Numerical multi-loop calculations with pySecDec

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In collaboration with:
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Numerical results for two-loop amplitudes

Differential equations

\[ pp \rightarrow t\bar{t} \] Czakon, Fiedler, Heymes, Mitov
('13,'16,'17)

\[ gg \rightarrow \gamma\gamma \] Mandal, Maltoni, Zhao (2019)

Sector decomposition

\[ pp \rightarrow HH \] Borowka, Greiner, Heinrich, Jones, Kerner, JS, Schubert, Zirke (2016)

\[ pp \rightarrow HJ \] Jones, Kerner, Luisoni (2018)

\[ pp \rightarrow HH \ (\text{partial EW}) \] Borowka, Duhr, Maltoni, Pagani, Shivaji, Zhao (2019)

Direct numerical integration

\[ pp \rightarrow HH \] Baglio, Campanario, Glaus, Mühleitner, Spira, Streicher (2018)
Numerical calculation of Feynman integrals using sector decomposition

Hepp (1966); Denner, Roth (1996); Binoth, Heinrich (2000)

\[
\int \prod_{i=1}^{L} \frac{d^D k_i}{D_1^{\nu_1} \cdots D_N^{\nu_N}} \sim \int_0^\infty \frac{dx}{x} x^\nu \delta(1-x_N) \frac{\mathcal{U}(x)^{N-(L+1)D/2}}{\mathcal{F}(x, s_{ij})^{N-LD/2}} = \frac{c_{-2L}}{\epsilon^{2L}} + \frac{c_{-2L+1}}{\epsilon^{2L-1}} + \ldots
\]

- Decompose integration region into sectors with simple singularity structure
- Contour deformation for multi-scale integrals in physical region Soper (2000); Binoth, Guillet, Heinrich, Pilon, Schubert (2005); Nagy, Soper (2006); Borowka, Heinrich (2012)
- Subtract divergences and expand in the regularization parameter \(\epsilon\)
- Integrate the finite coefficients (numerically)
- Applicable to loop integrals and more general parametric integrals
Geometric sector decomposition

Kaneko, Ueda (2010), Borowka, Heinrich, Jones, Kerner, JS, Zirke (2015)
other strategies: Binoth Heinrich (2000), Bogner, Weinzierl (2008), Smirnov, Tentyukov (2009)

\[ m \sim \int_0^\infty \frac{dx_1 dx_2}{x_1 x_2} x_1^{\nu_1} x_2^{\nu_2} \left( x_1^0 x_2^0 + x_1^1 x_2^1 + x_0^1 x_1^2 \right)^{-\frac{D}{2}} \]

\[ x_i = \prod_{F} y_F^{\langle n_F, \hat{e}_i \rangle} \]

\[ = \int_0^1 \frac{dy_1 dy_2 dy_3}{y_1 y_2 y_3} y_1^{-\nu_1 + \frac{D}{2}} y_2^{-\nu_2 + \frac{D}{2}} y_3^{\nu_1 + \nu_2 - \frac{D}{2}} \left( y_1 + y_2 + y_3 \right)^{-\frac{D}{2}} \sum_{i=1}^3 \delta(1 - y_i) \]
pySecDec


Other public tools


- FIESTA Smirnov, Smirnov Tentyukov ('09, '11, '14, '15)
Numerical Integration

\[ l_s(f) = \int_{[0,1]^s} \, d\mathbf{x} f(\mathbf{x}) \rightarrow Q_{s,n}(f) = \frac{1}{n} \sum_{i=0}^{n-1} f(x_i) \]

minimize error \( \epsilon = |l_s(f) - Q_{s,n}(f)| \)

Monte Carlo

- Integration points \( x_i \) randomly distributed
  \[ \epsilon = \frac{\sigma(f)}{\sqrt{n}} \sim \mathcal{O}(n^{-1/2}) \]
- Implemented in CUBA \(^\text{Hahn ('04, '14)}\)
Quasi Monte Carlo
Dick, Kuo, Sloan (2013)

Rank-1 lattice rule: \( x_i = \{ \frac{iz}{n} + \Delta_k \}, \quad i = 0, \ldots, n - 1 \)

- \( z \): generating vector
- \( \{ \ldots \} \): fractional part
- \( O(n^{-1}) \) error scaling for certain classes of smooth, periodic functions
- First application to sector decomposition by Li, Wang, Yan, Zhao (2015)
- Shift lattice by random vectors \( \Delta_k \) to obtain error estimate

\[
\tilde{Q}_{s,n,m}(f) = \frac{1}{m} \sum_{k=0}^{m-1} Q_{s,n}^{(k)} \quad Q_{s,n}^{(k)} = \frac{1}{n} \sum_{i=0}^{n-1} f\left( \left\{ \frac{iz}{n} + \Delta_k \right\} \right)
\]
Periodization

Dick, Kuo, Sloan (2013)

Functions can be periodized by change of variables $x = \psi(y)$:

$$I_s(f) = \int_{[0,1]^s} dxf(x) = \int_{[0,1]^s} \prod_{j=1}^s dy_j \omega(y_j)f(\psi(y))$$

with $\psi'(y) = \omega(y)$

- **Korobov**: $\omega_{\alpha,\beta}(y) = (\alpha + \beta + 1)\left(\frac{\alpha+\beta}{\alpha}\right) y^\alpha (1 - y)^\beta$
  
  Korobov (1963), Laurie (1996), Kuo, Sloan, Wozniakowski (2007)

- **Sidi**: $\omega_{\alpha}(y) = \frac{\pi}{2^\alpha} \frac{\Gamma(\alpha+1)}{\Gamma((\alpha+1)/2)^2} sin(\pi y)^\alpha$
  
  Sidi (1993)

- **Baker**: $\psi(y) = 1 - |1 - 2y|$
  
  Hickernell (2002)
Scaling

3-loop form-factor integral

relative error

3-loop form-factor integral

Korobov-1
(n 1)
Korobov-3
(n 2)

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Variance reduction

Flatten integrand by change of variables $x = p(y)$ with $p'(y) \sim f(p(y))^{-1}$

$$\int_0^1 dx f(x) = \int_0^1 dy p'(y) f(p(y))$$

- Smooth function ansatz for $p(y)$ to preserve smoothness of integrand
- Free parameters fitted to inverse of cumulative distribution function

$$p(x) = a_2 \cdot x \frac{a_0 - 1}{a_0 - x} + a_3 \cdot x \frac{a_1 - 1}{a_1 - x} + a_4 \cdot x + a_5 \cdot x^2 + \left(1 - \sum_{i=2}^{5} a_i\right) \cdot x^3$$
QMC implementation
Public implementation of Quasi Monte Carlo integration Borowka, Heinrich, Jahn, Jones, Kerner, JS (2018)

github.com/mppmu/qmc

- Single header C++11 library using CUDA
- Parallelization over multiple GPUs and CPUs on a single machine

<table>
<thead>
<tr>
<th>Device</th>
<th>M Func evals/s</th>
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<tr>
<td>Xeon 6140</td>
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<tr>
<td>GTX1080</td>
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<td>V100</td>
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Performance hugely dependent on integrand

Study and figure by Stephen Jones
Hyperelliptic integrals: 3 mass banana graph

- New class of analytic functions
- → talk by L. Tancredi
- Unproblematic for numerical calculation
- \( s = 20, m_1^2 = 1, m_2^2 = 1.3, m_3^2 = 0.7 \)
- \( \text{minn}=1000000, \text{transform}='\text{korobov2}' \)

\[
I = \left( 1.97000000000000264 \pm 9.85 \cdot 10^{-15} + i (1.84 \cdot 10^{-15} \pm 1.16 \cdot 10^{-15}) \right) \cdot \epsilon^{-3} \\
+ \left( -5.9281676367925620 \pm 6.52 \cdot 10^{-14} + i (1.07 \cdot 10^{-13} \pm 2.63 \cdot 10^{-14}) \right) \cdot \epsilon^{-2} \\
+ \left( 9.86757086818429 \pm 1.64 \cdot 10^{-12} - i (2.54 \cdot 10^{-11} \pm 9.83 \cdot 10^{-12}) \right) \cdot \epsilon^{-1} \\
- 89.066074732329 \pm 8.25 \cdot 10^{-10} + i (8.10892634289 \pm 2.37 \cdot 10^{-9}) \\
+ O(\epsilon) .
\]
High loop integrals: 6L bubble

- geometric decomposition
- minn=10**7, transform='baker', polysingular fit
- analytic result Kompaniets, Panzer (2017)

\[
B_{6L}^{\text{analyt.}} = \frac{1}{\epsilon^2} \frac{147}{16} \zeta_7 - \frac{1}{\epsilon} \left( \frac{147}{16} \zeta_7 + \frac{27}{2} \zeta_3 \zeta_5 + \frac{27}{10} \zeta_{3,5} - \frac{2063}{504000} \pi^8 \right) + \mathcal{O}(\epsilon^0)
\]

\[
B_{6L}^{\text{num.}} = + \left( 9.2642089624 \pm 1.58 \cdot 10^{-8} \right) \cdot \epsilon^{-2} + \left( 91.73175426 \pm 2.15 \cdot 10^{-6} \right) \cdot \epsilon^{-1} + \left( 1118.607204 \pm 1.31 \cdot 10^{-4} \right) + \mathcal{O}(\epsilon).
\]
\( m_{\text{int}} = m_{\text{ext}} \rightarrow \) numerically unstable

- Use split option to split integration region
- \( s = (p_1 + p_2)^2 = -1 \), \( t = (p_1 + p_3)^2 = -0.8 \), \( m^2 = 0.1 \)
- 8 to 11 digits precision

\[
\text{minn} = 10^{**7}, \quad \text{minn} = 10^{**9}, \quad \text{minn} = 15173222401,
\text{ transform='korobov4'}, \quad \text{transform='korobov6'}, \quad \text{transform='korobov6'}
\]

polysingular fit for \( H_a \), polysingular fit for \( H_b \), for \( H_c \).
Higgs boson pair production with full top quark mass dependence

$$\sigma^{NLO} = \sigma^{LO} + \sigma^{virt} + \sigma^{real}$$

analytic result known

Glover, van der Bij (1988)

requires two-loop amplitude

Catani, Seymour (1996) for the cancellation of IR divergences

Dipole subtraction


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Contributing diagrams

- 2-loop integrals with 4 mass scales \( \{ \hat{s}, \hat{t}, m_t^2, m_h^2 \} \)
- Only small subset known analytically:
  - \( gg \rightarrow h \) Spira et al. (1993); Anastasiou et al. (2006)
  - \( h \rightarrow Z\gamma \) Gehrmann, Guns, Kara (2015); Bonciani, Del Duca, Frellesvig, Henn, Moriello, Smirnov (2015)
  - Reducible (1-loop)\(^2\) contributions Degrassi, Giardino, Gröber (2016)
Integral reduction

- Integration-by-parts reduction \cite{Tkachov:1981as,Chetyrkin:1981qh}
- Choose 5 planar + 3 nonplanar integral families with 9 propagators
- Complete reduction of planar families with Reduze \cite{vonManteuffel:2012np} using numerical values for masses:

\[
\{\hat{s}, \hat{t}, m_t^2, m_h^2\} \rightarrow \{\hat{s}, \hat{t}, 173^2, 125^2\}
\]

- Nonplanar families not fully reduced
- Choose finite integrals where possible \cite{vonManteuffel:2014aha}
- Use dimension shift relations \cite{Tarasov:1995bw, Lee:2009nb}
- Improves stability of numerical integration
Integration

Phase-space

- unweighted events based on LO calculation
- originally computed 917 points, excluded 4 (now 6320)

Amplitude

- Precision for individual sector integrals set dynamically
- Target accuracy $F_1 : 3\%$, $F_2 : 5-20\%$
- GPU time/PS point: 80min - 2d (median 2h)

Figure by Stephen Jones
Results - Inclusive cross section

\[ \sigma^{NLO}(pp \rightarrow hh) = 32.91^{+13.6\%}_{-12.6\%} \, fb \pm 0.3\%(\text{stat.}) \pm 0.1\%(\text{int.}) \]

Borowka, Greiner, Heinrich, Jones, Kerner, JS, Schubert, Zirke (2016), Borowka, Greiner, Heinrich, Jones, Kerner, JS, Zirke (2016)

- LHC@14 TeV
- 7-point scale variation
  \[ \mu_F/R \in \{\mu_0/2, \mu_0, 2\mu_0\} \] with
  \[ \mu_0 = \frac{m_{hh}}{2} \]
- PDF4LHC15_nlo_30_pdfas
- \( m_h = 125 \) GeV, \( m_t = 173 \) GeV
- agreement with independent result Baglio, Campanario, Glaus, Mühlleitner, Spira, Streicher (2018)
Results - $m_{hh}$

The graph shows the differential cross section $d\sigma/dm_{hh}$ in fb/GeV for different models:

- **LO**: Leading Order
- **NLO HEFT**: Next-to-Leading Order Heavy Exponent Framework
- **NLO FTapprox**: Next-to-Leading Order FT Approximation
- **NLO**: Next-to-Leading Order

The $m_{hh}$ axis is labeled in GeV, with values ranging from 300 to 1000 GeV. The $K$ factor is shown at the bottom of the graph, with values ranging from 1.0 to 2.0.
Conclusion and Outlook

- Improvements in pySecDec:
  - Quasi Monte Carlo integration
  - GPU support
- NLO Higgs boson pair production with full top quark mass dependence

Outlook

- Apply pySecDec setup to other processes
- Further improvements to pySecDec:
  - Expansion by regions
  - Improvements for integrals with numerators
Backup
NLO Higgs boson pair production in gluon fusion

- (HL-)LHC: Determine Higgs boson properties
- Higgs self-couplings probe Higgs potential and mechanism of EW symmetry breaking

Higgs potential:

\[
V(\Phi) = -\mu^2 \Phi \dagger \Phi + \lambda \left( \Phi \dagger \Phi \right)^2
\]

\[
V(h) = \frac{m_h^2}{2} h^2 + \frac{m_h^2}{2v} h^3 + \frac{m_h^2}{8v^2} h^4
\]
The process $gg \rightarrow hh$

- **LO (1-loop) with full top quark mass dependence** Glover, van der Bij (1988)
- **NLO in $m_t \rightarrow \infty$ limit (HEFT)** Dawson, Dittmaier, Spira (HPAIR 1998)
  - + $\frac{1}{m_t}$ expansion Grigo, Hoff, Melnikov, Steinhauser (2013); Grigo, Hoff, Steinhauser (2015)
  - + full $m_t$ dependence in real radiation ($FT_{\text{approx}}$) Maltoni, Vryonidou, Zaro (2014)
- **NNLO in $m_t \rightarrow \infty$ limit** De Florian, Mazzitelli (2013)
  - + matching coefficients Grigo, Hoff, Melnikov, Steinhauser (2013)
  - + $\frac{1}{m_t}$ expansion Grigo, Hoff, Steinhauser (2015)
  - fully differential de Florian, Grazzini, Hanga, Kallweit, Lindert, Maierhöfer, Mazzitelli, Rathlev (2016)
  - real-virtual $\frac{1}{m_t}$ expansion Davies, Herren, Mishima, Steinhauser (2019)
- **NLO in high energy limit** Davies, Mishima, Steinhauser (2019)
- **NLO (2-loop) with full top quark mass dependence** Borowka, Greiner, Heinrich, Jones, Kerner, JS, Schubert, Zirke (2016), Borowka, Greiner, Heinrich, Jones, Kerner, JS, Zirke (2016)
  - Baglio, Campanario, Glaus, Mühlleitner, Spira, Streicher (2018)


Combination with NNLO in $m_t \to \infty$: Grazzini, Heinrich, Jones, Kallweit, Kerner, Lindert, Mazzitelli (2018),


Self coupling studies with PS: Heinrich, Jones, Kerner, Luisoni, Scyboz (2019)


Combination with high energy approximation: Davies, Heinrich, Jones, Kerner, Mishima, Steinhauser, Wellmann (2019) (→ talk by Stephen Jones)