Integral Reduction with Kira 2 and Finite Field Methods

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Introduction

- Kira is a linear solver for sparse linear system of equations with main application to **Feynman integral reduction**
- **The development of Kira** is dedicated to extend the range of feasible high precision calculations and help to study many state-of-the-art problems
- Kira should be used to built more advanced tools to compute Feynman integrals
- To do so, YAML allows to write human readable interface to Kira

Feynman integral reduction applications

- Integration-by-parts (IBP)[Chetyrkin, Tkachov, 1981] and Lorentz invariance [Gehrmann, Remiddi, 2000] identities for scalar Feynman integrals are very important in quantum field theoretical computations (multi-loop computations)
- **Reduce the number of Feynman integrals** to compute, which appear in scattering amplitude computations to a **small basis** of master integrals
- **Compute these integrals** analytically or numerically with the methods of
  - **differential equations** [Kotikov, 1991; Remiddi, 1997; Henn, 2013; Argeri et al., 2013; Lee, 2015; Meyer, 2016; Moriello, 2019; Hidding, 2020] or **difference equations**[Laporta, 2000; Lee, 2010]
  - Use the method of **sector decomposition** [Heinrich,2008] (pySecDec [Borowka et al., 2018] and Fiesta4 [Smirnov, 2016])
  - Use the **linear reducibility** of the integrals (HyperInt [Panzer, 2014]) to compute the Feynman integrals analytically or numerically
  - **Auxiliary mass flow integrals** [Xin Guan, Xiao Liu, Yan-Qing Ma, 2020]

Feynman integral

$$T(a_1,\ldots,a_N) = \int \left(\prod_{i=1}^{L} \mathrm{d}^d\ell_i\right) \frac{1}{P_1^{a_1} P_2^{a_2}\cdots P_N^{a_N}}, \qquad N = \frac{L}{2}(L+1) + LE \tag{1}$$

- $P_j = q_j^2 - m_j^2$, $j = 1,\ldots,N$, are the inverse propagators
- The momenta q_j are linear combinations of the loop momenta ℓ_i, $i = 1,\ldots,L$ for an L-loop integral, and external momenta p_k, $k = 1,\ldots,E$ for $E+1$ external legs
- The m_j are the propagator masses
- The a_j are the (integer) propagator powers
- sector number: $S = \sum_{j=1}^{N} 2^{j-1}\,\theta(a_j - \frac{1}{2})$

Integrals with the same sector number share the same number of positive propagator powers. **Example:** Integrals T(1,1,0,2) and T(1,2,-1,1) belong to the same sector, while the integral T(0,0,1,2) belongs to a different sector.

Relations from higher sectors

- Relations between the integrals in one sector exist which cannot be generated with the IBP- or LI-identities or symmetry relations for the same sector
- More relevant: the number of master integrals for one specific sector may be further reduced by taking symmetry relations from sectors with more positive propagator powers

Kira specific:

- In case a sector, which is missing the additional relation, is the same sector as listed in `top_level_sectors`, then the option `top_level_sectors` restricts Kira not to generate symmetry relations beyond the `top_level_sector` and we still miss the additional relation
- For this scenario the option `magic_relations` exists. It loosens the restrictions of the option `top_level_sectors` and allows Kira to built symmetry relations for sectors with more positive propagator powers, which generate the additional relation
- We will explain this in more detail in our gitlab Wiki

Automatic generation of equations

- The default behavior of Kira is to generate a system of equations for each integral in the list of preferred master integrals or master equations
- The idea is: Kira guarantees that for any choice of master integrals the integrals appearing in the system of differential equations are reduced to the minimal set of preferred master integrals
- Advanced trick: in the study of magic relations we may list one integral in the preferred list of master integrals, which represents the sector responsible for the generation of magic relations/ Which is needed if multi-topology reductions are considered
- We promise to bring up soon a feature to switch on/off this behavior

Laporta algorithm challenges

- The system of equations generated the Laporta way contains many redundant equations
- The number of equations may go up to billions and more
- The coefficients are polynomials in the dimension D and many different scales $\{s_{12}, s_{23}, m_1, m_2, ..\}$
- Solving linear system of equations generated with the Laporta algorithm are CPU, disk and memory expensive computations
- **Make trade offs to finish the reduction, e.g.: decrease the CPU costs but increase memory or disk costs**
- **Explore algorithmic improvements!**

Finite field reconstruction: Kira + FireFly

- Reconstruction of multivariate rational functions from **samples over finite integer fields** [Schabinger, von Manteuffel, 2014][T. Peraro, 2016]
- Public implementations available: FireFly [J. Klappert and F. Lange, 2019][Klappert, Klein, Lange, 2020], FIRE 6 [A. V. Smirnov and F. S. Chukharev, 2019] and FiniteFlow [T. Peraro, 2019]
- **FireFly has been combined with Kira's native finite field linear solver**
- Furthermore Kira supports MPI: to utilize the new parallelization opportunities now available with finite field methods
- **Side note:** the collaboration [Dominik Bendle, Janko Boehm, Murray Heymann, Rourou Ma, Mirko Rahn, Lukas Ristau, Marcel Wittmann, Zihao Wu, Yang Zhang, 2021] implements semi-numeric row reduced echelon form. They play with Laporta ordering in intermediate steps to improve the reduction time for the forward elimination!

What is special about FireFly I

- FireFly uses **Zippel algorithm** in the multivariate case instead of the nested Newton algorithm to interpolate the Polynomials
- In IBP reductions we will meet two kind of Polynomials:
- $E_1 = 1 + s + s^2 + t + t^2 + st$, homogeneous in the variables which are of the same mass dimension. Note: we set in this example one variable to 1.
- $(1+d+d^2)(1+s+s^2) = E_2 = 1+d+d^2+s+ds+d^2s+s^2+ds^2+d^2s^2$, again we set one variable to one
- For the polynomial E_1 the Zippel algorithm needs just 6+4 probes compared to the nested Newton 9+7 probes
- For the E_2 the nested Newton interpolation and the Zippel algorithm are of the same complexity
- In general the algorithmic complexity for Zippel is $O(n * D * T)$ and for nested Newton $O(D^n)$, with n number of variables, D the maximal degree and T the number of terms

What is special about FireFly II

- Main observation: IBP reductions involving 2 scales have the complexity of $E_2 = 1 + d + d^2 + s + ds + d^2s + s^2 + ds^2 + d^2s^2$, thus FIRE6 and FiniteFlow should be on par with FireFly (probably)
- IBP reductions involving 3 or more scales have the complexity of $E_1 = 1 + s + s^2 + t + t^2 + st$, thus FireFly should be better suited compared to other public codes.
- Further algorithmic improvements over brute force approaches implemented in FireFly are efficient algorithms for rational functions, racing algorithms, scan for univariate factors and many more

Kira + FireFly, strategy plans

- The run time for the sampling over finite field is **always** dominated by the forward elimination of the reduction
- **Strategy**: compute the rational functions appearing in the forward elimination phase first with Kiras native forward elimination algorithm using Fermat
- Use this system of equations in triangular form as an input to reconstruct the final rational functions appearing in the backward substitution

Combining algebraic forward elimination with finite field reduction - Hybrid I

$$P_1 = k_1^2,\quad P_2 = k_2^2,\quad P_3 = k_3^2,\quad P_4 = (p_1 - k_1)^2,\quad P_5 = (p_1 - k_2)^2,\quad P_6 = (p_1 - k_3)^2,\quad P_7 = (p_2 - k_1)^2,$$
$$P_8 = (p_2 - k_2)^2,\quad P_9 = (p_2 - k_3)^2,\quad P_{10} = (k_1 - k_2)^2,\quad P_{11} = (k_1 - k_3)^2,\quad P_{12} = (k_2 - k_3)^2,$$
$$p_1^2 = z z_b,\quad p_2^2 = 1,\quad p_1 p_2 = (1 - z)(1 - z_b)$$

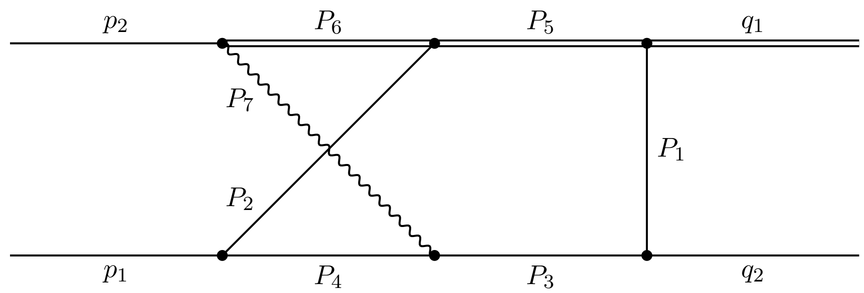
We chose $r = 17$ and $s = 0$ for the benchmark

Mode	Runtime	Memory	Probes	CPU time per probe	CPU time for probes
`run_initiate`	5 h 20 min	128 GiB	-	-	-
`run_triangular` + `run_back_substitution`	> 14 d	~ 540 GB	-	-	-
`run_firefly: true`	6 d 3 h	670 GiB	108500	370 s	100 %
`run_triangular: sectorwise`	36 min	4 GiB	-	-	-
`run_firefly: back`	4 h 54 min	35 GiB	108500	12.2 s	100 %

Combining algebraic forward elimination with finite field reduction - Hybrid II

- The complexity to generate the equations is in this example fixed (We documented in the most recent Kira paper how to optimize this step)
- The hybrid method is 20 times less expensive in main memory management and 27 times more efficient in CPU time usage
- The forward elimination generates a new system of equations which is smaller and faster to evaluate than the original IBP system of equations
- The hybrid method is usually good idea for reductions up to 3 scales
- We encourage everyone to play with different reduction strategies available within Kira to get the best results

Reducing the memory footprint with iterative reduction



$r = 7$ and $s = 4$

Mode	Iterative	Runtime	Memory
Kira ⊕ FireFly	-	18 h	40 GiB
	sectorwise	33 h 15 min	9 GiB

- iterative_reduction: sectorwise — one sector at a time
- iterative_reduction: masterwise — one master integral at a time
- Works well with the options run_back_substitution and run_firefly
- Independent study confirms the efficiency of this method

  [Chawdhry, Lim, Mitov, 2018]
- Sacrifice the CPU time for 4 times less main memory consumption

Runtime reduction with coefficient arrays

`--bunch_size=`	Runtime	Memory	CPU time per probe	CPU time for probes
1	18 h	40 GiB	1.73 s	95 %
2	14 h	41 GiB	1.30 s	94 %
4	11 h	46 GiB	1.00 s	93 %
8	10 h 15 min	51 GiB	0.91 s	92 %
16	9 h 45 min	63 GiB	0.85 s	92 %
32	9 h 30 min	82 GiB	0.84 s	92 %
64	9 h 30 min	116 GiB	0.83 s	92 %
`Kira` $\oplus$ `Fermat`	82 h	147 GiB	-	-

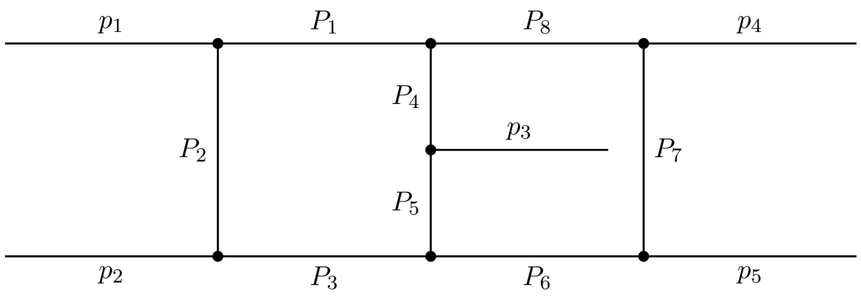
- The runtime of the probes is dominated by the forward elimination
- 48 cores each with hyper-threading disabled
- Coefficient arrays bring sizeable effects in exchange for main memory

Runtime reduction with MPI

# nodes	Runtime	Speed-up	CPU efficiency
1	18 h	1.0	95 %
2	10 h 15 min	1.8	87 %
3	7 h 15 min	2.5	82 %
4	5 h 45 min	3.1	76 %
5	5 h 30 min	3.3	65 %
`Kira` ⊕ `Fermat`	82 h	-	-

- Option `run_firefly: true` and `Intel`® `MPI` is used
- The first prime number suffers in the performance because FireFly cannot process arbitrary probes
- New probes are scheduled based on intermediate results
- **Remark:** the user should use less nodes for the first prime number

Double-pentagon topology in five-light-parton scattering I



Runtime	Memory	Probes	CPU time per probe	CPU time for probes
12 d	540 GiB	38278000	0.37 s	25 %

- Including d, the reduction of the double-pentagon topology is a six variable problem
- We use the system of equations is in block-triangular form taken from [Xin Guan, Xiao Liu, Yan-Qing Ma, 2019], which is of the size of 72 MB, best value I could find comparing to other methods. And no simplifications where yet applied.
- We benchmark the reduction of all integrals including five scalar products

Double-pentagon topology in five-light-parton scattering II

- FireFly's factor scan improves the denominators
- `-bunch_size = 128` option is used to improve the speed
- 40 cores with hyperthreading enabled
- The most complicated master integral coefficient has a maximum degree in the numerator of 87 and in the denominator of 50
- The database of the reduction occupies 25 GiB of disk space
- The number of required probes 10^7 is computed fast due to the block triangular structure of the system of equations

  [Xin Guan, Xiao Liu, Yan-Qing Ma, 2020]
- Main memory reduction can be achieved with the options `iterative_reduction` or by reducing the `-bunch_size` option
- We use Horner form to accelerate the parsing for the coefficients

Double-pentagon topology in five-light-parton scattering III

- The new option `insert_prefactors` would give a factor of 2 improvement in an overall performance if we use the denominators from [J.U, arXiv:2002.08173]. The method to compute these denominators is explained shortly in the summary of this paper, which relies on algebraic reconstruction methods pioneered in [arXiv:1805.01873, arXiv:1712.09737, arXiv:1511.01071]. A second approach to compute the denominator functions is available with finite field methods [Heller, von Manteuffel, arXiv:2101.0828].
- The **block triangular form** is much better suited for the reduction than a naive IBP system of equations as generated by Kira
- Reduction tables are available upon request

Upcoming Features in next Kira Version

Kira's, development release

Get Kira on gitlab: https://gitlab.com/kira-pyred/kira.git

- Interface to user defined IBP-identities
- Documentation to symbolic IBP-identities
- On https://hepforge.kira.org we provide a static linked Kira executable
- We have launched a Wiki and a best practice summary on gitlab

Summary and Outlook

- Many parallelization improvements
- Kira is an all-rounder for multi-scale as well as for multi-loop computations
- Kira utilize the finite field methods and helps to tailor it to your needs
- The examples should help you to find the balance yourself
- Bunches should be used if there is unused memory on the system
- `MPI` if there are more computers or cluster nodes available
- Many features are driven by the high energy physics community demands
- We plan to go for the block triangular form: `run_triangular: block`, which finds a small and fast to evaluate system of equations for general topologies [Xin Guan, Xiao Liu, Yan-Qing Ma, 2020]! It is a paper about auxiliary mass flow integrals, but the ideas to generate block triangular form relations are independent from this formalism
- Be prepared to find more algorithmic improvements in Kira in the near future