# Reconstructing Rational Functions with FireFly

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We present the open-source C++ library FireFly for the reconstruction of multivariate rational functions over finite fields. We discuss the involved algorithms and their implementation. As an application, we use FireFly in the context of integration-by-parts reductions and compare runtime and memory consumption to a fully algebraic approach with the program Kira.

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## 1 Introduction

The interpolation of polynomials has been researched since the 18th century and some of the algorithms, e.g. Newton's interpolation algorithm [1], are still used today. They use black-box probes, i.e. evaluations at numerical values, of the to be interpolated function, the black box, for the interpolation. However, these original algorithms were designed for univariate polynomials and are costly to generalize to the multivariate case. Interpolation algorithms specific for multivariate polynomials have been studied intensively for several decades, e.g. in Refs. [2–9].

The interpolation of rational functions is a younger field of research, even though Thiele's univariate interpolation formula [1] has been known for more than one hundred years. To our knowledge, the first multivariate algorithm came up in the early 1990s. Grigoriev, Karpinski, and Singer presented an algorithm to obtain a bound on the degrees of numerator and denominator, then build a system of equations, and solve it for all possible coefficients [10–12]. This is a dense algorithm, i.e. it assumes that all coefficients of the rational function up to the bounds are non-zero. The next algorithm was presented by Khodadad and Monagan in Ref. [13] in 2006 and is based on the Extended Euclidean Algorithm [14]. In the following year, Kaltofen and Zhang published an algorithm based on the separate evaluation of numerator and denominator [15]. It also exploits the sparsity of the rational function if only a small subset of possible coefficients is non-zero. The algorithm by Cuyt and Lee from 2010 first performs a univariate interpolation using Thiele's formula and then uses the coefficients as input for a multivariate polynomial interpolation [16]. In 2017, Huang and Gao [17] presented an algorithm which uses Kronecker substitution [14].

Most of the algorithms mentioned above rely on finite field arithmetic. Finite fields, e.g. integers modulo a prime number, are used for several hundred years. These calculations are done in an exact arithmetic environment which, however, avoids a number swell. This means that the coefficients of the polynomials and rational functions obtained by the interpolation algorithms are numbers in the finite field. In 1981, Wang presented an algorithm based on the Extended Euclidean Algorithm [14] which allows to reconstruct rational numbers from their image in a finite field [18].

We review finite fields, interpolation algorithms for both polynomials and rational functions, and the reconstruction algorithms for rational numbers in Sect. 2. The C++ library FireFly uses some of these algorithms. For the rational reconstruction we employ the algorithm by Cuyt and Lee [16] combined with Zippel's algorithm for the polynomial interpolation [2,3]. We also present some modifications to reduce the number of black-box probes. In Sect. 3 we present the implementation of FireFly and show how it can be used. We also present some benchmarks for the interpolation of multivariate rational functions.

As an application we apply FireFly to the reduction of Feynman integrals with integrationby-parts (IBP) relations [19,20], which are a standard calculation technique in multi-loop calculations of theoretical particle physics. They relate different integrals with each other through linear relations. The first solution strategy is to rearrange the IBP relations to recursion relations, which always express an integral through easier integrals. Applying the recursion relations repeatedly allows to express all integrals through master integrals. At three-loop level, this approach has been successfully applied for massless propagator-type diagrams [20–22], massive tadpoles [23, 24], and on-shell propagators [25–27]. However, at higher orders in perturbation theory it becomes unpractical to obtain such recursion relations. Nonetheless, some progress in deriving such relations automatically has been made in the last decade [28–31].

The second strategy was presented by Laporta in 2001 [32]. He suggested to build a system of equations out of the IBP relations by inserting values for the propagator powers and then solve this system. The Laporta algorithm and its modifications have been implemented in several public codes, AIR [33], FIRE [29, 34–36], Reduze [37, 38], and Kira [39, 40], as well as in numerous private codes. However, the systems of equations can become gigantic and, thus, expensive to solve both in terms of memory and runtime, which is partly related to large intermediate expressions.

To circumvent these problems, the use of finite-field techniques has been proposed by Kauers in 2008 together with a Mathematica package as an example [41]. In 2013, Kant proposed to solve the system of equations over a finite field before running the Laporta algorithm in order to reduce the size of the system by identifying and removing the linearly dependent equations [42]. This auxiliary use of finite fields has been implemented in Kira and led to significantly improved runtimes [39]. The use of the interpolation techniques over finite fields in the context of the Laporta algorithm has been advocated in Ref. [43]. In 2016, Peraro summarized some of the interpolation techniques from computer science in the context of generalized unitarity [44]. The first calculation using finite-field interpolation techniques for IBP reductions was accomplished by von Manteuffel and Schabinger in 2016 [45]. This was a one scale problem and, thus, also a one variable problem. Recently, three more one-scale calculations have been finished [46–48]. The recently published version 1.2 of Kira uses a multivariate Newton interpolation as supportive technique [40], albeit over  $\mathbb{Z}$  instead of a finite field. Shortly after, FIRE6 was published as first public implementation of a Laporta algorithm with a multivariate interpolation of rational functions over a finite field [36]. It supports the stable interpolation with two variables, i.e. two scales when setting one of them to one.

After a concise review of IBP reductions, we briefly describe our implementation with FireFly and compare it with the traditional reduction with Kira for some examples in Sect. 4. We also point out the advantages and disadvantages of the finite-fields-interpolation approach.

Another important method for multi-loop calculations is based on generalized unitarity. As mentioned above, Peraro pioneered the application of finite-field interpolation techniques for this method in 2016 [44]. This lead to several successful calculations in the last two years [49–56], where functions with up to four variables have been interpolated. However, we do not delve into this field in our paper.

## 2 Functional interpolation over finite fields

The interpolation of a function f of n variables  $\vec{z} = (z_1, \dots z_n)$  is based on the idea to require no knowledge about the function itself and only use its evaluations at different values of  $\vec{z}$  to construct an analytic form of the probed function or at least find an approximation formula. These kinds of interpolation problems are also called black-box interpolation problems, where the function to be interpolated serves as the black box. These interpolations are performed over a field. A set of particularly suited fields, due to their specific properties, are finite fields  $\mathbb{Z}_p$  with characteristic p, where p is the defining prime, on which we will focus in this paper. All calculations are thus carried out modulo p avoiding number swell and thus saving memory and runtime. The multiplicative inverse is unique and can be determined using the Extended Euclidean Algorithm [14].

In the following sections, we describe how polynomials and rational functions of in principle arbitrarily many variables can be efficiently interpolated and how one can promote elements of  $\mathbb{Z}_p$  to the field of rational numbers  $\mathbb{Q}$ .

#### 2.1 Interpolation of polynomials

To fix the notation, we start by defining multivariate polynomials as follows. Given a set of n variables  $\vec{z} = (z_1, \ldots, z_n)$  and an n-dimensional multi-index  $\alpha = (\alpha[1], \ldots, \alpha[n])$  containing integers  $\alpha[i] \geq 0$ , we define a monomial  $\vec{z}^{\alpha}$  as

$$\vec{z}^{\,\alpha} \equiv \prod_{i=1}^{n} z_i^{\alpha[i]} \tag{1}$$

with a degree r of

$$r = \sum_{i=1}^{n} \alpha[i]. \tag{2}$$

A polynomial f, which is a member of the polynomial ring  $\mathbb{Z}_p[\vec{z}]$  in the variables  $\vec{z}$ , is defined as

$$f(\vec{z}) = \sum_{i} c_{\alpha_j} \vec{z}^{\alpha_j}. \tag{3}$$

The coefficients  $c_{\alpha_i}$  are elements of  $\mathbb{Z}_p$  corresponding to different multi-indices  $\alpha_j$ .

Solving the black-box interpolation problem of a multivariate polynomial can be done by recursive interpolations of univariate polynomials. Thus, we briefly mention how to interpolate univariate polynomials before turning to the multivariate case. A well-known interpolation algorithm for univariate polynomial functions  $f = f(z_1) \in \mathbb{Z}_p[z_1]$  is given by the Newton interpolation which relies on Newton polynomials [1]. Given a sequence of distinct interpolation points  $y_{1,1}, \ldots, y_{1,R+1} \in \mathbb{Z}_p$ , the Newton polynomial for f of degree R can be written as

$$f(z_1) = a_0 + \sum_{i=1}^{R} a_i \prod_{j=1}^{i} (z_1 - y_{1,j+1}), \tag{4}$$

where the coefficients  $a_i$  can be recursively defined as

$$a_i \equiv a_{i,i},\tag{5}$$

$$a_{i,j} = \frac{a_{i,j-1} - a_{j-1}}{y_{1,i+1} - y_{1,j}},\tag{6}$$

$$a_{i,0} = f(y_{1,i+1}). (7)$$

A benefit of this algorithm is that the calculation of a new term does not alter the previously computed terms. This feature makes the Newton interpolation particularly suited for interpolations with an unknown degree R. The interpolation terminates if an  $a_i$  is equal to zero. As a check, one could evaluate further  $a_i$  with additional  $y_{1,i}$  which should also be zero.

There are two caveats which have to be mentioned. First, one has to be careful of spurious poles which can occur in the recursion formula. In this case one has to choose another value of  $y_{1,i}$  and proceed with the algorithm. To minimize the chance of spurious poles, we use random numbers for  $y_{1,i}$  and fields with a large characteristic. Secondly, the termination criterion of finding  $a_i = 0$  is just a probabilistic one when the interpolation is performed in  $\mathbb{Z}_p$ . Since there is only a finite number of elements, one could accidentally find a zero and the interpolation of f terminates wrongly. The probability can be reduced by calculating  $a_i$  multiple times for different random choices of  $y_{1,i}$  and by choosing a larger a characteristic for  $\mathbb{Z}_p$ . In our studies, no wrongly terminated interpolation was found when defining  $\mathbb{Z}_p$  with the largest 63-bit primes. Hence, for practical usage, it might be sufficient to omit additional checks for  $a_i$  after one encounters  $a_i = 0$ .

The algorithm can be easily generalized to the case of multivariate polynomials by a recursive application of the Newton interpolation for univariate functions, e.g. as proposed in Ref. [44]. Consider a generic multivariate polynomial  $f \in \mathbb{Z}_p[z_1, \ldots, z_n]$ . f can be reinterpreted as a univariate polynomial in  $z_1$  of degree R, with its coefficients being multivariate polynomials of n-1 variables  $(z_2, \ldots, z_n)$ . This promotes the coefficients  $a_i$  to be elements of the polynomial ring  $\mathbb{Z}_p[z_2, \ldots, z_n]$  such that

$$f(z_1, \dots, z_n) = \sum_{i=0}^{R} a_i(z_2, \dots, z_n) \prod_{j=1}^{i} (z_1 - y_{1,j}),$$
(8)

where  $y_{1,i} \in \mathbb{Z}_p$  are randomly chosen interpolation points for  $z_1$  as in the univariate case. Obviously, one can again use the same partition for  $a_i(z_2,\ldots,z_n)$  leading to new coefficients which are functions of n-2 arguments. After applying this procedure n-1 times, we are left with the univariate interpolation problem, which can be solved by the Newton interpolation. For later usage, we denote the numerical choices  $y_{i,j}$  for  $z_i$  as the corresponding value to  $z_i$  at order j. The orders of each variable form a tuple which we call  $z_i$  order, i.e. the numerical choices  $y_{2,2}, y_{3,3}$  form the  $z_i$  order (2,3).

For practicality, it is useful to transform the interpolated Newton polynomial to its canonical form defined in Eq. (3). This can be done by using additions of multivariate polynomials and multiplications of a multivariate polynomial by a linear univariate polynomial.

However, the Newton interpolation algorithm is a *dense* algorithm, i.e. it interpolates all possible terms of a polynomial even if it is *sparse* and only a small subset of coefficients

is non-zero. It requires  $\prod_i (R_i + 2)$  black-box probes of the polynomial  $f(z_1, \ldots, z_n)$  in general, where  $R_i$  is the maximal degree of  $z_i$ . Overall, the complexity of this algorithm is exponential in n and grows quickly as the number of variables and the individual maximal degrees increase, which is inefficient for sparse polynomials. Note that a degree bound on each variable can reduce the complexity to be  $\prod_i (R_i + 1)$ . This is still not preferable for sparse polynomials which are usually encountered in physical calculations.

A more efficient multivariate algorithm in terms of black-box probes is the Zippel algorithm [2,3], which in addition takes advantage of the sparsity of the polynomial. As in the previous algorithm, Zippel's algorithm interpolates one variable at a time. The interpolation of a variable is called a stage, i.e. stage one is the interpolation  $f(z_1, y_{2,1}, y_{3,1}, ...)$ , stage two the interpolation  $f(z_1, z_2, y_{3,1}, ...)$  and so on. After the first stage, one interpolates each coefficient of the previous stage as a univariate polynomial. The main advantage of the Zippel algorithm is the following. If a polynomial coefficient  $c_{\alpha}$  evaluates to zero at one stage, one assumes that it will also vanish at all other stages. This can avoid a sizable amount of black-box probes compared to a dense interpolator. Since this assumption is probabilistic, it is crucial to choose the numbers at which the polynomial is probed with great care in order for this assumption to hold. To make this choice more robust, one usually uses seed numbers which are called anchor points. The anchor points should be set to random numbers to minimize the chance of coincidental cancellations. All other  $z_i$  order values can be obtained by computing the corresponding power of the anchor point, i.e. if  $y_{i,1} = 2$  then the corresponding jth  $z_i$  order value is  $y_{i,j} = 2^j$ .

For illustration we provide an example of the Zippel algorithm. Consider the following polynomial to be interpolated

$$f(z_1, z_2, z_3) = c_{\alpha_1} z_1^5 + c_{\alpha_2} z_1 z_2^4 + c_{\alpha_3} z_1 z_2 z_3^3 + c_{\alpha_4} z_2^5.$$

$$\tag{9}$$

The indices  $\alpha_i$  are the multi-index of the corresponding monomial, i.e.  $\alpha_1 = (5,0,0)$ . In the first stage, one interpolates the univariate polynomial in  $z_1$  with Newton's algorithm by fixing  $z_2 = y_{2,1}$  and  $z_3 = y_{3,1}$ . This yields

$$f(z_1, y_{2,1}, y_{3,1}) = k_0(y_{2,1}, y_{3,1}) + k_1(y_{2,1}, y_{3,1}) \cdot z_1 + k_5(y_{2,1}, y_{3,1}) \cdot z_1^5$$
(10)

after six black-box probes. An additional probe is needed to verify the termination of this stage. The polynomial coefficients  $k_i(y_{2,1}, y_{3,1})$  are multivariate polynomials in the remaining variables  $z_2$  and  $z_3$  evaluated at  $y_{2,1}$  and  $y_{3,1}$ .

At stage two, the coefficients  $k_i(y_{2,1}, y_{3,1})$  are promoted to polynomials  $k_i(z_2, y_{3,1})$ . Since  $k_2 = k_3 = k_4 = 0$ , we also assume the corresponding polynomials  $k_i(z_2, z_3)$  to vanish. Therefore, only three polynomials have to be interpolated in  $z_2$  at stage two. The univariate interpolation in  $z_2$  is done by using the numerical values of  $k_i(y_{2,j}, y_{3,1})$  of the polynomials

$$f_i(z_1, y_{2,i}, y_{3,1}) = k_0(y_{2,i}, y_{3,1}) + k_1(y_{2,i}, y_{3,1}) \cdot z_1 + k_5(y_{2,i}, y_{3,1}) \cdot z_1^5, \tag{11}$$

as black-box probe for the univariate interpolation of  $k_i(z_2, y_{3,1})$ . The result of the first stage,  $f_1(z_1, y_{2,1}, y_{3,1})$  given by Eq. (10), can be reused. The other polynomials  $f_j(z_1, y_{2,j}, y_{3,1})$  can again be interpolated by a univariate Newton interpolation. However, since we already

know that only three coefficients contribute to the univariate polynomial  $f_j(z_1, y_{2,j}, y_{3,1})$ , it is more efficient to build a system of three equations and solve it. Zippel's original algorithm requests new polynomials  $f_j(z_1, y_{2,j}, y_{3,1})$  until all  $k_i(z_2, y_{3,1})$  are interpolated, i.e. six times in the example. This means that stage two would require  $6 \times 3 = 18$  black-box probes in total.

Kaltofen, Lee, and Lobo suggested to remove those  $k_i(z_2, y_{3,1})$  from the system where the Newton interpolation terminates, which reduces the size of the system for the remaining coefficients [7,8]. This procedure is called *temporary pruning*. In the example, the interpolation of  $k_3(z_2, y_{3,1})$  terminates after the second step, the evaluation of  $k_1(z_2, y_{3,1})$  after the sixth, and  $k_0(z_2, y_{3,1})$  after the seventh, which corresponds to  $3 + 4 \times 2 + 1 = 12$  black-box probes for stage two.

The result of stage two is

$$f(z_1, z_2, y_{3,1}) = \tilde{k}_0(y_{3,1}) \cdot z_2^5 + (\tilde{k}_1(y_{3,1}) \cdot z_2 + \tilde{k}_2(y_{3,1}) \cdot z_2^4) z_1 + \tilde{k}_5(y_{3,1}) \cdot z_1^5$$

$$= \tilde{k}_0(y_{3,1}) \cdot z_2^5 + \tilde{k}_1(y_{3,1}) \cdot z_1 z_2 + \tilde{k}_2(y_{3,1}) \cdot z_1 z_2^4 + \tilde{k}_5(y_{3,1}) \cdot z_1^5.$$
(12)

Stage three starts by promoting  $\tilde{k}_i(y_{3,1})$  to polynomials  $\tilde{k}_i(z_3)$  and proceeds exactly as stage two. The interpolations of  $\tilde{k}_0(z_3)$ ,  $\tilde{k}_2(z_3)$ , and  $\tilde{k}_5(z_3)$  terminate after the second step, and the interpolation of  $\tilde{k}_1(z_3)$  after the fifth. Thus, Zippel's original algorithm requires  $4 \times 4 = 16$  and the improved version  $4 + 3 \times 1 = 7$  black-box probes for stage three.

Therefore, the complete interpolation of Eq. (9) requires 7 + 18 + 16 = 41 black-box probes with the original version and 7 + 12 + 7 = 26 with the improved version using temporary pruning. In contrast, the recursive multivariate Newton interpolation needs  $(5 + 2) \times (5 + 2) \times (3 + 2) = 245$  probes.

The Zippel algorithm can be further improved by assuming knowledge of the maximal degree R, which always is the case when using it as part of the multivariate interpolation of rational functions as described in Sect. 2.2. Then, one can abort the univariate Newton interpolation of  $k_i$  after step j if  $j = R - r_i$ , where  $r_i$  is the total degree of the monomial corresponding to  $k_i$ . This procedure is called permanent pruning [57]. This reduces the total number of black-box probes to 20 for the given example, whereas the multivariate Newton algorithm only drops to  $(5+1) \times (5+1) \times (3+2) = 180$  probes. In contrast, there are  $\binom{3+5}{5} = 56$  possible coefficients and solving for them with a system of equations requires the same amount of black-box probes. This clearly shows the advantage of the Zippel algorithm compared to a recursive multivariate Newton interpolation.

Furthermore, if we know that all monomials have the same degree r=5, the example already finishes after stage two. From Eq. (12) we can deduce that  $c_{\alpha_3} = \tilde{k}_1(y_{3,1})/y_{3,1}^3$  is the coefficient for  $z_1 z_2 z_3^3$ . This prediction of the remaining powers is not used in our implementation of the Zippel algorithm, because it is closely related to the homogenization precedure [57] which will be done for the rational interpolation in Sect. 2.2.

Assuming a degree bound R, the Zippel algorithm scales as O(nRt), with t being the number of non-zero coefficients [2]. In the completely dense case, the improved version with pruning requires  $\binom{n+R}{R}$  probes with a degree bound, which is exactly one probe for every coefficient.

Without a degree bound, only a small number of additional probes is required to verify that the interpolation terminates.

An additional optimization regarding runtime can be achieved by noticing that the systems of equations which have to be solved during each stage in Zippel's algorithm are generalized transposed Vandermonde systems [3]

$$\begin{pmatrix}
1 & 1 & \dots & 1 \\
v_{\alpha_1} & v_{\alpha_2} & \dots & v_{\alpha_m} \\
\vdots & \vdots & \ddots & \vdots \\
v_{\alpha_1}^{m-1} & v_{\alpha_2}^{m-1} & \dots & v_{\alpha_m}^{m-1}
\end{pmatrix}
\begin{pmatrix}
c_{\alpha_1} \\
c_{\alpha_2} \\
\vdots \\
c_{\alpha_m}
\end{pmatrix} =
\begin{pmatrix}
f(\vec{y}^{\,0}) \\
f(\vec{y}^{\,1}) \\
\vdots \\
f(\vec{y}^{\,m-1})
\end{pmatrix},$$
(13)

where  $f(\vec{z})$  is a multivariate polynomial with m terms,

$$v_{\alpha_i} = \vec{y}^{\alpha_i} = \prod_{j=1}^n y_{j,1}^{\alpha_i[j]}, \qquad \vec{y}^i = \prod_{j=1}^n y_{j,1}^i.$$
 (14)

All  $v_{\alpha_i}$  have to be increasing monotonically with respect to  $\alpha_i$ , with  $\alpha_1$  being the lowest degree. Solving algorithms for Vandermonde systems are much more efficient compared to Gaussian elimination, since Vandermonde systems can be solved using only  $O(m^2)$  time and O(m) space, where m is the number of equations [3,5]. For usual Vandermonde systems presented in Eq. (13), the first evaluation of  $f(\vec{z})$  will be done while setting all variables equal to 1. This variable choice increases the probability that monomials cancel, which is especially dangerous if  $f(\vec{z})$  is the denominator of a rational function. To circumvent this problem, we propose to consider a modified version of generalized transposed Vandermonde systems:

$$\begin{pmatrix}
v_{\alpha_1} & v_{\alpha_2} & \dots & v_{\alpha_m} \\
v_{\alpha_1}^2 & v_{\alpha_2}^2 & \dots & v_{\alpha_m}^2 \\
\vdots & \vdots & \ddots & \vdots \\
v_{\alpha_1}^m & v_{\alpha_2}^m & \dots & v_{\alpha_m}^m
\end{pmatrix}
\begin{pmatrix}
c_{\alpha_1} \\
c_{\alpha_2} \\
\vdots \\
c_{\alpha_m}
\end{pmatrix} =
\begin{pmatrix}
f(\vec{y}^{\,1}) \\
f(\vec{y}^{\,2}) \\
\vdots \\
f(\vec{y}^{\,m})
\end{pmatrix}.$$
(15)

These systems preserve all properties of general Vandermonde systems and only require a modification of the solving algorithm, while making cancellations very unlikely. An algorithm to solve such systems is given in App. A.

Note that it is beneficial in terms of the number of black-box probes to choose the variable order descending in the maximal degrees, i.e. that the lowest degree variable should be the last one to interpolate and the highest the first. This follows from the nature of the Zippel algorithm in which intermediate systems of equations usually grow with every stage. Generally, the best order for a black-box function is not known a priori, but for physical calculations one can utilize problems which are similar but simpler to obtain a guess on how the individual degrees could be distributed. We will illustrate the impact on the number of black-box probes of such a choice in Sect. 3.3.

Instead of using a univariate Newton interpolation in Zippel's algorithm for the multivariate polynomial interpolation, Refs. [7,8] present a racing algorithm which races the sparse Ben-Or/Tiwari algorithm [4,6] against the dense Newton interpolation. This procedure may significantly reduce the number of black-box probes by combining the advantages of both

a sparse and a dense algorithm. Further optimizations of the Ben-Or/Tiwari algorithm are described in Ref. [9]. We leave these optimizations for future versions.

### 2.2 Interpolation of rational functions

Rational functions can be constructed by combining two polynomials. Given two polynomials  $P, Q \in \mathbb{Z}_p[\vec{z}]$ , we define a rational function  $f \in \mathbb{Z}_p(\vec{z})$ , where  $\mathbb{Z}_p(\vec{z})$  is the field of rational functions in the variables  $\vec{z}$ , as the ratio of P and Q:

$$f(\vec{z}) = \frac{P(\vec{z})}{Q(\vec{z})} = \frac{\sum_{i} n_{\alpha_i} \vec{z}^{\alpha_i}}{\sum_{j} d_{\beta_j} \vec{z}^{\beta_j}}.$$
 (16)

The coefficients  $n_{\alpha_i}, d_{\beta_j}$  are members of the field  $\mathbb{Z}_p$  corresponding to multi-indices  $\alpha_i$  and  $\beta_i$ .

Rational functions are not uniquely defined since their normalization is arbitrary. In order to provide a unique representation, we define the lowest degree coefficient in the denominator to be equal to one. If several monomials contribute to the lowest degree  $d_{\min}$ , we choose to define that coefficient of the monomial  $\vec{z}^{\alpha}$  to be equal to one whose multi-index  $\alpha$  is the smallest in a colexicographical ordering, e.g.

$$(1,1,0) < (1,0,1) < (0,1,1),$$
 (17)

for r=2.

The best strategy for interpolating rational functions is highly dependent on the available information. In the univariate case one can use Thiele's interpolation formula [1]. In the multivariate case, the best algorithm in terms of black-box probes is to solve a dense system of equations if one knows the terms of the rational function but not the values of the coefficients. Of course, this also works if one can restrict the number of terms by knowing bounds for the degrees of numerator and denominator. However, this is then a completely dense interpolation. In the early 1990s, Grigoriev, Karpinski, and Singer presented an algorithm to obtain bounds and then build a system of equations [10–12]. This approach can have a bad scaling behavior for many unknowns and high degrees since Gaussian elimination scales as  $O(m^3)$  in time and  $O(m^2)$  in space, with m being the number of equations.

In 2006, Khodadad and Monagan published an algorithm [13] which is based on the modified versions of the Extended Euclidean Algorithm [14, 18, 58]. The algorithm presented by Kaltofen and Zhang in 2007 [15] evaluates numerator and denominator separately [59, 60] and then uses a multivariate polynomial interpolation. It also exploits the sparsity of rational functions. Huang and Goa presented an algorithm in 2017 [17] based on Kronecker substitution [14]. These three algorithms all require bounds on the degrees of numerator and denominator.

In 2010, Cuyt and Lee presented an algorithm which uses the results of univariate interpolations with Thiele's interpolation formula as input for multivariate polynomial interpolations [16]. It is this algorithm which we adopt for FireFly, because it requires no information apart from the number of variables a priori and it utilizes the sparsity of a rational function.

Thus, we start by discussing how to interpolate a univariate rational function. According to Thiele [1] one can express a rational function  $f \in \mathbb{Z}_p(t)$  as a continued fraction

$$T(t) = b_0 + (t - t_1) \left( b_1 + (t - t_2) \left( b_2 + (t - t_3) \left( \dots + \frac{t - t_n}{b_n} \right)^{-1} \right)^{-1} \right)^{-1},$$
 (18)

with  $t_1, \ldots, t_{n+1}$  being distinct elements of  $\mathbb{Z}_p$ . The coefficients  $b_0, \ldots, b_n$  can be obtained recursively by numerical evaluations of the rational function f at  $t_1, \ldots, t_{n+1}$ ,

$$b_i \equiv b_{i,i},\tag{19}$$

$$b_{i,j} = \frac{t_{i+1} - t_j}{b_{i,j-1} - b_{j-1}},\tag{20}$$

$$b_{i,0} = f(t_{i+1}). (21)$$

The termination criterion is reached if one finds agreement between  $f(t_i)$  and  $T(t_i)$ . Note that this approach only scales optimally with the number of black-box probes if the degree of the polynomials of numerator and denominator differ at most by one.

The idea of the algorithm of Ref. [16] is to perform the multivariate rational function interpolation with a dense univariate rational function interpolation and a sparse multivariate polynomial interpolation. First, we assume a rational function  $f(\vec{z})$  of n variables which has a constant in the denominator and discuss the general case later. The constant is used to normalize the rational function and set to one. One starts by introducing a homogenization variable t and defining a new function  $\tilde{f}(t\vec{z})$  as [57]

$$\tilde{f}(t\vec{z}) = f(tz_1, \dots, tz_n). \tag{22}$$

We can interpret  $\tilde{f}$  as a univariate rational function in the variable t, whose coefficients are multivariate polynomials in  $\vec{z}$ . Their degrees are bounded by the corresponding degree of t. Thus, by interpolating  $\tilde{f}$  in t, we can use its coefficients for multivariate polynomial interpolation as described in Sect. 2.1. As optimization, we can set  $z_1 = 1$  and reconstruct its power by homogenizing with respect to the corresponding power of t. To interpolate  $\tilde{f}$ , we generate random anchor points  $y_{i,1}$  for the remaining  $z_i$  and perform a Thiele interpolation by evaluating  $\tilde{f}(t\vec{y}^1)$  for several random t until it terminates. We proceed for each variable sequentially  $(z_1 \to z_2 \to \cdots \to z_n)$  until the polynomial interpolation terminates. Ref. [16] uses the racing algorithm of Refs. [7,8] mentioned in Sect. 2.1 for the polynomial interpolation instead of Zippel's algorithm with a univariate Newton interpolation as we do.

Since Thiele's interpolation is not optimal for general rational functions in terms of the number of black-box probes, we use the knowledge gained during the first interpolation and subsequently only solve univariate systems of equations for all remaining coefficients. Additionally, we remove already solved coefficients from the system, to further reduce the number of black-box probes. The univariate system of equations can then easily be constructed by evaluating  $\tilde{f}(t\vec{y})$  for different t at a fixed  $\vec{z} = \vec{y}$  and construct each equation as

$$\sum_{i} n_{\mathbf{u},i}(\vec{y}) t^{r_i} - \tilde{f}(t, \vec{y}) \sum_{j} d_{\mathbf{u},j}(\vec{y}) t^{r_j} = \tilde{f}(t, \vec{y}) \sum_{j} d_{\mathbf{s},j}(\vec{y}) t^{r_j} - \sum_{i} n_{\mathbf{s},i}(\vec{y}) t^{r_i},$$
 (23)

where the subscripts s and u denote the solved and unsolved coefficients, respectively. In this notation the normalizing coefficient is included in the solved subset. Each of the solved coefficients can be computed by evaluating the corresponding multivariate polynomial at  $\vec{z} = \vec{y}$ . When enough equations have been obtained, the system can be solved for the unsolved coefficients. The time spent solving such univariate systems is usually negligible compared to the evaluation of the black-box function.

Until now, we have assumed that the denominator of f has a constant term. The generalization of the presented algorithm to arbitrary rational functions leads to a normalization problem. Assuming no constant term, we cannot set the coefficient of the the lowest degree monomial in the denominator of  $\tilde{f}$  to one since this coefficient is a polynomial and not a constant. The algorithm presented in Ref. [16] cures this problem by introducing a variable shift  $\vec{s} = (s_1, \ldots, s_n)$  such that  $f(\vec{z}) \to f(\vec{z} + \vec{s}) \equiv \hat{f}(\vec{z})$  and  $\hat{f}$  has a constant term in the denominator. A reliable way to fulfill this condition is to choose random but distinct values for all  $s_i$ . This shift comes with the caveat that  $\hat{f}$  will be a much denser rational function in general. Especially, aside from accidental cancellations, it will contain all univariate terms in t up to the maximal degrees of numerator and denominator.

For simplicity we will focus on the numerator, noting that the following procedure can be applied completely analogously to the denominator. Assume that the maximal degree of the numerator of  $\hat{f}$  in t is R with its corresponding coefficient  $n_R$ . Note that  $n_R$  will not be affected by the shift, thus, one starts by interpolating only this polynomial. The numerical values of  $n_i$  for i < R are stored for later usage. Once  $n_R$  has been interpolated, we can remove it from the system of equations as before to reduce the number of black-box probes, and additionally subtract the effect of the shift on the lower degree coefficients to preserve their sparsity. The latter can be achieved by analytically evaluating

$$n_R(\vec{z} + \vec{s}) - n_R(\vec{z}). \tag{24}$$

It is convenient to save the results of Eq. (24) split according to their corresponding degree in t. Subsequently, one moves to  $n_{R-1}$  and subtracts the term of Eq. (24) corresponding to the degree R-1 evaluated at the same  $y_{i,j}$  as the current interpolation point. This removes the shift from  $n_{R-1}$  and preserves its sparsity in the multivariate polynomial interpolation.

To illustrate the above algorithm, we present the following example which will be interpolated over  $\mathbb{Z}_{509}$ . Assume we want to interpolate the function

$$f(\vec{z}) = \frac{3z_1 + 7z_2}{z_1 + z_2 + 4z_1 z_2}. (25)$$

We start by choosing the anchor points  $\vec{y}^1$  for  $\vec{z}$ , and homogenize with t:

$$y_{1,1} = 1, y_{2,1} = 10 \Rightarrow \tilde{f}(t\vec{y}^1) = \frac{73t}{11t + 40t^2}.$$
 (26)

Since there is no constant term in the denominator, we perform a variable shift  $\vec{s}$  to find a unique normalization:

$$s_1 = 4, s_2 = 1 \Rightarrow \hat{f}(t\vec{y}^1) = \frac{316 + 464t}{1 + 178t + 317t^2}.$$
 (27)

The function  $\hat{f}$   $(t\vec{y}^{\,1})$  in Eq. (27), whose coefficients are already uniquely normalized, is the result of the Thiele interpolation in the first step of the algorithm. Since we now know the maximal degrees of numerator and denominator, we can proceed in the remaining stages by solving systems of equations instead of using Eq. (18) to reduce the number of black-box probes. The numerical coefficients of  $\hat{f}$   $(t\vec{y}^{\,1})$  are multivariate polynomials evaluated at  $t\vec{y}^{\,1} + \vec{s}$  and, thus, are used as the input for the following polynomial interpolation according to Sect. 2.1. We will now focus on the numerator. The denominator can be interpolated in an analogous way. Assume we have fully interpolated the highest degree of the numerator as

$$P_1' = 291 + 170z_2, (28)$$

which will yield

$$P_1 = 291z_1 + 170z_2 \tag{29}$$

after homogenization. The prime indicates the non-homogenized coefficient. To interpolate  $n_0$  without the shift, we have to remove its effect before performing the polynomial interpolation. The input for the latter will thus be

$$316 - (P_1(\vec{z} + \vec{s}) - P_1(\vec{z})) = 316 - (146 + 170) = 0.$$
(30)

This is expected since there is no constant term in the numerator of  $f(\vec{z})$ . In total it takes twelve black-box probes to interpolate Eq. (25) using this algorithm. One can also apply this example to the case where  $d_0 \neq 0$  with  $\vec{s} = 0$ . To further reduce the probes mandatory for this algorithm to succeed, the variable with the highest degree should be set to one and is thus only obtained by homogenization of the degrees after the polynomial interpolation finishes. This step requires neither additional black-box evaluations nor the use of interpolation algorithms.

Note that there is no need that the denominator comes with a constant. The same procedure can be applied if one finds a constant in the numerator after introducing a shift and using the latter for normalization. Additionally, one can apply algorithms to find a shift in fewer variables to reduce the higher complexity introduced by the normalization ambiguity. A straightforward algorithm is to test different shifts and apply the one, which shifts a minimal number of variables to obtain a unique normalization. To achieve this, in a first run the maximal degrees of numerator and denominator of the homogenized rational function have to be determined. Since we assume no knowledge about the black box, it is necessary to shift all variables to guarantee the existence of constants in numerator and denominator and thus prevent cancellations in the homogenization variable. Afterwards, one tests different shift configurations and checks if the maximal degrees of numerator and denominator coincide with the degrees obtained when shifting all variables. For practical usage, these steps may be important for sparse black-box functions with four or more variables since a shift including all arguments can lead to  $O(\binom{n+R}{R})$  additional terms, where n is the number of variables and R the maximal degree of numerator or denominator, which have to be calculated to remove the effect of the shift in the interpolation of multivariate polynomials.

#### 2.3 From finite fields to rational numbers

In the previous sections, we described how one can interpolate multivariate polynomials and rational functions over a finite field. Since their coefficients are only valid in the specific field used for the interpolation, one has to promote these numbers to rational numbers such that the corresponding functions are elements of  $\mathbb{Q}[\vec{z}]$  and  $\mathbb{Q}(\vec{z})$ , respectively. Therefore, we need to reconstruct the interpolated results over the rational field. Generally, there is no inversion of the mapping from rational numbers to members of a finite field, but one can use a method called rational reconstruction (RR). This method is based on the Extended Euclidean Algorithm [14] and the first algorithm was described by Wang in 1981 [18], which is presented in Alg. (1).

This algorithm leads to a guess for a rational number a = b/c, with b and c being integers, from its image

$$e = a \bmod p \in \mathbb{Z}_p. \tag{31}$$

It will succeed if  $|b|, |c| \leq \sqrt{p/2}$ . In Ref. [61] it was proven that a is unique if it is found for a given e and p. However, this does not mean that the a is the correct rational number in  $\mathbb Q$  which one desires to reconstruct, because the unique guess can be different in other prime fields. Also, the bound of  $\sqrt{p/2}$  could lead to failures of the RR if p is restricted to machine-size integers.

**Algorithm 1** Modified Euclidean Algorithm for rational reconstruction based on [18].

```
Input: A finite field member a, the defining prime of the finite field p.
```

**Output:** If succeeded a unique value of a in  $\mathbb{Q}$  else an error.

Both problems can be solved by the Chinese Remainder Theorem (CRT) [14], which comes with the cost of additional interpolations in other prime fields. The theorem states that one can uniquely reconstruct an element in  $\mathbb{Z}_p$  from its images  $\mathbb{Z}_{p_i}$  with  $i=1,\ldots,l$  by combining pairwise coprime numbers  $p_i$  to  $p=p_1\cdot p_2\cdot \cdots\cdot p_l$  and applying the RR using p. An algorithmic realization is shown in Alg. (2). To reconstruct a rational number, one can then combine as many prime numbers as are required to successfully perform the RR. We then consider the rational number to probably be the correct number in  $\mathbb{Q}$  if the RR yields the same result for two different fields. This guess will be tested later.

## Algorithm 2 Chinese Remainder Theorem algorithm CRT [14].

**Input:** Two pairs containing a prime p<sub>-</sub>i of a finite field and a coefficient c<sub>-</sub>i obtained by the functional reconstruction over this field.

Output: A pair consisting of the combined value of the c\_i's and p\_i's according to the CRT.

```
\begin{split} & \text{function CHINESE\_REMAINDER}((\texttt{c\_1}, \texttt{p\_1}), (\texttt{c\_2}, \texttt{p\_2})) \\ & p\_3 \leftarrow \texttt{p\_1} \ * \ \texttt{p\_2}; \\ & \texttt{m\_1} \leftarrow (\texttt{1} \ / \ \texttt{p\_2} \ \% \ \texttt{p\_1}) \ * \ \texttt{p\_2}; \\ & \texttt{m\_2} \leftarrow (\texttt{1} \ - \ \texttt{m\_1}) \ \% \ \texttt{p\_3}; \\ & \texttt{c\_3} \leftarrow (\texttt{m\_1} \ * \ \texttt{c\_1} \ + \ \texttt{m\_2} \ * \ \texttt{c\_2}) \ \% \ \texttt{p\_3}; \\ & \textbf{return} \ (\texttt{c\_3}, \texttt{p\_3}); \\ & \textbf{end function} \end{split}
```

Alg. (1) is not an optimal algorithm for arbitrary b and c because it will only succeed if both |b| and |c| are smaller than  $\sqrt{p/2}$ . Thus, in the worst case they differ by many orders in magnitude and only one of them fails the bound. In principle, it is possible to have different bounds for b and c. However, without additional knowledge one does not know a priori how to choose them. In Ref. [58] it was observed that the guess of the rational number comes together with a huge quotient in the Euclidean Algorithm. The suggested algorithm based on this observation is called Maximal Quotient Rational Reconstruction and presented in Alg. (4) in Sect. A. It can only be proven that it returns a unique solution if  $|b||c| \leq \sqrt{p}/3$ . However, it performs much better in the average case because large quotients from random input are rare. The parameter T allows to choose a lower bound for the quotients and, thus, the tolerance for false positive reconstructions. For FireFly we adjusted it to get roughly 1% false positive results.

We then race Alg. (1) against Alg. (4) and consider a guess for a rational number as probably correct if either of the two algorithms reconstructs the same number in two consecutive fields. Both algorithms can return false positive results, i.e. unique rational numbers which are not the correct number in  $\mathbb{Q}$ . However, we consider the probability to reconstruct the same false positive number in two different fields as negligible. We also consider a guess as probably correct if it is an integer fulfilling the condition of Alg. (1) or if the combined integer does not change after applying the CRT.

Combining the RR, the CRT, and the interpolation of functions over finite fields, the generic algorithm to obtain an interpolated function in  $\mathbb{Q}$  is shown in Alg. (3). The algorithm succeeds when the function build up by the probably correct coefficients in  $\mathbb{Q}$  coincides with the black-box probe evaluated in a new prime field. We also take all coefficients into account were either Alg. (1) or Alg. (4) was able to reconstruct a guess, which does not fulfill the criteria mentioned aboved, because it still could be correct.

After the first prime field, one obtains full knowledge about the functional form and only the coefficients have to be promoted to  $\mathbb{Q}$ . Thus, one can use this knowledge and only reconstruct those coefficients which cannot be promoted to  $\mathbb{Q}$  or are not valid in all used prime fields. This can be done most efficiently in numbers of black-box probes by solving systems of equations and remove all already known coefficients. Additionally, no variable

## **Algorithm 3** Functional reconstruction algorithm over $\mathbb{Q}$ based on [44].

```
Input: A sequence of primes p_1, \ldots, p_l and a black-box function f(\vec{z}).
Output: The result of f(\vec{z}) in \mathbb{Q} with high probability.
  for i \leftarrow 1; i \leq n do
       if i == 1 then
           Interpolate the function f over \mathbb{Z}_{p_1}(\vec{z}) and store the result;
           Use the RR to promote the stored result to a guess g \in \mathbb{Q}(\vec{z});
       else
           if the previous rational reconstruction succeeded then
                Evaluate g over the new field \mathbb{Z}_{p_i} for a given \vec{z};
                if g(\vec{z}) == f(\vec{z}) then
                    Terminate the algorithm and set g(\vec{z}) = f(\vec{z});
                end if
           else
                Reconstruct the function f in \mathbb{Z}_{p_i} and store the result;
                Use the CRT to combine the function in \mathbb{Z}_{p_i} with the stored result in \mathbb{Z}_{p_1\cdots p_{i-1}}
                and store the combined result;
                Use the RR to promote the stored result in \mathbb{Z}_{p_1\cdots p_i} to a guess g\in\mathbb{Q}(\vec{z});
           end if
       end if
       i \leftarrow i + 1;
  end for
```

shift is required to solve the normalization problem anymore.

However, the simple idea to construct a single system of equations for all coefficients which still need to be determined has a major drawback. It requires  $O(m^3)$  operations to solve this system with a standard algorithm. The size of the system can become quite large if the function has many variables and is densely populated. Solving this system can then become much more expensive than just interpolating the function from scratch if the time cost of the black-box probes is not too high. For polynomials, however, this is can be directly solved by using a generalized transposed Vandermonde system.

To circumvent this problem for rational functions, we break the system of equations down to several subsystems. We first build a univariate system of equations in the homogenization variable for all degrees which contain unsolved coefficients. This system is in general much smaller than a complete multivariate system and, thus, cheap to solve. The result for each univariate coefficient is again a multivariate polynomial in all remaining variables and thus used as input for the corresponding multivariate Vandermonde system. As soon as we have enough values to solve one of these systems, we solve it and remove the univariate degree from the following univariate systems of equations which are needed to calculate the remaining coefficients. Therefore, the number of black-box probes is the same as for the full multivariate system of equations without homogenization.

However, a rational function has to be normalized to one of the coefficients in order to yield unambiguous results after solving the homogenized univariate system. Since the functional

form is known after the interpolation over the first prime field, we check all univariate degrees for the number of contributing monomials and if their coefficients have already been promoted to  $\mathbb{Q}$ . If there is only a single contributing monomial for any degree, we choose its coefficient as normalization by setting it to one. For illustration, let its univariate degree be r. Afterwards, we check again which monomial coefficients can be promoted to  $\mathbb{Q}$  using this normalization. Therefore, the homogenized rational function evaluated at  $\vec{z} = \vec{y}$  is given by

$$\tilde{f}(t,\vec{y}) = \frac{\vec{y}^{\alpha}t^r + \sum_i n_i(\vec{y})t^{d_i}}{\sum_j d_j(\vec{y})t^{d_j}} \quad \text{or} \quad \tilde{f}(t,\vec{y}) = \frac{\sum_i n_i(\vec{y})t^{d_i}}{\vec{y}^{\alpha}t^r + \sum_j d_j(\vec{y})t^{d_j}}, \quad (32)$$

where  $n_i(\vec{y})$  and  $d_j(\vec{y})$  are the coefficients of the univariate rational function evaluated at  $\vec{z} = \vec{y}$ , which are multivariate polynomials. The univariate system can then be build exactly as in Eq. (23) and its solutions for  $n_{u,i}(\vec{y})$  and  $d_{u,j}(\vec{y})$  serve again as input for the generalized Vandermonde systems as described in Sect. 2.2.

In the application to IBP reductions as described in Sect. 4 a normalizing coefficient can be found sometimes. This is due to the fact that the variables are the space-time dimension d and variables with a mass dimension. The rational functions occuring have a fixed mass dimension and, thus, numerator and denominator have fixed mass dimensions as well. Different powers of d then distribute the monomials to different univariate degrees. The known mass dimensions also make it possible to set one of the massive variables to one, because it can be unambiguously reconstructed after the calculation. This distributes the monomial degrees further.

The normalization can also be fixed if the coefficient of a univariate degree is completely known represented as multivariate polynomial, i.e. all coefficients of the polynomial are already promoted to  $\mathbb{Q}$ . The numerical value of the coefficient can then always be computed for all  $\vec{z}$  and all prime fields, which allows us to use it as normalization.

Should there be no coefficient which can be used as normalization we reintroduce the shift so that we can normalize to the constant term. We then proceed as described above with the complication that we have to start with the highest degree and then remove the shift from lower degrees recursively as described in Sect. 2.2.

# 3 FireFly

We implemented the functional interpolation and rational number reconstruction algorithms described in the previous section in the C++ library FireFly, which is publicly available at

https://gitlab.com/firefly-library/firefly

It requires

- A C++ compiler supporting C++11
- CMake  $\geq 3.1$

- FLINT  $\geq 2.5$  (optional)
- GMP > 6.1

The dependency on the GNU Multiple Precision Arithmetic Library (GMP) [62] is needed to utilize the CRT if a single prime field is not sufficient to reconstruct the black-box function.

After downloading the library, FireFly can be configured and compiled by running

```
cd $FIREFLY_PATH
mkdir build
cd build
cmake -DWITH_FLINT=true .. # Without FLINT: -DWITH_FLINT=false
make
```

where \$FIREFLY\_PATH is the path to the FireFly directory. When the compilation has finished, the build directory will contain the static and shared libraries libfirefly.a and libfirefly.so, respectively. Calling

```
make install
```

will additionally copy the corresponding header files and libraries to a specified directory which is by default the system <code>include</code> and <code>lib</code> directory, respectively. The prefix of both installation directories can be set with

```
cmake -DCMAKE_INSTALL_PREFIX=$PREFIX ..
```

where \$PREFIX is the desired path prefix. The include and library files will then be installed to \$PREFIX/include and \$PREFIX/lib, respectively.

When using FLINT [63,64] additional flags have to be set if FLINTs header and library files cannot be found in the system include and lib directories. The configuration has thus to be provided with the absolute paths to the include directory and the shared library of FLINT. This can be done calling

```
cmake -DWITH_FLINT=true -DFLINT_INCLUDE_DIR=$FLINT_INC_PATH \
-DFLINT_LIBRARY=$FLINT_LIB_PATH
```

where \$FLINT\_INC\_PATH and \$FLINT\_LIB\_PATH are the absolute paths to the include directory to the shared library of FLINT, respectively.

In the following sections, we describe the library FireFly and give examples of its usage.

#### 3.1 Finite field integer and modular arithmetic

Most of the numerical computations are carried out over a finite field modulo a prime p. Since there is no built-in C++ implementation of such an object, we provide the class FFInt which denotes a finite field integer up to 64 bit. An FFInt holds basically three uint64\_t objects: n which is the element of the field, p to set the defining prime and p\_inv which is the inverse of p needed for modular arithmetic when using FLINT. To enable parallel interpolations of various functions over the same field and to save memory, the latter two are static variables. All basic arithmetic operations

relational operators

and unary operators

are implemented. The default implementation of modular arithmetic is given as an interface to routines of FLINT. Using the latter is optional but without this library, one has to provide own routines for all arithmetic operators and the pow member function which is mentioned in the next paragraph.

All public member functions and variables are summarized in the following:

#### static void set\_new\_prime(uint64\_t prime)

Static function that sets p = prime and calculates p\_inv. The latter is only set if one compiles FireFly with FLINT.

#### FFInt(const T n)

Creates an FFInt object by setting its value to  $n \mod p$  where the template T can be of type FFInt, mpz\_class, uint64\_t, std::string, or any other primitive integer type.

FFInt pow(const FFInt& e)

Returns  $a^e \mod p$ .

FFInt pow(const FFInt& a, const FFInt& e)

Returns  $a^e \mod p$ .

static uint64\_t p

The defining prime p of the field.

uint64\_t n

The element n of the prime field  $\mathbb{Z}_p$ .

set\_new\_prime has always to be called first before performing modular arithmetic to define a prime field. In the following code snippet, we show the exemplary usage of the FFInt class:

```
FFInt::set_new_prime(509);
FFInt a(10);
FFInt b(13);
FFInt c(3);
FFInt d = pow(c, a); // d is now 5
FFInt e = a.pow(b) + c/a; // e is now 355
```

All member functions are understood to be part of the firefly namespace. Firefly provides the user with an array of the 100 largest 63 bit primes which can be accessed through the function primes. To get the largest 63 bit prime, one calls primes()[0] and has to include the header ReconstHelper.hpp. Note that we are only using C++ STL containers apart from our custom container classes.

#### 3.2 Reconstructing functions with FireFly

FireFly offers the interface class Reconstructor for the reconstruction of rational functions and polynomials. It is provided with a thread pool<sup>1</sup> to allow for the parallel interpolation of various black-box functions over the same prime field and the promotion of their coefficients to  $\mathbb{Q}$ . Its member functions can be summarized as:

Reconstructor(uint32\_t n, uint32\_t thr\_n, uint32\_t verbosity = IMPORTANT)

Creates a Reconstructor object with n variables and thr\_n threads. The verbosity levels are SILENT, IMPORTANT, and CHATTY.

#### void enable\_scan()

Enables the scan for a sparse shift at the beginning of the reconstruction. As FireFly assumes a variable ordering by degree, i.e. the first variable has the highest degree, the possible shifts are scanned starting by shifting only the last variable and proceeding variable by variable until the first. After this two variables are scanned starting again with the last two proceeding to the first two etc.

#### void reconstruct()

Performs the reconstruction.

### vector<RationalFunction> get\_result()

Returns the reconstructed functions as RationalFunction objects (c.f. App. B).

#### void black\_box(vector<FFInt>& result, const vector<FFInt>& values)

The user-provided black-box function, which fills the probes for the variable values values into result. The vector result is required to have immutable ordering. values contains n entries corresponding to n variables.

#### void set\_tags(const vector<string>& tags)

Enables storing of intermediate results in the directory ./ff\_save. Each function state is stored under the name given by the corresponding entry in tags. The same immutable ordering as for the probes in black\_box is assumed.

<sup>&</sup>lt;sup>1</sup>We adapted the thread pool used in FlexibleSUSY 2.0 [65].

```
void set_tags()
```

Same as above but set generic tag numbers starting at 0.

```
void resume_from_saved_state(const vector<string>& file_paths)
```

Resumes the reconstruction with the saved files given at the absolute paths file\_paths.

To perform functional reconstructions, the user has to implement the function black\_box which is provided with an empty result vector and a tuple of values at which the black box should be evaluated. The result vector has then to be filled by calling user defined functions to probe the black box. The Reconstructor class demands an immutable ordering of the result vector to verify the consistency of the reconstruction.

Below we show an example how one could use the black\_box member function with dummy black boxes implemented in FireFly.

```
// Example of how one can use the black_box function of the interface
void Reconstructor::black_box(vector<FFInt>& result, const vector<FFInt>& \
  values) {
  result.emplace_back(singular_solver(values));
  result.emplace_back(n_eq_1(values[0]));
  result.emplace_back(n_eq_4(values));
  result.emplace_back(gghh(values));
  result.emplace_back(gghh(values));
  result.emplace_back(ggh(values));
}
```

To run the reconstruction for the above definded black-box function, the Reconstructor class could be used as follows:

```
// Construct the Reconstructor class with 4 variables and 4 threads
Reconstructor reconst(4, 4);
reconst.enable_scan(); // Enable the scan for a sparse shift
vector<string> tags = {"sing","n1","n4","gghh","pol","ggh"};
reconst.set_tags(tags); // Set tags to save states after each prime field
reconst.reconstruct(); // Reconstruct the functions
vector<RationalFunction> results = reconst.get_result(); // Get results
```

We first initialize the Reconstructor with four variables and four threads. Then, we enable the scan for a sparse shift and set tags to store intermediate results. reconstruct first scans the functions to check if a shift in a subset of the four variables is sufficient to always produce a constant term for the normalization and then performs the interpolation, manages the promotion to new prime fields and tries to reconstruct each coefficient over  $\mathbb{Q}$ . To parallelize the reconstruction, each probe is evaluated in its own thread and each black-box function is reconstructed by a RatReconst object (c.f. App. B) which itself performs the reconstruction single threaded.

Should the interpolation be aborted it can be resumed with

```
// Give the absolute paths to the intermediate results
vector<string> file_paths = {"ff_save/sing_3.txt", "ff_save/n1_2.txt", \
 "ff_save/n4_3.txt", "ff_save/gghh_4.txt", "ff_save/pol_1.txt", \setminus
 "ff_save/ggh_2.txt"};
// Enables to resume from a saved state
reconst.resume_from_saved_state(file_paths);
reconst.reconstruct();
```

The file names consist of the tag given above and the last prime counter for which the object was saved. These counters can differ between the tags because the corresponding reconstruction can finish at different counters and already reconstructed functions will not produce new intermediate states to save.

If the black-box function requires the numerical result to be in a different format, e.g. a matrix in the form of a nested vector instead of a vector, the user has two options. One could either parse the result to a vector or implement the Reconstruct object oneself and adjust a few lines of code. We follow the latter approach for our application to IBP reductions in Sect. 4. More information about FireFly can be found in App. B.

#### 3.3 Benchmarks

In this section we highlight the influence of different options which can strongly affect the time spent on a reconstruction and the corresponding memory consumption. For that purpose, we define the following benchmark functions:

$$f_1(z_1, \dots, z_{20}) = \frac{\sum_{i=1}^{20} z_i^{20}}{\sum_{i=1}^{5} (z_1 z_2 + z_3 z_4 + z_5 z_6)^i z_{20}^{35}},$$
(33)

$$f_{1}(z_{1},...,z_{20}) = \frac{\sum_{i=1}^{20} z_{i}^{20}}{\sum_{i=1}^{5} (z_{1}z_{2} + z_{3}z_{4} + z_{5}z_{6})^{i} z_{20}^{35}},$$

$$f_{2}(z_{1},...,z_{5}) = \frac{123456789109898799879870980 \left(\left(1 + \sum_{i=1}^{5} z_{i}\right)^{20} - 1\right)}{z_{4} - z_{2} + z_{1}^{10} z_{2}^{10} z_{3}^{10} z_{4}^{10} z_{5}^{10}},$$

$$f_{3}(z_{1},...,z_{5}) = \frac{z_{1}^{100} + z_{2}^{200} + z_{3}^{300}}{z_{1}z_{2}z_{3}z_{4}z_{5} + z_{1}^{4} z_{2}^{4} z_{3}^{4} z_{5}^{4}}.$$

$$(33)$$

$$f_3(z_1, \dots, z_5) = \frac{z_1^{100} + z_2^{200} + z_3^{300}}{z_1 z_2 z_3 z_4 z_5 + z_1^4 z_2^4 z_3^4 z_4^4 z_5^4}.$$
 (35)

We test a sparse function with 20 variables  $(f_1)$ , a dense function with five variables  $(f_2)$ which requires the usage of the CRT, and a sparse function with five variables and high individual degrees  $(f_3)$ . All functions need a shift in at least one variable.

For the benchmarks we measure the total time, the number of black-box probes, and the total memory consumption using a single threaded setup without a thread pool. We compare different variable orderings and the influence of the scan for a sparser shift to the default options. All calculations are done on an Intel Core i7-3770 and 8 GiB of RAM. FLINT is enabled for modular arithmetic. The results of the benchmark tests are shown in Tab. 1 using different kinds of possible optimizations. To reconstruct  $f_2$  we use the first five entries of the primes vector which can be found in the ReconstHelper.hpp file.

To fully reconstruct  $f_1$ , FireFly needs  $\sim 90000$  black-box probes using a parameter shift in all variables and a non-optimal ordering. This can be reduced to  $\sim 20000$  probes by using

**Table 1:** Benchmarks for  $f_1$ ,  $f_2$  and  $f_3$  defined in Eqs. (33)-(35) obtained with FireFly using different optimizations.

Function	Shift scan	Variable order	Probes	Runtime	Memory usage
$f_1$	×	$ (z_1,\ldots,z_{20}) $	87137	$3.6\mathrm{s}$	$27.9\mathrm{MiB}$
$f_1$	×	$(z_{20}, z_1, \ldots, z_{19})$	41628	2.1 s	$25.4\mathrm{MiB}$
$f_1$	✓	$(z_1,\ldots,z_{20})$	84569	4.0 s	$132.1\mathrm{MiB}$
$f_1$	✓	$  (z_{20}, z_1, \ldots, z_{19})  $	22617	$1.7\mathrm{s}$	127.3 MiB
$f_2$	×	$(z_1,\ldots,z_5)$	332893	$5 \min 30 s$	54.9 MiB
$f_2$	✓	$(z_1,\ldots,z_5)$	320800	4 min 58 s	$43.2\mathrm{MiB}$
$f_3$	×	$(z_1,\ldots,z_5)$	139710	42.4 s	13.7 MiB
$f_3$	×	$(z_3, z_2, z_1, z_4, z_5)$	54211	$9.5\mathrm{s}$	$9.4\mathrm{MiB}$
$f_3$	✓	$(z_1,\ldots,z_5)$	137493	$38.0\mathrm{s}$	$13.5\mathrm{MiB}$
$f_3$	✓	$(z_3, z_2, z_1, z_4, z_5)$	34349	2.8 s	7.7 MiB

an optimal ordering and scanning for a sparse shift. The ordering alone leads to a reduction of  $\sim 40000$  probes, the search for a sparse shift requests 184 black-box evaluations but additionally reduces the total number of probes by  $\sim 20000$  leading to a reduced runtime of more than 50% from 3.6 s to 1.7 s taking both optimizations into account. Note that the memory consumption drastically increases when performing a shift scan for  $f_1$  since we first calculate all possible permutations of the shift and store them in a vector. For 20 variables, this leads to  $O(10^6)$  entries occupying  $\sim 120$  MiB of memory. The memory consumption of the reconstruction itself only needs  $\sim 7$  MiB and is thus reduced by roughly a factor of 4. The generation of the permuted shift vector requires 1.3 s whereas the reconstruction only takes 0.4 s.  $f_1$  is constructed in a way that the ordering has a huge impact on the number of black-box probes required to reconstruct it. Thus, scanning only for a sparse shift and not reordering parameters leads to a shift in  $z_{20}$  which is the worst shift one could possibly choose. Therefore, almost non probes are avoided compared to shifting all variables and using the same variable ordering.

The optimization effects seen for  $f_1$  are not that drastic when reconstructing a dense function like  $f_2$  in which a parameter reordering is not helpful. Instead, only a scan for a sparser shift can avoid some probes and reduces the overall runtime in operations in which the shift needs to be removed. Thus, there is no significant benefit concerning memory consumption but a slightly faster runtime. Separated to different prime fields, the number of requested probes using a shift scan are: 204 to find a suitable shift, 213130 to interpolate the full functional dependence, 53130 for the second prime field since we can normalize to the univariate degree 50 term in the denominator, 53129 for the third prime field, 1206 for the fourth, and an additional probe to check that the reconstruction succeeded.

As for the reconstruction of  $f_1$ , one can observe similar benefits utilizing optimizations

for  $f_3$ . A reordering of variables can significantly reduce the number of black-box probes to approximately one third of the non-optimal ordered case and, additionally, shorten the runtime to almost one fifth. Scanning for a sparser shift without a reordering leads, by construction, only to a small number of black-box evaluations avoided compared to shifting all variables. The benefit of this option is reflected in the runtime which reduces by almost 4s due to the much simpler polynomials needed to remove the effects of the shift during the polynomial interpolation. Combining an optimal variable order and a sparse shift can further reduce the runtime to 2.8s while requiring only less than a quarter of the black-box probes needed using no optimizations.

Usually, there is no knowledge about the function to be interpolated. Therefore, a useful a priori assumption about the variable ordering cannot be made in general. However, for physical calculations it can be often useful to first study a similar but simpler problem to estimate the variable structure and apply a corresponding ordering to the actual calculation. It is always best to set the potentially highest degree variable to  $z_1$  which will thus not be interpolated directly.

If evaluating probes is time consuming or the black-box function only depends on two to three variables, the scan for a sparse shift can lead to an increased overall runtime and might not be beneficial anymore.

# 4 Application to IBP reductions

In multi-loop calculations in high-energy physics one ends up with scalar Feynman integrals after an appropriate tensor reduction. The general form of scalar Feynman integrals with L loops is given by

$$I(d, \{p_j\}, \{m_i\}, \{a_i\}) \equiv \int_{k_1, \dots, k_L} \frac{1}{P_1^{a_1} \dots P_N^{a_N}}$$
(36)

with

$$\int_{k} \equiv \int \frac{\mathrm{d}^{d}k}{(2\pi)^{d}}.$$
(37)

and the inverse propagators  $P_i = q_i^2 - m_i^2 + i\epsilon$  in Minkowski space or  $P_i = q_i^2 + m_i^2$  in Euclidean space. The  $q_i$  are linear combinations of the loop momenta  $k_l$  and the external momenta  $p_j$ . The integral  $I(d, \{p_j\}, \{m_i\}, \{a_i\})$  depends on the space-time dimension d, the set of masses  $\{m_i\}$ , the set of external momenta  $\{p_j\}$ , and the propagator powers  $a_i$  which take integer values. N can be computed from L and the number of external momenta E by

$$N = EL + \frac{L(L+1)}{2}. (38)$$

It is useful to define the sum of all positive powers of the propagators of an integral as

$$r \equiv \sum_{i=1}^{\text{\#prop.}} \theta \left( a_i - \frac{1}{2} \right) a_i \tag{39}$$

and the absolute value of the sum of all negative powers as

$$s \equiv \sum_{i=1}^{\text{\#prop.}} \theta\left(\frac{1}{2} - a_i\right) |a_i|, \tag{40}$$

where  $\theta(x)$  is the Heaviside step function. Usually, an integral with higher r or higher s is regarded more difficult than an integral with lower r or s. Therefore, r and s can be used to sort the occurring integrals by difficulty.

The integration-by-parts (IBP) algorithm of Chetyrkin and Tkachov [19, 20] is based on the observation that inserting the scalar product of a derivative with respect to a loop momentum with another momentum into Eq. (36) leads to a vanishing integral in dimensional regularization:

$$\int_{k_1,\dots k_L} \frac{\partial}{\partial k_i^{\mu}} \left( \tilde{q}_j^{\mu} \frac{1}{P_1^{a_1} \dots P_N^{a_N}} \right) = 0, \tag{41}$$

where  $\tilde{q}_{j}^{\mu}$  can either be another loop momentum or an external momentum. By explicitly evaluating the derivative one arrives at the linear relations

$$0 = \sum_{n} c_n I(d, \{p_j\}, \{m_i\}, \{a_i^{(n)}\})$$
(42)

with modified  $a_i^{(n)}$ , where the values change by the addition or subtraction of small integers. The coefficients  $c_n$  are polynomials in d,  $\{m_i\}$ , and  $\{p_j\}$  with a small degree and also depend on the  $a_i$  in general. These relations are called IBP relations.

They can be combined to recursion relations which express an integral through easier integrals. The recursive application of the relations then allows to reduce all integrals to a small set of master integrals, which have to be computed by other methods to get the final result. At three-loop level, this approach has been successfully applied for massless propagator-type diagrams [20–22], massive tadpoles [23,24], and on-shell propagators [25–27]. However, the recursion relations usually have to be derived manually which makes this procedure unfeasible for multi-loop calculations. On the other hand, the reduction is straightforward and fast should they be found. In the last decade, some progress in the automatic derivation of recursion relations has been made [28–31].

In 2001, Laporta presented a different strategy [32]. By inserting integer values for the  $a_i$  in Eq. (42), so-called *seeds*, one obtains a system of equations for the occuring integrals. These systems can be solved by standard procedures to yield the desired reduction to master integrals. Obviously, one has to choose a sufficient amount of seeds for the specific problem. There exist several public implementations of modified versions of the Laporta algorithm, AIR [33], FIRE [29, 34–36], Reduze [37, 38], and Kira [39, 40], and numerous private ones. However, the Laporta algorithm has some major drawbacks. The systems of equations for the state-of-the-art calculations become huge and expensive to solve both in terms of memory and runtime. This is partially related to large intermediate expressions which occur during the solution process.

Since the IBP relations are linear, the solution strategies only involve the addition, subtraction, multiplication, and division of the polynomial coefficients  $c_n$ . Therefore, the coefficients

of the master integrals are rational functions in d,  $\{m_i\}$ , and  $\{p_j\}$ . Thus, the problems of the Laporta algorithm can be eased by finite-field techniques as proposed by Kauers in 2008 [41]. One can replace all occurring variables by members of the finite field and the solve the system of equations numerically. This is in general orders of magnitude faster than solving the system analytically. The first realized application was to solve the system of equations over a finite field before the actual analytic reduction [42]. This allows to identify and remove the linearly dependent equations. By also performing the back substitution, one can additionally identify the master integrals and also select only those equations which suffice to reduce a requested subset of integrals. This procedure has been implemented in Kira [39].

Some of the finite-field-interpolation techniques from computer science described in Sect. 2 have been summarized before in a physical context in Refs. [43, 44]. The first pure finite-field IBP reduction was presented by von Manteuffel and Schabinger in 2016 [45]. Recently, three more calculations were concluded [46–48]. All of them are one scale problems and, thus, one variable problems, i.e. they only require univariate interpolation techniques, which has been implemented in private codes. The recently published Version 1.2 of Kira uses a multivariate polynomial interpolation at intermediate stages of the reduction if it seems useful [40]. This means that instead of multiplying some (sub-)coefficients algebraically, their numerical values are multiplied and the result is interpolated by Newton's interpolation formula. However, this interpolation is done over  $\mathbb Z$  and not in a finite field.

Recently, FIRE6 was published as first public implementation of the Laporta algorithm using the interpolation of rational functions over a finite field [36]. For polynomials it performs a multivariate Newton interpolation. The interpolation of rational functions works in several steps. First, univariate interpolations are performed for each variable separately using Thiele's interpolation formula. By assuming that the denominator of the final result can be factorized into functions depending only on one variable each, one can turn the rational function into a polynomial by multiplying it with the denominators obtained from the univariate interpolation. This allows to perform a multivariate Newton interpolation. However, it seems to only work for up to two variables at the moment and it is not clear whether the factorization assumption can be generalized to several kinematic variables.

For more details on IBP reductions we refer the reader to the Ref. [66] and Refs. [67,68] for an general overview about techniques for the calculation of multi-loop Feynman integrals.

#### 4.1 Implementation

Since Kira already utilizes the reduction over a finite field as a preliminary step, we chose it as a basis for our implementation. The idea is to use the built-in solver pyRed to solve the system of IBPs many times over several prime fields, extract the numerical values, and feed them to FireFly to reconstruct the rational functions. We thus added the option to start the reduction with an interpolation in finite fields using FireFly. Another important option is to choose the order of the variables of the problem including d. The order can have a major impact on the runtime as shown in Sect. 3.3.

Our implementation follows the Reconstructor class described in Sect. 3.2 with several

small modifications, e.g. the structure of the function black\_box. FireFly is compiled to use FLINT for the modular arithmetic. We start by loading the system of linearly-independent equations. The variables are replaced by the values requested by the reconstruction objects and the resulting numerical system is solved by pyRed. Additionally, we perform two integral selections. Even though the system only contains all required linearly-independent equations from the start, after the forward eliminations not all of these equations are required anymore for the back substitution in general. We thus select only those equations which are required for the reduction of the requested integrals. The same selection is performed in the analytic calculation with Kira. We perform a second selection after the back substitution which selects only the coefficients of the master integrals for the requested integrals. This selection does not offer any advantage in an analytic approach because everything is already solved at this point. In our approach this allows us to omit potentially difficult rational functions which are not required to get the desired result.

#### 4.2 Examples

To illustrate the validity of the reconstruction approach for Laporta's algorithm for multiscale Feynman integrals, we apply our private implementation described in the previous section to some example topologies. We compare it with the highly optimized algebraic program Kira  $1.2.^2$  It is important to stress that our link of FireFly to Kira has room for optimizations and that we leave real benchmarks for an official implementation. Therefore, we just compare the straight on calculations, i.e. we do not use some of the advanced features of Kira like the sectorwise forward elimination or the back substitution for subsets of master integrals. We also do not use the option algebraic\_reconstruction, i.e. we compare a fully algebraic calculation to the finite field approach. In both approaches, we restrict r and s of the seed integrals by  $r_{\rm max}$  and  $s_{\rm max}$  and select the integrals with the option select\_mandatory\_recursively in the same range.

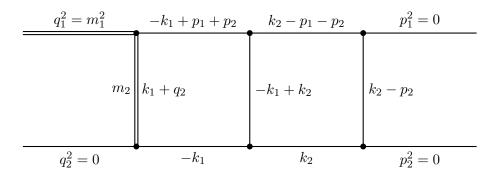


Figure 1: The planar double box topo7 which occurs, e.g., in single top production.

Our first example is topo7, which is one of the examples provided by Kira. This planar two-loop diagram is shown in Fig. 1. It occurs in single top production. We first set the masses  $m_1$  and  $m_2$  to zero so that the kinematic invariants  $s^3$  and t are the only massive parameters.

<sup>&</sup>lt;sup>2</sup>We use it in combination with version 6.21 of Fermat [69].

<sup>&</sup>lt;sup>3</sup>Not to be confused with the sum of all negative powers s defined in Eq. (40).

By setting s to one, only t and the space-time dimension d remain as parameters. For our reconstruction, we order them as d, t for the best performance, because d appears with higher powers in the result.

Table 2: Runtime and memory usage for Kira 1.2 and Kira with FireFly for topo7 without masses and with  $r_{\rm max}=7$ . We use the option select\_mandatory\_recursively, order the variables as d, s, t, and set s to one. The runtime only includes the time spent on the forward elimination and back substitution or the time for the reconstruction, respectively. These tests were run on a computer with an Intel Core i7-3770 and 8 GiB of RAM.

	Kira 1.2		Kira with FireFly		
$s_{\max}$	Runtime	Memory usage	Runtime	CPU time for pyRed	Memory usage
2	$7.9\mathrm{s}$	$0.3\mathrm{GiB}$	1.9 s	89 %	$0.3\mathrm{GiB}$
3	$10.2\mathrm{s}$	$0.5\mathrm{GiB}$	$5.2\mathrm{s}$	90%	$0.5\mathrm{GiB}$
4	14.1 s	$0.9\mathrm{GiB}$	14.3 s	90%	$0.9\mathrm{GiB}$

The results for different  $s_{\rm max}$  are shown in Tab. 2. For  $s_{\rm max}=2$ , the reconstruction is faster by a factor of four. However, it scales worse than the algebraic calculation when increasing  $s_{\rm max}$  with only eight threads available. Kira becomes slightly faster for the amplitude with  $s_{\rm max}=4$ . Kira has to reduce 2774, 7994, and 17548 equations for  $s_{\rm max}=2,3,4$ , whereas the reconstruction implementation selects only the 730, 1837, and 3970 mandatory equations, respectively. Most of the CPU time for the reconstruction is used for the numerical solutions of the system with pyRed, i.e. the black-box probes. For  $s_{\rm max}=2$ , the reconstruction requires about 120 black-box probes which take 0.07 s, 180 with 0.17 s each for  $s_{\rm max}=3$ , and 280 with 0.33 s each for  $s_{\rm max}=4$ . The forward elimination contributes with roughly 75% to these times. The memory consumption for both versions is dominated by the preliminary steps to construct the system of linearly independent equations.

The calculation becomes much more expensive in terms of CPU time when taking the masses into account. We again order the variables by the highest powers appearing in the result, which now is  $m_2$ , t, s, d,  $m_1$  and set the highest massive parameter  $m_2$  to one.

The two additional parameters lead to a drastic increase in the runtime up to two orders of magnitude for both approaches for higher  $s_{\rm max}$ , but the reconstruction approach suffers much more than the algebraic one as shown in Tab. 3. However, now the scaling with  $s_{\rm max}$  is inverted. The reconstruction approach is slower by a factor of 3.4 for  $s_{\rm max}=2$ , which reduces to a factor of 3.0 for  $s_{\rm max}=4$ . The memory consumption is almost entirely dominated by the actual reduction or reconstruction with  $s_{\rm max}=2$  for the reconstruction being the sole exception. Kira reduces 3902, 10216, and 22571 equations for  $s_{\rm max}=2,3,4$ , whereas our reconstruction implementation selects only the 949, 2439, and 5370 mandatory equations. The number of coefficients which have to be reconstructed increases from 2984 to 7428 to 15531. Since the complexity of the coefficients also increases when going to higher  $s_{\rm max}$ , they require a lot more memory to store input values, terms, and subtraction terms of the shift. The higher complexity also leads to a decreasing limitation through pyRed, because internal calculations in FireFly become more expensive. However, the numerical

Table 3: Runtime and memory usage for Kira 1.2 and Kira with FireFly for topo7 with  $r_{\text{max}} = 7$ . We use the option select\_mandatory\_recursively, order the variables as  $m_2$ , t, s, d,  $m_1$ , and set  $m_2$  to one. The runtime only includes the time spent on the forward elimination and back substitution or the time for the reconstruction, respectively. These tests were run on a computer with an Intel Core i7-3770 and 8 GiB of RAM.

	Kira 1.2		Kira with FireFly		
$s_{\max}$	Runtime	Memory usage	Runtime	CPU time for pyRed	Memory usage
2	$38\mathrm{s}$	$0.5\mathrm{GiB}$	128 s	94%	$0.4\mathrm{GiB}$
3	$270\mathrm{s}$	$0.8\mathrm{GiB}$	880 s	91%	$0.8\mathrm{GiB}$
4	$3000\mathrm{s}$	$1.6\mathrm{GiB}$	$9200\mathrm{s}$	89%	$3.6\mathrm{GiB}$

solutions with pyRed are still the main bottleneck by an order of magnitude. Roughly 9400 of them are required for  $s_{\text{max}} = 2$ , with each of them taking taking 0.1 s. These numbers increase to 25900 and 0.24 s for  $s_{\text{max}} = 3$  and 117000 and 0.54 s for  $s_{\text{max}} = 4$ . Again, the forward elimination is responsible for more than 75% of the solution times.

Table 4: Scaling of Kira 1.2 and Kira with FireFly with the number of threads for topo7 with  $r_{\rm max}=7$  and  $s_{\rm max}=4$ . We use the option select\_mandatory\_recursively, order the variables as  $m_2$ , t, s, d,  $m_1$ , and set  $m_2$  to one. The runtime only includes the time spent on the forward elimination and back substitution or the time for the reconstruction, respectively. These tests were run on a computer with two Intel Xeon Gold 6138 and 768 GiB of RAM.

	Kira 1.2		Kira with FireFly	
# Threads	Runtime Memory usage		Runtime	Memory usage
10	1900 s	1.9 GiB	7450 s	3.6 GiB
20	$1500\mathrm{s}$	$2.8\mathrm{GiB}$	$4350\mathrm{s}$	$3.9\mathrm{GiB}$
40	$1550\mathrm{s}$	$4.8\mathrm{GiB}$	$2950\mathrm{s}$	$4.1\mathrm{GiB}$
80	$1450\mathrm{s}$	$8.8\mathrm{GiB}$	$2050\mathrm{s}$	$4.9\mathrm{GiB}$

In Tab. 4 we show how both approaches scale with the number of CPU threads available. Note that these numbers are not directly comparable to the numbers in Tab. 3, because different computers were used. The CPUs not only differ in clock speed and architecture but also in the number of cores. The Intel Core i7-3770 used in Tab. 3 has four physical cores and four additional logical cores whereas the two Intel Xeon Gold 6138 used for Tab. 4 offer 20 physical and 20 additional logical cores each. Therefore, the calculations in Tab. 4 can run on physical cores for up to 40 threads.

Kira does not really profit from many threads in this example. Doubling the number from 10 to 20 only increases the performance by less than a factor of 1.3. A further increase basically does not impact the runtime anymore, since large parts of the back substitution run on one or two threads. However, the memory consumption increases drastically, because

each additional Fermat instance requires additional memory. On the other hand, doubling the number of threads from 10 to 20 increases the performance of the reconstruction approach by a factor of 1.7, doubling from 20 to 40 by a factor of 1.5, and doubling from 40 to 80 still by a factor of 1.4. Thus, while the reconstruction takes almost four times longer than the algebraic approach on 10 threads, this difference reduces to only 40 % on 80 threads. Additionally, the reconstruction approach could profit from even more threads. The performance gain only comes with a moderate increase in memory consumption.

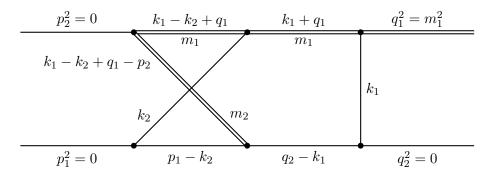


Figure 2: The non-planar double box topo5 which occurs, e.g., in single top production.

Our second example is topo5 of the Kira examples, which is a two-loop non-planar diagram occurring in single top production. The diagram is shown in Fig. 2. We order the parameters as  $m_1$ , s,  $m_2$ , t, d and set  $m_1$  to one.

Table 5: Runtime and memory usage for Kira 1.2 and Kira with FireFly for topo5 with  $r_{\text{max}} = 7$ . We use the option select\_mandatory\_recursively, order the variables as  $m_1$ , s,  $m_2$ , t, d, and set  $m_1$  to one. The runtime only includes the time spent on the forward elimination and back substitution or the time for the reconstruction, respectively. These tests were run on a computer with two Intel Xeon Gold 6138 and 768 GiB of RAM.

	Kira 1.2		Kira with FireFly		
$s_{\max}$	Runtime	Memory usage	Runtime	CPU time for pyRed	Memory usage
1	$4 \min$	$7.6\mathrm{GiB}$	$3 \min$	99%	$0.9\mathrm{GiB}$
2	1 h 53 min	$33\mathrm{GiB}$	1 h 42 min	97%	$3.3\mathrm{GiB}$
3	18 h 28 min	$102\mathrm{GiB}$	18 h 34 min	91%	$18\mathrm{GiB}$

Both versions perform the reductions in similar times as shown in Tab. 5. However, the reconstruction approach requires significantly less memory. Again, the CPU time is mainly used for pyRed. For  $s_{\rm max}=1,2,3$ , the reconstruction requires 15500 probes and one prime field, 269700 probes and two prime fields, 1090400 probes and three prime fields. Each probe takes 0.36 s, 0.91 s, or 2.1 s, respectively, and around 83 % of this is spent for the forward elimination. Kira reduces 3044, 10069, and 23670 equations whereas the reconstruction approach selects only 434, 1512, and 4086 mandatory equations.

As last example, we consider topo5 with a different mass configuration. The non-planar

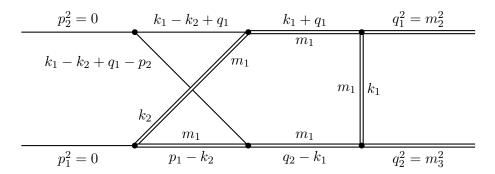


Figure 3: The non-planar double box topo5 $_{m}$  which occurs, e.g., in the gluon-induced production of a Higgs and a Z boson.

two-loop diagram shown in Fig. 3 occurs for example in HZ production through gluon fusion. In contrast to topo5 there are now five massive parameters:  $m_1$ , s,  $m_2$ ,  $m_3$ , and t. We can only guess the optimal order from the completed calculations with small  $s_{\text{max}}$ . There, their highest powers occur in the order stated above, with the additional space-time dimension d at the last position. Thus, we set  $m_1$  to one.

Table 6: Runtime and memory usage for Kira 1.2 and Kira with FireFly for topo5\_m with  $r_{\rm max}=7$ . We use the option select\_mandatory\_recursively, order the variables as  $m_1$ , s,  $m_2$ ,  $m_3$ , t, d, and set  $m_1$  to one. The runtime only includes the time spent on the forward elimination and back substitution or the time for the reconstruction, respectively. These tests were run on a computer with two Intel Xeon Gold 6138 and 768 GiB of RAM.

	Kira 1.2		Kira with FireFly		
$s_{ m max}$	Runtime	Memory usage	Runtime	CPU time for pyRed	Memory usage
1	22 h 40 min	$175\mathrm{GiB}$	7 h 35 min	88 %	$4.7\mathrm{GiB}$

Since this example is extremely complicated, we only consider  $s_{\rm max}=1$  in Tab. 6 to illustrate how both approaches perform. The reconstruction over finite fields is faster by a factor of four and still mainly limited by pyRed. Additionally, it requires one to two orders less memory than the algebraic approach. It selects only the 1785 mandatory equations in contrast to the 3140 equations Kira reduces. About  $1.5 \cdot 10^6$  black-box probes and two prime fields are needed to reconstruct all coefficients. Each pyRed solution takes  $0.32 \, {\rm s}$ , where the forward elimination contributes with 93 %.

## 4.3 Application to the perturbative gradient flow

The gradient-flow formalism [70–72] has proven to be a useful tool in lattice QCD. Additionally, there are several areas of potential cross fertilization between lattice and perturbative calculations. However, the perturbative side was only computed to a low order in perturbation theory in many cases. We want to use the IBP reduction as a systematic approach to higher-order calculations. As a verification of this approach we want to compute the same

observable as in Ref. [73], where the computation was performed by solving all integrals numerically. Furthermore, we want to compute two additional observables. Our results will be published in Ref. [74].

Our setup produces all Feynman diagrams, inserts the Feynman rules, and reduces the tensor structures. We also expand the integrals to the leading order in the quark masses and end up with massless three-loop vacuum integrals of the form

$$I(d, t, \{t_f^{\text{up}}\}, \{T_i\}, \{a_i\}) = \left(\prod_{f=1}^F \int_0^{t_f^{\text{up}}} dt_f\right) \int_{k_1, k_2, k_3} \frac{\exp[-(T_1 q_1^2 + \dots + T_6 q_6^2)]}{q_1^{2a_1} \dots q_6^{2a_6}},$$
(43)

where  $F \leq 4$  is the number of flow-time integrations and the upper limits  $t_f^{\text{up}}$  are either the flow-time scale t of the diagram or other flow-time variables  $t_{f'}$ . The  $T_i$  are nonnegative linear combinations of the flow variables, i.e.  $T_1 = t + t_1 - 2t_3$ . Due to the expansion in the quark masses, the flow-time scale t is the only massive scale appearing in the integrals.

Instead of evaluating the integrals numerically as in Ref. [73] we build a system of equations using IBP-like relations, where we set t=1 and, thus, the space-time dimension d is the only parameter. However, the analytic forward elimination with Kira 1.2 fills all our available memory of 768 GiB of RAM after running for five days and nine hours on the 80 threads of two Intel Xeon Gold 6138. The progress so far indicates that it probably would have to run for at least several days more if we had enough memory. It might be possible to complete the reduction by adapting the sectorwise forward elimination introduced in Kira 1.2 for the gradient flow integrals.

Our implementation with finite-field-interpolation techniques as described in Sect. 4.1 runs about two days and 20 hours on ten threads to obtain the complete analytic result. Each numerical system requires around 70 GiB of RAM and takes  $\sim 50\,\mathrm{s}$  to parse all analytic coefficients to numerical values,  $\sim 10400\,\mathrm{s}$  to complete the forward elimination, and  $\sim 16\,\mathrm{s}$  to complete the back substitution. We need three 63-bit prime numbers and 201 numerical solutions in total to reconstruct all rational functions with all rational coefficients and an additional solution with a fourth prime to verify the results.

The highest degree in the numerator is 32 and the highest degree in the denominator 34. At intermediate stages of the analytic forward elimination monomials with at least degree 508 occur.<sup>4</sup> Therefore, this is either a prime example for circumventing large intermediate expressions or of the possibility to neglect large coefficients which are not required for the desired result. However, this is a special problem with only one massive scale, which can be set to one, and, thus, only the space-time dimension d appears in the rational functions. The reduction is also heavily limited by the forward elimination. While this is the default case for numerical solutions, this also holds for the analytic reduction of gradient-flow integrals based on our experience. This is unusual for the reduction of Feynman integrals.

The reduction allows us to express the 3195 required integrals through 188 master integrals. We checked that our reduction yields the correct results by comparing the numerical values for the integrals expressed through the master integrals with the numerical values of the integrals computed directly.

<sup>&</sup>lt;sup>4</sup>We know this because we had to change the Fermat [69] settings to support higher degrees with Kira 1.1.

#### 5 Conclusions

We presented the open-source C++ library FireFly for the reconstruction of polynomials and rational functions, which is based on algorithms developed in computer science. Additionally, we made some modifications to reduce the number of black-box probes and avoid cancellations. We showed that FireFly is capable to reconstruct multivariate rational functions with many variables.

As an example, we applied FireFly to the Laporta algorithm for IBP reductions by linking it to Kira. In the example topologies, this approach proved to be competitive to the algebraic approach with Kira. Kira is usually faster for smaller problems. However, when the system of equations becomes huge and large intermediate expressions occur, the reconstruction with FireFly can become faster and require much less memory. The reconstruction approach does not need to compute the large intermediate expressions and can also strictly select only those coefficients which are requested, whereas the algebraic approach can neither circumvent the large intermediate expressions nor perform such a strict selection.

In both approaches, the reduction can be distributed to several computers or several sessions on the same machine, which require less memory. Kira allows to perform the back substitution for subsets of master integrals, which is of course limited by the number of master integrals. The reconstruction approach allows to reconstruct subsets of the coefficients or in principle each coefficient on its own. The number of coefficients is usually orders of magnitude larger than the number of master integrals. This also offers the possibility to choose the subsets such that all of them require a sparser shift than the complete set, which can speed up the reconstruction for the individual coefficients significantly. Even for the straight-on approach for quite simple problems, the reconstruction benefits much more from additional CPU threads at least up to several hundred of them. This scaling can even be improved by guessing the required black-box probes in advance. However, this could lead to unnecessary calculations.

Our implementation within Kira is strongly limited by the numerical solutions with pyRed, which require most of the CPU time in our examples. Therefore, it is desirable to reduce the number of black-box probes required for the reconstruction by algorithmic improvements in FireFly. We hope that racing the Ben-Or/Tiwari algorithm against Newton's algorithm as part of Zippel's algorithm as proposed in Refs. [7, 8] achieves this. Optimizations for pyRed would also help to widen this bottleneck. We also noted that performing the forward elimination is usually the most expensive step for pyRed. Since the algebraic forward elimination is often cheap compared to the back substitution, it might be worthwhile to perform it algebraically and perform only the back substitution numerically for the reconstruction if one expects to require many black-box probes.

Of course, FireFly can also be used for hybrid approaches. For example, Kira 1.2 already offers a multivariate Newton interpolation for (sub-)coefficients over  $\mathbb{Z}$  instead of multiplying them algebraically if this seems heuristically useful [40].

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The Feynman diagrams in this paper were drawn with TikZ-Feynman [75].

## **A** Algorithms

#### **Maximal Quotient Rational Reconstruction**

Wang's algorithm for the RR, Alg. (1) [18], only succeeds if the modulus of both numerator |b| and denominator |c| of the rational number are smaller than  $\sqrt{p/2}$ . However, the proof of the uniqueness of the result only requires  $p \geq 2|b||c|$  [14]. This bound is equally distributed to b and c in Alg. (1). In principle, one can adjust the bounds for every number separately, but this requires knowledge of the number before the RR.

Monagan observed that the guess of the rational number comes together with a huge quotient in the Euclidean algorithm [58]. Based on this observation he suggested the algorithm called Maximal Quotient Rational Reconstruction, which returns the rational number corresponding to the largest quotient encountered.

### Algorithm 4 Maximal Quotient Rational Reconstruction (MQRR) [58].

**Input:** A finite field member a, the defining prime of the finite field p, and the error tolerance parameter T.

**Output:** If succeeded a unique value of a in  $\mathbb{Q}$  else an error.

```
function MQRR(a, p)
   if a == 0 then
       if p > T then
           return 0;
       else
           Throw an error that the rational reconstruction failed;
       end if
   end if
   n \leftarrow 0; d \leftarrow 0;
   t \leftarrow 1; old_t \leftarrow 0;
   r \leftarrow a; old_r \leftarrow p;
   while r \neq 0 and old_r > T do
       quotient \leftarrow | \text{old}_r / r |;
       if quotient > T then
           n \leftarrow r; d \leftarrow t; T \leftarrow quotient;
       end if
       (old_r, r) \leftarrow (r, old_r - quotient * r);
       (old_t, t) \leftarrow (t, old_t - quotient * t);
   end while
   if d == 0 or gcd(n, d) \neq 1 then
       Throw an error that the rational reconstruction failed;
   end if
   return n / d;
end function
```

It can only be proven that it returns a unique solution if  $|b||c| \le \sqrt{p}/3$ . However, it performs much better in the average case because large quotients from random input are rare. The

parameter T allows to choose a lower bound for the quotients and the algorithm fails if the quotients are smaller. Of course, it has to increase with an increasing prime number p, because a random input will generate higher quotients as well. Monagan suggested to calculate it by the formula  $T = 2^c \lceil \log_2 p \rceil$  and choose c according to the required error tolerance. We choose c = 10 for FireFly, which roughly corresponds to 1% false positive reconstructions.

#### Solving modified transposed Vandermonde systems

The solution of modified transposed Vandermonde systems defined in Eq. (15) only requires small changes compared to the solution strategies for usual transposed Vandermonde systems given by Refs. [3,5]. Vandermonde matrices of size  $M \times M$  are completely determined by M evaluation points  $v_1, \ldots, v_M$ . Their  $M^2$  components are given by integer powers  $v_i^j$ ,  $i, j = 1, \ldots, M$  in the modified case. For simplicity, we only consider one variable. The solution method of such systems is closely related to Lagrange's polynomial interpolation formula.

Let  $B_i(z)$  be the polynomial of degree M defined by

$$B_{j}(z) = \frac{z}{v_{j}} \prod_{\substack{m=1\\m \neq j}}^{M} \frac{z - v_{m}}{v_{j} - v_{m}} = \sum_{k=1}^{M} A_{jk} z^{k}.$$
 (44)

 $A_{ij}$  is the matrix defined by the coefficients that arise when the product of Eq. (44) is multiplied out and like terms are collected. The polynomial  $B_j(z)$  is specifically designed so that it vanishes at all  $v_i$  with  $i \neq j$  and has a value of unity at  $z = v_j$ . Inserting  $v_i$  as an argument, one observes

$$B_j(v_i) = \delta_{ij} = \sum_{k=1}^{M} A_{jk} v_i^k.$$
 (45)

Eq. (45) states that  $A_{jk}$  is exactly the inverse of the matrix of components  $v_i^k$ . Therefore, the solution of the modified Vandermonde system in Eq. (15) is just that inverse times the right-hand side,

$$c_{\alpha_i} = \sum_{k=1}^{M} A_{ik} f(\vec{y}^k). \tag{46}$$

It is left to multiply the monomial terms in Eq. (44) out in order to get the components of  $A_{ik}$ . By defining a master polynomial B(z) by

$$B(z) \equiv \prod_{m=1}^{M} (z - v_m) = \sum_{i=0}^{M} d_i z^i$$
 (47)

one can evaluate its coefficients and then obtain the specific  $B_j$  via synthetic divisions by the one supernumerary term. Each division is of O(M) and the total procedure is thus of  $O(M^2)$ . To generalize the solution algorithm to a multivariate system one just needs to redefine  $v_i$  as defined in Eq. (15). The algorithm for generalized systems is summarized in Alg. (5).

## **Algorithm 5** Algorithm to solve modified Vandermonde systems motiviated by Refs. [3,5].

Input: An array of probes of a polynomial, an array of the corresponding inserted values and an array of the contributing degrees of the polynomial ordered (co)lexicographically.Output: An array with the coefficients of the contributing degrees.

```
function SOLVE_MOD_TRANSPOSED_VANDERMONDE(probes, values, degrees)
   num\_eqn \leftarrow probes length; cis; vis;
   i \leftarrow 0;
   for i < length of values do // Calculate v_i
       j \leftarrow 0;
       vi \leftarrow 1;
       for j < length of values[j] do</pre>
           vi ← vi * values[i][j] ** degrees[i][j];
           j \leftarrow j + 1;
       end for
       vis[i] = vi;
        i \leftarrow i + 1;
   end for
   if num_eqn is equal to 1 then
        cis[0] \leftarrow probes[0] / vi;
   else
        dis[num\_eqn - 1] = -vis[0]; // Calculate d_i
        i \leftarrow 1;
        for i < num_eqn do
           \texttt{j} \leftarrow \texttt{num\_eqn - 1 - i};
           for j < num_eqn - 1 do
               cis[j] \leftarrow dis[j] - vis[i] * dis[j + 1];
               j \leftarrow j + 1;
           end for
           dis[num\_eqn - 1] \leftarrow dis[num\_eqn - 1] - vis[0];
           i \leftarrow i + 1;
        end for
   end if
    i \leftarrow 0;
   for i < num_eqn do // Calculate A_{kj} and c_{\alpha_i}
                   b \leftarrow 1; s \leftarrow probes[num\_eqn - 1]; j \leftarrow num\_eqn - 1;
        t \leftarrow 1;
        for j > 0 do
           b \leftarrow dis[j] + vis[i] * b;
           s \leftarrow s + probes[j - 1] * b;
           t \leftarrow vis[i] * t + b;
       end for
        cis[i] = s / t / vis[i];
   end for
   return cis;
end function
```

# B Internals of FireFly

FireFly provides additional classes to the ones introduced in Sect. 3, which can be useful for the usage of FireFly or modifications of the parallelization. We briefly summarize them in the following:

#### BaseReconst

The base class of functional-reconstruction objects BaseReconst serves as a container class for different member variables and functions. Its members are summarized in the following:

## FFInt get\_rand()

Returns a random number in the current prime field using an implementation of the pcg\_32 algorithm [76].

```
uint32_t get_num_eqn()
```

Returns the number of equations that have to be solved at the current stage as a uint32\_t, which corresponds to the number of black-box probes for the current  $z_i$  order. This option is currently only used for RatReconst.

```
bool is_done()
```

Returns true if the interpolation is done.

```
bool is_new_prime()
```

Returns true if the interpolation object needs a new prime field.

```
uint32_t get_prime()
```

Returns the prime counter of the interpolation object.

```
vector<uint32_t> get_zi_order()
```

Returns a vector which contains the current tuple of  $z_i$  orders.

```
uint32_t get_zi()
```

Returns the i of the corresponding  $z_i$  which is currently interpolated.

## PolyReconst

The polynomial-reconstruction class PolyReconst is derived from the BaseReconst class and performs the functional interpolation and promotion of the polynomial coefficients to  $\mathbb{Q}$ . Its member variables and functions can be summarized as:

```
PolyReconst(uint32_t n, const int deg_inp)
```

Creates a PolyReconst object for n variables. The second argument deg\_inp is optional and sets an upper bound on the maximal degree of the black-box function to optimize its interpolation.

## 

Feeds the object with a numerical probe num of the black-box function, the corresponding  $z_i$  order fed\_zi\_ord and prime counter fed\_prime.

### void interpolate()

Starts the interpolation for all stored feeds.

### Polynomial get\_result()

Returns the reconstructed polynomial in  $\mathbb{Q}$  as a Polynomial object. It should only be called after is\_done() returns true.

## void generate\_anchor\_points()

Generates the initial values for all  $z_i$ .

#### FFInt get\_rand\_zi(uint32\_t zi, uint32\_t order)

If already stored, returns the randomized value of  $z_i$  corresponding to its  $z_i$  order order.

### vector<FFInt> get\_rand\_zi\_vec(const vector<uint32\_t>& orders)

If already stored, returns the randomized values of  $z_i$  corresponding to their  $z_i$  orders orders as a vector.

### static void reset()

Resets all static varibles to start new reconstruction jobs over different prime fields.

#### RatReconst

The rational-function reconstruction class RatReconst is derived from the BaseReconst class and performs the functional interpolation and promotion of the rational-function coefficients to  $\mathbb{Q}$ . Its member variables and functions can be summarized as:

## RatReconst(uint32\_t n)

Creates a RatReconst object for n variables.

```
void feed(const FFInt& new_ti, const FFInt& num, \
      const vector<uint32_t>& fed_zi_ord, const uint32_t fed_prime)
```

Feeds the object with a numerical value of the homogenization variable  $new_ti$ , a numerical probe num of the black-box function, the corresponding  $z_i$  order  $fed_zi_ord$  and prime counter  $fed_prime$ .

## bool interpolate()

Starts the interpolation for all stored feeds. Returns **true** if the interpolation is already running.

## RationalFunction get\_result()

Returns the reconstructed rational function in  $\mathbb{Q}$  as a RationalFunction object. If called when is\_done returns false it exits with an error message.

### void generate\_anchor\_points()

Generates the initial values for all  $z_i$  with i > 1.

#### void disable\_shift()

Sets all entries of the static variable shift to zero.

## FFInt get\_rand\_zi(uint32\_t zi, uint32\_t order)

If already stored, returns the randomized value of  $z_i$  corresponding to its  $z_i$  order order.

#### vector<FFInt> get\_rand\_zi\_vec(const vector<uint32\_t>& orders)

If already stored, returns the randomized values of  $z_i$  corresponding to their  $z_i$  orders orders as a vector.

## vector<FFInt> get\_zi\_shift(uint32\_t zi)

Returns the shift for a specific  $z_i$ .

## vector<FFInt> get\_zi\_shift\_vec()

Returns the shift for all  $z_i$  stored in a vector starting with  $z_1$  at position 0.

#### bool need\_shift()

Returns true if the objects needs the shift to interpolate the black box over additional prime fields.

## void set\_tag(const string& tag)

Allows the user to set a tag for a RatReconst object. If a tag is set, the state of the object will be written to ./ff\_save/tag\_<prime\_counter>.txt, where prime\_counter is the currently used entry of the provided prime array. The written file can then be used to resume an interpolation starting from this state.

## void start\_from\_saved\_file(string file\_path)

Passing the absolute path file\_path to a previously saved state of a RatReconst object, FireFly will continue the interpolation from this state.

#### void scan\_for\_sparsest\_shift()

Enables the scan variable for a sparser shift. Afterwards a normal interpolation takes place until one accepts a tested shift.

### bool is\_shift\_working()

Returns true if the current shift is sufficient to obtain a unique normalization. Additionally, all variables are resetted to probe another shift. Should be called during a scan after each interpolation.

#### set\_zi\_shift(const vector<uint32\_t>& shifted\_zis)

Set a new, random shift according to the vector  $shifted\_zis$ .  $shifted\_zis$  is filled with zeros and ones to indicate which variable should be shifted, i.e.  $\{0,1,0\}$  leads to a shift in  $z_2$ . This function has to be called after  $is\_shift\_working()$  and before the first interpolation after shifting all variables takes place.

### void accept\_shift()

Accepts the previously tested shift for the reconstruction of the black box.

```
static void reset()
```

Resets all static varibles to start new reconstruction jobs over different prime fields.

#### RationalNumber

A RationalNumber object is a container class which represents an element of  $\mathbb{Q}$ . The element is built by two arbitrarily precise integer values which are realized through mpz\_class objects. The latter can be accessed by the member variables numerator and denominator. For convenience, it also provides the << insertion operator for streams. Useful member functions are summarized in the following:

RationalNumber(const mpz\_class& numerator, const mpz\_class& denominator) Creates a RationalNumber object with a given numerator and denominator.

## Polynomial

A Polynomial object represents a multivariate polynomial over  $\mathbb{Q}$ . The data structure is an unordered\_map called coefs, whose key is a vector<uint32\_t> of length n where n is the number of variables. The entries of this vector are the degrees of each variable. This vector is the equivalent of the multi index  $\alpha_i$  introduced in Eq. (3). The values of the map are RationalNumber objects and correspond to the coefficient  $c_{\alpha_i}$  as defined in Eq. (3). For convenience, it provides the << insertion operator for streams. Useful member functions are summarized in the following:

Polynomial(const unordered\_map<vector<uint32\_t>, RationalNumber>& coefs)
Creates a Polynomial object with the given degrees and coefficients of coefs.

void clear()

Clears the polynomial.

string to\_string(const vector<string>& symbols)

Rewrites the polynomial by incorporating the given symbols and returns it as a string.

void sort()

Sorts the coefficient map of the polynomial in a lexicographical order with respect to the degrees.

### RationalFunction

A RationalFunction object is a container class which combines two Polynomial objects to a rational function by defining a numerator and denominator. For convenience, it provides the << insertion operator for streams. Useful member functions are:

RationalFunction(const Polynomial& numerator, const Polynomial&\ denominator)

Creates a RationalFunction object for the given Polynomial objects.

```
string to_string(const vector<string>& symbols)
```

Rewrites the rational function incorporating the given symbols and returns it as a string.

## ReconstHelper

The ReconstHelper file contains the hundred largest 63-bit prime numbers which can be accessed through the function primes() that returns a vector. The first element is the largest one and the last is the smallest.

#### utils

The utils file contains the implementation of some algorithms and a function to generate all possible tuples of zeros and ones needed for a full scan of all possible shifts with respect to the number of variables.

Combines the two pairs p1 and p2 of a number and a prime number to a new pair with the CRT given by Alg. (2).

Applies Alg. (1) for the integer a and the prime number p. It returns the pair of a bool which indicates if it suceeded and the reconstructed RationalNumber.

Applies Alg. (4) for the integer a and the prime number p. It returns the pair of a bool which indicates if it suceeded and the reconstructed RationalNumber.

```
vector<vector<uint32_t>> generate_possible_shifts(uint32_t r))
```

Returns a vector of all possible tuples of zeros and ones of length  ${\tt r}$  ordered from tuples containing only one one to at most  ${\tt r}$  - 1 ones.

### **Parallelization**

Let us finish this section by a few more words on the details of parallel computing. Each PolyReconst and RatReconst object possesses two mutexes, namely, mutex\_status and mutex\_statics. The former protects the status of the object, i.e. all member variables which can be accessed through getters. All changes to these variables only occur after mutex\_status was obtained and all getters obtain mutex\_status before accessing the variables. mutex\_statics protects the static variables which are used by all reconstruction objects, e.g. shift and rand\_zi, which are private members representing the used shift and a collection of numerical values for different  $z_i$  orders.

To interpolate a function, we follow a two step paradigm. In a first step, we provide the reconstruction class with a black-box probe at a given  $z_i$  order. This procedure is called a feed. If a reconstruction is not already done, the reconstruction class always accepts a feed if it is evaluated for the current prime number. All feeds are stored in a queue for later usage. The interpolation and reconstruction is done independently of the feed procedure. If the member function interpolate is called, the class tries to reconstruct the black-box function with all stored feeds in the queue and runs until it is done or a probe corresponding to a  $z_i$  order is requested, which is not present in the queue. During the interpolation, the object can be fed, but no additional interpolation job is accepted. Thus, the interpolate function checks whether another interpolation is already running and returns immediately should this be the case. Otherwise it takes feeds from the queue and proceeds with the interpolation until the queue is empty or the reconstruction is done. This procedure allows the user to start the interpolation for every feed without concerning whether the interpolation is already running or not.

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