Fighting the machine, the tale of two pQCD calculations

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LinApart: optimizing the univariate partial fraction decomposition

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The structure of the presentation

- Motivation
- Mathematical background
- Performance
  - Linear case
  - General case
  - Parallelization
- Conclusions and outlook

Motivation

- Univariate partial fraction decomposition is a standard tool in any calculation.
- This operation untangles and separates singularities, thus in modern QFT calculations it is vital in various contexts like:
  - during integration, where polylogarithms surface,
  - simplifying expressions, eg. after IBP reductions.
- Unfortunately nowadays, the complexity of individual terms and of the whole expression reached a point, where the standard publicly available tools could not provide results in a timely manner if at all.

Motivation

$$
\begin{aligned}
f(x_a, x_b; y) = \Big[&(-4+y)(1-y+x_b y)(2-y+x_b y)(4-y+x_b y)(1-x_a-y+x_b y)^3 \\
&\times (-1+x_a-y+x_b y)(-4-4x_b-y+x_b y)(-4x_b-y+x_b y) \\
&\times (-4x_a-4x_b-y+x_b y)(4x_a-4x_b-y+x_b y)(2+2x_b-y+x_b y)^3 \\
&\times (6+2x_b-y+x_b y)(2-4x_a+2x_b-y+x_b y)(2+4x_a+2x_b-y+x_b y) \\
&\times (-1+x_a-x_a y+x_a x_b y)(1+x_a-x_a y+x_a x_b y)(-2+2x_a-x_a y+x_a x_b y) \\
&\times (2+2x_a-x_a y+x_a x_b y)(-x_b+x_a x_b-x_a y+x_a x_b y)^3 \\
&\times (-4+2x_a+2x_a x_b-x_a y+x_a x_b y)(4+2x_a+2x_a x_b-x_a y+x_a x_b y) \\
&\times (1-2x_a+x_a^2-y-x_a y+x_b y+x_a x_b y) \\
&\times \left(2x_b-2x_a x_b+x_a y-x_b y-x_a x_b y+x_b^2 y\right)^3 \Big]^{-1}
\end{aligned}
$$

- Let us examine a rational function $f(x) = \frac{x^l}{Q(x)}$, where $Q = \prod_{i=1}^{n}(x - a_i)^{m_i}$ and $l < \deg Q$.
- The partial fraction decomposition means we have to separate the poles of said function.

$$f(x) = \sum_{i=1}^{n}\sum_{j=1}^{m_i}\frac{c_{ij}}{(x - a_i)^j}$$

- The task is the calculation of the c_{ij} coefficients.

Mathematical background

- The most well known method is the equation system method.
- The steps of its algorithm:
  1. write down the previously showed ansatz,
  2. multiply both sides with the denominators,
  3. compare the coefficient of monomials on both side,
  4. solve the given linear equation system.

Mathematical background

- Mathematician prefer the so called Euclidean-method.
- During this method we
  1. write down every possibly pair of denominators without multiplicities,
  2. calculate the extended GCD of every pair:

     $$a\ d_1 + b\ d_2 = 1\ ,$$

  3. divide both side of the equation to get a reduction rule:

     $$a/d_2 + b/d_1 = 1/d_1/d_2\ ,$$

  4. iteratively use the reduction rules until only one variable dependent denominator remains.

Mathematical background

- We use a third approach, which was to the best of our knowledge was not implemented before in a public code.
- The aforementioned ansatz is nothing else but the Laurent-expansion of the given fraction; thus we can use the residuum theorem:

$$c_{ij} = \mathrm{Res}(g_{ij}, a_i) = \frac{1}{(m_i - j)!} \lim_{x \to a_i} \frac{d^{m_i - j}}{dx^{m_i - j}} \Big((x - a_i)^{m_i} f(x) \Big)$$

Mathematical background

- Since we remove the pole at a_i we can easily take the limit and get:

$$c_{ij} = \frac{1}{(m_i - j)!} \frac{d^{m_i - j}}{da_i^{m_i - j}} a_i^l \prod_{\substack{k=1 \\ k \neq i}}^{n} \frac{1}{(a_i - a_k)^{m_k}}.$$

- The polynomial part of the Laurent-series can be acquired by taking the limit $x \to \infty$.

Mathematical background

- If we would like to treat non linear irreducible denominators wit the Laurent-series method, we must expand it.
- In this case we want to express our result as a function of the polynomial coefficient of the denominators rather than their roots.
- Since the roots are algebraically equivalent, it is sufficient to calculate the pole part of the Laurent-series with a symbolic α_i root.
- Reduce the given expression in the basis of the roots.
- Sum over all of the roots and express the final expression with the coefficients of the pole.

Performance

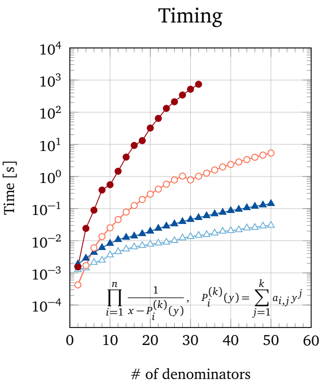
- Which formula or method to use is up to the nature of the problem and language choice.
- If our fraction is defined entirely over the rationals we can leverage finite field sampling methods coupled to the equation system method.
- The Euclidean-method has a clear advantage in FORM due to the possibility of rapid expansions and rule substitutions.
- The Laurent-series method is the most versatile and scales the best in most scenarios as we will see.

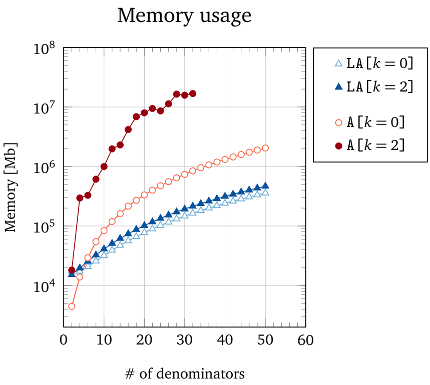
- In general, a rational fraction's complexity can come from several factors, for example from:

  1. the number of distinct denominator factors.
  2. the degree of each individual denominator.
  3. the algebraic complexity of the polynomial coefficients of the denominators.
  4. the multiplicity (the exponent) of the denominators.
  5. the degree of the numerator.

Performance

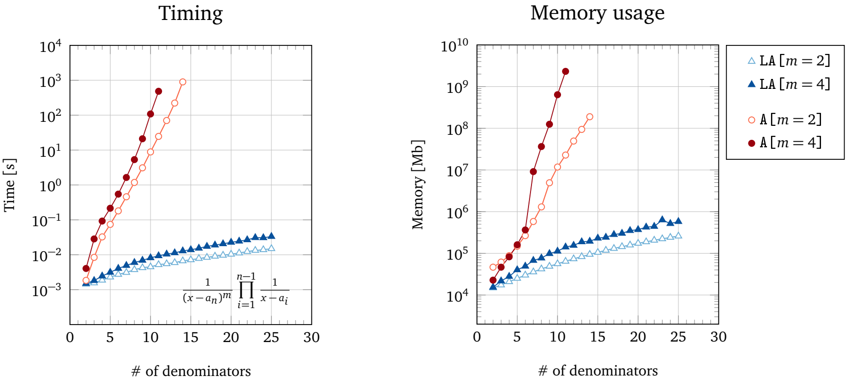
-The linear case





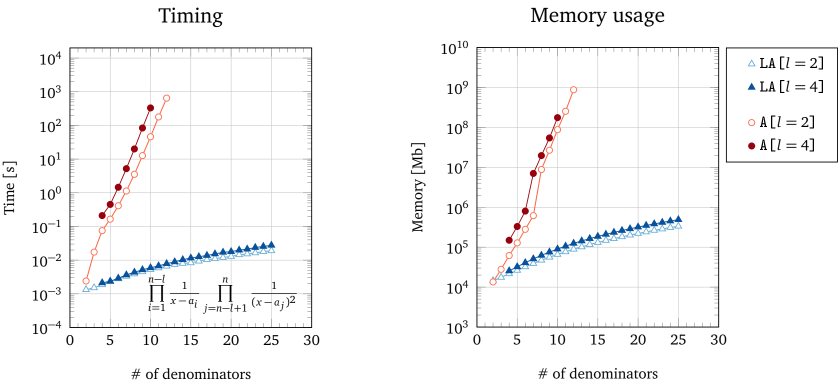
Performance

-The linear case



Performance

-The linear case



Performance

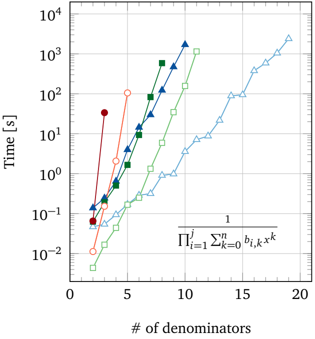
-The linear case

$$
\begin{aligned}
f(x_a, x_b; y) = \Big[& (-4+y)(1-y+x_b y)(2-y+x_b y)(4-y+x_b y)(1-x_a-y+x_b y)^3 \\
& \times (-1+x_a-y+x_b y)(-4-4x_b-y+x_b y)(-4x_b-y+x_b y) \\
& \times (-4x_a-4x_b-y+x_b y)(4x_a-4x_b-y+x_b y)(2+2x_b-y+x_b y)^3 \\
& \times (6+2x_b-y+x_b y)(2-4x_a+2x_b-y+x_b y)(2+4x_a+2x_b-y+x_b y) \\
& \times (-1+x_a-x_a y+x_a x_b y)(1+x_a-x_a y+x_a x_b y)(-2+2x_a-x_a y+x_a x_b y) \\
& \times (2+2x_a-x_a y+x_a x_b y)(-x_b+x_a x_b-x_a y+x_a x_b y)^3 \\
& \times (-4+2x_a+2x_a x_b-x_a y+x_a x_b y)(4+2x_a+2x_a x_b-x_a y+x_a x_b y) \\
& \times (1-2x_a+x_a^2-y-x_a y+x_b y+x_a x_b y) \\
& \times \left(2x_b-2x_a x_b+x_a y-x_b y-x_a x_b y+x_b^2 y\right)^3 \Big]^{-1}
\end{aligned}
$$

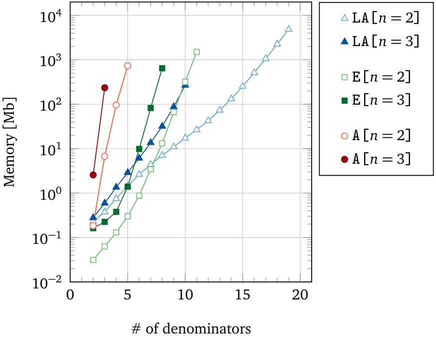
Performance

-The general case

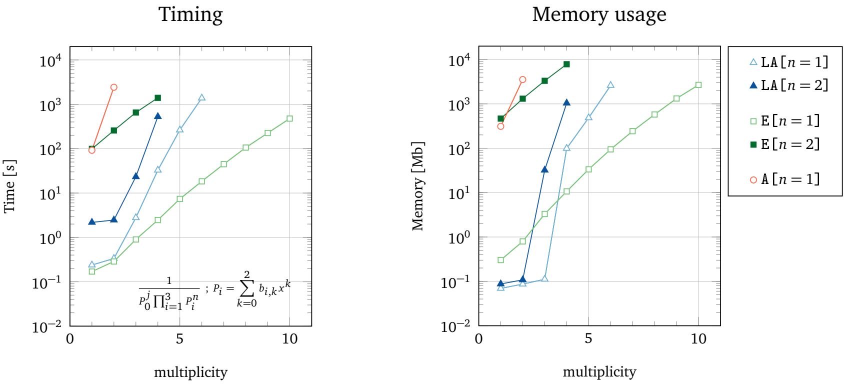
Timing



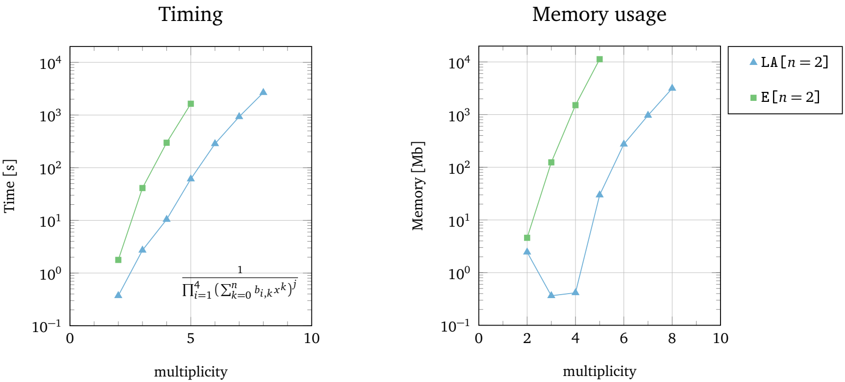
Memory usage



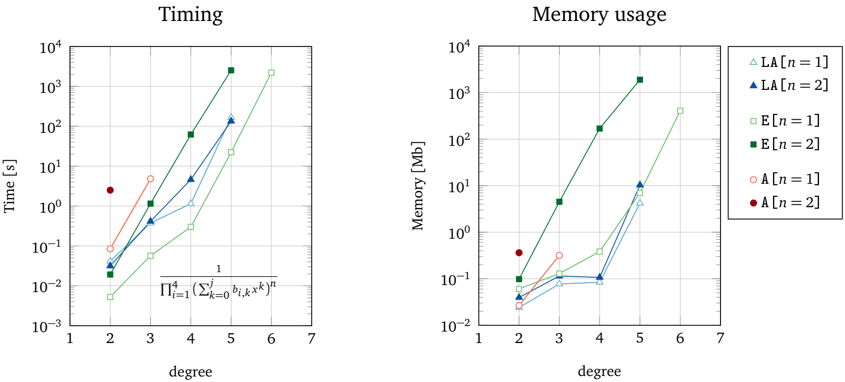
Performance
-The general case



Performance
-The general case



Performance
-The general case



In[1]:=

```
expr=x^2/Product[(x-b[i,1])^20,{i,1,15}];
expr//LinApart[#,x]&;//AbsoluteTiming
expr//LinApart[#,x,
        "Parallel"->{True,4,NotebookDirectory[]}
        ]&;//AbsoluteTiming
```

Out[1]=

```
{29.8126,Null}
```

Out[2]=

```
{13.6825,Null}
```

In[3]:=

```
expr=x^2/Product[Sum[b[i,j] x^j, {j,0,2}]^4, {i,1,5}];

expr//LinApart[#,x]&;//AbsoluteTiming
expr//LinApart[#,x,
        "Parallel"->{True,4,NotebookDirectory[]}
        ]&;//AbsoluteTiming
```

Out[3]=

```
{148.413, Null}
```

Out[4]=

```
{103.241, Null}
```

In[5]:=

```
expr=x^2/Product[Sum[b[i,j] x^j, {j,0,2}]^2, {i,1,8}];

expr//LinApart[#,x]&;//AbsoluteTiming
expr//LinApart[#,x,
        "Parallel"->{True,4,NotebookDirectory[]}
        ]&;//AbsoluteTiming
```

Out[5]=

```
{31.7012, Null}
```

Out[6]=

```
{30.7866, Null}
```

Conclusion and outlook
-Summary

- The univariate partial fraction decomposition is vital to QFT calculations. In some cases the publicly available native function of popular symbolic algebra programs are insufficient.
- We presented new implementations of the Laurent-expansion method, with which we were able to decrease the time and memory usage by magnitudes.
- We firmly believe the LinApart algorithm is a prime candidate for an efficient all-around single variable partial decomposition algorithm.

Direct calculation of time-like N3LO coefficient functions

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The structure of the presentation

- Motivation
- Theoretical background
  - Mass-refactorization
  - Outline of the calculation
- Challenges
  - Exploding complexity
  - Bottlenecks the technical side
  - Nuances
- Status of our research
  - What are we aiming for
  - What do we have right now
- Summary

Motivation

- One of the cleanest process to probe parton hadronization is the semi-inclusive electron-positron annihilation.
- Experimental uncertainties have reached the scale of theoretical uncertainties.
- Thus, in order to draw meaningful conclusions from data, we must reduce the theoretical uncertainties.
- This would open up not just the possibility of reanalyzing data from LEP, Belle, BaBar; but also lay the theoretical groundwork for the new colliders, like the FCC-ee.

Theoretical background

-Mass-refactorization: hard cross section

$$\sigma_p = C_p^{(0)} +$$

$$\alpha_s \left[-\frac{1}{\varepsilon} \boxed{P_{pp'}^{(0)}} \otimes C_{p'}^{(0)} + \boxed{C_p^{(1)}} + \varepsilon \boxed{A_p^{(1)}} + \varepsilon^2 \boxed{B_p^{(1)}} \right] +$$

$$\alpha_s^2 \left[\frac{1}{\varepsilon^2} \left(\frac{1}{2} P_{pi}^{(0)} \otimes P_{ip'}^{(0)} + \frac{\beta_0}{2} P_{pp'}^{(0)} \right) \otimes C_{p'}^{(0)} + \right.$$

$$\frac{1}{\varepsilon} \left(-\frac{1}{2} \boxed{P_{pp'}^{(1)}} \otimes C_{p'}^{(0)} - P_{pp'}^{(0)} \otimes C_{p'}^{(1)} \right) +$$

$$\left. \left(\boxed{C_p^{(2)}} - P_{pp'}^{(0)} \otimes A_{p'}^{(1)} \right) + \varepsilon \left(\boxed{A_p^{(2)}} - P_{pp'}^{(0)} \otimes B_{p'}^{(1)} \right) \right] +$$

$$\alpha_s^3 \left[\frac{1}{\varepsilon^3} \left(-\frac{\beta_0^2}{3} P_{pp'}^{(0)} - \frac{\beta_0}{2} P_{pi}^{(0)} \otimes P_{ip'}^{(0)} - \frac{1}{6} P_{pi}^{(0)} \otimes P_{ij}^{(0)} \otimes P_{jp'}^{(0)} \right) \otimes C_{p'}^{(0)} + \right.$$

$$\frac{1}{\varepsilon^2} \left\{ \left(\frac{\beta_0}{2} P_{pp'}^{(0)} + \frac{1}{2} P_{pi}^{(0)} \otimes P_{ip'}^{(0)} \right) \otimes C_{p'}^{(1)} + \right.$$

$$\left. \left(\frac{\beta_1}{3} P_{pp'}^{(0)} + \frac{\beta_0}{2} P_{pp'}^{(1)} + \frac{1}{3} P_{pi}^{(0)} \otimes P_{ip'}^{(1)} + \frac{1}{6} P_{pi}^{(1)} \otimes P_{ip'}^{(0)} \right) \otimes C_{p'}^{(0)} \right\} +$$

$$\frac{1}{\varepsilon} \left\{ -\frac{1}{3} \boxed{P_{pp'}^{(2)}} \otimes C_{p'}^{(0)} - \frac{1}{3} P_{pp'}^{(1)} \otimes C_{p'}^{(1)} - P_{pp'}^{(0)} \otimes C_{p'}^{(2)} + \left(\frac{\beta_0}{2} P_{pp'}^{(0)} + \frac{1}{2} P_{pi}^{(0)} \otimes P_{ip'}^{(0)} \right) \otimes A_{p'}^{(1)} \right\} +$$

$$\left. \left(\boxed{C_p^{(3)}} - P_{pp'}^{(0)} \otimes A_{p'}^{(2)} - \frac{1}{2} P_{pp'}^{(1)} A_{p'}^{(1)} + \left(\frac{\beta_0}{2} P_{pp'}^{(0)} + \frac{1}{2} P_{pi}^{(0)} \otimes P_{ip'}^{(0)} \right) \otimes B_{p'}^{(1)} \right) \right]$$

- The calculation is pretty straight forward. We have to:
  - calculate the relevant amplitudes,
  - reduce the integrals with an IBP software,
  - calculate the integrals,
  - do the renormalization of the amplitudes,
  - iteratively determine the splitting and coefficient functions.

- The 3-,4- and 5-particle-cut semi-inclusive integrals were calculated at 4 loops by dr. Vitaly Magerya during his PhD.
- He calculated the integrals with the exclusion method, meaning he restricted the phase space; put the final state particles on mass-shell and introduced the tag as a mass.

$$I = \int \prod_i \frac{d^d l_i}{(2\pi)^d} \mathrm{dPS}_n(q) \prod_j \frac{1}{D_j^{\nu_j}} \delta\left(x - 2\frac{qp}{q^2}\right)$$

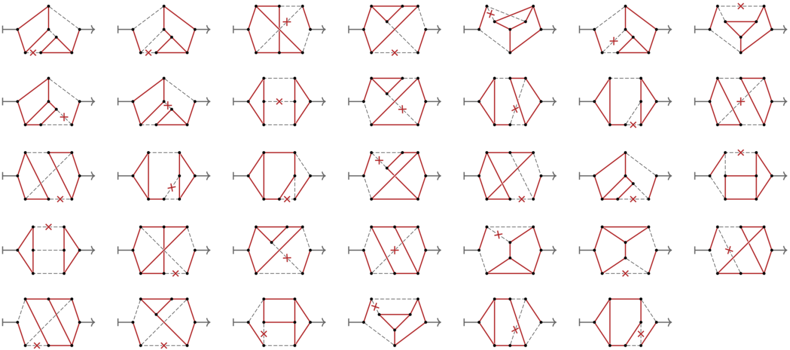

Figure: 3-particle-cut semi-inclusive integral families; source [1]

- The quark and gluon form factors contribute the part proportional to $\delta(1-x)$. Although, these can be found in the existing literature we have recalculated them. [2]

$$\Bigg[\Bigg\{\left(-\frac{\beta_0^3}{\varepsilon^3}-\frac{\beta_0\beta_1}{\varepsilon^2}\right)\langle M^{(0)}|M^{(0)}\rangle_{gg}+\left(\frac{\beta_0^2}{\varepsilon^2}-\frac{\beta_1}{\varepsilon}\right)\langle M^{(1)}|M^{(0)}\rangle_{gg}-\frac{\beta_0}{\varepsilon}\langle M^{(2)}|M^{(0)}\rangle_{gg}-$$

$$\frac{2\beta_0}{\varepsilon}\langle M^{(1)}|M^{(1)}\rangle_{gg}+\langle M^{(2)}|M^{(1)}\rangle_{gg}\Bigg\}_{[2\times 1]}+$$

$$\Bigg\{\left(-\frac{\beta_0^3}{\varepsilon^3}-\frac{2\beta_0\beta_1}{\varepsilon^2}-\frac{\beta_2}{\varepsilon}\right)\langle M^{(0)}|M^{(0)}\rangle_{gg}+\left(\frac{3\beta_0^2}{\varepsilon^2}-\frac{3\beta_1}{2\varepsilon}\right)\langle M^{(1)}|M^{(0)}\rangle_{gg}-$$

$$\frac{3\beta_0}{\varepsilon}\langle M^{(2)}|M^{(0)}\rangle_{gg}+\langle M^{(3)}|M^{(0)}\rangle_{gg}\Bigg\}_{[3\times 0]}\Bigg]_{\underline{2\ \mathrm{cut}}}$$

Challenges

-Exploding complexity: the hard cross-section

- The 3[1],4 and 5 cut cases were never calculated at N3LO order, thus these are completely new.

$$2\Bigg[\left\{\frac{9\beta_0^2}{4\varepsilon^2}\langle M^{(0)}|M^{(0)}\rangle_{q\bar{q}g}-\frac{3\beta_0}{\varepsilon}\langle M^{(1)}|M^{(0)}\rangle_{q\bar{q}g}+\langle M^{(1)}|M^{(1)}\rangle_{q\bar{q}g}\right\}_{[1\times1]}+$$

$$\left\{\left(\frac{15\beta_0^2}{8\varepsilon^2}-\frac{5\beta_0}{4\varepsilon}\right)-\frac{5\beta_0}{2\varepsilon}\langle M^{(1)}|M^{(0)}\rangle_{q\bar{q}g}+\langle M^{(2)}|M^{(0)}\rangle_{q\bar{q}g}\right\}_{[2\times1]}\Bigg]_{\underline{3\ \text{cut}}}+$$

$$2\Bigg[\left\{\frac{9\beta_0^2}{4\varepsilon^2}\langle M^{(0)}|M^{(0)}\rangle_{ggg}-\frac{3\beta_0}{\varepsilon}\langle M^{(1)}|M^{(0)}\rangle_{ggg}+\langle M^{(1)}|M^{(1)}\rangle_{ggg}\right\}_{[1\times1]}+$$

$$\left\{\left(\frac{15\beta_0^2}{8\varepsilon^2}-\frac{5\beta_0}{4\varepsilon}\right)-\frac{5\beta_0}{2\varepsilon}\langle M^{(1)}|M^{(0)}\rangle_{ggg}+\langle M^{(2)}|M^{(0)}\rangle_{ggg}\right\}_{[2\times1]}\Bigg]_{\underline{3\ \text{cut}}}$$

[2] During our calculation an independent group has published an article, where they calculate these parts. [3]

- From the computational perspective these diagrams pose no problem.
- The longest calculation is the $H \to ggggg$, which has $230^2 = 52900$ diagrams. However, since they are tree level they can be calculated in less than 4 days, with 4 cores per diagram and running 100 calculation parallel.

$$\left[\left\{-\frac{2\beta_0}{\varepsilon}\langle M^{(0)}|M^{(0)}\rangle_{q\bar{q}gg} + \langle M^{(1)}|M^{(0)}\rangle_{q\bar{q}gg}\right\}_{[1\times 0]}\right]_{4\ cut} +$$

$$\left[\left\{-\frac{2\beta_0}{\varepsilon}\langle M^{(0)}|M^{(0)}\rangle_{gggg} + \langle M^{(1)}|M^{(0)}\rangle_{gggg}\right\}_{[1\times 0]}\right]_{\underline{4\ \mathrm{cut}}} +$$

$$\left[\left\{\langle M^{(0)}|M^{(0)}\rangle_{ggggg} + \langle M^{(0)}|M^{(0)}\rangle_{q\bar{q}ggg} + \langle M^{(0)}|M^{(0)}\rangle_{q\bar{q}q\bar{q}g}\right\}_{[0\times 0]}\right]_{\underline{5\ \mathrm{cut}}}$$

Challanges

-Bottlenecks the technical side

- The number of families at four loops in the case of five final state particles reach above a hundred and the reduction of even one family requires great resources.
- The size and complexity of the results of the IBP reduction also increases;
  - expressions are not particularly huge, IBP results are at the order of $10^6 - 10^7$ fully expanded and maximum are a few tens of Gbs in Mathematica's own binary dump formats (.mx or .wxf).
  - however, even basic operations like series expansion and partial fractioning pose a challenge.
- We overcome these by two methods:
  - optimizing already existing algorithm,
  - heavy parallelization.

Challenges

-Bottlenecks the technical side

- Optimizing already existing algorithm:
  - LinApart for partial fractioning the IBP output for faster gathering and series expansion [4] ,
  - alibrary for harmonic polylogarithms and streamlining the calculation.
- heavy parallelization:
  - with KIRA2 some families require 1Tb+ memory and days of runtime on 30 cores (main bottleneck is the equation generation).
  - in order to get a result in a reasonable time-frame, we run the families parallel; this requires up to 300-400 cores and up to 10Tbs of memory.
  - due to the size of the IBP results, further operations must also be run on 100s of cores. We run the particularly time-consuming operations on 500 cores with basic load balancing in Wolfram Mathematica.

Challenges

-Nuances: plus-distribution with higher multiplicities

UHH ELTE

- In the case of higher multiplicities during the construction of the plus-distribution we must subtract the Laurent series of the singularity

$$\Big[(1-x)^{-n+k\varepsilon}\Big]_+ = \int_0^1 dx(1-x)^{-n+k\varepsilon}\left(F(x) - \sum_{i=0}^{n-1}(-1)^i(1-x)^i \lim_{x\to 1}\Big[F(x)^{(i)}\Big]\right) = \sum_{i=0}^{\infty}\varepsilon^i \frac{k^i}{i!}\left[\frac{ln^i(1-x)}{(1-x)^n}\right]_+$$

- But in this case even though $\lim_{x\to 1}\Big[F(x)\Big] = F(1)$, the derivatives can diverge in the limit; $\lim_{x\to 1}\Big[F(x)^{(i)}\Big] \to \infty$.

Challenges

-Nuances: plus-distribution with higher multiplicities

- Although this mathematical possibility exists, it would mean higher order terms in ε influence lower order terms, since:

$$\int_0^1 dx \ln(1-x)^a (1-x)^{-n+k\varepsilon} = -\frac{\Gamma(1+a)}{(-1+n-k\varepsilon)^{1+a}}$$

- For example a double pole, would mean that we still have double singularities like collinear-collinear, soft-soft or collinear-soft in our expression.
- We think that, these are spurious and in the end have to cancel; in the processes we have so far checked, these are indeed absent.

Challenges

-Nuances: not every pole cancels

- According to the KNL theorem UV and IR singularities cancel if one sums over ***all*** degenerate initial and final states.
- But since we tag particles we leave out some processes from the sum. In the N2LO, tagged g, Higgs mediated case, we have:

$\lvert\mathcal{M}_{gg}^{[1\times1]}\rvert^2$	$\lvert\mathcal{M}_{gg}^{[2\times0]}\rvert^2$	$\lvert\mathcal{M}_{qqg}^{[1\times0]}\rvert^2$	$\lvert\mathcal{M}_{qqqq}^{[0\times0]}\rvert^2$
$\frac{1}{9}\frac{Nf^2}{\varepsilon^2}$	$\frac{2}{9}\frac{Nf^2}{\varepsilon^2}$	$-\frac{4}{9}\frac{Nf^2}{\varepsilon^2}$	$\frac{1}{9}\frac{Nf^2}{\varepsilon^2}$

- Since we leave out the *qqqq* case, the Nf^2 parts do not cancel in the lower orders like $\frac{1}{\varepsilon^2}$.

Status of our research
-What are we aiming for

Process	γ		Z	H
Projection	Transversal	Longitudinal	Axial	
Tagged particle	$q\ g\ \gamma$	$q\ g\ \gamma$	$q\ g\ \gamma$	$q\ g\ \gamma$

- Our aim is plain and simple, we want to directly calculate the time-like N2LO splitting and N3LO coefficient functions.
- A direct calculation has never been done before, the existing results were acquired by the means of analytic continuation.
- With our results, we would confirm the already existing results and deliver all the other yet missing pieces.
- We also plan to publish our code base in order to facilitate future research in this direction.

Status of our research
-What do we have right now

- We have successfully recalculated all of the relevant fully-inclusive results at N3LO in terms of Ca, Cf, Nf. [5, 6]
- We have calculated the amplitudes for the tagged quarks and gluons in case of a mediating photon (both transversal and longitudinal), Z- and Higgs-boson.
- The IBP reduction for the 3- and 4-cut-particle cases have finished, the 5-cut is running.

Status of our research

-What do we have right now

- We have started the construction of the plus-distribution and the cross checks with the inclusive results.
- So far we have checked the following amplitudes:

Loops	Process	Tagged
1 x 1	$H \to q\bar{q}g$	q
1 x 1	$H \to q\bar{q}g$	g
1 x 1	$H \to ggg$	g
2 x 0	$H \to q\bar{q}g$	q
2 x 0	$H \to q\bar{q}g$	g

- We intend to publish the N3LO Higgs tagged quark coefficient functions in the near future; along with the recalculated inclusive results.

Summary

- A number of different coefficient functions are yet to be calculated at N3LO.
- These are accessible with a direct calculation, which would also serve as a strong check of the already existing results acquired by the means of analytic continuation.
- Our calculation is already in an advanced stage. However along the way we faced harsh, mostly technical difficulties.
- We overcome these, by writing new, faster software solutions and fully utilizing the available resources.

Thank you!

Thank you for your attention!

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