# Advances in computational methods for Quantum Field Theory calculations

Ruijl, B.J.G.

## SUMMARY

One of the primary goals of physics is to understand what the fundamental properties of Nature are. A highly successful tool to achieve this is Quantum Field Theory (QFT), which describes the interactions of indivisible particles. Built on the QFT framework, the Standard Model is the current best theory of the fundamental structure of Nature. Physics beyond the Standard Model will likely only lead to small deviations of the outcome of collisions in particle accelerators. Thus, very accurate predictions have to be made to detect new physics. This thesis will study the computational problems that arise when trying to improve precision.

In chapter 1 we define the research questions and the problem statement.

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

We focus on three computational and combinatorial problems of QFT calculations that we deemed the most urgent ones: (1) slowness of Monte Carlo integrations, (2) slowness in the computation of massless propagator integrals, and (3) slowness when computing the poles of Feynman diagrams.

PROBLEM 1 Monte Carlo methods are frequently used in QFT calculations. After the integrals are rewritten to a suitable polynomial representation, they are sampled millions of times. Some of these polynomials have more than a hundred thousand terms, making evaluation very slow. Thus, the first research question is as follows.

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

In chapter 2 we investigate ways to simplify expressions, using Horner schemes and Common Subexpression Elimination (CSEE). Our approach applies Monte Carlo Tree Search (MCTS), a search procedure that has been successful in AI. We use it to find near-optimal Horner schemes. Although MCTS finds good solutions, this approach gives rise to two further challenges. (1) MCTS (with UCT) introduces a constant, $C_p$ that governs the balance between exploration and exploitation. This constant has to be tuned manually. (2) There should be more guided exploration at the bottom of the tree, since the current approach reduces the quality of the solution towards the end of the expression. To address both issues, we investigate NMCS (Nested Monte Carlo Search), but find that NMCS is computationally infeasible for our problem. Then, we modify the UCT formula by introducing a dynamic exploration-exploitation parameter $T$ that decreases linearly with the iteration number. Consequently, we provide a performance analysis. We observe that a variable $C_p$ solves the two problems: it yields more exploration at the bottom and as a result the tuning problem has been simplified. The region in $C_p$ for which good values are found is increased by more than a tenfold.

Next, we consider Stochastic Local Search methods, since these methods do not have the problem of performing little optimisation in the order of the final variables. We investigate the state space properties of Horner schemes and find that the domain is relatively flat and contains only a few local minima. As a result, the Horner space is appropriate to be explored by Stochastic Hill Climbing (SHC), which has only two parameters: the number of iterations (computation time) and the neighbourhood structure. We find a suitable neighbourhood structure, leaving only the allowed computation time as a parameter. We perform a range of experiments. The results obtained by SHC are similar or better than those obtained by MCTS, which means that the number of operations is at least an order of magnitude smaller than the input. Furthermore, we show that SHC obtains the good results at least 10 times faster. Since the evaluation time of Monte Carlo integrators is proportional to the number of operations, their performance is improved.

PROBLEM 2 Most integrals that can be computed analytically, are calculated by using Integration by Parts (IBP) identities to express integrals into simpler ones. This method is generally quite slow and often requires months of computation time on a cluster. Hence, our second research question reads as follows.

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

In chapter 3, we explain the construction of FORCER, a FORM program for the reduction of four-loop massless propagator-type integrals to master integrals. The resulting program performs parametric IBP reductions similar to the three-loop MINCER program. We show how one can solve many systems of IBP identities parametrically in a computer-assisted manner. Next, we discuss the structure of the FORCER program, which involves recognizing reduction actions for each topology, applying symmetries, and transitioning between topologies after edges have been removed. This part is entirely precomputed and automatically generated. We give examples of recent applications of FORCER, and study the performance of the program. We show that the four-loop beta function can be computed in three minutes on a 32-core machine. Finally, we demonstrate how to use the FORCER package and sketch how to prepare physical diagrams for evaluation by FORCER.

In chapter 4 we have computed the self-energies and a set of three-particle vertex functions for massless QCD at the four-loop level in the $\overline{\text{MS}}$ renormalisation scheme, using the FORCER program. The vertex functions are evaluated at points where one of the momenta vanishes. Analytical results are obtained for a generic gauge group and with the full gauge dependence, which was made possible by extensive use of the FORCER program for massless four-loop propagator integrals. The bare results in dimensional regularisation are provided in terms of master integrals and rational coefficients; the latter are exact in any space-time dimension. Our results can be used for further precision investigations of the perturbative behaviour of the theory in schemes other than $\overline{\text{MS}}$.

Additionally, we compute Mellin moments of four-loop splitting functions and coefficient functions. These are used as basic ingredients for collision processes, such as Higgs production. We compute Mellin moments $N = 2, 4, 6$ for the non-singlet case and $N = 2, 4$ for the singlet case. Furthermore, we calculate $N = 1, 3, 5$ of vector-axial interference $F_3$. By computing to $N = 40$ and beyond, we reconstruct the all-$N$ $n_f^2$ contribution to the four-loop non-singlet splitting function and the $n_f^3$ contribution to the four-loop singlet splitting function. Using the OPE method, we calculate up to $N = 16$ for the non-singlet splitting function. For the large-$n_c$ limit, we compute up to $N = 19$. This allows for an all-$N$ reconstruction and yields a new term to the four-loop planar cusp anomalous dimension.

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. One way to compute the poles is with the $R^*$-operation, which is complicated and quite slow. Hence, we formulate our third research question as follows.

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

In chapter 5 we extend the $R^*$-operation to Feynman graphs with arbitrary numerators, including tensors. We also provide a novel way of defining infrared counterterms which closely resembles the definition of its ultraviolet counterpart. We further express both infrared and ultraviolet counterterms in terms of scaleless vacuum graphs with a logarithmic degree of divergence. By exploiting symmetries, integrand and integral relations, which the counterterms of scaleless vacuum graphs satisfy, we can vastly reduce their number and complexity. A FORM implementation of this method was used to compute the poles in the dimensional regulator of all top-level propagator graphs at five loops in four dimensional $\phi^3$ theory.

In chapter 6 we compute the five-loop corrections to the scale dependence of the renormalised coupling constant (the beta function) for QCD, its generalisation to non-Abelian gauge theories with a simple compact Lie group, and for QED. Our analytical result, obtained using the background field method, infrared rearrangement via the new diagram-by-diagram implementation of the $R^*$-operation and the FORCER program for massless four-loop propagators, confirms the QCD and QED results obtained by only one group before. The numerical size of the five-loop corrections is briefly discussed in the standard $\overline{\text{MS}}$ scheme for QCD with $n_f$ flavours and for pure SU($N$) Yang-Mills theory. Their effect in QCD is much smaller than the four-loop contributions, even at rather low scales. Additionally, we derive the five-loop beta function in a relatively common alternative, the minimal momentum subtraction (MiniMOM) scheme using the propagators and vertices computed in chapter 4. The computation of the five-loop beta function took six days on a 32-core machine.

CONCLUSION Finally, in chapter 7 we again consider the problem statement and research questions. Based on our findings, we may conclude that we have improved the performance of QFT calculations in three different regions. Since all our methods can be applied in practice to compare theory to experiment in colliders, we conclude that we have improved the precision of predictions.