The Les Houches Accord PDFs (LHAPDF) and LHAGLUE

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Abstract

We describe the development of the LHAPDF library from its initial implementation following the Les Houches meeting in 2001 to its present state as a functional replacement for PDFLIB. Brief details are given of how to install and use the library together with the PDF sets available. We also describe LHAGLUE, an add-on PDFLIB look-a-like interface to LHAPDF, which facilitates using LHAPDF with existing Monte Carlo generators such as PYTHIA and HERWIG.

1   LHAPDF – Introduction

Parton Density Functions (PDFs), which describe the partonic content of hadrons, need to be well understood and of sufficiently high precision if theoretical predictions are to match the experimental accuracies expected from future LHC data. These PDFs, which are produced by several different groups (e.g. MRST, CTEQ, Alekhin and more recently ZEUS and H1), are derived from fitting deep inelastic and related hard scattering data using parameterisations at low Q_0^2 ($\approx$ 1–7 (GeV/c)^2) and evolving these to higher Q^2. These PDFs are typically presented as grids in x-Q^2 with suitable interpolation codes provided by the PDF authors. The CERN PDFLIB library [1] has to date provided a widely used standard FORTRAN interface to these PDFs with the interpolation grids built into the PDFLIB code itself. However, it is realised that PDFLIB would be increasingly unable to meet the needs of the new generation of PDFs which often involve large numbers of sets ($\approx$20–40) describing the uncertainties on the individual partons from variations in the fitted parameters. As a consequence of this, at the Les Houches meeting in 2001 [2], the beginnings of a new interface were conceived — the so-call "Les Houches Accord PDF"— LHAPDF. This has further been developed over the course of the HERA-LHC workshop incorporating many new features to enable it to replace PDFLIB as the standard tool to use. The development is briefly described in this writeup together with LHAGLUE, an interface to LHAPDF, which provides PDF access using almost identical calling routines as PDFLIB.

2   LHAPDF – Development during the Workshop

In its initial incarnation (Version 1), LHAPDF had two important features which distinguished it from the methods used by PDFLIB in handling PDFs.

Firstly the PDFs are defined by the analytical formulae used in the original fitting procedures, with external files of parameters, which describe the momentum x distributions of the partons at the relevant Q_0^2. Evolution codes within LHAPDF then produce the PDF at any desired Q^2 at the users request. At present LHAPDF provides access to two evolution codes, EVLCTEQ for the CTEQ distributions and QCDNUM 16.12 [3] for the other PDF sets. This represents a radical difference from the existing methods used by the PDF authors to present their distributions where large grid files and interpolation routines are the norm. In PDFLIB these interpolation codes and grids are essentially compiled into a single FORTRAN library. The advantage of the LHAPDF method is that the compiled code is separate from the parameter files, which are typically small. Thus to add new PDF sets does not necessarily need the code to be recompiled and the library rebuilt.

Secondly, the concept is introduced of a "set" being a related collection of PDFs (e.g. an error set) all of which are accessible to the program after initialisation of that set. This allows LHAPDF to

handle the multi-set "error" PDFs produced in recent years which give predicted uncertainties to the PDF values. All the PDFs in a set are initialised together and are therefore available to the user.

V1 was written by Walter Giele of Fermilab who in 2002 released a working version which could be downloaded from a web-site together with the parameter files for a limited number of PDF sets. There was also a manual and example files. One of the present authors MRW became involved and took over maintenance and development of LHAPDF in March 2003. The limitations of the idealised situation in V1 with respect to making LHAPDF a replacement tool for PDFLIB soon became apparent.

The primary problem was that V1 contained only a limited number of PDF sets and, since the method was reliant on the x parameterisations at Q_0^2 being available, it would be virtually impossible to include many of the older sets which are still needed for comparisons. A second and serious problem is the compute time taken in the initialisation phase of the individual members of a PDF set (i.e. calling the routine InitPDF described later). This can take in the region of 2 seconds per call on a 1GHz machine and is therefore unacceptable in the situation of a program which makes repeated use of the different members. [1]

A solution introduced in LHAPDF Version 2, which helps to solve the above problems, was to include the option to make the original grid files and interpolation codes available in LHAPDF **in addition** to the V1 method of parameter files and "on-the-fly" evolution. For some PDF sets both methods would be available and for others only the latter. The operation of the program was made identical for both methods with the content of the input file (with extension ".LHpdf" for the former and ".LHgrid" for the latter) dictating which is used. Not only does this allow all the older PDF sets to be included but also there is no time penalty in changing between members of the same set since all are loaded in the initialisation phase. LHAPDF V2 was released in March 2004 including many of the older PDF sets as well as some new ones.

LHAPDF Version 3 was released in September 2004 and, as well incorporating more older and some new PDF sets (e.g. ZEUS and H1), it also included the code for LHAGLUE, a newly developing add-on interface to LHAPDF which provides PDFLIB look-alike access. In addition to having subroutine calls identical to those in PDFLIB it also incorporates a PDF numbering scheme to simplify usage. It should be noted however that, because of the greatly increased number of new PDF sets, it was not possible to follow the original numbering scheme of PDFLIB and a new one was devised. This is described in more detail in Section 5.

The major feature of Version 4, which was released in March 2005, was the incorporation of the photon and pion PDFs. All the photon and pion PDFs that were implemented in PDFLIB were put into LHAPDF using identical code and using the ".LHgrid" method. The LHAGLUE numbering scheme in these cases more closely resembles that of PDFLIB than it does for the protons.

In addition in V4 there were new proton PDFs (MRST2004 and an updated Alekhin's a02m), a new simpler file structure with all the source files being in a single "src" directory, some code changes to incorporate access to $\Lambda_{4/5}^{QCD}$ and a more rigorous implementation of the α_s evolution as being exactly that used by the PDF author.

All the LHAPDF and LHAGLUE data and code, in addition to being made available on the new web site (http://hepforge.cedar.ac.uk/lhapdf/), is also included in the GENSER subproject of the LHC Computing Grid.

3 LHAPDF – Development after the Workshop

Since the last HERA-LHC meeting there has been one minor release of LHAPDF (Version 4.1 in August 2005). In this version the installation method has changed to be more standard with the "configure; make;

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[1]A third problem reported at the workshop concerning small differences (up to $\approx 0.5\%$) between the PDFs produced by LHAPDF for MRST and the authors' code directly is now believed to be due to slight mismatches of grid boundaries at the heavy quark thresholds and will be corrected in future MRST grids.

make install" sequence familiar to many and also a small amount of code has been altered to be more compliant with proprietary FORTRAN 95 compilers. As mentioned in the previous section the web site for public access to LHAPDF from which the source code can be obtained has changed. Since this is the current and most recent version we assume V4.1 in the following referring to earlier versions where necessary.

4 Using LHAPDF

Once the code and PDF data sets have been downloaded from the relevant web site and installed following the instructions given therein, using LHAPDF is simply a matter of linking the compiled FORTRAN library **libLHAPDF.a** to the users program. Table 1 lists the LHAPDF routines available to the user, which are of three types:

– Initialisation (selecting the required PDF set and its member)
– Evolution (producing the momentum density functions (f) for the partons at selected x and Q)
– Information (displaying for example α_s, descriptions, etc.)

Table 1: LHAPDF commands

Command	Description
call InitPDFset(name **)**	Initialises the PDF set to use.
call InitPDF(member **)**	Selects the member from the above PDF set.
call evolvePDF(x,Q,f **)**	Returns the momentum density function, $f(x, Q)$, for protons or pions.
call evolvePDFp(x,Q,P2,ip2,f **)**	Returns the momentum density function for photons[2].
call numberPDF(num **)**	Returns the number (num) of PDF members in the set.
call GetDesc( )	Prints a description of the PDF set.
alphasPDF(Q **)**	Function giving the value of α_s at Q GeV.
call GetLam4(mem,qcdl4 **)**	Returns the value of Λ_4^{QCD} for the specific member.
call GetLam5(mem,qcdl5 **)**	Returns the value of Λ_5^{QCD} for the specific member.
call GetOrderPDF(order **)**	Returns the order of the PDF evolution.
call GetOrderAs(order **)**	Returns the order of the evolution of α_s .
call GetRenFac(muf **)**	Returns the renormalisation factor.
call GetQmass(nf,mass **)**	Returns the mass of the parton of flavour nf.
call GetThreshold(nf,Q **)**	Returns the threshold value for parton of flavour nf.
call GetNf(nfmax **)**	Returns the number of flavours.

The evolution commands utilise a double precision array *f(-6:6)* where the arguments range from -6 to +6 for the different (anti)partons as shown in Table 2 below.

Table 2: The flavour enumeration scheme used for *f(n)* in LHAPDF

parton	$\bar{t}$	$\bar{b}$	$\bar{c}$	$\bar{d}$	$\bar{u}$	$\bar{d}$	g	d	u	s	c	b	t
n	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6

Specifying the location of the PDF sets in the code should be especially mentioned at this point. The argument (*name*) in **InitPDFset** should specify the complete path (or at least to a symbolic link to this

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[2]In **evolvePDFp** $P2$ is the vitruality of the photon in GeV ^{2}, which should by 0 for an on-shell photon, and *ip2* is the parameter to evaluate the off-shell anomalous component. See the PDFLIB manual [1] for details.

path). From version 4.1 onwards, however, a new routine **InitPDFsetByName** can be used in which only the name of the PDF set need by specified. This works in conjunction with the script 'lhapdf-config' which is generated at the configure stage of the installation which provides the correct path to the PDF sets. The location of this script must therefore be in the users execution path. Tables 3 and 4 list the complete range of PDF set available. The equivalent numbers to use in LHAGLUE, as described in the next section, are also listed in these tables.

Table 3: The Proton PDF sets available in LHAPDF.

Ref	Prefix	Suffix (number of sets)	type	LHAGLUE numbers
[4]	alekhin‗	100 (100), 1000 (1000)	p	**40100-200, 41000-1999**
[5]	a02m‗	lo (17), nlo (17), nnlo (17)))	g	40350-67, 40450-67, 40550-67
[6]	botje‗	100 (100),1000 (1000)	p	**50100-200, 51000-1999**
[7]	cteq	61 (41)	p,g	**10100-40**, 10150-90
[8]	cteq	6 (41)	p,g	**10000-40**, 10050-90
	cteq	6m, 6l, 6ll	p	**10000, 10041, 10042**
[9]	cteq	5m, 5m1, 5d, 5l	g	19050, 19051, 19060, 19070
[10]	cteq	4m, 4d, 4l	g	19150, 19160, 19170
[11]	fermi2002‗	100 (100), 1000 (1000)	p	**30100-200, 31000-2000**
[12]	GRV98	lo, nlo(2)	g	80060, 80050-1
[13]	H12000	msE (21), disE (21), loE (21)	g	70050-70, 70150-70, 70250-70
[14]	MRST2004	nlo	p,g	**20400**, 20450
	MRST2004	nnlo	g	20470
[15]	MRST2003	cnlo	p,g	**20300**, 20350
	MRST2003	cnnlo	g	20370
[16]	MRST2002	nlo (2)	p,g	**20200**, 20250
	MRST2002	nnlo	g	20270
	MRST2001	E (31)	p,g	**20100-130**, 20150-180
[17]	MRST2001	nlo(4)	p,g	**20000-4**, 20500-4
	MRST2001	lo, nnlo	g	20060, 20070
[18]	MRST98	(3)	p	**29000-3**
	MRST98	lo (5), nlo (5) dis (5), ht	g	29040-5, 29050-5,29060-5,29070-5
[19]	ZEUS2002‗	TR (23), FF (23), ZM (23)	p	**60000-22, 60100-22, 60200-22**
[20]	ZEUS2005‗	ZJ (23)	p	**60300-22**

Notes:
    LHAPDF → PrefixSuffix.LHpdf (type p),   filename → PrefixSuffix.LHgrid (type g).
    Where both p and g are present (p,g) the user has the choice of either.
    LHAGLUE numbers in **bold** are the type p (.LHpdf) sets.

5 LHAGLUE

The LHAGLUE interface [21] to LHAPDF is designed along the lines of the existing interface from PYTHIA to PDFLIB. [3]. For both HERWIG and PYTHIA the existing 'hooks' for PDFLIB have been utilised for the LHAGLUE interface. This makes it possible to link it exactly like PDFLIB with no further changes to PYTHIA's or HERWIG's source code needing to be implemented.

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[3]DB would like to thank T. Sjöstrand and S. Mrenna for discussions on this topic.

Table 4: The Pion and Photon PDF sets available in LHAPDF.

Prefix	Suffix	LHAGLUE numbers	Prefix	Suffix	LHAGLUE numbers
Pion PDFs			**Photon PDFs**		
OWPI	(2)	211-12	DOG	0, 1	311, 312
SMRSPI	(3)	231-3	DGG	(4)	321-4
GRVPI	0, 1	251, 252	LACG	(4)	331-4
ABFKWPI	(3)	261-3	GSG	0 (2), 1	341-2, 343
All filenames are PrefixSuffix.LHgrid			GSG96	0, 1	344, 345
The nomenclature used here is			GRVG	0 (2), 1 (2)	351-2, 353-4
essentially the same as in PDFLIB and			ACFGPG	(3)	361-3
the relevant publication references			WHITG	(6)	381-6
can be found in the PDFLIB manual [1].			SASG	(8)	391-8

The interface contains three subroutines (similar to PDFLIB) and can be used seamlessly by Monte Carlo generators interfaced to PDFLIB or in standalone mode. These are described in Table 5. In addition any of the LHAPDF routines, **except** the initialisation routines **InitPDFset** and **InitPDF**, described in Table 1, can also be used, for example to return the value of the strong coupling constant α_s (**alphasPDF**(Q)), or to print the file description (**call GetDesc()**).

There are also several CONTROL switches specified through the 20 element character array LHA-PARM and COMMON blocks which determine how the interface operates.

– Location of the LHAPDF library of PDFs (pathname):
  From version LHAPDF v4.1 onwards, and the LHAGLUE routines distributed with it, the location of the PDFsets data files is set automatically using the "lhapdf-config" script as described in the previous section, provided that the prescribed installation instructions have been used.
  For previous versions (4.0 and earlier) the common block **COMMON/LHAPDFC/LHAPATH** is used where **LHAPATH** is a **character*132** variable containing the full path to the PDF sets. The default path is subdir 'PDFsets' of the current directory.

– Statistics on under/over-flow requests for PDFs outside their validity ranges in x and Q^2.
  a) **LHAPARM(16) .EQ. 'NOSTAT'** → No statistics (faster)
  b) **LHAPARM(16) .NE. 'NOSTAT'** → Default: collect statistics
  c) **call PDFSTA** at the end to print out statistics.

– Option to use the values for α_s as computed by LHAPDF in the Monte Carlo generator as well in order to ensure uniform α_s values throughout a run
  a) **LHAPARM(17) .EQ. 'LHAPDF'** → Use α_s from LHAPDF
  b) **LHAPARM(17) .NE. 'LHAPDF'** → Default (same as LHAPDF V1/V3)

– Extrapolation of PDFs outside the LHAPDF validity range given by $x_{min/max}$ and $Q^2_{min/max}$.
  a) Default → PDFs "frozen" at the boundaries.
  b) **LHAPARM(18) .EQ. 'EXTRAPOLATE'** → Extrapolate PDFs at own risk

– Printout of initialisation information in PDFSET (by default)
  a) **LHAPARM(19) .EQ. 'SILENT'** → No printout (silent mode).
  b) **LHAPARM(19) .EQ. 'LOWKEY'** → Print 5 times (almost silent).

– Double Precision values of $\Lambda^{QCD}_{4/5}$ applicable to the selected PDF are available (as read-only) in the COMMON block: **COMMON/W50512/QCDL4,QCDL5** → as in PDFLIB.

Table 5: LHAGLUE commands

Command	Description
call PDFSET(*parm,value)*	For initialisation (called once) where PARM and VALUE are LOCAL arrays in the calling program specified as **CHARACTER*20 PARM(20)** **DOUBLE PRECISION VALUE(20)**
call STRUCTM(*X,Q,UPV,DNV,USEA,DSEA,STR,CHM,BOT,TOP,GLU)*	For the proton (and pion) PDFs: where X and Q are the input kinematic variables and the rest are the output PDF of the valence and sea quarks and the gluon.
call STRUCTP(*X,Q2,P2,IP2,UPV,DNV,USEA,DSEA,STR,CHM,BOT,TOP,GLU)*	For the photon PDFs: as above with the additional input variables P2 and IP2 [2].

The LHAGLUE interface can be invoked in one of 3 ways, Standalone, PYTHIA or HERWIG, depending on the value of *parm(1)* when calling **PDFSET**(*parm,value).*

- **Standalone** mode
  PARM(1)= 'DEFAULT'
  VALUE(1) = "*PDF number*"
- **PYTHIA mode**
  PARM(1) = 'NPTYPE' ← set automatically in PYTHIA
  In this case the user must supply MSTP(51) and MSTP(52) in the PYTHIA common block
  COMMON/PYPARS/MSTP(200),PARP(200),MSTI(200).PARI(200)
  MSTP(52) = 2 ← to use an external PDF library
  MSTP(51)= "*PDF number*"
- **HERWIG mode**
  PARM(1) = 'HWLHAPDF'← set by the user.
  In this case one sets for the beam and target particles separately
  AUTPDF(1) = 'HWLHAPDF'
  AUTPDF(2) = 'HWLHAPDF'
  MODPDF(1) = "*PDF number*"
  MODPDF(2) = "*PDF number*"
  Note that HERWIG specifies the"*PDF number*" for each of the colliding particles separately and care should be taken that the same PDF members are used when appropriate.

The user then simply links their own standalone code, or the HERWIG/PYTHIA main program and the HERWIG/PYTHIA code [4], with the LHAPDF library **libLHAPDF.a** making sure the 'PDFsets' directory is specified as described above.

The LHAGLUE interface has been tested extensively at TEVATRON and LHC energies for the proton PDFs and with HERA examples for the photon PDFs. Results with new and legacy PDF sets, using LHAPDF, PDFLIB or internal implementations in the Monte Carlo generators, and comparing cross sections produced with PYTHIA and HERWIG, give us confidence in the consistency of the LHAGLUE interface and the underlying LHAPDF library [22].

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[4]It is important when starting with a fresh PYTHIA or HERWIG download the user must first rename the 'dummy' subroutines **STRUCTM**, **STRUCTP** and **PDFSET** in the PYTHIA/ HERWIG source codes exactly as if one were to link to PDFLIB.

6 Summary and Future Development

Both LHAPDF and the interface LHAGLUE have been developed over the period of the Workshop to a point where they can now be used as a serious replacement for PDFLIB. Indeed, except for the PDF authors' own code, they are the only place to obtain the latest PDFs. There is however still considerable development in progress and the latest PDF sets will be incorporated as and when they become available. One major development area is to include the possibility of having more than one PDF set initialised concurrently. This may be necessary in interactions between different beam and target particles types and also including photon and pion PDFs. This will be the aim of the next LHAPDF release.

Acknowledgements

References

[1] H. Plothow-Besch, Comput. Phys. Commun. **75**, 396 (1993).

[2] W. Giele *et al.*, in *The QCD/SM working group: Summary report*. 2002. Also in preprint hep-ph/0204316.

[3] M. Botje, *QCDNUM version 16.12* (unpublished). Available on http://www.nikhef.nl/ h24/qcdcode/index.html.

[4] S. I. Alekhin, Phys. Rev. **D63**, 094022 (2001).

[5] S. I. Alekhin, Phys. Rev. **D68**, 014002 (2003).

[6] M. Botje, Eur. Phys. J. **C14**, 285 (2000).

[7] D. Stump *et al.*, JHEP **10**, 046 (2003).

[8] J. Pumplin *et al.*, JHEP **07**, 012 (2002).

[9] H. L. Lai *et al.*, Eur. Phys. J. **C12**, 375 (2000).

[10] H. L. Lai *et al.*, Phys. Rev. **D55**, 1280 (1997).

[11] W. T. Giele, S. A. Keller and D. A. Kosower, *Parton distribution function uncertainties*. Preprint hep-ph/0104052, 2001.

[12] M. Glück, E. Reya and A. Vogt, Eur. Phys. J. **C5**, 461 (1998).

[13] C. Adloff *et al.* [H1 Collaboration], Eur. Phys. J. **C30**, 1 (2003).

[14] A. D. Martin, R. G. Roberts, W. J. Stirling and R. S. Thorne, Eur. Phys. J. **C39**, 155 (2005).

[15] A. D. Martin, R. G. Roberts, W. J. Stirling and R. S. Thorne, *Mrst partons and uncertainties*. Preprint hep-ph/0307262, 2003.

[16] A. D. Martin, R. G. Roberts, W. J. Stirling and R. S. Thorne, Eur. Phys. J. **C28**, 455 (2003).

[17] A. D. Martin, R. G. Roberts, W. J. Stirling and R. S. Thorne, Eur. Phys. J. **C23**, 73 (2002).

[18] A. D. Martin, R. G. Roberts, W. J. Stirling and R. S. Thorne, Eur. Phys. J. **C4**, 463 (1998).

[19] S. Chekanov *et al.* [ZEUS Collaboration], Phys. Rev. **D67**, 012007 (2003).

[20] S. Chekanov *et al.* [ZEUS Collaboration], *An NLO QCD analysis of inclusive cross-section and jet- production data from the ZEUS experiment - DESY-05-050.* (unpublished). Preprint hep-ph/0503274, 2005.

[21] D. Bourilkov, *Study of parton density function uncertainties with LHAPDF and PYTHIA at LHC* (unpublished). Preprint hep-ph/0305126, 2003.

[22] DB, CG, MRW. Note in preparation.