

# Modern multiloop calculations.

Search for new algorithms and fast computer algebra systems

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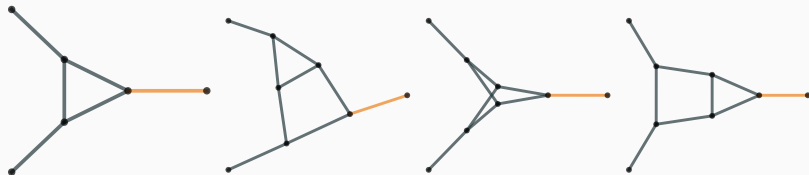
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- High-precision theoretical description of Standard Model processes is of crucial importance. In particular, the New Physics — new particles and interactions — is likely to appear as small deviations from SM and therefore can be detected only with high precision of theoretical predictions at hand.
- From the computational point of view, our ability to obtain high-precision results depends crucially on multiloop calculation techniques. Complexity grows both qualitatively and quantitatively in an explosive way with the number of loops and/or scales.
- New methods and approaches are always required. Using computer power is a must for at least two last decades. Insights from various fields of mathematics help a lot.

## 2 loops:



- Dispersion relation
  - Feynman parametrization
  - Mellin-Barnes parametrization
  - ${}_pF_q$  expansion in indices, HypExp
- } [Matsuura, van der Marck, and van Neerven, 1989; Harlander, 2000]
- } [Gehrmann, Huber, and Maitre, 2005]

## 3 loops:

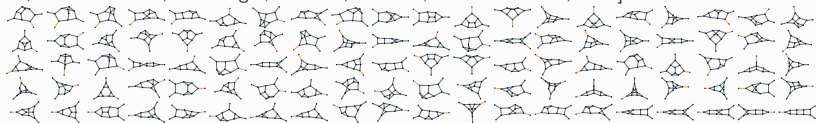
[Gehrmann, Heinrich, Huber, and Studerus, 2006; Heinrich, Huber, and Maître, 2008; RL, Smirnov, and Smirnov, 2010]



- Feynman parametrization
- Mellin-Barnes parametrization, MB, AMBRE [Czakon, 2006; Gluza et al., 2007]
- Recurrence+analyticity in  $d$ , [Tarasov, 1996; RL, 2010]
- PSLQ recognition [Ferguson et al., 1998]

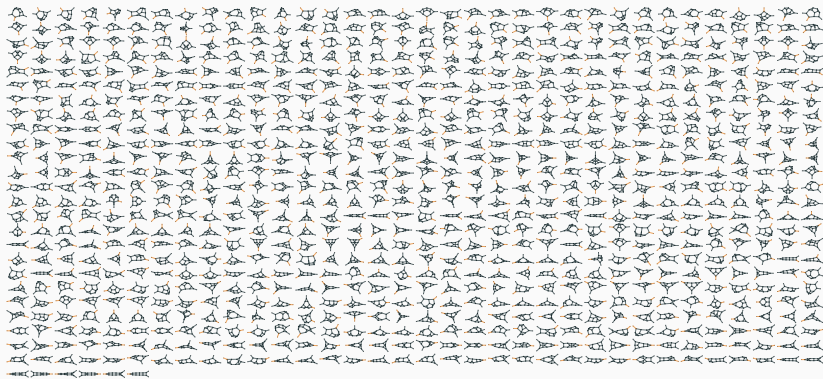
## 4 loops:

[Henn, Smirnov, Smirnov, and Steinhauser, 2016; RL, Smirnov, Smirnov, and Steinhauser, 2019; RL, von Manteuffel, Schabinger, Smirnov, Smirnov, and Steinhauser, 2021]



- $\sim 100$  big topologies.
- Linear reducibility, HyperInt [Panzer, 2013]
- Parallelization for IBP reduction, finite fields reconstruction [von Manteuffel and Schabinger, 2015; Smirnov and Chuharev, 2020]
- Differential equations, reduction to  $\epsilon$ -form [Henn, 2013; RL, 2015], Libra [RL, 2021]
- PSLQ recognition

## 5 loops:



- $\sim 1000$  big topologies.
- It looks like no available techniques can help.

- But from the experimental point of view less loops and more scales are even more important. In particular NNLO (two-loop) corrections to the cross sections processes are of a great interest.
- Only very recently multiloop methods have grown to NNLO calculations for more than 2 scales:  $2 \rightarrow 2$  processes with massive particles,  $2 \rightarrow 3$  processes with massless particles.
- Partial results start to appear. One example:  $e - \mu$  scattering at NNLO [Banerjee et al., 2020].

Computational complexity crucially depends on the number of loops and on the number of scales.

loops \ scales	1 loop	2 loops	3 loops	4 loops	5 loops	> 6
1	✓	✓	✓	many	a few	
2	✓	✓	some	a few		
3	✓	some	a few			
> 3	✓	a few				

- Massive internal lines add extra complexity.
- State-of-the-art examples:
  - 5-loop massless propagators [Georgoudis, Gonçalves, Panzer, Pereira, Smirnov, and Smirnov, 2021].
  - 4-loop  $g - 2$  integrals (onshell massive propagators) [Laporta, 2017]
  - 4-loop  $\mathcal{N} = 4$  SYM form factors [RL, von Manteuffel, Schabinger, Smirnov, Smirnov, and Steinhauser, 2021]
  - 3-loop massless boxes [Henn, Mistlberger, Smirnov, and Wasser, 2020]
  - 2-loop 5 legs [Badger, Chicherin, Gehrmann, Heinrich, Henn, Peraro, Wasser, Zhang, and Zoia, 2019]
- Massive internal lines add more complexity than just an extra scale:
  - 3-loop massive form factors not yet calculated.
  - results for two-loop boxes with inner massive lines are mostly not available.  
This is basically the minimal complexity of the diagrams required for NNLO precision of differential cross section for  $2 \rightarrow 2$  processes with massive particles.



## 1. Diagram generation

Generate diagrams contributing to the chosen order of perturbation theory.

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Tools: qgraf [Nogueira, 1993], FeynArts [Hahn, 2001],...

## 2. IBP reduction

Setup IBP reduction, derive differential system for master integrals.

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Tools: FIRE6 [Smirnov and Chuharev, 2020], Kira2 [Klappert et al., 2021], LiteRed [RL, 2012], Reduze2 [von Manteuffel and Studerus, 2012],...

## 3. DE Solution

Reduce the system to  $\epsilon$ -form, write down solution in terms of polylogarithms.  
Fix boundary conditions by auxiliary methods.

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Tools: Fuchsia [Gituslar and Magerya, 2017], epsilon [Prausa, 2017], Libra [RL, 2021]

## **IBP reduction: new ideas**

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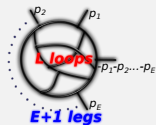
Given a Feynman diagram, consider a family

$$j(\mathbf{n}) = \int d\mu_L \prod_{k=1}^N D_k^{-n_k}, \quad d\mu_L = \prod_{k=i}^L d^d l_i$$

$D_1, \dots, D_M$  — denominators of the diagram,

$D_{M+1}, \dots, D_N$  — irreducible numerators, such that

$$N = L(L+1)/2 + L \cdot E.$$



From  $0 = \int d\mu_L \frac{\partial}{\partial l_i} \cdot q_m \prod_{k=1}^N D_k^{-n_k}$  one obtains

IBP identities

$$[c_{kl} B_k A_l + c_l A_l] j(\mathbf{n}) = 0.$$

Here  $c_{kl}$ ,  $c_l$  are some coefficients.

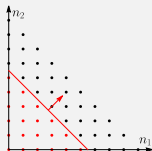
$$A_{lj} j(n_l) = n_l j(n_l + 1),$$

$$B_{lj} j(n_l) = j(n_l - 1)$$

IBP identities allow one to express any integral in the family via a finite # of master integrals. They also allow to construct differential and difference equations for the latter.

## Laporta algorithm (FIRE, Kira, Reduze, ...)

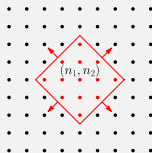
- generate identities for many numeric  $\mathbf{n} \in \mathbb{Z}^N$ .
- use Gauss elimination and collect reduction rules to database.
- twist: mapping to finite fields  $\mathbb{F}_p$  + reconstruction.  $\Leftarrow$  naturally parallelizable



## Heuristic search (LiteRed)

1. Generate identities for shifts around  $\mathbf{n}$  with *symbolic* entries.
2. Use Gauss elimination until acceptable rule is found.
3. Solve Diophantine equations to derive applicability condition.

Observation: only a small fraction of identities finally contribute to the reduction rule.



# IBP reduction in parametric representation

Note that  $N = L(L + 1)/2 + L \cdot E$  grows quadratically with  $L$ , while  $M$ , the # of lines in the diagram, grows only linearly. Parametric representation: only  $M$  indices.

Parametric representation

$$\tilde{j}^{(d)}(n_1, \dots, n_M) = \int \frac{\prod_{k=1}^M dx_k x_k^{n_k-1}}{G(\mathbf{x})^{d/2}}$$

$G = U + F$ , where  $U$  and  $F$  are Feynman graph polynomials.

IBP identities relating integrals with the same  $d$  require constructing *syzygy module* for ideal generated by  $\langle G, \partial_1 G, \partial_M G \rangle$ .

IBP identities from syzygies [RL, 2014]. Baikov rep.: [Zhang, 2014]

Syzygy  $QG + Q_1 \partial_1 G + \dots + Q_M \partial_M G = 0$  leads to IBP identity

$$\left[ \frac{d}{2} Q(\mathbf{A}) + Q_k(\mathbf{A}) B_k \right] \tilde{j}(\mathbf{n}) = 0$$

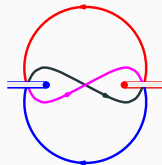
Quite promising, but a fast algorithm for constructing a *minimal* (rather than Groebner) basis of syzygy module is very desirable.

# IBP reduction with intersection theory?

[Mastrolia and Mizera, 2019]: use intersection theory for IBP reduction.

- Integral in parametric representation is understood as bilinear pairing between integration cycle  $C$  and differential form  $\phi$ .

$$\int_C G^{-\nu} \phi = \langle \phi | C \rangle ,$$



- $\langle \phi | C \rangle$  is invariant under  $\phi \rightarrow \phi + \nabla_\nu \tilde{\phi}$  and/or  $C \rightarrow C + \partial \tilde{C}$ , where  $\nabla_\nu = d - \nu G^{-1} dG$  is twisted differential and  $\partial \tilde{C}$  is a boundary (contractable) cycle.
- Therefore,  $\langle \cdot | \cdot \rangle$  is defined on the elements of twisted de Rham cohomology and twisted homology. Those are finite-dimensional spaces, therefore we can use basis expansion as IBP.
- Ref. [Cho and Matsumoto, 1995] introduced pairing  $\langle \phi_1 | \phi_2 \rangle$ , correctly defined for  $\nabla_\nu$ - and  $\nabla_{-\nu}$ - de Rham cohomologies.
- Unfortunately,  $\langle \phi_1 | \phi_2 \rangle$  is still very difficult to calculate in general. Perspectives of this approach are quite unclear to me.

## Differential equations

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- Differential equations for master integrals have the form

$$\partial_x \mathbf{j} = M(x, \epsilon) \mathbf{j}$$

- One can try to simplify the equation by transformation  $\mathbf{j} = T \tilde{\mathbf{j}}$ , so that

$$\partial_x \tilde{\mathbf{j}} = \tilde{M} \tilde{\mathbf{j}}, \quad \tilde{M} = T^{-1} [MT - \partial_x T]$$

- [Henn, 2013]: there is often a “canonical” basis  $\mathbf{J} = T^{-1} \mathbf{j}$  such that

$$\partial_x \mathbf{J} = \epsilon S(x) \mathbf{J} \quad (\epsilon\text{-form})$$

- General solution is easily expanded in  $\epsilon$ :

$$U = \text{Pexp} \left[ \epsilon \int dx S(x) \right] = \sum_n \epsilon^n \int \int \int_{x > x_n > \dots > x_0} dx_n \dots dx_1 S(x_n) \dots S(x_1)$$

- Algorithm of finding transformation to  $\epsilon$ -form: [RL, 2015]. Implemented in 3 publicly available codes: Fuchsia [Gituliar and Magerya, 2017], epsilon [Prausa, 2017], and recently in Libra [RL, 2021].



# General structure of reduction algorithm

Algorithm proceeds in three major stages, each involving a sequence of “elementary” transformations.

## 1. *Fuchsification*: Eliminating higher-order poles

Input: Rational matrix  $M(x, \epsilon)$

Output: Rational matrix with only simple poles on the extended complex plane,

$$M(x, \epsilon) = \sum_k \frac{M_k(\epsilon)}{x-a_k}.$$

## 2. *Normalization*: Normalizing eigenvalues

Input: Matrix from the previous step,  $M(x, \epsilon) = \sum_k \frac{M_k(\epsilon)}{x-a_k}$ .

Output: Matrix of the same form, but with the eigenvalues of all  $M_k(\epsilon)$  being proportional to  $\epsilon$ .

## 3. *Factorization*: Factoring out $\epsilon$

Input: Matrix from the previous step.

Output: Matrix in  $\epsilon$ -form,  $M(x, \epsilon) = \epsilon S(x) = \epsilon \sum_k \frac{S_k}{x-a_k}$ .

- Libra is a *Mathematica* package useful for treatment of differential systems which appear in multiloop calculations.
- Tools for reduction to  $\epsilon$ -form
  - Visual interface
  - Algebraic extensions
  - Birkhoff-Grothendieck factorization
- Tools for constructing solution
  - Determining boundary constants.
  - Constructing  $\epsilon$ -expansion of  $P_{\text{exp}}$ .
  - Constructing Frobenius expansion of  $P_{\text{exp}}$ .

- Fuchsification and normalization.

- Automatic tool (useful for simple cases)

```
In[1]: t=Rookie[M,x,ε];
```

- Interactive tool (useful for most cases)

```
In[1]: t=VisTransformation[M,x,ε];
```

Apply balance transformation (7b)

Paste overall transformation

0-dimensional u-space and 0-dimensional v-space

- Factorization.

```
In[2]: t=FactorOut[M,x,ε,μ];
```

- General solution

```
In[3]: U=PexpExpansion[{M,6},x];
```

## Boundary conditions

Suppose we have found a transformation  $T(x) = T(x, \epsilon)$  to  $\epsilon$ -form,  $j = TJ$ . Then we can write

$$J(x) = U(x, x_0)J(x_0),$$
$$j(x) = T(x)U(x, x_0)[T(x_0)]^{-1}j(x_0)$$

But the point  $x_0$  should be somewhat special to simplify the evaluation of  $j(x_0)$  as compared to  $j(x)$ . As a rule, "special" boils down to "singular", i.e., we can expect simplifications for  $x_0$  being a singular point of the differential system. Let it be  $x_0 = 0$  for simplicity.

### Problem

$U(x, x_0)$  diverges when  $x_0$  tends to zero. Therefore, we have to consider not the values, but the asymptotics of  $j(x_0)$  at  $x = 0$ .

Libra can determine which asymptotic coefficients,  $c$ , are sufficient to calculate and find the "adapter" matrix  $L$  relating those with the column of boundary constants,  $C = Lc$ .

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```
In[4]: {L, cs}=GetLcs[M, T, {x, 0}];
```

## Algebraic extensions and non-polylogarithmic integrals

- Sometimes, in order to find the transformation to  $\epsilon$ -form, one has to extend the class of transformations by passing from  $x$  to  $y$ , such that  $x = x(y)$  is some rational function. `Libra` has tool for it:

```
In[1]: ChangeVar[ds,x→(4 y*y)/(1 - y*y),y];
```

- Moreover, in many cases there is no common rationalizing variable. Thus, `Libra` implements a more powerful way to treat such algebraic extensions, with

```
In[1]: AddNotation[ds,y → x(1-y*y) - 4 y*y];
```

One may add as many notations as needed, and `Libra` will take care of them (minimizing their appearance, correctly treating their differentiation).

- Unfortunately, there are cases when the system can not be reduced to  $\epsilon$ -form even with algebraic extensions. `Libra` implements Birkhoff-Grothendieck factorization to help to detect such cases (see [RL and Pomeransky, 2017]):

```
In[1]: {L,T,R}=BirkhoffGrothendieck[t,x];
```

There is no general approach for such cases in this case. Proper treatment of transcendental extensions is needed?

## Example of using Libra

One of many 4-loop massless vertex topologies with two off-shell legs.

- Differential system

$$\partial_{x_j} = \left( \begin{array}{c} \text{[Diagram of a 374 x 374 matrix with a diagonal line and a triangular block structure]} \end{array} \right) j, \quad \text{where } j = \left( \begin{array}{c} \text{[Diagram of a vertical vector with a circle at the top and a triangle at the bottom]} \end{array} \right)$$

374 × 374 matrix

- Maximum size of the diagonal blocks is “only”  $11 \times 11$ .
- No global rationalizing variable. Three algebraic extensions are needed for the reduction to  $\epsilon$ -form:

$$x_1 = \sqrt{x}, \quad x_2 = \sqrt{x - 1/4}, \quad x_3 = \sqrt{1/x - 1/4}$$

- Each step towards increasing the # of loops and/or # of scales requires new methods. Those involve both technological advances (e.g. massive parallelization) and new algorithms coming various fields of mathematics.
- IBP reduction still remains a bottleneck for many calculations. New ideas of IBP reduction appear, whether they will be successful is yet to find out.
- Differential equations method is already in very good shape. Exception: the systems irreducible to  $\epsilon$ -form.

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Thank you!



## References

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- S. Badger, D. Chicherin, T. Gehrmann, G. Heinrich, J. M. Henn, T. Peraro, P. Wasser, Y. Zhang, and S. Zoia. Analytic form of the full two-loop five-gluon all-plus helicity amplitude. *Phys. Rev. Lett.*, 123(7):071601, 2019. doi: 10.1103/PhysRevLett.123.071601.
- P. A. Baikov and K. G. Chetyrkin. Four Loop Massless Propagators: An Algebraic Evaluation of All Master Integrals. *Nucl. Phys. B*, 837: 186–220, 2010. doi: 10.1016/j.nuclphysb.2010.05.004.
- Pulak Banerjee et al. Theory for muon-electron scattering @ 10 ppm: A report of the MUonE theory initiative. *Eur. Phys. J. C*, 80(6):591, 2020. doi: 10.1140/epjc/s10052-020-8138-9.
- Koji Cho and Keiji Matsumoto. Intersection theory for twisted cohomologies and twisted riemann’s period relations i. *Nagoya Mathematical Journal*, 139:67–86, 1995.
- M. Czakon. Automatized analytic continuation of Mellin-Barnes integrals. *Comput. Phys. Commun.*, 175:559–571, 2006. doi: 10.1016/j.cpc.2006.07.002.
- Helaman RP Ferguson, David H Bailey, and Paul Kutler. A polynomial time, numerically stable integer relation algorithm. Technical report, 1998.
- T. Gehrmann, T. Huber, and D. Maitre. Two-loop quark and gluon form-factors in dimensional regularisation. *Phys. Lett. B*, 622: 295–302, 2005. doi: 10.1016/j.physletb.2005.07.019.
- T. Gehrmann, G. Heinrich, T. Huber, and C. Studerus. Master integrals for massless three-loop form-factors: One-loop and two-loop insertions. *Phys. Lett. B*, 640:252–259, 2006. doi: 10.1016/j.physletb.2006.08.008.
- Alessandro Georgoudis, Vasco Gonçalves, Erik Panzer, Raul Pereira, Alexander V. Smirnov, and Vladimir A. Smirnov. Glue-and-cut at five loops. *JHEP*, 09:098, 2021. doi: 10.1007/JHEP09(2021)098.
- Oleksandr Gituliar and Vitaly Magerya. Fuchsia: a tool for reducing differential equations for Feynman master integrals to epsilon form. *Comput. Phys. Commun.*, 219, 2017.
- J. Gluza, K. Kajda, and T. Riemann. AMBRE: A Mathematica package for the construction of Mellin-Barnes representations for Feynman integrals. *Comput. Phys. Commun.*, 177:879–893, 2007. doi: 10.1016/j.cpc.2007.07.001.

- Thomas Hahn. Generating Feynman diagrams and amplitudes with FeynArts 3. *Comput. Phys. Commun.*, 140:418–431, 2001. doi: 10.1016/S0010-4655(01)00290-9.
- Robert V. Harlander. Virtual corrections to  $g g \rightarrow H$  to two loops in the heavy top limit. *Phys. Lett. B*, 492:74–80, 2000. doi: 10.1016/S0370-2693(00)01042-X.
- G. Heinrich, T. Huber, and D. Maître. Master integrals for fermionic contributions to massless three-loop form factors. *Physics Letters B*, 662(4):344–352, 2008. ISSN 0370-2693. doi: <https://doi.org/10.1016/j.physletb.2008.03.028>. URL <https://www.sciencedirect.com/science/article/pii/S0370269308003341>.
- Johannes Henn, Bernhard Mistlberger, Vladimir A Smirnov, and Pascal Wasser. Constructing d-log integrands and computing master integrals for three-loop four-particle scattering. *arXiv preprint arXiv:2002.09492*, 2020.
- Johannes M. Henn. Multiloop integrals in dimensional regularization made simple. *Phys.Rev.Lett.*, 110(25):251601, 2013. doi: 10.1103/PhysRevLett.110.251601.
- Johannes M. Henn, Alexander V. Smirnov, Vladimir A. Smirnov, and Matthias Steinhauser. A planar four-loop form factor and cusp anomalous dimension in QCD. *JHEP*, 05:066, 2016. doi: 10.1007/JHEP05(2016)066.
- Jonas Klappert, Fabian Lange, Philipp Maierhöfer, and Johann Usovitsch. Integral reduction with Kira 2.0 and finite field methods. *Comput. Phys. Commun.*, 266:108024, 2021. doi: 10.1016/j.cpc.2021.108024.
- Stefano Laporta. High-precision calculation of the 4-loop contribution to the electron  $g-2$  in QED. *Phys. Lett. B*, 772:232–238, 2017. doi: 10.1016/j.physletb.2017.06.056.
- Pierpaolo Mastrolia and Sebastian Mizera. Feynman integrals and intersection theory. *JHEP*, 02:139, 2019. doi: 10.1007/JHEP02(2019)139.
- T. Matsuura, S.C. van der Marck, and W.L. van Neerven. The calculation of the second order soft and virtual contributions to the drell-yan cross section. *Nuclear Physics B*, 319(3):570–622, 1989. ISSN 0550-3213. doi: [https://doi.org/10.1016/0550-3213\(89\)90620-2](https://doi.org/10.1016/0550-3213(89)90620-2). URL <https://www.sciencedirect.com/science/article/pii/0550321389906202>.
- Paulo Nogueira. Automatic Feynman graph generation. *J. Comput. Phys.*, 105:279–289, 1993. doi: 10.1006/jcph.1993.1074.
- Erik Panzer. On the analytic computation of massless propagators in dimensional regularization. *Nuclear Physics, Section B 874 (2013)*, pp. 567-593, May 2013. doi: 10.1016/j.nuclphysb.2013.05.025.

- Mario Prausa. epsilon: A tool to find a canonical basis of master integrals. *Comput. Phys. Commun.*, 219:361–376, 2017. doi: 10.1016/j.cpc.2017.05.026.
- RL. Space-time dimensionality  $d$  as complex variable: Calculating loop integrals using dimensional recurrence relation and analytical properties with respect to  $d$ . *Nucl. Phys. B*, 830:474, 2010. ISSN 0550-3213. doi: DOI:10.1016/j.nuclphysb.2009.12.025. URL <http://www.sciencedirect.com/science/article/B6TVC-4Y34PW6-2/2/bd2b4965b69dc349aa8f5f9040fc5d30>.
- RL. Presenting litered: a tool for the loop integrals reduction, 2012.
- RL. Modern techniques of multiloop calculations. In Etienne Augé and Jacques Dumarchez, editors, *Proceedings, 49th Rencontres de Moriond on QCD and High Energy Interactions*, pages 297–300, Paris, France, 2014. Moriond, Moriond.
- RL. Reducing differential equations for multiloop master integrals. *J. High Energy Phys.*, 1504:108, 2015. doi: 10.1007/JHEP04(2015)108.
- RL. Libra: A package for transformation of differential systems for multiloop integrals. *Computer Physics Communications*, 267:108058, 2021. ISSN 0010-4655. doi: <https://doi.org/10.1016/j.cpc.2021.108058>. URL <https://www.sciencedirect.com/science/article/pii/S0010465521001703>.
- RL and Andrei A. Pomeransky. Normalized Fuchsian form on Riemann sphere and differential equations for multiloop integrals. 2017.
- RL, V. Smirnov, and A. Smirnov. Analytic results for massless three-loop form factors. *Journal of High Energy Physics*, 2010(4):1–12, 2010.
- RL, Alexander V. Smirnov, Vladimir A. Smirnov, and Matthias Steinhauser. Four-loop quark form factor with quartic fundamental colour factor. *JHEP*, 02:172, 2019. doi: 10.1007/JHEP02(2019)172.
- RL, Andreas von Manteuffel, Robert M. Schabinger, Alexander V. Smirnov, Vladimir A. Smirnov, and Matthias Steinhauser. The Four-Loop  $\mathcal{N} = 4$  SYM Sudakov Form Factor. 10 2021.
- A. V. Smirnov and F. S. Chuharev. FIRE6: Feynman Integral REduction with Modular Arithmetic. *Comput. Phys. Commun.*, 247:106877, 2020. doi: 10.1016/j.cpc.2019.106877.
- O. V. Tarasov. Connection between feynman integrals having different values of the space-time dimension. *Phys. Rev. D*, 54:6479, 1996. doi: 10.1103/PhysRevD.54.6479.
- A. von Manteuffel and C. Studerus. Reduze 2 - Distributed Feynman Integral Reduction. 1 2012.
- Andreas von Manteuffel and Robert M. Schabinger. A novel approach to integration by parts reduction. *Phys. Lett. B*, 744:101–104, 2015. doi: 10.1016/j.physletb.2015.03.029.
- Yang Zhang. Integration-by-parts identities from the viewpoint of differential geometry. In *19th Itzykson Meeting on Amplitudes 2014*, 8 2014.