Short User Guide for nPDFs in xFitter

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1 Introduction

A new QCD analysis for nuclear parton distribution functions (nPDFs) at next-to-leading order (NLO) and next-to-next-to-leading order (NNLO) was published in [1]. The framework of the analysis, including the form of the parameterization as well as the included DIS datasets, are discussed there. Also the results of that QCD analysis are compared to the existing nPDF sets and to the fitted data in reference [1]. The presented framework is based on xFitter [2, 3] which has been modified to be applicable also for a nuclear PDF analysis. The purpose of this documentation is to provide a short user guide for nPDFs in xFitter. For the general xFitter manual please refer to [4]. A summary of the required modifications can be found in [1].

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2 nPDF Parameterization

Usually, the information on the mass number A and the proton number Z is individual per dataset since different nuclei can be involved in the measured scattering reaction. Therefore, it is recommended to provide A and Z for the particular nucleus inside the dataset file. This option is described in section 3.

In order to activate the nPDF analysis one needs to set the following parameters in the **steering.txt** file:

1. PDFType = 'nucleus'
2. Anucleus = 1.0 [Mass number A, =1 for proton]
3. Znucleus = 1.0 [Proton number Z, =1 for proton]

Please note: there are several nuclei, and not a single one, involved in a global analysis. Therefore, it is strongly recommended to provide the information on the individual combinations of A and Z inside the data files. Here, in the steering.txt file, the parameters Anucleus, Znucleus are used only in case that this information is *not* provided in the data files.

2.1 TUJU19 Framework

As per the current implementation, the nPDFs are available only for the following combination of flags:

4. PDFStyle = 'CTEQ'
5. nTUJU = True [Flag to activate constraints, like e.g. sum rules, in the TUJU19 style [1]]

The extension 'n' in the name of the flag 'nTUJU' symbolizes that 'TUJU' framework has been developed for *nuclear* PDFs. However, the flag 'nTUJU' can be used for both PDFTypes proton and nucleus. If the user does not set the flag 'nTUJU = True' the program will run, but the results might be potentially inconsistent.

By selecting PDFStyle = 'CTEQ' the following parameterization is applied:

$$x f_i^{p/A}\left(x, Q_0^2\right) = c_0\, x^{c_1} (1-x)^{c_2} \left(1 + c_3\, x + c_4\, x^2\right) \tag{1}$$

with $i = g$, u_v d_v $\bar{u}$, $\bar{d}$, s as per TUJU19 framework. A similar ansatz has been used to derive [5]. Note: For 'nTUJU=True' the number of parameters per parton flavour is limited to 5 (c_i with $i = 0, ..., 4$).

The same form of the parameterization (1) is valid for both, proton and nuclear PDFs. The difference appears in regards to the parameters c_i $(i = 0, ..., 4)$. For nuclear PDFs the coefficients in equation (1) are further parameterized to be dependent on the nuclear mass number A as

$$c_k \;\rightarrow c_k(A) = c_{k,0} + c_{k,1}\left(1 - A^{-c_{k,2}}\right) \tag{2}$$

with $k = 0, \ldots, 4$. This form of A-dependent coefficients was used in the nCTEQ15 analysis [6]. This A-dependent parameterization has the advantage that in case of a free proton ($A = 1$) the term $(1 - A^{-c_{k,2}})$ in equation (2) becomes zero and the functional form of a free proton is automatically retained. Here, again $k = 0, \ldots, 4$ is valid only for 'nTUJU=True' setting.

As per the current implementation, nuclear, i.e. A-dependent coefficients are implemented only for the PDFStyle='CTEQ' as described above. For each coefficient in equation (1) one can have two additional A-dependent parameters as per equation (2).

In order to provide the initial parameters the **minuit.in.txt** file is used. The input format of coefficients $c_k \equiv c_{k,0}$ remains unchanged, i.e.:

Parameters	Parton
$1 - 9$	g
$11 - 19$	u_v
$21 - 29$	d_v
$31 - 39$	$\bar{u}$
$41 - 49$	$\bar{d}$
$81 - 89$	s
$90 - 100$	others

These parameters are what one could call coefficients of the PDF for the *free* proton. What is new for nPDFs are the A-dependent coefficients $c_{k,1}$ and $c_{k,2}$. For those the following parameter numbers have been reserved in the **minuit.in.txt** file:

Parameter #	Parameter name	Parton
111, 112	$c_{0,1}$, $c_{0,2}$	g
113, 114	$c_{1,1}$, $c_{1,2}$	
115, 116	$c_{2,1}$, $c_{2,2}$	
117, 118	$c_{3,1}$, $c_{3,2}$	
119, 120	$c_{4,1}$, $c_{4,2}$	
131, 132	$c_{0,1}$, $c_{0,2}$	u_v
133, 134	$c_{1,1}$, $c_{1,2}$	
135 - 140	...	
151, 152	$c_{0,1}$, $c_{0,2}$	d_v
153, 154	$c_{1,1}$, $c_{1,2}$	
155 - 160	...	

and

Parameter #	Parameter name	Parton
171, 172	$c_{0,1}$, $c_{0,2}$	$\bar{u}$
173, 174	$c_{1,1}$, $c_{1,2}$	
175 - 180	...	
189, 190	$c_{0,1}$, $c_{0,2}$	$\bar{d}$, in TUJU19 $\bar{d} = \bar{u}$
191, 192	$c_{1,1}$, $c_{1,2}$	
193 - 198	...	

The $c_{k,1}$ and $c_{k,2}$ parameters for $\bar{d}$ are determined by the constrain $\bar{d} = \bar{u}$ if the parameters for $\bar{d}$ are left empty, i.e. if the normalization parameter $c_{0,0}$ (no 41) is left empty. Due to the limited maximum number of parameter allowed in **minuit.in.txt** file, the $c_{k,1}$ and $c_{k,2}$ coefficients for s have been assigned to the following parameter space:

Parameter #	Parameter name	Parton
129, 130	$c_{0,1}$, $c_{0,2}$	$s = \bar{s}$
149, 150	$c_{1,1}$, $c_{1,2}$	
169, 170	$c_{2,1}$, $c_{2,2}$	
184, 185	$c_{3,1}$, $c_{3,2}$	
186, 187	$c_{4,1}$, $c_{4,2}$	

Please note, that the implemented routine has been validated only for 'nTUJU=True' and 'PDF-STyle =CTEQ' with $c_{k,\max} = 4$. In the general case ('nTUJU=False') the according assignment might change or overlap (especially for s quarks).

Furthermore, please note, that with 'nTUJU=True' the number sum rule and the momentum sum rule are used to constrain the normalizations of d_v, u_v and $\bar{u}$. Furthermore, the constraint $\bar{u} = \bar{d} = s = \bar{s}$ is applied.

The nuclear parton distribution function $f_i^{N/A}$ for a *bound* nucleon inside a nucleus with mass number A is constructed from the *bound* proton's PDF $f_i^{p/A}$ (not from a free proton's PDF f^p). In particular for the distribution of partons in a bound nucleon we write

$$f_i^{N/A}\left(x, Q^2\right) = \frac{Z \cdot f_i^{p/A} + (A - Z) \cdot f_i^{n/A}}{A}\,, \tag{3}$$

where Z is the number of protons in the nucleus. The PDF of the *bound* neutron $f_i^{n/A}$ is determined from the fitted proton's PDF using the isospin symmetry.

This nucleon decomposition has been implemented in xFitter for the calculation of DIS cross sections by using the following heavy-quark schemes only: '**ZMVFNS**' scheme and '**FONLL**' scheme. For the other schemes available in xFitter, the nucleon decomposition has not been implemented/validated.

2.2 TUJU19 Example

The first nuclear PDFs 'TUJU19' obtained with xFitter have been published in [1]. The according minuit.in.TUJU19-(N)NLO.txt and the steering.TUJU19-(N)NLO input files are placed inside the folder 'input_steering'. The minuit.in.txt files include the final parameters obtained during the fit (*not* the initial values used for that). Furthermore, in order to run the according calculations it is necessary to configure xFitter with the settings '–enable-apfel' (since FONLL scheme has been used in the TUJU19 fit) and also '–enable-lhapdf'.
Please note that the results published in [1] have been obtained by the numerical tool set based on xFitter version 2.0.0, whereas the released version is based on xFitter 2.0.1. Therefore, minor numerical deviations in the χ^2 values are possible.

2.3 nCTEQ Flags

The parameterization described in subsection 2.1 has been tested, verified and the results have been published officially [1]. However, during the code modification and testing phase, also parts of the nCTEQ15 framework [6] have been implemented in xFitter for *testing* purposes only. The according flags and options are described in this subsection. Please note: that the results do *not* reflect the full nCTEQ15 framework nor the officially published results. They provide only an additional setup for testing purposes.

The available nCTEQ flags are meant to be used in conjunction with the flags $1-4$ described in subsection 2.1. The flag

5. nCTEQ = True

needs to be used instead of nTUJU, i.e. with nTUJU=False. The combination of PDFStyle = 'CTEQ' and nCTEQ = True leads to the PDF parameterization of the form

$$x f_i^{p/A}\left(x, Q_0^2\right) = c_0\, x^{c_1} (1-x)^{c_2} e^{c_3 x}\, (1 + e^{c_4}\, x)^{c_5} \tag{4}$$

for $i = u_v$, d_v, g, $\bar{u}$, $\bar{d}$, $s + \bar{s}$ with A-dependentn coefficients c_i $(i = 0, \ldots, 5)$ as given in equation (2).

The flag 'nCTEQ=True' activates all options described in the following. Alternatively, also subsets can be used by setting

- nCTEQparams = True, or
- nCTEQframework = True

only. The flag '**nCTEQframework**' activates the sum rules of the style as given in equations (2.10) and (2.11) of the original publication [6] and the constraint $s = \bar{s} = \frac{\kappa(A)}{2}\left(\bar{u} + \bar{d}\right)$ with $\kappa(A) = c_{0,0}^{s+\bar{s}} + c_{0,1}^{s+\bar{s}}\left(1 - A^{-c_{0,2}^{s+\bar{s}}}\right)$. Here, one needs to mention that especially the latter relation could *not* be reproduced completely for all nuclei, but was fixed manually by reverse engineering for a set of selected nuclei, which was sufficient for testing purposes. This flag can be activated intependent of the nCTEQ=True setting, if required.

The flag '**nCTEQparams**' changes how the input parameters from minuit.in.txt file are interpreted. Here, the following logic is applied:

Parameter #	Parameter name	Parton
$1-6$	$c_{i,0}$	g
7	M_g	as used in Eq. (2.10) in Ref. [6]
$11-19$	$c_{i,0}$	u_v
$21-29$	$c_{i,0}$	d_v
$31-39$	$c_{i,0}$	$\bar{u}+\bar{d}$
$41-49$	$c_{i,0}$	$\bar{d}/\bar{u}$
$81-89$	$c_{i,0}$	$s+\bar{s}$
$90-100$	others	-

and

Parameter #	Parameter name	Parton
113, 114	$c_{1,1}$, $c_{1,2}$	g
115, 116	$c_{2,1}$, $c_{2,2}$	
117, 118	$c_{3,1}$, $c_{3,2}$	
119, 120	$c_{4,1}$, $c_{4,2}$	
123	$c^g_{0,0}$	as used in Eq. (2.10) in Ref. [6]
124	$c^g_{0,1}$	as used in Eq. (2.10) in Ref. [6]
125	$c^g_{0,2}$	as used in Eq. (2.10) in Ref. [6]
131, 132	$c_{0,1}$, $c_{0,2}$	u_v
133, 134	$c_{1,1}$, $c_{1,2}$	
135 - 140	...	
151, 152	$c_{0,1}$, $c_{0,2}$	d_v
153, 154	$c_{1,1}$, $c_{1,2}$	
155 - 160	...	
171, 172	$c_{0,1}$, $c_{0,2}$	$\bar{u}+\bar{d}$
173, 174	$c_{1,1}$, $c_{1,2}$	
175 ...	...	
155 - 160	...	
189, 190	$c_{0,1}$, $c_{0,2}$	$\bar{d}/\bar{u}$
191, 192	$c_{1,1}$, $c_{1,2}$	
193 ...	...	
129, 130	$c_{0,1}$, $c_{0,2}$	$s+\bar{s}$
149, 150	$c_{1,1}$, $c_{1,2}$	
169, 170	$c_{2,1}$, $c_{2,2}$	
184, 185	$c_{3,1}$, $c_{3,2}$	
186, 187	$c_{4,1}$, $c_{4,2}$	

as per Tab. V. in Ref. [6]. The input parameters of the form $\bar{u} + \bar{d}$ and $\bar{d}/\bar{u}$ are used to construct the output for $\bar{u}$ and $\bar{d}$. If input parameters for $s + \bar{s}$ are left empty in the minuit.in.txt file the constraint $s = \bar{s} = \frac{\kappa(A)}{2}\left(\bar{u} + \bar{d}\right)$ is applied.

Summary: The flag 'nCTEQ=True' activates all options described in this subsection. Alternatively, also a subset can be activated by using the flags 'nCTEQparams' and/or 'nCTEQframework'. Please note that the results do *not* reflect the full nCTEQ15 framework nor the officially published results [6]. They provide only an additional setup for testing purposes only.

3 Nuclear Data

For nuclear data, the experimental measurements are often published for a ratio of a cross section measured on one nucleus with mass number A_1 to the cross section of the other nuclear target A_2, i.e. $\sigma(A_1)/\sigma(A_2)$ for cross sections or $F_2(A_1)/F_2(A_2)$ for structure functions. In such a case, inside the data file one would not provide a single observable, but a ratio of two observables. As part of the fitting routine, the quantities inside the data files are compared to the calculated theoretical values. In order to have a consistent comparison one needs to identify inside the data file if the bin 'Sigma' is a ratio or not. For a ratio it needs to be set:

CInfo = 'ratio'

DataInfo = 1.0 [and 0.0 for an absolute cross section].

The information on Z_1, A_1 and Z_2, A_2 (if applicable) is also provided inside the data file:

CInfo = 'A1', 'Z1', 'A2', 'Z2'

DataInfo = 56., 26.0, 12.0, 6.0 [an example for $\sigma(Fe)/\sigma(C)$].

Besides that, some experiments apply isoscalar corrections to the measured data and publish only the modified information. Thus, the analysis procedure has been adapted so that the theoretically calculated quantities are consistent with the iso-corrected experimental data. For this purpose, different flags were introduced in xFitter for the different forms of isoscalar corrections, which are specific to the corresponding experiments (CInfo='NMC', 'EMC', 'SLAC'). For the explicit form of the isoscalar correction please refer to the TUJU19 publication [1]. The information if or if not an isoscalar flag needs to be applied is provided by the particular experimental publication. In order to set the corresponding flag CInfo and DataInfo are used:

CInfo = 'NMC' [or 'EMC' or 'SLAC' respectively]

DataInfo = 1.0 [if True, and 0.0 if False].

Eventually, another modification on xFitter was necessary for the treatment of charged current DIS processes measured in neutrino-nucleus scattering reactions. As part of this framework, the differential cross sections $\mathrm{d}\sigma^2/\mathrm{d}y\mathrm{d}Q$ were used for the analysis. In order to identify the corresponding reaction one needs to specify inside the data file:

Reaction = 'antineutrino+p CC' [or Reaction = 'neutrino+p CC'].

Please note that these additional processes have been implemented only for the two heavy-quark schemes 'ZMVFNS' and 'FONLL'. When using another scheme available in xFitter an error message might probably occur.

4 Output and Error Analysis

When running the analysis routine for nPDFs in xFitter the file minuit.out.txt will automatically contain all final parameters (proton and nuclear parameters). Files containing PDFs, originally named 'pdfs_q2val_0i.txt', are named 'A-XXX_pdfs_q2val_0i.txt' where XXX is the nuclear mass number (e.g. 2 for D, and 208 for Pb). During the Hessian error analysis, there are also PDF files generated, those do not carry an A-dependent extension, but are valid for the nucleus used last in the series of data files. This is due to the reason, that one would need an additinal loop over all nuclei in the error analysis routine which is not implemented yet. A workaround exists by running the error analysis part ('DoBands=True') changing the series of data files, so that every time another nucleus is listed last. The same is valid for the generated output in the LHAPDF format. The central PDF members and the *.info files are generated for all nuclei and are stored in folders named 'A-XXX_xfitter_pdf', whereas the error set members are created only for the last nucleus on the list. This is valid for the Hessian error analysis only. If the Monte Carlo (MC) error analysis method is used, all nuclei are covered simultaneously. The text files containing PDFs and the grids in LHAPDF format are generated for the partons in a nucleon (*not* proton).

For nuclear PDFs the Hessian error analysis is usually performed with $\Delta\chi^2 > 1$. The error bands routine has been modified accordingly so that scaling based on the quadratic approximation is applied (please refer to [1] for more details). In order to set the $\Delta\chi^2$ parameter the command

set errdef 10.0 [for example]

can be used in the minuit.in.txt file.

5 Change Log

The modifications described here have been applied on xFitter versoin 2.0.1.

Modified header and include files:

- include/c_interface.inc
- include/dimensions.h
- include/indata.inc
- include/pdfparam.inc
- include/qcdnumhelper.inc

- include/steering.inc
- include/theo.inc
- include/theorexpr.inc
- include/xfitter_cpp.h

Modified source code files (bold items have been modified largely):

- interfaces/src/hf_pdf_calls.f
- src/c_interface.f
- src/chi2scan.cc
- src/dataset_tools.f
- **src/dis_sigma.f**
- src/error_bands_pumplin.f
- src/evolution.f
- **src/fcn.f**
- src/lhapdf6_output.c
- src/lhapdferrors.cc
- **src/pdf_param.f**
- src/read_data.f
- src/read_steer.f
- **src/sumrules.f**
- src/theory_dispatcher.f

New source code files:

- src/nucl_pdf.f
- src/nucl_pdfcc.cc (optional, requires gsl libraries)

Additionally, files Makefile.in and Makefile.am in the src/ folder have been modified in order to add new source code files.

References

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