PFD-PARALLEL, a Singular/GPI-Space package for massively parallel multivariate partial fractioning

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Abstract

Multivariate partial fractioning is a powerful tool for simplifying rational function coefficients in scattering amplitude computations. Since current research problems lead to large sets of complicated rational functions, performance of the partial fractioning as well as size of the obtained expressions are a prime concern. We develop a large scale parallel framework for multivariate partial fractioning, which implements and combines an improved version of Leinartas' algorithm and the MultivariateApart algorithm. Our approach relies only on open source software. It combines parallelism over the different rational function coefficients with parallelism for individual expressions. The implementation is based on the Singular/GPI-Space framework for massively parallel computer algebra, which formulates parallel algorithms in terms of Petri nets. The modular nature of this approach

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allows for easy incorporation of future algorithmic developments into our package. We demonstrate the performance of our framework by simplifying expressions arising from current multiloop scattering amplitude problems.

Keywords: multivariate partial fraction; massive parallelization; scattering amplitudes; integration-by-parts reduction;

PROGRAM SUMMARY

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Program Title: pfd-parallel

CPC Library link to program files: (to be added by Technical Editor)

Developer's repository link: https://github.com/singular-gpispace/pfd-parallel

Code Ocean capsule: (to be added by Technical Editor)

Licensing provisions(please choose one): GPLv3

Programming language: Singular language, GPI-Space Petri net

Computer(s) for which the program has been designed: from personal computer to HPC cluster

Operating system(s) for which the program has been designed: Linux Supplementary material: none

Nature of problem: In scattering amplitude computation, we often encounter complicated rational functions, which may be simplified using the multivariate partial fraction decomposition. With the consideration of the increasing complexity of the problems, an efficient implementation of such a method is needed.

Solution method: We present the package PFD-PARALLEL, which is a large-scale parallelized framework for multivariate partial fractioning. Our package relies only on open source software. It combines different algorithms and provides parallelization based on the Singular/GPI-Space framework [1, 2, 3]. The package combines both the improved Leinartars' algorithm [4], as well as the MultivariateApart algorithm [5], and combines parallelism over the different rational function coefficients and parallelism for individual expressions. Using this approach cutting-edge computations can be handled in an efficient way.

Additional comments including restrictions and unusual features (approx. 50-250 words): The software, including all dependencies like Singular, GPI-2, GPI-Space, and the Singular/GPI-Space framework, is distributed via the supercomputing package manager Spack, which allows for convenient installation of scientific software, in particular in HPC environments. The code has been tested on Centos 7 and 8, Ubuntu 18.04 LTS and 20.04 LTS.

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1. Introduction

Higher order perturbative quantum field theory correction is a very important theoretical tool in high energy physics. The higher order correction is usually obtained by the computation of multi-loop scattering amplitudes. One difficulty in scattering amplitude computations arises from the complicated rational function coefficients in terms of the kinematic variables. Complicated rational functions are difficult to handle algebraically to evaluate numerically.

Algorithmic multivariate partial fractioning, originating from the mathematical work of Leinartas [1, 2], is a powerful tool which can simplify many kinds of rational function expressions in scattering amplitude computations. See the recent improved Leinartas' algorithm in ref. [3]. On the other hand, the MultivariateApart [4] algorithm, based on computation algebraic geometry, is significantly different from Leinartas' and has strong performance.

Multivariate partial fractioning was used in the algorithm in [5] for finding Feynman integrals with uniform transcendental weights [6], in simplifying integration-by-parts (IBP) reduction coefficients [3], and, with a multitude of applications, in simplifying the rational function coefficients in the final expressions of multiloop scattering amplitudes [7, 8, 9, 10, 11, 12, 13, 14].

In multiloop amplitude computations, both the number and complexity of rational functions to be handled can be very significant. Therefore the performance of the multivariate partial fraction implementation is important. A large scale parallelization of multivariate partial fractioning, over different rational function coefficients is obviously a necessity. Furthermore, the rational function coefficients from a scattering amplitude computation typically have quite uneven size and thus dramatically different running times for the partial fraction decomposition. A naive parallelization over batches of different rational functions is then not efficient. For very complicated rational functions, a parallelization of the decomposition of individual functions would be helpful. Realizing both types of parallelism simultaneously in an efficient way requires to model a non-trivial workflow.

There are several publicly available programs for applying multivariate partial fraction methods, like PFD [3], MULTIVARIATEAPART [4], as well as private codes. In this paper, we present a large-scale parallel implementation of the two algorithms in [3] and [4], based on the Singular/GPI-Space framework¹ introduced in [15]. Our package is solely based on open source software. It can be conveniently installed via the widely-used supercomputing package manager Spack [16], and is usable on homogeneous and heterogenous computing environments from a personal computer to a high-performance cluster.

In our approach, the open source computer algebra system SINGULAR [17] provides efficient tools for handling algebraic structures, and in particular Gröbner bases. We rely on the powerful task-based workflow management system GPI-SPACE [18] to model our parallel algorithm. This system has also been made open source. By formulating the algorithm in GPI-SPACE in the language of Petri nets leads to automated parallelization. The parallelization is realized not just on the level of different coefficients, but also within the partial fraction computation of individual coefficients. This feature is very useful for simplifying rational function coefficients if the sizes of

¹https://www.mathematik.uni-kl.de/~boehm/singulargpispace/

these coefficients are quite uneven, which is typically the case. Due to the internal parallelization, complicated coefficients do not dominate any more the run-time. In particular, a very good parallel efficiency is achieved.

Our package also provides convenient strategies to choose different partial fractioning algorithms and types of parallelism based on the sizes of the input functions. The package and the realization of the parallelism are designed with a modular structure in mind, allowing for easy integration of improvements and algorithms which might become available in the future.

To demonstrate the power of our package, we present two examples of simplifying (1) IBP reduction coefficients for two-loop five-point massless Feynman integrals with degree 5 numerators, and (2) rational functions from two-loop leading colour helicity amplitudes for $W\gamma + j$ production [14]. Both cases can be handled with our package in a highly efficient way, and the resulting representation of the data is significantly shorter.

This paper is organized in the following way: In Section 2, we introduce our improved Leinartas' algorithm equipped with polynomial division and syzygy reduction computations, for the multivariate partial fraction. The parallel structures are also mentioned. In Section 3, we discuss our new large-scale parallel implementation of our partial fraction algorithm based on the Singular/GPI-Space framework. In Section 4, we provide a note on the installation and a short manual for our program.² In Section 5, we apply our multivariate partial fractioning framework in the case of our examples (1) and (2), and analyze timings and compression ratios. We observe that the IBP coefficients for the two-loop five-point non-planar Feynman integral with degree 5 numerators are compressed by more than two orders of magnitudes and are put into a usable form, moreover, that the amplitude example achieves similar compression ratios. Finally, in Section 6, we summarize our paper and provide some outlook.

2. Partial fraction decomposition

The algorithm we use to reduce the size of rational functions is an improved version of Leinartas' algorithm for multivariate partial fraction decomposition [1, 2]. Since our approach for parallelization of the decomposition of individual functions relies on it, we start out with a short account of

²More details can be found in the online manual in the GitHub repository https://github.com/singular-gpispace/pfd-parallel.

the improved Leinartas algorithm. For more details refer to Section 3 of our paper [3]. For the MULTIVARIATEAPART algorithm, of which we also provide an implementation, we refer to [4].

Let in the following $K[x_1, \ldots, x_d]$ or short $K[\mathbf{x}]$ be the ring of polynomials over some field K in d variables $\mathbf{x} = (x_1, \ldots, x_d)$ and let \overline{K} be the algebraic closure of K (e.g. $\overline{\mathbb{R}} = \mathbb{C}$). The goal is to write a rational function f/g $(f, g \in K[\mathbf{x}])$ where the polynomial $g = q_1^{e_1} \cdot \ldots \cdot q_m^{e_m}$ factors into many small³ irreducible factors q_i , as a sum of functions with "smaller" numerators and denominators. The algorithm consists of 3 main steps:

2.1. Nullstellensatz decomposition

In the first step of the algorithm we search for relations of the form

$$1 = h_1 q_1^{e_1} + \dots + h_m q_m^{e_m} \tag{1}$$

where $h_i \in K[\mathbf{x}]$ are polynomials. By multiplying (1) with f/g, we get the decomposition

$$\frac{f}{g} = \frac{f \cdot \sum_{k=1}^{m} h_k q_k^{e_k}}{\prod_{i=1}^{m} q_i^{e_i}} = \sum_{k=1}^{m} \frac{f \cdot h_k}{\prod_{i=1, i \neq k}^{m} q_i^{e_i}}.$$
 (2)

in which each denominator contains only m-1 different irreducible factors. Now we repeat this step with each summand in the decomposition (2) until we obtain a sum of rational functions where each denominator contains only factors, that do not admit a relation as in (1). By Hilbert's weak Nullstellensatz [3, Lemma 3.6], such a relation exists if and only if the polynomials q_i do not have a common zero in \overline{K}^d and can be computed by calculating a Gröbner basis [3, Definition 3.3] of the ideal generated by the polynomials $q_i^{e_i}$ [3, Algorithm 1].

2.2. Algebraic dependence decomposition

If the polynomials $q_1^{e_1}, \ldots, q_m^{e_m}$ are algebraically dependent, i.e. there exists a polynomial $p \in K[y_1, \ldots, y_m]$ in m variables called an annihilating

 $^{^3}$ In rational functions arising from IBP reductions most of the denominator factors are of degree 1.

polynomial for $q_1^{e_1}, \ldots, q_m^{e_m}$, such that $p(q_1^{e_1}, \ldots, q_m^{e_m}) = 0 \in K[\mathbf{x}]$, then we can use this equation to derive a decomposition similar to (2). For this, write

$$p = c_{\alpha} \mathbf{y}^{\alpha} + \sum_{\substack{\beta \in \mathbb{N}^m \\ \deg(p) \ge |\beta| \ge |\alpha|}} c_{\beta} \mathbf{y}^{\beta} \qquad (c_{\alpha}, c_{\beta} \in K, c_{\alpha} \ne 0)$$
(3)

such that $c_{\alpha}\mathbf{y}^{\alpha}$ is one of the terms of smallest degree (using multi-indices $\beta \in \mathbb{N}^m$, so $\mathbf{y}^{\beta} = y_1^{\beta_1} \cdot \ldots \cdot y_m^{\beta_m}$ and $\deg(\mathbf{y}^{\beta}) = |\beta| = \beta_1 + \cdots + \beta_m$). Writing \mathbf{q} for the vector $(q_1^{e_1}, \ldots, q_m^{e_m})$, it holds

$$0 = p(\mathbf{q}) \quad \Leftrightarrow \quad c_{\alpha} \mathbf{q}^{\alpha} = -\sum_{\beta} c_{\beta} \mathbf{q}^{\beta}$$

$$\Leftrightarrow \quad 1 = -\sum_{\beta} \frac{c_{\beta} \mathbf{q}^{\beta}}{c_{\alpha} \mathbf{q}^{\alpha}} = -\sum_{\beta} \frac{c_{\beta}}{c_{\alpha}} \prod_{i=1}^{m} \frac{q_{i}^{e_{i}\beta_{i}}}{q_{i}^{e_{i}\alpha_{i}}}$$

$$\Rightarrow \quad \frac{f}{g} = -\sum_{\beta} \frac{c_{\beta}}{c_{\alpha}} f \prod_{i=1}^{m} \frac{q_{i}^{e_{i}\beta_{i}}}{q_{i}^{e_{i}(\alpha_{i}+1)}}$$

$$(4)$$

and since \mathbf{y}^{α} has minimal degree, for each β in the sum in Equation (4) it holds $\beta_i \geq \alpha_i + 1$ for at least one index i, i.e. the factor q_i does not appear in the denominator of the corresponding term and thus the denominators of the rational functions in the decomposition each have at most m-1 different irreducible factors.

As with the Nullstellensatz decomposition, this step is repeated with each summand in (4). This leads to a decomposition where each denominator contains only algebraically independent factors q_i , since it can be shown [3, Corollary 3.8], that polynomials q_1, \ldots, q_m are algebraically dependent if and only if $q_1^{e_1}, \ldots, q_m^{e_m}$ are (for any $e_i \in \mathbb{N}_{\geq 1}$).

The problem of calculating annihilating polynomials can be reduced to the computation of the Gröbner basis of a certain ideal [3, Lemma 3.9, 3.10 and Algorithm 2]. But there is a simpler way of determining beforehand, whether an annihilating polynomial exists: The Jacobian criterion states, that a set of polynomials $\{g_1, \ldots, g_m\}$ is algebraically independent if an only if the Jacobian $m \times d$ -matrix of polynomials $\left(\frac{\partial g_i}{\partial x_j}\right)_{i,j}$ has full row rank over the field $K(\mathbf{x})$ of rational functions [3, Lemma 3.7]. From this it also follows, that after the algebraic dependence decomposition, in each denominator the

number of different irreducible factors is at most d (the number of variables) since an $m \times d$ -matrix with m > d cannot have full row rank and thus any d+1 polynomials are algebraically dependent.

2.3. Numerator decomposition

Note that in the previous two steps, the denominators become simpler (with respect to the number of different factors in their factorisation), but the numerators do not. In (2) and (4) the original numerator f still appears in each summand. To also shorten the numerators, it makes sense to do a division with remainder by the factors in the denominator. For a rational function f/g with factorisation $g = q_1^{e_1} \cdot \ldots \cdot q_m^{e_m}$ as above we can calculate a division expression

$$f = r + \sum_{k=1}^{m} a_k q_k \tag{5}$$

where $a_i \in K[\mathbf{x}]$ are polynomials and $r \in K[\mathbf{x}]$ is a "small" remainder. More precisely, by making use of a Gröbner basis of the ideal $I = \langle q_1, \ldots, q_m \rangle$ generated by the irreducible factors q_i we can ensure, that each term of the polynomial r is not divisible by the lead term of any element of I [3, Definition 3.4 and Algorithm 3]. We say, that r is "reduced" with respect to I. Simply multiplying (5) by f/g yields

$$\frac{f}{g} = \frac{r}{\prod_{i=1}^{m} q_i^{e_i}} + \sum_{k=1}^{m} \frac{a_k}{q_k^{(e_k - 1)} \prod_{i=1}^{m} i \neq k} q_i^{e_i}$$
 (6)

where the first term has a particularly small numerator and in each of the other terms one of the factors in the denominator cancels. Thus repeatedly applying this decomposition step results in a sum of rational functions where the numerator of any function is reduced (as defined above) with respect to (the ideal generated by the irreducible factors of) its denominator.

Note that the division expression (5) depends on the choice of a monomial ordering, i.e. a total ordering on the set $\{\mathbf{x}^{\alpha} | \alpha \in \mathbb{N}^d\}$ of monomials, that is compatible with multiplication [3, Definition 3.2]. This ordering is needed to define the "lead term" of a multivariate polynomial in the division-with-remainder algorithm. In our SINGULAR implementation we used the graded reverse lexicographic ordering [3, (3.5)] which sorts first by the degree of the monomial.

2.4. The resulting algorithm

If we do the Nullstellensatz decomposition, the algebraic dependence decomposition and the numerator decomposition one after the other, we obtain a sum of rational functions where each summand is of the form

$$\frac{f_S}{\prod_{i \in S} q_i^{b_i}} \tag{7}$$

where $S \subseteq \{1, ..., m\}$ is some set of indices, $b_i \in \mathbb{N}$, $f_S \in K[\mathbf{x}]$ and by the above

- (1) the polynomials $\{q_i|i\in S\}$ have a common zero in \overline{K}^d ,
- (2) the polynomials $\{q_i|i\in S\}$ are algebraically independent,
- (3) f_S is reduced with respect to the ideal $\langle q_i | i \in S \rangle \subseteq K[\mathbf{x}]$.

(This is Theorem 3.5 in [3].)

Since in practice, the computation of annihilating polynomials can become very slow if the degrees of the polynomials $q_i^{e_i}$ get too big, we make the following two modifications to the algorithm. Firstly, before the algebraic dependence decomposition we insert a short version of the numerator decomposition step described in 2.3, which only decomposes further if the remainder r in (5) is zero. This eliminates some of the denominator factors before going into the more complicated algebraic dependence decomposition (see also Remark 1.2 and Algorithm 4 in [3]). Secondly, the algebraic dependence decomposition step itself can be changed to using an annihilating polynomial for q_1, \ldots, q_m rather than $q_1^{e_1}, \ldots, q_m^{e_m}$. Instead of (4), we then get

$$\frac{f}{g} = -\sum_{\beta} \frac{c_{\beta}}{c_{\alpha}} f \prod_{i=1}^{m} \frac{q_i^{\beta_i}}{q_i^{\alpha_i + e_i}}.$$
 (8)

Now the number of different irreducible denominator factors does not have to decrease in every step, since it is possible, that $\beta_i < \alpha_i + e_i$ for all i. However, if in (3) we always choose α minimal with respect to the graded reverse lexicographic ordering, it can be shown, that the algorithm still terminates (see Remark 1.3 in [3]).

In our implementation of the final algorithm [3, Algorithm 5], we make use of the computer algebra system SINGULAR, which provides efficient algorithms for Gröbner basis computations as well as polynomial factorization and division with remainder.

2.5. A simple example

To demonstrate the algorithm described in 2.4 consider the rational function

$$\frac{f}{g} = \frac{x_1 + x_2}{x_1 x_2 (x_2 + 1) x_3 (x_1 - x_3)} \in \mathbb{R}[x_1, x_2, x_3]$$
(9)

with m = 5 denominator factors $q_1 = x_1$, $q_2 = x_2$, $q_3 = x_2 + 1$, $q_4 = x_3$, $q_5 = x_1 - x_3$.

In the first step (Nullstellensatz decomposition) we observe, that q_2 and q_3 have no common zeros and find the relation $1 = 1 \cdot q_3 + (-1) \cdot q_2$. Multiplying with f/g yields

$$\frac{f}{g} = \frac{x_1 + x_2}{q_1 q_2 q_4 q_5} + \frac{-x_1 - x_2}{q_1 q_3 q_4 q_5}. (10)$$

Now q_1, q_2, q_4, q_5 have the common zero $x_1 = x_2 = x_3 = 0$ and also q_1, q_3, q_4, q_5 have a common zero, namely $x_1 = x_3 = 0$, $x_2 = -1$. So condition (1) is fulfilled.

In the short numerator decomposition described in Section 2.4 we see that only the first numerator $x_1 + x_2$ has remainder 0 when dividing by the denominator factors q_1, q_2, q_4, q_5 : $x_1 + x_2 = 1 \cdot q_1 + 1 \cdot q_2 + 0$. Thus in the first term, we can cancel q_1 and q_2 respectively:

$$\frac{f}{g} = \frac{1}{q_2 q_4 q_5} + \frac{1}{q_1 q_4 q_5} + \frac{-x_1 - x_2}{q_1 q_3 q_4 q_5}.$$
 (11)

Next, in the algebraic dependence decomposition, the factors in the second and third denominator of (11) are found to be algebraically dependent, since $0 = q_1 - q_4 - q_5$. Thus $1 = \frac{q_1}{q_5} + \frac{-q_4}{q_5}$ and multiplying this to the second and third term gives the decomposition

$$\frac{f}{g} = \frac{1}{q_2 q_4 q_5} + \frac{1}{q_4 q_5^2} + \frac{-1}{q_1 q_5^2} + \frac{-x_1 - x_2}{q_3 q_4 q_5^2} + \frac{x_1 + x_2}{q_1 q_3 q_5^2}$$
(12)

in which all denominators consist of algebraically independent factors, so (2) is fulfilled.

Finally, in the numerator decomposition, the first three numerators are already reduced with respect to the denominator factors since they are just ± 1 . For the fourth numerator we get the division expression $-x_1 - x_2 = (-1) \cdot q_3 + (-1) \cdot q_4 + (-1) \cdot q_5 + 1$ and for the fifth numerator it holds

 $x_1 + x_2 = 1 \cdot q_1 + 1 \cdot q_3 + (-1)$. Substituting this into (12) yields

$$\begin{split} \frac{f}{g} &= \frac{1}{q_2 q_4 q_5} + \frac{1}{q_4 q_5^2} + \frac{-1}{q_1 q_5^2} + \frac{-1}{q_4 q_5^2} + \frac{-1}{q_3 q_5^2} + \frac{-1}{q_3 q_4 q_5} + \frac{1}{q_3 q_4 q_5^2} + \frac{1}{q_3 q_4 q_5^2} \\ &+ \frac{1}{q_1 q_5^2} + \frac{-1}{q_1 q_3 q_5^2} \\ &= \frac{1}{q_2 q_4 q_5} + \frac{-1}{q_3 q_4 q_5} + \frac{1}{q_3 q_4 q_5^2} + \frac{-1}{q_1 q_3 q_5^2} \end{split} \tag{13}$$

which now also satisfies condition (3). Note, that for this simple example the partial fraction decomposition (13) does not seem "shorter" than the original fraction f/g. However, as described in the following, for the large functions occurring in amplitude and IBP problems, this algorithm can reduce the size of rational functions by factors of more than 100.

2.6. Parallel structures in the algorithm

To reduce the runtime, it is of course possible to run the partial fractioning algorithm in parallel for all functions occurring in the problem under consideration. However, it is often the case that a small number of large functions dominate and hence determine the total runtime. Therefore it makes sense to also parallelize the PFD algorithm itself, at least for the most complicated functions in the given problem set.

In the implementation of the algorithm described above we work with a list D of terms representing a sum and start with D containing only the input rational function as single entry. Then each step of the algorithm consists of decomposing all terms in D individually into a sum/list of terms itself (as in equations (2), (6) and (8)) and then replacing D by the concatenation of these lists as well as merging terms that have the same denominator (see lines 4, 7, 10, 13 in [3, Algorithm 5]). The processing of summands can be done in parallel over all elements of D, leading to Fork/Join patterns, which can be used for parallelization. We discuss parallelism in detail in the subsequent sections.

3. Parallel computing using the Singular/GPI-Space framework

The implementation of our RREF algorithm and the partial fraction decomposition algorithm is part of the SINGULAR/GPI-SPACE framework project for massively parallel computations in computer algebra [15]. This

framework combines the open source computer algebra system SINGULAR [17] with the workflow management system GPI-SPACE [18], developed at the Fraunhofer Institute ITWM. It originates in an effort to realize massively parallel computations computer algebra, and has bee used for a variety of problems, for example, from commutative algebra, algebraic geometry, and tropical geometry [15, 19, 20, 21, 22].

In the present section, we discuss the application of the SINGULAR/GPI-SPACE framework to the partial fraction decomposition. The application of the framework to the RREF problem has already been addressed in [23]. Though our aim is an efficient parallel implementation of the partial fraction decomposition problem, the programming constructs developed along our way in terms of Petri nets are in fact useful in its own right and may be used in other algorithmic problems with a similar structure: While the WaitAll workflow is obviously essential in countless settings where the problem splits into independent (possibly very unevenly sized) subproblems, the Fork/Join workflow will, for example, also be applicable to modular computations relying on a Chinese Remainder lift.

3.1. GPI-SPACE AND SINGULAR

The task-based workflow management system GPI-SPACE is based on Gelernter's approach of separating coordination and computation [24]. The idea is that through a coordination language, a computation can convey information to another computation whose state is evolving and unpredictable.

To realize an implementation of this approach, GPI-SPACE provides three main components: a distributed runtime system, that manages the resources (assigning jobs to cores); a virtual memory layer, which allows computations to access common data, and a workflow engine, which provides the coordination layer. In the coordination layer, the user specifies a program relying on the language of Petri nets [25]:

Definition 3.1. A Petri net is a bipartite directed graph N = (P, T, F), where where P and T are disjoint, finite sets, and

$$F \subseteq (P \times T) \cup (T \times P).$$

The set P contains the *places* of the net, the set T the *transitions*. The set F is called the *flow relation* of the net. If $(p,t) \in F$ then we say p is an *input* of t and if $(t,p) \in F$ we say p is an *output* of t.

In addition to this static part of the concept of Petri nets, there are dynamic aspects describing the execution of the net.

Definition 3.2. A marking of N is a map $M: P \to \mathbb{N}_0$.

A marking defines the state of the Petri net, and may be thought of as a map that counts a number of tokens on a given place.

Definition 3.3. We say that M enables the transition t of N if, for all p such that $(p,t) \in F$, we have M(p) > 0.

If a Petri net equipped with a marking has an enabled transition, the transition can be *fired*. Firing is a process which maps a given marking marking M to a new marking M', defined by

$$M'(p) := M(p) - |\{(p,t)\} \cap F| + |\{(t,p)\} \cap F|.$$

for all $p \in P$. Firing a transition can be thought of as that transition consuming a token from each input and placing a new token on each output. A Petri net with a marking is *executed* by firing random enabled transitions.

In its implementation, GPI-SPACE expands the concept of a Petri net in the sense that tokens can be complex data structures. Transitions run code on that data and the result usually determines the data carried by the tokens placed on the output places of the respective transition. GPI-SPACE also allows the user to put conditionals on transitions: A transition can inspect the contents of an input token without consuming it (yet) and only accept it provided the stated conditions are met.

Fundamental functionality of our SINGULAR library that implements the algorithmic building blocks of the partial fraction decomposition is executed by the C-library version of SINGULAR and is then wrapped into transitions of a GPI-SPACE Petri net that models the coordination level structure of the algorithm. Our implementation in GPI-SPACE is, in turn, configured and called from a standard SINGULAR for transparent and convenient user interaction.

3.2. Algorithmic realization of the partial fraction decomposition based on Petri nets

The elements of a set of rational function coefficients are decomposed using a workflow implemented in GPI-SPACE. Parallelism is achieved by two mechanisms: first, the Petri net processes different functions in parallel

using a WaitAll approach, which is depicted in Figure 1, and second, by parallelizing the algorithmic sub-steps of the PFD algorithm applied to an individual function using a Fork/Join approach on the terms, which is implemented in the Petri nets shown in Figures 2 and 3. Note that the concept a of Petri net is modular, and the Petri net in Figure 3 is a subnet of that depicted in Figure 2, taking the place of the transition/subnet depicted as a cloud. The net in Figure 2 is in turn a subnet of that in Figure 1. The overall Petri net leads to an intertwined form of parallelism which is able to handle the decomposition of terms of different IBP coefficients at different stages of the PFD algorithm in parallel, which leads to an efficient utilization of the resources und thus a good parallel efficiency.

We remark that Figures 1 and 3 have a similar structure, with the major addition of a parallel merge mechanism in the latter. In Figure 3, the results of the parallel computations are all part of the same problem and hence need to be recombined, whereas in Figure 1, the results are unrelated and treated individually.

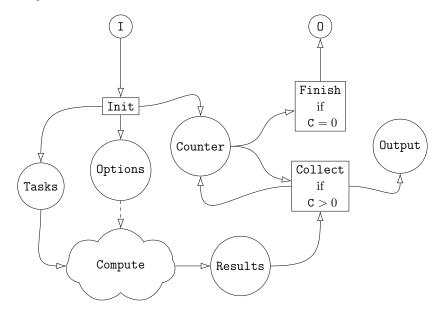


Figure 1: The WaitAll Petri net to parallelize over an input tuple

In the following, we briefly discuss each Petri net by listing first the places, followed by the transitions that connect to the various places.

We begin with Figure 1. Place I is initialized with an input token provided by the client program (SINGULAR implementing the user interface),

and contains, in particular, the given set of rational functions. The transition Init then uses this data to set up various other places: The tokens on Tasks each represent a function to be decomposed. The single token on the place Counter has a field storing the total number of computations to be performed and a field counting the number of finished computations which is initialized with zero. The place Options holds a token with read-only input data and auxiliary technical data for the compute transition.⁴ Tokens on the place Results will represent finished computations. These finished computations will be passed to the place Output, where the client program can then collect them. The place O will be used to indicate by the presence of a token that the Petri net has finished with all computations ready for collection at Output.⁵ In our application, the transition/subnet Compute calls the Petri net depicted in Figure 2. The transition/subnet consumes a token from Tasks and reads the values at Options. This information is then used to perform the desired partial fraction decomposition for the respective function. Once a computation has finished, a token is placed on Results. The Collect transition fires conditionally on the token on Counter being strictly greater than 0, that is, that not all computations that were started have finished. In that case, it consumes a token from Results, decrements the token on Counter by one, and passes the token on to the place Output. Once the value of C equals 0, the condition for the transition Finish is met, and the transition places a token on 0. The client program then collects the results on the place Output.

The net in Figure 2 is a subnet of Figure 1 representing Compute and, hence, must take as input and output the same token types as the Compute transition/subnet in Figure 1. The place I in Figure 2 takes rational functions. Although not displayed explicitly, information on the place Options of Figure 1 is used by transitions in Figure 2. Tokens on the place Tasks hold two fields, one corresponding to the rational function and a boolean flag status, indicating that no further computation on this function is needed. The places between the computational steps are unmarked, as these only hold the tokens passed on between the steps. Once all the steps are completed for a given function, the corresponding result is placed on 0.

⁴Note that, if we want to copy data from an input token of a transition to an output token, it is possible and typically preferable to only copy a reference to the actual data.

 $^{^5\}mathrm{Data}$ in the token may be used to pass, for example, debugging information to SINGULAR.

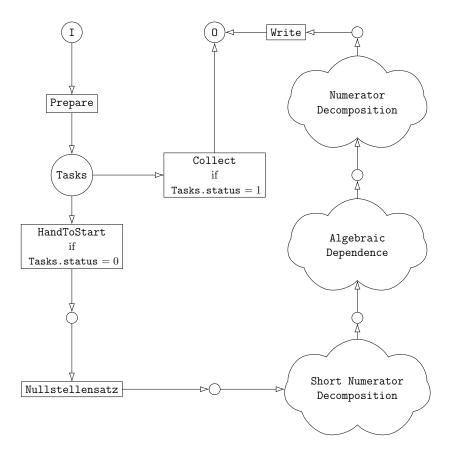


Figure 2: The subnet calculating the partial fraction decomposition.

The transition Prepare consumes the input token provided on I and prepares the input data so that we can work in the decomposition steps with a consistent input/output format. As part of this process, it checks whether the rational function is zero or has constant denominator, in which case the the data field status of the token put on Tasks is given the value 1 to indicate that no further computation is needed. In this case, the Collect transition consumes the token at Tasks and passes it on to 0. Otherwise, Prepare assigns the status value 0 to the token (indicating the computation is not yet complete), which is then handed on to the input place for the transition Nullstellensatz. This transition computes the Nullstellensatz decomposition in SINGULAR by applying the respective function provided in our library pfd.lib.

The Petri net depicted in Figure 3 is used to realize each of the decom-

position steps ShortNumeratorDecomposition, AlgebraicDependence and NumeratorDecomposition in a parallel way over the summands received as input, relying on a Fork/Join approach: The list of input summands is split into individual tokens, which are then decomposed in parallel. The resulting lists of summands are merged before being handed over to the next transition. The merge step at the end of such a decomposition often leads to cancelation, which reduces the size of the output and speeds up the computation. Note that, as the fork process is done in our approach with respect to the summands of the input, this does not lead to additional parallelism for the Nullstellensatz transition, that is, this transition is parallel only over the different rational functions. Finally, the Write transition writes the resulting decomposition in various serialization formats, before handing a token to 0 to signal that the algorithm has finished.

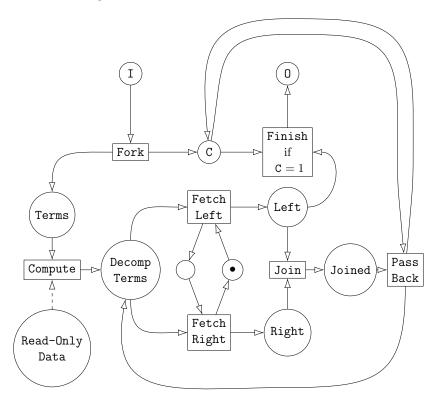


Figure 3: The Fork/Join subnet to parallelize over the decomposition of terms.

We discuss the Fork/Join process illustrated in Figure 3 in more detail.

The aim is to fork into a number of parallel computations, and join two results into one via a parallel approach until only a single token is left, which then is put on the output place. The Fork step takes a token representing a list of terms (corresponding to a sum) and splits it into a partition of sublists of approximately equal length, which in turn are handled in parallel. Once a Compute task has been finished, the corresponding token with a list of terms is put on DecompTerms. A pair of transitions - FetchLeft and Fetch Right - are responsible for dividing these summands evenly into the two input places for the Join transition, which combines the two lists into one (with possibly cancellation occurring) and puts the resulting token on its output place Joined. The place C is used to keep count of the number of tokens still to be merged and to enable the Finish transition once there is only a single token remaining. Consuming a token from Joined, the transition PassBack decrements the counter for the number of parallel results to still to be merged by one and places the token onto DecompTerms.

The fetch transitions ensure that whenever a token is put on Left, the following token is placed on Right by passing a control token between two control places. A trivial inductive argument on the number of tokens on Left, Right and DecompTerms shows that once all the summands have been merged together, the final token will be placed at Left. At this point, the Finish step will collect the token and place a finishing token at O.

Remark 3.4. If the input sizes of the rational functions are varying significantly, the randomized nature of the execution of the Petri net will lead to some drop in efficiency due to late scheduling of long-running jobs. This can be remedied by scheduling the hardest problems first. In Figure 4 we provide a variation of the WaitAll net that provides a simple but useful realization of this strategy. The transition Init generates a token with a list with the rational functions on the place TaskList such that the entries are sorted by byte size. The transition Extract extracts and deletes the entry of largest byte size, places it on Tasks and decrements TaskList.count by one.

4. Instructions on how to use the massively parallel PFD application

Our framework can be used from the interactive SINGULAR command line or from within SINGULAR libraries. In order to do so, the PFD-PARALLEL

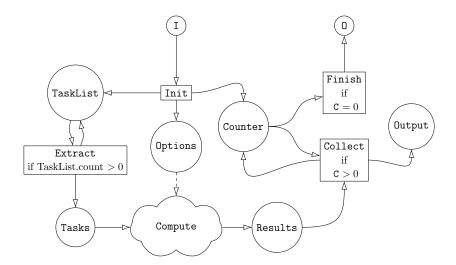


Figure 4: The WaitAll Petri net with pre-sorting by input file size

package and its dependencies have to be installed. This includes GPI-SPACE, GPI-2, and SINGULAR.

We provide a one-line-installation for Linux environments based on the SPACK package manager [16]. Detailed instructions can be found in the Github repository of our application:

https://github.com/singular-gpispace/pfd-parallel

These instructions are self contained in the sense that they include the installation of SPACK, and the installation of our package with installation of all dependencies. The project has been tested on Centos 7 and 8 and Ubuntu 18.04 LTS and 20.04 LTS. While we also provide manual installation instructions, we recommend the use of Spack, since it takes care of all dependencies automatically.

Assume that \${example_ROOT} has been set to some directory accessible from all nodes involved in the installation and computation. The Spack install will set, relying on \${example_ROOT}, the following environment variables: \$PFD_INSTALL_DIR, which is the directory where our application was installed, and \$SINGULAR_INSTALL_DIR, which is the directory where SINGULAR was installed. Change directory to \${example_ROOT}:

cd \${example_ROOT}

To run our example, we have to create some configuration and input data in ${\text{example}_R00T}$:

• A nodefile with the machines to be used as nodes (one line per node). For example, the following command generates such a file with just the current machine:

```
hostname > hostfile
```

• Optionally, the GPI-SPACE Monitor can be started to display computations in form of a Gantt diagram (to use the monitor, you need an X-Server running). In case you do not want to use the monitor, you should not set in SINGULAR the fields options.loghostfile and options.logport of the GPI-SPACE configuration token (see below). In order to use the GPI-SPACE monitor, we need a loghostfile with the address of the machine running the monitor.

```
hostname > loghostfile
```

On this machine, we start the monitor, specifying a TCP port where the monitor will receive information from GPI-SPACE. The same port has to be specified in the configuration token in the field options.logport (see below).

```
${PFD_INSTALL_DIR}/libexec/bundle/gpispace/bin/gspc-monitor --port 9876
```

• To create some example files with input, we copy data included in the PFD install directory:

```
mkdir -p ${example_ROOT}/input
mkdir -p ${example_ROOT}/results
cp -v ${PFD_INSTALL_DIR}/example_data/* ${example_ROOT}/
input
```

These files contain the entries of a 1x10 row of matrix of rational functions for which the partial fraction decomposition should be computed.

• Finally, a directory for temporary files is need. This directory will be used during runtime, and should be accessible from all machines involved in the computation:

```
mkdir ${example_ROOT}/tempdir
```

We can now start SINGULAR, telling it where to find the library and the shared object file for the PFD application:

```
SINGULARPATH="$PFD_INSTALL_DIR/LIB" $SINGULAR_INSTALL_DIR/bin/Singular
```

In the SINGULAR interpreter shell, enter the following code to setup the framework (or make similar code part of a library you are writing):

```
LIB "pfd_gspc.lib";
configToken gspcconfig = configure_gspc();
gspcconfig.options.tempdir = "tempdir";
gspcconfig.options.nodefile = "hostfile";
gspcconfig.options.procspernode = 8;
```

If the GPI-SPACE monitor is supposed to be used then also do:

```
gspcconfig.options.loghostfile = "loghostfile";
gspcconfig.options.logport = 9876;
```

We also define a configuration token for the PFD algorithm:

```
configToken pfdconfig = configure_pfd();
pfdconfig.options.inputdir = "input";
pfdconfig.options.filename = "xb_deg5";
pfdconfig.options.suffix = "ssi";
pfdconfig.options.parallelism = "intertwined";
pfdconfig.options.algorithm = "Leinartas";
pfdconfig.options.outputformat = "ssi,cleartext,
    indexed_numerator_denominator";
pfdconfig.options.outputdir = "results";
```

This will

- load the Singular library providing access to the PFD-PARALLEL application,
- add information where to store temporary data (in the corresponding field options.tempdir of the GPI-SPACE configuration token) with the path corresponding to the directory created above,
- specify where to find the nodefile (in the field options.nodefile of the GPI-SPACE configuration token), and
- set how many processes per node⁶ should be started (in the corresponding field options.procspernode of the GPI-SPACE configuration token,

⁶A version of the framework which allows the user to set the number of cores individually for each node is under development.

usually one process per core, not taking hyper-threading into account; you may have to adjust according to your available resources),

- specify the address of the GPI-SPACE monitor (this step is optional),
- specify a base file name used for accessing the array of input files by appending the indices, along with the path where the input files are located, and the path where the output files should be written (in the respective fields options.filename, options.inputdir, and options.outputdir of the PFD configuration token)⁷,
- specify the input format (field options.inputformat), see Remark 4.1 below for a discussion of the formats⁸,
- specify the output formats (field options.outputformat, see again Remark 4.1 below; note that multiple output formats can be requested at the same time),
- specify the parallelization strategy to be used (by specifying the field options.parallelism of the PFD configuration token), where the field can take the values waitAll, intertwined, or size_strategy for a parallelization over the different rational functions, for using in addition parallelism for the individual rational functions, and for handling the rational functions serially or in parallel depending on the size of the input coefficient, respectively; in the latter case, options.percentage has to be set to an integer $0 \le p \le 100$ to specify that the p/100 largest of all input functions should be processed with parallelism per individual function, and
- choose the algorithm to be used (Leinartas or MultivariateApart for our SINGULAR implementations of the respective algorithms) by specifying the field options.algorithm of the PFD configuration token; note that

⁷Note that in more complex environments like a cluster, it is usually preferable to specify absolute paths, in particular, for the nodefile and the temporary directory. Specifying the results directory is optional, and only necessary if the result directory should be different from the input directory.

⁸Note that if ssi is specified the program assumes that the data is available in the high-performance SINGULAR serialization format ssi, while if txt is specified, and the respective ssi file is not present in the input folder, the program automatically converts the text format to ssi, and continues with the ssi format.

this option affects only the sequential processing of individual functions, while parallel processing of individual functions is always done with our parallel Leinartas algorithm (since the MultivariateApart algorithm is not parallel).

Remark 4.1. Note that the input can be specified in one of two formats: a human-readable text-based format, or a data structure encoded in the high-performance SINGULAR ssi serialization format. Our implementation outputs results in a number of formats: the same ssi based format as used for input; a self contained, human-readable text-based mathematical expression (cleartext); a human-readable, indexed, text-based mathematical expression, where the numerators and denominators are factorized and the unique factors represented by indexed variables (indexed_numerator_denominator); and a similar format, where only the denominators are factorized and indexed (indexed_denominator). The correspondence between the indexed variables and the factors is encoded in an additional file, so the output in the indexed formats consist of two files. When analyzing the byte size of the results of our algorithms, we usually consider the sum of the size of both files in the indexed_numerator_denominator format.

Once the framework and the algorithm are configured, we can run the computation, specifying the indices of the array of input files (generated above) which should be processed:

5. Examples for partial fraction via large scale parallelizations

In this section, we apply our multivariate partial fractioning framework in the case two examples, simplifying rational functions occurring in IBP reduction coefficients and in analytic multiloop scattering amplitudes. We provide timings and an analysis of compression ratios to demonstrate the power of our framework.

⁹While the ssi format contains the information about the polynomial ring containing the numerators and denominators, using the text format requires that in the controlling SINGULAR instance the polynomial ring is already defined

5.1. Simplifying IBP reduction coefficients

We consider in this section the nonplanar two-loop five-point diagram (Figure 5) as an example. All external and internal lines are massless. The

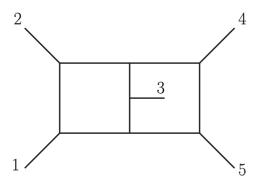


Figure 5: Two-loop five-point nonplanar "double pentagon" diagram

kinetic conditions are $2p_1 \cdot p_2 = s_{12}$, $2p_2 \cdot p_3 = s_{23}$, $2p_3 \cdot p_4 = s_{34}$, $2p_4 \cdot p_5 = s_{45}$ and $2p_1 \cdot p_5 = s_{15}$. The propagators are

$$D_{1} = l_{1}^{2}, \quad D_{2} = (l_{1} - p_{1})^{2}, \quad D_{3} = (l_{1} - p_{12})^{2}, \quad D_{4} = l_{2}^{2},$$

$$D_{5} = (l_{2} - p_{123})^{2}, \quad D_{6} = (l_{2} - p_{1234})^{2}, \quad D_{7} = (l_{1} - l_{2})^{2},$$

$$D_{8} = (l_{1} - l_{2} + p_{3})^{2}, \quad D_{9} = (l_{1} - p_{1234})^{2}, \quad D_{10} = (l_{2} - p_{1})^{2},$$

$$D_{11} = (l_{2} - p_{12})^{2},$$

$$(14)$$

where $p_{i...j} = \sum_{k=i}^{j} p_k$. For this diagram, the UT basis and the corresponding symbol form was given in refs. [26, 27], while refs. [27, 28] provided the analytic evaluations. In ref. [23], the analytic IBP reduction coefficients for the integrals with ISP up to the degree 4 in the top sector were calculated. In ref. [3], using the improved Leinartas' algorithm in Section 2, the size of the IBP coefficients up to degree 4 with respect to the UT basis was decreased from 700MB to 19MB by rewriting the rational functions in terms of a partial fraction decomposition. Recently, integrals for this diagram with irreducible scalar product (ISP) of degree 5 have been reduced to a well-chosen basis in ref. [29], making use of the systems of block triangular system given in refs. [30, 31, 32]. In the choice of basis of ref. [29], the analytic reduction coefficients have a size of ~ 25 GB.

In this section, we reduce the relevant target integrals, that is, the 47 topsector integrals with ISPs up to degree 5, to a UT basis, and show that the coefficients can be greatly simplified further by relying on our PFD-PARALLEL package.

We use the module intersection method [23] to obtain a simple IBP system for reducing target integrals. As has been already observed for the relations up to degree four, the number of IBP relations and corresponding size is much smaller than those generated by the traditional Laporta algorithm. As shown with some more detail in Table 1, the total size of the system is only 17 MB. The IBP generation step finishes within one hour on a single core. See also ref. [32] for generating a simple integral relation system for the same diagram.

Table 1: The IBPs system for the "double-pentagon" integrals with numerator degree up to 5, generated on the spanning cuts, relying on the module intersection method.

Cut	# relations	# integrals	size
{1,5,7}	2723	2749	1.4 MB
$\{1,5,8\}$	2753	2777	1.6 MB
$\{1,6,8\}$	2817	2822	2.1 MB
${2,4,8}$	2918	2921	2.1 MB
$\{2,5,7\}$	2796	2805	1.5 MB
$\{2,6,7\}$	2769	2814	1.2 MB
$\{2,6,8\}$	2801	2821	1.6 MB
${3,4,7}$	2742	2771	1.4 MB
${3,4,8}$	2824	2849	1.9 MB
${3,6,7}$	2662	2674	1.5 MB
$\{1,3,4,5\}$	1600	1650	$0.72~\mathrm{MB}$

We solve the IBP system generated via the module intersection method by numeric linear algebra and interpolation. Since the IBP reduction coefficients tend to have simple denominators in a UT basis [3], we interpolate the coefficients for a UT basis. The coefficients are rational functions in $s_{12}, s_{23}, s_{23}, s_{23}, s_{23}, s_{23}, \epsilon$ and ϵ_5 , where $\epsilon_5 = 4\sqrt{-1}\epsilon_{\mu_1\mu_2\mu_3\mu_4}p_1^{\mu_1}p_2^{\mu_2}p_3^{\mu_3}p_4^{\mu_4}$ is from the UT integral definition.

As illustrated in [3], the denominators of the IBP reduction coefficients

for this diagram when using a UT basis contain factors either in ϵ or symbol letters. With a semi-numeric computation, we determine all irreducible factors in the denominators of the IBP reduction coefficients and their expression in terms of the factors. For the example under consideration, the factors are:

$$\epsilon - 1, \quad 2\epsilon - 1, \quad 3\epsilon - 1, \quad 4\epsilon - 1, \quad 4\epsilon + 1, \quad s_{12}, \quad s_{15}, \quad s_{15} - s_{23}, \quad s_{23},
s_{12} + s_{23}, \quad s_{12} - s_{34}, \quad s_{12} + s_{15} - s_{34}, \quad s_{15} - s_{23} - s_{34}, \quad s_{34}, \quad s_{23} + s_{34}
s_{12} - s_{45}, \quad s_{23} - s_{45}, \quad s_{12} + s_{23} - s_{45}, \quad s_{12} - s_{15} + s_{23} - s_{45}, \quad s_{12} - s_{34} - s_{45},
s_{12} + s_{15} - s_{34} - s_{45}, \quad s_{45}, \quad s_{15} - s_{23} + s_{45}, \quad s_{34} + s_{45}, \quad \epsilon_{5}$$
(15)

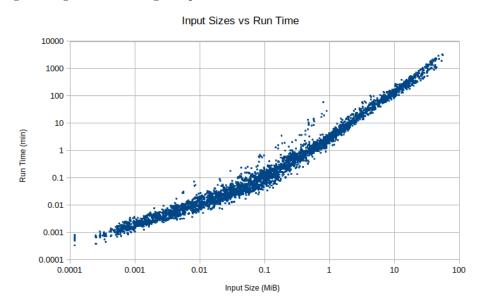
Knowing the denominators, we analytically calculate the numerators via polynomial interpolation (which is computationally easier than rational function interpolation). To perform the computation, we take $s_{12}=1$, and determine the maximum degrees in the other variables by numertic tests. We then do the reduction with symbolic variables s_{45} and ϵ , and 307200 numerical tuples of values for the remaining variables. Via polynomial interpolation, the analytic expressions of the IBP reduction coefficients are obtained. The variable s_{12} is then restored. The interpolation of the numerators finishes within 3 hours on 210 CPU cores. Restoring s_{12} by dimensional analysis can be done within 3 hours on 20 CPU cores. The resulting analytic expressions for the reduction coefficients form a 47×108 matrix, which takes about 19.6 GB of disk space.

We then use PFD-PARALLEL to simplify this huge set of coefficients. When using one layer of parallelization over the different coefficients, our implementation of the improved Leinartas algorithm can simplify the 19.6 GB data set of the original reduction coefficients to expressions of a total size of 186 MB within 68 hours of parallel computation on 350 cores. We remark that using the improved Leinartas algorithm or the MULTIVARIATEAPART algorithm (both implemented in our framework and available as computational backend) produce a similar output size and computation time. Figure 6 shows a scatterplot of the run times of the improved Leinartas algorithm against the input file sizes for the IBP reduction coefficients

While this form of parallelism of course provides a significant speedup

 $^{^{10}\}mathrm{We}$ use a cluster consisting of 10 nodes with two Intel Xeon Gold 6230R CPUs and 768 GB RAM each.

Figure 6: A scatterplot of the run times of the improved Leinartas algorithm against the input file sizes for the IBP reduction coefficients for the five-point non-planar "double pentagon" diagram for the degree up to 5.



compared to a sequential computation as well as compared to a parallel computation relying on an a priori partitioning of the set of jobs into batches, the approach is not as efficient as one would desire: Most of the coefficients require only less then 3 hours to finish, and our implementation achieves almost full utilization of the available resources as long as there are unprocessed tokens to fill the cores. However, there are various long-running IBP coefficients, including one which decomposes in about 68 hours and thus dominates the overall run-time. As a result, this form of parallelism is exhausted in the above mentioned computation and increasing the number of cores cannot lead to a further speedup.

Therefore, we use a second layer of parallelism available for the improved Leinartas algorithm (and described in Sections 2.6 and 3.2) to speed up the decomposition of the individual IBP coefficients. This Petri-net based approach (detailed in Figures 2 and 3) can decompose the most complicated coefficient in less than 12 hours. We remark that the best achieved with standard task-based parallelism in Singular was about 19 hours. Applying the Petri net based parallelization with two layers of parallelism, PFD-PARALLEL

finishes the decomposition for the complete set of IBP coefficients in about 22 hours and 15 minutes on 520 cores.¹¹

Table 2 shows the size of the IBP coefficients before and after applying the partial fraction decomposition, specified for different numerator degrees of the Feynman integral. We observe that the compression ratio for the IBP reduction coefficients increases with the numerator degree.

Table 2: Compression ratio of UT basis IBP reduction coefficients of the "double-pentagon" integral with different numerator degrees

degree	original size	compressed size	compression ratio
2	73.1KB	52.4KB	1.4
3	23.6MB	1.69MB	14
4	1.19GB	20.7MB	59
5	18.4GB	163MB	115
total	19.6GB	186MB	108

Figure 7 shows a scatterplot of the output file sizes against the input file sizes, and Figure 8 details the compression ratios vs the input file sizes. The final result for the IBP coefficients in the setting of this example can be downloaded from

https://www.dropbox.com/s/v64rp4saphi1czh/double_pentagon_deg5_ IBP.tar.gz

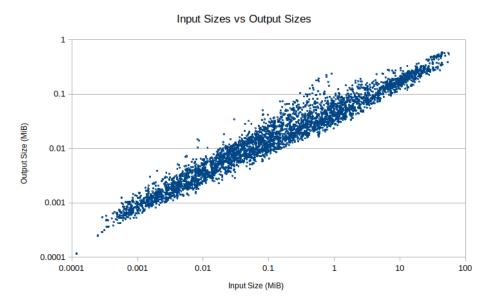
containing a file with a 47×108 matrix where each row corresponds to a target integral being reduced and each column corresponds to an UT integral in the basis. The UT basis and the target integrals are also provided under this link.

5.2. Simplifying analytic multi-loop scattering amplitudes

Our program can in the same way be used to simplify analytic coefficients in the results of multi-loop scattering amplitude computations. In this sec-

¹¹We expect that increasing the resources for the computation will lead to a further speedup, limited by the performance of the parallel computation of the most difficult coefficient.

Figure 7: A scatterplot of the output file sizes against the input file sizes for the IBP reduction coefficients for the five-point non-planar "double pentagon" diagram for the degree up to 5.



tion, we consider the complicated coefficients arising in the result of [14] on the two-loop leading colour helicity amplitudes for $W\gamma+j$ production at the LHC.

Our goal is to simplify the most complicated coefficients of the finite remainder in ref. [14]. These coefficients explicitly are 452 rational functions in terms of the kinematic variables,

$$s_{12}, s_{123}, s_{23}, s_{234}, s_{34}, s_{56}$$
 (16)

The denominators of the rational functions are factored. Among them, there are 20 linear denominator factors as

$$s_{12}, s_{23}, s_{12} + s_{23} - s_{123}, s_{23} - s_{234}, s_{12} - s_{34} - s_{123},$$
 (17)

$$s_{12} + s_{23} - s_{34} - s_{123}, -s_{34} + s_{234}, s_{12} - s_{34} + s_{234}, s_{34},$$
 (18)

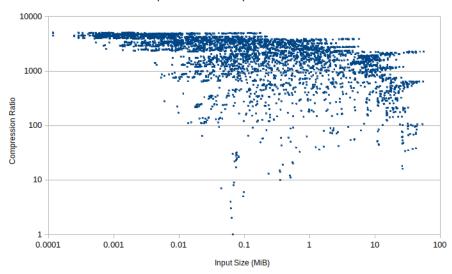
$$s_{23} + s_{34}, s_{34} - s_{234}, s_{23} + s_{34} - s_{234}, -s_{56} + s_{123}, -s_{56} + s_{234},$$
 (19)

$$s_{12} - s_{56} + s_{234}, -s_{23} - s_{56} + s_{123} + s_{234}, s_{12} - s_{34} - s_{56} + s_{234},$$
 (20)

$$s_{56} - s_{234}, s_{23} + s_{56} - s_{123} - s_{234}, -s_{12} + s_{34} + s_{56} - s_{234},$$
 (21)

Figure 8: A scatterplot of the compression ratios against the input file sizes for the IBP reduction coefficients for the five-point non-planar "double pentagon" diagram for the degree up to 5.

Input Sizes vs Compression Ratio



12 quadratic denominator factors as

$$s_{12}s_{56} - s_{12}s_{123} + s_{34}s_{123} - s_{56}s_{123} + s_{123}^2, (22)$$

$$s_{12}s_{123} - s_{34}s_{123} + s_{56}s_{123} - s_{123}^2 - s_{12}s_{56}, (23)$$

$$s_{123}s_{234} - s_{23}s_{56}, s_{23}s_{56} - s_{123}s_{234}, (24)$$

$$s_{12}^2 - 2s_{12}s_{34} + s_{34}^2 + s_{23}s_{56} - s_{12}s_{123} + s_{34}s_{123} + s_{12}s_{234}$$

$$-s_{34}s_{234} - s_{123}s_{234}, (25)$$

$$s_{34}s_{234} + s_{123}s_{234} - s_{12}s_{234} - s_{23}s_{56} - s_{34}s_{56}, (26)$$

$$s_{34}s_{234} + s_{56}s_{234} - s_{12}s_{234} - s_{234}^2 - s_{34}s_{56}, (27)$$

$$s_{12}s_{23} - s_{23}s_{34} - s_{23}s_{56} - s_{34}s_{56} - s_{12}s_{234} + s_{23}s_{234} + s_{34}s_{234} + s_{56}s_{234} - s_{234}^2,$$

$$(28)$$

$$s_{34}s_{56} + s_{12}s_{234} + s_{23}s_{234} - s_{34}s_{234} - s_{123}s_{234}, (29)$$

$$s_{23}s_{56} + s_{34}s_{56} + s_{12}s_{234} - s_{34}s_{234} - s_{123}s_{234}, \tag{30}$$

$$s_{34}s_{56} + s_{12}s_{234} - s_{34}s_{234} - s_{56}s_{234} + s_{234}^2, (31)$$

$$s_{12}^2 - 2s_{12}s_{34} + s_{34}^2 - 2s_{12}s_{56} - 2s_{34}s_{56} + s_{56}^2, (32)$$

and a degree-4 denominator factor as

$$s_{12}^{2}s_{23}^{2} - 2s_{12}s_{23}^{2}s_{34} + s_{23}^{2}s_{34}^{2} - 2s_{12}s_{23}^{2}s_{56} - 4s_{12}s_{23}s_{34}s_{56} - 2s_{23}^{2}s_{34}s_{56} + s_{23}^{2}s_{56}^{2} + 2s_{12}s_{23}s_{34}s_{123} - 2s_{23}s_{34}^{2}s_{123} + 2s_{23}s_{34}s_{56}s_{123} + s_{34}^{2}s_{123}^{2} - 2s_{12}^{2}s_{23}s_{234} + 2s_{12}s_{23}s_{34}s_{234} + 2s_{12}s_{23}s_{56}s_{234} + 2s_{12}s_{23}s_{123}s_{234} + 2s_{12}s_{34}s_{123}s_{234} + 2s_{23}s_{34}s_{123}s_{234} - 2s_{23}s_{56}s_{123}s_{234} - 2s_{34}s_{123}^{2}s_{234} + s_{12}^{2}s_{234}^{2} - 2s_{12}s_{123}s_{234}^{2} + s_{123}^{2}s_{234}^{2}$$

$$(33)$$

We observe that the representation of the functions can be significantly simplified by our PFD-PARALLEL package, thus reducing the size of the data by a large factor. We rely on our implementation of the MULTIVARIATEAPART algorithm, since the Leinartas algorithm does not perform well with regard to compression ratio and hence computation time in this example. We remark, that an automatism is under development to run different algorithmic strategies competitively using a wait-first parallelism to automatically obtain the best possible computation time or compression factor.

The computation was run on a single node with 48 CPU cores and 385 GB of RAM. The byte sizes of the input and output, along with the total runtime and compression ratio, are shown in Table 3.

Table 3: Input and output sizes of the rational functions in the two-loop leading colour helicity amplitudes for $W\gamma + j$ production. Here "ssi" means the data file format of SINGULAR. The words "indexed text" means results with abbreviated names of irreducible factors.

Compression ratio	Time	Output size (MB)		ze (MB)	Input size (MB)	
		indexed text	text	ssi	ssi	text
187.60	5h34m	5.85	9.24	9.20	392.30	1096.76

The indexed text output byte size vs the text input byte size is illustrated as a scatter plot in Figure 10. The the compression ratio vs the text input byte size (for the indexed output format) are shown in a similar fashion in Figure 11. The output result after the partial fraction, can be downloaded from,

 $\verb|https://www.dropbox.com/s/xgfj6x1qg25n44w/pfd_W_FiniteRemainder.tar.gz|$

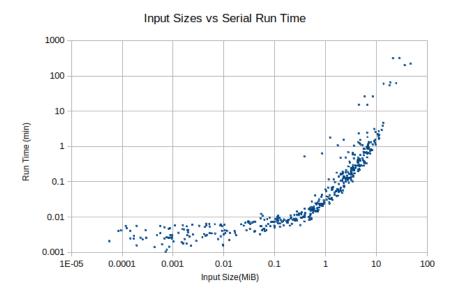


Figure 9: Scatterplot of computation times vs input byte size for the two-loop leading colour helicity amplitudes for $W\gamma + j$ production.

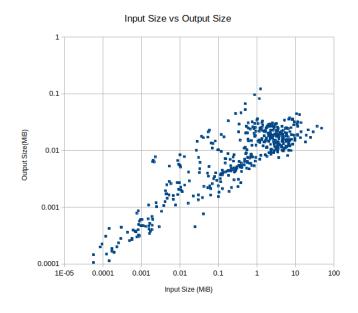


Figure 10: Scatterplot of output byte size vs input byte size for two-loop leading colour helicity amplitudes for $W\gamma+j$ production.

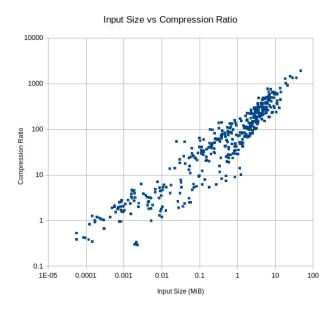


Figure 11: Scatterplot the compression ratio vs the input byte size for the two-loop leading colour helicity amplitudes for $W\gamma + j$ production.

6. Summary

In this paper, we present a massively parallel implementation of the multivariate partial fraction algorithms from [3] and [4]. Our implementation relies only on open source software. Based on the Singular/GPI-Space framework for parallel computations in computer algebra, it combines parallelisation over different target coefficients, and a parallel decomposition of individual coefficients. Using this approach, problems where individual coefficients dominate the overall run-time can be handled in an efficient way. In the paper, we demonstrate the power of our package by cutting-edge examples: (1) simplifying very complicated IBP reduction coefficients (2) rational function coefficients in analytic multiloop scattering amplitudes. We expect that our package can be of essential use in multiloop amplitudes computations.

The workflow of multivariate partial fraction computation with several levels of parallelism is realized in an efficient way using the workflow management system GPI-SPACE. The approach is based on the idea of separation of coordination and computation, and models the fundamental algorithmic structure in form of a Petri net. This allows for automated parallelisation,

makes the code easily maintainable and suitable for transparently incorporating future improvements. The Petri net based parallelisation methods developed in this paper are expected to be useful in a much broader sense, for example, for applications in modular computations. Respective code is under development.

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