

handyG – rapid numerical evaluation of generalised polylogarithms in Fortran

L. Naterop¹, A. Signer^{1,2}, and Y. Ulrich^{*1,2}

¹*Physik-Institut, Universität Zürich,
Winterthurerstrasse 190, CH-8057 Zürich, Switzerland*

²*Paul Scherrer Institut
CH-5232 Villigen PSI, Switzerland*

Abstract

Generalised polylogarithms naturally appear in higher-order calculations of quantum field theories. We present handyG, a Fortran 90 library for the evaluation of such functions, by implementing the algorithm proposed by Vollinga and Weinzierl. This allows fast numerical evaluation of generalised polylogarithms with currently relevant weights, suitable for Monte Carlo integration.

Keywords: numerical evaluation, Feynman integrals, polylogarithms

*Corresponding author.

E-mail address: yannick.ulrich@psi.ch

PROGRAM SUMMARY *Program Title:* handyG

Licensing provisions: GPLv3

Programming language: Fortran 90

Operating system: Linux (tested on Ubuntu 18.04 and Scientific Linux 7.6), macOS. Code optimisation is only available with recent compilers

Distribution format: <https://gitlab.psi.ch/mcmule/handyG>

E-mail: yannick.ulrich@psi.ch

Other programs called: none, Mathematica interface available

Nature of problem: Numerical evaluation routine for generalised (or Goncharov [1]) polylogarithms that is fast enough for Monte Carlo integration.

Solution method: Implementing the algorithm presented by Vollinga and Weinzierl [2] in Fortran 90, providing a Fortran module and a Mathematica interface.

Typical running time: Dependent on the complexity of the function. GPLs with typical weight up to five evaluate in the millisecond range.

Limitations: There are no theoretical limitations of the weight through the algorithm. However, for arbitrary parameters there are limits through runtime for increasing weight.

References

- [1] A. B. Goncharov, *Multiple polylogarithms, cyclotomy and modular complexes*, *Math. Res. Lett.* **5** (1998) 497 [[1105.2076](#)].
- [2] J. Vollinga and S. Weinzierl, *Numerical evaluation of multiple polylogarithms*, *Comput. Phys. Commun.* **167** (2005) 177 [[hep-ph/0410259](#)].

1 Introduction

It is well known that analytic calculations of higher-order corrections in quantum field theory give rise to polylogarithms. In the calculation of master integrals this usually happens when solving complicated Mellin-Barnes integrals or differential equations. For processes involving many scales, these are not just harmonic polylogarithms [1] any more. Instead, generalised or Goncharov polylogarithms (GPL) are required [2].

Much effort has been dedicated to harmonic polylogarithms [3–6], making their numerical evaluation fast and effortless. Unfortunately, the same cannot quite be said for generalised polylogarithms. Worse yet, as we enter the era of high-precision fully-differential NNLO and N³LO calculations, being able to merely evaluate these functions is not sufficient anymore. We need to be able to integrate over GPLs numerically within a Monte Carlo code, meaning that speed ceases to be just a luxury – it becomes critical.

There are two public methods that deal with the numeric aspect of GPLs: a general implementation in the computer algebra system GiNaC [7] and a set of reduction rules to reduce GPLs to known functions [8]. The latter is implemented in Mathematica and can be difficult to use if the choice of branch cuts matters. The former, written in C++, on the other hand, can be cumbersome to interface with Monte Carlo programs which are usually written in Fortran. The computer algebra library GiNaC performs the numerical evaluation symbolically, resulting in performance unsuitable for Monte Carlo integration. The algorithm employed by GiNaC is also implemented in Maple [9].

Hence, we present handyG, an easy-to-use Fortran implementation of the algorithm presented in [7], enjoying the raw speed of the compiled language’s complex number arithmetic without sacrificing simplicity.

This paper is structured as follows: in Section 2 we formally introduce GPLs and the different notations we are using as well as some general properties. Next, in Section 3 we discuss how to obtain, install and use handyG. For the inclined reader, Section 4 discusses the algorithm used by GiNaC and handyG in detail, providing examples. Finally, we compare the code’s performance on a set of test cases in Section 5 before we conclude in Section 6.

2 Notation and properties of GPLs

GPLs are complex-valued functions that depend on m complex parameters z_1, \dots, z_m as well as an argument y . We can define a GPL as a nested integral with $z_m \neq 0$

$$G(z_1, \dots, z_m ; y) \equiv \int_0^y \frac{dt_1}{t_1 - z_1} \int_0^{t_1} \frac{dt_2}{t_2 - z_2} \dots \int_0^{t_{m-1}} \frac{dt_m}{t_m - z_m}. \quad (1)$$

Alternatively, they can also be defined in recursive form as

$$G(z_1, \dots, z_m ; y) = \int_0^y \frac{dt_1}{t_1 - z_1} G(z_2, \dots, z_m ; t_1), \quad (2)$$

where the base case of $m = 1$ is just a logarithm

$$G(z; y) = \log \left(1 - \frac{y}{z} \right). \quad (3)$$

To also cover the case of $z_m = 0$ we define

$$G(\underbrace{0, \dots, 0}_m; y) \equiv G(0_m; y) = \frac{(\log y)^m}{m!}, \quad (4)$$

where we denote a string of m zeros as 0_m .

We call $G(z_1, \dots, z_m; y)$ *flat* since all parameters are explicit. However, this notation can be cumbersome if many of the z_i are zero. In this case we introduce the *condensed* notation which uses partial weights m_i in order to keep track of the number of zeros in front of the parameter z_i

$$G_{m_1, \dots, m_k}(z_1, \dots, z_k; y) \equiv G(0_{m_1-1}, z_1, \dots, z_{k-1}, 0_{m_k-1}, z_k; y). \quad (5)$$

Both notations will be used interchangeably. We say that this GPL is of depth k as it has k non-zero parameters (not counting y). Its total weight is $m = \sum m_i$.

2.1 Multiple polylogarithms

Multiple polylogarithms (MPLs) are a related class of functions that also generalise logarithms. They are defined as an infinite nested series

$$\text{Li}_{m_1, \dots, m_k}(x_1, \dots, x_k) \equiv \sum_{i_1 > \dots > i_k} \frac{x_1^{i_1}}{i_1^{m_1}} \dots \frac{x_k^{i_k}}{i_k^{m_k}}, \quad (6)$$

where m_1, \dots, m_k are integer weights. If there is only one argument present, they reduce to classical polylogarithms $\text{Li}_m(x)$.

MPLs are closely related to GPLs through

$$\text{Li}_{m_1, \dots, m_k}(x_1, \dots, x_k) = (-1)^k G_{m_1, \dots, m_k} \left(\frac{1}{x_1}, \frac{1}{x_1 x_2}, \dots, \frac{1}{x_1 \dots x_k}; 1 \right). \quad (7)$$

This can be inverted by performing an iterated substitution

$$u_1 = \frac{1}{x_1}, \quad u_2 = \frac{1}{x_1 x_2} = \frac{u_1}{x_1}, \quad \dots \quad u_k = \frac{1}{x_1 \dots x_k} = \frac{u_{k-1}}{x_k}, \quad (8)$$

allowing us to write the GPLs in terms of MPLs

$$G_{m_1, \dots, m_k}(u_1, \dots, u_k; 1) = (-1)^k \text{Li}_{m_1, \dots, m_k} \left(\frac{1}{u_1}, \frac{u_1}{u_2}, \dots, \frac{u_{k-1}}{u_k} \right). \quad (9)$$

In (9), the left-hand side is an integral representation whereas the right-hand side is a series representation.

GPLs with arbitrary parameters satisfy the scaling relation

$$G(z_1, \dots, z_m; y) = G(\kappa z_1, \dots, \kappa z_m; \kappa y) \quad (10)$$

for any complex number $\kappa \neq 0$. (9) assumes the argument of G is equal to one. Using the scaling relation we can normalise $G(z_1, \dots, z_m; y)$ with $\kappa = 1/y$ to guarantee that the argument is indeed one.

For the numerical evaluation the main idea will be to compute G -functions by reducing them to their corresponding series representation (9).

2.2 Convergence properties

If we want to use an infinite series for numerical evaluation of GPLs, the series needs to be convergent. It can be shown [7] that an MPL $\text{Li}_{m_1, \dots, m_k}(x_1, \dots, x_k)$ is convergent if the conditions

$$|x_1 \cdots x_k| < 1 \quad \text{and} \quad (m_1, x_1) \neq (1, 1) \quad (11)$$

are satisfied. Using the relation (9), this translates to a sufficient convergence criterion for the integral representation. We find that if

$$|y| < |z_i| \quad \forall i = 1, \dots, k \quad \text{and} \quad (m_1, y/z_1) \neq (1, 1), \quad (12)$$

$G_{m_1, \dots, m_k}(z_1, \dots, z_k; y)$ is convergent.

In Section 4 we will review the algorithm developed by [7] to transform any GPL into this form.

2.3 Shuffle algebra and trailing zeros

If the last parameter z_k of a GPL $G_{m_1, \dots, m_k}(z_1, \dots, z_k; y)$ vanishes, the convergence criterion (12) is not fulfilled. Hence, any algorithm that intends to exploit (6) for numerical evaluation needs to remove trailing zeros.

We can exploit the fact that GPLs satisfy two Hopf algebras: a shuffle algebra and a stuffle algebra [7, 8, 10]. Here, we will only be needing the former. It allows us to write the product of two GPLs with parameters \vec{a} and \vec{b} as

$$G(\vec{a}; y) \cdot G(\vec{b}; y) = \sum_{\vec{c} = \vec{a} \sqcup \vec{b}} G(\vec{c}; y). \quad (13)$$

The sum in the right-hand side of (13) runs over all elements of the the shuffle product of the list \vec{a} with \vec{b} . This shuffle product gives the set of all permutations of the elements in \vec{a} and \vec{b} that preserve the respective orderings of \vec{a} and \vec{b} . For practical implementations, a recursive algorithm exists [11].

3 Installation and usage

The code is available in a public GitLab repository hosted by the Paul Scherrer Institut at

```
https://gitlab.psi.ch/mcmule/handyG
```

From this URL a release version can be downloaded in compressed form. Alternatively, handyG can be obtained by cloning using the git command

```
git clone https://gitlab.psi.ch/mcmule/handyG.git
```

This will download handyG into a subfolder called handyG. Within this folder

```
git pull
```

can be used to update handyG.

3.1 Installation

handyG should run on a variety of systems though this can obviously not be guaranteed. The code follows the conventional installation scheme¹

```
./configure # Look for compilers and make a guess at
             # necessary flags
make all     # Compiles the library
make check  # Performs a variety of checks (optional)
make install # Installs library into prefix (optional)
```

handyG has a Mathematica interface (activate with `--with-mcc`) and a GiNaC interface (activate with `--with-ginac`) that can be activated by supplying the necessary flags to `./configure`. The latter is only used for testing purposes and is not actually required for running. Another important flag is `--quad` which enables quadruple precision in Fortran. Note that this will slow down handyG, so that it should only be used if double-precision is indeed not enough.

The compilation process creates the following results

<code>libhandyg.a</code>	the handyG library
<code>handyg.mod</code>	the module files for Fortran 90
<code>geval</code>	a binary file for quick-and-dirty evaluation
<code>handyG</code>	the Mathematica interface

An overview of systems on which the code was successfully tested can be found in Table 1 (see Section 5 for performance).

¹Despite the name, `./configure` has nothing to do with autotools

Operating System	Processor	Compiler	math
Scientific Linux 6.0	Xeon E3 Sandy Bridge 3.3GHz	gcc 4.4.4*	N/A
Scientific Linux 6.4	Xeon E5 Broadwell 2.1GHz	gcc 8.2.0 intel 14.0.2	11.0.0 N/A
Scientific Linux 7.6	Xeon E3 Sandy Bridge 3.3GHz	gcc 8.2.0 intel 19.0.3	11.0.0 N/A
Ubuntu 18.04.2	i5 Kaby Lake R 1.7GHz	gcc 7.4.0	11.3.0
macOS 10.12.6	i5 Broadwell 1.6GHz	gcc 5.1.0	11.0.1
macOS 10.14.5	Core M Broadwell 0.9GHz i5 Ivy Bridge 2.5GHz	gcc 8.3.0 gcc 8.3.0	11.3.0 11.3.0

Table 1: An overview of systems under which handyG works as expected. All processors are manufactured by Intel. math indicated the version of Mathematica used. The * indicates that for this version of gcc no optimisation is available.

3.2 Usage in Fortran

handyG is written with Fortran in mind. We provide a module `handyg.mod` containing the following objects

- `prec`: the working precision as a Fortran kind. This is read-only, the code needs to be reconfigured for a change to take effect. Note that this does not necessarily increase the result's precision without also changing the next options.
- `set_options`:
a subroutine to set runtime parameters of handyG. `set_options` takes the following arguments
 - `real(kind=prec) :: MPLdel = 1e-15`: difference between two successive terms at which the series expansion (6) is truncated.
 - `integer LiInf = 1000`: number of terms in the expansion of classical polylogarithms.
 - `real(kind=prec) :: hCircle = 1.1`: the size of the Hölder circle λ (see Section 4.4).

For an example of how to use `set_options`, see Listing 2.

- `inum`:
a datatype to handle $i0^+$ -prescription (see Section 3.4).
- `clearcache`:
handyG caches a certain number of classical polylogarithms (see Section 3.5). This resets the cache (in a Monte Carlo this should be called at every phase space point).
- `G`:
the main interface for generalised polylogarithms.

```
real(kind=prec) :: delta, circle
integer inf
delta = 1e-15
inf = 1000
circle = 1.1
call set_options(MPLdel = delta , &
                LiInf   = inf   , &
                hCircle = circle)
```

Listing 2: The default values of the options of handyG

In Listing 3 we show an example program to calculate the following GPLs

$$\begin{aligned}
 \text{res}(1) &= G(1, 2; 1), \\
 \text{res}(2) &= G\left(1, 0, \frac{1}{2}; x\right) = G_{1,2}\left(1, \frac{1}{2}; x\right), \\
 \text{res}(3) &= G\left(1, 0, \frac{1}{2}, 1+i; x\right) = G_{1,2,1}\left(1, \frac{1}{2}, 1+i; x\right), \\
 \text{res}(4) &= G\left(1_+, 0, 5; \frac{1}{x}\right), \\
 \text{res}(5) &= G\left(1_-, 0, 5; \frac{1}{x}\right),
 \end{aligned}
 \tag{14}$$

with $x = 0.3$ and 1_{\pm} indicating $1 \pm i0^+$.

The easiest way to compile the code is with `pkg-config`. Assuming `handyG` has been installed with `make install`, the example program `example.f90` can be compiled as (assuming you are using `GFortran`)

```

$ gfortran -o example example.f90 \
    'pkg-config --cflags --libs handyg'
$ ./example
res(1) = -0.822467+ 0.000000i
res(2) =  0.128388+ 0.000000i
res(3) = -0.003748+ 0.003980i
res(4) = -0.961279+-0.662888i
res(5) = -0.961279+ 0.662888i

```

If `pkg-config` is not available and/or for non-standard installations it might be necessary to specify the search paths²

```

$ gfortran -o example example.f90 \
> -I/absolute/path/to/handyG -fdefault-real-8 \
> -L/absolute/path/to/handyG -lhandyg

```

3.3 Usage in Mathematica

Mathematica is arguably one of the most used computer algebra system among particle physicists. Hence, we have interfaced our code to Mathematica using Wolfram's MathLink interface (for a review on how this works, see [12]). In Listing 4 we show how to calculate the functions in (14) in Mathematica, assuming that the code was installed with `make install`. The subscript 1_{\pm} , indicating the side of the branch cut, can be entered using `SubPlus` (`SubMinus`) or using `ctrl_` and `+`, (`ctrl_` and `-`). When using `handyG` in Mathematica, keep in mind that it uses Fortran which means that computations are performed with fixed precision.

²Some versions of `GFortran` specify a search path for modules. `ifort` does this automatically.

```

PROGRAM gtest
  use handyG
  complex(kind=prec) :: res(5), x, weights(4)
  call clearcache

  x = 0.3 ! the parameter

  ! flat form with integers
  res(1) = G(/ 1, 2, 1 /)

  ! very flat form for real numbers using F2003 arrays
  res(2) = G([ 1., 0., 0.5, real(x)])
  ! this is equivalent to the flat expression
  res(2) = G([ 1., 0., 0.5 ], real(x))
  ! or in condensed form
  res(2) = G(/1, 2/), (/ 1., 0.5 /), real(x))

  ! flat form with complex arguments
  weights = [(1.,0.), (0.,0.), (0.5,0.), (1.,1.) ]
  res(3) = G(weights, x)

  ! flat form with explicit i0-prescription
  res(4) = G([inum(1.,+1),inum(0,+1),inum(5,+1)], &
             inum(1/x,di0))
  res(5) = G([inum(1.,-1),inum(0,+1),inum(5,+1)], &
             inum(1/x,di0))
  ! this is equivalent to
  res(5) = G(/1,2/),[inum(1.,-1),inum(5,+1)], &
             inum(1/x,+1))

  do i =1,5
    write(*,900) i, real(res(i)), aimag(res(i))
  enddo
900 FORMAT("res(",I1,")=□",F9.6,"+",F9.6,"i")
END PROGRAM gtest

```

Listing 3: The example program example.f90 to calculate the example in (14)

```

In[1]:= Install["handyG"];
handyG by L. Naterop, Y. Ulrich, A. Signer

In[2]:= x=0.3;

In[3]:= res[1] = G[1,2,1]

Out[3]= -0.822467

In[4]:= res[2] = G[1,0,1/2,x]

Out[4]= 0.128388

In[5]:= res[3] = G[1,0,1/2,1+I,x]

Out[5]= -0.003747969 + 0.00398002 I

In[6]:= res[4] = G[1+,5,1/x]

Out[6]= -1.12732 - 0.701026 I

In[7]:= res[5] = G[1-,5,1/x]

Out[7]= -1.12732 + 0.701026 I

```

Listing 4: An example of how to use handyG in Mathematica to calculate the functions of (14).

3.4 Proper $i0^+$ prescription

To evaluate integrals in the physical kinematic region, we often need to prescribe on which side of any potential branch cut a parameter lies. This is done by adding an infinitesimal imaginary part to the parameter. In handyG this is implemented using a custom data type³ that keeps track of both the (potentially complex) number c and the sign of the imaginary part $i0$

```
type inum
  complex(kind=prec) :: c
  integer(1) :: i0
end type inum
```

There are a few constants and procedures implemented for the user's convenience

```
integer(1), parameter :: di0 = +1
type(inum), parameter :: izero=inum( 0.,di0)

FUNCTION TOINUM(z, s)
real(kind=prec) :: z(:)
type(inum) :: toinum(size(z))
integer(1), optional :: s
...
END FUNCTION TOINUM

FUNCTION TOCMPLX
type(inum) :: z
complex(kind=prec) tocmplx
...
END FUNCTION TOCMPLX
```

The variable `di0` specifies the default imaginary part that will be used if nothing is specified explicitly. The functions `toinum` and `tocmplx` can be used to convert lists and numbers to `inum` objects and complex numbers, respectively.

Finally, `real`, `aimag` and `abs` work as expected even on objects of type `inum`.

3.5 Cache system

handyG has a cache system for classical polylogarithms. This is controlled through the parameter

```
integer, parameter :: PolyLogCacheSize(2) = (/ n, m_max /)
```

³Note that, due to padding, the actual size of `inum` may be as large as 24 byte

in `globals.f90`. This caches n polylogarithms of the form $\text{Li}_m(x)$ for $2 \leq m \leq m_{\max}$ each. The default values are $n = 100$ and $m_{\max} = 5$.

The cache system consumes

$$n \times m_{\max} \times (2 \times \text{sizeof}(\text{complex}(\text{kind}=\text{prec})) + 1\text{byte} + \text{padding}) = 12 \text{ kB}$$

bytes of memory in the default settings. This is a very small price to pay for improving the evaluation speed considerably.

The gain from a similar system for convergent MPLs or even entire GPLs is presently not worth the effort.

4 The algorithm

The central idea to numerically evaluate GPLs is to first map their parameters to the domain where the corresponding series representation is convergent (12) and to then use the series expansion up to some finite order. Thus, we will first look at how to remove trailing zeros in Section 4.1, and then how to make a GPL without trailing zeros convergent in Section 4.2 as presented in [7]. In Section 4.4, we comment on accelerating the convergence of already convergent GPLs. Finally, in Section 4.5 we apply the algorithm to an explicit example.

4.1 Removal of trailing zeros

Consider a GPL of weight m with $m-j$ trailing zeros

$$G(z_1, \dots, z_j, 0_{m-j}; y).$$

We now shuffle $\vec{a} = (z_1, \dots, z_j, 0_{m-j-1})$ with $\vec{b} = (0)$. This results in $m-j$ times the original GPL as well as terms with less trailing zeros

$$G(0; y) \cdot G(z_1, \dots, z_j, 0_{m-j-1}; y) = (m-j)G(z_1, \dots, z_j, 0_{m-j}; y) + \sum_{\vec{s}} G(s_1, \dots, s_j, z_j, 0_{m-j-1}; y), \quad (15)$$

where the sum runs over all shuffle $\vec{s} = (z_1, \dots, z_{j-1}) \sqcup (0)$. We now solve (15) for $G(z_1, \dots, z_j, 0_{m-j}; y)$ and obtain an expression with fewer trailing zeros. By applying this strategy recursively, we can remove all trailing zeros.

4.2 Making GPLs convergent

4.2.1 Reduction to pending integrals

Consider a GPL of the form

$$G(a_1, \dots, a_{i-1}, s_r, a_{i+1}, \dots, a_m ; y) \quad (16)$$

where $s_r (= a_i)$ has the smallest absolute value among all the non-zero parameters in G . If $|s_r| < |y|$, (16) has no convergent series expansion. In order to remove the smallest weight s_r , we apply the fundamental theorem of calculus to generate terms where s_r is either integrated over or not present anymore

$$\begin{aligned} G(a_1, \dots, a_{i-1}, s_r, a_{i+1}, \dots, a_m ; y) &= G(a_1, \dots, a_{i-1}, 0, a_{i+1}, \dots, a_m ; y) \\ &+ \int_0^{s_r} ds_{r+1} \frac{\partial}{\partial s_{r+1}} G(a_1, \dots, a_{i-1}, s_{r+1}, a_{i+1}, \dots, a_m ; y). \end{aligned} \quad (17)$$

For the second term we use partial fraction decomposition and integration by parts. Then we obtain different results depending on where s_r is in the parameter list:

- If s_r appears first in the list (i.e. $i = 1$ and $s_r = a_1$) we find

$$\begin{aligned} G(s_r, a_{i+1}, \dots, a_m ; y) &= G(0, a_{i+1}, \dots, a_m ; y) + \underbrace{\int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - y} G(a_{i+1}, \dots, a_m ; y)}_{G(y; s_r)} \\ &+ \underbrace{\int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i+1}} G(s_{r+1}, a_{i+2}, \dots, a_m ; y)}_{\text{pending integral}} - \underbrace{\int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i+1}} G(a_{i+1}, \dots, a_m ; y)}_{G(a_2 ; s_r)}. \end{aligned} \quad (18)$$

In the first term on the right-hand side, s_r is absent. Therefore the resulting GPL is simpler. It might still be non-convergent, but we can use this method recursively on the resulting GPLs until we end up with convergent GPLs.

In the second and fourth terms the integration variable s_{r+1} does not appear in the parameters of the GPL, so that the integral can be solved (we write the solution as a GPL instead of a logarithm to be able to continue recursively).

The third term does have the integration variable s_{r+1} among the weights and therefore yields what we refer to as a pending integral. This object can be written as a linear combination of simpler GPLs as we will see in Section 4.3.

Note that all GPLs on the right-hand side have depth reduced by one.

- If s_r appears in the middle of the list, i.e. $1 < i < m$, we find

$$\begin{aligned}
G(a_1, \dots, a_{i-1}, s_r, a_{i+1}, \dots, a_m; y) = & \\
& + G(a_1, \dots, a_{i-1}, 0, a_{i+1}, \dots, a_m; y) \\
& - \int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i-1}} G(a_1, \dots, a_{i-2}, s_{r+1}, a_{i+1}, \dots, a_m; y) \\
& + \underbrace{\int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i-1}} G(a_1, \dots, a_{i-1}, a_{i+1}, \dots, a_m; y)}_{G(a_{i-1}; s_r)} \\
& + \int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i+1}} G(a_1, \dots, a_{i-1}, s_{r+1}, a_{i+2}, \dots, a_m; y) \\
& - \underbrace{\int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i+1}} G(a_1, \dots, a_{i-1}, a_{i+1}, \dots, a_m; y)}_{G(a_{i+1}; s_r)}.
\end{aligned} \tag{19}$$

Again we obtain simpler GPLs (without s_r or lower depth) as well as pending integrals.

- If s_r appears last in the list, i.e. $i = m$, we use the shuffle algebra to remove s_r from the last place, just as we have done to removed trailing zeros.

We repeat these steps also for GPLs that are already under a pending integral.

4.3 Evaluation of pending integrals

The most general term created by the procedure of the last section is of the form

$$\text{PI}\left(\vec{p} = (y', \vec{b}), i, \vec{g} = (\vec{a}, y)\right) \equiv \int_0^{y'} \frac{ds_1}{s_1 - b_1} \int_0^{s_1} \frac{ds_2}{s_2 - b_2} \dots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} \tag{20}$$

$$G(a_1, \dots, a_{i-1}, s_r, a_{i+1}, \dots, a_m; y).$$

Here we have adopted the convention that $i = 0$ implies that the integration variable does not appear inside the GPL. For example

$$\begin{aligned}
\text{PI}\left(\vec{p} = (1, 2, 3), 0, (4, 5)\right) &= \int_0^1 \frac{ds_1}{s_1 - 2} \int_0^{s_1} \frac{ds_2}{s_2 - 3} G(4; 5) \\
\text{PI}\left(\vec{p} = (1, 2, 3), 2, (4, 5)\right) &= \int_0^1 \frac{ds_1}{s_1 - 2} \int_0^{s_1} \frac{ds_2}{s_2 - 3} G(4, s_2; 5).
\end{aligned}$$

As we use the algorithm, we need a way to collapse the pending integrals back down again. As an example, consider the case $i = 1$

$$\begin{aligned}
\text{PI}\left(\vec{p} = (y', \vec{b}), 1, \vec{g} = (\vec{a}, y)\right) &= \int_0^{y'} \frac{ds_1}{s_1 - b_1} \cdots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} G(s_r, a_{i+1}, \dots, a_m; y) = \\
&\underbrace{\int_0^{y'} \frac{ds_1}{s_1 - b_1} \cdots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} G(0, a_{i+1}, \dots, a_m; y)}_{\text{PI}(\vec{p}, 0, 0)} \\
&+ \underbrace{\int_0^{y'} \frac{ds_1}{s_1 - b_1} \cdots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} \int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - y} G(a_{i+1}, \dots, a_m; y)}_{\text{PI}(\vec{p}, y, 0, 0)} \\
&+ \underbrace{\int_0^{y'} \frac{ds_1}{s_1 - b_1} \cdots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} \int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i+1}} G(s_{r+1}, a_{i+2}, \dots, a_m; y)}_{\text{PI}(\vec{p}, a_{i+1}, 1, (a_{i+2}, \dots, a_m; y))} \\
&- \underbrace{\int_0^{y'} \frac{ds_1}{s_1 - b_1} \cdots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} \int_0^{s_r} \frac{ds_{r+1}}{s_{r+1} - a_{i+1}} G(a_{i+1}, \dots, a_m; y)}_{\text{PI}(\vec{p}, a_{i+1}, 0, 0)} \\
&= \text{PI}(\vec{p}, 0, 0) G(0, a_{i+1}, \dots, a_m; y) + \text{PI}(\vec{p}, y, 0, 0) G(a_{i+1}, \dots, a_m; y) \\
&+ \text{PI}(\vec{p}, a_{i+1}, 1, (a_{i+2}, \dots, a_m; y)) - \text{PI}(\vec{p}, a_{i+1}, 0, 0) G(a_{i+1}, \dots, a_m; y).
\end{aligned} \tag{21}$$

The other combinations follow similarly

$$\begin{aligned}
\text{PI}\left(\vec{p}, i, (\vec{a}; y)\right) &= +\text{PI}\left(\vec{p}, 0, 0\right) G(a_1, \dots, a_{i-1}, 0, a_{i+1}, \dots, a_m; y) \\
&- \text{PI}\left(\vec{p}, a_{i-1}, i-1, (a_{i+1}, \dots, a_m; y)\right) \\
&+ \text{PI}\left(\vec{p}, a_{i-1}, 0, 0\right) G(a_1, \dots, a_{i-1}, a_{i+1}, \dots, a_m; y) \\
&+ \text{PI}\left(\vec{p}, a_{i+1}, i, (a_1, \dots, a_{i-1}, a_{i+2}, \dots, a_m; y)\right) \\
&- \text{PI}\left(\vec{p}, a_{i+1}, 1, 0\right) G(a_1, \dots, a_{i-1}, a_{i+1}, \dots, a_m; y).
\end{aligned} \tag{22}$$

As we recursively apply the algorithm, we increase the number of pending integrals

in front but decrease the depth of the G -functions by one unit in every recursion step. We do this until

- (a) the only GPLs remaining under pending integrals are of depth one, i.e. $G_m(s_r, y)$,
- (b) s_r is the argument, i.e. $G(\dots; s_r)$, or
- (c) there are no GPLs under pending integrals.

We now discuss all these cases in turn:

- (a) For GPLs of depth one, i.e. $G_m(s_{r\pm}; y)$, we will be working with explicit logarithms. Hence, we need to indicate the infinitesimal imaginary part. We have to distinguish two cases: $m = 1$ and $m > 1$. For $m = 1$ we have

$$G_1(s_{r\pm}; y) = G_1(y_{2\mp}; s_r) - G(0; s_r) + \log(-y). \quad (23)$$

Note that we will most likely have pending integrals in front, thus each term gives again a simpler pending integral

$$\text{PI}\left(\vec{p} = (y'_{\pm}, \vec{b}), 1, (y)\right) = G(\vec{b}, y_{\mp}; y') - G(\vec{b}, 0; y') + \log(-y_{\mp})G(\vec{b}, y') \quad (24)$$

The first and second terms have been reduced to case (b) and the third term to case (c).

For $m > 1$, we note

$$G_m(s_{r\pm}; y) = -\zeta(m) + \int_0^y \frac{dt}{t} G_{m-1}(t_{\pm}; y) - \int_0^{s_r} \frac{dt}{t} G_{m-1}(t_{\pm}; y). \quad (25)$$

The second and third terms are now longer pending integrals, albeit with reduced weight

$$\begin{aligned} \text{PI}\left(\vec{p}, m, (0_{m-1}, y)\right) &= -\zeta(m)\text{PI}\left(\vec{p}, 0, ()\right) \\ &\quad + \text{PI}\left((y, 0), m-1, (0_{m-2}; y)\right)\text{PI}\left(\vec{p}, 0, ()\right) \\ &\quad - \text{PI}\left(\vec{p}, 0, m-1, (0_{m-2}; y)\right). \end{aligned} \quad (26)$$

- (b) In this case we end up simply with one large GPL

$$\int_0^{y'} \frac{ds_1}{s_1 - b_1} \dots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} G(\vec{a}; s_r) = G((\vec{b}, \vec{a}); y'). \quad (27)$$

In terms of pending integrals this is written as

$$\text{PI}\left(\vec{p} = (y', \vec{b}), m+1, \vec{g}\right) = G(\vec{b}, \vec{g}; y'). \quad (28)$$

(c) If there is no GPL under the pending integral, the integral evaluates to a GPL

$$\int_0^y \frac{ds_1}{s_1 - b_1} \dots \int_0^{s_{r-1}} \frac{ds_r}{s_r - b_r} = G(b_1, \dots, b_r; y'). \quad (29)$$

In each case we end up with GPLs that are simpler in the sense that s_r has been eliminated. These might still be non-convergent due to other (non-zero) z_i elements being smaller in absolute value than y . But applying the removal of s_r recursively we can eliminate all z_i for which $|z_i| < |y|$. Therefore in the end we always obtain convergent GPLs.

4.4 Increase rate of convergence

Even though we have now only convergent GPLs, that does not imply that the convergence is fast enough for numerical applications. From now on we will only consider $y = 1$, as we can normalise any convergent GPL using (10). Convergence of such a GPL is slow if some z_i is close to the unit circle, i.e.

$$1 \leq |z_i| \leq \lambda < 2, \quad (30)$$

where λ is a parameter to be chosen.

Only for such z_i we apply the following strategy: to increase the rate of convergence we can use the fact that GPLs satisfy the Hölder convolution equation [13]

$$G(z_1, \dots, z_k; 1) = \sum_{j=0}^k (-1)^j G\left(1 - z_j, \dots, 1 - z_1; 1 - \frac{1}{p}\right) G\left(z_{j+1}, \dots, z_k; \frac{1}{p}\right), \quad (31)$$

where p is an arbitrary non-zero complex number. Separating the first and last term of this sum we obtain for $p = 2$ and again normalising the GPLs on the right-hand side

$$G(z_1, \dots, z_k; 1) = G(2z_1, \dots, 2z_k; 1) + (-1)^k G(2(1 - z_k), \dots, 2(1 - z_1); 1) \quad (32)$$

$$+ \sum_{j=1}^{k-1} (-1)^j G\left(2(1 - z_j), \dots, 2(1 - z_1); 1\right) G\left(2z_{j+1}, \dots, 2z_k; 1\right). \quad (33)$$

The first term has now better convergence as all parameters are twice as big. The GPL appearing in the sum all have reduced weight and are therefore not relevant for the present discussion.

The second term may or may not be convergent. If not, we repeat the algorithm outlined in Section 4.2, including if necessary, Hölder convolution. At this stage it is not obvious why this recipe does indeed lead to a final answer and not to an infinite recursion. This can be shown by noting that the algorithm does only replace parameters with zero or permutes them; it does not introduce new non-trivial parameters. By carefully

considering all possible behaviours under transformation $z \mapsto 2(1 - z)$, [7] proved that this method indeed works.

The choice of λ is a trade-off between accuracy and speed. A typical choice would be $\lambda = 1.1$ which is the default in `handyG`. λ can be changed using the `hCircle` option in `set_options`.

4.5 An example reduction

To illustrate the various aspects discussed so far, we include here an example of how the algorithm works in practice. For this purpose we reduce $G(1, 0, 3; 2)$ according to this algorithm until we end up with logarithms, polylogarithms and convergent MPLs. In our notation of a non-convergent GPL we have

$$G(\underbrace{1}_{s_r}, \underbrace{0}_{a_2}, \underbrace{3}_{a_3}; \underbrace{2}_y) = G(0, 0, 3; 2) + \int_0^1 ds_1 \frac{\partial}{\partial s_1} G(s_1, 0, 3; 2). \quad (34)$$

The first term corresponds to $G_3(3; 2)$ and therefore it is a convergent trilogarithm. The second term has s_r appearing at the first place. Using (18) we obtain for the second term

$$\begin{aligned} \int_0^1 ds_1 \frac{\partial}{\partial s_1} G(s_1, 0, 3; 2) &= \int_0^1 \frac{ds_1}{s_1 - 2} G(0, 3; 2) + \int_0^1 \frac{ds_1}{s_1 - 0} G(s_1, 3; 2) \\ &\quad - \int_0^1 \frac{ds_1}{s_1 - 0} G(0, 3; 2). \end{aligned} \quad (35)$$

The first and last terms are both conventional functions. Hence, we only need to worry about the second term which involves a pending integral. In order to evaluate it, we apply again (18) to the GPL under the pending integral to find

$$\begin{aligned} G(s_1, 3; 2) &= G(0, 3; 2) + \int_0^{s_1} \frac{ds_2}{s_2 - 2} G(3; 2) + \int_0^{s_1} \frac{ds_2}{s_2 - 3} G(s_2; 2) \\ &\quad - \int_0^{s_1} \frac{ds_2}{s_2 - 3} G(3; 2). \end{aligned} \quad (36)$$

Substituting this back into (35) gives

$$\begin{aligned} \int_0^1 \frac{ds_1}{s_1 - 0} G(s_1, 3; 2) &= \int_0^1 \frac{ds_1}{s_1} G(0, 3; 2) + \int_0^1 \frac{ds_1}{s_1} \int_0^{s_1} \frac{ds_2}{s_2 - 2} G(3; 2) \\ &\quad + \int_0^1 \frac{ds_1}{s_1} \int_0^{s_1} \frac{ds_2}{s_2 - 3} G(s_2; 2) - \int_0^1 \frac{ds_1}{s_1} \int_0^{s_1} \frac{ds_2}{s_2 - 3} G(3; 2). \end{aligned} \quad (37)$$

Here only the third term is interesting, as the others are (poly)logarithms. The third term is a pending integral over a GPL of depth one. Thus,

$$\begin{aligned} & \int_0^1 \frac{ds_1}{s_1} \int_0^{s_1} \frac{ds_2}{s_2-3} G(s_2; 2) \\ &= \int_0^1 \frac{ds_1}{s_1} \int_0^{s_1} \frac{ds_2}{s_2-3} \left(G(2; s_2) - G(0; s_2) + \log(-2) \right) \end{aligned} \quad (38)$$

The first two terms have s_r as the argument and hence they are GPLs. The last term is independent of s_r , making the integration trivial. Unfortunately, the second term $G(0, 3, 0; 1)$ has a trailing zero. To remove it, we shuffle $G(0, 3; 1)$ with $G(0; 1)$ to find

$$G(0, 3; 1)G(0; 1) = \sum_{\vec{c}=(0,3)\sqcup(0)} G(\vec{c}; 1) = G(0, 3, 0; 1) + 2 \times G(0, 0, 3; 1), \quad (39)$$

which we solve for $G(0, 3, 0; 1)$.

Gathering all terms we obtain with $G(0; 1) = \log 1 = 0$

$$\begin{aligned} G(1, 0, 3; 2) &= \underbrace{G(0, 0, 3; 2)}_{-\text{Li}_3(2/3)} + \underbrace{G(2; 1)}_{\log(1/2)} \underbrace{G(0, 3; 2)}_{-\text{Li}_2(2/3)} - \cancel{G(0; 1)G(0, 3; 2)} \\ &+ \cancel{G(0; 1)G(0, 3; 2)} + \underbrace{G(0, 2; 1)}_{-\text{Li}_2(1/3)} \underbrace{G(3; 2)}_{\log(1/3)} - \underbrace{G(0, 3; 1)}_{-\text{Li}_2(2/3)} \underbrace{G(3; 2)}_{\log(1/3)} \\ &+ \underbrace{G(0, 3, 2; 1)}_{\text{Li}_{2,1}(1/3, 3/2)} + \underbrace{G(0, 3; 1)}_{-\text{Li}_2(1/3)} \log(-2) - \cancel{G(0; 1)G(0, 3; 1)} \\ &+ 2 \underbrace{G(0, 0, 3; 1)}_{-\text{Li}_3(1/3)} = -0.81809 - 1.15049i. \end{aligned} \quad (40)$$

5 Validation and performance

We have validated handyG for some practical examples of GPLs, namely

0. the GPLs entering the heavy-to-light form factor with full mass dependence after simplification [14] (540 GPLs up to weight four),
1. all GPLs appearing in the master integrals computed [15] for the heavy-to-light form factor (1399 functions up to weight four, including the 540 above),
2. the planar integrals for muon-electron scattering in the unphysical region $s < 0$ and $t < 0$ with vanishing electron mass [16] (198 functions up to weight four), and
3. the non-planar integrals for the same process [17] (1732 GPLs up to weight four).

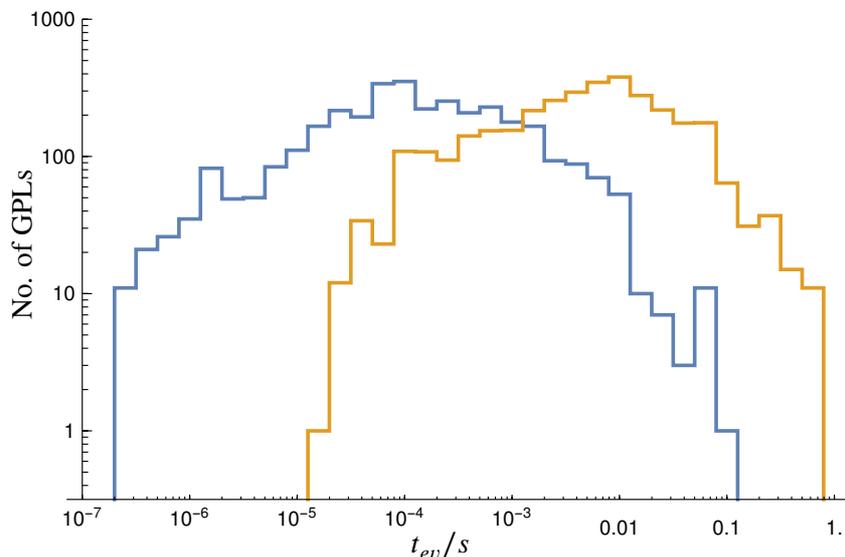


Figure 5: Histogram of average evaluation time of the GPLs needed in [15–17] using handyG (blue) and GiNaC (yellow)

In all four test cases we find complete agreement with GiNaC⁴.

Of course the speed of any numerical routine strongly depends on the complexity of the requested function. Hence, comparing total runtime, while important, does not provide many insights. Instead, one should study how handyG and GiNaC perform for different GPLs. This is done in Figure 5, where we have calculated a total of 3329 GPLs, using both GiNaC and handyG and histogrammed the average evaluation time of five successive calls. On average our code is approximately twenty times faster (1100 GPL/s v. 60 GPL/s). However, one should keep in mind that the GiNaC implementation was never intended to be directly used in a Monte Carlo [18]. Instead, GiNaC would generate C code that evaluates expressions using double precision. Of course this is only possible for elementary functions that are implemented in C and not for, say, GPLs. handyG fills this gap by providing a low-level implementation of GPLs suitable for Monte Carlo applications.

Additionally, we studied in Figure 6 how the different sets of GPLs in the list above compare. For the muon-electron scattering case, it is perhaps unsurprising that the planar integrals give rise to easier GPLs than the non-planar integrals.

As a last example we considered GPLs of higher weight. While there is in principle no limitation for the number of parameters that can be evaluated with the implemented algorithm, in practice the evaluation can become very slow for weights above $m > 7$,

⁴In some rare cases, depending on the GiNaC installation make check may still fail.

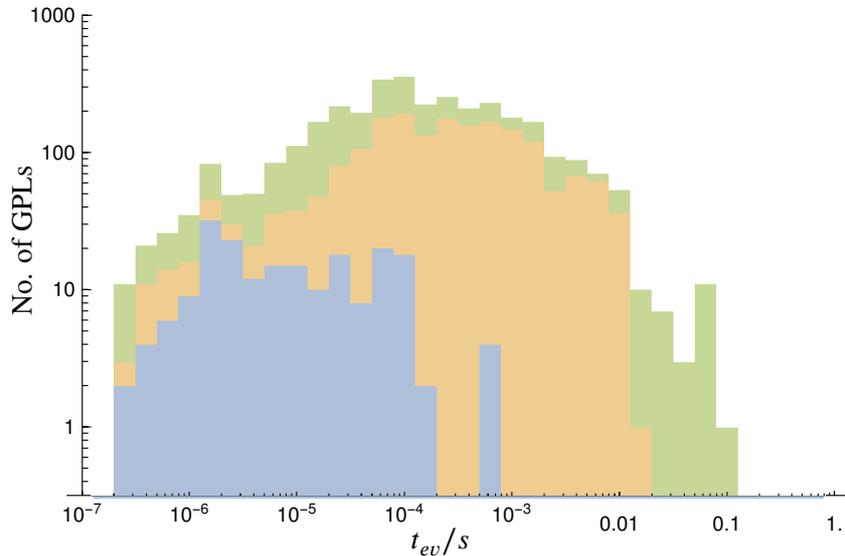


Figure 6: Histogram of average evaluation time of the GPLs using handyG broken down by their source: planar $\mu-e$ scattering (2, blue), non-planar $\mu-e$ scattering (3, yellow) and the heavy-to-light form factor (1, green)

depending on the complexity of the parameters. We have created some more or less realistic examples for high-weight GPLs by shuffling parameters of the GPLs appearing in the zeroth set tested above, i.e. the GPLs entering the heavy-to-light form factor [14]. The average evaluation times are plotted in Figure 7 as a function of m .

All of these tests were performed on a computer with Intel i5 Kaby Lake R 1.7GHz processor.

6 Conclusion

We have presented handyG, a numerical routine for the fast evaluation of GPLs. Compared to the current state-of-the-art, handyG does not require a framework for symbolic manipulation and is therefore much faster. GPLs of weight ≤ 5 can now be evaluated fast enough to allow numerical integration in a Monte Carlo framework.

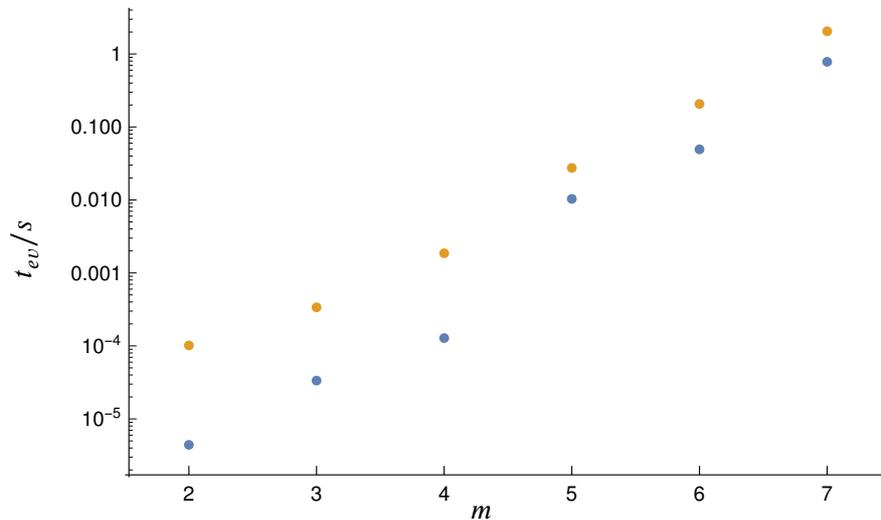


Figure 7: Average evaluation time of GPLs as a function of the weight m using handyG (blue) and GiNaC (yellow). Even though handyG remains faster, the lead decreases with increasing weight.

Acknowledgement

We would like to thank Emanuele Bagnaschi, Pulak Banerjee, Tim Engel, Lukas Fritz, Thomas Gehrmann and William J. Torres Bobadilla for comments on the usability of the code as well as the manuscript.

YU acknowledges support by the Swiss National Science Foundation (SNF) under contract 200021_178967.

References

- [1] E. Remiddi and J. A. M. Vermaseren, *Harmonic polylogarithms*, *Int. J. Mod. Phys. A* **15** (2000) 725 [[hep-ph/9905237](#)].
- [2] A. B. Goncharov, *Multiple polylogarithms, cyclotomy and modular complexes*, *Math. Res. Lett.* **5** (1998) 497 [[1105.2076](#)].
- [3] S. Buehler and C. Duhr, *CHAPLIN - Complex Harmonic Polylogarithms in Fortran*, *Comput. Phys. Commun.* **185** (2014) 2703 [[1106.5739](#)].
- [4] T. Gehrmann and E. Remiddi, *Numerical evaluation of harmonic polylogarithms*, *Comput. Phys. Commun.* **141** (2001) 296 [[hep-ph/0107173](#)].

- [5] T. Huber and D. Maitre, *HypExp: A Mathematica package for expanding hypergeometric functions around integer-valued parameters*, *Comput. Phys. Commun.* **175** (2006) 122 [[hep-ph/0507094](#)].
- [6] D. Maitre, *HPL, a mathematica implementation of the harmonic polylogarithms*, *Comput. Phys. Commun.* **174** (2006) 222 [[hep-ph/0507152](#)].
- [7] J. Vollinga and S. Weinzierl, *Numerical evaluation of multiple polylogarithms*, *Comput. Phys. Commun.* **167** (2005) 177 [[hep-ph/0410259](#)].
- [8] H. Frellesvig, D. Tommasini and C. Wever, *On the reduction of generalized polylogarithms to Li_n and $Li_{2,2}$ and on the evaluation thereof*, *JHEP* **03** (2016) 189 [[1601.02649](#)].
- [9] H. Frellesvig, *Generalized Polylogarithms in Maple*, [1806.02883](#).
- [10] C. Duhr, *Mathematical aspects of scattering amplitudes*, in *Proceedings, Theoretical Advanced Study Institute in Elementary Particle Physics: Journeys Through the Precision Frontier: Amplitudes for Colliders (TASI 2014): Boulder, Colorado, June 2-27, 2014*, pp. 419–476, 2015, [1411.7538](#), [DOI](#).
- [11] C. Duhr and F. Dulat, *PolyLogTools - Polylogs for the masses*, [1904.07279](#).
- [12] T. Hahn, *The High-Energy Physicist's Guide to MathLink*, *Comput. Phys. Commun.* **183** (2012) 460 [[1107.4379](#)].
- [13] J. M. Borwein, D. M. Bradley, D. J. Broadhurst and P. Lisonek, *Special values of multiple polylogarithms*, *Trans. Am. Math. Soc.* **353** (2001) 907 [[math/9910045](#)].
- [14] T. Engel, C. Gnendiger, A. Signer and Y. Ulrich, *Small-mass effects in heavy-to-light form factors*, *JHEP* **02** (2018) 118 [[1811.06461](#)].
- [15] L.-B. Chen, *Two-Loop master integrals for heavy-to-light form factors of two different massive fermions*, *JHEP* **02** (2018) 066 [[1801.01033](#)].
- [16] P. Mastrolia, M. Passera, A. Primo and U. Schubert, *Master integrals for the NNLO virtual corrections to μe scattering in QED: the planar graphs*, *JHEP* **11** (2017) 198 [[1709.07435](#)].
- [17] S. Di Vita, S. Laporta, P. Mastrolia, A. Primo and U. Schubert, *Master integrals for the NNLO virtual corrections to μe scattering in QED: the non-planar graphs*, *JHEP* **09** (2018) 016 [[1806.08241](#)].
- [18] C. Bauer, C. Dams, A. Frink, V. Kisil, R. Kreckel, V. Magerya, A. Sheplyakov, M. Vala and J. Vollinga, *GiNaC, an open framework for symbolic computation within the C++ programming language*, June, 2019, <https://ginac.de/tutorial/>.