# pySecDec: a toolbox for the numerical evaluation of multi-scale integrals 

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#### Abstract

We present pySecDec, a new version of the program SECDEC, which performs the factorisation of dimensionally regulated poles in parametric integrals, and the subsequent numerical evaluation of the finite coefficients. The algebraic part of the program is now written in the form of python modules, which allow a very flexible usage. The optimization of the C++ code, generated using FORM, is improved, leading to a faster numerical convergence. The new version also creates a library of the integrand functions, such that it can be linked to user-specific codes for the evaluation of matrix elements in a way similar to analytic integral libraries.


Key words: Perturbation theory, Feynman diagrams, multi-loop, numerical integration

## PROGRAM SUMMARY

Manuscript Title: pySecDec: a toolbox for the numerical evaluation of multi-scale integrals
Authors: S. Borowka, G. Heinrich, S. Jahn, S. P. Jones, M. Kerner, J. Schlenk,T .Zirke
Program Title: pySecDec
Journal Reference:
Catalogue identifier:
Licensing provisions: GNU Public License v3
Programming language: python, FORM, C++
Computer: from a single PC/Laptop to a cluster, depending on the problem
Operating system: Unix, Linux
RAM: depending on the complexity of the problem
Keywords: Perturbation theory, Feynman diagrams, multi-loop, numerical integration
Classification: 4.4 Feynman diagrams, 5 Computer Algebra, 11.1 General, High Energy Physics and Computing.
External routines/libraries: catch [1], gsl [2], numpy [3], sympy [4], Nauty [5], Cuba [6], FORM [7], Normaliz [8]. The program can also be used in a mode which does not require Normaliz.
Journal reference of previous version: Comput. Phys. Commun. 196 (2015) 470-491. Nature of the problem:
Extraction of ultraviolet and infrared singularities from parametric integrals appearing in higher order perturbative calculations in quantum field theory. Numerical integration in the presence of integrable singularities (e.g. kinematic thresholds).

## Solution method:

Algebraic extraction of singularities within dimensional regularization using iterated sector decomposition. This leads to a Laurent series in the dimensional regularization parameter $\epsilon$ (and optionally other regulators), where the coefficients are finite integrals over the unit-hypercube. Those integrals are evaluated numerically by Monte Carlo integration. The integrable singularities are handled by choosing a suitable integration contour in the complex plane, in an automated way. The parameter integrals forming the coefficients of the Laurent series in the regulator(s) are provided in the form of libraries which can be linked to the calculation of (multi-) loop amplitudes.
Restrictions: Depending on the complexity of the problem, limited by memory and CPU time.
Running time: Between a few seconds and several days, depending on the complexity of the problem.
References:
[1] https://github.com/philsquared/Catch/.
[2] http://www.gnu.org/software/gsl/.
[3] http://www.numpy.org/.
[4] http://www.sympy.org/.
[5] http://pallini.di.uniroma1.it/.
[6] T. Hahn, "CUBA: A Library for multidimensional numerical integration," Comput. Phys. Commun. 168 (2005) 78 [hep-ph/0404043], http://www.feynarts.de/cuba/.
[7] J. Kuipers, T. Ueda and J. A. M. Vermaseren, "Code Optimization in FORM," Comput. Phys. Commun. 189 (2015) 1 [arXiv:1310.7007], http://www.nikhef.nl/ form/.
[8] W. Bruns, B. Ichim, B. and T. Römer, C. Söger, "Normaliz. Algorithms for rational cones and affine monoids." http://www.math.uos.de/normaliz/.

## 1 Introduction

The current experiments at the Large Hadron Collider as well as future collider experiments will explore TeV energy scales, posing new challenges for both the experiments and the theoretical predictions. Radiative corrections play an important role in this situation, making it necessary to develop calculational methods and tools which can facilitate the task of calculating higher orders in perturbation theory; both virtual (loop) corrections and real corrections, the latter of which involve extra radiation leading to infrared singularities when unresolved.

The analytic calculation of loop integrals beyond one loop has seen an enormous progress in the last few years, to a large extent due to new insights [1] into the method of differential equations [2,3]. However, as the number of mass scales increases, the analytic evaluation of two-loop integrals and beyond becomes a very challenging and tedious task. At high energies, however, where massive loops are more likely to be resolved, and where electro-weak corrections become important, multi-scale problems are ubiquitous.

In such cases, numerical approaches may be the method of choice. A method which is particularly useful in the presence of dimensionally regulated singularities is sector decomposition [4-7], as it provides an algorithm to factorise such singularities in an automated way. The coefficients of the resulting Laurent series in the regularization parameter are in general complicated, but can be integrated numerically. This has been implemented in the program SECDEc [8-10], where from version 2.0 [9] the restriction to Euclidean kinematics was lifted by combining sector decomposition with a method to deform the multi-dimensional integration contour into the complex plane [11,12. Other implementations of the sector decomposition algorithm can be found in Refs. 13 20.

In this paper, we present a completely new version of the SECDEC program, called pySECDEc. The algebraic part is now coded in python and FORM 21, 22 rather than Mathematica. As a consequence, the new program is entirely based on open source software and allows maximal flexibility due to its modular structure. The python code writes FORM files to produce optimized $C++$
functions which can be numerically integrated with Cuba 23,24 . The $C++$ functions are by default combined into a library and thus can be linked to the calculation of, for example, a full amplitude. Therefore pySECDEC can be used in a similar manner as analytic one-loop integral libraries. This opens up new possibilities for the calculation of multi-loop amplitudes where analytic results for most of the master integrals are not known.

The outline of the paper is as follows. In Section 2 we describe the structure of the program and its new features. In Section 3 we explain the installation and usage of the program. Section 4 describes a number of examples, before we conclude in Section 5. An appendix contains an overview of possible parameter settings, where their default values are also listed.

## 2 Description of pySecDec



Fig. 1. Flowchart showing the main building blocks of pySecDec. Steps 1-6 are done in python. FORM is used in step 7 to produce optimized $C++$ code.

The program consists of two main parts, an algebraic part, based on python and FORM [21,22], and a numerical part, based on $C++$ code. A flowchart is shown in Fig. 1. The isolation of endpoint singularities and the subsequent numerical integration can act on general polynomial functions, as indicated in the box (1b). Loop integrals (after Feynman parametrisation) can be considered as special cases of these more general polynomial integrands. In the python code, this is reflected by the following structure: The python function make_package accepts a list of polynomials raised to their individual powers as input - corresponding to the box (1b). In contrast, loop_package takes a loop integral (e.g. from its graph or propagator representation), which corresponds
to to box (1a). After Feynman parametrizing the loop integral, loop_package calls make_package for further processing. The steps (1) to (6) are performed in python and FORM, where FORM, after step (6), produces optimized $C++$ code. The compiled integrand functions are by default combined into a library. For the numerical integration, we provide a simple interface to integrators from the Cuba [23] library. The user also has direct access to the integrand functions for example to pass them to an external integrator.

The pySECDEC distribution comes with a very detailed documentation both in html and in pdf format. The manual is also available in both formats on the webpage http://secdec.hepforge.org.

### 2.1 Algebraic part

The algebraic part consists of several modules that provide functions and classes for the purpose of the generation of the integrand, performing the sector decomposition, contour deformation, subtraction and expansion in the regularization parameter(s). The algebra modules contained in pySECDEC use both sympy and numpy, but also contain the implementation of a computer algebra system tailored to the sector decomposition purposes, in order to be competitive in speed with the previous implementation in Mathematica. For example, since sector decomposition is an algorithm that acts on polynomials, a key class contained in pySecDec.algebra is the class Polynomial.

Acting on general polynomials, pySECDEC is not limited to loop integrals. It can take as an integrand any product of polynomials, raised to some power, provided that the endpoint singularities are regulated by regularisation parameters, and that integrable singularities away from the integration endpoints can be dealt with by a deformation of the integration path into the complex plane. We should point out that pySECDEC can perform the subtraction and expansion in several regulators, see the description of example 4.8.

For loop integrals, the program contains the module pySecDec.loop_integral. There are two ways to define a loop integral in pySECDEC: (a) from the list of propagators, and (b) from the adjacency list defining the graph, which is roughly the list of labels of vertices connected by propagators. Examples for both alternatives to define loop integrals are given in Sections 3.2 and 4 .

The availability of python functions which can be called individually by the user allows for a very flexible usage of pySecDec. The html documentation describes all the available modules and functions in detail, and also contains a "quick search" option.

### 2.1.1 Sector decomposition strategies

When using loop_package, which facilitates the definition and calculation of Feynman integrals, one can choose between the following sector decomposition strategies:

- iterative: Default iterative method [6,7].
- geometric: Algorithm based on algebraic geometry (G2 in SECDEC 3). Details can be found in Refs. [10, 25, 26].
- geometric_ku: Original algorithm based on algebraic geometry introduced by Kaneko and Ueda (G1 in SecDec 3) [16, 27].

The recommended sector decomposition algorithm based on algebraic geometry is geometric, since it improves on the original geometric algorithm. For general parametric integrals there are additionally the following options which can be set in make_package:

- iterative_no_primary: Iterative method without primary sector decomposition.
- geometric_no_primary: Geometric decomposition according to Kaneko and Ueda without primary sector decomposition.


### 2.2 Producing $C++$ code and numerical results

The module pySecDec.code_writer is the main module to create a $C++$ library. It contains the function pySecDec.code_writer.make_package which can decompose, subtract and expand any polynomial expression and return the produced set of finite functions as a $C++$ package, where FORM has been employed to write out optimised expressions. Simple examples of how to use make_package are described in Sections 4.7 and 4.8 .

A more advanced example is given in Section 4.9, which shows how the user can define any number of additional finite functions. These functions need not be polynomial. Furthermore, the user is free to define arbitrary $C++$ code (for example, a jet clustering routine) to be called by the integrand during the numerical integration. Templates for such user-defined functions will be created automatically if the field functions, where the names of such functions are given, is non-empty in make_package.

If a loop integral should be calculated, the function loop_package can be used, which contains methods specific to loop integrals, for example the construction of the Symanzik polynomials $\mathcal{F}$ and $\mathcal{U}$ from the list of propagators or from the adjacency list of a graph. Examples how to use the loop package are given in Sections 4.1 to 4.5 .

Both make_package and loop_package will create a directory (with the name given by the user in the field name) which contains the main $C++$ integration files and a Makefile to generate the $C++$ source code and the libraries (static and dynamic) containing the integrand functions.

The library can be linked against a user-specific code, or it can be called via a python interface, as described in Section 4.1.

### 2.3 New features

In addition to the complete re-structuring, which opens up new possibilities of usage, there are various new features compared to SECDEC 3:

- The functions can have any number of different regulators, not only the dimensional regulator $\epsilon$.
- The treatment of numerators is much more flexible. Numerators can be defined in terms of contracted Lorentz vectors or inverse propagators or a combination of both.
- The distinction between "general functions" and "loop integrands" is removed in the sense that all features are available for both general polynomial functions and loop integrals (except those which only make sense in the loop context).
- The inclusion of additional "user-defined" functions which do not enter the decomposition has been facilitated and extended.
- The treatment of poles which are higher than logarithmic has been improved.
- A procedure has been implemented to detect and remap singularities at $x_{i}=1$ which cannot be cured by contour deformation.
- A symmetry finder 28 has been added which can detect isomorphisms between sectors.
- Diagrams can be drawn (optionally, based on neato [29]; the program will however run normally if neato is not installed).
- The evaluation of multiple integrals or even amplitudes is now possible, using the generated $C++$ library, as shown in Example 4.10.


## 3 Installation and usage

Here we describe briefly the installation and usage of the program. For more details we refer to the manual and to the examples.

### 3.1 Installation

The program can be downloaded from http://secdec.hepforge.org.

It relies on python and runs with versions 2.7 and 3 . Further the packages numpy (http://www.numpy.org) and sympy (http://www. sympy.org) are required. The former is a package for scientific computing with python, the latter is a python library for symbolic mathematics.

To install pySECDEC, perform the following steps

```
tar -xf pySecDec-<version>.tar.gz
cd pySecDec-<version>
make
<copy the highlighted output lines into your .bashrc>
```

The make command will automatically build further dependencies in addition to pySecDec itself. These are the Cuba library [23, 24] needed for multidimensional numerical integration, FORM 21,22$]$ for the algebraic manipulation of expressions and to produce optimized $C++$ code, and Nauty 28] to find sector symmetries, thereby reducing the total number of sectors to be integrated. The lines to be copied into the .bashrc define environment variables which make sure that pySECDEC is found by python and finds its aforementioned dependencies.

With our effort of shipping external dependencies with our program, we want to make sure the installation is as easy as possible for the user. The pySecDec user is strongly encouraged to cite the additional dependencies when using the program.

### 3.1.1 Geometric sector decomposition strategies

The program Normaliz [30, 31] is needed for the geometric decomposition strategies geometric and geometric_ku. In pySECDEC version 1.0, the versions 3.0.0, 3.1.0 and 3.1.1 of Normaliz are known to work. Precompiled executables for different systems can be downloaded from
https://www.normaliz.uni-osnabrueck.de. We recommend to export its path to the environment of the terminal such that the normaliz executable is always found. Alternatively, the path can be passed directly to the functions that call it, see the manual for more information. The strategy iterative can be used without having Normaliz installed.

### 3.2 Usage

Due to its highly modular structure, modules of the program pySECDEC can be combined in such a way that they are completely tailored to the user's needs. The individual building blocks are described in detail in the manual. The documentation is shipped with the tarball in pdf (doc/pySecDec.pdf) and html (doc/html/index.html) format.

We provide python scripts for the two main application directions of the program. One is to use pySECDEC in a "standalone" mode to obtain numerical results for individual integrals. This corresponds to a large extent to the way previous SEcDec versions were used. The other allows the generation of a library which can be linked to the calculation of amplitudes or other expressions, to evaluate the integrals contained in these expressions. The different use cases are explained in detailed examples in Section 4.

To get started, we recommend to read the section "getting started" in the online documentation. The basic steps can be summarized as follows:
(1) Write or edit a python script to define the integral, the replacement rules for the kinematic invariants, the requested order in the regulator and some other options (see e.g. the one-loop box example box1L/generate_box1L.py).
(2) Run the script using python. This will generate a subdirectory according to the name specified in the script.
(3) Type make -C <name>, where <name> is your chosen name. This will create the $C++$ libraries.
(4) Write or edit a python script to perform the numerical integration using the python interface (see e.g. box1L/integrate_box1L.py).

Further usage options such as looping over multiple kinematic points are described in the documentation as well as in section 4.1.

The algebra package can be used for symbolic manipulations on integrals. This can be of particular interest when dealing with non-standard loop integrals, or if the user would like to interfere at intermediate stages of the algebraic part.

For example, the Symanzik polynomials $\mathcal{F}$ and $\mathcal{U}$ resulting from the list of propagators can be accessed as follows (example one-loop bubble):

```
>>> from pySecDec.loop_integral import *
>>> propagators = ['k**2', '(k - p)**2']
>>> loop_momenta = ['k']
>>> li = LoopIntegralFromPropagators(propagators,loop_momenta)
```

Then the functions $\mathcal{U}$ and $\mathcal{F}$ including their powers can be called as:

```
>>> li.exponentiated_U
( + x0 + x1)**(2*eps - 2)
>>> li.exponentiated_F
( + (-p**2)*x0*x1)**(-eps)
```

Numerators can be included in a much more flexible way than in SEcDEc 3, see the example in Section 4.3 and the manual.

An example where $\mathcal{F}$ and $\mathcal{U}$ are calculated from the adjacency list defining a graph looks as follows (for a one-loop triangle with two massive propagators):

```
>>> from pySecDec.loop_integral import *
>>> internal_lines = [['0', [1,2]], ['m', [2,3]], ['m', [3,1]]]
>>> external_lines = [['p1',1],['p2',2],['-p12',3]]
>>> li = LoopIntegralFromGraph(internal_lines, external_lines)
```

Finally, we should point out that the conventions for additional prefactors defined by the user have been changed between SecDec 3 and pySecDec. The prefactor will now be multiplied automatically to the result. For example, if the user defines additional prefactor $=\Gamma(3-2 \epsilon)$, this prefactor will be expanded in $\epsilon$ and included in the numerical result returned by pySECDEC.

## 4 Examples

All the examples listed below can be found in subdirectories of the examples folder.

### 4.1 One-loop box

This example is located in the folder box1L. It calculates a 1-loop box integral with one off-shell leg $\left(p_{1}^{2} \neq 0\right)$ and one massive propagator connecting the external legs $p_{1}$ and $p_{2}$.

The user has basically two possibilities to perform the numerical integrations: (a) using the python interface to call the library or
(b) using the $C++$ interface by inserting the numerical values for the kinematic point into integrate_box1L.cpp.

The commands to run this example in case (a) above are
python generate_box1L.py

```
make -C box1L
python integrate_box1L.py
```

In case (b) above the commands are
python generate_box1L.py
<edit kinematic point in box1L/integrate_box1L.cpp>
make -C box1L integrate_box1L
./box1L/integrate_box1L
The make command can optionally be passed the jobs $(-j)$ command to run multiple FORM jobs and then multiple compilation jobs in parallel, for example make -j 8 -C box1L would run 8 jobs in parallel where possible.

Other simple examples can be run in their corresponding folders by replacing the name box1L in the above commands with the name of the example.

In more detail, running the python script generate_box1L.py will create a folder called box1L (the "name" specified in generate_box1L.py) which will contain the following files and subdirectories:

| box1L.hpp | integrate_box1L.cpp | Makefile | pylink/ |
| :--- | :--- | :--- | :--- |
| box1L.pdf | src/ codegen/ | Makefile.conf | README |

Inside the generated box1L folder typing 'make' will create the source files for the integrand and the libraries 'libbox1L.a' and 'box1L_pylink.so', which can be linked to an external program calling these integrals.

Note that pySECDEC automatically creates a pdf file with the diagram picture if LoopIntegralFromGraph is used as input format.

In case (a) the python file integrate_box1L.py is used to perform the numerical integration, the user may edit the kinematic point and integration parameter settings directly at python level.

In case (b), the user has to insert the values for the kinematic point in
box1L/integrate_box1L.cpp at the line
const std::vector[box1L::real_t](box1L::real_t) real_parameters = \{\};
which can be found at the beginning of int main(). Complex parameters should be given as a list of the real and imaginary part. For box1L, the complex numbers $1+2 i$ and $2+1 i$ are written as
const std::vector[box1L::complex_t](box1L::complex_t) complex_parameters=\{ \{1.0,2.0\}, $\{2.0,1.0\}\} ;$
If no complex parameters are present, the list complex_parameters should be left empty. The command 'make -C box1L box1L/integrate_box1L' pro-
duces the executable integrate_box1L which can be run to perform the numerical integration using the $C++$ interface.

## Loop over multiple kinematic points

The file integrate_box1L_multiple_points.py shows how to integrate a number of kinematic points sequentially. The points are defined in the file kinematics.input. They are read in by the python script (line by line).
The first entry of each line in the kinematics data file kinematics.input should be a string, the "name" of the kinematic point, which can serve to label the results for each point. The results are written to the file results_box1L.txt.

### 4.2 Two-loop three-point function with massive propagators

The example triangle2L calculates the two-loop diagram shown in Fig. 2 , The steps to perform to run this example (using the python interface) are analogous to the ones given in the previous section:
python generate_triangle2L.py \&\& make -C triangle2L \&\&
python integrate_triangle2L.py
Results for this diagram can be found e.g. in 3235 .


Fig. 2. A two-loop vertex graph containing a massive triangle loop. Solid lines are massive, dashed lines are massless. The vertices are labeled to match the construction of the integrand from the topology.
The result of pySECDEC is shown in Tab. 1. We would like to point out that the default accuracy in this example is set to $10^{-2}$ in order to keep the runtimes low. This does not reflect the accuracy pySEcDEc can actually reach.

A comparison of the timings with SECDEC 3 and Fiesta 4.1 for the evaluation of the finite part can be found in Table 5.

### 4.3 Two-loop four-point function with numerators

The example box2L_numerator shows how numerators can be treated in pySECDEC. It calculates a massless planar on-shell two-loop 7-propagator box in two different ways:

Table 1
Result for the two-loop triangle P126 at $p_{3}^{2}=9$ and $m^{2}=1$ compared to the analytic result of Ref. 33 .

| $\epsilon$ order | pySECDEC result |
| :--- | :--- |
| $\epsilon^{-2}$ | $(-0.0379735-\mathrm{i} 0.0747738) \pm(0.000375449+\mathrm{i} 0.000695892)$ |
| $\epsilon^{-1}$ | $(0.2812615+\mathrm{i} 0.1738216) \pm(0.003117778+\mathrm{i} 0.002358655)$ |
| $\epsilon^{0}$ | $(-1.0393673+\mathrm{i} 0.2414135) \pm(0.011940978+\mathrm{i} 0.004604699)$ |
|  | analytic result |
| $\epsilon^{-2}$ | $-0.038052884394-\mathrm{i} 0.0746553844162$ |
| $\epsilon^{-1}$ | $0.279461083591+\mathrm{i} 0.1746609123993$ |
| $\epsilon^{0}$ | $-1.033851309109+\mathrm{i} 0.2421265865644$ |

(a) with the numerator defined as an inverse propagator (box2L_invprop.py), (b) with the numerator defined in terms of contracted Lorentz vectors (box2L_contracted_tensor.py).

This example is run with the following commands
make (will run both python scripts and compile the libraries)
./integrate_box2L (will calculate the integral in both ways and
print the results as well as the difference between the two results, which should be numerically zero).

The result for $s=-3$ and $t=-2$ is listed in Tab. 2,

The integral is given by

$$
\begin{align*}
& I_{a_{1} \ldots a_{8}}=\int \frac{d^{D} k_{1}}{i \pi^{\frac{D}{2}}} \frac{d^{D} k_{2}}{i \pi^{\frac{D}{2}}} \frac{1}{\left[D_{1}\right]^{a_{1}}\left[D_{2}\right]^{a_{2}}\left[D_{3}\right]^{a_{3}}\left[D_{4}\right]^{a_{4}}\left[D_{5}\right]^{a_{5}}\left[D_{6}\right]^{a_{6}}\left[D_{7}\right]^{a_{7}}\left[D_{8}\right]^{a^{8}}}  \tag{1}\\
& D_{1}=k_{1}^{2}, D_{2}=\left(k_{1}+p_{2}\right)^{2}, D_{3}=\left(k_{1}-p 1\right)^{2}, D_{4}=\left(k_{1}-k_{2}\right)^{2} \\
& D_{5}=\left(k_{2}+p_{2}\right)^{2}, D_{6}=\left(k_{2}-p_{1}\right)^{2}, D_{7}=\left(k_{2}+p_{2}+p_{3}\right)^{2}, D_{8}=\left(k_{1}+p_{3}\right)^{2} .
\end{align*}
$$

In case (a), the integral $I_{1111111-1}$ is specified by powerlist $=[1,1,1,1,1,1,1,-1]$ in box2L_invprop.py.
In case (b), the same integral is specified (in box2L_contracted_tensor.py) by powerlist $=[1,1,1,1,1,1,1,0]$ and numerator $=' \mathrm{k} 1(\mathrm{mu}) * \mathrm{k} 1(\mathrm{mu})+2 * \mathrm{k} 1(\mathrm{mu}) * \mathrm{p} 3(\mathrm{mu})+\mathrm{p} 3(\mathrm{mu}) * \mathrm{p} 3(\mathrm{mu})$ '.

Table 2
Result for the two-loop four-point function with numerators at the kinematic point $s=-3, t=-2$.

| $\epsilon$ order | pySECDEC result |
| :---: | :---: |
| $\epsilon^{-4}$ | $-0.2916 \pm 0.0022$ |
| $\epsilon^{-3}$ | $0.7410 \pm 0.0076$ |
| $\epsilon^{-2}$ | $-0.3056 \pm 0.0095$ |
| $\epsilon^{-1}$ | $-2.2966 \pm 0.0313$ |
| $\epsilon^{0}$ | $1.1460 \pm 0.0504$ |



Fig. 3. Three-loop massless 7-propagator graph.

### 4.4 Three-loop triangle integral

The example triangle3L demonstrates how the symmetry finder can reduce the number of sectors. We consider the seven-propagator 3-loop 3-point integral depicted in Fig. 3, which is the figure that is automatically created by the code. This integral has been calculated to order $\epsilon$ in Ref. [36] and to order $\epsilon^{4}$ in Ref. 37. Here we also calculate it to order $\epsilon^{4}$.

This example is run as usual by the commands
python generate_triangle3L.py \&\& make -C triangle3L \&\& python integrate_triangle3L.py

It shows that the symmetry finder reduces the number of primary sectors to calculate from 7 to 3 , and the total number of sectors from 212 to 122 . For comparison, SECDEC 3 produces 448 sectors using strategy X.

### 4.5 Integrals containing elliptic functions

In the examples elliptic2L_euclidean and elliptic2L_physical an integral is calculated which is known from Refs. 38,39 to contain elliptic func-
tions. We consider the integrals $I_{a_{1} \ldots a 9}$

$$
\begin{align*}
& I_{a_{1} \ldots a_{9}}=\int \frac{d^{D} k_{1}}{i \pi^{\frac{D}{2}}} \frac{d^{D} k_{2}}{i \pi^{\frac{D}{2}}} \frac{D_{8}^{-a 8} D_{9}^{-a 9}}{\left[D_{1}\right]^{a_{1}}\left[D_{2}\right]^{a_{2}}\left[D_{3}\right]^{a_{3}}\left[D_{4}\right]^{a_{4}}\left[D_{5}\right]^{a_{5}}\left[D_{6}\right]^{a_{6}}\left[D_{7}\right]^{a_{7}}}  \tag{2}\\
& D_{1}=k_{1}^{2}-m^{2}, D_{2}=\left(k_{1}+p_{1}+p_{2}\right)^{2}-m^{2}, D_{3}=k_{2}^{2}-m^{2}, \\
& D_{4}=\left(k_{2}+p_{1}+p_{2}\right)^{2}-m^{2}, D_{5}=\left(k_{1}+p_{1}\right)^{2}-m^{2}, D_{6}=\left(k_{1}-k_{2}\right)^{2}, \\
& D_{7}=\left(k_{2}-p_{3}\right)^{2}-m^{2}, D_{8}=\left(k_{2}+p_{1}\right)^{2}, D_{9}=\left(k_{1}-p_{3}\right)^{2} .
\end{align*}
$$

The topology for $I_{110111100}$ is depicted in Fig. (4. Here we calculate the integral $f_{66}^{A}=\left(-s / m^{2}\right)^{\frac{3}{2}} I_{110111100}$ discussed in Ref. [38].

In elliptic2L_euclidean we calculate the kinematic point $s=-4 / 3, t=$ $-16 / 5, p_{4}^{2}=-100 / 39, m=1$ (Euclidean point) with the settings epsrel $=10^{-5}$, maxeval $=10^{7}$ and obtain

$$
\begin{equation*}
f_{66}^{A}=0.2470743601 \pm 6.9692 \times 10^{-6} \tag{3}
\end{equation*}
$$

The analytic result $\sqrt{1}$ is given by

$$
f_{66, \text { analytic }}^{A}=0.247074199140732131068066
$$

In elliptic2L_physical we calculate the non-Euclidean point $s=90, t=$ $-2.5, p_{4}^{2}=1.6, m^{2}=1$ and find with epsrel $=10^{-4}$, maxeval $=10^{7}$ :

$$
\left.\left(\frac{-s}{m^{2}}\right)^{-\frac{3}{2}} f_{66}^{A}=-0.04428874+i 0.01606818 \pm(2.456+i 2.662) \times 10^{-5}\right)
$$



Fig. 4. Two-loop 6-propagator graph leading to elliptic functions. Curly lines denote massless particles. The box contains massive propagators with mass $m$. One leg ( $p_{4}$ ) has $p_{4}^{2} \neq 0$.

### 4.6 Two-loop vertex diagram with special kinematics

In the example triangle2L_split we calculate an integral entering the twoloop corrections to the $Z b \bar{b}$ vertex, calculated in Refs. 40, 41], where it is called $N_{3}$.
${ }^{1}$ We thank Francesco Moriello and Hjalte Frellesvig for providing us the result.

This example is run as usual by the commands
python generate_triangle2L_split.py \&\& make -C triangle2L_split \&\& python integrate_triangle2L_split.py

The diagram produced by pySECDEC is shown in Fig. 5.


Fig. 5. The integral $N_{3}$ with one massive propagator $\left(m_{Z}\right)$ and $s=p_{3}^{2}=m_{Z}^{2}$.
The kinematic condition $s=M_{Z}^{2}$ leads to an integrand which is particularly difficult for the sector decomposition method because it does not have a Euclidean region. As a consequence, the integral has both endpoint singularities as well as singularities due to the fact that the second Symanzik polynomial $\mathcal{F}$ can vanish on some hyperplane in Feynman parameter space, rather than only at the origin. The remappings done by the standard sector decomposition algorithm would turn this into singularities at $x_{i}=1$. In SecDec 3, singularities at $x_{i}=1$ were treated by a split of the integration domain at $x_{i}=0.5$ and subsequent remapping to the unit hypercube. However, this can lead to an infinite recursion of the problem.
pySECDEC can detect and remap such "hyperplane singularities" into singularities at the origin by a dedicated spitting procedure, where a splitting at the symmetric point $x_{i}=0.5$ is avoided.

The results obtained for this example are listed in Table 3 .
Table 3
Numerical result from pySECDEC for the integral $N_{3}$.

| $\epsilon$ order | pySECDEC result |
| :---: | :--- |
| $\epsilon^{-2}$ | $\left(1.23370112+\mathrm{i} 5.76 \times 10^{-7}\right) \pm(0.00003623+\mathrm{i} 0.00003507)$ |
| $\epsilon^{-1}$ | $(2.89050847+\mathrm{i} 3.87659429) \pm(0.00060165+\mathrm{i} 0.00070525)$ |
| $\epsilon^{0}$ | $(0.77923028+\mathrm{i} 4.13308243) \pm(0.00815782+\mathrm{i} 0.00923315)$ |

### 4.7 Hypergeometric function ${ }_{5} F_{4}$

An example of a general dimensionally regulated parameter integral, which can also have endpoint-singularities at $z_{i}=1$, can be found in hypergeo5F4. We consider the hypergeometric function ${ }_{5} F_{4}\left(a_{1}, \ldots, a_{5} ; b_{1}, \ldots, b_{4} ; \beta\right)$.

This example is run by the usual commands
python generate_hypergeo5F.py \&\& make -C hypergeo5F4 \&\&
python integrate_hypergeo5F.py
The considered function has the integral representation

$$
\prod_{i=1}^{4}\left[\frac{\Gamma\left[b_{i}\right]}{\Gamma\left[a_{i}\right] \Gamma\left[b_{i}-a_{i}\right]} \int_{0}^{1} d z_{i}\left(1-z_{i}\right)^{-1-a_{i}+b_{i}} z_{i}^{-1+a_{i}}\right]\left(1-\beta z_{1} z_{2} z_{3} z_{4}\right)^{a_{5}}
$$

The potential singularities at $z_{i}=1$ are automatically detected by the program and remapped to the origin if the flag split=True is set. Results for values $a_{5}=-\epsilon, a_{2}=-\epsilon, a_{3}=-3 \epsilon, a_{4}=-5 \epsilon, a_{5}=-7 \epsilon, b_{1}=2 \epsilon, b_{2}=4 \epsilon, b_{3}=6 \epsilon, b_{4}=$ $8 \epsilon, \beta=0.5$ are shown in Tab. 4 .

Table 4
Comparison of the exact result for ${ }_{5} F_{4}$ with the evaluation of pySECDEC, maximally using $10^{9}$ integrand evaluations.

| $\epsilon$ order | Exact result (using HypExp 42]) | pySECDEC result |
| :---: | :---: | :---: |
| $\epsilon^{0}$ | 1 | $1 \pm \times 10^{-15}$ |
| $\epsilon^{1}$ | 0.1895324 | $0.18953239 \pm 0.0002$ |
| $\epsilon^{2}$ | -2.2990427 | $-2.2990377 \pm 0.0016$ |
| $\epsilon^{3}$ | 55.469019 | $55.468712 \pm 0.084$ |
| $\epsilon^{4}$ | -1014.3924 | $-1014.3820 \pm 0.89$ |

### 4.8 Function with two different regulators

The example two_regulators demonstrates the sector decomposition and integration of a function with multiple regulators. We consider the integra ${ }^{2}$

[^0]\[

$$
\begin{align*}
I=e^{-\gamma_{E}(2 \epsilon+\alpha)} \int_{0}^{1} d z_{0} & \int_{0}^{1} d z_{1} z_{0}^{-1-2 \epsilon-\alpha}\left(1-z_{0}\right)^{-1+2 \epsilon+\alpha} z_{1}^{-\epsilon+\frac{\alpha}{2}} e^{-z_{0} /\left(1-z_{0}\right)}  \tag{4}\\
& =\frac{2}{\alpha} \Gamma(-2 \epsilon-\alpha) e^{-\gamma_{E}(2 \epsilon+\alpha)} \\
= & -\frac{1}{\alpha \epsilon}+\frac{1}{2 \epsilon^{2}}-\frac{\pi^{2}}{6}+\mathcal{O}(\alpha, \epsilon) .
\end{align*}
$$
\]

This example can be run using the usual commands
python generate_two_regulators.py \&\& make -C two_regulators \&\& python integrate_two_regulators.py

The regulators are specified in a list as regulators = ['alpha', 'eps']. The orders to be calculated in each regulator are defined in a list where the position of each entry matches the one in the regulator list. For example, if the integral should be calculated up to the zeroth order in the regulator $\alpha$ and to first order in $\epsilon$, the corresponding input would be requested_orders $=[0,1]$.

### 4.9 User-defined additional functions

The user has several possibilities to define functions which are not included in the decomposition procedure itself and which can therefore be non-polynomial or be defined by an arbitrary $C++$ function, for example a jet algorithm or the definition of an event shape variable. Three examples (dummyI, dummyII and thetafunction) which demonstrate the use of user defined functions are contained in the subdirectory userdefined_cpp.

### 4.9.1 Analytic functions not entering the decomposition

The example dummy I demonstrates how a result can be multiplied by an analytic function of the integration variables which should not be decomposed. The example can be run with the usual commands python generate_dummyI.py \&\& make -C dummyI \&\&
python integrate_dummyI.py
The functions which are to be multiplied onto the result are listed in generate_dummy I py on the line functions = ['dum1', 'dum2']. The user can give functions any name which is not a reserved python function name.
The dependence of these functions on a number of arguments is given on the line

```
remainder_expression =
'(dum1(z0,z1,z2,z3) + 5*eps*z0)**(1+eps) *
dum2(z0,z1,alpha)**(2-6*eps)'.
```

Note that the remainder_expression is an explicitly defined function of the integration variables but that the functions dum1 and dum2 are left implicit in the python input file.

Any functions left implicit in the python input (in this example dum1 and dum2) are to be defined later in the file <name>/src/functions.hpp. A template for this file will be created automatically together with the process directory. In our example, for the user's convenience, the appropriate functions are copied to the process directory in the last line of generate_dummyI.py. Note that the arguments in functions.hpp are the ones that occur in the argument list of the function in generate_dummyI.py, in the same order. The function arguments can be both integration variables and parameters. Derivatives of the functions are needed if higher than logarithmic poles appear in the decomposition of the integrand. The definition of the derivatives are named following the pattern $\mathrm{d}<$ function>d<argument>, for example 'ddum1d0' means the first derivative of the function with name 'dum1' with respect to its first argument.

Alternatively, if the extra functions are simple, they can be defined explicitly in the python input file in remainder_expression $=$ 'define explicit function here'. The example dummyII demonstrates this. It can be run with the usual commands
python generate_dummyII.py \&\& make -C dummyII \&\&
python integrate_dummyII.py
In this case, the definition of functions like dum1,dum2 is obsolete. The definitions given in remainder_expression will be multiplied verbatim to the polynomials to decompose.

### 4.9.2 Non-analytic or procedural functions not entering the decomposition

The user can also multiply the result by $C++$ functions which are not simple analytic functions, for example they may contain if statements, for loops, etc., as may be needed to define measurement functions or observables. An example of this is given in generate_thetafunction.py which shows how a theta-function can be implemented in terms of a $C++$ if statement. This example can be run with the usual commands
python generate_thetafunction.py \&\& make -C thetafunction \&\& python integrate_thetafunction.py

In the python input file the name of the $C++$ function is given on the line functions = ['cut1']. The line
remainder_expression $=$ 'cut1 (z1, delt)'
instructs pySECDEC to multiply the function onto the result, without decomposition. Note that the implementation of the function cut1 is not given in the python input file. Once the process directory is created, the func-
tion cut1 should be defined in <name>/src/functions.hpp. In our example, the appropriate function is copied to the process directory in the last line of generate_thetafunction.py for the user's convenience. The theta-function may be defined as follows:

```
template<typename T0, typename T1>
integrand_return_t cut1(T0 arg0, T1 arg1)
{
    if (arg0 < arg1) {
        return 0.;
    } else {
        return 1.;
    }
};
```

The first argument $(\arg 0)$ corresponds to $z 1$, the second one $(\arg 1)$ is the cut parameter delta.

### 4.10 Four-photon amplitude

This example, contained in 4photon1L_amplitude, calculates the one-loop four-photon amplitude $\mathcal{M}^{++--}$. The example may be run using the commands:
make \&\& ./amp
The Makefile will produce the libraries for the two-point and four-point functions entering the amplitude and compile the file amp.cpp which defines the amplitude. Executing './amp' evaluates the amplitude numerically and prints the analytic result for comparison.

The amplitude for 4-photon scattering via a massless fermion loop can be expressed in terms of three independent helicity amplitudes, $\mathcal{M}^{++++}, \mathcal{M}^{+++-}$, $\mathcal{M}^{++--}$, out of which the remaining helicity amplitudes forming the full amplitude can be reconstructed using crossing symmetry, Bose-symmetry and parity. Omitting an overall factor of $\alpha^{2}$, the analytic expressions read (see e.g. 43|)

$$
\begin{align*}
& \mathcal{M}^{++++}=8 \quad, \quad \mathcal{M}^{+++-}=-8 \\
& \mathcal{M}^{++--}=-8\left[1+\frac{t-u}{s} \log \left(\frac{t}{u}\right)+\frac{t^{2}+u^{2}}{2 s^{2}}\left(\log \left(\frac{t}{u}\right)^{2}+\pi^{2}\right)\right] \tag{5}
\end{align*}
$$

Up to an overall phase factor, the amplitude $\mathcal{M}^{++--}$can be expressed in
terms of one-loop integrals as

$$
\begin{equation*}
\mathcal{M}^{++--}=-8\left\{1+\frac{t^{2}+u^{2}}{s} I_{4}^{D+2}(t, u)+\frac{t-u}{s}\left(I_{2}^{D}(u)-I_{2}^{D}(t)\right)\right\} . \tag{6}
\end{equation*}
$$

The purpose of our simple example is to show how pySECDEC can be used to calculate the master integrals occurring in the amplitude $\mathcal{M}^{++--}$.

### 4.11 Comparison of timings

Table 5
Comparison of timings (algebraic, numerical) using pySecDec, SecDec 3 and Fiesta 4.1.

|  | pySECDEC time (s) | SECDEC 3 time (s) | FIESTA 4.1 time (s) |
| :---: | :---: | :---: | :---: |
| triangle2L | $(40.5,9.6)$ | $(56.9,28.5)$ | $(211.4,10.8)$ |
| triangle3L | $(110.1,0.5)$ | $(131.6,1.5)$ | $(48.9,2.5)$ |
| elliptic2L_euclidean | $(8.2,0.2)$ | $(4.2,0.1)$ | $(4.9,0.04)$ |
| elliptic2L_physical | $(21.5,1.8)$ | $(26.9,4.5)$ | $(115.3,4.4)$ |
| box2L_invprop | $(345.7,2.8)$ | $(150.4,6.3)$ | $(21.5,8.8)$ |

We compare the timings for several of the above mentioned examples between pySecDec, SecDec 3 and Fiesta 4.1, where we distinguish between the time needed to perform the algebraic and the numeric part. In Tab. 5, the compilation of the generated $C++$ functions is included in the algebraic part, because it needs to be done only once. The timings for the numerical part are the wall clock times for the evaluation of the $C++$ functions.

The timings were taken on a four-core (eight hyper-thread) Intel(R) Core(TM) i7-4770 CPU @ 3.40 GHz machine. We set the parameter number_of_presamples in pySEcDec, optlamevals in SEcDec 3 and LambdaIterations in FiESTA 4.1, which controls the number of samples used to optimise the contour deformation, to the Fiesta 4.1 default of 1000. The default decomposition strategy of each tool was used, STRATEGY_S for FIESTA 4.1 and $X$ for pySECDEC and SecDec 3. The integrands were summed before integrating in the following way: setting together=True in pySECDEC and togetherflag=1 in SECDEC 3 sums all integrands contributing to a certain pole coefficient before integrating. SeparateTerms=False in Fiesta 4.1 sums the integrands in each sector which appears after pole resolution before integrating. For the examples considered on our test platform these settings were found to be optimal for all three tools. The integration is performed using the default settings of pySecDec and the same settings in SecDec 3 and Fiesta 4.1. In particular, this implies a rather low desired relative accuracy of $10^{-2}$.

The numerical integration times in pySECDEC are generally reduced with respect to SECDEC 3, which is mostly due to a better optimization during the algebraic part, and partly also due to a more efficient deformation of the integration contour in pySEcDEc. For the test cases considered we found that Fiesta 4.1 is the fastest to perform the algebraic (decomposition) step when contour deformation is not required. We would like to stress that although we endeavoured to keep all relevant settings identical across the tools we are not experts in the use of Fiesta 4.1 and we expect that it is possible to obtain better timings by adjusting settings away from their default values. Furthermore, which tool is fastest strongly depends on the case considered and whether one prefers faster decomposition or numerical evaluation of the resulting functions.

## 5 Conclusions

We have presented a new version of the program SEcDEc, called pySEcDec, which is publicly available at http://secdec.hepforge.org. The program pySECDEC is entirely based on open source software (python, FORM, CUBA) and can be used in various contexts. The algebraic part can isolate poles in any number of regulators from general polynomial expressions, where Feynman integrals are a special case of. For the numerical part, a library of $C++$ functions is created, which allows very flexible usage, and in general outperforms SecDec 3 in the numerical evaluation times. In particular, it extends the functionality of the program from the evaluation of individual (multi-)loop integrals to the evaluation of larger expressions containing multiple analytically unknown integrals, as for example two-loop amplitudes. Such an approach already has been used successfully for the two-loop integrals entering the full NLO corrections to Higgs boson pair production. Therefore pySecDec can open the door to the evaluation of higher order corrections to multi-scale processes which are not accessible by semi-analytical approaches.

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## A Parameter settings

## A. 1 Algebraic part

The settings for the algebraic part are listed and explained in detail in the section "Code Writer/Make Package" in the documentation, as well as in the section "Loop Integral" for settings which are specific to loop integrals.

## A.1.1 Loop package

The parameters for loop_package are:
name : string. The name of the $C++$ namespace and the output directory.
loop_integral : The loop integral to be computed, defined via pySecDec.loop_integral.LoopIntegral (see below).
requested_orders : integer. The expansion in the regulator will be computed to this order.
real_parameters : iterable of strings or sympy symbols, optional. Parameters to be interpreted as real numbers, e.g. Mandelstam invariants and masses.
complex_parameters : iterable of strings or sympy symbols, optional. Parameters to be interpreted as complex numbers, e.g. masses in a complex mass scheme.
contour_deformation (True) : bool, optional. Whether or not to produce code for contour deformation.
additional_prefactor (1) : string or sympy expression, optional. An additional factor to be multiplied to the loop integral. It may depend on the regulator, the real parameters and the complex parameters.
form_optimization_level (2) : integer out of the interval [0,3], optional. The optimization level to be used in FORM.
form_work_space ('500M') : string, optional. The FORM WorkSpace.
decomposition_method : string, optional. The strategy for decomposing the polynomials. The following strategies are available:

- 'iterative' (default)
- 'geometric'
- 'geometric_ku'
normaliz_executable ('normaliz') : string, optional. The command to run normaliz. normaliz is only required if decomposition_method is set to 'geometric' or 'geometric_ku'.
enforce_complex (False) : bool, optional. Whether or not the generated integrand functions should have a complex return type even though they might be purely real. The return type of the integrands is automatically complex if contour_deformation is True or if there are complex parame-
ters. In other cases, the calculation can typically be kept purely real. Most commonly, this flag is needed if the logarithm of a negative real number can occur in one of the integrand functions. However, pySECDEC will suggest setting this flag to True in that case.
split (False) : bool, optional. Whether or not to split the integration domain in order to map singularities at 1 back to the origin. Set this option to True if you have singularities when one or more integration variables are equal to one.
ibp_power_goal (-1) : integer, optional. The power_goal that is forwarded to the integration by parts routine. Using the default setting, integration by parts is applied until no linear or higher poles remain in the integral. We refer to the documentation for more detailed information.
use_dreadnaut (True) : bool or string, optional. Whether or not to use dreadnaut to find sector symmetries.

The main keywords to define loop integrals from a "graphical representation" (LoopIntegralFromGraph) are:
internal_lines : list defining the propagators as connections between labelled vertices, where the first entry of each element denotes the mass of the propagator, e.g. [['m', [1,2]], ['0', $[2,1]]]$.
external_lines : list of external line specifications, consisting of a string for the external momentum and a string or number labelling the vertex, e.g. [['p1', 1], ['p2', 2]].
replacement_rules : symbolic replacements to be made for the external momenta, e.g. definition of Mandelstam variables. Example: [('p1*p2', ' $s$ '), ('p1**2', 0 )] where p 1 and p 2 are external momenta. It is also possible to specify vector replacements, e.g. [('p4', ' $\left.\left.-(\mathrm{p} 1+\mathrm{p} 2+\mathrm{p} 3)^{\prime}\right)\right]$.
Feynman_parameters ('x') : iterable or string, optional. The symbols to be used for the Feynman parameters. If a string is passed, the Feynman parameter variables will be consecutively numbered starting from zero.
regulator ( $\epsilon$ ) : string or sympy symbol, optional. The symbol to be used for the dimensional regulator. Note: If you change this symbol, you have to adapt the dimensionality accordingly.
regulator_power (0) : integer. The numerator will be multiplied by the regulator $(\epsilon)$ raised to this power. This can be used to ensure that the numerator is finite in the limit $\epsilon \rightarrow 0$.
dimensionality (4-2 $\epsilon$ ) : string or sympy expression, optional. The dimensionality of the loop momenta.
powerlist : iterable, optional. The powers of the propagators, possibly dependent on the regulator. The ordering must match the ordering of the propagators given in internal_lines.

For LoopIntegralFromPropagators:
propagators : iterable of strings or sympy expressions. The propagators in momentum representation, e.g. ['k1**2', '(k1-k2)**2-m1**2'].
loop_momenta : iterable of strings or sympy expressions. The loop momenta, e.g. ['k1', 'k2'].
external_momenta : iterable of strings or sympy expressions, optional. The external momenta, e.g. ['p1', 'p2']. Specifying the external momenta is only required when a numerator is to be constructed.
Lorentz_indices : iterable of strings or sympy expressions, optional. Symbols to be used as Lorentz indices in the numerator.
numerator (1) : string or sympy expression, optional. The numerator of the loop integral. Scalar products must be passed in index notation, e.g. $\mathrm{k} 1(\mathrm{mu}) * \mathrm{k} 2(\mathrm{mu})+\mathrm{p} 1(\mathrm{mu}) * \mathrm{k} 2(\mathrm{mu})$. All Lorentz indices must be explicitly defined using the parameter Lorentz_indices.
metric_tensor ('g') : string or sympy symbol, optional. The symbol to be used for the (Minkowski) metric tensor $g^{\mu \nu}$.

Note: The parameters replacement_rules, regulator, dimensionality, powerlist, regulator_power are available for both, LoopIntegralFromGraph and LoopIntegralFromPropagators.

## A.1.2 Make package

The parameters for make package are:
name : string. The name of the $C++$ namespace and the output directory. integration_variables : iterable of strings or sympy symbols. The variables that are to be integrated from 0 to 1 .
regulators : iterable of strings or sympy symbols. The (UV/IR) regulators of the integral.
requested_orders : iterable of integers. Compute the expansion in the regulators to these orders.
polynomials_to_decompose : iterable of strings or sympy expressions. The polynomials to be decomposed.
polynomial_names : iterable of strings. Assign symbols for the polynomials to decompose. These can be referenced in the other_polynomials.
other_polynomials : iterable of strings or sympy expressions. Additional polynomials where no decomposition is attempted. The symbols defined in polynomial_names can be used to reference the polynomials_to_decompose. This is particularly useful when computing loop integrals where the numerator can depend on the first and second Symanzik polynomials. Note that the polynomial_names refer to the polynomials_to_decompose without their exponents.
prefactor : string or sympy expression, optional. A factor that does not depend on the integration variables. It can depend on the regulator(s) and
the kinematic invariants. The result returned by pySECDEC will contain the expanded prefactor.
remainder_expression : string or sympy expression, optional. An additional expression which will be considered as a multiplicative factor.
functions : iterable of strings or sympy symbols, optional. Function symbols occurring in remainder_expression. Note: The power function pow and the logarithm log are already defined by default. The log uses the nonstandard continuation from a negative imaginary part on the negative real axis (e.g. $\log (-1)=-i \pi)$.
form_insertion_depth (5) : non-negative integer, optional. How deep FORM should try to resolve nested function calls.
contour_deformation_polynomial : string or sympy symbol, optional. The name of the polynomial in polynomial_names that is to be continued to the complex plane according to a $-i \delta$ prescription. For loop integrals, this is the second Symanzik polynomial F, and this will be done automatically in loop_package. If not provided, no code for contour deformation is created.
positive_polynomials : iterable of strings or sympy symbols, optional. The names of the polynomials in polynomial_names that should always have a positive real part. For loop integrals, this applies to the first Symanzik polynomial U. If not provided, no polynomial is checked for positiveness. If contour_deformation_polynomial is None, this parameter is ignored.

Note: All parameters (except loop_integral) described under loop_package are also available in make_package.

## A. $2 C++$ part

The default settings for the numerical integration are listed in the section "Integral Interface" in the documentation. We also list the defaults and a short description for the main parameters here. The values in brackets behind the keywords denote the defaults.

## A.2.1 Contour deformation parameters and general settings

real_parameters : iterable of float. The real parameters of the library (e.g. kinematic invariants in the case of loop integrals).
complex_parameters : iterable of complex. The complex parameters of the library (e.g. complex masses).
together (True) : bool. Determines whether to integrate the sum of all sectors or to integrate the sectors separately.
number_of_presamples (100000) : unsigned int, optional. The number of samples used for the contour optimization. This option is ignored if the
integral library was created with contour deformation set to 'False'.
deformation_parameters_maximum (1.0) : float, optional. The maximal value the deformation parameters $\lambda_{i}$ can obtain. If number_of_presamples $=0$, all $\lambda_{i}$ are set to this value. This option is ignored if the integral library was created without deformation.
deformation_parameters_minimum $\left(10^{-5}\right)$ : float, optional. The minimal value for the deformation parameters $\lambda_{i}$. This option is ignored if the integral library was created without deformation.
deformation_parameters_decrease_factor (0.9) : float, optional. If the sign check (the imaginary part always must be negative) with the optimized $\lambda_{i}$ fails, all $\lambda_{i}$ are multiplied by this value until the sign check passes. This option is ignored if the integral library was created without deformation.
real_complex_together (False) : If true, real and imaginary parts are evaluated simultaneously. If the grid should be optimally adapted to both real and imaginary part, it is more advisable to evaluate them separately.

## A.2.2 Cuba parameters

Table 6
Default settings for integrator-specific parameters.

| Vegas | Suave | Divonne | Cuhre |
| :--- | :--- | :--- | :--- |
| nstart (1000) | nnew (1000) | key1 (2000) | key (0) |
| nincrease (500) | nmin (10) | key2 (1), key3 (1) |  |
| nbatch (1000) | flatness (25.0) | maxpass (4) <br> border (0.0) <br> maxchisq (1.0) <br> mindeviation (0.15) |  |

Common to all integrators:
epsrel (0.01) : The desired relative accuracy for the numerical evaluation.
epsabs $\left(10^{-7}\right)$ : The desired absolute accuracy for the numerical evaluation.
flags (0) : Sets the Cuba verbosity flags. The flags=2 means that the Cuba input parameters and the result after each iteration are written to the log file of the numerical integration.
seed (0) : The seed used to generate random numbers for the numerical integration with Cuba.
maxeval (1000000) : The maximal number of evaluations to be performed by the numerical integrator.
mineval (0) : The number of evaluations which should at least be done before the numerical integrator returns a result.

For the description of the more specific parameters, we refer to the Cuba
manual. Our default settings are given in Table 6. When using Divonne, we strongly advise to use a non-zero value for border, e.g. $10^{-8}$.

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