6 Numerical Multi-loop Calculations: Sector Decomposition & QMC Integration in pySecDec

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The FCC-ee will allow the experimental uncertainties on several important observables, such as the Electroweak Pseudo-Observables (EWPOs), to be reduced by up to two orders of magnitude compared to the previous generation LEP/SLC experiments [1, 2]. In order to be able to best exploit this unprecedented boost in precision, it is necessary also for theoretical predictions to be known with sufficient accuracy. In practice, this means that very high order perturbative corrections to electroweak precision observables and other processes will be required both in the Standard Model (SM) and potentially also in BSM scenarios.

One of the key challenges for computing perturbative corrections is our ability to compute the Feynman integrals that appear in these multi-loop corrections. There has been very significant progress in this direction in recent years ranging from purely analytic approaches [3–17] to semi-analytic approaches based on expansions [18–23] and also via purely numerical methods [24–32].

So far, the method of sector decomposition has already proved to be useful for computing the complete electroweak two-loop corrections to Z-boson production and decay [33], which is of direct relevance to the FCC-ee, as well as several processes of significant interest at the LHC [34–37] and also BSM corrections [38, 39]. The latter calculations were based on SecDec 3 [40]. Another code based on sector decomposition, Fiesta [41–43], has also been used successfully in various multi-loop calculations, for example for numerical checks of recent evaluations of four-loop three-point functions [13–16].

In this contribution we will briefly describe the essential aspects of this method and provide a short update regarding some of the recent developments [26, 44] that have enabled state of the art predictions to be made using this technique.

In Section 6.1 we will introduce the method of sector decomposition as we use it for computing Feynman integrals and describe how it leads to integrals that are suitable for numerical evaluation. In Section 6.2 we will discuss a particular type of Quasi-Monte-Carlo integration that allows us to efficiently numerically integrate the sector decomposed loop integrals. Finally, in Section 6.3 we will give a short outlook for the field of numerical multi-loop calculations.

6.1 Feynman Integrals & Sector Decomposition

A general scalar Feynman integral I in $D = 4 - 2\epsilon$ dimension with L loops and N propagators P_j, each raised to a power ν_j, can be written in momentum space as

$$I = \int_{-\infty}^{\infty} \prod_{l=1}^{L} \left[\mathrm{d}^D k_l\right] \frac{1}{\prod_{j=1}^{N} P_j^{\nu_j}}, \quad \text{where} \quad \left[\mathrm{d}^D k_l\right] = \frac{\mu^{4-D}}{i\pi^{\frac{D}{2}}} \mathrm{d}^D k_l, \qquad P_j = (q_j - m_j^2 + i\delta), \quad (6.131)$$

and q_j are linear combinations of external momenta p_i and loop momenta k_l. After introducing Feynman parameters the momentum integrals can be performed straightforwardly and the integral can be recast in the following form

$$I = (-1)^{N_\nu} \frac{\Gamma(N_\nu - LD/2)}{\prod_{j=1}^{N} \Gamma(\nu_j)} \int_0^\infty \prod_{j=1}^{N} \mathrm{d}x_j \; x_j^{\nu_j - 1} \delta(1 - \sum_{i=1}^{N} x_i) \frac{\mathcal{U}^{N_\nu - (L+1)D/2}(\vec{x})}{\mathcal{F}^{N_\nu - LD/2}(\vec{x}, s_{ij})}, \tag{6.132}$$

where the momentum integrals have been replaced by an N-fold parameter integral. Here $\mathcal{U}$ and $\mathcal{F}$ are the 1st and 2nd Symanzik polynomials, they are homogeneous polynomials in the Feynman parameters of degree L and $L+1$, respectively, and $N_\nu = \sum_j \nu_j$. The above procedure can be extended to support also Feynman integrals with tensor numerators. There are 3 possibilities for poles in the dimensional regulator ϵ to arise:

1. The overall $\Gamma(N_\nu - LD/2)$ can diverge, resulting in a single UV pole,
2. $\mathcal{U}(\vec{x})$ vanishes for some $x = 0$ and has a negative exponent, resulting in a UV sub-divergence,
3. $\mathcal{F}(\vec{x}, s_{ij})$ vanishes on the boundary and has a negative exponent, giving rise to an IR divergence.

After integrating out the δ-distribution and extracting a common factor of $(-1)^{N_\nu}\Gamma(N_\nu - LD/2)$ we are faced with integrals of the form

$$I_i = \int_0^1 \prod_{j=1}^{N-1} \mathrm{d}x_j x_j^{\nu_j - 1} \frac{\mathcal{U}_i(\vec{x})^{\mathrm{expo}\mathcal{U}(\epsilon)}}{\mathcal{F}_i(\vec{x}, s_{ij})^{\mathrm{expo}\mathcal{F}(\epsilon)}}. \tag{6.133}$$

The sector decomposition algorithm(s) aim to factorise, via integral transforms, the polynomials $\mathcal{U}_i$ and $\mathcal{F}_i$ (or more generally any product of polynomials $\mathcal{P}(\{x_j\})$) as products of a monomial and a polynomial with non-zero constant term, explicitly

$$\mathcal{P}(\{x_j\}) \to \prod_j x_j^{\alpha_j} \left(c + p(\{x_j\})\right), \tag{6.134}$$

where $\{x_j\}$ is the set of Feynman parameters, c is a constant and the polynomial p has no constant term. After this procedure, singularities in ϵ resulting from the region where one or more $x_j \to 0$ can appear only from the monomials $x_j^{\alpha_j}$. In this factorised form, the integrand can now be expanded in ϵ and the coefficients of the expansion can be numerically integrated, for an overview see [25].

If we consider only integrals for which the Mandelstam variables and masses can be chosen such that the $\mathcal{F}$ polynomial is positive semidefinite (i.e. with a Euclidean region), the above procedure is sufficient to render the integrals numerically integrable[†]. However, not all integrals of interest have a Euclidean region in this sense. Consider, for example, the three-point function depicted in Figure C.5 which appears in the two-loop electroweak corrections to the $Zb\bar{b}$ vertex [48, 49]. The $\mathcal{F}$ polynomial is given by,

$$\begin{aligned} \mathcal{F}/m_Z^2 &= x_3^2 x_5 + x_3^2 x_4 + x_2 x_3 x_5 + x_2 x_3 x_4 + x_1 x_3 x_5 + x_1 x_3 x_4 \\ &+ x_1 x_3^2 + x_1 x_2 x_3 + x_0 x_3 x_4 + x_0 x_3^2 + x_0 x_2 x_3 \\ &- x_1 x_2 x_4 - x_0 x_1 x_5 - x_0 x_1 x_4 - x_0 x_1 x_2 - x_0 x_1 x_3. \end{aligned} \tag{6.135}$$

[†]In the physical region such integrals may still require the integration contour to be deformed into the complex-plane in accordance with the causal $i\delta$ Feynman prescription [45–47].

where m_Z is the Z-boson mass and x_j are the Feynman parameters. Note that the massive propagator has the same mass as the external Z-boson which gives rise to terms in the $\mathcal{F}$ polynomial of differing sign regardless of the value chosen for m_Z.

After sector decomposition, integrals for which the $\mathcal{F}$ polynomial is not positive semidefinite can diverge not only as some $x_j \to 0$ but also as some $x_j \to 1$. One solution for dealing with such integrals is to split the integration domain in each Feynman parameter and then map the integration boundaries back to the unit hypercube such that the divergences at $x_j \to 1$ are mapped to divergences at $x_j \to 0$. Sector decomposition can then resolve the singularities at $x_j \to 0$ as usual. Such a splitting procedure was introduced in earlier versions of SecDec [50, 51], and also in Fiesta [42, 43].

However, prior to pySecDec [44], integrals were always split at $x_j = 1/2$ and, as shown in Ref. [52], this can again lead to problems if the $\mathcal{F}$ polynomial vanishes at this point (which happens to be the case for the polynomial in Eq. 6.135). The proposed solution in [52] was therefore to split the integrals at a random point, such that, if one run produces a problematic result, it is always possible to re-run the code and avoid a problematic split.

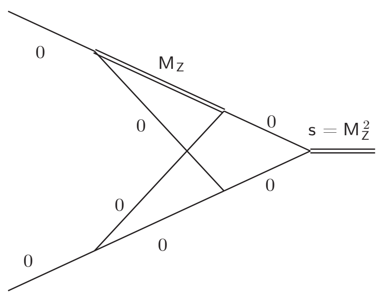

Fig. C.5: A $Zb\bar{b}$ vertex diagram with no Euclidean region and which can give rise to poorly convergent numerical integrals after sector decomposition. Figure taken from [49].

Alternatively, it is often possible to avoid having to evaluate such problematic integrals, as well as integrals that have poor numerical convergence properties, through the use of integration by parts identities (IBPs) [53, 54]. In particular, it is usually possible to express Feynman integrals in terms of a sum of (quasi-)finite integrals‡ with rational coefficients [55,56]. Typically, choosing a basis of (quasi-)finite integrals leads to significantly improved numerical properties, see for example [57]. The choice of a quasi-finite basis proved advantageous for the numerical evaluation of the $gg \to HH$ and $gg \to Hg$ amplitudes [34–36].

6.2 QMC Integration

The numerical integration of the sector decomposed finite integrals can be a computationally intensive process. One of the most widely used tools for numerical integration is the Cuba package [58, 59] which implements several different numerical integration routines relying on pseudo-random sampling, quasi-random sampling or cubature rules.

‡Here, quasi-finite integrals are integrals for which the overall $\Gamma(N_\nu - LD/2)$ can give rise to poles in ϵ but for which no poles arise from the integration over the $\mathcal{U}$ and $\mathcal{F}$ polynomials.

In the last few years, it was found that a particular type of Quasi-Monte-Carlo (QMC) integration based on Rank-1 Shifted Lattice (R1SL) rules has particularly good convergence properties for the numerical integration of Feynman parametrised integrals [60–62]. An unbiased R1SL estimate $\bar{Q}_{n,m}[f]$ of the integral $I[f]$ can be obtained from the following (QMC) cubature rule [63]:

$$I[f] \approx \bar{Q}_{n,m}[f] \equiv \frac{1}{m} \sum_{k=0}^{m-1} Q_n^{(k)}[f], \qquad Q_n^{(k)}[f] \equiv \frac{1}{n} \sum_{i=0}^{n-1} f\left(\left\{ \frac{i\mathbf{z}}{n} + \mathbf{\Delta}_k \right\}\right). \tag{6.136}$$

Here, the estimate of the integral depends on the number of lattice points n and the number of random shifts m. The generating vector $\mathbf{z} \in \mathbb{Z}^d$ is a fixed d-dimensional vector of integers coprime to n. The shift vectors $\mathbf{\Delta}_k \in [0,1)^d$ are d-dimensional vectors with components consisting of independent, uniformly distributed random real numbers in the interval $[0,1)$. Finally, the curly brackets indicate that the fractional part of each component is taken, such that all arguments of f remain in the interval $[0,1)$. An unbiased estimate of the mean-square error due to the numerical integration can be obtained by computing the variance of the different random shifts $Q_n^{(k)}[f]$.

The latest version of pySecDec provides a public implementation of a R1SL (QMC) integrator. The implementation is capable of performing numerical integration also on multiple CUDA compatible Graphics Processing Units (GPUs), which can accelerate the evaluation of the integrand significantly. The integrator, which is distributed as a header-only C++ library, can also be used as a standalone integration package [26]. The generating vectors distributed with the package are generated using the component-by-component (CBC) construction [64].

6.3 Summary and Outlook

We have presented new developments for the numerical calculation of multi-loop integrals, focusing on the sector decomposition approach in combination with Quasi-Monte-Carlo (QMC) integration. We described a new feature present in pySecDec, which allows to calculate integrals with special (non-Euclidean) kinematic configurations as they occur e.g. in electroweak two-loop corrections, which previously had shown poor convergence in SecDec 3. We also described a QMC integrator, developed in conjunction with pySecDec as well as for standalone usage, which can lead to considerably more accurate results in a given time compared to standard Monte Carlo integration. This integrator is also capable of utilising CUDA compatible Graphics Processing Units (GPUs).

In view of the need for high-precision calculations with many mass scales at future colliders, as they occur for example in electroweak corrections, numerical methods are a promising approach, and are being actively developed to best utilise recent progress in computing hardware. Several further developments towards the automation of numerical multi-loop calculations, with sector decomposition as an ingredient, could be envisaged. For example, to provide boundary conditions for numerical solutions to differential equations, along the lines of [29, 65], or for automated asymptotic expansions similar to [20, 66], or aiming at fully numerical evaluations of both virtual and real corrections.

Acknowledgements

We would like to thank Tom Zirke for his contributions to earlier versions of the code and Oliver Schulz for providing GPU computing support.

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