SecDec: a versatile tool for multi-loop/leg calculations

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New Physics?

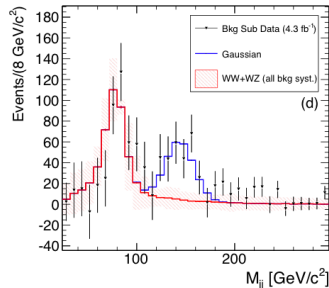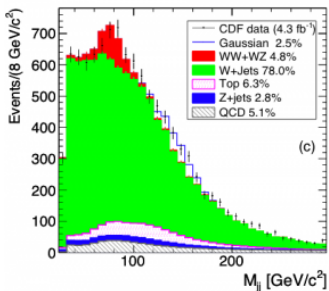

Figure: CDF collaboration, arXiv:1104.0699

In order to discover new physics, we need to know signal and background processes to a high degree of accuracy.

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Higher Order Corrections

Knowledge of backgrounds to a high degree of accuracy requires

calculations involving integrals (over loop momenta for virtual

corrections, and over phase space). Thus multi-dimensional

parameter integrals occur widely in these calculations.

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Basic Concept (I)

Multi-dimensional parameter integrals can have complicated singularity structures.
Sector decomposition is an algorithmic approach to extracting regulated IR/UV singularities.
Consider

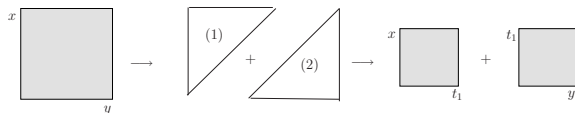$$I = \int_0^1 dx \int_0^1 dy \; x^{-1-a\epsilon} y^{b\epsilon} (x+y)^{-1}$$

Here we have a singularity when x and y $\rightarrow$ 0 simultaneously. We split the integration region in two, with x>y in one half, y>x in the other

$$I = \left(\int_0^1 dx \int_0^x dy + \int_0^1 dy \int_0^y dx\right) x^{-1-a\epsilon} y^{b\epsilon} (x+y)^{-1}$$

In the first we set $y = x t_1$, and the second $x = y t_1$

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Basic Concept (II)

$$I = \int_0^1 dx \; x^{-1-(a+b)\epsilon} \int_0^1 dt_1 \; t_1^{-b\epsilon}(1+t_1)^{-1}$$

$$+ \int_0^1 dy \; y^{-1-(a+b)\epsilon} \int_0^1 dt_1 \; t_1^{-1-a\epsilon}(1+t_1)^{-1}$$

The singularities are now factorised and can be read off from the powers of simple monomials in the integration variables. The polynomial in the denominator $\rightarrow$ constant as the integration variables $\rightarrow 0$

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Components of an NLO calculation

For an n-particle observable, there are 2 types of processes to be considered at NLO

- 1-loop correction to n-particle process
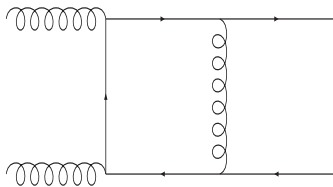- Tree-level (n+1)-particle process, where 1 particle can be unresolved
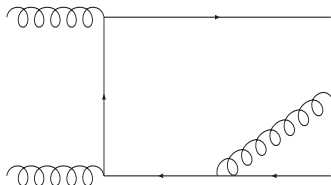

Figure: $gg \rightarrow t\bar{t}$

Figure: $gg \rightarrow t\bar{t}+g$

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Components of an NNLO calculation

For an n-particle observable, there are 3 types of process to be considered at NNLO

- 2-loop correction to n-particle process
- 1-loop correction to (n+1)-particle process, where 1 particle can be unresolved
- Tree-level (n+2)-particle process, where up to 2 particles can be unresolved.
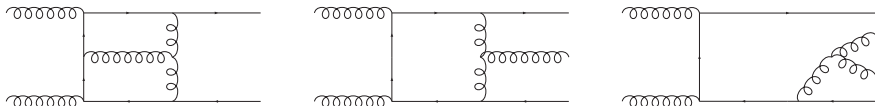
Each of these contains IR singularities. The soft and final-state collinear singularities cancel when the sum is taken.

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Analytic methods

- At NLO, various methods have been successfully applied to these calculations. Extension of these methods to NNLO (and beyond) has been attempted, with varying levels of success.
- For multi-loop integration, Mellin-Barnes representation has proved successful, eg in the calculation of the massless 3-loop form factor(Baikov et al 2009, Heinrich et al 2009, Lee/Smirnov 2010, Gehrman et al 2010)
- For double real radiation, Antenna Subtraction at NNLO has been developed (A. Gehrmann–De Ridder, T. Gehrmann, E.W.N. Glover hep-ph/0501291), and has been successfully applied to $e^+e^- \to 3j$ (Gehrmann et al. 2007-11, Weinzierl et al 2008-2011). Antenna subtraction requires analytic integration of subtraction terms, which for cross-sections involving massive particles is particularly difficult.

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Benefits of Sector Decomposition

- Doesn't require analytic integration

- Can be used for real corrections

- Can be used for virtual corrections for 1-scale problems, or multi-scale problems in the Euclidean region.

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Current Status of Sector Decomposition

A number of public programs exist for virtual corrections, including

- FIESTA2 (A.V Smirnov et al, arXiv:0912.0518)
- sector_decomposition (C. Bogner & S. Weinzierl arXiv:0709.4092), written in C++
- CSectors (Gluza, Kajda, Riemann, Yundin, arXiv:1010.1667), a Mathematica interface to sector_decomposition
- SecDec (JC & Heinrich, arXiv:1011.5493)

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Current Status of Sector Decomposition

A few examples of calculations of cross sections using sector decomposition, and further developments

- Hadronic $t\bar{t}+$ double real radiation(Czakon arXiv:1101.0642), using sector decomposition guided by knowledge of the singularity structure

- NNLO QCD predictions for $H \to WW \to l\nu l\nu$ (Anastasiou et al. arXiv:0707.2373)

- EW gauge boson production at hadron colliders to NNLO (Melnikov & Petriello, hep-ph/0609070)

- Second order QCD corrections to inclusive semileptonic $b \to X_c l\bar{\nu}_l$ (Biswas & Melnikov, arXiv:0911.4142)

- Non-linear transformations have been used alongside sector decomposition to reduce the number of produced sectors (Anastasiou et al, arXiv:1011.4867)

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What are Multi-Dimensional Parameter Integrals?

In general, we wish to calculate integrals of the form

$I = \int_0^1 d^N \mathbf{x} \prod_{j=1}^{k} f_j(\mathbf{x})^{a_j + b_j \epsilon}$

where the f_j are polynomials, and ϵ is the regulator

(cf dimensional regularisation $\epsilon = \frac{4-D}{2}$)

Some of the f_j may contain overlapping singularities such that

$f_j(\mathbf{x}) \rightarrow 0$ as some subset of the $x_i \rightarrow 0$

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Feynman Parameters

- Write down amplitude using Feynman rules
- Employ reduction methods to give the amplitude as a sum of certain master integrals with various coefficients
- Use Feynman parameters and integrate over loop momenta
- These master integrals are of the form
  $I = \int_0^1 (\prod_{i=1}^N dx_i)\delta(1 - \sum_{i=1}^N x_i)\mathcal{U}(\mathbf{x})^{a+b\epsilon}\mathcal{F}(\mathbf{x})^{c+d\epsilon}$
- N is the number of propagators, $\mathcal{U}$ is a function of $\mathbf{x}$, and $\mathcal{F}$ is a function of $\mathbf{x}$ and external invariants (s,m^2,...). Both can have zeroes when all or some of $x_i \to 0$

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Example

Figure: Non-Planar 2-loop massless box

$\mathcal{F}(\mathbf{x}) = -x_1(s_{13}x_5x_6 + s_{23}x_4x_7) - s_{12}(x_3x_4x_5 + x_2(x_6x_7 + x_3(x_4 + x_5 + x_6 + x_7)))$

$\mathcal{U}(\mathbf{x}) = x_5x_6 + x_7x_6 + x_4(x_5 + x_7) + x_1(x_4 + x_5 + x_6 + x_7) + x_2(x_4 + x_5 + x_6 + x_7) + x_3(x_4 + x_5 + x_6 + x_7)$

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Simple Example (I)

The phase space of a $2 \to n$ process is given by

$$d\Phi_{2\to n} = \prod_{j=3}^{n} \left(\frac{d^D p_j}{(2\pi)^{D-1}} \delta^+(p_j^2 - m_j^2) \right)(2\pi)^D \delta^{(D)}(p_1 + p_2 - \sum_{k=3}^{n} p_k)$$

1 or more particles becoming unresolved (soft or collinear) can lead to singularities, which must be extracted so that we can compute them numerically.

As a simple example, consider $\gamma(p_1)\gamma(p_2) \to t(p_3)\bar{t}(p_4)g(p_5)$
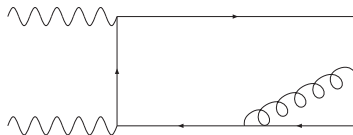
The only possible singularity comes from the gluon becoming soft, so we should parametrise the phase space in such a way that E_5 is simple

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Simple Example (II)

A convenient parametrisation gives us the phase space

$$\int d\Phi_{2\to 3} \sim s^{D-3} \int_0^1 du\, u^{D-3} (1-u)^{\frac{D-4}{2}} R_m$$

$$\int_0^1 dx_2 \int_0^1 dx_3 [x_2(1-x_2)x_3(1-x_3)]^{\frac{D-4}{2}} \int_0^1 dx_4 [x_4(1-x_4)]^{\frac{D-5}{2}}$$

Where $E_5 = uE_5^{max}$ and R_m is non-zero at $u = 0$

The only 2 denominators in the matrix element which can become zero are $D_1 = (p_3 + p_5)^2 - m_t^2$ and $D_2 = (p_4 + p_5)^2 - m_t^2$, and these $\sim u(1 + ...)$ so the singularities will be factorised already.
More complicated processes lead to more complicated singularity structures. Eg if we considered a *gg* initial state instead, then the final state gluon could become collinear with an initial gluon.

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More Complicated Example

When 2 final particles can become unresolved the singularity structure is significantly more complex. Eg
$g(p_1)g(p_2) \rightarrow H(p_h)g(p_3)g(p_4)$
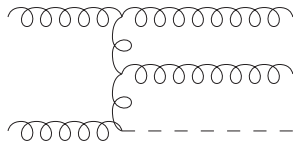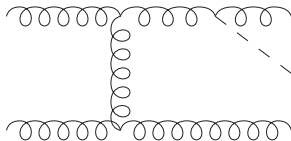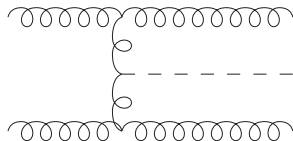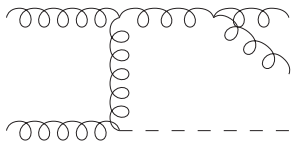
Can have singular denominators s_{34}, s_{ih} and s_{if}

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Iterative Decomposition

Consider the integral $I = \int_0^1 d^N \mathbf{x} \prod_{j=1}^k f_j(\mathbf{x})^{a_j + b_j \epsilon}$

- Find an f_j which requires decomposition. If no such f_j exists then the iteration terminates.
- Find a minimal subset of integration variables $\mathcal{S} = \{x_{i_1}, ..., x_{i_m}\}$ such that $f_j(\mathbf{x}) \to 0$ as $\mathcal{S} \to \mathbf{0}$
- Split $I = I_1 + ... + I_m$ where I_p has $x_{i_p} > x_{i_q} \forall x_{i_q} \in \mathcal{S}$
- For each I_p, remap the variables of $\mathcal{S}$ such that $x_{i_q} \to x_{i_p} x_{i_q} \forall p \neq q$
- Factorize x_{i_p} from all polynomials
- Repeat the iteration until the process terminates

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Termination of Iteration

In general the choice of subset $\{x_{i_1}, ... x_{i_p}\}$ is not unique.

It has been shown (arXiv:0709.4092 Bogner & Weinzierl, arXiv:0812.4700 Smirnov & Smirnov) that strategies exist which guarantee that the iteration terminates, but such strategies tend to lead to a large number of subsectors.

A deterministic algorithm based on methods from computational geometry has been devised by Kaneko & Ueda (arXiv:0908.2897)

Following certain heuristic rules leads to fewer subsectors, and has worked well in a multitude of practical applications.

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Subtraction (I)

- After the iteration terminates and the subsectors are relabelled we have $I = \sum_{m=1}^{\#subsectors} I_m$
- Each I_m is of the form $\int_0^1 (\prod_{i=1}^N dx_i x_i^{\alpha_i+\beta_i\epsilon}) \prod_{j=1}^k \tilde{f}_j(\mathbf{x})^{a_j+b_j\epsilon}$
- Each $\tilde{f}_j$ is non-zero as $\mathbf{x} \to \mathbf{0}$ so we rewrite
  $\prod_{j=1}^k \tilde{f}_j(\mathbf{x})^{a_j+b_j\epsilon} \equiv g(\mathbf{x}, \epsilon)$

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Subtraction (II)

- All the singularities are contained in the $\prod_{i=1}^{N} dx_i x_i^{\alpha_i + \beta_i \epsilon}$
- If $\alpha_i > -1$ then there is no singularity in x_i
- If $\alpha_i = -1$, subtraction is needed.

  Write $g(x, \epsilon) \equiv g(0, \epsilon) + (g(x, \epsilon) - g(0, \epsilon))$

  $\int_0^1 x^{-1+\beta\epsilon} g(0, \epsilon) dx = \frac{g(0,\epsilon)}{\beta\epsilon} \int_0^1 dx$

  $\int_0^1 x^{\beta\epsilon} \frac{g(x,\epsilon) - g(0,\epsilon)}{x} = O(1)$

- If $\alpha_i <= -2$ then more terms of the Taylor expansion are required

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Numerical Integration

- $I(\epsilon) = \sum_m I_m(\epsilon)$

- Perform the Laurent Expansion in ϵ

- For each order of ϵ the coefficient is a sum of well-behaved integrals over the *N* dimensional unit hypercube, each of which can be integrated numerically to yield the full result

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Numerical Stability (I)

Consider the integral $I = \int_0^1 x^{-2+\epsilon} f(x) dx$ After subtraction, we have an integral of the form $\int_0^1 x^\epsilon \frac{f(x) - f(0) - f'(0)x}{x^2}$

This is integrable, but as $x \to 0$, we get something which is $O(\frac{0^2}{0^2})$, which is numerically unstable.

In practice this example is coped with easily by numerical integrators, for complicated problems with many subtractions, the problem is magnified.

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Numerical Stability (II)

One can use integration by parts to explicitly remove the $\frac{1}{x^2}$.

$I = [\frac{x^{-1+\epsilon}}{-1+\epsilon} h(x)]_0^1 + \frac{1}{1-\epsilon} \int_0^1 x^{-1+\epsilon} h'(x)dx$

By construction, $h(x)$ is at least $O(x^2)$ as $x \to 0$, so $h'(x)$ is at least $O(x)$

$I = \frac{h(1)}{-1+\epsilon} + \frac{1}{1-\epsilon}([\frac{x^\epsilon}{\epsilon} h'(x)]_0^1 - \frac{1}{\epsilon} \int_0^1 x^\epsilon h''(x)dx)$

We expand $x^\epsilon = 1 + \epsilon log(x) + ...$ and explicitly integrate the first term:

$I = \frac{h(1)}{-1+\epsilon} + \frac{1}{\epsilon(1-\epsilon)} \int_0^1 (1 - x^\epsilon)h''(x)dx$

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Numerical Stability (III)

The downside to this is that expressions can become large. However the method gives a solution to this problem:
If we consider $h(x) = \sum_m g_m(x)$, then the integral after IBP is

$$I = \frac{\sum_m g_m(1)}{-1+\epsilon} + \frac{1}{\epsilon(1-\epsilon)} \int_0^1 (1 - x^\epsilon)(\sum_m g_m(x))'' dx$$

$$I = \sum_m (\frac{g_m(1)}{-1+\epsilon}) + \sum_m \frac{1}{\epsilon(1-\epsilon)} \int_0^1 (1 - x^\epsilon) g_m''(x) dx$$

where each of these integrals is finite, and so can be performed separately, thus large expressions can be split down into many smaller ones.

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Singularities for $x_i \neq 0$

The above method requires the f_j to only have zeros for some $x_i \to 0$. Often this is not the case. Trivially if a variable x_i causes a singularity at $x_i = 1$ only, one can remap $x_i \to 1 - x_i$. If x_i can cause a singularity at both 0 and 1, we split the integration region into $x_i < \frac{1}{2}$ and $x_i > \frac{1}{2}$.

There can also be line singularities of the form $\frac{1}{|f(x)-g(x)|}$. These f and g are non-negative functions, and have $f(x) = g(x)$ on a line $x_i = x_i(x_j)$. We split the integration region into $x_i < x_i(x_j)$ and $x_i > x_i(x_j)$, and now the singularity lies on the boundary of the integration.

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Singularities for $x_i \neq 0$

For multi-scale loop integrals the kinematics determine the singularity structure of the integral. Eg a term in the integrand might be $\frac{1}{(-s_{12}t_1t_2-s_{13})^2}$, which can only be integrated numerically if the denominator is non-zero throughout the integration region.

This cannot be solved in general by splitting the hypercube, as the splitting would depend on the kinematic point. A solution can be contour integration in the complex plane (see e.g. work by Binoth et al, Anastasiou et al, Weinzierl et al)

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

- Documentation and examples can be found at Comput. Phys.
  Commun. 182(2011)1566 (JC & Heinrich)

- Review article on Sector Decomposition
  Int.J.Mod.Phys.A23:1457-1486 (2008) (Heinrich)

- Original article on multi-loop integrals Nucl.Phys.B585:741
  (2000) (Binoth & Heinrich)

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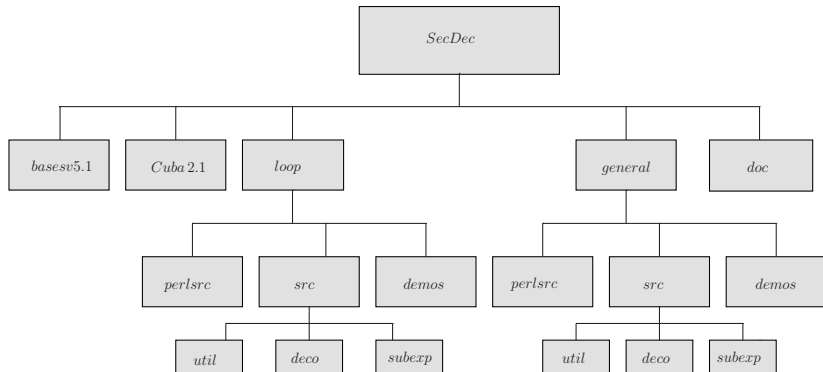Sector Decomposition
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Structure

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Loop Template File

To perform the calculation, SecDec requires 2 files: a template file and a parameter file.

The template file contains

- A list of propagators
- A list of loop momenta
- A list containing the numerator (eg $\{1\}$ or $\{p_1 k_1, k_1 k_2\}$)
- The dimension (usually Dim=4-2eps)

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Template Example

For the 1-loop box:

momlist$= \{k1\}$;

proplist$= \{k1^2, (k1 + p1)^2, (k1 + p1 + p3)^2, (k1 - p2)^2\}$;

numerator$= \{1\}$

Dim$= 4 - 2 * eps$;

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Loop Parameter File

The parameter file contains

- The name of the graph
- Number of legs
- Number of loops
- Number of propagators
- Required order in the ϵ expansion
- Further parameters, all of which can be unassigned and take default values

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Parameter Example

For the 1-loop box:

graph=box

legs=4

loops=1

propagators=4

epsord=2

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Template for General Parameter Integrals

The template file contains

- A list of integration variables
- The integrand, in the form $\{\{f_1, a_1 + b_1\,eps\}, ...\{f_k, a_k + b_k\,eps\}\}$
  (which represents $\prod_{j=1}^{k} f_j^{a_j + b_j\epsilon}$)
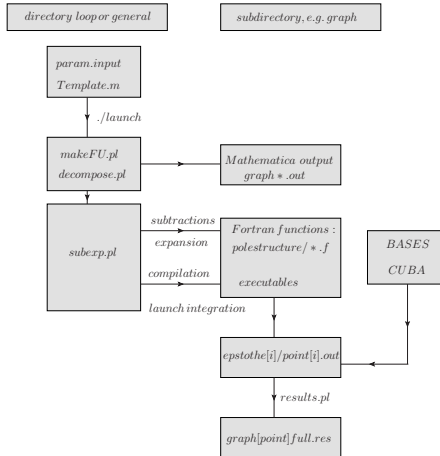- A list of variables which can cause singularities at both 0 and 1

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General Parameter File

The parameter file contains

- The name of the integrand
- Required order in the ϵ expansion
- Further parameters, all of which can be unassigned and take default values

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Current Features

SecDec currently includes a number of useful features

- Parameters (eg invariant masses) can be left implicit up until the numerical integration. This means that the algebraic part needs to only be run once, and then various numerical points can be calculated

- Contracted tensors in the numerator and non-integer powers of propagators in the denominator allowed for loop integrals

- Choice of integrators - BASES (Kawabata, Comput. Phys. Commun. 88 (1995) 309) and the Cuba library (Hahn, Comput.Phys.Commun.168(2005)78) are available, with full control over parameters used (eg desired accuracy)

- Simple to use with Portable Batch System for parallel processing, and readily adjusted to work for different batch syntax

- Subtraction with non-integer powers of variables

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Non-planar 2-loop Corrections for $t\bar{t}$ (I)

Analytic results for these diagrams are not yet available.

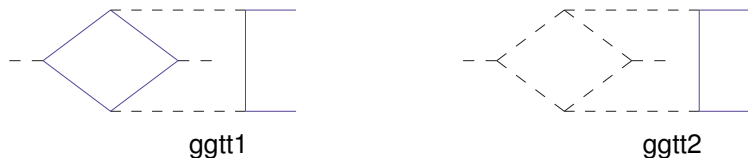An overall factor of $\Gamma(1 + \epsilon)^2$ is extracted.

ggtt1   ggtt2

Figure: Non-planar graphs ocurring in the calculation of $gg \rightarrow t\bar{t}$ at NNLO.
Blue (solid) lines denote massive particles.

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Non-planar 2-loop Corrections for $t\bar{t}$ (II)

ggtt1		
(s, t, u, m_1^2, m_2^2)	(-0.5,-0.4,-0.1,0.17,0.17)	(-1.5,-0.3,-0.2,3,1)
P_0	-38.0797±0.0027	-0.19904±1.5×10^{-5}
P_1	-263.22± 0.015	-0.71466±6×10^{-5}
P_2	-936.86± 0.06	-1.45505± 0.0002
ggtt2		
(s, t, u, m_1^2, m_2^2)	(-0.5,-0.4,-0.1,0.17,0)	(-1.5,-0.3,-0.2,3,0)
P_{-4}	-10.9159 ± 0.0006	-0.13678±1.46×10^{-5}
P_{-3}	-43.5213 ± 0.0075	-0.2087 ±0.00024
P_{-2}	165.384 ± 0.048	3.3417 ±0.0014
P_{-1}	20.842±0.268	-6.593±0.007
P_0	2117.5 ± 1. 57	20.42±0.04

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3-loop Form Factors (I)

9-propagator master integrals for massless 3-loop form factors have been calculated using Mellin-Barnes representation and sector decomposition (Heinrich, Huber, Kosower & Smirnov '09, Baikov, Chetyrkin, Smirnov, Smirnov & Steinhauser '09, Lee, Smirnov & Smirnov '10). These result are reproduced using SecDec.
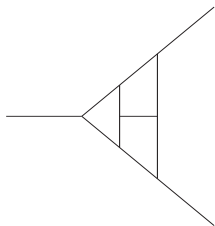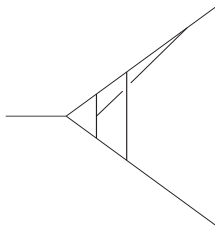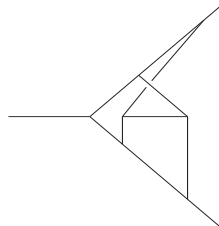

Figure: $A_{9,1}$

Figure: $A_{9,2}$

Figure: $A_{9,4}$

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3-loop Form Factors (II)

$A_{9,*} = i\Gamma(1-\epsilon)^{-3}(-q^2 - i\eta)^{-3-3\epsilon}(C_{-6}/\epsilon^6 + C_{-5}/\epsilon^5 + C_{-4}/\epsilon^4 + C_{-3}/\epsilon^3 + C_{-2}/\epsilon^2 + C_{-1}/\epsilon + C_0)$

$A_{9,4}$	Analytic	SecDec	Longest time(s)	Total time(s)
C_{-6}	0.111111	0.11111	8	17
C_{-5}	0.888889	0.8889	60	154
C_{-4}	-4.65541	-4.652	529	1397
C_{-3}	-33.1607	-33.14	5705	16297
C_{-2}	-42.8359	-42.83	7879	93598
C_{-1}	117.400	117.5	15375	382138
C_0	1948.17	1948	20330	1371382

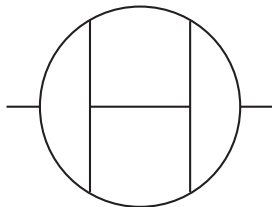Longest algebraic calculation took 40173 seconds, total algebraic time was 108190 seconds.

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4-loop Propagator (I)

Figure: A four-loop two-point master integral

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4-loop Propagator (II)

Stage	Longest time	Total time (secs)
Sector Decomposition	615	2160
Subtraction & ϵ-expansion	809	3767
Numerical integration ϵ^{-1}	156	508
Numerical integration ϵ^{0}	422	4720
Numerical integration ϵ^{1}	492	5946
Numerical integration ϵ^{2}	2172	8123
Full Calculation	-	25224

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4-loop Propagator (III)

Order	Analytical result	Numerical result
ϵ^{-1}	-10.3692776	-10.371 ± 0.002
ϵ^{0}	-70.99081719	-71.002 ± 0.013
ϵ^{1}	-21.663005	-21.65 ± 0.12
ϵ^{2}	Unknown	2833.79 ± 0.92

Analytical results calculated by Baikov & Chetyrkin
(arXiv:1004.1153v2)
This has also been calculated using FIESTA 2, with a lower stated
error 0.17 for ϵ^2, however this takes almost 9 days to run, compared
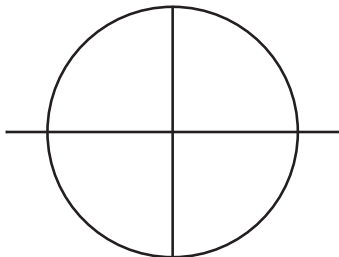to SecDec's 7 hours on a single core.

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4-loop Propagator (IV)

Figure: M_{36}, $O(\epsilon^2)$
Total time (s)
SecDec: 976, FIESTA2: 10565

Figure: M_{41}, $O(\epsilon^2)$
Total time (s)
SecDec: 10595, FIESTA2: 22778

Calculation performed by M. Zentile

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Higher loop calculations

SecDec has recently been applied to a number of 4-loop vertex and 5-loop propagator master integrals (G. Welsh & M. Zentile), many of which have not been calculated analytically.

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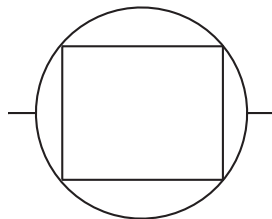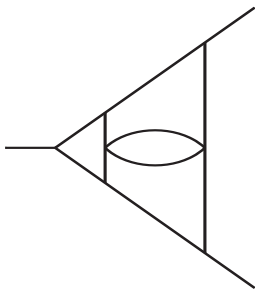
Hypergeometric $_4F_3$ (I)

This example demonstrates half-integer exponents. The analytic result was calculated using HypExp 2
(Huber & Maitre, arXiv:0708.2443)

$$\frac{\Gamma\left(2\epsilon-\frac{1}{2}\right)\Gamma\left(4\epsilon-\frac{1}{2}\right)\Gamma\left(6\epsilon+\frac{1}{2}\right)(1-x_1)^{3\epsilon-1}x_1^{-\epsilon-\frac{3}{2}}(1-x_2)^{6\epsilon}x_2^{-2\epsilon-\frac{5}{2}}(1-x_3)^{9\epsilon-1}x_3^{-3\epsilon-\frac{1}{2}}(1-\beta x_1 x_2 x_3)^{4\epsilon}}{\Gamma\left(\frac{1}{2}-3\epsilon\right)\Gamma\left(-2\epsilon-\frac{3}{2}\right)\Gamma\left(-\epsilon-\frac{1}{2}\right)\Gamma(3\epsilon)\Gamma(9\epsilon)\Gamma(6\epsilon+1)}$$

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Hypergeometric $_4F_3$ (II)

ϵ order	analytic result	numerical result	time taken (secs)
ϵ^0	1	$1.000000 \pm 1.6 \times 10^{-5}$	0.01
ϵ^1	-4.27969	-4.2823 ± 0.0013	0.33
ϵ^2	-26.6976	-26.734 ± 0.075	1.32

Table: $_4F_3(-4\epsilon, -\frac{1}{2} - \epsilon, -\frac{3}{2} - 2\epsilon, \frac{1}{2} - 3\epsilon; -\frac{1}{2} + 2\epsilon, -\frac{1}{2} + 4\epsilon, \frac{1}{2} + 6\epsilon; \beta)$ at $\beta = 0.5$.

Algebraic part of the calculation took 4.8 seconds.

Summary

- Higher order calculations require the evaluation of multi-dimensional parameter integrals.
- Sector decomposition algorithm can be used to compute these integrals.
- I presented the public program SecDec, and demonstrated how it performs very well, both for complicated loop diagrams and general parameter integrals.

Future Features

- Interface with matrix element generator to calculate real radiation contributions
- Implementation of an efficient way to include measurement functions, user-defined observables, kinematic cuts etc and to produce distributions
- Implementation of contour deformation to calculate loop integrals for physical kinematics