Laporta algorithm for multi-loop vs multi-scale problems

(with Philipp Maierhöfer)

Workshop: Mathtematics of Linear Relations between Feynman Integrals

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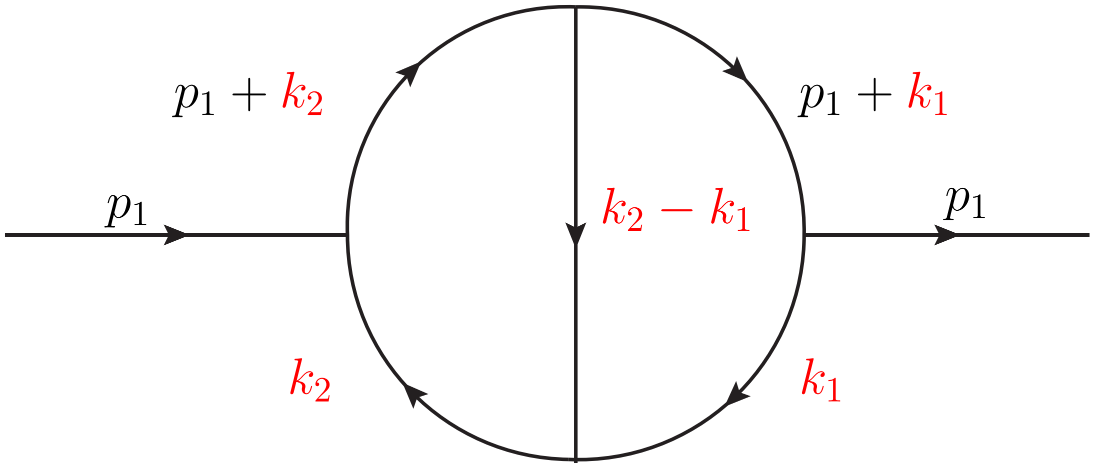
Outline

Integration-by-parts identities 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
- Compute the integrals analytically or numerically with the method of differential equations [Kotikov, 1991; Remiddi, 1997; Henn, 2013; Argeri et al., 2013; Lee, 2015; Meyer, 2016] or difference equations[Laporta, 2000; Lee, 2010] (these require basis change and IBP reductions)
- Use the method of sector decomposition [Heinrich,2008] (pySecDec [Borowka et al., 2018] and Fiesta4 [Smirnov, 2016]) or use the linear reducibility of the integrals (HyperInt [Panzer, 2014]) to compute the Feynman integrals analytically or numerically (these require basis change and IBP reductions).
- Application to the cappricious integrals (Mellin-Barnes integrals) is very non trivial, see works [J.U., Ievgen Dubovyk and Tord Riemann]

Scalar Integrals



$$I(a_1, \ldots, a_5) = \int \frac{d^D k_1 d^D k_2}{[{k_1}^2]^{a_1}[(p_1 + k_1)^2]^{a_2}[{k_2}^2]^{a_3}[(p_1 + k_2)^2]^{a_4}[(k_2 - k_1)^2]^{a_5}}$$

- Integral depends explicitly on the exponents a_f
- Loop momenta: $k_1,\ k_2$, $L = 2$
- Number of propagators: $N = 5$

IBP Identities

$$I(a_1,\ldots,a_5)=\int\frac{d^Dk_1\,d^Dk_2}{[k_1{}^2]^{a_1}[(p_1+k_1)^2]^{a_2}[k_2{}^2]^{a_3}[(p_1+k_2)^2]^{a_4}[(k_2-k_1)^2]^{a_5}}$$

Integration-by-parts (IBP) identities:

$$\begin{aligned}\int d^D\boldsymbol{k_1}\ldots d^D\boldsymbol{k_L}\frac{\partial}{\partial(\boldsymbol{k_i})_\mu}\left((q_j)_\mu\frac{1}{[P_1]^{a_1}\ldots[P_N]^{a_N}}\right) &=0\\ c_1(\{a_f\})I(a_1,\ldots,a_N\mathbf{-1})+\cdots+c_m(\{a_f\})I(a_1\mathbf{+1},\ldots,a_N) &=0\end{aligned}$$

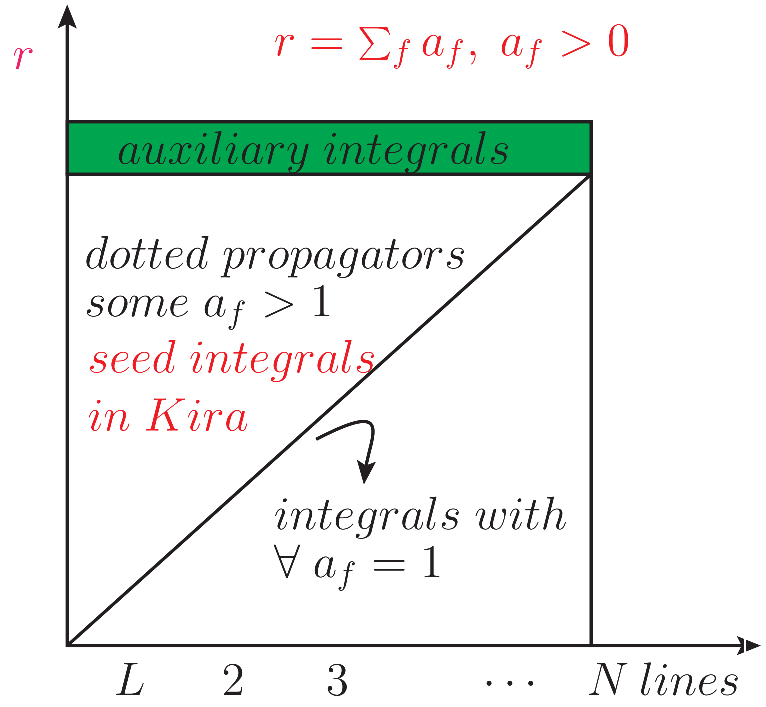
$$q_j=p_1,\ldots,p_E,k_1,\ldots,k_L$$

Express all integrals with the same set of propagators but with different exponents a_f as a linear combination of some basis integrals (master integrals)

- Gives relations between the scalar integrals with different exponents a_f
- Number of $L(E+L)$ IBP equations, $i=1,\ldots,L$ and $j=1,\ldots,E+L$
- a_f = symbols: Seek for recursion relations, LiteRed [Lee, 2012]
- a_f = integers: Sample a system of equations, Laporta algorithm [Laporta, 2000]

System of Equations the Laporta Way

- Seeds:



- Sectors: $S = \sum_{i=1}^{N} \theta_j \times 2^{j-1} \begin{cases} \theta_j = 1, & \text{for each } a_f > 0 \\ \theta_j = 0, & \text{else} \end{cases}$ (one way to tell a computer whether a propagator exists in an integral)
- System of equations: generate IBPs for all seeds
- Auxiliary integrals come from the IBPs applied to the seeds at the edge

Laporta Algorithm [Laporta, 2000]

Scalar integrals $I(a_1, \dots, a_5)$ with integer values a_f

Boundary conditions to sample the IBP equations

- $r = \sum_{f=1}^{N} a_f$ with $a_f > 0, \ f = 1, \dots, N$
- $s = -\sum_{f=1}^{N} a_f$ with $a_f < 0, \ f = 1, \dots, N$
- Seed integrals: $r \in [r_{\min}, r_{\max}], \quad s \in [s_{\min}, s_{\max}]$
- T topology number

- Reduce only a chosen set of integrals to a fixed number of basis integrals
- Public implementations: Air [Lazopoulos, Anastasiou, 2004], FIRE [A. V. Smirnov et al., 2008, 2013, 2014, 2019] and Reduze [Studerus, 2010] and Reduze 2 [Studerus, von Manteuffel, 2012] and Kira [Maierhöfer, Usovitsch, Uwer, 2017]

Laporta Algorithm Challenges

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

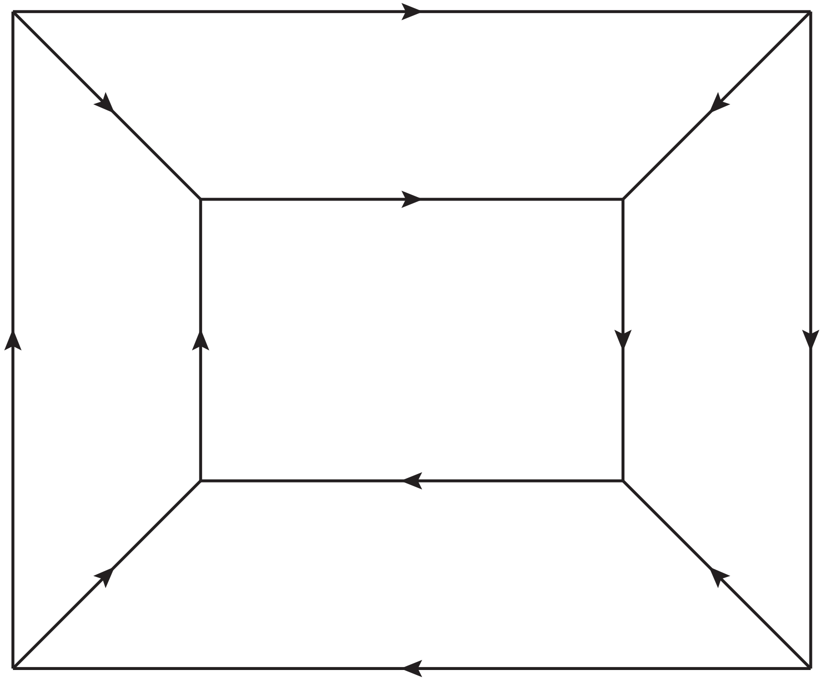
Features of Kira Version 1.2

Kira, release notes: arXiv:1812.01491

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

- The equation generator is $\sim 10^L$ faster than Kira 1.1 multi-loop
- Improved parallelization - no openMP
- Support for Mac OX / New build system: Meson
- Get relations from higher sectors – minimize the number of master integrals / faster symmetry and trivial sectors detection than in Kira 1.1
- Start a reduction with a preferred list of master integrals
- Focus the reduction only to a subset of master integrals — set all other coefficients to zero, since Kira 1.0 and Kira 1.1
- More flexible seed notation is introduced, while the old is preserved
- Choose between 8 different integral integral orderings
- Coefficient simplifications are based on heuristics
- Algebraic reconstruction multi-scale
- User defined system of equations
- ...

Example Symmetry Finder



- 15 minutes on one core to find all trivial sectors, sector relations / symmetries for the complete topology + subsectors
- This time we use the Pak algorithm [Pak, 2011]
- New efficient loop momenta mapper

Reduction to a Subset of Master Integrals

- The idea is simple and is probably used by many others with available public codes of FIRE and Reduze 2
- Reduction to a subset of master integrals is to apply if at least two trash collector integrals exist.
- Trash collector integrals: master integrals with big coefficients in front
- Good synergy with the option algebraic reconstruction and the parallelization across multiple computer nodes
- Kira provides an interface to do so since Kira 1.0
- This strategy allows to increase the CPU and the RAM performance simultaneously

User Defined System of Equations

- Case 1: Take an arbitrary linear system of equations and bring it in a echelon row reduced form
- Case 2: Generate symmetries and trivial sectors with Kira, but provide your own linear system of equations, e.g.: system generated via Syzygy IBP equations (source terms, IBPs without dotted propagators) and not with the usual IBP identities
- Case 3: Reduce to a UT basis

gg→H at 3-loops: integralfamilies.yaml

```
integralfamilies:
  - name: Xhiggs3l1_mmmmmmm00
    loop_momenta: [ l1, l2, l3 ]
    top_level_sectors: [511] # important option
    propagators:
      - [ "l1", "m^2" ]
      - [ "l2", "m^2" ]
      - [ "l3", "m^2" ]
      - [ "l1 - q1", "m^2" ]
      - [ "l2 - q1 - q2", "m^2" ]
      - [ "l1 - l2", 0 ]
      - [ "-l2 + l3 + q1 + q2", 0 ]
      - [ "l1 - l2 + l3", "m^2" ]
      - [ "l1 - l2 + l3 + q2", "m^2" ]
      - { bilinear: [ [ "l1", "l3" ], 0 ] }
      - { bilinear: [ [ "l2", "q1" ], 0 ] }
      - { bilinear: [ [ "l3", "q1" ], 0 ] }
```

gg→H at 3-loops: Old v.s. New jobs.yaml Interface

```
jobs:
  - reduce_sectors:
     sector_selection: # Old
      select_recursively: # Old
       - [Xhiggs3l1_mmmmmmm00,511] # Old
     identities: # Old
      ibp: # Old
       - { r: [t, 10], s: [0, 4] } # Old
     reduce: # New
      - {r: 10, s: 4} # New
     select_integrals: # important option
      select_mandatory_recursively: # important option
       - {r: 10, s: 4, d: 1} # important option
```

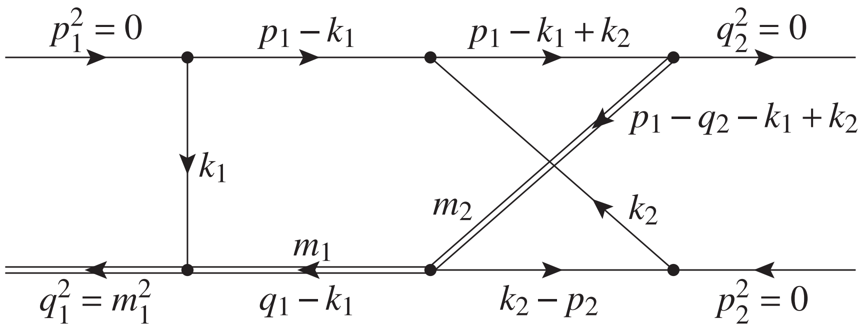
- Kira implicitly knows from integralfamilies.yaml that the user wants to reduce the topology named: Xhiggs3l1_mmmmmmm00
- From `top_level_sectors: [511]`, Kira assumes that the user wants to reduce the sector: 511

Reduction of a gg$\rightarrow$H at 3-loops Non-planar Topology

Algorithm	**Kira 1.1** (32 cores)	**Kira 1.2** (16 cores)
Generate system of equations	7.9 h	-
Reduce numerically	3.6 h	-
Generate and reduce numerically	-	3.4 h
Build triangular form (thread pools)	26 h	4.8 h
Backward substitution (heuristics)	18.8 d	4.1 d

- Seed specification: {r: 10, s: 4, d: 1}
- Speedup comes from less calls to Fermat: 382.502.520 x 5 (Kira 1.1) v.s. 981 (Kira 1.2)
- After the numerical reduction over the finite field (integers modulo 64 Bit prime number) is finished, you know the master integrals

Algebraic Coefficient Simplification



Type	$T_{\text{Kira}}^{m_2^2=\frac{3}{14}m_1^2}$	T_{Kira}	$T_{\text{FIRE 6}}^{m_2^2=\frac{3}{14}m_1^2}$
default	22 min	4 h	-
B	6.7 min	1 h	2.5 h

- default: `select_mandatory_recursively: [{r: 7, s: 4}]`
- B: `select_mandatory_list:` [1,1,1,1,1,1,1,-4,0] [1,1,1,1,1,1,1,-1,-3] [1,1,1,1,1,1,1,-2,-2] [1,1,1,1,1,1,1,-3,-1] [1,1,1,1,1,1,1,0,-4]
- FIRE 6 [A. V. Smirnov, F. S. Chukharev (2019)] in C++ and using the same Fermat executable as in Kira.
- Kira is used with the option -integral_ordering=2 (same master integral basis as in FIRE 6)

Algebraic Reconstruction

Backward substitution gives: $I(\{a_i\}) = \sum_j^M C_j M_j$, M_j master integral

- $C_j = \sum_{i=1}^N c_i$,
- $N \approx \mathcal{O}(10^2) - (10^5)$
- Naiv sum gives a snow ball effect: Intermediate sum grows to more complicated terms then the final result.
- One solution since Kira 1.0 is to constantly sort the terms c_i and the intermediate sums in their string length. **Extremely powerful!**

Second solution since Kira 1.2 is the algebraic reconstruction

- Sample $\sum_{i=1}^N c_i$ by setting at least one parameter $\{\frac{s}{m_1^2}, \frac{t}{m_1^2}, \frac{m_{i\neq 1}^2}{m_1^2}, \ldots\}$ to integer numbers
- Interpolate the final result from these samples

Implementation Part 1

Dependence on at least 2 parameters, e.g.: $\{D, x\}$, $x = \frac{s}{m_1^2}$

- Sample once $C(D, x)$ for numeric value in D
- Get $C(x)$ rational function
- Get the degree of the polynomials (numerator and denominator) of $C(x)$ in x: d_N and d_D
- Interpolate the numerator and denominator in x individually with Newtonian approach
- Use $C(x)$ later as a reference point to eliminate sign and numeric prefactor ambiguities
- Original work in this field is based on, see arXiv: 1805.01873 1712.09737 1511.01071 by Yang Zhang and his collaborators

Implementation Part 2

Sample $C(D,x)$ $\max(d_N+2, d_D+2)$ for numeric values x_j in x

- Get multiple functions $C(D,x) \rightarrow \{C(D,x_j)\}$
- Test that all numerators and denominators have the same number of terms, if not, resample

Interpolate the numerator and the denominator of $C(D,x)$ individually, e.g. use the Newtonian interpolation formula

- $C(D,x) = \sum_{i=1}^{d_N+1, d_D+1} a_i \prod_{j=1}^{i-1} (x - x_j)$
- $a_1 = C(D,x_1)$
- $a_2 = \frac{C(D,x_2)-a_1}{x_2-x_1}$
- $a_3 = (\frac{C(D,x_3)-a_1}{x_3-x_1} - a_2)\frac{1}{x_3-x_2}$
- $\ldots$
- $a_{d_N+1} = ((\frac{C(D,x_{d_N+1})-a_1}{x_{d_N+1}-x_1} - a_2)\frac{1}{x_{d_N+1}-x_2} - \cdots - a_{d_N})\frac{1}{x_{d_N+1}-x_{d_N}}$

Implementation Part 3

- To activate the algebraic reconstruction use:
  `algebraic_reconstruct: true`
- Kira decides based on heuristics to use the algebraic reconstruction algorithm or not
- Heuristics are: number of terms in a sum, length of the biggest coefficients
- All implementation details are "hidden under the hood" — await improvements and more benchmarks (code is public)
- At present algebraic reconstruction kicks in only for the coefficients during the backward substitution
- Next Kira version will include the algebraic reconstruction of the whole reduction
- Possible usage: Treat coefficients of the master integrals individually

Challenges

- We experience that Kira is very RAM hungry for 5 loop computations, because we generate all possible IBPs for all possible seeds
- Numerical solver is going to use more disk less RAM, which will reduce the speed performance during the initiation of the reduction problem
- Use of Syzygy equations to generate IBP equations without dots
- Use of algebraic reconstruction to the complete reduction process
- Algebraic reconstruction will receive more and more improvements
- Fusion of two algorithms for coefficient simplification
- More Sophisticated interpolation of polynomials than the Newton algorithm
- Getting rid of the external calls to the program Fermat, e.g. use it as a library

Summary and Outlook

- Kira version 1.2 is available: https://gitlab.com/kira-pyred/kira.git and includes:
- Fast equation generator
- Improved parallelization
- New flexible seed notation, while the old is preserved
- New feature: Algebraic reconstruction
- Todo list:
- Algebraic reconstruction for the whole system, parallelization across different machines.
- Kira is an all-rounder competitive in all disciplines: multi-loop, multi-scale and user defined system of equations reductions