# Modern methods for multi-loop multi-scale amplitudes

## High Precision for Hard Processes 2022

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# Introduction

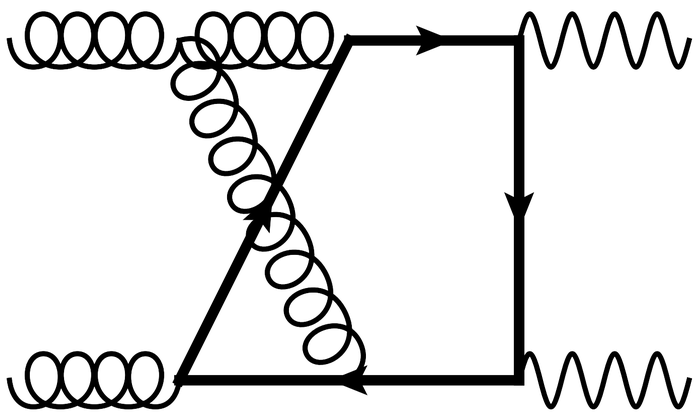
- With HL-LHC starting, $\sim 1\,\%$ precision to be achieved for many important observables → theory needs to catch up
- Higher order corrections needed to achieve theoretical precision; NLO already automated, NNLO corrections achieved for many processes
- Requires calculation of scattering amplitudes with many loops and scales (kinematic variables)
- Development of many new methods in recent years to push the state-of-the-art
- Talk mostly based on two papers:

  *Two-loop helicity amplitudes for $gg \to ZZ$ with full top-quark mass effects;* **BA**, Jones, von Manteuffel; [https://doi.org/10.1007/JHEP05(2021)256]

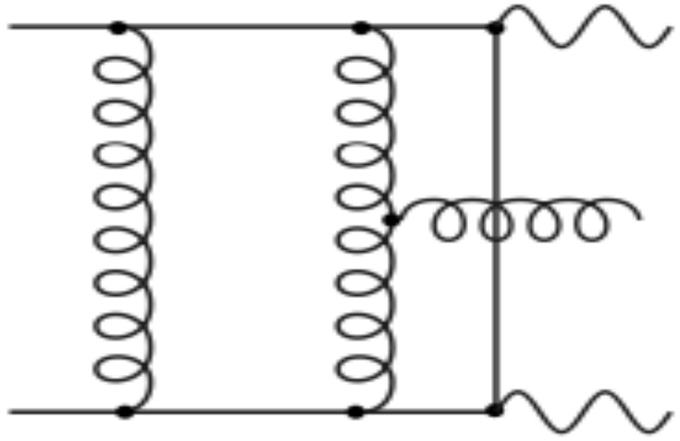
  *Two-Loop Helicity Amplitudes for Diphoton Plus Jet Production in Full Color;* **BA**, Buccioni, von Manteuffel, Tancredi; [https://doi.org/10.1103/PhysRevLett.127.262001]

- Not meant to be a comprehensive overview, rather a short description of methods that made the above calculations possible. Also see talks on related processes:
  - Ryan Moodie - $jjj$ and $\gamma\gamma + j$ (gluon fusion) production
  - Giuseppe De Laurentis - $q\bar{q} \to \gamma\gamma\gamma$ at 2-loops
  - Matthias Kerner - $ZH$ production through gluon fusion

# Loop Amplitudes



- $2 \to 2$ scattering process with internal masses
- Up to $s = 4$ integrals
- 2 scales $s, t$ ($m_t, m_Z$ set to numbers)
- Extremely complicated due to internal masses



- $2 \to 3$ scattering process
- Up to $s = 5$ integrals
- 4 scales $s_{23}, s_{34}, s_{45}, s_{51}$ ($s_{12} = 1$)
- Complicated color structure

# Loop Amplitudes

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Recipe for a multi-loop amplitude:

1. Generation of unreduced amplitude
2. IBP reduction
   - Major bottleneck for processes with many scales and/or legs
   - Significant progress with syzygy based approaches and finite-field methods
3. Insertion of IBP identities into the amplitude
   - Significant blow-up for intermediate results and final reduced amplitude
   - Numerical instabilities in final coefficients
   - Use of multivariate partial fractioning to tame the computational complexity and improve numerical performance
4. Evaluation of master integrals
   - Express in terms of multiple polylogarithms; internal masses => Functions beyond multiple polylogarithms
   - Use of numerical methods instead, improved with the use of finite integrals

# Integration-By-Parts reduction using Syzygies

- Integration-By-Parts reduction to reduce all the integrals to a basis set
- Generate linear relations between integrals [Chetyrkin & Tkachov (1981)]
- Systematically construct and reduce a linear system to a basis set of master integrals -> Laporta's algorithm [Laporta (2000)]. Public codes available *AIR, FIRE6, Kira, LiteRed, Reduze 2*, etc.
- In Baikov representation [Baikov (1996)] :

$$0 = \int \left( \prod_i^L dz_i \right) \sum_i^N \frac{\partial}{\partial z_i} \left( f_i(z_1, \ldots, z_N) P^{(d-L-E-1)/2} \prod_i^N \frac{1}{z_i^{\nu_i}} \right)$$

$$0 = \int \left( \prod_i^L dz_i \right) \sum_i^N \left( \frac{\partial f}{\partial z_i} + \boxed{\frac{d-L-E-1}{2P} f_i \frac{\partial P}{\partial z_i}} - \boxed{\frac{\nu_i f_i}{z_i}} \right) P^{(d-L-E-1)/2}$$

Dimension shifting term  Doubled propagators

- Require:
  - No dimension-shifting terms
  - No integrals with doubled propagators

# Integration-By-Parts reduction using Syzygies

Disadvantages:

- Such integrals don't appear in amplitudes
- Significantly larger linear system to reduce for the appearance of auxiliary integrals

Would like to avoid doubled propagators:

- Generating vectors using Groebner basis [Gluza, Kajda, Kosower (2010)]
- Linear algebra based approach [Schabinger (2011)]
- Differential geometry [Zhang (2014)]

$$\boxed{f_i \frac{\partial P}{\partial z_i} \sim P}$$

Dimension shifting term

- Explicit solutions known [Boehm, Georgoudis, Larsen, Schulze, Zhang (2017)] [Abreu, Cordero, Ita, Page, Zeng (2017)]
- Polynomials of degree 1 in Baikov parameters
- Straightforward to write

$$\boxed{f_i \sim z_i}$$

Doubled propagator term

- Trivial to write explicit solutions

# Integration-By-Parts reduction using Syzygies

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- Simultaneous solution for the two constraints highly non-trivial
- Compute module intersection of the two syzygy modules using e.g. *Singular*
- Conventional approaches insufficient for our purpose [Larsen, Zhang (2015)] [Boehm, Georgoudis, Larsen, Schoenemann, Zhang (2018)]
  - Syzygies for top-level topologies inaccessible for $gg \to ZZ$

- Developed a new **linear algebra approach based on finite fields** [BA, Jones, von Manteuffel (2020)]
  - Map the problem of module intersection to row reduction of a matrix; use *Finred* - IBP solver based on finite field methods [von Manteuffel, Schabinger (2014)], [Peraro (2016)] for the linear algebra
  - Solutions produced up to a requested degree in $z_i$
  - **Much faster** for our purpose than the Groebner basis approach; can run in a highly distributed manner
  - Able to generate the required syzygies for this calculation

- Use *Finred* to compute the required IBP reductions
- Also use this approach for the 2-loop amplitudes for $\gamma\gamma + j$ [BA, Buccioni, von Manteuffel, Tancredi (2021)], [BA, Buccioni, von Manteuffel, Tancredi (2021)]

# Denominator Guessing

- Predetermine the denominator factors to reduce reconstruction cost [Abreu, Dormans, Febres Cordero, Ita, Page (2018)] [Heller, von Manteuffel (2021)]

- Write the reduced amplitude as:

$$\mathscr{M} = \Sigma_l R_l(\{s_{ij}\}, \{m_i^2\}, \epsilon) F_l(\{s_{ij}\}, \{m_i^2\}, \epsilon)$$

with $F_i$ the master integrals and $R_i$ the rational functions in kinematics $\{s_{ij}\}$ and masses $\{m_i^2\}$

- Can determine all the factors appearing in the rational functions by performing IBP reductions on cuts - much simpler than computing full reduction

- Determine the exponent of each denominator factor by performing an IBP reduction for large prime values for kinematic variables and analysing the prime factors of the resulting rational numbers

- Naively, expect a reduction in number of samples required by $2^n$ where $n$ is the number of independent scales (including $d$), assuming roughly equal degrees for both the numerator and denominator polynomials; actual improvement is less and depends on the process; e.g. $\sim 20$ for diphoton plus jet production at full color compared to ideally 32

# Multivariate partial fractioning

- Certain basis choices lead to spurious poles with denominators depending on both kinematics and $d$; want to avoid such poles, e.g.

$$1250 - 500\,d - 9000\,t + 3600\,d\,t + 16200\,t^2 - 6480\,d\,t^2 - 4050\,s + 1575\,d\,s + 19440\,s\,t - 8100\,d\,s\,t - 52488\,s\,t^2 + 20412\,d\,s\,t^2 - 29160\,s^2\,t + 11664\,d\,s^2\,t$$

In $d \to 4$ this becomes :$-125 + 375\,s + 900\,t - 2160\,s\,t + 2916\,s^2\,t - 1620\,t^2 + 4860\,s\,t^2$

- Spurious poles may lead to numerical instabilities in the physical phase-space region
- Choose $d$-factoring basis to avoid such denominators [Smirnov, Smirnov (2020)], [Usovitsch(2020)]; for $\gamma\gamma + j$ not necessary since canonical basis already known
- Amplitudes for $gg \to ZZ$ reduced to such a basis of finite integrals; still need to insert the identities into the unreduced amplitude
- This is computationally very difficult; IBPs size of over 200 GB with intermediate steps requiring TB of disk space
- Employ multivariate partial fractioning [Pak (2011)], [Abreu, Dormans, Febres Cordero, Ita, Page, Sotnikov (2019)], [Böhm, Wittman, Wu, Xu, Zhang (2020)], [Bendle, Böhm, Heymann, Ma, Rahn, Ristau, Wittmann, Wu, Zhang (2021)]; Mathematica package *MultivariateApart* [Heller, von Manteuffel (2021)]
- Also see Ben Page's talk for another approach to partial fractioning

# Multivariate partial fractioning

- Use Singular to perform partial fractioning using a Gröbner basis to prevent new denominators from appearing. E.g. naive partial fractioning in Mathematica:

$$\frac{1}{(25-270\,t+324\,s\,t)}\,\frac{1}{(-5+18\,t+9\,s)}=\frac{-1}{(5+18\,t)(-5+36\,t)(-5+18\,t+9\,s)}+\frac{36\,t}{(5+18\,t)(-5+36\,t)(25-270\,t+324\,s\,t)}$$

- Instead use a Gröbner basis approach; find relations between all appearing denominators to reduce them to simpler ones
- Unique decomposition for a chosen ordering of denominator polynomials
- Handle nasty degree 6 denominators:

$$105625-468000\,t-797850\,t^2+3863700\,t^3+2001105\,t^4-5904900\,t^5+2125764\,t^6-3676500\,s+17309700\,s\,t$$
$$-19260180\,s\,t^2+25850340\,s\,t^3-35901792\,s\,t^4+8503056\,s\,t^5+25891650\,s^2-73614420\,s^2\,t^2-75149694\,s^2\,t^3$$
$$+12754584\,s^2\,t^4-50490540\,s^3+80752788\,s^3\,t-60466176\,s^3\,t^2+8503056\,s^3\,t^3+29452329\,s^4-18187092\,s^4\,t$$
$$+2125764\,s^4\,t^2$$

# Multivariate partial fractioning

- For a choice of basis of master integrals that are finite in $d = 4$, further simplification can be obtained
  1. Partial fraction in $d$ to separate the poles (as usual)
  2. Set $d = 4$ (allowed since the basis is finite) everywhere except the poles

Factorised form: $\frac{1}{(-1+d)(-3+d)^2(-4+d)(-7+2d)} = (\frac{1}{3} + \frac{2\epsilon}{9})(1+2\epsilon)^2(\frac{-1}{2\epsilon})(1+4\epsilon)$ ~16 terms

Partial fractioned: $\frac{1}{3(-4+d)} + \frac{5}{4(-3+d)} + \frac{1}{2(-3+d)^2} + \frac{1}{60(-1+d)} + \frac{-16}{5(-7+2d)} = \frac{-1}{6\epsilon} + \frac{-13}{9}$ 2 terms

- Prevents proliferation of terms
- Partial fraction in kinematics to arrive at final form
- Resulting coefficients smaller than 1MB in size with total size of all coefficients $O(100)$ MB (started from $O(100)$ GB of coefficients)
- Very fast numerical evaluation; coefficients evaluated as exact rationals in ~30 s and a few s for double precision reals

# Multivariate partial fractioning

- Similar approach used in $\gamma\gamma + j$ production with the added benefit of the master integrals being expressed in terms of special functions with fast numerical evaluation [Chicherin, Sotnikov (2020)]
- Polynomials appearing in the denominator much simpler due to lack of internal masses; only 1 degree 2 polynomial appears i.e. the Gram determinant, rest are linear in kinematics [BA, Buccioni, vonManteuffel, Tancredi (2021)]. Use *MultivariateApart* [Heller, von Manteuffel (2021)] as frontend for the partial fractioning procedure
- Express the amplitude as linear combination of Pentagon functions with rational functions in kinematics only as coefficients, and exploit linear relations between the coefficients for further simplification
- Additionally, observed that canonical basis generates simpler factors than e.g. a naive choice based on numerator degree, with a reduction by a factor of 2
- Reduction of up to a factor of 100 in disk space for the coefficients, particularly significant for the complicated topologies; resulting coefficients less than 100 MB

# Finite Integrals

- Feynman integrals often have UV and IR divergences
- Sector decomposition standard method to resolve IR poles [Binoth, Heinrich (2000)] [Bogner, Weinzierl (2007)]
- Public codes: *Fiesta4*, *pySecDec*, etc.

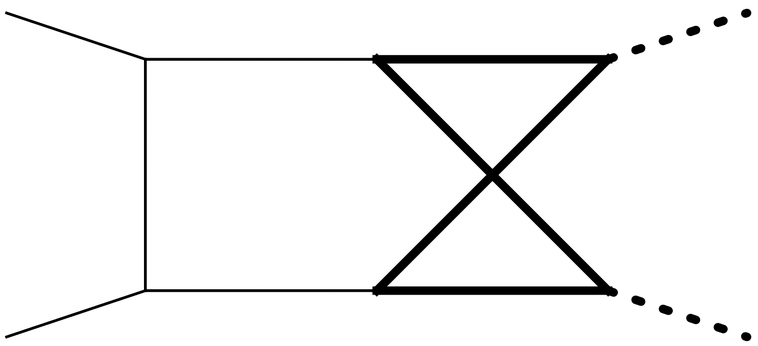
Why use finite integrals instead?

- Much better behaved numerically
- Require fewer orders in epsilon expansion in general
- Poles drop out into the coefficients => Easier to take $d \to 4$ limit

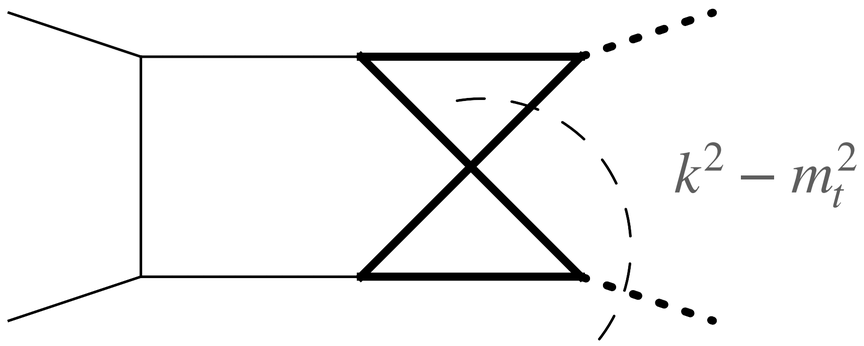
Constructing finite integrals:

- Dimension shifted integrals [Bern, Dixon, Kosower (1992)]
- Existence of a finite basis [Panzer (2014)] [von Manteuffel, Panzer, Schabinger (2014)]
- *Reduze 2* to find such integrals, usually involving higher propagator powers (dots) and dimension shifts

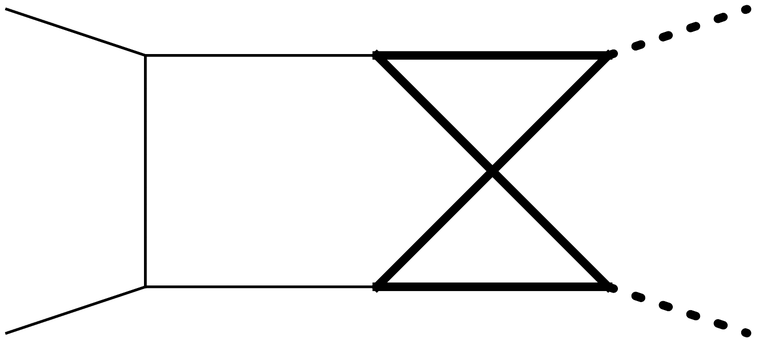
# Finite Integrals



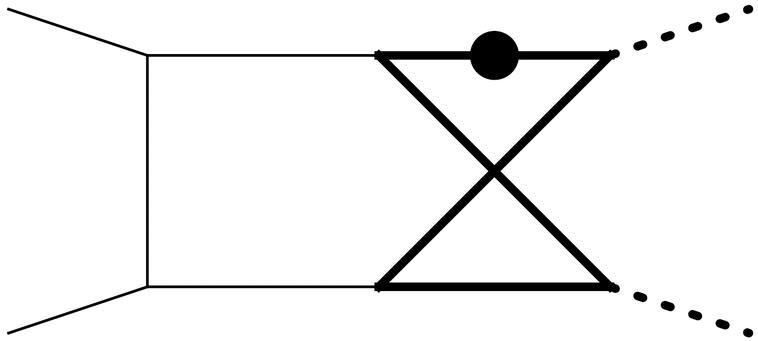
Divergent integral in $d = 4 - 2\epsilon$




Divergent integral in $d = 4 - 2\epsilon$ with a numerator



Finite integral in $d = 6 - 2\epsilon$



Finite integral in $d = 6 - 2\epsilon$ with a dot

# Finite Integrals

However:

- Integrals with dots and dimension-shifts often hard to reduce e.g. need reductions for integrals with 4 dots for the required finite integrals
- Higher dots implies higher powers of $\mathscr{F}$ polynomial in the denominator => worse contour deformation which leads to numerical instabilities

Alternate approach - combining divergent integrals into **finite linear combinations**. Advantages:

- Integrals often already appearing in the amplitude => avoid computing extra reductions
- More "natural" $d = 4$ representation
- Finite at the integrand level i.e. integrand free of non-integrable divergences

- In general a highly non-trivial task to find these numerators
- Algorithmically construct finite linear combinations in $d = 4$ from a list of seed integrals [BA, Jones, von Manteuffel (2020)]
- Arbitrary integrals with numerators, dots, dimension shifts, subsector integrals etc allowed as seed integrals

# Finite Integrals

$$\text{Integrand} = a_1 \frac{1}{D_1 \dots D_N} + a_2 \frac{D_{N+1}}{D_1 \dots D_N} + a_3 \frac{D_j}{D_1 \dots D_j \dots D_N} + \dots$$

- Combine over a common denominator using the general formula for Feynman parametric representation [BA, Jones, von Manteuffel (2020)] , embedding the subsector integrals in the parent topology

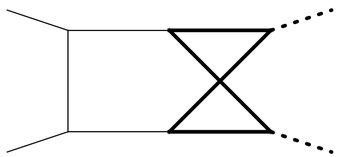
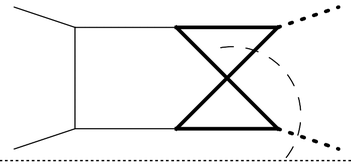
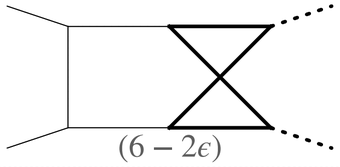
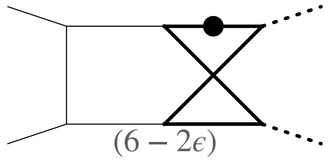
$$I(\nu_1, \dots, \nu_N) = (-1)^{r+\Delta t}\, \Gamma(\nu - L\, d/2) \int \left( \prod_{j \in \mathcal{N}_T} dx_j \right) \left( \prod_{j \in \mathcal{N}_t} \frac{x^{\nu_j - 1}}{\Gamma(\nu_j)} \right) \delta\left( 1 - \sum_{j \in \mathcal{N}_T} x_j \right)$$

$$\left[ \left( \prod_{j \in \mathcal{N}_{\setminus T}} \frac{\partial^{|\nu_j|}}{\partial x_j^{|\nu_j|}} \right) \left( \prod_{j \in \mathcal{N}_{\Delta t}} \frac{\partial^{|\nu_j|+1}}{\partial x_j^{|\nu_j|+1}} \right) \frac{\mathcal{U}^{\nu - (L+1)d/2}}{\mathcal{F}^{\nu - L\, d/2}} \right]_{x_j = 0\ \forall\, j \in \mathcal{N}_{\setminus T}} \qquad (\nu_j \in \mathbb{Z})$$

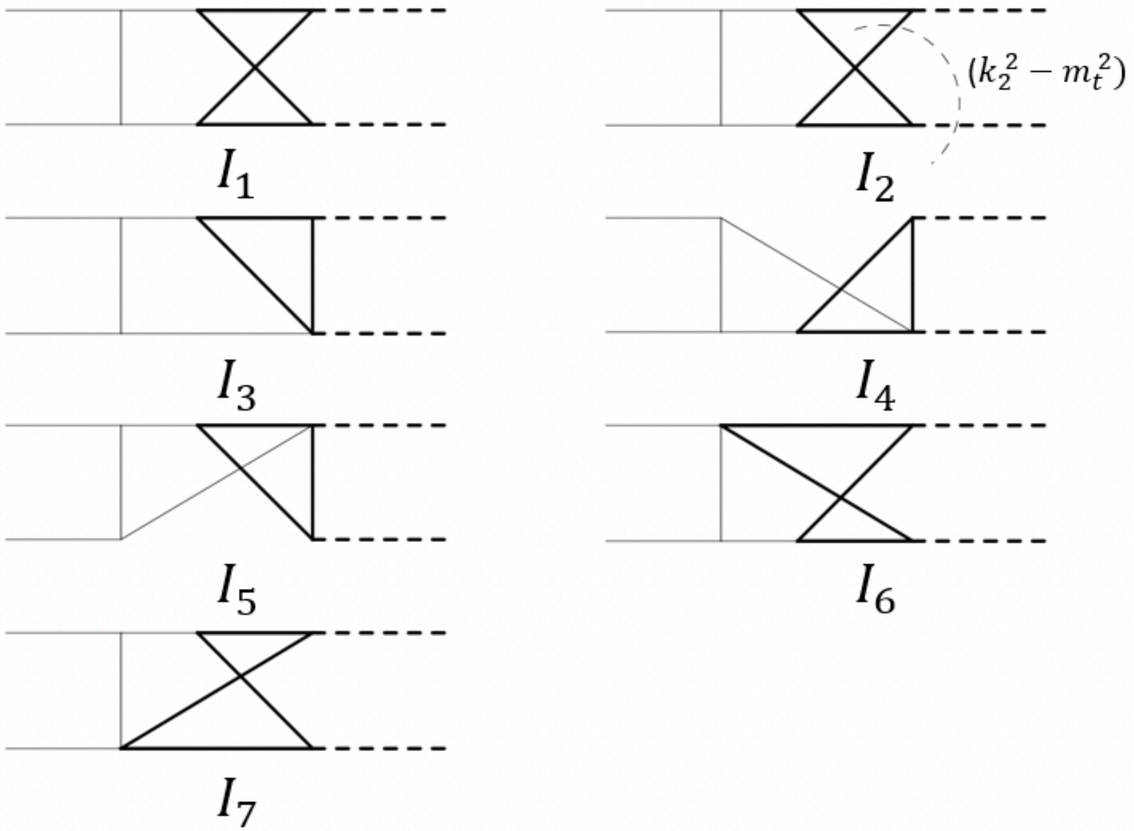
$\mathcal{N}_T$ : Parent sector
$\mathcal{N}_t$ : Current integral propagators
$\mathcal{N}_{\setminus T}$ : Numerators
$\mathcal{N}_{\Delta t}$ : Pinched propagators

- Constrain $a_i$ requiring absence of non-integrable divergences in the integrand

# Finite Integrals

| Integral | Rel. err. leading term | Timing (s) | |
|---|---|---|---|
|  | ~2*10^-3 | 45 | |
|  | ~4*10^-2 | 63 | |
|   | ~8*10^-6 | 55 | $\sim \frac{1}{\mathcal{F}}$ |
|   | ~8*10^-4 | 60 | $\sim \frac{1}{\mathcal{F}^2}$ |
| Linear Combination | ~1*10^-4 | 18 | $\sim \frac{1}{\mathcal{F}^3}$ |

Naively expected to be much worse




$$I = (m_z^2 - s - t)(sI_1 - I_6) + s(I_2 + I_3 - I_4 - I_5) - (m_z^2 - t)I_7$$

# Finite Integrals

- Calculation of the four-loop collinear anomalous dimension in QCD and $\mathcal{N} = 4$ SYM using finite integrals [BA, von Manteuffel, Panzer, Schabinger (2021)]

- Using pySecDec to numerically evaluate the leading term of the remaining (analytically unsolved) finite integral (in $d = 6 - 2\,\epsilon$) to 11 significant digits

- Guess the analytic solution in terms of Multiple Zeta Values with the help of PSLQ algorithm and certain assumptions for the $\mathcal{N} = 4$ part

- Full result verified analytically [Lee, von Manteuffel, Schabinger, Smirnov, Smirnov, Steinhauser (2021)]

# Conclusions

- Use of syzygies and finite field methods for IBP reduction including presenting our **new algorithm for constructing syzygies**
- Significantly reducing the complexity of rational reconstruction by "inferring" the denominator
- Method of finite integrals with **new general approach to construct finite integrals** for faster converging numerical integration
- Multivariate partial fractioning to drastically simplify amplitude coefficients
- Allow the calculation of some challenging processes

# Backup

# Denominator Guessing

- E.g. with $d+2$, $d+3$, and $d-1$ as the denominators, use $d = 1197433$

$$d + 2 = 1197435 = 3 \text{ x } 5 \text{ x } 79829$$

$$d + 3 = 1197436 = 2^2 \text{ x } 299359$$

$$d - 1 = 1197432 = 2^3 \text{ x } 3^2 \text{ x } 16631$$

Perform IBP reduction with $d = 1197433$ and read off the powers of $79829, 299359, 16631$ in the denominators of the rational coefficients to determine the exponents of the corresponding denominator factors

# Integration-By-Parts reduction using Syzygies

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- It is observed that syzygies of a certain degree are sufficient for IBP reduction, instead of the complete syzygy module
- However, the current approach still not feasible to use for many difficult processes
- Putting kinematic variables in the variable field (like the Baikov parameters) reduces the effective degree e.g. $z_2 z_3\, x_{12}^2 x_{23} x_{35}$ is formally degree 6 but only degree 2 in the Baikov parameters
- Slightly modified version of the algorithm to put kinematics in the coefficient field; reconstruct the coefficients using finite field methods