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The MC@NLO 3.4 Event Generator

Stefano Frixione[†]

PH Department, TH Unit, CERN, CH-1211 Geneva 23, Switzerland
ITPP, EPFL, CH-1015 Lausanne, Switzerland
E-mail: Stefano.Frixione@cern.ch

Bryan R. Webber

Cavendish Laboratory, J.J. Thomson Avenue, Cambridge CB3 0HE, U.K.
E-mail: webber@hep.phy.cam.ac.uk

Abstract: This is the user's manual of MC@NLO 3.4. This package is a practical implementation, based upon the HERWIG event generator, of the MC@NLO formalism, which allows one to incorporate NLO QCD matrix elements consistently into a parton shower framework. Processes available in this version include the hadroproduction of single vector and Higgs bosons, vector boson pairs, heavy quark pairs, single top, single top in association with a W, lepton pairs, and Higgs bosons in association with a W or Z. Spin correlations are included for all processes except ZZ and WZ production. This document is self-contained, but we emphasise the main differences with respect to previous versions.

Keywords: QCD, Monte Carlo, NLO Computations, Resummation, Hadronic Colliders.

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[†] On leave of absence from INFN, Sez. di Genova, Italy

Contents

1. Generalities

In this document, we briefly describe how to run the MC@NLO package, implemented according to the formalism introduced in ref. [1]. The production processes now available are listed in tables 1 and 2. The process codes IPROC and the variables IV and IL will be explained below. $H_{1,2}$ represent hadrons (in practice, nucleons or antinucleons). The information given in refs. [1, 2] allows the implementation in MC@NLO of any production process, provided that the formalism of refs. [3, 4] is used for the computation of cross sections to NLO accuracy. The production matrix elements have been taken from the following references: vector boson pairs [5, 6, 7], heavy quark pairs [8], Standard Model Higgs [9, 10], single vector boson [11], lepton pairs [12], associated Higgs [13] and single-top s- and t-channel [14]; those for single-top production in association with a W have been re-derived and thoroughly compared to those of ref. [15].

This documentation refers to MC@NLO version 3.4. This version includes the upgrades of sub-version 3.31, which was not released officially but was distributed to several experiments. Single-top production in association with a W has been added since sub-version 3.31, including spin correlations. Top hadron decays (at the leading order) with spin correlations are now included. New Monte Carlo subtraction terms have been implemented in single-top production (all channels) – they were already implemented in $Q\bar{Q}$ production in sub-version 3.31, and they coincide with the old ones for all other processes. The automatic assignment of $\Lambda_{\rm QCD}$ in conjunction with LHAPDF has been improved. As a standalone package, MC@NLO version 3.4 should be easier to link to any external libraries (such as Root, for which we provide a Fortran interface [16]) and to recent versions of LHAPDF. For precise details of version changes, see app. A.1–A.8.

1.1 Citation policy

When using MC@NLO, please cite ref. [1]. In addition to ref. [1], if $t\bar{t}$ or $b\bar{b}$ events are generated, please also cite ref. [2]; if s- or t-channel single-top events are generated, please also cite ref. [17]; if Wt single-top events are generated, please also cite ref. [18]. The current user manual, or any other user manuals relevant to past versions, should not be cited unless the relevant papers mentioned above are cited too.

1.2 Mode of operation

In the case of standard MC, a hard kinematic configuration is generated on a event-by-event basis, and it is subsequently showered and hadronized. In the case of MC@NLO, all of the hard kinematic configurations are generated in advance, and stored in a file (which we call event file – see sect. 3.2); the event file is then read by HERWIG, which showers and hadronizes each hard configuration. Since version 2.0, the events are handled by the "Les Houches" generic user process interface [19] (see ref. [2] for more details). Therefore, in MC@NLO the reading of a hard configuration from the event file is equivalent to the generation of such a configuration in a standard MC.

The signal to HERWIG that configurations should be read from an event file using the Les Houches interface is a negative value of the process code IPROC; this accounts for the negative values in tables 1 and 2. In the case of heavy quark pair, Higgs, Higgs in association with a W or Z, and lepton pair (through Z/γ exchange) production, the codes are simply the negative of those for the corresponding standard HERWIG MC processes. Where possible, this convention will be adopted for additional MC@NLO processes. Consistently with what happens in standard HERWIG, by subtracting 10000 from IPROC one generates the same processes as in tables 1 and 2, but eliminates the underlying event[1].

Higgs decays are controlled in the same way as in HERWIG, that is by adding −ID to the process code. The conventions for ID are the same as in HERWIG, namely ID $= 1 \ldots 6$ for $u\bar{u} \ldots t\bar{t}$; 7, 8, 9 for e^+e^-, $\mu^+\mu^-$, $\tau^+\tau^-$; 10, 11 for W^+W^-, ZZ; and 12 for $\gamma\gamma$. Furthermore, ID = 0 gives quarks of all flavours, and ID = 99 gives all decays. It should be stressed that the event file does not contain the Higgs decay products, and therefore is independent of the value of ID; the decay is dealt with by HERWIG.[2]

Process codes IPROC= −1360−IL and −1370−IL do not have an analogue in HERWIG; they are the same as −1350−IL, except for the fact that only a Z or a γ respectively is exchanged. The value of IL determines the lepton identities, and the same convention as in HERWIG is adopted: IL= $1, \ldots, 6$ for $l_{IL} = e, \nu_e, \mu, \nu_\mu, \tau, \nu_\tau$ respectively. At variance with HERWIG, IL cannot be set equal to zero. Process codes IPROC= −1460−IL and −1470−IL are the analogue of HERWIG 1450+IL; in HERWIG either W^+ or W^- can be produced, whereas MC@NLO treats the two vector bosons separately. For these processes, as in HERWIG, IL= $1, 2, 3$ for $l_{IL} = e, \mu, \tau$, but again the choice IL = 0 is not allowed.

The lepton pair processes IPROC= −1350−IL, …, −1470−IL include spin correlations when generating the angular distributions of the produced leptons. However, if spin correlations are not an issue, the single vector boson production processes IPROC= −1396, −1397, −1497, −1498 can be used, in which case the vector boson decay products are distributed (by HERWIG, which then generates the decays) according to phase space.

There are a number of other differences between the lepton pair and single vector boson processes. The latter do not feature the γ–Z interference terms. Also, their cross sections are fully inclusive in the final-state fermions resulting from γ, Z or W. The user can still select a definite decay mode using the variable MODBOS (see sect. 3.5), but the relevant branching ratio will not be included by MC@NLO.

In NLO computations for single-top production, it is customary to distinguish between three production mechanisms, conventionally denoted as s channel, t channel, and Wt mode. Starting from the current version 3.4, all three mechanisms are implemented in MC@NLO; s- and t-channel single top production correspond to setting IC= 10 and IC= 20 respectively. For example, according to tables 1 and 2, t-channel single-t events will be generated by entering IPROC= −2021. These two channels can also be simulated simultaneously (by setting IC= 0). We point out that Wt cross section is ill-defined beyond the leading order in QCD. See sect. 3.4 for more details.

[1] The same effect can be achieved by setting the HERWIG parameter PRSOF = 0.

[2] In the current version of HERWIG (6.510), spin correlations between the products of Higgs decays are neglected. In version 6.520, to be released shortly, spin correlations in decays to vector boson pairs are included. Please check the Fortran HERWIG wiki at http://projects.hepforge.org/fherwig/trac/report for pre-release reports on this and other improvements.

IPROC	IV	IL_1	IL_2	Spin	Process
−1350−IL				X	$H_1H_2 \to (Z/\gamma^* \to) l_{IL}\bar{l}_{IL} + X$
−1360−IL				X	$H_1H_2 \to (Z \to) l_{IL}\bar{l}_{IL} + X$
−1370−IL				X	$H_1H_2 \to (\gamma^* \to) l_{IL}\bar{l}_{IL} + X$
−1460−IL				X	$H_1H_2 \to (W^+ \to) l^+_{IL}\nu_{IL} + X$
−1470−IL				X	$H_1H_2 \to (W^- \to) l^-_{IL}\bar{\nu}_{IL} + X$
−1396					$H_1H_2 \to \gamma^* (\to \sum_i f_i\bar{f}_i) + X$
−1397					$H_1H_2 \to Z^0 + X$
−1497					$H_1H_2 \to W^+ + X$
−1498					$H_1H_2 \to W^- + X$
−1600−ID					$H_1H_2 \to H^0 + X$
−1705					$H_1H_2 \to b\bar{b} + X$
−1706		7	7		$H_1H_2 \to t\bar{t} + X$
−2000−IC		7			$H_1H_2 \to t/\bar{t} + X$
−2001−IC		7			$H_1H_2 \to \bar{t} + X$
−2004−IC		7			$H_1H_2 \to t + X$
−2030		7	7		$H_1H_2 \to tW^-/\bar{t}W^+ + X$
−2031		7	7		$H_1H_2 \to \bar{t}W^+ + X$
−2034		7	7		$H_1H_2 \to tW^- + X$
−2600−ID	1	7			$H_1H_2 \to H^0W^+ + X$
−2600−ID	1	i		X	$H_1H_2 \to H^0(W^+ \to) l^+_i\nu_i + X$
−2600−ID	−1	7			$H_1H_2 \to H^0W^- + X$
−2600−ID	−1	i		X	$H_1H_2 \to H^0(W^- \to) l^-_i\bar{\nu}_i + X$
−2700−ID	0	7			$H_1H_2 \to H^0Z + X$
−2700−ID	0	i		X	$H_1H_2 \to H^0(Z \to) l_i\bar{l}_i + X$
−2850		7	7		$H_1H_2 \to W^+W^- + X$
−2860		7	7		$H_1H_2 \to Z^0Z^0 + X$
−2870		7	7		$H_1H_2 \to W^+Z^0 + X$
−2880		7	7		$H_1H_2 \to W^-Z^0 + X$

Table 1: Some of the processes implemented in MC@NLO 3.4 (see also table 2). $H_{1,2}$ represent nucleons or antinucleons. H^0 denotes the Standard Model Higgs boson and the value of ID controls its decay, as described in the HERWIG manual and in the text. The values of IV, IL, IL_1, and IL_2 control the identities of vector bosons and leptons, as described in the text. In single-t production, the value of IC controls the production processes (s- and/or t-channel), as described in the text. For more details on Wt production, see sect. 3.4. IPROC−10000 generates the same processes as IPROC, but eliminates the underlying event. A void entry indicates that the corresponding variable is unused. The 'Spin' column indicates whether spin correlations in vector boson or top decays are included (X), neglected ( ) or absent (void entry); when included, spin correlations are obtained by direct integration of the relevant NLO matrix elements. Spin correlations in Higgs decays to vector boson pairs (e.g. $H^0 \to W^+W^- \to l^+\nu l^-\bar{\nu}$) are included in HERWIG versions 6.520 and higher.

IPROC	IV	IL_1	IL_2	Spin	Process
–1706		i	j	X	$H_1H_2 \to (t \to) b_k f_i f'_i (t \to) b_l f_j f'_j + X$
–2000–IC		i		X	$H_1H_2 \to (t \to) b_k f_i f'_i / (t \to) b_k f_i f'_i + X$
–2001–IC		i		X	$H_1H_2 \to (t \to) b_k f_i f'_i + X$
–2004–IC		i		X	$H_1H_2 \to (t \to) b_k f_i f'_i + X$
–2030		i	j	X	$H_1H_2 \to (t \to) b_k f_i f'_i (W^- \to) f_j f'_j /$ $(t \to) b_k f_i f'_i (W^+ \to) f_j f'_j + X$
–2031		i	j	X	$H_1H_2 \to (t \to) b_k f_i f'_i (W^+ \to) f_j f'_j + X$
–2034		i	j	X	$H_1H_2 \to (t \to) b_k f_i f'_i (W^- \to) f_j f'_j + X$
–2850		i	j	X	$H_1H_2 \to (W^+ \to) l_i^+ \nu_i (W^- \to) l_j^- \nu_j + X$

Table 2: Some of the processes implemented in MC@NLO 3.4 (see also table 1). $H_{1,2}$ represent nucleons or antinucleons. For more details on Wt production, see sect. 3.4. Spin correlations for the processes in this table are implemented according to the method presented in ref. [20]. b ($\bar b$) can either denote a b (anti)quark or a generic down-type (anti)quark. f and f' can denote a (anti)lepton or an (anti)quark. See sects. 3.3 and 3.5 for fuller details.

In the case of vector boson pair production, the process codes are the negative of those adopted in MC@NLO 1.0 (for which the Les Houches interface was not yet available), rather than those of standard HERWIG.

Furthermore, in the case of $t\bar t$, single-t, $H^0W^\pm$, H^0Z and W^+W^- production, the value of IPROC alone may not be sufficient to fully determine the process type (including decay products), and variables IV, IL_1, and IL_2 are also needed (see tables 1 and 2). In the case of top decays (and of the decay of the hard W in Wt production), the variables IL_1 and IL_2 have a more extended range of values than that of the variable IL, which is relevant to lepton pair production and to which they are analogous (notice, however, that in the latter case IL is not an independent variable, and its value is included via IPROC). In addition, $IL = 7$ implies that spin correlations for the decay products of the corresponding particle are not taken into account, as indicated in table 1. More details are given in sect. 3.5.

Apart from the above differences, MC@NLO and HERWIG behave in exactly the same way. Thus, the available user's analysis routines can be used in the case of MC@NLO. One should recall, however, that MC@NLO always generates some events with negative weights (see refs. [1]); therefore, the correct distributions are obtained by summing weights with their signs (i.e., the absolute values of the weights must NOT be used when filling the histograms).

With such a structure, it is natural to create two separate executables, which we improperly denote as NLO and MC. The former has the sole scope of creating the event file; the latter is just HERWIG, augmented by the capability of reading the event file.

1.3 Package files

The package consists of the following files:

- Shell utilities
  - MCatNLO.Script

MCatNLO.inputs
MCatNLO_dyn.Script
MCatNLO_rb.inputs
Makefile
Makefile_dyn

Utility codes
MEcoupl.inc
alpha.f
dummies.f
linux.f
mcatnlo_date.f
mcatnlo_hbook.f
mcatnlo_helas2.f
mcatnlo_hwdummy.f
mcatnlo_int.f
mcatnlo_libofpdf.f
mcatnlo_mlmtolha.f
mcatnlo_mlmtopdf.f
mcatnlo_pdftomlm.f
mcatnlo_str.f
mcatnlo_uti.f
mcatnlo_utilhav4.f
mcatnlo_uxdate.c
rbook_be.cc
rbook_fe.f
sun.f
trapfpe.c

General HERWIG routines
mcatnlo_hwdriver.f
mcatnlo_hwlhin.f

Process-specific codes
mcatnlo_hwanxxx.f
mcatnlo_hwanxxx_rb.f
mcatnlo_hgmain.f
mcatnlo_hgxsec.f
mcatnlo_llmain.f
mcatnlo_llxsec.f
mcatnlo_qqmain.f
mcatnlo_qqxsec.f
mcatnlo_sbmain.f
mcatnlo_sbxsec.f

mcatnlo_stmain.f
mcatnlo_stxsec.f
mcatnlo_vbmain.f
mcatnlo_vbxsec.f
mcatnlo_vhmain.f
mcatnlo_vhxsec.f
mcatnlo_wtmain_dr.f
mcatnlo_wtmain_ds.f
mcatnlo_wtxsec_dr.f
mcatnlo_wtxsec_ds.f
hgscblks.h
hvqcblks.h
llpcblks.h
stpcblks.h
svbcblks.h
vhgcblks.h

These files can be downloaded from the web page:

http://www.hep.phy.cam.ac.uk/theory/webber/MCatNLO

The files mcatnlo_hwanxxx.f (which use a version of HBOOK written by M. Mangano that outputs plots in TopDrawer format) and mcatnlo_hwanxxx_rb.f (which use front-end Fortran routines written by W. Verkerke [16] for filling histograms in Root format) are sample HERWIG analysis routines. They are provided here to give the user a ready-to-run package, but they should be replaced with appropriate codes according to the user's needs. Examples of how to use these analysis files in MC@NLO are given in the (otherwise identical) MCatNLO.inputs and MCatNLO_rb.inputs files (see sect. 3 for more details on input cards).

In addition to the files listed above, the user will need a version of the HERWIG code [21, 22, 23]. As stressed in ref. [1], for the MC@NLO we do not modify the existing (LL) shower algorithm. However, since MC@NLO versions 2.0 and higher make use of the Les Houches interface, first implemented in HERWIG 6.5, the version must be 6.500 or higher. On most systems, users will need to delete the dummy subroutines UPEVNT, UPINIT, PDFSET and STRUCTM from the standard HERWIG package, to permit linkage of the corresponding routines from the MC@NLO package. As a general rule, the user is strongly advised to use the most recent version of HERWIG (currently 6.510 – with versions lower than 6.504 problems can be found in attempting to specify the decay modes of single vector bosons through the variable MODBOS. Also, crashes in the shower phase have been reported when using HERWIG 6.505, and we therefore recommend not to use that version).

1.4 Working environment

We have written a number of shell scripts and a Makefile (all listed under Shell utilities above) which will simplify the use of the package considerably. In order to use them, the computing system must support bash shell, and gmake[3]. Should they be unavailable on the user's computing system, the compilation and running of MC@NLO requires more detailed instructions; in this case, we refer the reader to app. B. This appendix will serve also as a reference for a more advanced use of the package.

1.5 Source and running directories

We assume that all the files of the package sit in the same directory, which we call the source directory. When creating the executable, our shell scripts determine the type of operating system, and create a subdirectory of the source directory, which we call the running directory, whose name is Alpha, Sun, Linux, or Darwin, depending on the operating system. If the operating system is not known by our scripts, the name of the working directory is Run. The running directory contains all the object files and executable files, and in general all the files produced by the MC@NLO while running. It must also contain the relevant grid files (see sect. 3.1), or links to them, if the library of parton densities provided with the MC@NLO package is used.

2. Prior to running

Before running the code, the user must be aware of the fact that the files:

mcatnlo_hwdriver.f
mcatnlo_hwlhin.f
mcatnlo_hwanxxx.f
mcatnlo_hwanxxx_rb.f

contain the statement INCLUDE HERWIG65.INC, which indicates that the code will link to HERWIG version 6.500 or higher, for the reasons explained above. In the current MC@NLO release, the file HERWIG65.INC contains the statement

INCLUDE 'herwig6510.inc'

We do not assume that the user will adopt version 6.510, which is the latest release of HERWIG; for this reason, the user will in general have to edit the file HERWIG65.INC, and change the statement above into

INCLUDE 'herwig65nn.inc'

with 65nn the HERWIG version chosen by the user (this must be consistent with the value of the input parameter HERWIGVER, see sects. 3 and 4).

The file mcatnlo_hwdriver.f contains a set of read statements, which are necessary for the MC to get the input parameters (see sect. 3 for the input procedure); these read statements must not be modified or eliminated. Also, mcatnlo_hwdriver.f calls the HERWIG routines which perform showering, hadronization, decays (see sect. 3.5 for more details on this issue), and so forth; the user can freely modify this part, as customary in MC runs. Finally, the sample codes mcatnlo_hwanxxx.f and mcatnlo_hwanxxx_rb.f contain analysis-related routines: these files must be replaced by files which contain the user's analysis routines. We point out that, since version 2.0, the Makefile need not be edited any

[3] For Macs running under OSX v10 or higher, make can be used instead of gmake.

longer, since the corresponding operations are now performed by setting script variables (see sect. 4).

3. Running

It is straightforward to run MC@NLO. First, edit[4]

    MCatNLO.inputs

and write there all the input parameters (for the complete list of the input parameters, see sect. 4). As the last line of the file MCatNLO.inputs, write

    runMCatNLO

Finally, execute MCatNLO.inputs from the bash shell. This procedure will create the NLO and MC executables, and run them using the inputs given in MCatNLO.inputs, which guarantees that the parameters used in the NLO and MC runs are consistent. Should the user only need to create the executables without running them, or to run the NLO or the MC only, he/she should replace the call to runMCatNLO in the last line of MCatNLO.inputs by calls to

    compileNLO
    compileMC
    runNLO
    runMC

which have obvious meanings. We point out that the command runMC may be used with IPROC=1350+IL, 1450+IL, 1600+ID, 1699, 1705, 1706, 2000–2008, 2600+ID, 2699, 2700+ID, 2799, 2800, 2810, 2815, 2820, 2825 to generate Z= , W , Higgs, bb, tt, single top, H^0W, H^0Z, and vector boson pair events with standard HERWIG (see the HERWIG manual for more details).

We stress that the input parameters are not solely related to physics (masses, CM energy, and so on); there are several of them which control other things, such as the number of events generated. These must also be set by the user, according to his/her needs: see sect. 4.

Two such variables are HERWIGVER and HWUTI, which were moved in version 2.0 from the Makefile to MCatNLO.inputs. The former variable must be set equal to the object file name of the version of HERWIG currently adopted (matching the one whose common blocks are included in the files mentioned in sect. 2). The variable HWUTI must be set equal to the list of object files that the user needs in the analysis routines.

The sample input file MCatNLO.inputs provided in this package is relevant to tt production and subsequent t and t leptonic decays. Similar sample inputs are given in the file MCatNLO_rb.inputs, which is identical to the former, except that at the end of the MC run an output file in Root format will be produced (as opposed to the output file in TopDrawer format produced by MCatNLO.inputs); for this to happen, the user will have to edit MCatNLO_rb.inputs in order to insert the path to the Root libraries for the machine on which the run is performed (shell variables EXTRAPATHS and INCLUDEPATHS). We stress that,

[4] See below for comments on MCatNLO_rb.inputs

apart from the differences in the output formats, MCatNLO.inputs and MCatNLO_rb.inputs have exactly the same meaning. Thus, although for the sake of brevity we shall often refer only to MCatNLO.inputs in this manual, all the issues concerning the inputs apply to MCatNLO_rb.inputs as well.

If the shell scripts are not used to run the codes, the inputs are given to the NLO or MC codes during an interactive talk-to phase; the complete sets of inputs for our codes are reported in app. B.2 for vector boson pair production.

3.1 Parton densities

Since the knowledge of the parton densities (PDFs) is necessary in order to get the physical cross section, a PDF library must be linked. The possibility exists to link the (now obsolete) CERNLIB PDF library (PDFLIB), or its replacement LHAPDF [24]; however, we also provide a self-contained PDF library with this package, which is faster than PDFLIB, and contains PDF sets released after the last and final PDFLIB version (8.04; most of these sets are now included in LHAPDF). A complete list of the PDFs available in our PDF library can be downloaded from the MC@NLO web page. The user may link one of the three PDF libraries; all that is necessary is to set the variable PDFLIBRARY (in the file MCatNLO.inputs) equal to THISLIB if one wants to link to our PDF library, and equal to PDFLIB or to LHAPDF if one wants to link to PDFLIB or to LHAPDF. Our PDF library collects the original codes, written by the authors of the PDF fits; as such, for most of the densities it needs to read the files which contain the grids that initialize the PDFs. These files, which can also be downloaded from the MC@NLO web page, must either be copied into the running directory, or defined in the running directory as logical links to the physical files (by using ln -sn). We stress that if the user runs MC@NLO with the shell scripts, the logical links will be created automatically at run time.

As stressed before, consistent inputs must be given to the NLO and MC codes. However, in ref. [1] we found that the dependence upon the PDFs used by the MC is rather weak. So one may want to run the NLO and MC adopting a regular NLL-evolved set in the former case, and the default HERWIG set in the latter (the advantage is that this option reduces the amount of running time of the MC). In order to do so, the user must set the variable HERPDF equal to DEFAULT in the file MCatNLO.inputs; setting HERPDF=EXTPDF will force the MC to use the same PDF set as the NLO code.

Regardless of the PDFs used in the MC run, users must delete the dummy PDFLIB routines PDFSET and STRUCTM from HERWIG, as explained earlier.

3.1.1 LHAPDF

As mentioned above, by setting THISLIB=LHAPDF in the input file the code is linked to the LHAPDF library. By default, MC@NLO will link to the static LHAPDF library. If one wants to link to the dynamic LHAPDF library (which will produce a smaller executable but otherwise identical results), one needs to replace

```
  . $thisdir/MCatNLO.Script
```

in MCatNLO.inputs with

```
  . $thisdir/MCatNLO_dyn.Script
```

In order for the Makefile (or Makefile_dyn, in the case of dynamic libraries) to be able to find the LHAPDF library, the variable LHAPATH in MCatNLO.inputs should be set equal to the name of the directory where the local version of LHAPDF is installed. This is typically the name of the directory where one finds the files libLHAPDF.a and libLHAPDF.so, except for the final /lib in the directory name.

As is well known, a given PDF set has a preferred value of Λ_{QCD}, which should be used in the computation of short-distance cross sections. Upon setting LAMBDAFIVE in MCatNLO.inputs equal to a negative value, this choice is made automatically. However, when linking to PDFLIB or LHAPDF, the code has to rely on the value Λ_{QCD} stored (by the PDF libraries) in a common block. This is far from ideal, since Λ_{QCD} is not a physical parameter, and in particular is dependent upon the form adopted for α_s, which may not be the same as that used in MC@NLO. Starting from version 3.4, the above automatic choice has been rendered more solid in the case of a linkage to LHAPDF; the code now reads the value of $\alpha_s(M_Z)$ (i.e., of a physical quantity) from the PDF library, and converts it into a value for Λ_{QCD} using the form of $\alpha_s(Q^2)$ used internally in MC@NLO. MC@NLO will print out on the standard output when running the NLO code (FPREFIXNLO.log if using the scripts) the value of Λ_{QCD} used in the computation. Such a value is now expected to be quite close to that listed under the column labeled with $\Lambda^{(5)}_{QCD}$ (MeV) on our PDF library manual (which can be found on the MC@NLO web page).

Version 3.4 of MC@NLO has been tested to link and run with several versions of LHAPDF. In particular, the user is not supposed to edit the Makefile if linking with LHAPDF version 5.0 or higher. If one is interested into linking with earlier versions of LHAPDF, then one must replace the string mcatnlo_uti.o in the variable LUTIFILES in the Makefile (or Makefile_dyn, in the case of dynamic libraries) with the string mcatnlo_utilhav4.o.

3.2 Event file

The NLO code creates the event file. In order to do so, it goes through two steps; first it integrates the cross sections (integration step), and then, using the information gathered in the integration step, produces a set of hard events (event generation step). Integration and event generation are performed with a modified version of the SPRING-BASES package [25].

We stress that the events stored in the event file just contain the partons involved in the hard suprocesses. Owing to the modified subtraction introduced in the MC@NLO formalism (see ref. [1]) they do not correspond to pure NLO configurations, and should not be used to plot physical observables. Parton-level observables must be reconstructed using the fully-showered events.

The event generation step necessarily follows the integration step; however, for each integration step one can have an arbitrary number of event generation steps, i.e., an arbitrary number of event files. This is useful in the case in which the statistics accumulated with a given event file is not sufficient.

Suppose the user wants to create an event file; editing MCatNLO.inputs, the user sets BASES=ON, to enable the integration step, sets the parameter NEVENTS equal to the number of events wanted on tape, and runs the code; the information on the integration step (unreadable to the user, but needed by the code in the event generation step) is written on files whose name begin with FPREFIX, a string the user sets in MCatNLO.inputs; these files (which we denotes as data files) have extensions .data. The name of the event file is EVPREFIX.events, where EVPREFIX is again a string set by the user.

Now suppose the user wants to create another event file, to increase the statistics. The user simply sets BASES=OFF, since the integration step is not necessary any longer (however, the data files must not be removed: the information stored there is still used by the NLO code); changes the string EVPREFIX (failure to do so overwrites the existing event file), while keeping FPREFIX at the same value as before; and changes the value of RNDEVSEED (the random number seed used in the event generation step; failure to do so results in an event file identical to the previous one); the number NEVENTS generated may or may not be equal to the one chosen in generating the former event file(s).

We point out that data and event files may be very large. If the user wants to store them in a scratch area, this can be done by setting the script variable SCRTCH equal to the physical address of the scratch area (see sect. 3.6).

3.3 Inclusive NLO cross sections

MC@NLO integrates NLO matrix elements in order to produce the event file, and thus computes (as a by-product) the inclusive NLO cross section. This cross section (whose value is given in pb) can be obtained from an MC@NLO run in three different ways[5]:

a) It is printed out at the end of the NLO run (search for Total for fully inclusive in the standard output).

b) It is printed by HERWIG at the end of the MC run (search for CROSS SECTION (PB) in the standard output).

c) It is equal to the integral of any differential distribution which covers the whole kinematically-accessible range (e.g. $0 \le p_T \le \infty$) and on which no cuts are applied.

These three numbers are the same (up to statistics, which here means the number of generated events – see the bottom of this section for further comments) for the processes listed in table 1. For the processes listed in table 2, on the other hand, the results of b) and c) are equal to that of a), times the branching ratio(s) for the selected decay channel(s), times (in the case of top decays) other factors due to kinematic cuts specified in input (see below). This is so because for the processes of table 2 spin correlations are obtained as described in ref. [20]. For these processes, we shall denote in what follows the cross section obtained in a) as the undecayed cross section, and those obtained in b) or c) as the decayed cross sections. We note that, both for the processes in table 1 and for those in table 2, the results of b) and c) are equal to the sum of the weights of all events stored in the event file (possibly up to the contributions of those few events which HERWIG is unable to shower and hadronize, and which are therefore discarded with error messages in the MC run).

[5] This is true only if WGTTYPE=1.

The branching ratios used in the computation are determined by the values of the branching ratios for individual decay channels. The following variables are relevant to top decays:

$$\mathrm{BRTOPTOLEP} = \frac{\sum_j \Gamma(t \to \nu_l l b_j)}{\Gamma_t}\,; \qquad \mathrm{BRTOPTOHAD} = \frac{\sum_{ij} \Gamma(t \to u \bar{d}_i b_j)}{\Gamma_t}\,; \tag{3.1}$$

with b_j and $\bar{d}_i$ any down-type quark and antiquark respectively, u an up-type quark, and l a charged lepton; lepton and flavour universality are assumed. In the case of W decays, one has the analogous variables

$$\mathrm{BRWTOLEP} = \frac{\Gamma(W \to l \nu_l)}{\Gamma_W}\,; \qquad \mathrm{BRWTOHAD} = \frac{\sum_i \Gamma(W \to u \bar{d}_i)}{\Gamma_W}\,. \tag{3.2}$$

The variables in eqs. (3.1) and (3.2) can either be given a numerical value in input, or computed at the LO in the SM by the code – see sect. 3.5 for details. The numerical values of these variables are then combined to obtain the overall branching ratio for the decay channels selected, which is done by setting the variables IL and TOPDECAY as explained in sect. 3.5 (see in particular table 3). For example, for a top decaying into a W and any down-type quarks, with the W decaying in an electron, muon, or any quarks, one sets IL = 6, TOPDECAY=ALL, and the resulting branching ratio will be 2 × BRTOPTOLEP + 2 × BRTOPTOHAD.

As mentioned above, in the case of top decays (as opposed to hard W decays in Wt or W^+W^- production) the decayed cross section will include kinematic factors in addition to the branching ratios. These factors are due to the fact that in general the range for the invariant mass of the pair of particles emerging from the W decay (i.e. the virtuality of the W) does not coincide with the maximum that is kinematically allowed. For each top that decays, the following kinematic factor will therefore be included in the decayed cross section

$$\frac{\Gamma(t \to f f' b \,|\, q_W(\mathrm{inf}), q_W(\mathrm{sup}))}{\Gamma(t \to f f' b \,|\, 0, m_t)}\,, \tag{3.3}$$

with

$$\Gamma\left(t \to f f' b \,|\, m, M\right) = \int_{m^2}^{M^2} dq_W^2 \, \frac{d\Gamma(t \to f f' b)}{dq_W^2}\,, \tag{3.4}$$

and $q_W(\mathrm{inf})$, $q_W(\mathrm{sup})$ the lower and upper limits of the W virtuality, which can be chosen in input. In particular, if V1GAMMAX > 0, one will have

$$q_W(\mathrm{inf}) = \mathrm{WMASS} - \mathrm{V1GAMMAX} \times \mathrm{WWIDTH}\,; \qquad q_W(\mathrm{sup}) = \mathrm{WMASS} + \mathrm{V1GAMMAX} \times \mathrm{WWIDTH}\,. \tag{3.5}$$

On the other hand, if V1GAMMAX < 0, one has

$$q_W(\mathrm{inf}) = \mathrm{V1MASSINF}\,; \qquad q_W(\mathrm{sup}) = \mathrm{V1MASSSUP}\,. \tag{3.6}$$

The ranges in eqs. (3.5) or (3.6) apply to the W emerging from the decay of the top quark in $t\bar{t}$ production, and of the top or antitop in single-top production (all channels). The corresponding ranges for the W emerging from the decay of the antitop quark in $t\bar{t}$ production are identical to those above, except for the replacement of V1 with V2.

The user is also allowed to generate events by fixing the virtuality of the W emerging from top/antitop decays equal to the W pole mass, by setting xGAMMAX= 0, with x=V1,V2. In such a case, the decayed cross section will be equal to the undecayed cross section, times the branching ratios, times a factor

$$\left.\frac{d\Gamma(t\to f\bar{f}'b)}{dq_W^2}\right|_{q_W^2=M_W^2}, \tag{3.7}$$

for each decaying top quark. The decayed cross section will have therefore to be interpreted as differential in the W virtuality squared (doubly differential in the case of $t\bar{t}$ production), and will be expressed in pb GeV^{-2} (or pb GeV^{-4} for $t\bar{t}$ production) units.

The branching ratios and kinematics factors for each decaying particles are multiplied to give a single number (always less than or equal to one), which is by definition the ratio of the decayed over the undecayed cross section. This number is printed out at the end of the NLO run (search for Normalization factor due to decays in the standard output).

We conclude this section by stressing that, while the result of a) is always computed with a typical relative precision of 10^{-4}, those of b) and c) depend on the number of events generated. Although it has been checked that, upon increasing the number of events generated, the results of b) and c) do approach that of a) (possibly times the branching ratios and kinematic factors), option a) has clearly to be preferred. As mentioned above, the decayed cross section of b) or c) can be obtained without any loss of accuracy by multiplying the undecayed cross section of a) by the normalization factor printed out by the code at the end of the NLO run.

3.4 Wt production

Owing to the interference with $t\bar{t}$ production, which occurs in the gg and $q\bar{q}$ partonic channels starting at the NLO, the Wt cross section is ill-defined beyond the leading order in QCD. One can still give an operative meaning to NLO Wt production, but one must always be aware of the potential biases introduced in this way. This issue and its potential physics implications are discussed at length in ref. [18], which the reader is strongly advised to consult before generating Wt events.

In MC@NLO version 3.4, we have implemented two different definitions of the Wt cross section, which we denoted by diagram removal and diagram subtraction in ref. [18]. The former computation is carried out by setting WTTYPE=REMOVAL in MCatNLO.inputs, while the latter corresponds to WTTYPE=SUBTRACTION.

In Wt production, the factorization (renormalization) scale is assigned the value of the variable PTVETO (whose units are GeV) if FFACT< 0 (FREN< 0). This option should be used for testing purposes only; it is not recommended in the generation of event samples for experimental studies.

3.5 Decays

MC@NLO is intended primarily for the study of NLO corrections to production cross sections and distributions; NLO corrections to the decays of produced particles are not included. As for spin correlations, the situation in version 3.4 is summarized in tables 1 and 2: they are included for all processes except ZZ and WZ production[6]. For the latter processes, quantities sensitive to the polarisation of produced particles are not given correctly even to leading order. For such quantities, it may be preferable to use the standard HERWIG MC, which does include leading-order spin correlations.

Following HERWIG conventions, spin correlations in single-vector-boson processes are automatically included using the process codes (IPROC) relevant to lepton pair production (in other words, if one is interested in including spin correlations in e.g. W^+ production and subsequent decays into $^+$, one needs to use IPROC= 1461 rather than IPROC= 1497 and MODBOS(1)= 3). In order to avoid an unnecessary proliferation of IPROC values, this strategy has not been adopted in other cases (tt, single-t, H^0W , H^0Z, W^+W), in which spin correlations are included if the variables IL_1 and IL_2 (the latter is used only in tt, Wt, and W^+W production) are assigned certain values. In the case of individual lepton decays, these range from 1 to 3 if the decaying particle is a W or a top, or from 1 to 6 if the decaying particle is a Z. For these cases, the value of IL fully determines the identity of the leptons emerging from the decay, and the same convention as in HERWIG is adopted (see the HERWIG manual and sect. 1.2).

In tt and single-top production, i.e. for all processes listed in table 2, the top quark and/or antiquark, and the hard W in the case of Wt production, can also decay hadronically. In such cases, therefore, the variables IL can be assigned more values than for the other processes; the situation is summarized in table 3. When generating the decays, lepton and avour universalities are assumed. The relative probabilities of individual hadronic decays (e.g. $W^+ \to ud$ vs $W^+ \to us$) are determined using the CKM matrix elements entered by the user (variables Vud in MCatNLO.inputs). The relative probabilities of leptonic vs hadronic decays are on the other hand determined using the values of the corresponding branching ratios entered by the user: variables BRTOPTOLEP and BRTOPTOHAD for top/antitop decays, and BRWTOLEP and BRWTOHAD for the decays of the hard W emerging from the hard process in Wt production[7] – see eqs. (3.1) and (3.2) for the de nitions of these variables.

In the case of top/antitop decays, it is also possible to generate events in which the top decays into a W and any down-type quark (hence the notations b and b in table 2). The identity of the latter is determined according to the CKM matrix values. For this to happen, one needs to set TOPDECAY=ALL in MCatNLO.inputs. If, on the other hand, one wants to always generate $t \to Wb$ decays, one needs to set TOPDECAY=Wb; in such a case, event weights (and thus the decayed cross section, as de ned in sect. 3.3) will be multiplied by a factor $V_{tb}^2/(V_{td}^2 + V_{ts}^2 + V_{tb}^2)$.

For the processes in table 2 it is also possible to force the code to use the LO values of the relevant leptonic and hadronic branching ratios, by entering negative values for the top and W widths (variables TWIDTH and WWIDTH in MCatNLO.inputs). In such a case, the

[6] Non-factorizable spin correlations of virtual origin are not included in W^+W , tt, and single-t production. See ref. [20].

[7] BRWTOLEP is also used in W^+W production. W hadronic decays are not implemented in this process, hence the branching ratio is only used as a rescaling factor for event weights.

IL	Decay
0	e+ + + q
1	e
2	
3	
4	e+
5	q
6	e+ + q
7	no decay

Table 3: Decays of the W's originating from top/antitop decay or from the hard process in Wt production. The symbol q denotes all hadronic W decays. Values different from 1, 2, or 3 are only allowed in tt and single-top production (all channels).

values of BRTOPTOLEP, BRTOPTOHAD, BRWTOLEP and BRWTOHAD given in the input file will be ignored, and replaced by 1=9, 1=3, 1=9 and 1=3 respectively. The top and W widths will be computed using the LO SM formulae.

Spin correlations are implemented in the processes in table 2 according to the method of ref. [20], which is based on a zero-width approximation for the decaying particles. Nevertheless, the top quark and antiquark in tt production (IPROC= 1706), and the vector bosons in W^+W production (IPROC= 2850) can be given masses different from the pole masses. These off-shell effects are modeled by re-weighting the cross section with skewed Breit-Wigner functions (in order to take into account the fact that by changing the invariant mass of the system produced one probes different values of Bjorken x's). This re-weighting is unitary, i.e. it does not change the inclusive cross section. For tt production, the ranges of top and antitop masses are controlled by the parameters TiGAMMAX, TiMASSINF, and TiMASSSUP (with i= 1,2 for top and antitop respectively). For W^+W, one needs to use instead ViGAMMAX, ViMASSINF, and ViMASSSUP, with i= 1,2 for W^+ and W respectively. In both cases, the mass ranges will be defined by formulae formally identical to those of eqs. (3.5) and (3.6). In version 3.4, off-shell effects are not implemented in the other processes in table 2, i.e. all channels of single-top production.

Finally, we point out that since spin correlations for the processes in table 2 are implemented according to the method of ref. [20], tree-level matrix elements for leptonic final states are needed. The codes for these have been generated with MadGraph/MadEvent [26, 27], and embedded into the MC@NLO package.

When IL = 7, the corresponding particle is left undecayed by the NLO code, and is passed as such to the MC code; the information on spin correlations is lost. However, the user can still force particular decay modes during the MC run. In the case of vector bosons, one proceeds in the same way as in standard HERWIG, using the MODBOS variables – see sect. 3.4 of ref. [22]. However, top decays cannot be forced in this way because the decay is treated as a three-body process: the W boson entry in HEPEVT is for information only. Instead, the top branching ratios can be altered using the HWMODK subroutine

– see sect. 7 of ref. [22]. This is done separately for the t and $\bar{t}$. For example, CALL HWMODK(6,1.D0,100,12,-11,5,0,0) forces the decay $t \to \nu_e e^+ b$, while leaving $\bar{t}$ decays unaffected. Note that the order of the decay products is important for the decay matrix element (NME = 100) to be applied correctly. The relevant statements should be inserted in the HERWIG main program (corresponding to mcatnlo_hwdriver.f in this package) after the statement CALL HWUINC and before the loop over events. A separate run with CALL HWMODK(-6,1.D0,100,-12,11,-5,0,0) should be performed if one wishes to symmetrize the forcing of t and $\bar{t}$ decays, since calls to HWMODK from within the event loop do not produce the desired result.

3.6 Results

As in the case of standard HERWIG the form of the results will be determined by the user's analysis routines. However, in addition to any files written by the user's analysis routines, the MC@NLO writes the following files:

- FPREFIXNLOinput: the input file for the NLO executable, created according to the set of input parameters defined in MCatNLO.inputs (where the user also sets the string FPREFIX). See table 4.
- FPREFIXNLO.log: the log file relevant to the NLO run.
- FPREFIXxxx.data: xxx can assume several different values. These are the data files created by the NLO code. They can be removed only if no further event generation step is foreseen with the current choice of parameters.
- FPREFIXMCinput: analogous to FPREFIXNLOinput, but for the MC executable. See table 6.
- FPREFIXMC.log: analogous to FPREFIXNLO.log, but for the MC run.
- EVPREFIX.events: the event file, where EVPREFIX is the string set by the user in MCatNLO.inputs.
- EVPREFIXxxx.events: xxx can assume several different values. These files are temporary event files, which are used by the NLO code, and eventually removed by the shell scripts. They MUST NOT be removed by the user during the run (the program will crash or give meaningless results).

By default, all the files produced by the MC@NLO are written in the running directory. However, if the variable SCRTCH (to be set in MCatNLO.inputs) is not blank, the data and event files will be written in the directory whose address is stored in SCRTCH (such a directory is not created by the scripts, and must already exist at run time).

4. Script variables

In the following, we list all the variables appearing in MCatNLO.inputs; these can be changed by the user to suit his/her needs. This must be done by editing MCatNLO.inputs. For fuller details see the comments in MCatNLO.inputs.

ECM The CM energy (in GeV) of the colliding particles.

FREN The ratio between the renormalization scale, and a reference mass scale.

FFACT As FREN, for the factorization scale.

HVQMASS The mass (in GeV) of the top quark, except when IPROC= −(1)1705, when it is the mass of the bottom quark. In this case, HVQMASS must coincide with BMASS.

xMASS The mass (in GeV) of the particle x, with x=HGG,W,Z,U,D,S,C,B,G.

xWIDTH The physical (Breit-Wigner) width (in GeV) of the particle x, with x=HGG,W,Z,T for H^0, $W^\pm$, Z, and t respectively.

BRTOPTOx Branching ratio for top decay channels $\sum_j t \to l\nu_l b_j$ (when x=LEP) and $\sum_{ij} t \to u d_i b_j$ (when x=HAD). Lepton and flavour universality is assumed.

BRWTOx Branching ratio for W decay channels $W \to l\nu_l$ (when x=LEP) and $\sum_i W \to u d_i$ (when x=HAD). Lepton and flavour universality is assumed.

IBORNHGG Valid entries are 1 and 2. If set to 1, the exact top mass dependence is retained at the Born level in Higgs production. If set to 2, the $m_t \to \infty$ limit is used.

xGAMMAX If xGAMMAX > 0, controls the width of the mass range for Higgs (x=H), vector bosons (x=V1,V2), and top (x=T1,T2): the range is MASS ± (GAMMAX × WIDTH). Off-shell effects for top are only implemented in $t\bar{t}$ production.

xMASSINF Lower limit of the Higgs (x=H), vector boson (x=V1,V2), and top (x=T1,T2) mass range; used only when xGAMMAX < 0.

xMASSSUP Upper limit of the Higgs (x=H), vector boson (x=V1,V2), and top (x=T1,T2) mass range; used only when xGAMMAX < 0.

Vud CKM matrix elements, with u=U,C,T and d=D,S,B. Set VUD=VUS=VUB=0 to use values of PDG 2003.

AEMRUN Set it to YES to use running α_{em} in lepton pair and single vector boson production, set it to NO to use $\alpha_{em} = 1/137.0359895$.

IPROC Process number that identifies the hard subprocess: see tables 1 and 2 for valid entries.

IVCODE Identifies the nature of the vector boson in associated Higgs production. It corresponds to variable IV of table 1.

ILxCODE Identify the nature of the particles emerging from vector boson or top decays. They correspond to variables IL_1 and IL_2 (for $x = 1, 2$ respectively) of tables 1, 2 and 3.

TOPDECAY Valid entries are ALL and Wb. Controls the type of top decay. See sect. 3.5.

WTTYPE Valid entries are REMOVAL and SUBTRACTION. Determines the definition of the Wt cross section at the NLO. See sect. 3.4.

PTVETO Used in conjunction with FFACT and/or FREN to set mass scales in Wt production. See sect. 3.4.

PARTn The type of the incoming particle #n, with $n=1,2$. HERWIG naming conventions are used (P, PBAR, N, NBAR).

PDFGROUP The name of the group fitting the parton densities used; the labeling conventions of PDFLIB are adopted. Unused when linked to LHAPDF.

PDFSET The number of the parton density set; according to PFDLIB conventions, the pair (PDFGROUP,PDFSET) identifies the densities for a given particle type. When linked to LHAPDF, use the numbering conventions of LHAGLUE [24].

LAMBDAFIVE The value of $\Lambda_{\rm QCD}$, for five flavours and in the $\overline{\rm MS}$ scheme, used in the computation of NLO cross sections. A negative entry sets $\Lambda_{\rm QCD}$ equal to that associated with the PDF set being used.

LAMBDAHERW The value of $\Lambda_{\rm QCD}$ used in MC runs; this parameter has the same meaning as $\Lambda_{\rm QCD}$ in HERWIG.

SCHEMEOFPDF The subtraction scheme in which the parton densities are defined.

FPREFIX Our integration routine creates files with name beginning by the string FPREFIX. Most of these files are not directly accessed by the user. See sects. 3.2 and 3.6.

EVPREFIX The name of the event file begins with this string. See sects. 3.2 and 3.6.

EXEPREFIX The names of the NLO and MC executables begin with this string; this is useful in the case of simultaneous runs.

NEVENTS The number of events stored in the event file, eventually processed by HERWIG.

WGTTYPE Valid entries are 0 and 1. When set to 0, the weights in the event file are ± 1. When set to 1, they are $\pm w$, with w a constant such that the sum of the weights gives the total inclusive NLO cross section (see sect. 3.3 for more details). Note that these weights are redefined by HERWIG at MC run time according to its own convention (see HERWIG manual).

RNDEVSEED The seed for the random number generation in the event generation step; must be changed in order to obtain statistically-equivalent but different event files.

BASES Controls the integration step; valid entries are ON and OFF. At least one run with BASES=ON must be performed (see sect. 3.2).

PDFLIBRARY Valid entries are PDFLIB, LHAPDF, and THISLIB. In the former two cases, PDFLIB or LHAPDF is used to compute the parton densities, whereas in the latter case the densities are obtained from our self-contained PDF library.

HERPDF If set to DEFAULT, HERWIG uses its internal PDF set (controlled by NSTRU), regardless of the densities adopted at the NLO level. If set to EXTPDF, HERWIG uses the same PDFs as the NLO code (see sect. 3.1).

HWPATH The physical address of the directory where the user's preferred version of HERWIG is stored.

SCRTCH The physical address of the directory where the user wants to store the data and event files. If left blank, these files are stored in the running directory.

HWUTI This variables must be set equal to a list of object files, needed by the analysis routines of the user (for example, HWUTI=''obj1.o obj2.o obj3.o'' is a valid assignment).

HERWIGVER This variable must to be set equal to the name of the object file corresponding to the version of HERWIG linked to the package (for example, HERWIGVER=herwig6510.o is a valid assignment).

PDFPATH The physical address of the directory where the PDF grids are stored. Effective only if PDFLIBRARY=THISLIB.

LHAPATH Set this variable equal to the name of the directory where the local version of LHAPDF is installed. See sect. 3.1.1.

LHAOFL Set LHAOFL=FREEZE to freeze PDFs from LHAPDF at the boundaries, or equal to EXTRAPOLATE otherwise. See LHAPDF manual for details.

EXTRALIBS Set this variable equal to the names of the libraries which need be linked. LHAPDF is a special case, and must not be included in this list.

EXTRAPATHS Set this variable equal to the names of the directories where the libraries which need be linked are installed.

INCLUDEPATHS Set this variable equal to the names of the directories which contain header files possibly needed by C++ files provided by the user (via HWUTI).

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Appendices

A. Version changes

A.1 From MC@NLO version 1.0 to version 2.0

In this appendix we list the changes that occurred in the package from version 1.0 to version 2.0.

The Les Houches generic user process interface has been adopted.

As a result, the convention for process codes has been changed: MC@NLO process codes IPROC are negative.

The code mcatnlo_hwhvvj.f, which was specific to vector boson pair production in version 1.0, has been replaced by mcatnlo_hwlhin.f, which reads the event file according to the Les Houches prescription, and works for all the production processes implemented.

The Makefile need not be edited, since the variables HERWIGVER and HWUTI have been moved to MCatNLO.inputs (where they must be set by the user).

A code mcatnlo_hbook.f has been added to the list of utility codes. It contains a simplified version (written by M. Mangano) of HBOOK, and it is only used by the sample analysis routines mcatnlo_hwanxxx.f. As such, the user will not need it when linking to a self-contained analysis code.

We also remind the reader that the HERWIG version must be 6.5 or higher since the Les Houches interface is used.

A.2 From MC@NLO version 2.0 to version 2.1

In this appendix we list the changes that occurred in the package from version 2.0 to version 2.1.

Higgs production has been added, which implies new process-specific files (mcatnlo_hgmain.f, mcatnlo_hgxsec.f, hgscblks.h, mcatnlo_hwanhgg.f), and a modification to mcatnlo_hwlhin.f.

Post-1999 PDF sets have been added to the MC@NLO PDF library.

Script variables have been added to MCatNLO.inputs. Most of them are only relevant to Higgs production, and don't affect processes implemented in version 2.0. One of them (LAMBDAHERW) may affect all processes: in version 2.1, the variables LAMBDAFIVE and LAMBDAHERW are used to set the value of Λ_{QCD} in NLO and MC runs respectively, whereas in version 2.0 LAMBDAFIVE controlled both. The new setup is necessary since modern PDF sets have Λ_{QCD} values which are too large to be supported by HERWIG. (Recall that the effect of using LAMBDAHERW different from LAMBDAFIVE is beyond NLO.)

The new script variable PDFPATH should be set equal to the name of the directory where the PDF grid files (which can be downloaded from the MC@NLO web page) are stored. At run time, when executing runNLO, or runMC, or runMCatNLO, logical links to these files will be created in the running directory (in version 2.0, this operation had to be performed by the user manually).

Minor bugs corrected in mcatnlo_hbook.f and sample analysis routines.

A.3 From MC@NLO version 2.1 to version 2.2

In this appendix we list the changes that occurred in the package from version 2.1 to version 2.2.

Single vector boson production has been added, which implies new process-specific files (mcatnlo_sbmain.f, mcatnlo_sbxsec.f, svbcblks.h, mcatnlo_hwansvb.f), and a modification to mcatnlo_hwlhin.f.

The script variables WWIDTH and ZWIDTH have been added to MCatNLO.inputs. These denote the physical widths of the W and Z^0 bosons, used to generate the mass distributions of the vector bosons according to the Breit–Wigner function, in the case of single vector boson production (vector boson pair production is still implemented only in the zero-width approximation).

A.4 From MC@NLO version 2.2 to version 2.3

In this appendix we list the changes that occurred in the package from version 2.2 to version 2.3.

Lepton pair production has been added, which implies new process-specific files (mcatnlo_llmain.f, mcatnlo_llxsec.f, llpcblks.h, mcatnlo_hwanllp.f), and modifications to mcatnlo_hwlhin.f and mcatnlo_hwdriver.f.

The script variable AEMRUN has been added, since the computation of single vector boson and lepton pair cross sections is performed in the $\overline{MS}$ scheme (the on-shell scheme was previously used for single vector boson production).

The script variables FRENMC and FFACTMC have been eliminated.

The structure of pseudo-random number generation in heavy flavour production has been changed, to avoid a correlation that affected the azimuthal angle distribution for the products of the hard partonic subprocesses.

A few minor bugs have been corrected, which affected the rapidity of the vector bosons in single vector boson production (a 2–3% effect), and the assignment of Λ_{QCD} for the LO and NLO PDF sets of Alekhin.

A.5 From MC@NLO version 2.3 to version 3.1

In this appendix we list the changes that occurred in the package from version 2.3 to version 3.1.

Associated Higgs production has been added, which implies new process-specific files (mcatnlo_vhmain.f, mcatnlo_vhxsec.f, vhgcblks.h, mcatnlo_hwanvhg.f), and modifications to mcatnlo_hwlhin.f and mcatnlo_hwdriver.f.

Spin correlations in W^+W^- production and leptonic decay have been added; the relevant codes (mcatnlo_vpmain.f, mcatnlo_vhxsec.f) have been modified; the sample analysis routines (mcatnlo_hwanvbp.f) have also been changed. Tree-level matrix elements have been computed with MadGraph/MadEvent [26, 27], which uses HELAS [28]; the relevant routines and common blocks are included in mcatnlo_helas2.f and MEcoupl.inc.

The format of the event file has changed in several respects, the most relevant of which is that the four-momenta are now given as (p_x, p_y, p_z, m) (up to version 2.3 we had

$(p_x;p_y;p_z;E)$). Event files generated with version 2.3 or lower must not be used with version 3.1 or higher (the code will prevent the user from doing so).

The script variables GAMMAX, MASSINF, and MASSSUP have been replaced with xGAMMAX, xMASSINF and xMASSSUP, with x=H, V1, V2.

New script variables IVCODE, IL1CODE, and IL2CODE have been introduced.

Minor changes have been made to the routines that put the partons on the HERWIG mass shell for lepton pair, heavy quark, and vector boson pair production; effects are beyond the fourth digit.

The default electroweak parameters have been changed for vector boson pair production, in order to make them consistent with those used in other processes. The cross sections are generally smaller in version 3.1 wrt previous versions, the dominant effect being the value of $\sin\theta_W$: we have now $\sin^2\theta_W = 0.2311$, in lower versions $\sin^2\theta_W = 1 - m_W^2/m_Z^2$. The cross sections are inversely proportional to $\sin^4\theta_W$.

A.6 From MC@NLO version 3.1 to version 3.2

In this appendix we list the changes that occurred in the package from version 3.1 to version 3.2.

Single-t production has been added, which implies new process-specific files (mcatnlo_stmain.f, mcatnlo_stxsec.f, stpcblks.h, mcatnlo_hwanstp.f), and modifications to mcatnlo_hwlhin.f and mcatnlo_hwdriver.f.

LHAPDF library is now supported, which implies modifications to all *main.f files, and two new utility codes, mcatnlo_lhauti.f and mcatnlo_mlmtolha.f.

New script variables Vud, LHAPATH, and LHAOFL have been introduced.

A bug affecting Higgs production has been fixed, which implies a modification to mcatnlo_hgxsec.f. Cross sections change with respect to version 3.1 only if FFACT$\neq$ 1 (by $O(1\%)$ in the range $1/2 \le$ FFACT ≤ 2).

A.7 From MC@NLO version 3.2 to version 3.3

In this appendix we list the changes that occurred in the package from version 3.2 to version 3.3.

Spin correlations have been added to $t\bar{t}$ and single-t production processes, which imply modifications to several codes (mcatnlo_qqmain.f, mcatnlo_qqxsec.f, mcatnlo_stmain.f, mcatnlo_stxsec.f, mcatnlo_hwlhin.f and mcatnlo_hwdriver.f). Tree-level matrix elements have been computed with MadGraph/MadEvent [26, 27].

The matching between NLO matrix elements and parton shower is now smoother in Higgs production, which helps eliminate one unphysical feature in the p_T spectra of the accompanying jets. The code mcatnlo_hgmain.f has been modified. Technical details on this matching procedure will be posted on the MC@NLO web page.

The new script variable TWIDTH has been introduced.

All instances of HWWARN('s',i,*n) have been replaced with HWWARN('s',i) in HERWIG-related codes. This is consistent with the definition of HWWARN in HERWIG versions 6.510 and higher; the user must be careful if linking to HERWIG versions, in which the former form of HWWARN is used. Although HERWIG 6.510 compiles with g95 or gfortran, MC@NLO 3.3 does not.

A.8 From MC@NLO version 3.3 to version 3.4

In this appendix we list the changes that occurred in the package from version 3.3 to version 3.4.

Wt production has been implemented, which implies new process-specific codes (mcatnlo_wtmain_dr.f, mcatnlo_wtmain_ds.f, mcatnlo_wtxsec_dr.f and mcatnlo_wtxsec_ds.f).

Owing to the implementation of Wt production and of top hadronic decays, the Les Houches interface (mcatnlo_hwlhin.f) and the driver (mcatnlo_hwdriver.f) have been upgraded.

New script variables (BRTOPTOx and BRWTOx, with x=LEP,HAD; yGAMMAX, yMASSINF and yMASSSUP with y=T1,T2; TOPDECAY; WTTYPE; PTVETO) have been introduced.

The new script variables EXTRALIBS, EXTRAPATHS, and INCLUDEPATHS can be used to link to external libraries. Their use has only been tested on a recent Scientific Linux release, and they may be not portable to other systems.

The ranges of variables ILxCODE have been extended for several processes, in order to account for the newly-implemented hadronic decays.

MCatNLO.inputs and MCatNLO.Script have been upgraded to reflect the changes above. A new sample input file (MCatNLO_rb.inputs) is included, which documents the use of an analysis producing plots in Root format. Finally, the possibility is given to link to a dynamic LHAPDF library (through MCatNLO_dyn.Script and Makefile_dyn).

Front-end Fortran routines (rbook_fe.f) are provided, to produce plots in Root format, using the same syntax as for calling our HBOOK-type routines. A companion C++ code is needed (rbook_be.cc). These codes have been written by W. Verkerke. Examples of analysis routines using Root format have been added (mcatnlo_hwanxxx_rb.f). A call to a release-memory routine (RCLOS) has been added to mcatnlo_hwdriver.f; this is only needed when using a Root-format output, and a dummy body of RCLOS has been added to HBOOK-format analysis files mcatnlo_hwanxxx.f.

The linking to LHAPDF has been upgraded, assuming the use of LHAPDF version 5.0 or higher. The file mcatnlo_lhauti.f has been eliminated, and replaced with mcatnlo_utilhav4.f, which is however necessary only if the user wants to link with LHAPDF versions 4.xx (in such a case, the user will also need to edit the Makefile).

The automatic assignment of Λ_{QCD} when using LHAPDF is now to be considered robust. This implies changes to mcatnlo_mlmtolha.f, the insertion of a dummy routine into mcatnlo_mlmtopdf.f and mcatnlo_pdftomlm.f, and very minor changes to all *main*.f files.

Minor changes to mcatnlo_hbook.f, mainly affecting two-dimensional plot outputs.

A bug has been fixed, which prevented one from choosing properly the W mass ranges in W^+W^- production and subsequent decays in the case of ViGAMMAX< 0 (thanks to F. Filthaut).

A bug has been fixed, which affected the computation of branching ratios in $t\bar{t}$ and single-top production; $\alpha_{em}(q^2)$ was previously called with argument m_{top} rather than m^2_{top}. This only affects event weights (i.e. not distributions), and is numerically very small.

A bug in HERWIG versions 6.500 – 6.510 can lead to occasional violation of momentum conservation when the HERWIG parameter PRESPL=.FALSE. (hard subprocess rapidity preserved), as is formally assumed in MC@NLO. Therefore at present we leave this parameter at its default value, PRESPL=.TRUE. (hard subprocess longitudinal momentum preserved). We have checked that this formal inconsistency has negligible actual consequences. The bug will be fixed in HERWIG version 6.520; meanwhile, the fix may be found on the Fortran HERWIG wiki at http://projects.hepforge.org/fherwig/trac/report (ticket 33). When this fix is implemented, the statement PRESPL=.FALSE. must be inserted in mcatnlo_hwdriver.f at the place indicated by the comments therein.

It has been found that a simpler form for the MC subtraction terms with respect to that of eq. (B.43) of ref. [2] can be adopted; this form is now implemented in version 3.4. This change is relevant only to $Q\bar{Q}$ and single-top production, since for the other processes the new form and that of eq. (B.43) (which is implemented in MC@NLO version 3.3 or earlier) coincide. The differences between the two forms are equivalent to power-suppressed terms. This has been verified by comparing results obtained with version 3.4 for $t\bar{t}$ and single-top (s- and t-channel) production at the Tevatron and the LHC, and for $b\bar{b}$ production at the Tevatron, with analogous results obtained with version 3.3. On the other hand, $b\bar{b}$ production at the LHC does display large differences, owing to the fact that the old form of MC subtraction terms has a pathology which affects this process. Starting from version 3.4 $b\bar{b}$ production at the LHC may be considered safe. Technical details on the new form of the MC subtraction terms will be posted on the MC@NLO web page.

B. Running the package without the shell scripts

In this appendix, we describe the actions that the user needs to take in order to run the package without using the shell scripts, and the Makefile. Examples are given for vector boson pair production, but only trivial modifications are necessary in order to treat other production processes.

B.1 Creating the executables

An MC@NLO run requires the creation of two executables, for the NLO and MC codes respectively. The files to link depend on whether one uses PDFLIB, LHAPDF, or the PDF library provided with this package; we list them below:

- NLO with private PDFs: mcatnlo_vbmain.o mcatnlo_vbxsec.o mcatnlo_helas2.o mcatnlo_date.o mcatnlo_int.o mcatnlo_uxdate.o mcatnlo_uti.o mcatnlo_str.o mcatnlo_pdftomlm.o mcatnlo_libofpdf.o dummies.o SYSFILE

- NLO with PDFLIB: mcatnlo_vbmain.o mcatnlo_vbxsec.o mcatnlo_helas2.o mcatnlo_date.o mcatnlo_int.o mcatnlo_uxdate.o mcatnlo_uti.o mcatnlo_str.o mcatnlo_mlmtopdf.o dummies.o SYSFILE CERNLIB

NLO with LHAPDF: mcatnlo_vbmain.o mcatnlo_vbxsec.o mcatnlo_helas2.o mcatnlo_date.o mcatnlo_int.o mcatnlo_uxdate.o mcatnlo_lhauti.o mcatnlo_str.o mcatnlo_mlmtolha.o dummies.o SYSFILE LHAPDF

MC with private PDFs: mcatnlo_hwdriver.o mcatnlo_hwlhin.o mcatnlo_hwanvbp.o mcatnlo_hbook.o mcatnlo_str.o mcatnlo_pdftomlm.o mcatnlo_libofpdf.o dummies.o HWUTI HERWIGVER

MC with PDFLIB: mcatnlo_hwdriver.o mcatnlo_hwlhin.o mcatnlo_hwanvbp.o mcatnlo_hbook.o mcatnlo_str.o mcatnlo_mlmtopdf.o dummies.o HWUTI HERWIGVER CERNLIB

MC with LHAPDF: mcatnlo_hwdriver.o mcatnlo_hwlhin.o mcatnlo_hwanvbp.o mcatnlo_hbook.o mcatnlo_str.o mcatnlo_mlmtolha.o dummies.o HWUTI HERWIGVER LHAPDF

The process-specific codes mcatnlo_vbmain.o and mcatnlo_vbxsec.o (for the NLO executable) and mcatnlo_hwanvbp.o (the HERWIG analysis routines in the MC executable) need to be replaced by their analogues for other production processes, which can be easily read from the list given in sect. 1.3.

The variable SYSFILE must be set either equal to alpha.o, or to linux.o, or to sun.o, according to the architecture of the machine on which the run is performed. For any other architecture, the user should provide a file corresponding to alpha.f etc., which he/she will easily obtain by modifying alpha.f. The variables HWUTI and HERWIGVER have been described in sect. 4. In order to create the object files eventually linked, static compilation is always recommended (for example, g77 -Wall -fno-automatic on Linux).

B.2 The input files

Here, we describe the inputs to be given to the NLO and MC executables in the case of vector boson pair production. The case of other production processes is completely analogous. When the shell scripts are used to run the MC@NLO, two files are created, FPREFIXNLOinput and FPREFIXMCinput, which are read by the NLO and MC executable respectively. We start by considering the inputs for the NLO executable, presented in table 4. The variables whose name is in uppercase characters have been described in sect. 4. The other variables are assigned by the shell script. Their default values are given in table 5. Users who run the package without the script should use the values given in table 5. The variable zi controls, to a certain extent, the number of negative-weight events generated by the MC@NLO (see ref. [1]). Therefore, the user may want to tune this parameter in order to reduce as much as possible the number of negative-weight events. We stress that the MC code will not change this number; thus, the tuning can (and must) be done only by running the NLO code. The variables nitn_i control the integration step (see sect. 3.2), which can be skipped by setting $\mathrm{nitn}_i = 0$. If one needs to perform the integration step, we suggest setting these variables as indicated in table 5.

We now turn to the inputs for the MC executable, presented in table 6. The variables whose names are in uppercase characters have been described in sect. 4. The other variables

```
'FPREFIX'                                 ! prefix for BASES files
'EVPREFIX'                                ! prefix for event files
ECM FFACT FREN FFACTMC FRENMC              ! energy, scalefactors
IPROC                                     ! -2850/60/70/80=WW/ZZ/ZW+/ZW-
WMASS ZMASS                               ! M_W, M_Z
UMASS DMASS SMASS CMASS BMASS GMASS       ! quark and gluon masses
'PART1' 'PART2'                           ! hadron types
'PDFGROUP' PDFSET                         ! PDF group and id number
LAMBDAFIVE                                ! Lambda_5, <0 for default
'SCHEMEOFPDF'                             ! scheme
NEVENTS                                   ! number of events
WGTTYPE                                   ! 0 => wgt=+1/-1, 1 => wgt=+w/-w
RNDEVSEED                                 ! seed for rnd numbers
zi                                        ! zi
nitn_1 nitn_2                             ! itmx1,itmx2
```

Table 4: Sample input file for the NLO code (for vector boson pair production). FPREFIX and EVPREFIX must be understood with SCRTCH in front (see sect. 4).

Variable	Default value
zi	0.2
$\mathtt{nitn}_i$	10/0 (BASES=ON/OFF)

Table 5: Default values for script-generated variables in FPREFIXNLOinput.

are assigned by the shell script. Their default values are given in table 7. The user can freely change the values of esctype and pdftype; on the other hand, the value of beammom must always be equal to half of the hadronic CM energy.

When LHAPDF is linked, the value of PDFSET is sufficient to identify the parton density set. In such a case, PDFGROUP must be set in input equal to LHAPDF if the user wants to freeze the PDFs at the boundaries (defined as the ranges in which the fits have been performed). If one chooses to extrapolate the PDFs across the boundaries, one should set PDFGROUP=LHAEXT in input.

In the case of γ^*/Z, $W^\pm$, Higgs or heavy quark production, the MC executable can be run with the corresponding positive input process codes IPROC = 1350, 1399, 1499, 1600+ID, 1705, 1706, 2000–2008, 2600+ID or 2700+ID, to generate a standard HERWIG run for comparison purposes[8]. Then the input event file will not be read: instead, parton configurations will be generated by HERWIG according to the LO matrix elements.

[8] For vector boson pair production, for historical reasons, the different process codes 2800–2825 must be used.

'EVPREFIX.events'	! event file
NEVENTS	! number of events
pdftype	! 0->Herwig PDFs, 1 otherwise
'PART1' 'PART2'	! hadron types
beammom beammom	! beam momenta
IPROC	! -2850/60/70/80=WW/ZZ/ZW+/ZW-
'PDFGROUP'	! PDF group (1)
PDFSET	! PDF id number (1)
'PDFGROUP'	! PDF group (2)
PDFSET	! PDF id number (2)
LAMBDAHERW	! Lambda_5, < 0 for default
WMASS WMASS ZMASS	! M_W+, M_W-, M_Z
UMASS DMASS SMASS CMASS BMASS GMASS	! quark and gluon masses

Table 6: Sample input file for the MC code (for vector boson pair production), resulting from setting HERPDF=EXTPDF, which implies pdftype=1. Setting HERPDF=DEFAULT results in an analogous file, with pdftype=0, and without the lines concerning PDFGROUP and PDFSET. EVPREFIX must be understood with SCRTCH in front (see sect. 4). The negative sign of IPROC tells HERWIG to use Les Houches interface routines.

Variable	Default value
esctype	0
pdftype	0/1 (HERPDF=DEFAULT/EXTPDF)
beammom	EMC/2

Table 7: Default values for script-generated variables in MCinput.

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