Loop integral evaluation with pySecDec

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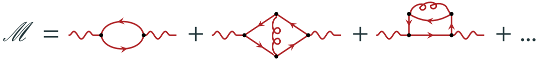
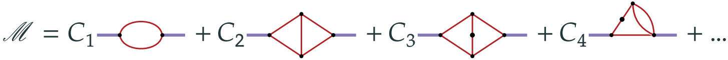
Where does pySecDec fit in?

Basic steps of calculating scattering matrix elements:

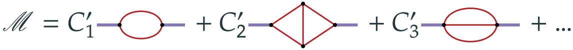
1. Generate Feynman diagrams for the process.

   * 

2. Project the diagrams onto scalar integrals.

   * 

3. Reduce the number of integrals using IBP relations.

   * 

4. *Evaluate the loop integrals.*

   * Analytically: hard to impossible at two loops if masses are present.
   * *Numerically:*
     * *Sector decomposition:* pySecDec, Fiesta.
     * Mellin-Barnes representation: MB, Ambre.
     * Numerical differential equations: e.g. DiffExp + pySecDec/Fiesta/MB.

5. Integrate over kinematics.

   * A whole field of study by itself.

Sector decomposition in short

$$I = \int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \, \left(x+y\right)^{-2+\varepsilon} = ?$$

Problem: the integrand diverges at $x, y \to 0$, can't integrate numerically.

Solution: [Heinrich '08; Binoth, Heinrich '00]

1. Factorize the divergence in x and y with sector decomposition:
   - $I = \int \cdots \times \Big(\underbrace{\theta\left(x > y\right)}_{\text{Sector 1}} + \underbrace{\theta\left(x < y\right)}_{\text{Sector 2}}\Big) = \int_0^1 \mathrm{d}x \int_0^x \mathrm{d}y \, \left(x+y\right)^{-2+\varepsilon} + \begin{pmatrix} x \\ \updownarrow \\ y \end{pmatrix}$
2. Rescale the integration region in each sector back to a hypercube:
   - $I \overset{y \to x\,y}{=} \int_0^1 \mathrm{d}x \, \underbrace{x^{-1+\varepsilon}}_{\text{Factorized pole}} \int_0^1 \mathrm{d}y \left(1+y\right)^{-2+\varepsilon} + \begin{pmatrix} x \\ \updownarrow \\ y \end{pmatrix}$
3. Extract the pole at $x \to 0$ analytically, expand in ε:
   - $I = -\frac{2}{\varepsilon} \int_0^1 \mathrm{d}y \left(1+y\right)^{-2+\varepsilon} = -\frac{2}{\varepsilon} \int_0^1 \mathrm{d}y \left(\frac{1}{\left(1+y\right)^2} - \frac{\ln\left(1+y\right)}{\left(1+y\right)^2} \varepsilon + \mathcal{O}\left(\varepsilon^2\right) \right)$
4. Integrate each term in ε numerically (they all converge now).

pySecDec overview

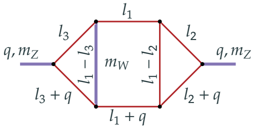
pySecDec: library for *numerically evaluating parametric integrals* via sector decomposition and Monte Carlo integration. [Heinrich et al '21, '18, '17]

- https://github.com/gudrunhe/secdec
- Written in *Python*, C++, Form.
- Multiple sector decomposition methods: iterative, geometric.
- Multiple integration algorithms:
  - Best: *Randomized Quasi-Monte Carlo* (Qmc); [Borowka et al '18]
    - Integration error $\sim \frac{1}{N_{\text{samples}}}$ (classical Monte Carlo has $\sim \frac{1}{N_{\text{samples}}^{1/2}}$);
    - Works on CPUs and GPUs (with CUDA);
  - Classic: Vegas/Suave/Divonne/Cuhre (Cuba), Cquad (Gsl).
- Installation via the *standard Python package* installer (Linux, Mac):
  - `pip3 install --user pySecDec`

Recent new features:

- Adaptive sampling of whole amplitudes (weighted sums of integrals).
- Builtin asymptotic expansion of integrals.

Using pySECDEC for a single Feynman integral



$= ?$

Generate the integration library:

```
import pySecDec as psd
if __name__ == "__main__":
    psd.loop_package(
        name="dia1",
        loop_integral=
            psd.LoopIntegralFromPropagators(
                loop_momenta=["l1", "l2", "l3"],
                propagators=[
                    "(l1)**2",
                    "(l2)**2",
                    "(l3)**2",
                    "(l1 + q)**2",
                    "(l2 + q)**2",
                    "(l3 + q)**2",
                    "(l1 - l2)**2",
                    "(l1 - l3)**2 - mw2"
                ],
                powerlist=[1,1,1,1,1,1,1,1],
                replacement_rules=[
                    ("q*q", "mz2")
                ]),
        real_parameters=["mz2", "mw2"],
        requested_orders=[0],
        decomposition_method="geometric")
```

Inspect the generated code:

```
$ ls dia1/
dia1_data/              dia1_integral/  pylink/
src/                    Makefile        Makefile.conf
README                  dia1.hpp        integral_names.txt
integrate_dia1.cpp
```

Compile it for the CPU:

```
$ cd dia1 && make
```

or for both CPU and GPU (with CUDA):

```
$ export SECDEC_WITH_CUDA_FLAGS="-arch=sm_80" CXX=nvcc
$ cd dia1 && make
```

Run it:

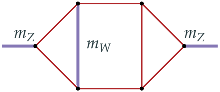
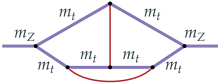
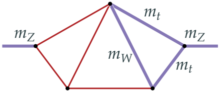
```
from pySecDec.integral_interface import IntegralLibrary
if __name__ == "__main__":
    lib = IntegralLibrary("dia1/dia1_pylink.so")
    lib.use_Qmc(verbosity=1)
    mz2 = 1.0
    mw2 = 0.78
    _, _, result = lib([mz2, mw2], epsrel=1e-7, verbose=True)
    print(result)
```

The result:

```
+ ((6.82645729748523067e+00,-1.60711801420445148e+01)
+/- (8.07205205949069617e-07,7.55815020343424309e-07))
+ O(eps)
```

Expected performance for 3-loop EW integrals

pySecDec[1] + QMC *integration times* for 3-loop self-energy integrals:[2]

<table>
<tr><th colspan="2">Diagram \ Relative precision</th><th>10^{-3}</th><th>10^{-4}</th><th>10^{-5}</th><th>10^{-6}</th><th>10^{-7}</th><th>10^{-8}</th></tr>
<tr><td rowspan="2"></td><td>GPU</td><td>15s</td><td>20s</td><td>40s</td><td>200s</td><td>13m</td><td>50m</td></tr>
<tr><td>CPU</td><td>10s</td><td>50s</td><td>400s</td><td>4000s</td><td>180m</td><td>1200m</td></tr>
<tr><td rowspan="2"></td><td>GPU</td><td>18s</td><td>19s</td><td>30s</td><td>20s</td><td>1.2m</td><td>2m</td></tr>
<tr><td>CPU</td><td>5s</td><td>14s</td><td>60s</td><td>50s</td><td>12m</td><td>16m</td></tr>
<tr><td rowspan="2"></td><td>GPU</td><td>6s</td><td>11s</td><td>12s</td><td>30s</td><td>3m</td><td>24m</td></tr>
<tr><td>CPU</td><td>5s</td><td>10s</td><td>50s</td><td>800s</td><td>60m</td><td>800m</td></tr>
</table>

[Same diagrams as in Dubovyk, Usovitsch, Grzanka '21]

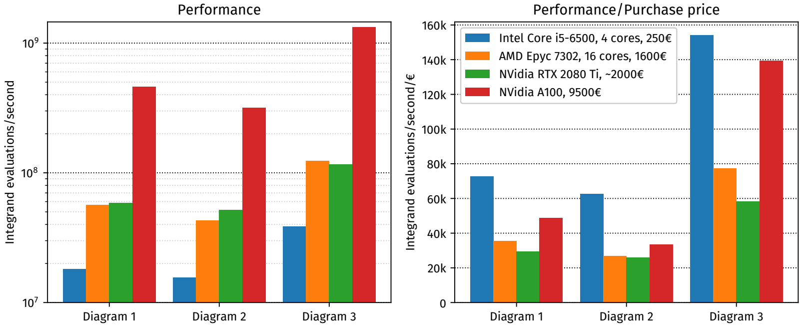
In short: *seconds to minutes per integral* to achieve practical precision.

[1] Version 1.5 + work-in-progress + AVX2.

[2] *GPU*: NVidia A100 40GB; *CPU*: AMD Epyc 7302 with 32 threads.

CPU vs GPU with pySecDec

pySecDec[3] integrand sampling speed on different devices:

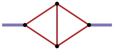


In short:

- Top consumer-grade GPU (RTX 2080 Ti) ≈ server-grade CPU.
- Top server-grade GPU (A100) ≈ $10\times$ server-grade CPU.

[3]Version 1.5 + work-in-progress + AVX2.

Adaptive sampling of amplitudes

Amplitude term	Naive sampling	Naive error	Better sampling	Better error
1 	10^6 samples	$1 \cdot 10^{-6}$	$\frac{1}{2} \cdot 10^6$ samples	$2 \cdot 10^{-6}$
10 	10^6 samples	$10 \cdot 10^{-6}$	$\frac{1}{2} \cdot 10^6$ samples	$20 \cdot 10^{-6}$
50 	10^6 samples	$50 \cdot 10^{-6}$	$2 \cdot 10^6$ samples	$25 \cdot 10^{-6}$
Total:	$3 \cdot 10^6$	$51 \cdot 10^{-6}$	$3 \cdot 10^6$	$32 \cdot 10^{-6}$

[Example assumes integration error = $1/n$]

pySecDec now automatically optimizes the total integration time based on

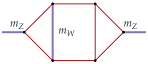
- how fast each integral can be sampled,
- how well it converges,
- how large its coefficient is.

$\Rightarrow$ Automatic *speedup for amplitudes* (weighted sums of integrals).

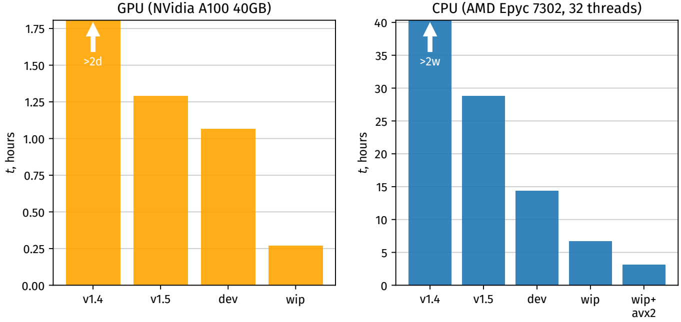
$\Rightarrow$ Automatic speedup for single integrals too (sums of sectors).

$\Rightarrow$ Used in e.g. 2-loop $gg \to ZZ$ (2011.15113) and $gg \to ZH$ (2011.12325); see also: talk by Chaitanya Paranjape on Thursday.

Performance improvements by pySecDec version

Time to integrate 

to 7 digits of precision with pySecDec + QMC:

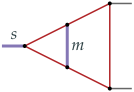


Speedup sources:

- *v1.5:* adaptive sampling, automatic contour deformation adjustment;
- *dev:* separation of real and complex variables in the integrand code;
- *wip:* removal of the indirection from the integrand code, vectorization.

The latest release is fast; *the next release will be faster.*

Asymptotic expansion, briefly

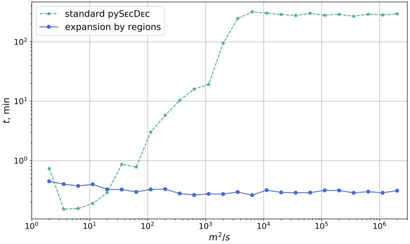
$I \equiv$  $= ?$

Problem: when $s/m^2 \ll 1$ numerical integration converges poorly.

- General problem when scale ratios are not ≈ 1.

Solution: asymptotic expansion in scale ratios. [Beneke, Smirnov '98, Jantzen '11]

- Takes out extreme ratios from the integrand:
  - $I = (\cdots + \cdots)\left(\frac{s}{m^2}\right)^{-1} + (\cdots + \cdots + \cdots + \cdots)\left(\frac{s}{m^2}\right)^{0} + \mathcal{O}\left(\frac{s}{m^2}\right)$
- Now implemented in pySecDec (through `pySecDec.loop_regions`).
- E.g. time to integrate the above triangle to 10^{-3} accuracy:



Summary

pySecDec provides:

- Numerical evaluation of *massive multi-loop integrals*.
  - 3-loop massive integrals at 6 digits in seconds to minutes.
- Dependable results when other methods fail.

The latest release (v1.5) introduces: [Heinrich '21]

- Optimized evaluation of *amplitudes* (weighted sums of integrals).
  - Proven in several 2-loop calculations.
  - Automatically applicable to single integrals too.
- *Asymptotic expansion* of integrals for extreme kinematics.

Future releases will bring:

- Even better performance.

Summary

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Thank you for your attention.

Backup slides

The need for higher loop corrections

Error predictions on key electroweak parameters: [Freitas '21]

Errors		Γ_Z, MeV	m_W, MeV	R_b, 10^{-5}	$\sin^2\theta^l_{\text{eff}}$, 10^{-5}
Experimental	current	2.3	12	66	14
	FCC-ee	0.1	0.7	6.0	0.5
	CEPC	0.5	1.0	4.3	2.3
Theoretical	current, ≤ 2 loops	0.4	4	10	4.5
	future?, ≤ 3 loops	0.15	1.0	5	1.5

Up to *3-loop theory is needed* to match the experimental precision of the future colliders.

Using pySecDec for amplitudes

Generate the integration library:

```
import pySecDec as psd
if __name__ == "__main__":
    # First term
    term1 = psd.LoopPackage(
        name="integral1",
        loop_integral=
            psd.LoopIntegralFromPropagators(
                ...
            ),
        real_parameters=[...])
    coeff1 = psd.Coefficient(
        numerators=['1 + 2*eps^3', ...],
        denominators=['-3 + 2*eps', '-1 + 2*eps', ...],
        parameters=[])
    # Second term
    term2 = ...
    coeff2 = ...
    ...
    # The amplitude
    psd.sum_package('amplitude',
        [term1, term2, ...],
        regulators=['eps'],
        requested_orders=[0],
        coefficients=[[coeff1, coeff2, ...]],
        real_parameters=[...]
    )
```

Compile an *run*: same as for a single integral.

$\Longrightarrow$ Under the hood single integrals are implemented the same as sums.

Using pySecDec with asymptotic expansion

Generate the integration library:

```
import pySecDec as psd
if __name__ == "__main__":
    # find the regions and expand the integral up to O(s)
    terms = psd.loop_regions(
        name="triangle2L",
        loop_integral=
            psd.LoopIntegralFromPropagators(
                loop_momenta=["l1", "l2"],
                external_momenta=["p1", "p2"],
                propagators=[
                    "(l1 + p1)**2",
                    "(l1 - p2)**2",
                    "(l2 + p1)**2",
                    "(l2 - p2)**2",
                    "l2**2",
                    "(l1 - l2)**2 - msq"
                ],
                replacement_rules=[
                    ("p1*p1", 0),
                    ("p2*p2", 0),
                    ("p1*p2", "s/2")
                ]),
        smallness_parameter="s",
        decomposition_method="geometric",
        expansion_by_regions_order=0)
    # generate the library
    psd.sum_package("triangle2L_by_regions",
        terms,
        regulators=["eps"],
        requested_orders=[0],
        real_parameters=["s", "msq"])
```

Compile an *run*: same as for a single integral.

⇒ Adaptive amplitude optimization is enabled automatically.