hessian method: The technique developed by [70] presents 649 an estimate of PDF uncertainties reflecting the experimental precision of data used in the QCD fit by examining the behaviour of  $\chi^2$  with the nuisance parameter representation (see section 5.2) in the neighborhood of the minimum. The systematic shift nuisance parameters  $b_j$  (Eq. 12) as well as the PDF parameters are free parameters of the fit. Thus the fit determines the best fit to the data taking into account correlated systematic shifts of the data. This is known as Hessian or error matrix method. The Hessian matrix is build by the second derivatives of  $\chi^2$  at the minimum. The PDF eigenvectors are obtained through an iterative procedure used to diagonalise the Hessian matrix and rescale the eigenvectors to adapt the step sizes to their natural scale.

### Offset method:

There is another method to propagate the correlated systematic experimental uncertainties from the measurements to PDFs [71], which has the practical advantage that does not require the inversion of a large measurement covariance matrix. It uses also the  $\chi^2$  function for the central fit for which only uncorrelated uncertainties are taken into account to get the best PDF parameters. The goodness of fit can no longer be judged from the  $\chi^2$  since correlated uncertainties are ignored. The correlated systematic uncertainties of the data are then used to esti- 650 mate the errors on the PDF parameters as follows. The cross section is varied by one sigma shift from the central value for each systematic source and the fit is performed. This is done for both postive and negative one sigma shifts. After this has been done for all sources the resulting deviations of each of these fits from the central PDF parameters are added in quadrature.

In most cases, the uncertainties estimated through the offset method are larger than those from the Hessian method, as the offset method does not use the information on correlated systematic uncertainties optimally.

Monte Carlo method: The PDF uncertainties can be estimated using a Monte Carlo technique [72, 73]. The method consists in preparing replicas of data sets by allowing the central values of the cross sections to fluctuate within their systematic and statistical uncertainties taking into account all point-to-point correlations. The preparation of the data is repeated for a large N > 100 times) and for each of these replicas a NLO QCD fit is performed to extract the PDF set. The PDF central values and uncertainties are estimated using the mean values and RMS over the replicas.

The MC method was checked against the standard error estimation of the PDF uncertainties as used by the Hessian method. A good agreement was found between the methods when employing for the MC approach the assumption that uncertainties (statistical and systematic)

follow Gauss distribution [18]. This comparison is illustrated in Fig. 10.

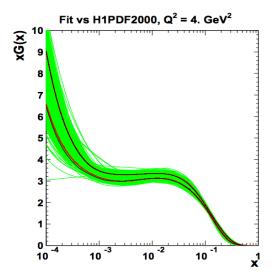


Fig. 10 Comparison between the standard error calculations as employed by the Hessian approach (black lines) and the MC approach assuming Gauss distribution for uncertainty distributions, shown here for each replica (green lines) together with the evaluated the root-mean-square (red lines).

Generally, the experimental uncertainties are symmetrised when QCD fits are performed, however often the provided uncertainties are rather asymmetric. HERAFitter provides possibility to use asymmetric systematic uncertainties. The technical implementation relies on assumption that asymmetric uncertainties can be described by a parabolic function, as given below:

$$f_i(b_j) = \omega_{ij}b_j^2 + \gamma_{ij}b_j, \tag{13}$$

where the coefficients  $\omega_{ij}$ ,  $\gamma_{ij}$  are defined as up and down shifts of the cross sections to a nuisance parameter,  $S_{ij}^{\pm}$ ,

$$\omega_{ij} = \frac{1}{2} \left( S_{ij}^- + S_{ij}^+ \right), \qquad \quad \gamma_{ij} = \frac{1}{2} \left( S_{ij}^- + S_{ij}^+ \right)$$
 (14)

For this case the definition of the  $\chi^2$  from Eq. 12 is extended with the parabolic approximation for asymmetric uncertainties, such that the expected cross section is adjusted to be

$$m_i(1+\sum_j b_j \gamma_{ij}) \to m_i \left(1+\sum_j (b_j(\boldsymbol{\omega}_{ij}b_j+\gamma_{ij})\right).$$
 (15)

The minimisation is performed using x number of iterations, with typical rapid convergence.

## 5.4 Treatment of the Theoretical Input Parameters

The results of a QCD fit depends not only on the input data but also on the input theoretical ansatz, which is also uncertain. Nowadays, modern PDFs try to address the impact of the choices of theoretical parameters by providing alternative PDFs with different choices of the mass of charm  $m_c$ , mass of the bottom quarks  $m_b$  and the value of  $\alpha_S(M_Z)$ , etc. 695 The above mentioned features make HERAFitter a powerfor the PDFs at the starting scale and indeed the value of the starting scale itself. HERAFitter provides a platform in 698 which such choices can readily be varied within a common 699 framework.

## 5.5 Reweighting Techniques

As an alternative to a complete QCD fit, the reweighting  $method \ (Bayesian \ Reweighting) \ is \ available \ in \ HERAFitter. \ _{706} \ tions, fast \ evolution \ kernels, and usage \ of the \ open MP \ (Open \ Appendix \ Appendix$ Because no fit is performed, the method provides a fast estimate of the impact of new data. It was originally developed 708 tions of some of the heavy flavour scheme theory predictions by the NNPDF collaboration [74, 75] and later extended [76] <sub>709</sub> in DIS. to work not only on the NNPDF replicas, but also on the eigenvectors provided by most PDF groups.

The Bayesian Reweighting technique uses the PDF probability distributions which are modified with weights to ac- 710 6 Alternative to DGLAP formalisms count for the difference between theory prediction and new data. In the NNPDF method the PDFs are constructed as 711 Different approaches that are alternative to the DGLAP forage of the predictions obtained from the ensemble  $\langle \mathcal{O}(\text{PDF}) \rangle_{\mp 8}$  of transverse momentum dependent, or unintegrated PDFs,  $\frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} \mathcal{O}(\text{PDF}_k)$ . In the case of PDF uncertainties pro- 715 uPDFs. These approaches are discussed below. vided by standard Hessian eigenvector error sets, this can be achieved by creating the k-th random replica by introducing random fluctuations around the central PDF set.

As a next step, the initial PDF probability distributions are updated by applying weights  $w_k$ , calculated as:

$$w_k = \frac{(\chi_k^2)^{\frac{1}{2}(N_{\text{data}}-1)} \exp^{-\frac{1}{2}\chi_k^2}}{\frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} (\chi_k^2)^{\frac{1}{2}(N_{\text{data}}-1)} \exp^{-\frac{1}{2}\chi_k^2}},$$
(16)

where  $N_{\rm data}$  is the number of new data points, k denotes 722 the specific replica for which the weight is calculated and  $\chi_k^2$ is a difference between a given data point  $y_i$  and its theoretical prediction obtained with the k-th PDF replica:

$$\chi^{2}(y, PDF_{k}) = \sum_{i,j=0}^{N_{\text{data}}} (y_{i} - y_{i}(PDF_{k})) \sigma_{ij}^{-1}(y_{j} - y_{j}(PDF_{k}))$$

based upon a smaller number of PDF sets compared to the 733 called the Bartels-Golec-Kowalski (BGK) dipole model [80].

input because replicas that are incompatible with the data are discarded in order to create a more stream-lined PDF set.

### 5.6 Performance Optimisation

Another important input is the choice of the functional form 696 ful project that encapsulates state of the art developments to debates on reaching the ultimate experimental precision.

> An important factor for a feasible QCD fit which is performed by iterative  $\chi^2$  minimisation, is performance in terms of how long a calculation takes for each given data point. The performance of the HERAFitter code is greatly improved with several special built-in options including the k - factor techniques (see section 4) and the grid techniques 704 for the fast calculation of cross sections of particular pro-705 cesses for arbitrary sets of PDFs. There are also cache op-707 Multi-Processing) interface which allows parallel applica-

ensembles of  $N_{rep}$  parton distribution functions and observ- 712 malism can be used to analyse DIS data in HERAFitter. ables  $\mathcal{O}(PDF)$  are conventionally calculated from the aver- 713 These include several different dipole models and the use

## 716 6.1 DIPOLE models

The dipole picture provides an alternative approach to virtual photon-proton scattering at low x which allows the de-<sub>719</sub> scription of 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 [77]. The dipoles can be viewed as quasi-stable quantum mechanical states, which have very long life time  $\propto 1/m_p x$  and a size which is not changed by scattering. The dynamics of the interaction are embedded in the dipole scattering amplitude.

Several dipole models which assume different behav-127 ior of the dipole-proton cross sections are implemented in HERAFitter: the Golec-Biernat-Wüsthoff (GBW) dipole sat-<sup>729</sup> uration model [78], the colour glass condensate approach (17) 730 to the high parton density regime called the Iancu-Itakura-Munier (IIM) dipole model [79] and a modified GBW model The new, reweighted PDFs commonly are chosen to be 732 which takes into account the effects of DGLAP evolution

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**GBW model:** In the GBW model the dipole-proton cross 764 Generally, the evolution of  $\tilde{\mathscr{A}}(x,k_t,p)$  can proceed via the section  $\sigma_{dip}$  is given by

$$\sigma_{\text{dip}}(x, r^2) = \sigma_0 \left( 1 - \exp\left[ -\frac{r^2}{4R_0^2(x)} \right] \right), \tag{18}$$

here r corresponds to the transverse separation between the quark and the antiquark, and  $R_0^2$  is an x-dependent  $^{\scriptscriptstyle{770}}$ scale parameter which represents the spacing of the gluons in the proton.  $R_0^2(x) = (x/x_0)^{\lambda}$  is called the saturation radius. The fitted parameters are the cross-section normalisation  $\sigma_0$  and  $x_0$  and  $\lambda$ . This model gives exact Bjorken scaling when the dipole size r is small.

**IIM model:** The IIM model assumes an improved expression for the dipole cross section which is based on the for  $\sigma_{\rm dip}$  can be found in [79]. The fitted parameters are an alternative scale parameter  $\tilde{R}$ ,  $x_0$  and  $\lambda$ .

**BGK model:** The BGK model modifies the GBW model 775 density. The dipole cross section is given by

$$\sigma_{\rm dip}(x, r^2) = \sigma_0 \left( 1 - \exp\left[ -\frac{\pi^2 r^2 \alpha_s(\mu^2) x g(x, \mu^2)}{3\sigma_0} \right] \right). \quad (19)$$

The factorization scale  $\mu^2$  has the form  $\mu^2 = C_{bgk}/r^2 +$  $\mu_0^2$ . This model relates to the GBW model using the idea that the spacing  $R_0$  is inverse to the gluon density. The gluon density parametrized at some starting scale  $Q_0^2$  by  $xg(x) = A_g x^{-\lambda_g} (1-x)^{C_g}$  is evolved to larger scales using  $_{780}$ this model are  $\sigma_0$ ,  $\mu_0^2$  and three parameters for the gluon <sub>782</sub> the starting scale  $Q_0$ , of the following form is used: density:  $A_g$ ,  $\lambda_g$ ,  $C_g$ . The parameter  $C_{bgk}$  is kept fixed:  $C_{bgk} = 4.0.$ 

### **BGK** model with valence quarks:

The dipole models are valid in the low-x region only, 784 PDF fits and added to the original BGK model, this is 789 quarks taken from [89]. uniquely possible within the HERAFitter framework.

# <sup>763</sup> 6.2 Transverse Momentum Dependent PDFs with CCFM

Here another alternative approach to collinear DGLAP evolution is presented. In high energy factorization [82] the mea- 793 sections. At HERA about 10% of deep inelastic interactions sured cross section is written as a convolution of the partonic cross section  $\hat{\sigma}(k_t)$ , which depends on the transverse momentum  $k_t$  of the incoming parton, with the  $k_t$ -dependent proton appears well separated from the rest of the hadronic parton distribution function  $\tilde{\mathscr{A}}(x,k_t,p)$  (transverse momen- 797 final state by a large rapidity gap and this is interpreted as tum dependent (TMD) or unintegrated uPDF):

$$\sigma = \int \frac{dz}{z} d^2 k_t \hat{\sigma}(\frac{x}{z}, k_t) \tilde{\mathscr{A}}(x, k_t, p)$$
 (20)

BFKL[?] DGLAP or via the CCFM evolution equations. In HERAFitter, an extension of the CCFM [83–86] evolution has been implemented. Since the evolution cannot be easily obtained in a closed form, first a kernel  $\mathcal{A}(x'', k_t, p)$  is determined from the MC solution of the CCFM evolution equation, and is then folded with a non-perturbative starting distribution  $\mathcal{A}_0(x)$  [87]:

$$x\mathscr{A}(x,k_t,p) = x \int dx' \int dx'' \mathscr{A}_0(x) \widetilde{\mathscr{A}}(x'',k_t,p) \, \delta(x' \cdot x'' - x)$$

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

$$= \int dx' \mathscr{A}_0(x') \cdot \frac{x}{x'} \widetilde{\mathscr{A}}(\frac{x}{x'},k_t,p). \tag{21}$$

Balitsky-Kovchegov equation [81]. The explicit formula  $_{772}$  The kernel  $\mathcal{A}$  includes all the dynamics of the evolution, Sudakov form factors and splitting functions and is determined in a grid of  $50 \otimes 50 \otimes 50$  bins in  $x, k_t, p$ .

The calculation of the cross section according to Eq.(20)by taking into account the DGLAP evolution of the gluon 776 involves a multidimensional Monte Carlo integration which 777 is time consuming and suffers from numerical fluctuations, and therefore cannot be used directly in a fit procedure. Instead the following procedure is applied:

$$\sigma_r(x, Q^2) = \int_x^1 dx_g \mathscr{A}(x_g, k_t, p) \hat{\sigma}(x, x_g, Q^2)$$
$$= \int_x^1 dx' \mathscr{A}_0(x') \cdot \tilde{\sigma}(x/x', Q^2). \tag{22}$$

The kernel  $\tilde{\mathscr{A}}$  has to be provided separately and is not LO or NLO DGLAP evolution. The fitted parameters for  $_{781}$  calculable within the program. A starting distribution  $\mathcal{A}_0$ , at

$$x\mathcal{A}_0(x, k_t) = Nx^{-B_g} \cdot (1 - x)^{C_g} (1 - D_g x)$$
(23)

with free parameters  $N, B_g, C_g, D_g$ .

The calculation of the ep cross section follows eq.(20), where the valence quark contribution is small, of the 785 with the off-shell matrix element including quark masses order of 5%. The new HERA  $F_2$  data have a precision 786 taken from [82] in its implementation in CASCADE [88]. In which is better than 2 %. Therefore, in HERAFitter 787 addition to the boson gluon fusion process, valence quark the contribution of the valence quarks is taken from the 788 initiated  $\gamma q \to q$  processes are included, with the valence

## 790 6.3 Diffractive PDFs

791 Similarly to standard DIS, diffractive parton distributions 792 (DPDFs) can be derived from QCD fits to diffractive cross are diffractive leading to events in which the interacting proton stays intact  $(ep \rightarrow eXp)$ . In the diffractive process the 798 the diffractive dissociation of the exchanged virtual photon 799 to produce a hadronic system X with mass much smaller (20) 800 than W and the same net quantum numbers as the exchanged approach is assumed where diffractive DIS is mediated by 843 PDF sets [91]). the exchange of hard Pomeron or a secondary Reggeon. The 844 factorisable pomeron picture has proved remarkably suc- 845 platform include the following SM processes studied at the cessful in the description of most of these data.

sider the squared four-momentum transfer t (the undetected 848 sults of QCD analyses using HERAFitter are published for momentum transfer to the proton system) and the mass  $M_X$  849 inclusive H1 measurements [27] and the recent combinaof the diffractively produced final state. In practice, the vari- 850 tion of charm production measurements in DIS [28]. The able  $M_X$  is often replaced by  $\beta = \frac{Q^2}{M_X^2 + Q^2 - t}$ . In models based 851 HERAFitter framework also provides an unique possibility to make impact studies for future colliders as illustrated on a factorisable Pomeron,  $\beta$  may be viewed as the fraction <sup>852</sup> ity to make impact studies for future colliders as illustrated of the pomeron longitudinal momentum which is carried by 853 by the QCD studies that have been performed to explore the the struck parton,  $x = \beta x_{IP}$ .

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For the inclusive case, the diffractive cross-section can 855 be expressed as:

$$\frac{d\sigma}{dB\,dO^2 dx_{IP} dt} = \frac{2\pi\alpha^2}{B\,O^4} \left( 1 + (1 - y)^2 \right) \overline{\sigma}^{D(4)}(\beta, Q^2, x_{IP}, t) \quad (24)$$

where the "reduced cross-section",  $\overline{\sigma}$ , is defined as

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

With  $x = x_{IP}\beta$  we can relate this to the standard DIS formula. The diffractive structure functions can be expressed as convolutions of the calculable coefficient functions with diffractive quark and gluon distribution functions, which in general depend on all of  $x_{IP}$ ,  $Q^2$ ,  $\beta$ , t.

The diffractive PDFs in HERAFitter are implemented following the prescription of ZEUS publication [90] and can be used to reproduce the main results.

### 7 Application of HERAFitter

The HERAFitter project has successfully incorporated a wide variety of tools to facilitate investigations of the HEP experimental data and theoretical calculations. It provides data and the derived PDFs in the context of precision QCD 878 We also would like to thank R. Thorne for fruitful discussions theory. The HERAFitter platform not only allows the extraction of PDFs but also of theory parameters such as the strong coupling and heavy quark masses. The parameters and distributions are ouput with a quantitative asssessment of the fit quality with fully detailed information on exper- 880 imental and theoretical uncertainties. The results are also 881 output to PDF grids that can be used to study predictions 882 for SM or beyond SM processes, as well as for the study of 883 the impact of future collider measurements (using pseudo- 884

So far the HERAFitter platform has been used to pro- 886 duce grids from the QCD analyses performed at HERA (HER \*87 APDF series [21]), and their extension to the LHC using 888

photon. For such processes, the proton vertex factorisation 842 measurements from ATLAS [22, 23] (the first ever ATLAS

New results that have been based on the HERAFitter 846 LHC: inclusive Drell-Yan and Wand Z production [22, 24, In addition to the usual variables x,  $Q^2$ , one must con- 847 25]; inclusive jets [23, 26] production. At HERA, the repotential of the LHeC data [92].

In addition, a recent study based on a set of parton dis-856 tribution functions determined with HERAFitter program using HERA data was performed [93]. It addresses the is- $\frac{d\sigma}{d\beta dQ^2 dx_{IP} dt} = \frac{2\pi\alpha^2}{\beta Q^4} \left(1 + (1 - y)^2\right) \overline{\sigma}^{D(4)}(\beta, Q^2, x_{IP}, t)$  (24) 858 sue of correlations between uncertainties for the LO, NLO and NNLO sets. These sets are then propagated to study un-860 certainties for ratios of cross sections calculated at different 861 order in QCD and a reduction of overall theoretical uncer-862 tainty is observed.

### 863 8 Summary

The HERAFitter project is a unique platform for QCD analyses to study the structure of the proton. It incorporates not only the crucial data on Deep Inelastic Scattering from HERA but also data from the hadron colliders which are sensitve to Parton Distribution Functions. A variety of up-to-date the-869 ory calculations are available for each process at LO, NLO and NNLO when possible. HERAFitter has flexible mod-871 ular structure and contains many different useful tools for PDF interpretation. HERAFitter is the first open source platform which is optimal for benchmarking studies.

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### 879 References

- 1. G. Aad et al. [ATLAS Collaboration], Phys.Lett. B716, 1 (2012), [1207.7214].
- 2. S. Chatrchyan et al. [CMS Collaboration], Phys.Lett. **B716**, 30 (2012), [1207.7235].
- 3. J. C. Collins et al. (1989), Factorization of Hard Processes (in QCD in Perturbative Quantum Chromodinamics), ISBN: 9971-50-564-9, 9971-50-565-7.
- 4. E. Perez and E. Rizvi, Rep.Prog.Phys. 76, 046201 (2013), [1208.1178].

897

898

90

920

- (2013), [1301.6754].
- 6. A. Martin, W. Stirling, R. Thorne, and G. Watt, Eur. 943 Phys. J. C 63, 189 (2009), [arXiv:0901.0002], URL 944 http://mstwpdf.hepforge.org/.
- 7. J. Gao, M. Guzzi, J. Huston, H.-L. Lai, Z. Li, et al., 946 http://hep.pa.msu.edu/cteq/public/.
- 8. R. D. Ball, V. Bertone, S. Carrazza, C. S. Deans, 949 34. R. Demina, S. Keller, M. Kramer, S. Kretzer, R. Martin, L. Del Debbio, et al., Nucl. Phys. **B867**, 244 (2013), 950 [1207.1303], URL https://nnpdf.hepforge.org/. 951
- 9. S. Alekhin, J. Bluemlein, and S. Moch (2013), 952 [1310.3059].
- 10. P. Jimenez-Delgado and E. Reya, Phys.Rev. 954 902 D80. 114011 (2009),[0909.1711], URL 955 http://www.het.physik.tu-dortmund.de/ pdfserver/index.html.
- V. N. Gribov and L. N. Lipatov, Sov. J. Nucl. Phys. 15, 958 906 438 (1972).
- 12. V. N. Gribov and L. N. Lipatov, Sov. J. Nucl. Phys. 15, 960 675 (1972). 909
  - 13. L. N. Lipatov, Sov. J. Nucl. Phys. 20, 94 (1975).
- 14. Y. L. Dokshitzer, Sov. Phys. JETP 46, 641 (1977). 911
- 913
- 16. M. Botje (2010), http://www.nikef.nl/h24/qcdnum/index.htm42. H. Spiesberger, Private communication. [arXiv:1005.1481]. 915
- 17. F. James and M. Roos, Comput. Phys. Commun. 10, 968 916 343 (1975).
- 18. M. Dittmar, S. Forte, A. Glazov, G. Moch, S. (conven- 970 918 ers) Altarelli, and others (contributing authors) (2009), [arXiv::0901.2504].
- 19. M. R. Whalley, D. Bourilkov, and R. Group (2005), 973 921 [hep-ph/0508110]. 922
- 20. LHAPDF, URL http://hepforge.cedar.ac.uk/ 923 lhapdf/.
- 21. F. Aaron et al. [H1 and ZEUS Collaborations], JHEP 925 1001, 109 (2010), [arXiv:0911.0884].
- G. Aad et al. [ATLAS Collaboration], Phys. Rev. Lett. 979 927 **109**, 012001 (2012), [arXiv:1203.4051].
- 23. G. Aad et al. [ATLAS Collaboration], Eur. Phys. J. 73, 981 929 2509 (2013), [arXiv:1304:4739]. 930
- 24. G. Aad et al. [ATLAS Collaboration], Phys. Lett. **B725**, 983 931 223 (2013), [arXiv::1305.4192]. 932
- 25. S. Chatrchyan et al. [CMS Collaboration], submitted to 985 Phys. Rev. **D** (2014), [arXiv:1312.6283]. 934
- 26. S. Chatrchyan et al. [CMS Collaboration], CMS PAS 987 SMP-12-028 (2014). 936
- (2012), [arXiv:1206.7007]. 938
- 939 Eur. Phys. J. C73, 2311 (2013), [arXiv:1211.1182].

- 5. S. Forte and G. Watt, Ann.Rev.Nucl.Part.Sci. 63, 291 941 29. R. Devenish and A. Cooper-Sarkar (2011), Deep Inelastic Scattering, ISBN: 0199602255,9780199602254.
  - 30. E. L. et al., Phys. Lett. **B291**, 325 (1992).
  - 31. E. L. et al., Nucl. Phys. **B392**, 162, 229 (1993).
  - 945 32. S. Riemersma, J. Smith, and van Neerven. W.L., Phys. Lett. **B347**, 143 (1995), [hep-ph/9411431].
  - Phys.Rev. **D89**, 033009 (2014), [1302.6246], URL 947 33. J. C. Collins and W.-K. Tung, Nucl. Phys. B **278**, 934 (1986).
    - et al. (1999), [hep-ph/0005112].
    - 35. S. Alekhin, *OPENQCDRAD*, a program description and the code are available via: http://wwwzeuthen.desy.de/~alekhin/OPENQCDRAD.
    - S. Alekhin and S. Moch, Phys. Lett. **B699**, 345 (2011), [arXiv:1011.5790].
    - 37. K. H., N. Lo Presti, S. Moch, and A. Vogt, Nucl. Phys. B864, 399 (2012).

956

965

990

- R. S. Thorne and R. G. Roberts, Phys. Rev. D 57, 6871 (1998), [hep-ph/9709442].
- 39. R. S. Thorne, Phys. Rev. D73, 054019 (2006), [hepph/0601245].
- R. S. Thorne, Phys. Rev. D 86, 074017 (2012), 40. [arXiv:1201.6180]. 963
- 15. G. Altarelli and G. Parisi, Nucl. Phys. B 126, 298 964 41. J. C. Collins, Phys.Rev. D58, 094002 (1998), [hepph/9806259].

  - 43. Jegerlehner, Proceedings, LC10 Workshop DESY 11-**117** (2011).
  - 44. H. Burkhard, F. Jegerlehner, G. Penso, and C. Verzegnassi, in CERN Yellow Report on "Polarization at LEP" 1988.
  - 45. S. D. Drell and T.-M. Yan, Phys. Rev. Lett. 25, 316 (1970).
  - 46. M. Yamada and M. Hayashi, Nuovo Cim. A70, 273 (1982).
  - 47. J. M. Campbell and R. K. Ellis, Phys. Rev. **D60**, 113006 (1999), [arXiv:9905386].
  - 48. J. M. Campbell and R. K. Ellis, Nucl. Phys. Proc. Suppl. 205-206, 10 (2010), [arXiv:1007.3492].
  - J. M. Campbell and R. K. Ellis, Phys. Rev. **D62**, 114012 (2000), [arXiv:0006304].
  - 50. Y. Li and F. Petriello, Phys.Rev. D86, 094034 (2012), [arXiv:1208.5967].
  - 984 51. G. Bozzi, J. Rojo, and A. Vicini, Phys.Rev. **D83**, 113008 (2011), [arXiv:1104.2056].
  - 986 52. A. Gehrmann-De Ridder, T. Gehrmann, E. Glover, and J. Pires, Phys. Rev. Lett. 110, 162003 (2013), [arXiv:1301.7310].
- 27. F. Aaron et al. [H1 Collaboration], JHEP 1209, 061 989 53. E. Glover and J. Pires, JHEP 1006, 096 (2010), [arXiv:1003.2824].
- 28. H. Abramowicz et al. [H1 and ZEUS Collaborations], 991 54. Z. Nagy, Phys.Rev.Lett. 88, 122003 (2002), [hepph/0110315].

- 55. Z. Nagy and Z. Trocsanyi, Phys.Rev. D59, 014020 1046 80. J. Bartels, K. Golec-Biernat, and H. Kowalski, Phys. (1999), [hep-ph/9806317].
- 56. M. Czakon, P. Fiedler, and A. Mitov, Phys. Rev. Lett. 1048 **110**, 252004 (2013), [1303.6254]. 1049

100

101

1029

- 57. M. Aliev, H. Lacker, U. Langenfeld, S. Moch, P. Uwer, 1050 et al., Comput.Phys.Commun. 182, 1034 (2011), 1051 [arXiv:1007.1327].
- 58. J. M. Campbell, R. Frederix, F. Maltoni, and F. Tramon-1053 tano, Phys.Rev.Lett. **102**, 182003 (2009), [0903.0005]. 1054
- 1002 109 (2005), [hep-ph/0506289]. 1003
- 60. J. M. Campbell, R. K. Ellis, and F. Tramontano, 1057 Phys.Rev. **D70**, 094012 (2004), [hep-ph/0408158].
- 61. J. M. Campbell and R. K. Ellis (2012), report 1059 1006 FERMILAB-PUB-12-078-T, [1204.1513].
- 62. T. Carli et al., Eur. Phys. J. C66, 503 (2010), 1061 1008 [arXiv:0911.2985].
- T. Kluge, K. Rabbertz, and M. Wobisch, pp. 483–486 1063 1010 (2006), [hep-ph/0609285].
- 64. M. Wobisch, D. Britzger, T. Kluge, K. Rabbertz, 1065 1012 and F. Stober [fastNLO Collaboration] (2011), 1066 1013 [arXiv:1109.1310].
- 65. D. Britzger, K. Rabbertz, F. Stober, and M. Wobisch 1068 1015 [fastNLO Collaboration] (2012), [arXiv:1208.3641]. 1016
- 66. Z. Nagy and Z. Trocsanyi, Phys.Rev.Lett. 87, 082001 1070 1017 (2001), [hep-ph/0104315].
- Z. Nagy, Phys.Rev. **D68**, 094002 (2003), [hep-1072 1019 ph/0307268]. 1020
- 68. N. Kidonakis and J. Owens, Phys.Rev. D63, 054019 (2001), [hep-ph/0007268]. 1023
- A. Glazov, S. Moch, and V. Radescu, Phys. Lett. B 695, 69. 238 (2011), [arXiv:1009.6170]. 1024
- 70. J. Pumplin, D. Stump, R. Brock, D. Casey, J. Hus-1025 ton, et al., Phys.Rev. D65, 014013 (2001), [hep-1026 ph/0101032].
  - M. Botje, J.Phys. G28, 779 (2002), [hep-ph/0110123].
    - 72. W. T. Giele and S. Keller, Phys.Rev. **D58**, 094023 (1998), [hep-ph/9803393].
- W. T. Giele, S. Keller, and D. Kosower (2001), [hep-73. 1031 ph/0104052].
- 74. R. D. Ball, V. Bertone, F. Cerutti, L. Del Deb-1033 bio, S. Forte, et al., Nucl. Phys. B855, 608 (2012), 1034 [arXiv:1108.1758]. 1035
- 75. R. D. Ball et al. [NNPDF Collaboration], Nucl. Phys. 1036 **B849**, 112 (2011), [arXiv:1012.0836].
- 76. G. Watt and R. Thorne, JHEP 1208, 052 (2012), 1038 [arXiv:1205.4024].
- 77. N. N. Nikolaev and B. Zakharov, Z.Phys. C49, 607 1040 (1991).
- 78. K. Golec-Biernat and M. Wüsthoff, Phys. Rev. D 59, 1042 014017 (1999), [hep-ph/9807513]. 1043
- 79. E. Iancu, K. Itakura, and S. Munier, Phys. Lett. B590, 1044 199 (2004), [hep-ph/0310338]. 1045

- Rev. D 66, 014001 (2002), [hep-ph/0203258].
- 81. I. Balitsky, Nucl. Phys. B 463, 99 (1996), [hepph/9509348].
- 82. S. Catani, M. Ciafaloni, and F. Hautmann, Nucl. Phys. B 366, 135 (1991).
- 1052 83. M. Ciafaloni, Nucl. Phys. B 296, 49 (1988).
  - 84. S. Catani, F. Fiorani, and G. Marchesini, Phys. Lett. B **234**, 339 (1990).
- 59. J. M. Campbell and F. Tramontano, Nucl. Phys. B726, 1055 85. S. Catani, F. Fiorani, and G. Marchesini, Nucl. Phys. B **336**, 18 (1990).
  - 86. G. Marchesini, Nucl. Phys. B **445**, 49 (1995).
  - 87. H. Jung and F. Hautmann (2012), [arXiv:1206.1796].
  - 88. H. Jung, S. Baranov, M. Deak, A. Grebenyuk, F. Hautmann, et al., Eur. Phys. J. C70, 1237 (2010), [arXiv:1008.0152].
  - 89. M. Deak, F. Hautmann, H. Jung, and K. Kutak, Forward-Central Jet Correlations at the Large Hadron Collider (2010), [arXiv:1012.6037].
  - 90. S. Chekanov et al. [ZEUS Collaboration], Nucl. Phys. **B831**, 1 (2010), [hep-ex/09114119].
  - NNLO **ATLAS** epWZ12, availble via: https://lhapdf.hepforge.org/pdfsets.
  - 92. J. L. Abelleira Fernandez et al. [LHeC Study Group], Journal of Phys. G, 075001 (2012), [arXiv:1206.2913].
  - 93. H. Pirumov, M. Lisovyi, A. Glazov, and HERAFitter (2014), [arXiv::1404.XXXX].