Advances in computational methods for Quantum Field Theory calculations

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1 INTRODUCTION

Understanding how Nature works on a fundamental level is one of the key goals of physics. Consequently, physicists try to identify what the smallest building blocks of our universe are and how they interact. The ideas about these fundamental building blocks have undergone many revolutions, each radically changing the way we describe Nature.

The ancients reasoned that all objects were composed of the elements fire, earth, water, and air. As technology progressed, scientists discovered cells, molecules, and atoms. Atoms only have a radius of about 30 trillionths of a meter. For a while it was believed that the atom was the smallest component (the Greek name means *indivisible*). This idea lasted until the early 20th century with the discoveries of the electron and proton. Six decades later, it turned out that even protons and neutrons were not fundamental, but consisted of quarks [15, 16].

From the invention of quantum mechanics in the early 1920s, it became clear that these small particles behave differently from everyday experience: particles could be in two places at once, act like waves, or spontaneously emerge from the vacuum, and quickly disappear again [17]. The fact that the fundamental building blocks had both particle-like and wave-like features was later unified by the framework of Quantum Field Theory (QFT) [18]. The new quantum field theoretic description of the electromagnetic interaction, Quantum Electrodynamics (QED), was hugely successful and is still used to this day.

Below we provide a brief introduction to the world of QFT. We describe the Standard Model in section 1.1, the aim for precise predictions in section 1.2, computer methods in section 1.3, and Feynman diagrams in section 1.4. Then we formulate our Problem Statement (PS) in section 1.5, and the Research Questions (RQs) in section 1.6. In section 1.7 we list our contributions and in section 1.8 we outline the structure of the thesis.

1.1 THE STANDARD MODEL

In the early 1960s, the first version of the Standard Model was constructed [19]. The goal was to capture all fundamental particles and interactions in this model. The first version contained several particles, such as quarks and electrons, and the electromagnetic and weak forces. The electromagnetic force governs the interactions of photons (light) with charged particles. The weak forces govern nuclear decay and are mediated by the W and Z bosons. The Higgs boson, which is responsible for giving elementary particles mass, was added to the model shortly after, in 1964 [20–22]. Finally, the strong force, mediated by gluons, was added in 1973 [23, 24]. The theory for the strong interaction, Quantum Chromodynamics (QCD), explained why quarks of opposite charge can stay in a stable configuration in the nucleus of an

atom. In figure 1 the modern-day Standard Model is displayed [25]. It contains six quarks, six leptons, and four force carriers. The shading signifies which particles are susceptible to which force. All non-fundamental particles in the universe are composed of these quarks. For example, the proton, which is part of the core of an atom, consists of two up quarks and a down quark.

The theories behind the Standard Model describe many properties of the particles, such as their charge and spin, and whether they have mass. However, the actual mass is not predicted by the Standard Model and has to be experimentally determined.

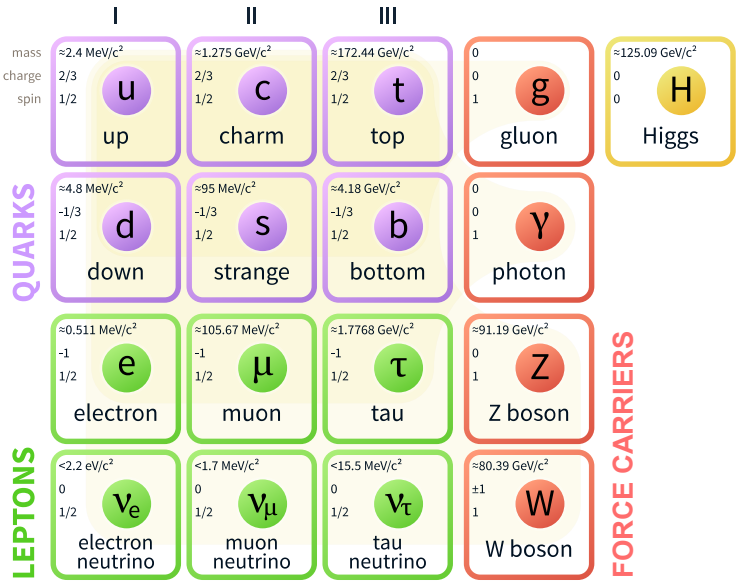


Figure 1: The Standard Model of elementary particles [25]. It contains 6 quarks and 6 leptons. The gluon is the force carrier of the strong force, the photon of the electromagnetic force, and Z/W bosons of the weak force. The shading signifies which particles are involved with which force. The Higgs particle is responsible for the mass of all massive particles.

Most features of the Standard Model are measured in particle accelerators, such as the Large Hadron Collider (LHC) [26]. At the LHC clusters of protons are accelerated in opposite directions in a 27 km long circular tunnel to almost the speed of light and are made to collide. From the energy of the collisions, new particles may be created, which are measured by detectors.

Over the last decades, many measurements have been performed that confirm the successful match of the Standard Model with Nature. The most famous measurement is the discovery of the Higgs boson in 2012 at the LHC [27, 28]. A second impressive measurement is the value of the fine-structure constant [29, 30] which governs the strength of the electromagnetic interaction. Theory and experiment are in agreement

to within ten parts per billion. This staggering precision constitutes one of the best predictions of mankind.

1.2 PRECISE PREDICTIONS

The Standard Model is extremely successful and has remained virtually unmodified for the last thirty years. So far, there have been no measurements that conclusively contradict the Standard Model. However, we know that it cannot be the final model, since it for instance does not include gravity or explain dark matter. The question then arises: how can we find physics beyond the Standard Model if we do not find discrepancies?

One of the reasons why experiments at the LHC may not find discrepancies is that the effects of new physics may only change the results of high-energy scattering experiments by a tiny fraction. For gravity this scenario is likely, since quantum gravity effects are believed to occur at the Planck scale, which is 10^{15} times higher than the energy that the LHC can produce. For dark matter, some candidates derived from Supersymmetry could be measured by the LHC, and those would lead to small discrepancies.

Therefore, extremely precise predictions are imperative to detect minuscule differences between what is expected and what is observed. Obtaining precise predictions will be the subject of the thesis.

1.3 COMPUTER METHODS

Precise predictions are hard to compute by hand, since performing the algebra is a laborious exercise. With the rise of computers in the 1960s, software started to be developed to perform calculations for quantum field theories.

In 1963 the computer program SCHOONSCHIP was created by Veltman for the symbolic computation of the early Standard Model [31]. The program had to process an expression with 50 000 terms, which at the time could only be done by storing intermediate results on tape.

The development of the symbolic manipulation toolkit FORM was started in 1984. It was designed to efficiently handle large expressions. A notable package was MINCER, originally developed for SCHOONSCHIP [32] and later ported to FORM [33]. Using MINCER and FORM, the evolution of unpolarized combinations of quark densities has been computed to next-to-next-to-leading order [34, 35].

Computer methods were also developed for numerical integration, which for complicated integrals is almost impossible to do by hand. Monte Carlo integrators, such as the popular VEGAS [36] program, became the preferred way to compute complicated scattering processes.

The fields of computer algebra and particle physics have developed hand in hand. Even though new computational methods have been designed and the hardware has had spectacular improvements, combinatorial and algorithmic challenges have not

disappeared due to the need for more precision. In the 1960s a calculation involving proton interactions was considered a success if the order of magnitude agreed with the experiment. Nowadays, the goal is to achieve 1% accuracy. As a result, we will encounter expressions with billions of terms, taking up more than a terabyte of memory.

We are going to study some of these computational challenges. First, we will have a slightly more detailed look at the objects that we wish to compute.

1.4 FEYNMAN DIAGRAMS

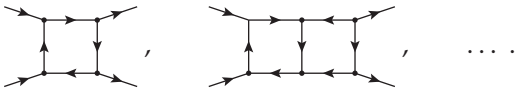
In particle colliders such as the LHC, fast moving protons collide with each other. The new particles that are created are measured by detectors. Quantum Chromodynamics is the theory that describes these collisions, in the same way that Newton's equations describe how two macroscopic objects collide [37].

In Quantum Chromodynamics, a scattering process can be described in pictures called Feynman diagrams [38]. An example of a Feynman diagram is

(1)

which signifies a process where two initial-state particles annihilate, creating a new particle, which then splits up into two new particles. Each particle is represented by a line, and each interaction by a vertex (a point where lines meet). The arrows represent whether the particle is moving to or from a vertex. The two final-state particles are measured by a detector.

One could imagine many more diagrams with two particles in the initial state and two in the final state. For example:



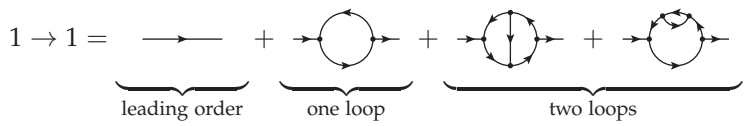
(2)

Each diagram with more particles (edges), more interactions (vertices), and more loops describes a more intricate process. From the rules of quantum mechanics, we know that in order to describe a scattering process, we need to take into account *all* the interactions that could happen in between [39]. This implies that we need to compute an infinite series of Feynman diagrams.

Computing the infinite series up to a certain number of loops leads to a reasonable estimate (i.e., the problem is suitable for perturbation theory). This is due to the fact that every interaction is suppressed by the interaction strength, called the 'coupling constant', which is smaller than one. Every diagram with the same number of loops has the same suppression factor. Contrary to what its name suggests, the coupling

constant is actually dependent on the energy of the collision. For low-energy QED, the coupling constant is about $1/137$. For the experimentally viable energies of QCD, the coupling constant varies from 0.1 to 0.3. Consequently, for a two-loop process the relative suppression of QED over QCD is 10^4, which means that for QCD more diagrams have to be computed to obtain the same accuracy as for QED.

Below we consider a single particle moving in space-time (1 in and 1 out) expanded up to two loops:



(3)

The number of possible diagrams increases exponentially with the number of loops. By simply constructing all possible graphs with vertices of degree three (where we enforce that a graph remains connected when one edge is removed), we see that at two loops we have two diagrams and at four loops 95 diagrams. If we also allow vertices with degree four, the number of diagrams at four loops is 1536.

For one-to-one reactions in QCD, the state-of-the-art is currently at four and five loop accuracy [2, 4, 40, 41]. For processes in QCD, each particle in the diagram could be of a different type (quark, gluon, etc.), which makes the number of diagrams much higher. Additionally, each individual diagram represents many fundamental integrals (also called scalar integrals). For example, at five loop accuracy one difficult diagram of the gluon propagator (with 160 500 diagrams) generates twelve million scalar integrals. This is an enormous number, which demands carefully constructed algorithms to be able to get an answer without running out of memory or time.

Having thus described the field of my research, we are now ready to state the overall problem statement of this thesis.

1.5 PROBLEM STATEMENT

Achieving higher precision, and thus going to a higher number of loops, creates at least three computational challenges: (1) billions of terms may be created, (2) the terms themselves may get large coefficients (fractions with more than a hundred digits), and (3) for some Feynman diagrams it is unknown how to compute them within a few months (or at all).

As we have reasoned in section 1.2, precise predictions are necessary to advance our understanding of Nature, which means these challenges have to be overcome. We now formulate our problem statement.

> **Problem statement:** *In what way can we improve the performance of QFT calculations with respect to obtaining more precise predictions?*

In this research we focus on three computational and combinatorial problems of QFT calculations that we deemed the most urgent ones.

Problem 1 Slowness of Monte Carlo integrations.

Monte Carlo integrators often take months on modern supercomputers to obtain high-quality results. This is caused by the large size of the input expression.

Problem 2 Slowness in the computation of massless propagator integrals.

Current methods based on Laporta-style algorithms [42] are notoriously slow. Often computations run for months or years on clusters with more than forty workstations.

Problem 3 Slowness when computing the singular parts of Feynman diagrams.

Computing the singular parts (poles) of diagrams is generally easier than computing the finite pieces. There exists a complicated R^* method that is not used often, in part due to combinatorial blow-up.

Below we derive three research questions, one for each problem.

1.6 THREE RESEARCH QUESTIONS

PROBLEM 1 Monte Carlo methods are frequently used in QFT calculations, since some integrals cannot be computed analytically. After the integrals are rewritten to a suitable polynomial representation, they are sampled millions of times. Some of these polynomials will have more than twenty variables and hundreds of thousands of terms, making evaluation very slow. Simplification of these polynomials will speed up integration. Thus, the first research question is as follows.

> **Research question 1 (RQ1):** *To what extent can the number of arithmetic operations of large multivariate polynomials be reduced?*

PROBLEM 2 Most integrals that can be computed analytically, are calculated by using Integration by Parts (IBP) identities to express integrals into simpler ones [43]. This method is generally quite slow and often requires months of computation time on a cluster. The MINCER program for three-loop massless propagator diagrams solves the IBP systems in a parametric way, which is more difficult to construct, but yields faster reductions [32, 33]. A four-loop equivalent of MINCER would mean that computations that currently take months, could be done in hours. Hence, our second research question reads as follows.

> **Research question 2 (RQ2):** *How can we construct a program that can compute four-loop massless propagator integrals more efficiently?*

PROBLEM 3 For five-loop calculations in QCD, so far only the poles of integrals have been computed, as the finite pieces are too difficult [40, 44]. There are several methods involving infrared rearrangement that allows one to compute the poles of five-loop integrals using only four-loop integral computations. One of these is the

R^*-operation [45], which is complicated and quite slow. Hence, we formulate our third research question as follows.

> **Research question 3 (RQ3):** *To what extent can we compute the poles of five-loop diagrams using only four-loop diagrams more efficiently?*

1.7 Research methodology and four contributions

The four main contributions of this thesis are listed below. After each bullet, we summarise the research methodology.

- The improvement of expression simplification for large expressions.

  We provide an algorithm that simplifies large expressions faster than the state-of-the-art and with slightly improved quality. The simplifications result in a speed-up of Monte Carlo integrations [11].

- The construction of Forcer, a program to compute massless four-loop propagators.

  The Forcer program has already been used in many large calculations, including the computation of four-loop Mellin moments of structure functions. These quantities are important ingredients for processes such as Higgs production at the LHC. So far, the calculations of these objects could not be performed in a reasonable amount of time by any other existing program [1].

- The generalisation of the R^*-operation to integrals with generic numerator structure.

  The R^*-operation can be used to compute the poles of Feynman diagrams using an infrared-rearranged version of the diagram. We have extended the R^*-operation to include Feynman diagrams with arbitrary numerator structure, which makes the method more suitable for practical use. We have written a computer code that can compute the poles of five-loop massless propagator diagrams efficiently [3].

- The computation of the five-loop beta function for Yang-Mills theory with fermions.

  The five-loop beta function of QCD describes how the strength of the strong coupling evolves with the energy scale. Precise determination is relevant for many processes, as well as for studying theoretical properties of QFTs. We have verified the QCD beta function presented in [40] and generalized the result to an arbitrary colour group. Our more general computation took only six days on a single 32-core machine using the methods developed in this thesis [4]. The computation in [40] took 1.5 years on 20 computers with 8 cores each.

1.8 STRUCTURE OF THE THESIS

In chapter 1 we formulated the problem statement, stated the three research questions, and alluded to the contributions of this thesis. In chapter 2 we will address **RQ1**. Chapter 3 is devoted to **RQ2**. Next, chapter 4 shows new four-loop results, obtained by answering **RQ2**. Chapter 5 addresses **RQ3**. Finally, in chapter 6 we compute the five-loop beta function for Yang-Mills theory with fermions, which was only possible by using the methods developed to answer **RQ2** and **RQ3**.