QCDLoop: a comprehensive framework for one-loop scalar integrals

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Abstract

We present a new release of the QCDLoop library based on a modern object-oriented framework. We discuss the available new features such as the extension to the complex masses, the possibility to perform computations in double and quadruple precision simultaneously, and useful caching mechanisms to improve the computational speed. We benchmark the performance of the new library, and provide practical examples of phenomenological implementations by interfacing this new library to Monte Carlo programs.
Program Summary

*Name of the program:* QCDLoop

*Version:* 2.0.0

*Program obtainable from:* [http://cern.ch/qcdloop](http://cern.ch/qcdloop)

*Distribution format:* compressed tar file from the GitHub git repository

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*License:* GNU Public License GPLv3

*Computers:* all

*Operating systems:* all with a c++11 compliant compiler with quadmath support, see Sect. 3

*Program language:* c/c++, fortran 77/90, and python

*Memory required to execute:* \( \lesssim 2 \) MB

*Other programs called:* None

*External files needed:* None

*Number of bytes in distributed program, including test data etc.:* \( \sim 1.0 \) MB

*Keywords:* one-loop scalar integrals, tadpole, bubble, triangle, box, numerical evaluation, QCD, Feynman integrals

*Nature of the physical problem:* Computation of one-loop scalar integrals

*Solution Method:* Numerical evaluation of one-loop scalar integrals such as tadpole, bubble, triangle and box through analytic expressions.

*Typical running time:* detailed performance benchmark presented in Sect. 4
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1 Introduction

The requirements of precision physics at the LHC and future experiments demand high precision theoretical predictions. In this context perturbative expansions in the coupling constant play a prominent role. The field of next-to-leading order (NLO) QCD corrections has undergone a revolution in the last 10-15 years, see e.g. Refs. [1, 2] and references therein. This revolution resulted in computational tools that allow one to obtain NLO results for generic processes in a semi- or fully automated way [3–6]. One longstanding bottleneck in NLO calculations has been the computation of virtual corrections. Recently, it was understood how to use algebraic methods to write any virtual amplitude as a product of coefficients (that can be computed essentially as products of tree level amplitudes) and of one-loop scalar master integrals. Still, for complicated final states often several CPU years are required to obtain distributions that are smooth both at low and high momentum scales. Practically, this means that one needs to run codes for several days on computer farms. Obviously any improvement in the performance of these tools would be welcome.

In more recent years, a NNLO (next-to-next-to-leading) revolution has also started, and now almost all $2 \rightarrow 2$ Standard Model processes are known to this accuracy. One of the ingredients required to achieve NNLO accuracy for $pp \rightarrow X$ is a pure NLO prediction $pp \rightarrow X + 1$ parton in the kinematic configuration where the parton becomes unresolved. Hence, one loop scalar integrals are a crucial ingredient for both NLO and NNLO calculations, and a fast computation of these integrals, that remains stable also in kinematic regions where external partons become soft or collinear, is required. In the original paper by two of us (Ellis and Zanderighi [7]) an algorithm was provided to calculate all the divergent one-loop integrals. The algorithm proceeds by defining a basis set of divergent integrals, some of which were available in the literature prior to ref. [7], and some of which were calculated $ab initio$. The results for all the divergent integrals in the basis set were given in ref. [7] and they were implemented in a fortran code, dubbed QCDLoop. For finite triangle- and box-integrals QCDLoop relied on $\text{ff}$ [8]. One-loop scalar integrals have been implemented also in a number of other packages: LoopTools [9], OneLoop [10] and Collier [11]. In the case of unstable particles, calculations are often performed in the complex mass scheme [12]. So far, the QCDLoop library was limited to real masses in the propagators. Here we present an extension of the package to deal with complex masses. More generally, the aim of this paper is to present QCDLoop 2.0 [13], a new library written in $c++$ and based on the QCDLoop 1.96 formalism documented in Ref. [7]. This new framework includes, new features such as the extension to complex masses, the possibility to switch precision from double to quadruple precision on the fly. Furthermore this new framework provides an abstract object-oriented inheritance mechanism which simplifies the implementation of caching algorithms which is useful when high performance is required.

The outline of this paper is the following. In Section 2 we present a short summary of the analytic expressions and relative diagrams implemented in QCDLoop. In Section 3 we describe the library structure and we introduce the main functionalities of QCDLoop and describe the standard user interface. In Section 4 we present a detailed performance benchmark followed by results obtained with the integration of QCDLoop in a few public Monte Carlo simulation codes. Finally, in Section 5 we summarize the features and advantages of the new QCDLoop package.
2 One-loop scalar integral formalism

The QCDLoop library provides the numerical evaluation of one-loop scalar integrals such as tadpole, bubble, triangle and box through analytic expressions. This set of integrals constitutes a basis for one-loop scalar integrals. In Fig. 1 we provide a graphical representation for the definition of the following integrals:

- **Tadpole:**
  \[ I_1^D(m_1^2) = \frac{\mu^{4-D}}{i\pi^2 r_\Gamma} \int d^Dl \frac{1}{(l^2 - m_1^2 + i\epsilon)}, \]  
  (1)

- **Bubble:**
  \[ I_2^D(p_1; m_1^2, m_2^2) = \frac{\mu^{4-D}}{i\pi^2 r_\Gamma} \int d^Dl \frac{1}{(l^2 - m_1^2 + i\epsilon) \left((l + q_1)^2 - m_2^2 + i\epsilon\right)}, \]  
  (2)

- **Triangle:**
  \[ I_3^D(p_1^2, p_2^2, p_3^2; m_1^2, m_2^2, m_3^2) = \frac{\mu^{4-D}}{i\pi^2 r_\Gamma} \times \int d^Dl \frac{1}{(l^2 - m_1^2 + i\epsilon) \left((l + q_1)^2 - m_2^2 + i\epsilon\right) \left((l + q_2)^2 - m_3^2 + i\epsilon\right)}, \]  
  (3)

- **Box:**
  \[ I_4^D(p_1^2, p_2^2, p_3^2, p_4^2; s_{12}, s_{23}; m_1^2, m_2^2, m_3^2, m_4^2) = \frac{\mu^{4-D}}{i\pi^2 r_\Gamma} \times \int d^Dl \frac{1}{(l^2 - m_1^2 + i\epsilon) \left((l + q_1)^2 - m_2^2 + i\epsilon\right) \left((l + q_2)^2 - m_3^2 + i\epsilon\right) \left((l + q_3)^2 - m_4^2 + i\epsilon\right)}, \]  
  (4)

where \( q_n \equiv \sum_{i=1}^n p_i \) and \( s_{ij} = (p_i + p_j)^2 \). The above expressions are in the Bjorken-Drell metric so that \( l^2 = l_1^2 - l_2^2 - l_3^2 \). In this paper we consider momenta to be real, but the masses to be either real or complex. Near four dimensions we use \( D = 4 - 2\epsilon \) and \( \mu \) is a scale introduced so that the integrals preserve their natural dimensions, despite excursions away from \( D = 4 \). We have also removed the overall constant term which occurs in \( D \)-dimensional integrals

\[ r_\Gamma \equiv \frac{\Gamma^2(1 - \epsilon)\Gamma(1 + \epsilon)}{\Gamma(1 - 2\epsilon)} = \frac{1}{\Gamma(1 - \epsilon)} + O(\epsilon^3) = 1 - \epsilon\gamma + \epsilon^2 \left[ \frac{\gamma^2}{2} - \frac{\pi^2}{12} \right] + O(\epsilon^3). \]  
(5)

The explicit expressions for all the divergent integrals in QCDLoop 2.0 are presented in detail in the original paper of Ellis and Zanderighi [7]. As noted in that paper, some of the results for the divergent integrals were new, but many of them were not. We refer the reader to Ref. [7] for details and the appropriate references. These expressions have been adjusted for performance optimization and the proper analytical continuation has been performed to deal with complex masses. The finite integrals for the bubble topology are taken from Refs. [13,14]. Finite integrals for the triangle topology with real masses are obtained from Refs. [15,16] following the LoopTools implementation. Expressions for complex masses can be derived from Refs. [13,15,17]. We
found that the expressions of Ref. [17], as implemented in\texttt{OneLoop}, had the best performance and hence this was the approach that we followed in our implementation. Finally, the finite box integrals are based on Ref. [17], following the\texttt{LoopTools} implementation. We invite the reader to examine the \texttt{QCDLoop 2.0} source code and documentation for further details.

3 \textbf{QCDLoop library documentation}

In this section we present the user manual for the \texttt{QCDLoop} library. First of all, we discuss how to download and install \texttt{QCDLoop}. After that, we illustrate the new framework design in \texttt{c++}, explaining how objects are organized and how to run a simple program. We conclude the discussion by presenting the available caching mechanisms and the \texttt{fortran} and \texttt{python} wrappers.

3.1 Download and installation

The \texttt{QCDLoop} library is available from the website:

\url{http://cern.ch/qcdloop}

The installation of the \texttt{QCDLoop} library can be easily performed using the standard \texttt{autotools} sequence:
which automatically installs QCDLoop in /usr/local/. Note that the QCDLoop library requires a c++11 compliant compiler with quadmath support, such as g++ 4.7\(^2\), icpc 13\(^3\) and or more recent versions of these compilers. The configure script will check for these and other system requirements before building the makefiles. In order to use a different installation path one can use the option:

```bash
./configure --prefix=<path to the installation folder>
```

In this case, the QCDLoop installation path should be included to the environment variables PATH and LD_LIBRARY_PATH, adding to the local .bashrc file (or .profile file on Mac) the string:

```bash
export PATH=$PATH:<installation folder>/bin
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:<installation folder>/lib
```

If the system provides more than one c++ compiler we suggest to set the preferable choice when running configure:

```bash
./configure CXX=<compiler name / path>
```

Finally, this package provides a qcdloop-config tool which simplifies the usage of the library when linking and compiling with user’s codes. We provide the following flags: --help: shows the help message; --prefix: shows the installation prefix; --incdir: shows the path to the qcdloop header directory; --libdir: shows the path to the qcdloop library directory; --cppflags: gets compiler flags for use with the C preprocessor stage of c++ compilation; --ldflags: gets compiler flags for use with the linker stage of any compilation; --version: returns qcdloop release version number

### 3.2 The framework design

The development of a new framework for QCDLoop is motivated by the following needs:

- generalization of the code to support complex masses;
- provision of the ability to provide double and quadruple precision results simultaneously;
- the removal of code dependencies such as the ff library [8];
- improvement of performance by implementing more sophisticated LRU cache algorithms;
- provision of a modern framework based on an object-oriented language, such as c++, which simplifies future developments and native integration with modern codes.

\(^2\)https://gcc.gnu.org/
\(^3\)https://software.intel.com/
The new QCDLoop framework design is presented schematically in Fig. 2. The core of the code is the Topology class which inherits common methods from Tools and LRUCache classes. Topology is a templated class which provides the public pure virtual integral method for the specialization of the one-loop scalar integrals, together with the basic mechanism for load and storage of cached results. The Tools templated class initializes real and complex constants based on the allocated precision type, and it provides a common set of functions which are shared by the specialization of topologies. It is important to highlight that this template class reduces to a minimum the duplication of code when a method or constant is required by several specializations. The LRUCache class implements a “latest recent used” (LRU) caching algorithm for dynamic caching sizes which are discussed in detail in Sec. 3.2.3.

The specialization of the one-loop scalar integrals are implemented in four classes, one for each topology: Tadpole, Bubble, Triangle and Box. These classes implement the public pure virtual integral method from Topology. For each topology the integral method triggers automatically the kinematics and selects the appropriate function call, when possible it also provides the public methods for the direct computation of the specific kinematics. A detailed summary of the function calls and the corresponding class methods are shown in Table 1 using the notation from Ref. [7].

On top of the specialized topologies we provide the QCDLoop class. This is a high-level user interface which detects the topology by checking the size of the integral arguments. This function verifies the consistency of the input arguments and calls the respective topology.
The trigger mechanism employed by the QCDLoop class is the safest and simplest way to access all the library functionalities, however when maximum performance is required the user is invited to allocate the specific topology in order to remove the overhead due to the triggering procedure.

We conclude the description of the framework design by highlighting the availability of c++ wrappers to fortran, c and python, further details about these interfaces are presented in Sect. 3.2.4. The native c++ interface of the QCDLoop library is thread-safe only when the caching algorithms are switched off. It is particularly important to highlight that the fortran wrapper is not thread-safe by construction.

Further details about the code are fully documented using the doxygen syntax. The respective documentation is located in the qcdloop/doc folder.

3.2.1 The namespace ql: types, typedefs and templates

From a technical point of view all objects of the QCDLoop library are implemented in the ql namespace. In this namespace we define also aliases for double and quadruple precision real and complex types so that the primitive ql types are double, qdouble, complex and qcomplex:

```cpp
namespace ql {
  typedef __float128 qdouble; // quadruple precision real type
  typedef __complex128 qcomplex; // quadruple precision complex type
  typedef std::complex<double> complex; // double precision complex type
}
```

The quadruple real and complex types are standard quadmath objects, and the double complex type corresponds to the std::complex type. Specialized mathematical operations are implemented for each type in the inline header qcdloop/math.h.

In order to allocate simultaneously double and quadruple precision objects, all classes presented in Fig. 2 are templated with three typenames: TOutput the output type, TMass the mass type and TScale the scale and momenta type. The accepted types for each typename is listed below:

```cpp
ql::QCDLoop<TOutput,TMass,TScale>::integral(vector<TOutput> &res,
    TScale const & mu2,
    vector<TMass> const & m,
    vector<TScale> const & p) const;
```
| Function | Short name | Method specialization |
|----------|------------|-----------------------|
| $F^R_4(m^2)$ | Tadpole | TadPole::<::integral() |
| $I^F_2(s, m_1^2, m_2^2)$ | Bubble finite (B00) | Bubble::<::BB0() |
| $I^F_3(m; 0, m^2)$ | Bubble BB1 | Bubble::<::BB1() |
| $I^F_2(0; 0, m^2)$ | Bubble BB2 | Bubble::<::BB2() |
| $I^F_2(s; 0, 0)$ | Bubble BB3 | Bubble::<::BB3() |
| $I^F_2(s; 0, m^2)$ | Bubble BB4 | Bubble::<::BB4() |
| $I^F_2(0, 0, 0; m_1, m_2, m_3^2)$ | Triangle finite (TIN0) | Triangle::<::TIN0() |
| $I^F_3(0, p_1^2, p_2^2, p_3^2; m_1^2)$ | Triangle finite (TIN1) | Triangle::<::TIN1() |
| $I^F_3(p_1^2, p_2^2, p_3^2; m_1^2, m_2^2, m_3^2)$ | Triangle finite (TIN2) | Triangle::<::TIN2() |
| $I^F_3(p_1^2, p_2^2, p_3^2; m_1^2, m_2^2, m_3^2)$ | Triangle finite (TIN3) | Triangle::<::TIN3() |
| $I^F_3(0, 0, p_3^2; 0, 0, 0)$ | Triangle T1 | Triangle::<::T1() |
| $I^F_3(0, p_2^2, p_3^2; 0, 0, 0)$ | Triangle T2 | Triangle::<::T2() |
| $I^F_3(0, p_2^2, p_3^2; 0, 0, m^2)$ | Triangle T3 | Triangle::<::T3() |
| $I^F_3(p_3^2, m; 0, 0, m^2)$ | Triangle T4 | Triangle::<::T4() |
| $I^F_3(0, m^2, m^2, 0; 0, m^2)$ | Triangle T5 | Triangle::<::T5() |
| $I^F_3(m_1^2, s, m_2^2; 0, m_2^2, m_3^2)$ | Triangle T6 | Triangle::<::T6() |

Table 1: Summary of the function calls and the corresponding class methods in QCDLoop following the notation from Ref. [7]. The second column refers to the labels used in Figs. 3 and 4. Note that finite configurations do not require D dimension.
// Typenames and possible combinations (columns)

typename TOutput -> complex | qcomplex | complex | qcomplex
typename TMass -> double | qdouble | complex | qcomplex
typename TScale -> double | qdouble | double | qdouble

Template classes are locked to these combinations. The compiler prevents the allocation of wrong combinations at compilation time. Further extensions for the typenames are possible if required.

### 3.2.2 Code examples

A simple example of code usage in C++ is presented in the code snippet given below. The code shows how to compute a tadpole double precision integral first by using the QCDLoop trigger and then the direct allocation of the TadPole class. A similar example is then illustrated for the quadruple precision and complex mass calculation, see comments in the code. In order to change the topology it is sufficient to modify the content and size of the squared momenta and mass vectors and the initialization of the specific topology class if a direct computation is desired. Further examples are available and are build at the compilation time in the examples/ folder.

```cpp
#include <qcdloop/qcdloop.h>
using namespace ql;

int main() {
  // double precision variables
  double mu2 = ql::Pow(1.7, 2);
  std::vector<double> p = {};
  std::vector<double> m = {5.0};
  std::vector<complex> res(3);

  // Trigger example - Tadpole double precision with real mass
  ql::QCDLoop<complex, double, double> auto_trigger;
  auto_trigger.integral(res, mu2, m, p);

  // Tadpole direct call - double precision with real mass
  ql::TadPole<complex, double, double> tp;
  tp.integral(res, mu2, m, p);

  // quadruple precision and complex mass variables
  qdouble mu2q = ql::Pow(1.7q, 2);
  std::vector<qdouble> pq = {};
  std::vector<qcomplex> mq = {{5.0q, -1.0q}};
  std::vector<qcomplex> resq(3);

  // Trigger example - Tadpole quadruple precision with complex mass
  ql::QCDLoop<qcomplex, qcomplex, qdouble> auto_trigger_q;
  auto_trigger_q.integral(resq, mu2q, mq, pq);

  // Tadpole direct call - quadruple precision with complex mass
  ql::TadPole<qcomplex, qcomplex, qdouble> tpq;
  tpq.integral(resq, mu2q, mq, pq);

  return 0; }
```
3.2.3 Caching mechanisms

We provide two caching algorithms for fast retrieval of previously computed one-loop scalar integrals. By default the Topology class implements and allocates a “last-used” LU cache, with dimension $N = 1$, where only the last computed result is stored. Such a caching mechanism is similar to the previous QCDLoop 1.96 version, however a faster argument comparison algorithm parser is employed. Note that this approach is the fastest method when using a small cache with $N = 1$.

Due to the practical limitations of this approach we implement a dynamic size “last-recent-used” (LRU) algorithm in the LRUCache class. Such approach provides a simple and fast method to store the last $N$ computed integrals, where $N$ is chosen by the user. The algorithm first computes a key associated with the integral arguments by using the Murmur hash algorithm from the std::Hash function available from the c++ standard library. We have verified explicitly that the rate of hash collisions is negligible in the context of one-loop scalar integral computations. Secondly, the result of the integral is stored in an unordered map so that the searching mechanism is based on a single key search. Performance results are presented and discussed in detail in Sec. 4.1.

In order to activate the different caching algorithms the user should call the setCacheSize(int const& size) method which is available from all inherited classes from Topology and QCDLoop. The code automatically selects the appropriate caching algorithm based on the size parameter:

```cpp
q1::TadPole<complex, double, double> tp; // default cache size N = 1
tp.setCacheSize(10); // sets the cache to N=10
```

Note the possibility to switch off the caching algorithm by setting size = 0.

3.2.4 Fortran and python wrappers

The QCDLoop library provides wrappers to fortran (77/90) and c based on the same syntax of QCDLoop 1.96 in [7]. Table 2 lists the available functions for different topologies and argument types. We enlarge the previous q1Ij ($j = 1, 2, 3, 4$) syntax with extra functions identified by new prefixes: q1Ijc computes integrals in double precision and complex masses, q1Ijq computes integrals in quadruple precision and real masses, q1Iqc computes integrals in quadruple precision and complex masses. In parallel to these functions we included the new q1cachesize(size) function which provides the interface to modify the cache size. Further details of these wrappers are available in the header qcdloop/wrapper.h

We also provide a basic python interface to the library through cython which can be extended by the user easily. In order to build and install the python module for QCDLoop the user should first install the library following the instructions in Sect. 3.1 (and exporting the PATH and LD_LIBRARY_PATH environment variables) and then perform the following operations:

```bash
1 cd pywrap
2 python setup.py install
```

The last command invokes the cython compiler and installs the module to the system PYTHONPATH.
| Integral | fortran function | Description |
|----------|------------------|-------------|
| -        | qlinit()         | initializes the library |
| -        | qlcachesize(size) | sets the cache size |

| Precision | Masses |
|-----------|--------|
| double    | real   |
| double    | complex|
| quadruple | real   |
| quadruple | complex|

| $I_1^D$      | $\text{ql1}(m_1,\mu_2,\ep)$ | double | real   |
| $I_2^D$      | $\text{ql1c}(m_1,\mu_2,\ep)$ | double | complex|
| $I_3^D$      | $\text{ql1q}(m_1,\mu_2,\ep)$ | quadruple | real |
| $I_4^D$      | $\text{ql1qc}(m_1,\mu_2,\ep)$ | quadruple | complex|

| $I_1^D$      | $\text{qlI2}(p_1,m_1,m_2,\mu_2,\ep)$ | double | real   |
| $I_2^D$      | $\text{qlI2c}(p_1,m_1,m_2,\mu_2,\ep)$ | double | complex|
| $I_3^D$      | $\text{qlI2q}(p_1,m_1,m_2,\mu_2,\ep)$ | quadruple | real |
| $I_4^D$      | $\text{qlI2qc}(p_1,m_1,m_2,\mu_2,\ep)$ | quadruple | complex|

| $I_1^D$      | $\text{qlI3}(p_1,p_2,p_3,m_1,m_2,m_3,\mu_2,\ep)$ | double | real   |
| $I_2^D$      | $\text{qlI3c}(p_1,p_2,p_3,m_1,m_2,m_3,\mu_2,\ep)$ | double | complex|
| $I_3^D$      | $\text{qlI3q}(p_1,p_2,p_3,m_1,m_2,m_3,\mu_2,\ep)$ | quadruple | real |
| $I_4^D$      | $\text{qlI3qc}(p_1,p_2,p_3,m_1,m_2,m_3,\mu_2,\ep)$ | quadruple | complex|

| $I_1^D$      | $\text{qlI4}(p_1,p_2,p_3,p_4,s_{12},s_{23},m_1,m_2,m_3,m_4,\mu_2,\ep)$ | double | real   |
| $I_2^D$      | $\text{qlI4c}(p_1,p_2,p_3,p_4,s_{12},s_{23},m_1,m_2,m_3,m_4,\mu_2,\ep)$ | double | complex|
| $I_3^D$      | $\text{qlI4q}(p_1,p_2,p_3,p_4,s_{12},s_{23},m_1,m_2,m_3,m_4,\mu_2,\ep)$ | quadruple | real |
| $I_4^D$      | $\text{qlI4qc}(p_1,p_2,p_3,p_4,s_{12},s_{23},m_1,m_2,m_3,m_4,\mu_2,\ep)$ | quadruple | complex|

Table 2: fortran and c wrapper functions.

The python wrapper contains the qcdloop.QCDLoop object which reflects exactly the class ql::QCDLoop from the library. One can obtain results by querying the python console with:

```python
# Tadpole computation in python
from qcdloop import QCDLoop as ql
m = [0.5]
mu2 = 1.7**2
out = ql.integral(mu2, m)
```

## 4 Validation and benchmarks

In this section we quantify and benchmark the performance of the new QCDLoop library in terms of computational time and then in terms of phenomenological results.

### 4.1 Performance tests

All the topologies implemented in QCDLoop 2.0 have been validated successfully by direct comparison with QCDLoop 1.96 [7] for configurations with real masses and OneLoop 3.6 [10] for complex masses.

The performance benchmark is based on a common setup: all libraries compiled with gcc-5.2.1 using -O2 optimization flags on a i7-6500U CPU @ 2.50GHz. Kinematical configurations are constructed before the computation of the scalar integrals in order to avoid
copy-assignment operations during the computation loop. We use the native language of each library when performing the benchmark in order to avoid eventual overhead due to wrapper manipulation. We remove the initialization time of OneLoop from the results.

In Figure 3 we present four performance tests. In the upper left plot we compare the two versions of QCDLoop, i.e. the new C++ library QCDLoop 2.0 (red triangles) and the previous Fortran library QCDLoop 1.96 (yellow circles), to OneLoop 3.6 (blue boxes). Computations are performed with disabled cache over $10^7$ random configurations using real masses and double precision accuracy. Results are quoted in terms of average time in milliseconds for each topology and specific kinematics, following the notation of Table 1. The right inset shows the ratio to QCDLoop 1.96 where we notice that, on average, the new library provides the best performance for tadpole, bubble and triangle integrals, but we obtain similar timings to OneLoop for box configurations. Overall we conclude that the new library provides an improvement in comparison to past releases, in particular when considering finite boxes computed in QCDLoop 1.96 through the ff library. The upper right plot compares the LRU cache between the two versions of QCDLoop. We perform $10^7$ trials of the same configuration for all topologies using real masses and double precision. The new library cache is 20 to 30% faster than the previous one for tadpoles, bubbles and triangles, meanwhile we observe a consistent speed-up of 70% for boxes. In the lower left plot we compare the performance of the new QCDLoop library when using the LRU cache with $N = 10$ in comparison to the direct computation of 10 configurations repeated $10^7$ times. Results show a great performance improvement when using this caching mechanism. For some simple topologies like the tadpole the caching algorithm has similar performance in comparison to the direct computation, however when considering the most time consuming configurations, like BIN4, differences of a factor 40 are observed. Finally, in the lower right plot we compare the performance of the new QCDLoop library when computing results in double and quadruple precision. In this case the same configuration is repeated $10^7$ times with double and quadruple variables. Differences are proportional to the complexity of the integral. We always observe a slowdown factor in the range 1.8 to 3 when using quadruple precision.

In Figure 4 we compare the performance of the new QCDLoop library when computing one-loop scalar integrals with real and complex masses. We observe a performance loss above 50% when activating complex masses for non finite integrals. Differences are smaller for finite triangles and boxes due to the fact that those implementations rely on complex objects for both mass types.

4.2 Phenomenological applications

In this section we test the new QCDLoop library in Monte Carlo environments. We first show results for real masses using simulations obtained with the MCFM 7.0.1 [18,19] interface. We then test complex masses using interfaces to Ninja [20,21] and GoSam [22] in a Sherpa 2.2.0 [23,24] simulation.

4.2.1 MCFM interface

The interface to the new QCDLoop library and MCFM is straightforward, thanks to the backward compatible Fortran wrapper presented in Section 3.2.4. The only technical requirement in MCFM consists in editing the makefile and updating the links and paths to the new library.

Simulations are performed for the LHC setup at $\sqrt{s} = 13$ TeV, using NNPDF3.0 NLO [25] set of PDFs and the default parameters of the MCFM 7.0.1 input card. Here we focus on the
Figure 3: Performance comparisons. Upper left: QCDLoop 2.0 vs QCDLoop 1.96 vs OneLoop 3.6 performance for real masses and double precision for $10^7$ configurations. Upper right: QCDLoop 2.0 vs QCDLoop 1.96 cache $N=1$ with real masses and double precision, for $10^7$ trials of the same configuration. Lower left: QCDLoop 2.0 cache $N > 1$ vs no cache for $10^7$ trials of ten configurations. Lower right: QCDLoop 2.0 double vs quadruple precision performance for $10^7$ trials of the same configuration.
predictions of three processes which cover a large range of topologies, including massive and massless loops, namely: $WW$ (nproc=61), $ZZ$ (nproc=81) and $\gamma\gamma\gamma\gamma$ (nproc=289) production. The aim of the results presented here is to show that fully compatible results are obtained when running the MC simulation with both versions of the library, i.e. $QCDLoop$ 1.96 and 2.0.

In Figure 5 we plot the inclusive cross-section for $WW$, $ZZ$ and $\gamma\gamma\gamma\gamma$ processes respectively for both versions of $QCDLoop$. Numerical results are in agreement for all processes. In terms of performance we observe 10% improvement with the new library for $WW$ and $ZZ$ production meanwhile 5% improvement for $\gamma\gamma\gamma\gamma$ production.

In Figure 6 we show differential distributions for the three processes described above, always comparing both versions of the $QCDLoop$ library. In the top left panel we show the $WW$-pair transverse mass, $m_{TT}^{WW}$, distribution. The top right panel presents the rapidity of the lepton-pair $y_Z$ for the $ZZ$ production. Finally, the bottom plot highlights the photon $p_T^\gamma$ distribution in the $\gamma\gamma\gamma\gamma$ production. In all cases the agreement is very good; for the $p_T^\gamma$ distribution we have performed a simulation of few hours (low statistics) in order to check that even with a low number of iterations the final agreement between both codes is excellent.

4.2.2 Ninja and GoSam interface

For the validation of complex masses in a Monte Carlo environment we considered the Ninja library [20,21], which provides the integrand reduction via Laurent expansion method for the computation of one-loop integrals, and the GoSam [22] automated package.

First, we expanded the Ninja library with the new $QCDLoop$ interface. We then verified the consistency of the new interface by comparing the output between OneLoop 3.6 and $QCDLoop$ 2.0 for the examples provided by the Ninja test codes. Second, this new version of Ninja was linked to GoSam granting access of matrix elements to Monte Carlo simulation tools.

In order to provide quantitative results we used Sherpa 2.2.0 to simulate $H+2j$ process at NLO, for the LHC setup at $\sqrt{s} = 13$ TeV with the NNPDF3.0 NLO PDF set. Such process is interesting for our tests because it calls several topologies with complex masses. We performed two simulations, the first with OneLoop and the second with $QCDLoop$. Table 3 shows the inclusive cross-section values obtained with both codes with 50M events, and Figure 7 presents the corresponding rapidity $y_H$ and $p_T^H$ distributions for the Higgs boson. This simulation shows
that numerical results are in agreement for all distributions within Monte Carlo uncertainties. In terms of performance, both codes require $\sim 10$ CPU hours to complete the simulation.

| Library         | $H + 2j$ cross-section (Sherpa 2.2.0) |
|-----------------|--------------------------------------|
| OneLoop 3.6     | $5.5867 \pm (0.0121 = 0.21\%) \text{ pb}$ |
| QCDLoop 2.0     | $5.5838 \pm (0.0121 = 0.21\%) \text{ pb}$ |

Table 3: Inclusive cross-section for $H+2j$ at NLO obtained with 5M events from Sherpa 2.2.0 interfaced with OneLoop 3.6 and QCDLoop 2.0 through the Ninja and GoSam interfaces.

Finally, other interfaces to Monte Carlo codes are possible, users are invited to interface their own code with QCDLoop.

5 Conclusions

In this work we presented a new object-oriented framework for the QCDLoop library. The new features compared with the fortran version are

- QCDLoop 2.0 calculates all integrals using native implementations. The reliance on the external library ff is no longer present.
Figure 6: Examples of differential distributions obtained with \texttt{MCFM 7.0.1} using both versions of \texttt{QCDLoop}, for the $m_W^T$ transverse mass in $WW$ production, the average $y_Z$ rapidity distribution in $ZZ$ production and the average $p_T^\gamma$ distribution in 4-$\gamma$ production. Simulations performed for LHC @ 13 TeV, using NNPDF3.0 NLO.

- Full implementation of double and quadruple precision for the whole library, including the possibility of switching between the two dynamically. This can be useful in regions of phase space in which double precision is not sufficient. This can occur in corners of phase space, for example, in the context of NNLO calculations when unresolved regions of phase space are probed.

- Improvements in the evaluation time with respect to the Fortran version.

- Improvements in the caching algorithm. For certain applications, in which the same integrals are needed several times, this can lead to great improvements in evaluation time with respect to the Fortran version. In the new version one can adjust the size of the cache to yield the best performance.

The new \texttt{QCDLoop} library is publicly available from the webpage:
Figure 7: Examples of differential distribution obtained with Sherpa 2.2.0 using Oneloop and QCDLoop through the Ninja/GoSam interfaces. Simulations performed for LHC @ 13 TeV, using NNPDF3.0 NLO. http://cern.ch/qcdloop

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