

Feynman Integral Evaluation by a Sector decomposition Approach (FIESTA)

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Abstract

Up to the moment there are two known algorithms of sector decomposition: an original private algorithm of Binoth and Heinrich and an algorithm made public last year by Bogner and Weinzierl. We present a new program performing the sector decomposition and integrating the expression afterwards. The program takes a set of propagators and a set of indices as input and returns the epsilon-expansion of the corresponding integral.

PACS: 02.60.Jh; 02.70.Wz; 11.10.Gh.

Key words: Feynman diagrams; Sector decomposition; Numerical integration; Data-driven evaluation.

PROGRAM SUMMARY

Manuscript Title: Feynman integral evaluation by a sector decomposition approach

Authors: A.V. Smirnov, M.N. Tentyukov

Program Title: FIESTA

Journal Reference:

Catalogue identifier:

Licensing provisions: GPLv2

Programming language: Wolfram Mathematica 6.0 and C

Computer: from a desktop PC to a supercomputer

Operating system: Unix, Windows

RAM: depends on the complexity of the problem

Number of processors used: the program can successfully work with a single processor, however it is ready to work in a parallel environment, and the use of multi-kernel processor and multi-processor computers significantly speeds up the calculation

Keywords: Feynman diagrams; Sector decomposition; Numerical integration; Data-driven evaluation.

PACS: 02.60.Jh; 02.70.Wz; 11.10.Gh.

Classification: 4.4 Feynman diagrams, 4.12 Other Numerical Methods, 5 Computer Algebra, 6.5 Software including Parallel Algorithms

External routines/libraries: **QLink** [1], **Vegas** [2]

Nature of problem: The sector decomposition approach to evaluating Feynman integrals falls apart into the sector decomposition itself, where one has to minimize the number of sectors; the pole resolution and epsilon expansion; and the numerical integration of the resulting expression

Solution method: The sector decomposition is based on a new strategy. The sector decomposition, pole resolution and epsilon-expansion are performed in **Wolfram Mathematica** 6.0 [3]. The data is stored on hard disk via a special program, **QLink** [1]. The expression for integration is passed to the C-part of the code, that parses the string and performs the integration by the **Vegas** algorithm [2]. This part of the evaluation is perfectly parallelized on multi-processor computers.

Restrictions: The complexity of the problem is mostly restricted by CPU time required to perform the evaluation of the integral, however there is currently a limit of maximum 11 positive indices in the integral; this restriction is to be removed in future versions of the code.

Running time: depends on the complexity of the problem

References:

[1] <http://qlink08.sourceforge.net>, open source

[2] G. P. Lepage, the Cornell preprint CLNS-80/447,1980.

[3] <http://www.wolfram.com/products/mathematica/index.html>

LONG WRITE-UP

1 Introduction

Sector decomposition in alpha (Feynman) parametric representations of Feynman integrals originated as a tool for analyzing the convergence and proving theorems on renormalization and asymptotic expansions of Feynman integrals [1]. The goal of this procedure is to decompose the initial integration domain into appropriate subdomains (sectors) and introduce, in each sector, new variables in such a way that the integrand factorizes, i.e. becomes equal to a monomial in new variables times a non-singular function. General mathematical results on Feynman integrals exist up to now only in the case where all the external momenta are Euclidean. However, in practice, one often deals with Feynman integrals on a mass shell or at threshold.

Sector decomposition became a practical tool for evaluating Feynman integrals numerically with the growth of computer power. Practical sector decomposition was introduced in [2] and was used to verify several analytical results for multiloop Feynman integrals, including three-loop [3,4,5] results. For a good review on the sector decomposition we refer to Ref. [6].

The first public algorithm has been published by Bogner and Weinzierl [7]. It proposes four strategies for the sector decomposition; three of those are guaranteed to terminate. Strategy A [8] is conceptually the simplest, however it results in too many sectors; strategy B (Spivakovsky's strategy) has been described in [9], strategy C has been created by Bogner and Weinzierl and is an improvement of strategy B. Strategy X is likely to share the ideas of Binoth and Heinrich [2] It is not guaranteed to terminate but results in less sectors, than the other strategies.

This paper presents a new algorithm **FIESTA** for evaluating Feynman integrals with the use of sector decomposition. We reproduced the strategies A, B and X in the code and presented a new strategy S, based on original ideas. Our strategy is also guaranteed to terminate, but results in more sectors than strategy X, however the difference is between S and X is not so significant as with B and X. We provide an example where the strategy X does not terminate. For details and the table comparing the various strategies please refer to Appendix A.

Our algorithm can successfully work with a single processor, however it is ready to work in a parallel environment, and the use of multi-kernel processors and multi-processor computers significantly speeds up the calculation.

To benchmark the power of **FIESTA**, we evaluated the triple box diagram [3] (which starts from ε^{-6} poles) up to the finite part. We used the strategy X and took the symmetries of the diagram into account (see section 6 for the syntax). A Xeon double processor computer was used (8 cores Intel(R) Xeon(R) CPU E5472, 3.00GHz, 1600FSB, 2x6MB L2 cache, 32 GB RAM, 4.6TB local hard drive). The evaluation took less than 3 days (62.4 hours); the job used maximally 1GB of RAM and 40GB on hard drive. All the answers are within the 1 percent error estimate from the existing analytical result.

We tested **FIESTA** only on Windows and Linux platforms but there are no Linux-specifics; it should be possible to compile the sources on any Unix platform. However, we provide the pre-compiled binary files only for Windows on x86 and Linux on x86-64.

2 Theoretical background

FIESTA calculates Feynman integrals with the sector decomposition approach. It is based on the α -representation of Feynman integrals. After performing Dirac and Lorentz algebra one is left with a scalar dimensionally regularized Feynman integral [10]

$$F(a_1, \dots, a_n) = \int \dots \int \frac{d^d k_1 \dots d^d k_l}{E_1^{a_1} \dots E_n^{a_n}}, \quad (1)$$

where $d = 4 - 2\varepsilon$ is the space-time dimension, a_n are indices, l is the number of loops and $1/E_n$ are propagators. We work in Minkowski space where the standard propagators are the form $1/(-p^2 + m^2 - i0)$. Other propagators are permitted, for example, $1/(v \cdot k \pm i0)$ may appear in diagrams contributing to static quark potentials or in HQET where v is the quark velocity. Substituting

$$\frac{1}{E_i^{a_i}} = \frac{e^{ai\pi/2}}{\Gamma(a)} \int_0^\infty d\alpha \alpha^{a_i-1} e^{-iE_i\alpha}, \quad (2)$$

changing the integration order, performing the integration over loop momenta, replacing α_i with $x_i\eta$ and integrating over η one arrives at the following formula (see e.g. [11]):

$$F(a_1, \dots, a_n) = \frac{\Gamma(A - ld/2)}{\prod_{j=1}^n \Gamma(a_j)} \int_{x_j \geq 0} dx_1 \dots dx_n \delta\left(1 - \sum_{i=1}^n x_i\right) \left(\prod_{j=1}^n x_j^{a_j-1}\right) \frac{U^{A-(l+1)d/2}}{F^{A-l d/2}}, \quad (3)$$

where $A = \sum_{i=1}^n a_i$ and U and F are constructively defined polynomials of x_i . The formula (3) has no sense if some of the indices are non-positive integers, so in case of those the integration is performed according to the rule

$$\int_0^\infty dx \frac{x^{(a-1)}}{\Gamma(a)} f(x) = f^{(n)}(0)$$

where a is a non-positive integer.

After performing the decomposition of the integration region into the so-called *primary sectors* [2] and making a variable replacement, one results in a linear combination of integrals of the following form:

$$\int_{x_j=0}^1 dx_i \dots dx_{n'} \left(\prod_{j=1}^{n'} x_j^{a_j-1} \right) \frac{U^{A-(l+1)d/2}}{F^{A-l d/2}} \quad (4)$$

If the functions $\frac{U^{A-(l+1)d/2}}{F^{A-l d/2}}$ had no singularities in ε , one would be able to perform the expansion in ε and perform the numerical integration afterwards. However, in general one has to resolve the singularities first, which is not possible for general U and F . Thus, one starts a process the sector decomposition aiming to end with a sum of similar expressions, but with new functions U and F which have no singularities (all the singularities are now due to the part $\prod_{j=1}^n x_j^{a_j-1}$). Obviously it is a good idea to make the sector decomposition process constructive and to end with a minimally possible number of sectors. The way sector decomposition is performed is called a *sector decomposition strategy* and is an essential part of the algorithm.

After performing the sector decomposition one can resolve the singularities by evaluating the first terms of the Taylor series: in those terms one integration is taken analytically, and the remainder has no singularities. Afterwards the ε -expansion can be performed and finally one can do the numerical integration and return the result.

Please keep in mind that this approach works only using numerical integration: the values for all invariants should be substituted at the very early stage, after generating the functions U and F .

3 Overview of the software structure

FIESTA is written in Wolfram Mathematica 6.0 and C. The user is not sup-

posed to use the C part directly as it is launched from **Mathematica** via the Mathlink protocol. The C part is performing the numerical integration with the use of the **Vegas** [13,14] algorithm implemented as a FORTRAN program. The **Mathematica** part can work independently, however the C-integration is much more powerful than the **Mathematica** built-in one. Hence to calculate complicated integrals one should use the C-integration.

4 Description of the individual software components

The **Mathematica** part is a *.m* file that is loaded into **Mathematica** simply by `<<FIESTA_1.0.0.m`¹.

The **Mathematica** part of the program takes as input the set of loop momenta, the set of propagators, the set of indices and the required order of ε -expansion to be evaluated. It performs the differentiation (in case of negative indices), the sector decomposition, the resolution of singularities, the ε -expansion and prepares the expressions for the numerical integration. The numerical integration can both be performed by **Mathematica** or by the C-part of **FIESTA**. The **Mathematica** integration has the advantage of being able to work with complex numbers (in future version this feature will also be added to the C-part), however, the C-integration is much more powerful and should be used if one goes for complicated integrals.

The C-integration is called from **Mathematica** via the Mathlink protocol. This part of the algorithm can perfectly work in a parallel environment: one simply has to specify the number of copies of **CIntegrate** to be launched. The **Mathematica** part distributes the integration tasks between those copies and collects the result, preparing the expression of the next order at the same time.

The C-integration comes as a set of source files and should be compiled first. The binary files of **CIntegrate** for Linux and Windows can be downloaded from the web-page of the project
<http://www-ttp.particle.uni-karlsruhe.de/~asmirnov/FIESTA!.htm>

The C-integration is using **Vegas** [13,14] to perform the integration. It takes a string with the expression from **Mathematica** as input, and performs an internal compilation of this string to be able to evaluate the expression fast afterwards. No external compiler is required and no files are used for data exchange.

In complicated cases one should use the **QLink** program [15] to store intermedi-

¹ The paths to the **CIntegrate** binary, to the **QLink**[15] and the database should be specified beforehand; see section 5 for details.

atedata from **Mathematica** on disk instead of RAM. **QLink** can be downloaded as a binary or as a source (it comes under the terms of GNU GPLv2).

5 Installation instructions

In order to install **FIESTA**, the user has to download the installation package from the following URL:

<http://www-ttp.particle.uni-karlsruhe.de/~asmirnov/data/FIESTA.tar.gz>,
unpack it and follow the instructions in the file **INSTALL**.

The **Mathematica** part of **FIESTA** requires almost no installation, one only needs to copy the **FIESTA_1.0.0.m** file and edit the default paths **QLinkPath**, **CIntegratePath** and **DataPath** in this file, e.g.:

- **QLinkPath**="/home/user/QLink/QLink";
- **CIntegratePath**="/home/user/FIESTA/CIntegrate";
- **DataPath**="/tmp/user/temp";

Here **QLinkPath** is a path to the executable **QLink** file, **CIntegratePath** is a path to the executable **CIntegrate** file, and **DataPath** is a path to the database directory. For the Windows system, these paths should look like

- **QLinkPath**="C:/programs/QLink/QLink.exe"²;
- **CIntegratePath**="C:/programs/FIESTA/CIntegrate.exe";
- **DataPath**="D:/temp";

Note, the program will create a big IO traffic to the directory **DataPath**, thus it is better to put this directory on a fast local disk.

Alternatively, one can specify all these paths manually after loading the file **FIESTA_1.0.0.m** into **Mathematica**.

Please note that the code requires **Wolfram Mathematica 6.0** to be installed and will not work correctly under lower versions of **Mathematica**.

In order to work with nontrivial integrals, the user must install **QLink** and the C-part of **FIESTA**, the **CIntegrate** program. The **QLink** [15] can be downloaded as a binary file or compiled from the sources. If the user decides to use pre-compiled **CIntegrate** executable file, he has to place the file to some location and edit the paths in the file **FIESTA_1.0.0.m** as it is described above. If the user wants to compile the executable file himself he must have the **Mathematica Developer Kit** installed on his computer.

² **Mathematica** uses normal slashes for paths both in Unix and Windows.

Under Unix, the user must edit the file `comdef.h` to be sure that the macro `WIN` is not defined, i.e., comment the macrodefinition `#define WIN 1`. Then the self-explanatory file `Makefile` can be used by means of running the “make” command (the path to the Mathematica Developer Kit libraries should be provided). As a result, the binary file `CIntegrate` appears.

For the Windows installation, the user must edit the file `comdef.h` to ensure that the macro `WIN` is defined, `#define WIN 1`. The Windows makefile is provided in the package; it is named “`CIntegrate.mak`” and is used with the “`nmake /f CIntegrate.mak`”; To run this command one has to have the Microsoft Visual C++ installed (an express edition of Microsoft Visual C++ can be downloaded for free from the Microsoft site). As an addition to the programs and packages mentioned above, the user should install the Microsoft Platform Software Developer Kit (It can also be downloaded freely after validating a genuine copy of Microsoft Windows) and the Intel Fortran compiler (an evaluation copy is also available from the Intel site).

6 Test run description

To run FIESTA load the `FIESTA_1.0.0.m` into Wolfram Mathematica 6.0. To evaluate a Feynman integral one has to use the command

```
SDEvaluate[{U,F,1},indices,order],
```

where `U` and `F` are the functions from formula (3), `1` is the number of loops, `indices` is the set of indices and `order` is the required order of the ε -expansion.

To avoid manual construction of U and F one can use a build-in function `UF` and launch the evaluation as

```
SDEvaluate[UF[loop_momenta,propagators,subst],indices,order],
```

where `subst` is a set of substitutions for external momenta, masses and other values (note, the code performs numerical integrations. Thus the functions `U` and `F` should not depend on any external values).

Example:

```
SDEvaluate[UF[{k},{-k^2,-(k+p1)^2,-(k+p1+p2)^2,-(k+p1+p2+p4)^2},
{p1^2→0,p2^2→0,p4^2→0,p1 p2→-S/2,p2 p4→-T/2,p1 p4→(S+T)/2,
S→3,T→1}],{1,1,1,1},0]
```

performs the evaluation of the massless on-shell box diagram (Fig. 1) where the Maldestam variables are equal to $S = 3$ and $T = 1$. A complete log of this

example follows in Appendix B.

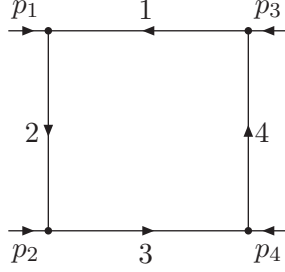


Fig. 1. The massless on-shell box diagram.

To clear the results from memory use the `ClearResults[]` command.

The code has the following options:

- `UsingC`: specifies whether the C-integration should be used; default value: `True`;
- `CIntegratePath`: path to the `CIntegrate` binary;
- `NumberOfLinks`: number of the `CIntegrate` programs to be launched; default value: 1;
- `UsingQLink`: specifies whether `QLink` should be used to store data on disk; works only with `UsingC=True`; default value: `True`; please refer to Appendix D on the use of `QLink`;
- `QLinkPath`: path to the `QLink` binary;
- `DataPath`: path to the place where `QLink` stores the data; for example, if `DataPath=/temp/temp`, then the code three directories: `/temp/temp1`, `/temp/temp2` and `/temp/temp3`; those directories will be erased if existent; the directory `/temp` should exist;
- `PrepareStringsWhileIntegrating`: specifies whether the code should prepare expressions of next order in epsilon at the same time with integrating; works only with `UsingC=True` and `UsingQLink=True`; should be set to `False` on slow machines; default value: `True`;
- `IntegrationCut`: the actual low boundary of the integration domain (instead of zero); default value: 0;
- `IfCut` and `VarExpansionDegree`: if `IfCut` is nonzero then the expression is expanded up to order `VarExpansionDegree` over some of the integration variables; the integration function is evaluated exactly if the integration variable is greater than `IfCut`, otherwise the expansion is taken instead; the default value of `IfCut` is zero, the default value of `VarExpansionDegree` is 1;
- `ForceMixingOfSectors`: if set to `True`, forces the code to perform one integration only for a given order of ε ; default value is `False`; please refer to Appendix G;

- **PrimarySectorCoefficients**: The usage of this option allows to take the symmetries of the diagram into account. If the diagram has symmetries, then the primary sectors corresponding to symmetrical lines result in equal contributions to the integration result. Hence it makes sense to speed up the calculation by specifying the coefficients before the primary sector integrands. For example, if two lines in the diagram are symmetrical, one can have a zero coefficient before one of those and 2 before the second. **PrimarySectorCoefficients** defines those coefficients if set; the size of this list should be equal to the number of primary sectors;
- **STRATEGY**: defines which sector decomposition strategy is used; **STRATEGY_0** is not exactly a strategy, but an instruction not to perform the sector decomposition; **STRATEGY_A** and **STRATEGY_B** are the two strategies from Ref. [7] guaranteed to terminate; **STRATEGY_S** (default value) is our strategy, producing better results than the preceding ones; **STRATEGY_X** is an heuristic strategy from [7]; likely to share the ideas of Binoth and Heinrich [2]: powerful but not guaranteed to terminate;
- **ResolveNegativeTerms**: defines whether an attempt to get rid of negative terms in F should be performed; default value: **True**; see Appendix C;
- **VegasSettings**: a list of 4 numbers $\{p_1, r_1, p_2, r_2\}$, instructs the code to evaluate the integral r_1 times with p_1 sampling points for warm-up and r_2 times with p_2 sampling points for the final integration; default value: $\{10000, 5, 100000, 15\}$.

The code sometimes returns **Indeterminate** as a result. There are the following reasons possible:

- *Negative function F provided*;
This might happen if the propagators in the input for UF are of the form $-1/(-p^2 + m^2 - i0)$ instead of $1/(-p^2 + m^2 - i0)$;
Solution: change the sign of the propagators;
- *Complex number as an answer*;
If the integrand has complex values, then the C integration cannot be used with the current version of FIESTA. If complex numbers are explicitly encountered in the integrand, the integration will produce a syntax error. Otherwise, if the expressions like $\log(-1)$ are encountered in the integrand, it the integration program returns **Indeterminate**;
Solution: One can try to use the **UsingC=False** option, however the built-in **Mathematica** integration cannot work in complicated examples and we don't guarantee correct results if complex numbers are used. The support for complex numbers will be provided in future versions of FIESTA;
- *Special singularities*;
The standard sector decomposition approach works only for singularities for small values of variables. Our code can resolve some extra singularities (see Appendix C), but surely all types of singularities could not be covered.

Solution: One can try different values of the `ResolveNegativeTerms` option. If the singularity is of a special type, one can try contact the authors in order to try to make the resolution of singularities of this type automatic.

- *Numerical instability;*

If all the singularities are for small values of integration variables, they are resolved in the code. However, the numerical integration may experience problems with small values of variables (see Appendix E).

Solution: One should use the `IntegrationCut` or `IfCut` together with `VarExpansionDegree` options. See Appendix E for details.

7 Acknowledgements

The authors would like to thank V.A. Smirnov and M. Steinhauser for posing the problem of sector decomposition and for testing in on various examples, to P. Uwer for the consultation on `Vegas` and numerical integration and to G. Heinrich for useful discussions.

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Appendix

A Sector decomposition strategies

The sector decomposition goal may be reformulated the following way: suppose we have a polynomial P of n variables and a unitary hypercube \mathcal{U} as integration area. The task is to separate the integration region into a number of sectors so that each of those sectors after a variable replacement turns into a unitary cube and P in those variables turns into a product of a monomial M and a polynomial of a *proper form*, i.e. having 1 as one of the summands. This requirement is often sufficient for the polynomial P to have no zeros apart from the ones due to M (this is valid for a wide class of integrals including those with the same sign for all kinematic invariants).

The sector decomposition is usually performed recursively; for a given polynomial P one has an algorithm to define how to perform a single sector decomposition step. Such an algorithm is also called a *sector decomposition strategy*.

All known strategies separate \mathcal{U} into parts the following way: a subset $I =$

$\{i_1, \dots, i_m\}$ of $\{1, \dots, n\}$ is chosen and m sectors are defined by

$$S_l = \{(x_1, \dots, x_n) \in \mathcal{U} | x_{i_l} \geq x_{i_k} \forall i_k \in I\},$$

($l = 1 \dots m$). The variable replacement in S_l is defined by

$$x_i = x'_i \forall i \notin I$$

$$x_{i_l} = x'_{i_l}$$

$$x_{i_k} = x'_{i_l} x'_{i_k} \forall i \in I, k \neq l$$

It is easy to verify that the integration region in the new variables x' is again a unitary cube.

We are extending the set of possible regions and variable replacements the following way: for any vector (v_1, \dots, v_n) in the positive quadrant with at least two non-zero coordinates we consider the set $I = \{i | v_i \neq 0\}$ and separate \mathcal{U} into m parts by

$$S_l = \{(x_1, \dots, x_n) \in \mathcal{U} | x_{i_l}^{a_{i_l}} \geq x_{i_k}^{a_{i_k}} \forall i_k \in I\},$$

where $\{i_1, \dots, i_m\} = I$ and the exponents a_i are defined by

$$\begin{pmatrix} a_{i_1} \\ a_{i_2} \\ a_{i_3} \\ \vdots \\ a_{i_m} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & 1 & \dots & 1 \\ 1 & 1 & 0 & \dots & 1 \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & 1 & 1 & \dots & 0 \end{pmatrix}^{-1} \begin{pmatrix} v_{i_1} \\ v_{i_2} \\ v_{i_3} \\ \vdots \\ v_{i_m} \end{pmatrix} \quad (\text{A.1})$$

The variable replacement in S_l is defined by

$$x_i = x'_i \forall i \notin I$$

$$x_{i_l} = x_{i_l}^{v_{i_l}}$$

$$x_{i_k} = x_{i_l}^{v_{i_k}} x'_{i_k} \forall i \in I, k \neq l.$$

It is only a little bit more complicated to verify that the integration region in the variables x' is still the unite hypercube.

Now let us describe how we choose the vector v . We consider the set of weights W of the polynomial P defined as the set of all possible (a_1, \dots, a_n) where $cx_1^{a_1} \dots x_n^{a_n}$ is one of the monomials of P . We will say that a weight is higher than another one if their difference is a set of non-negative numbers. If P had a unique lowest weight, a monomial could be factorized out and we would represent P in the required form. Hence it becomes reasonable to try to minimize the number of lowest weights of P . We consider the convex hull of W and choose one of its facets F visible from the origin. Now v is chosen to be the normal vector to F .

The reason of choosing such a vector is rather simple: the vectors formed by the weights of the vectors x'_{i_k} for $k \neq l$ are orthogonal to v , therefore are lying in the facet F . Hence there is a good chance that after a single sector decomposition step only one of the vertices of F is left to be a lowest weight.

Such a sector decomposition step is guaranteed not to increase the norm defined in the strategy A of [7] (the Zeillinger strategy [8]). If we can't find a facet such that the corresponding step decreases the norm, we fall back to the strategy A and perform one step. Hence our strategy is also guaranteed to terminate. Practice shows that the strategy A steps are applied in no more than in five percent cases.

The following table shows the number of sectors produced by different strategies on various examples:

Diagram	A	B	C	S	X
Box	12	12	12	12	12
Double box	755	586	586	362	293
Triple box	M	114256	114256	22657	10155
D420	8898	564	564	180	F

D420 is a diagram contributing to the 2-loop static quark potential on Fig. A.1 with the following set of propagators: $\{-k^2, -(k-q)^2, -l^2, -(l-q)^2, -(k-l)^2, -vk, -vl\}$, where k and l are loop momenta, $q^2 = -1$, $qv = 0$ and $v^2 = 1$.

“F” means that the sector decomposition fails (we suppose an infinite loop). “M” means that the memory overflow happened during the sector decomposition on a 8Gb machine. We suspect D420 to be a counterexample to the STRATEGY_X

Hence we recommend leaving the default option `STRATEGY=STRATEGY_S` (our strategy) or experimenting with `STRATEGY=STRATEGY_X` (based on the ideas of Binoth and Heinrich [2], not guaranteed to terminate).

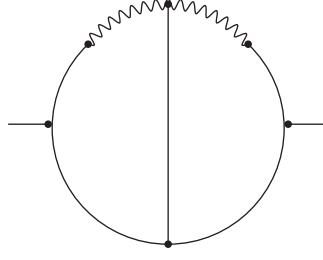


Fig. A.1. A diagram contributing to the 2-loop static quark potential

B An example

Here we provide the listing of the `Mathematica` session for evaluation of the massless on-shell box diagram with $S = 3$ and $T = 1$ (we split some long lines).

```
In[1]:= << FIESTA_1.0.0.m
FIESTA, version 1.0.0

In[2]:= UsingQLink=False;

In[3]:= SDEvaluate[UF[{k},{-k^2,-(k+p1)^2,-(k+p1+p2)^2,
-(k+p1+p2+p4)^2},{p1^2->0,p2^2->0,p4^2->0,
p1 p2->-S/2,p2 p4->-T/2,p1 p4->(S+T)/2,S->3,
T->1}],{1,1,1,1},0]
External integration ready! Use CIntegrate to perform calls
FIESTA, version 1.0.0
UsingC: True
NumberOfLinks:1
UsingQLink: False
IntegrationCut: 0
IfCut: 0.
Strategy: STRATEGY_S
Integration has to be performed up to order 0
Sector decomposition.....0.0138 seconds; 12 sectors.
Variable substitution.....0.0055 seconds.
Decomposing ep-independent term.....0.0025 seconds
Pole resolution.....0.0081 seconds; 40 terms.
Expression construction.....0.0021 seconds.
Replacing variables.....0.0063 seconds.
Epsilon expansion.....0.0123 seconds.
Expanding.....0.0002 seconds.
Counting variables: 0.0002 seconds.
Preparing integration string.....0.0004 seconds.
Terms of order -2: 8 (1-fold integrals).
Numerical integration: 8 parts; 1 links;
Integrating.....0.106322 seconds; returned answer:
```

```

1.333333
Integration of order -2: 1.333333
(1.333333)/ep^2
Expanding.....0.0005 seconds.
Counting variables: 0.0005 seconds.
Preparing integration string.....0.001 seconds.
Terms of order -1: 28 (2-fold integrals).
Numerical integration: 12 parts; 1 links;
Integrating.....0.409080 seconds; returned answer:
-2.065743 +- 5.*^-6
Integration of order -1: -2.065743 +- 5.*^-6
(1.333333)/ep^2 + (-0.73241 +- 5.*^-6)/ep
Expanding.....0.0008 seconds.
Counting variables: 0.0009 seconds.
Preparing integration string.....0.0022 seconds.
Terms of order 0: 40 (2-fold integrals).
Numerical integration: 12 parts; 1 links;
Integrating.....0.862786 seconds; returned answer:
-3.417375 +- 0.000012
Integration of order 0: -3.417375 +- 0.000012
(1.333333)/ep^2 + (-0.73241 +- 5.*^-6)/ep +
(-4.386496 +- 0.000013)
Total time used: 1.52991 seconds.

Out[3]= -4.3865 +  $\frac{1.33333}{\epsilon^2}$  +  $\frac{-0.73241 + 5. \cdot 10^{-6}}{\epsilon}$ 
+ 0.000013 pm47
In[4]:= Quit

```

The analytical answer for this integral is

$$\frac{4}{3\epsilon^2} - \frac{2\log(3)}{3\epsilon} - \frac{4\pi^2}{9}$$

which is equal to

$$1.333333\frac{1}{\epsilon^2} - 0.7324081\frac{1}{\epsilon} - 4.3864908.$$

C Dealing with negative terms in F

FIESTA has been used to verify master integrals for the three-loop static quark

potential [12]. A typical phenomenon when evaluating those integrals is that the function F can involve terms like $(x_i - x_j)^2 = x_i^2 - 2x_i x_j + x_j^2$. As a result, not all monomials of F have positive signs, resulting in extra singularities for the integration.

To overcome those problems we added an additional feature to **FIESTA**: an attempt to get rid of negative summands in F before performing the sector decomposition (those summands may lead to additional singularities that are not treated properly by the basic approach). The code tries to find two variables, x_i and x_j , split the unitary cube into two regions with $x_i \leq x_j$ and $x_i \geq x_j$ and do a variable replacement (e.g. for $x_i \leq x_j$ we make the replacement $x'_i = x_j - x_i$). In case of success, we result in a new function F without monomials with negative sign.

The ideas of this type are not original; it is a common situation when certain classes of integrals require a special treatment, in the papers of Binoth and Heinrich [2] one can find various examples where special operations preceding the sector decomposition are performed. Still we consider our automatic approach to the problem to be original: one does not require to specify the singularities of this type for the code to resolve them.

D Avoiding memory limits in Mathematica

Wolfram Mathematica, being a powerful CAS³ is widely used among researchers nowadays. However, a significant drawback of the **Mathematica** usage is the lack of RAM that is often encountered. **FIESTA** also had memory problems at the ε -expansion stage: an expression for a single sector can become huge after the expansion, and in complicated examples one can have many thousands of sectors. To avoid memory problems we used the **QLink** program to store data on hard disk.

After performing the sector decomposition we store all the expressions in a database via **QLink**. Afterwards the code never loads the whole set of expressions into RAM. On the contrary, the code works with sectors one by one: it loads an expression from the database, performs an operation with it and writes it back to the database. The operation might be one of the following: singularity resolution, ε -expansion, applying the **Expand** function or applying “if conditions” (see appendix E).

It is worth noting that the ε -expansion does not use the **Mathematica Series** function but explicit differentiation instead. This has two reasons: first of all,

³ Computer Algebra System

differentiation with subsequent expansion works faster in `Mathematica` 6.0 for the expressions we consider (remember that `FIESTA` uses `Mathematica` 6.0 because of the powerful build-in integration methods that were absent in 5.2). The second reason is to perform differentiation at the very beginning but to wait with applying the `Expand` function (which takes more time than the differentiation!). The latter function can be applied simultaneously with the integration at a later stage: we prepare expressions of order $o + 1$ while integrating expressions of order o .

Such an approach allows to keep the memory usage by `Mathematica` minimal and to leave most of the memory to the `CIntegrate` copies.

E Resolution of singularities and its influence on the convergence of numerical integration

As it has been noted in section 2, the integrals

$$\int_{x_j=0}^1 dx_i \dots dx_n \left(\prod_{j=1}^n x_j^{a_j-1} \right) Z, \quad (\text{E.1})$$

where Z has no singularities might have singularities because of non-positive a_j . Let us assume that $a_i \leq 0$ and treat the integrand as a function $x^{a_i-1}Y(a_i)$ with coefficients being polynomials of other variables. For readability we will omit the index i . We replace $x^{a-1}Y(a)$ by

$$Y(0)x^{a-1} + Y'(0)x^a + \dots + \frac{1}{a!}Y^{(-a)}(0)x^{-1} + \\ x^{a-1}(Y(a) - Y(0) - Y'(0)x - \dots - \frac{1}{a!}Y^{(-a)}(0))$$

The items in the first line of the expression can be analytically integrated over x leaving us with one integration less. As for the expression $R(a) = x^{a-1}(Y(a) - Y(0) - Y'(0)x - \dots - \frac{1}{a!}Y^{(-a)}(0))$, it is known to have no singularities at $x = 0$, however it might result in numerical instabilities at a later stage.

After performing the resolution of singularities and the ε -expansion, one obtains a set of integrands depending only on integration variables over the unit hypercube. The integrands arise from the expressions like R (or even more complicated ones in case of several integration variables).

Those integrands have no singularities, so one could expect that the integration is performed with ease. However, one can see that for small x the x^{a-1} is huge

and the remainder is small. Hence the remainder can't be evaluated exactly because it is a difference of not-so-small numbers stored with a finite number of digits.

The first step to the solution is to expand the expressions before evaluating. It leaves similar problems (a difference of huge numbers resulting in a normal number), but with a smaller numerical instability. Still, in highly degenerate examples the problem persists and prevents the code from evaluating the function when the variables turn small.

FIESTA has two methods to deal with the numerical instability. The first method is the usage of the `IntegrationCut` option. This option sets the low integration limit to `IntegrationCut` (instead of zero). This approach may lead to high error estimate, so there is a more advanced method (slower but providing better results).

The idea of the second method is to expand the integration function over the integration variables around zero up to a certain order (not all integration variables require the expansion, but only the ones with a negative exponent in the preceding monomial). Then one can integrate the original function for values greater than some fixed number and the expanded one for smaller values. The code is instructed to work this way by the `IfCut` and `VarExpansionDegree` options. Please note that even for `IfCut=10-2` and `VarExpansionDegree=1` one results in an 10^{-6} relative error estimate for the remainder that is smaller than the integration error estimate for complicated examples.

There is one more technical problem in the second approach: the usage of the `Mathematica Series` command can be quite slow. Hence to expand the function we need to substitute $x = 0$ into the function and its derivatives. The direct substitution is impossible for the same numerical reasons. The solution comes with finding the minimal possible s such that $(x^s f)(0)$ can be evaluated numerically. Now we can define a new function $g = \frac{(x^s f)^{(s)}}{s!}$ and use the fact that $f^{(l)}(0) = C_s^{l+s} g^{(l)}(0)$ to expand the function.

Please note that the error estimate in the output is the one that comes from the integration; if the cuts are used, one should keep in mind that the real error might be greater for the reason that a function different from the original one is integrated.

F External integration

F.1 Overview

For the integration we use the well-known **Vegas** algorithm [13,14] which is based on importance sampling. It samples points from the probability distribution described by the function $|f|$, so that the points are concentrated in the regions that make the largest contribution to the integral. In the present version of **FIESTA** we use the FORTRAN code linked with the C interface to **Mathematica**. The VEGAS routine requires an integrand as a reference to a function of an array of the integration variables x , the number of repetitions and the number of sampling points.

The **Mathematica** part provides the integrand in a form of a long symbolic algebraic expression consisting of the integration variables, powers and logarithm⁴, e.g.:

$$(1+x[1])*p[x[1]+x[1]*x[2],-3]+1[x[3]]/33$$

where $p[x[1]+x[1]*x[2],-3]$ stands for $(x[1] + x[1] * x[2])^{-3}$ and $1[x[3]]$ for $\log(x[3])$.

The common approach is based on generating the corresponding C (or FORTRAN) code, compiling it, linking with some integration routine (VEGAS in our case), running the resulting program and reading back the answer. However, in our case this approach does not work properly: it is specific to the sector decomposition that there can be many thousands of sectors. This leads to a big overhead for loading a compiler, a linker, writing the results to a file, loading and starting the resulting program and reading the results back.

Next, the size of the corresponding expressions to be integrated may vary from several bytes to hundreds of megabytes. Unfortunately, all of the existing C or FORTRAN compilers are strongly nonlinear with respect to the length of the input expression. The reason is that these compilers usually use the so-called AST (Abstract Syntax Tree, see [16]) which is a tree representation of the syntax: each node represents constants or variables (leaves) and operators or statements (inner nodes). The complexity of this tree grows rapidly with the size of the incoming expression. In practice, it is nearly impossible to compile an expression of more than a few megabytes length.

In order to compile a huge expression one can use some stack-based program-

⁴ For the **IfCut** method (see Appendix E) the **if-then-else** construction is also used, in the form **if(condition)(first branch)(second branch)**.

ming language like FORTH [17] but the performance of programs written on these languages is usually not so good as the performance of C or FORTRAN programs.

One of the standard approaches consists in optimizing the algebraic expression by means of some CAS tool like the Maple package “CodeGeneration” (formerly “codegen”)[18] and compiling the resulting C (or FORTRAN) code without optimization. This cannot solve our problem since the number of expressions is too big, anyway, and the resulting (optimized) code sometimes is still rather large. Moreover, the time the CAS spends to generate such an optimized code is too large. So we decided to develop an interpreter which is able to evaluate a given expression in a “data-driven” manner: a translator translates the incoming expression into some internal representation⁵ and then an interpreter evaluates the expression many times for various input data. It is worth noting that no intermediate AST is generated, only the linear sequence of triples. This permits our translator to be almost linear w.r.t. the length of the incoming expression.

F.2 Translation

The incoming expression consists of (many) terms. Each term is a product of a coefficient and a number of integration variables (possibly zero) in some powers, some prescribed functions of these variables and subexpressions of the same structure (recursively). The translator converts this expression into a sequence of triples, being “an operation”, “first operand” and “second operand”; e.g. the expression $1+x[1]+x[1]*x[3]$ will be represented as a following sequence of triples:

```
1: '+', 1, x[1]
2: '*', x[1], x[3]
3: '+', ^1, ^2
```

where ^1 is a reference to the result of the first triple evaluation, ^2 to the second one. A term may involve some functions and subexpressions, e.g. $x[1]+p[x[1],-2]*(x[2]+x[3])$ will be translated to

```
1: 'p', x[1], -2
2: '+', x[2], x[3]
3: '*', ^1, ^2
4: '+', x[1], ^3
```

⁵ We use the triple form, see [16].

During translation, the subexpression optimization is performed in the following way: the translator searches for each new triple in the dictionary. If the triple has already occurred, the translator does not put the triple into the resulting sequence, referencing the old one instead. Note, the translator input is already *sorted* since we get it from *Mathematica* so at least all coinciding monomials will be evaluated only once.

This simple prefix optimization is surely not perfect. Let us consider the following expression:

$$(1+x[1]+x[2]*x[4])*(1+x[2]*x[4]+x[2]*x[3]*x[4])$$

The terms are sorted but the subexpressions $1+x[2]*x[4]$ in brackets will not be recognized, and $x[2]*x[4]$ in $x[2]*x[3]*x[4]$ also will not be identified. Of course, we might have implemented all possible combinations, but the resulting time would grow factorially w.r.t. the length of the input string, which is unacceptable for us. Hence we implemented the following strategy:

Let us consider a term. Let us assume it has an implicit coefficient 1 in front. We consider every factor as a “commuting diad” of a form “operation”, “operand”, e.g. $3*x[1]*x[3]/x[2]$ will be considered as a set of the following commuting diads:

```
'*', 3
'*, x[1]
'*, x[3]
'/', x[2]
```

Now we can re-order all these diads without affecting the result. We try to evaluate such a sequence in some “native” order, e.g. in the above example this would be like the following:

```
'*', x[1]
'/', x[2]
'*, x[3]
'*, 3
```

We put the coefficient to the end, so terms differing by a coefficient will be evaluated only once. It is also worth noting that in each subexpression *Mathematica* already sums up all similar terms.

The same idea works out (even better) for summands, the only difference is the implicit initial value 0 instead of 1.

This works well, reducing the number of generated triples by an order of magnitude. The translation procedure is in the worst case quadratic w.r.t. to

the length of the input string, in average it is a bit worse than linear. Typically, in a 3GHz Xeon processor the translator spends about 30 seconds to translate a gigabyte expression, which is incomparably less than the integration time.

F.3 Evaluation

The sequence of the translated triples is completely platform independent, and it is rather straightforward to generate (directly to the memory) the binary executable code for any existing architecture, and execute it. For the moment, we've restricted ourselves by developing the interpreter suitable for every platform.

First of all, the triple sequence we have from the translation stage, is translated into the array of quadruples: "operation", "operand 1", "operand 2" and "result". The fields "operand 1" and "operand 2" are pointers to some memory addresses. The "result" field is either the result of the quadruple evaluation (`double` type in C), or the address of the memory cell in which the result must be stored. The point is that the size of the address field on 64 bit platforms is the same as the size of `double`, and the usage of indirect references is rather slow, so it seems to be reasonable to use a new memory cell for each intermediate result.

However, on a modern CPU such an approach appears to be completely wrong. Modern processors have a big write-back cache memory (megabytes), and provided the same memory address is permanently updated it is never written to RAM but stays in the cache. On the other hand, if we write intermediate results every time to a new address, all this data is sooner or later written to RAM (after the cache exhausted). That is why for "small" jobs, when all intermediate results fit into the processor cache, the interpreter stores results directly to the "result" field of a quadruple, while for "large-scale" jobs the translator creates some buffers and provides the quadruples with re-usable addresses of elements of these buffers.

The algorithm switches from the "small" to "large" model when the number of generated triples reaches some threshold which strongly depends on the size of the processor L2 (L3) cache per active core and it is a subject for tuning for every specific architecture. The corresponding value is hard-coded, it can be changed in the file `scanner.h`, the macro `INDIRECT_ADDRESSING_THRESHOLD`.

The complete structure of the C-part is as follows. The routine `AddString()` builds the integrand step by step collecting the incoming lines. Every moment the process may be canceled by invoking the function `ClearString()`. After (almost) all of the lines are collected, the routine `Integrate()` adds the rest

and invokes the translator. After the incoming expression is translated into the quadruple array the routine `Integrate()` invokes the VEGAS routine for 5 repetitions with 10000 sampling points in order to “warmup” the grid. Finally, the VEGAS routine is invoked by the `Integrate()` routine for 15 repetitions with 100000 sampling points for the real integration⁶.

G Integration of sums vs sums of integrations

The current version of FIESTA integrates in each sector separately (each sector, not just each primary sector). The results are summed up and the error estimate is calculated with a mean-square norm. This approach might encounter a natural suspicion: the errors add up and might result in an absurd result. However practice shows that the real error of this method is normally only about 20 percent greater than the error of the other approach — integrating the sum of expressions.

The reason lies within the adaptable integration algorithms: if each of the terms is integrated individually, the algorithm can adapt to all the peaks of the given term. Hence the error estimate for the individual terms might be good enough. However when one tries to evaluate the whole sum at once, the peaks and other peculiarities of the different terms collide and the integration algorithm cannot adapt to all of them properly.

Another reason to integrate in each sector individually is obviously the economy of RAM. And even more, this approach suits well for parallel environments due to much better load balancing.

For the `CIntegrate` interpreter short (but not *so*-short) expressions are also preferable.

At first sight, long expressions could be optimized much better than the short ones for the following reason: the longer the expression, the more common subexpressions are encountered, and all the subexpressions should be evaluated only once. But for a long expression the program must use the indirect referencing for quadruple results (see Appendix F.3) which can slowdown the interpreter considerably.

In general, all these effects speedup the evaluation up to an order of magnitude when each individual sector is integrated independently on others.

⁶ This is the default behavior; the exact number of sampling points can be set by the `VegasSettings` option, see Section 6.

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