



Universiteit  
Leiden  
The Netherlands

## **Advances in computational methods for Quantum Field Theory calculations**

Ruijl, B.J.G.

### **Citation**

Ruijl, B. J. G. (2017, November 2). *Advances in computational methods for Quantum Field Theory calculations*. Retrieved from <https://hdl.handle.net/1887/59455>

Version: Not Applicable (or Unknown)

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/59455>

**Note:** To cite this publication please use the final published version (if applicable).

Cover Page



Universiteit Leiden



The following handle holds various files of this Leiden University dissertation:

<http://hdl.handle.net/1887/59455>

**Author:** Ruijl, B.J.G.

**Title:** Advances in computational methods for Quantum Field Theory calculations

**Issue Date:** 2017-11-02

# **Advances in computational methods for Quantum Field Theory calculations**

Ben Ruijl

ISBN: 978-94-6233-746-6  
Printed by: Gildeprint, Enschede  
Cover: thesisexpert.nl



Universiteit  
Leiden



SIKS Dissertation Series No. 2017-31. The research reported in this thesis has been carried out under the auspices of SIKS, the Dutch Research School for Information and Knowledge Systems.

This work is supported by the ERC Advanced Grant no. 320651, "HEPGAME".

# Advances in computational methods for Quantum Field Theory calculations

Proefschrift

ter verkrijging van  
de graad van Doctor aan de Universiteit Leiden,  
op gezag van Rector Magnificus prof. mr. C.J.J.M. Stolker,  
volgens besluit van het College voor Promoties  
te verdedigen op donderdag 2 november 2017  
klokke 15.00 uur

door

Ben Jacobus Gertruda Ruijl

geboren te Geleen  
in 1989

Promotores: Prof. dr. H.J. van den Herik

Prof. dr. A. Plaat

Co-promotor: dr. J.A.M. Vermaseren (Nikhef)

Promotiecommissie: Prof. dr. J.N. Kok

Prof. dr. A. Achúcarro

Prof. dr. H.H. Hoos

Prof. dr. J.W. van Holten

Prof. dr. C. Anastasiou (ETH Zürich)

Prof. dr. E.L.P.M. Laenen (Universiteit van Amsterdam)

Prof. dr. A. Vogt (University of Liverpool)

dr. G. Heinrich (MPP München)

Isn't it a noble, an enlightened way of spending our brief time in the sun,  
to work at understanding the universe and how we have come to wake  
up in it?

Richard Dawkins





## PREFACE

---

This PhD thesis is the result of work I performed as part of the HEPGAME (High Energy Physics and Games) project. The HEPGAME project is supported by the ERC Advanced Grant no. 320651 and its primary goal is to apply methods from artificial intelligence to solve problems in high energy physics. The symbolic manipulation toolkit FORM plays a key role in the investigation.

During the PhD I worked in three different locations. The first half year I mostly worked at Tilburg University. The next few years I have worked at Leiden University and Nikhef. At Leiden University, I taught a course, supervised a student, and worked on the computer science aspect of this thesis with my close colleagues Jaap van den Herik, Aske Plaat, and Ali Mirsoleimani. This mainly involved expression simplification, which turned into chapter 2.

At Nikhef, I focused on physics, and worked on designing computer programs with my close colleagues Jos Vermaseren and Takahiro Ueda. This resulted in the FORCER program, described in chapter 3. Later, Andreas Vogt joined to compute new physical quantities with FORCER. The results formed the basis of chapter 4.

Together with Franz Herzog we decided to aim for something we had not thought possible: computing the five-loop beta function. After a year of puzzling, we understood the  $R^*$ -method which could help us achieve our goal. The method is explained in chapter 5.

Finally, after combining the FORCER program and the computer code for the  $R^*$ -method, we were able to compute the five-loop beta function for Yang-Mills theory with fermions. This formed the basis for chapter 6.

I have had the pleasure to work with experts in the fields of Artificial Intelligence, Computer Science, and Theoretical Physics. This enriching experience has helped shape this thesis, for which I am grateful.



## LIST OF ABBREVIATIONS

---

|        |                                                                                                                                                                         |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| CSEE   | Common Subexpression Elimination 11–15, 17, 35, 38                                                                                                                      |
| HEP    | High Energy Physics 15, 16, 18–21, 24, 26–36                                                                                                                            |
| IBP    | Integration by Parts 8, 39, 40, 42, 43, 45, 46, 48, 49, 52–55, 59, 60, 103, 128, 147, 161, 190                                                                          |
| IR     | Infrared 85, 103–110, 113, 118–127, 129–135, 181, 187, 188                                                                                                              |
| IRR    | Infrared Rearrangement 104, 118                                                                                                                                         |
| LHC    | Large Hadron Collider 4–6, 9, 39                                                                                                                                        |
| LTVG   | Logarithmic Tensor Vacuum Graph 105, 120, 123, 125, 127, 128, 133, 135                                                                                                  |
| MCTS   | Monte Carlo Tree Search 11, 12, 16–22, 35–37, 61, 161, 189, 190                                                                                                         |
| QCD    | Quantum Chromodynamics 3, 7–9, 39, 41, 80–82, 85–87, 90, 95, 97, 101, 104, 105, 114, 115, 129, 130, 135, 137, 138, 146, 150, 151, 153–157, 159, 160, 162, 190, 191, 195 |
| QED    | Quantum Electrodynamics 3, 7, 87, 137, 150–152, 159, 191, 195                                                                                                           |
| QFT    | Quantum Field Theory 3, 7–9, 39, 95, 103, 104, 129, 162, 189, 192                                                                                                       |
| SA     | Simulated Annealing 22, 25–27, 32–34                                                                                                                                    |
| SA-UCT | Simulated Annealing - UCT 11, 12, 16, 18, 21–24, 36                                                                                                                     |
| SDD    | Superficial Degree of Divergence 106, 116, 118, 120–123, 126, 129, 133                                                                                                  |
| SHC    | Stochastic Hill Climbing 22, 25–28, 30–37, 190                                                                                                                          |
| UCT    | Upper Confidence bounds applied to Trees 11, 16, 17, 20–24, 36, 189                                                                                                     |
| UV     | Ultraviolet 103–109, 111, 113, 115, 118–135, 139, 185, 187, 188                                                                                                         |



# CONTENTS

---

|                                                                 |     |
|-----------------------------------------------------------------|-----|
| PREFACE                                                         | vii |
| LIST OF ABBREVIATIONS                                           | ix  |
| 1 INTRODUCTION                                                  | 3   |
| 1.1 The Standard Model . . . . .                                | 3   |
| 1.2 Precise predictions . . . . .                               | 5   |
| 1.3 Computer methods . . . . .                                  | 5   |
| 1.4 Feynman diagrams . . . . .                                  | 6   |
| 1.5 Problem statement . . . . .                                 | 7   |
| 1.6 Three research questions . . . . .                          | 8   |
| 1.7 Research methodology and four contributions . . . . .       | 9   |
| 1.8 Structure of the thesis . . . . .                           | 10  |
| 2 EXPRESSION SIMPLIFICATION                                     | 11  |
| 2.1 Horner schemes and common subexpression elimination . . . . | 12  |
| 2.1.1 Horner Schemes . . . . .                                  | 12  |
| 2.1.2 Common subexpression elimination . . . . .                | 13  |
| 2.1.3 The evaluation function . . . . .                         | 13  |
| 2.1.4 Interplay . . . . .                                       | 14  |
| 2.2 Experimental setup . . . . .                                | 15  |
| 2.3 Tree search methods . . . . .                               | 16  |
| 2.3.1 Monte Carlo Tree Search . . . . .                         | 16  |
| 2.3.2 Nested Monte Carlo Search . . . . .                       | 19  |
| 2.3.3 SA-UCT . . . . .                                          | 20  |
| 2.4 Stochastic Local Search . . . . .                           | 22  |
| 2.4.1 SHC versus SA . . . . .                                   | 22  |
| 2.4.2 Neighbourhood structure . . . . .                         | 27  |
| 2.4.3 Two state space properties . . . . .                      | 31  |
| 2.5 Performance of SHC vs. MCTS . . . . .                       | 35  |
| 2.6 Chapter conclusion . . . . .                                | 36  |
| 2.6.1 Findings and conclusions . . . . .                        | 37  |
| 2.6.2 Future research . . . . .                                 | 37  |
| 3 FOUR LOOP FEYNMAN DIAGRAM CALCULATIONS                        | 39  |
| 3.1 Generalised Feynman diagrams . . . . .                      | 40  |
| 3.2 Integration of one-loop two-point functions . . . . .       | 42  |
| 3.3 Carpet rule . . . . .                                       | 43  |
| 3.4 Integration by parts . . . . .                              | 45  |
| 3.4.1 The rule of the triangle . . . . .                        | 46  |
| 3.4.2 The rule of the diamond . . . . .                         | 47  |
| 3.4.3 Custom solutions . . . . .                                | 52  |

|        |                                                                   |     |
|--------|-------------------------------------------------------------------|-----|
| 3.5    | Solving parametric IBP identities by heuristics . . . . .         | 53  |
| 3.5.1  | Heuristics and equation generation . . . . .                      | 54  |
| 3.5.2  | Reduction rules beyond $S_0$ . . . . .                            | 55  |
| 3.5.3  | Identities for topologies with insertions . . . . .               | 59  |
| 3.5.4  | Solving strategy . . . . .                                        | 60  |
| 3.6    | The 21 topologies that need custom reductions . . . . .           | 61  |
| 3.7    | The FORCER framework . . . . .                                    | 66  |
| 3.7.1  | Reduction graph generation . . . . .                              | 66  |
| 3.7.2  | Reduction graph execution . . . . .                               | 69  |
| 3.7.3  | Example . . . . .                                                 | 69  |
| 3.8    | Usage . . . . .                                                   | 72  |
| 3.9    | Expansions . . . . .                                              | 73  |
| 3.10   | From physical diagrams to FORCER . . . . .                        | 74  |
| 3.10.1 | Self-energy filtering . . . . .                                   | 77  |
| 3.10.2 | Colour split-off . . . . .                                        | 78  |
| 3.10.3 | Diagram database . . . . .                                        | 79  |
| 3.10.4 | Momentum substitutions . . . . .                                  | 79  |
| 3.11   | Examples and performance . . . . .                                | 80  |
| 3.12   | Chapter conclusion . . . . .                                      | 83  |
| 3.12.1 | Findings and main conclusion . . . . .                            | 83  |
| 3.12.2 | Future research . . . . .                                         | 83  |
| 4      | RESULTS FOR FOUR-LOOP COMPUTATIONS . . . . .                      | 85  |
| 4.1    | Group notations . . . . .                                         | 86  |
| 4.2    | Propagators and vertices . . . . .                                | 87  |
| 4.2.1  | Self energies . . . . .                                           | 87  |
| 4.2.2  | Triple-gluon vertex . . . . .                                     | 88  |
| 4.2.3  | Ghost-gluon vertex . . . . .                                      | 89  |
| 4.2.4  | Quark-gluon vertex . . . . .                                      | 90  |
| 4.2.5  | Renormalisation . . . . .                                         | 90  |
| 4.2.6  | Anomalous dimensions . . . . .                                    | 92  |
| 4.2.7  | Computations and checks . . . . .                                 | 93  |
| 4.3    | Splitting functions and coefficient functions . . . . .           | 94  |
| 4.3.1  | Optical theorem method . . . . .                                  | 96  |
| 4.3.2  | Operator method . . . . .                                         | 97  |
| 4.3.3  | Axial vector current . . . . .                                    | 98  |
| 4.4    | Chapter conclusion . . . . .                                      | 101 |
| 4.4.1  | Findings and main conclusion . . . . .                            | 101 |
| 4.4.2  | Future research . . . . .                                         | 102 |
| 5      | INFRARED REARRANGEMENT . . . . .                                  | 103 |
| 5.1    | Divergences in Euclidean non-exceptional Feynman graphs . . . . . | 105 |
| 5.1.1  | UV divergences in Feynman graphs . . . . .                        | 106 |
| 5.1.2  | IR divergences in Feynman graphs . . . . .                        | 107 |

|       |                                                                   |     |
|-------|-------------------------------------------------------------------|-----|
| 5.2   | The R-operation in the MS-scheme . . . . .                        | 110 |
| 5.2.1 | Definition of the R-operation in the MS-scheme . . . . .          | 111 |
| 5.2.2 | Examples of R-operations . . . . .                                | 113 |
| 5.3   | The R-operation for generic Feynman graphs in MS . . . . .        | 114 |
| 5.3.1 | Contraction anomalies and tensor reduction . . . . .              | 116 |
| 5.3.2 | Contraction anomalies and counterterm factorisation . . . . .     | 117 |
| 5.4   | The $R^*$ -operation . . . . .                                    | 118 |
| 5.4.1 | Definition of the $R^*$ -operation . . . . .                      | 119 |
| 5.4.2 | The infrared counterterm operation . . . . .                      | 122 |
| 5.4.3 | Examples of $R^*$ for generic Feynman graphs . . . . .            | 123 |
| 5.4.4 | Properties of logarithmic vacuum graphs . . . . .                 | 127 |
| 5.5   | Applications of $R^*$ . . . . .                                   | 128 |
| 5.6   | Discussion of the literature . . . . .                            | 132 |
| 5.7   | Chapter conclusion . . . . .                                      | 134 |
| 5.7.1 | Findings and main conclusion . . . . .                            | 135 |
| 5.7.2 | Future research . . . . .                                         | 135 |
| 6     | THE FIVE-LOOP BETA FUNCTION . . . . .                             | 137 |
| 6.1   | Optimisations . . . . .                                           | 138 |
| 6.1.1 | Treatment of propagator insertions . . . . .                      | 138 |
| 6.1.2 | Delayed Feynman rule substitution . . . . .                       | 140 |
| 6.1.3 | Rules to make Feynman diagrams logarithmic . . . . .              | 140 |
| 6.1.4 | Canonical forms for Feynman diagrams . . . . .                    | 142 |
| 6.1.5 | Efficient tensor reduction . . . . .                              | 143 |
| 6.2   | The background field . . . . .                                    | 145 |
| 6.3   | Diagram computations and analysis . . . . .                       | 147 |
| 6.4   | Results and discussion . . . . .                                  | 149 |
| 6.4.1 | Analysis of $n_f$ -dependence in QCD . . . . .                    | 153 |
| 6.4.2 | Analysis of $N$ -dependence in $SU(N)$ . . . . .                  | 154 |
| 6.4.3 | Cumulative effects of the QCD beta function corrections . . . . . | 154 |
| 6.5   | QCD beta function in the MiniMOM scheme . . . . .                 | 154 |
| 6.6   | Chapter conclusions . . . . .                                     | 159 |
| 6.6.1 | Findings and main conclusion . . . . .                            | 160 |
| 6.6.2 | Future work . . . . .                                             | 160 |
| 7     | CONCLUSIONS . . . . .                                             | 161 |
| 7.1   | Answers to the research questions . . . . .                       | 161 |
| 7.2   | Answer to the problem statement . . . . .                         | 162 |
| 7.3   | Future research . . . . .                                         | 162 |
|       | REFERENCES . . . . .                                              | 165 |
|       | APPENDICES . . . . .                                              | 181 |
|       | A CUTVERTEX RULE FOR SCALAR DIAGRAMS . . . . .                    | 183 |

|                                      |     |
|--------------------------------------|-----|
| B CUTVERTEX RULE FOR TENSOR DIAGRAMS | 185 |
| C IR SUBGRAPH SEARCH                 | 187 |
| SUMMARY                              | 189 |
| SAMENVATTING                         | 193 |
| CURRICULUM VITAE                     | 197 |
| ACKNOWLEDGEMENTS                     | 199 |
| SIKS DISSERTATION SERIES             | 201 |



The material presented in this thesis is based on the following works.

1. B. Ruijl, T. Ueda and J.A.M. Vermaseren, *Forcer, a FORM program for the parametric reduction of four-loop massless propagator diagrams*, [arXiv:1704.06650](#)
2. B. Ruijl, T. Ueda, J.A.M. Vermaseren and A. Vogt, *Four-loop QCD propagators and vertices with one vanishing external momentum*, *JHEP* **2017** (2017) 1, [http://dx.doi.org/10.1007/JHEP06\(2017\)040](http://dx.doi.org/10.1007/JHEP06(2017)040)
3. F. Herzog and B. Ruijl, *The  $R^*$ -operation for Feynman graphs with generic numerators*, *JHEP* **2017** (2017) 37, [http://dx.doi.org/10.1007/JHEP05\(2017\)037](http://dx.doi.org/10.1007/JHEP05(2017)037)
4. F. Herzog, B. Ruijl, T. Ueda, J.A.M. Vermaseren and A. Vogt, *The five-loop beta function of Yang-Mills theory with fermions*, *JHEP* **02** (2017) 090 [[arXiv:1701.01404](#)]
5. J. Davies, A. Vogt, B. Ruijl, T. Ueda and J.A.M. Vermaseren, *Large- $n_f$  contributions to the four-loop splitting functions in QCD*, *Nucl. Phys.* **B915** (2017) 335
6. F. Herzog, B. Ruijl, T. Ueda, J.A.M. Vermaseren and A. Vogt, *FORM, Diagrams and Topologies*, *PoS LL2016* (2016) 073 [[arXiv:1608.01834](#)]
7. T. Ueda, B. Ruijl and J.A.M. Vermaseren, *Forcer: a FORM program for 4-loop massless propagators*, *PoS LL2016* (2016) 070 [[arXiv:1607.07318](#)]
8. B. Ruijl, T. Ueda, J.A.M. Vermaseren, J. Davies and A. Vogt, *First Forcer results on deep-inelastic scattering and related quantities*, *PoS LL2016* (2016) 071, <https://arxiv.org/abs/1605.08408>
9. T. Ueda, B. Ruijl and J.A.M. Vermaseren, *Calculating four-loop massless propagators with Forcer*, *J. Phys. Conf. Ser.* **762** (2016) 012060 [[arXiv:1604.08767](#)]
10. B. Ruijl, T. Ueda and J. Vermaseren, *The diamond rule for multi-loop Feynman diagrams*, *Phys. Lett.* **B746** (2015) 347 [[arXiv:1504.08258](#)]
11. B. Ruijl, J. Vermaseren, A. Plaata and H.J. van den Herik, *Why Local Search Excels in Expression Simplification*, <http://arxiv.org/abs/1409.5223>, 2014, [arXiv:1409.5223](#)
12. B. Ruijl, J. Vermaseren, A. Plaata and J. van den Herik, *Problems and New Solutions in the Boolean Domain*, ch. Simplification of Extremely Large Expressions, p. 76. Cambridge Scholars Publishing, 2016
13. B. Ruijl, J. Vermaseren, A. Plaata and H.J. van den Herik, *HEPGAME and the Simplification of Expressions*, *Proceedings of the 11th International Workshop on Boolean Problems* (2014), <http://arxiv.org/abs/1405.6369>
14. B. Ruijl, J. Vermaseren, A. Plaata and H.J. van den Herik, *Combining Simulated Annealing and Monte Carlo Tree Search for Expression Simplification*, *Proceedings of ICAART Conference 2014* **1** (2014) 724 [[arXiv:1312.0841](#)], <http://arxiv.org/abs/1312.0841>



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