6 Numerical multiloop calculations: sector decomposition and QMC integration in pySecDec,

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The FCC-ee will allow the experimental uncertainties on several important observables, such as the electroweak precision observables (EWPOs), to be reduced by up to two orders of magnitude compared with the previous generation LEP and SLC experiments [1, 2]. To be able to best exploit this unprecedented boost in precision, it is also necessary 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 multiloop corrections. There has been very significant progress in this direction in recent years, ranging from purely analytic approaches [3–17] to semi-analytical 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 multiloop 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 numerically integrate the sector-decomposed loop integrals efficiently. Finally, in Section 6.3, we will give a short outlook for the field of numerical multiloop calculations.

6.1 Feynman integrals and sector decomposition

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

$$I = \int_{-\infty}^{\infty} \prod_{l=1}^{L} \left[\mathrm{d}^D k_l\right] \frac{1}{\prod_{j=1}^{N} P_j^{\nu_j}}, \quad \text{where} \quad \left[\mathrm{d}^D k_l\right] = \frac{\mu^{4-D}}{\mathrm{i}\pi^{\frac{D}{2}}} \mathrm{d}^D k_l, \qquad P_j = \left(q_j - m_j^2 + \mathrm{i}\delta\right), \quad (6.1)$$

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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 form

$$I = (-1)^{N_\nu} \frac{\Gamma(N_\nu - LD/2)}{\prod_{j=1}^{N} \Gamma(\nu_j)} \int_0^\infty \prod_{j=1}^{N} \mathrm{d}x_j \; x_j^{\nu_j - 1} \delta\left(1 - \sum_{i=1}^{N} x_i\right) \frac{\mathcal{U}^{N_\nu - (L+1)D/2}(\vec{x})}{\mathcal{F}^{N_\nu - LD/2}(\vec{x}, s_{ij}, m_j^2)}, \tag{6.2}$$

where the momentum integrals have been replaced by an N-fold parameter integral. Here, $\mathcal{U}$ and $\mathcal{F}$ are the first and second Symanzik polynomials; they are homogeneous polynomials in the Feynman parameters of degree L and $L+1$, respectively, and $N_\nu = \sum_j \nu_j$. This procedure can be extended to support Feynman integrals with tensor numerators. There are three possibilities of poles in the dimensional regulator ϵ arising.

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 subdivergence.
3. $\mathcal{F}(\vec{x}, s_{ij}, m_j^2)$ 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

$$I_i = \int_0^1 \prod_{j=1}^{N-1} \mathrm{d}x_j x_j^{\nu_j - 1} \frac{\mathcal{U}_i(\vec{x})^{\mathrm{expo}\mathcal{U}(\epsilon)}}{\mathcal{F}_i(\vec{x}, s_{ij}, m_j^2)^{\mathrm{expo}\mathcal{F}(\epsilon)}}. \tag{6.3}$$

The sector decomposition algorithms 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

$$\mathcal{P}(\{x_j\}) \to \prod_j x_j^{\alpha_j} \left(c + p(\{x_j\})\right), \tag{6.4}$$

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 Ref. [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), this 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 Fig. C.6.1, which appears in the two-loop electroweak corrections to the $\mathrm{Zb\bar{b}}$ vertex [48,49]. The $\mathcal{F}$ polynomial is given by

$\mathcal{F}/m_{\mathrm{Z}}^2$

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

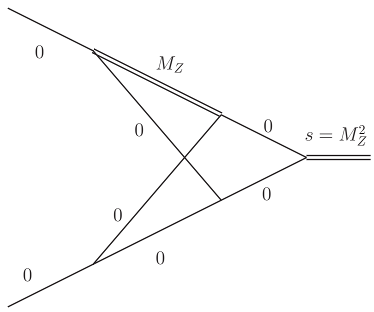

Fig. C.6.1: A Zb$\bar{\text{b}}$ vertex diagram with no Euclidean region, which can give rise to poorly convergent numerical integrals after sector decomposition. Figure taken from Ref. [49].

$$= x_3^2x_5 + x_3^2x_4 + x_2x_3x_5 + x_2x_3x_4 + x_1x_3x_5 + x_1x_3x_4 + x_1x_3^2 + x_1x_2x_3 + x_0x_3x_4 + x_0x_3^2 + x_0x_2x_3 - x_1x_2x_4 - x_0x_1x_5 - x_0x_1x_4 - x_0x_1x_2 - x_0x_1x_3\,, \quad (6.5)$$

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. (6.5)). The proposed solution in Ref. [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 rerun the code and avoid a problematic split.

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, Ref. [57]. The choice of a quasi-finite basis proved advantageous for the numerical evaluation of the gg → HH and gg → Hg amplitudes [34–36].

6.2 Quasi-Monte Carlo integration

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 parametrized 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]:

$$I[f] \approx \bar{Q}_{n,m}[f] \equiv \frac{1}{m} \sum_{k=0}^{m-1} Q_n^{(k)}[f], \qquad Q_n^{(k)}[f] \equiv \frac{1}{n} \sum_{i=0}^{n-1} f\left(\left\{\frac{i\mathbf{z}}{n} + \mathbf{\Delta}_k\right\}\right). \tag{6.6}$$

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 also capable of performing numerical integration on a number of CUDA-compatible graphics processing units (GPUs), which can significantly accelerate the evaluation of the integrand. The integrator, which is distributed as a header-only C++ library, can also be used as a stand-alone integration package [26]. The generating vectors distributed with the package are generated using the component-by-component construction [64].

6.3 Summary and outlook

We have presented new developments for the numerical calculation of multiloop 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 integrals with special (non-Euclidean) kinematic configurations to be calculated 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 stand-alone usage, which can lead to considerably more accurate results in a given time compared with 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 actively being developed to best utilise recent progress in computing hardware. Several further developments towards the automation of numerical multiloop 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 Refs. [29, 65], for automated asymptotic expansions, similar to Refs. [20, 66], or aiming at fully numerical evaluations of both virtual and real corrections.

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