

Recent developments in multiscale loop scattering amplitudes

Vasily Sotnikov

University of Zurich

Ringberg 2024:
2nd Workshop on Tools for High Precision LHC Simulations,
Castle Ringberg, Kreuth (Germany)

10th May 2024



European Research Council
Established by the European Commission



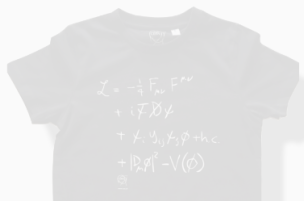
**Universität
Zürich**^{UZH}

The usual picture

General motivation

Success of the LHC physics program relies on precise theoretical understanding of the Standard Model.

[talks by Federico and Fabrizio].



Fixed order partonic cross sections

Collinear factorization:

$$d\sigma_{h_1 h_2 \rightarrow X}(p_1, p_2) = \sum_{i,j} \int dx_1 dx_2 f_i(x_1, \mu) f_j(x_2, \mu) \boxed{d\hat{\sigma}_{ij \rightarrow X}(x_1 p_1, x_2 p_2, \mu)} + \mathcal{O}(\Lambda_{\text{QCD}}/Q)$$

"Hard" partonic cross section

$$d\hat{\sigma}_0 \left(1 + \alpha_s \sigma^{(1,0)} + \alpha_s^2 \sigma^{(2,0)} + \alpha_s \sigma^{(0,1)} + \alpha_s^3 \sigma^{(3,0)} + \alpha_s \alpha_s \sigma^{(1,1)} + \dots \right)$$

Series truncation uncertainty

$\alpha_s(M_Z) \sim 0.1$
 $\alpha(M_Z) \sim 0.01$

At least **NNLO QCD** and **NLO EW** corrections must be included to achieve **percent level** theory uncertainties (\oplus PDFs, parton showers, resummations).

This talk: recent advances in **multi-scale** NNLO QCD corrections.

Ultimate goal:

fully differential NNLO cross sections for all (interesting) SM processes

NNLO QCD $2 \rightarrow 3$
current frontier

$$\sigma_{\text{NNLO}}^{F+X} = \sigma_{\text{NLO}}^{F+X} +$$

One-loop stable in IR,
e.g. OpenLoops2
[Buccioni et al. '19]

$$\int_{\Phi_{F+2}} d\sigma_{\text{RR}} + \int_{\Phi_{F+1}} d\sigma_{\text{RV}} + \int_{\Phi_F} d\sigma_{\text{VV}}$$

IR divergences

Two-loop amplitudes

Cancellation of IR divergences at NNLO
automated in principle

[Czakon '11] [Czakon, Heymes '14]

[Chen, Gehrmann, Glover, Huss, Marcoli '22]

[Grazzini, Kallweit, Wiesemann '17]

[Gehrmann, Glover, Marcoli '23]

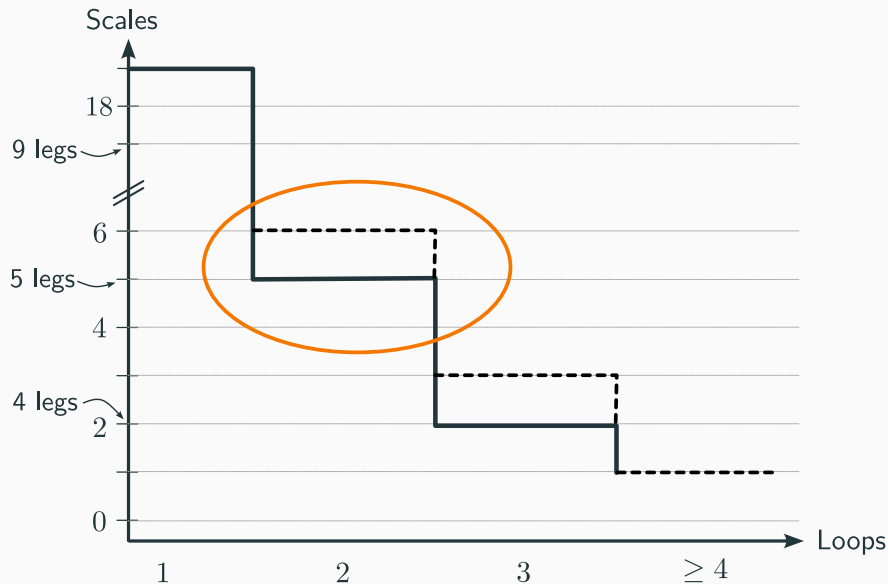
But:

- Doing it **efficiently** is hard
- General purpose **public codes** still missing

- Main missing ingredient, no automation in sight
- Both **technical** and **conceptual** challenges

Two-loop multi-scale amplitudes: state of the art

Loops & legs: state of the art



Two-loop five-point amplitudes: massless

Complete since the end of last year 🎉

	Comment	Complete analytic results	Public code	Cross sections
$pp \rightarrow \gamma\gamma\gamma$	l.c.*	[4, 5]	[4]	[11, 12]
$pp \rightarrow \gamma\gamma j$	l.c.*	[2, 3]	[2]	[10]
$pp \rightarrow jjj$	l.c.	[1]	[1]	[8, 9]
$pp \rightarrow \gamma\gamma\gamma$	NLO loop induced	[14]	[14]	
$pp \rightarrow \gamma\gamma j$		[6]		
$gg \rightarrow \gamma\gamma g$		[7]	[7]	[13]
$pp \rightarrow \gamma jj$		[15]		[15]
$pp \rightarrow jjj$		[16,17,18]	[17]	
$pp \rightarrow t\bar{t}H$		$m_t, m_H \rightarrow 0$ limit	[19]	

- | | | |
|---|--|---|
| [1] [Abreu, Febres Cordero, Ita, Page, VS '21] | [7] [Badger, Brønnum-Hansen, Chicherin, Gehrmann, Hartanto, Henn, Marcoli, Moodie, Peraro, Zoia '21] | [13] [Badger, Gehrmann, Marcoli, Moodie '21] |
| [2] [Agarwal, Buccioni, von Manteuffel, Tancredi '21] | [8] [Czakon, Mitov, Poncelet '21] | [14] [Abreu, de Laurentis, Ita, Klinkert, Page, VS '23] |
| [3] [Chawdry, Czakon, Mitov, Poncelet '21] | [9] [Chen, Gehrmann, Glover, Huss, Marcoli '21] | [15] [Badger, Czakon, Hartanto, Moodie, Peraro, Poncelet, Zoia '23] |
| [4] [Abreu, Page, Pascual, VS '20] | [10] [Chawdry, Czakon, Mitov, Poncelet '21] | [16] [de Laurentis, Ita, Klinkert, VS '23] |
| [5] [Chawdry, Czakon, Mitov, Poncelet '20] | [11] [Chawdry, Czakon, Mitov, Poncelet '19] | [17] [de Laurentis, Ita, VS '23] |
| [6] [Agarwal, Buccioni, von Manteuffel, Tancredi '21] | [12] [Kallweit, VS, Wiesemann '20] | [18] [Agarwal, Buccioni, Devoto, Gambuti, von Manteuffel, Tancredi '23] |
| | | [19] [Wang, Xia, Yang, Ye '24] |

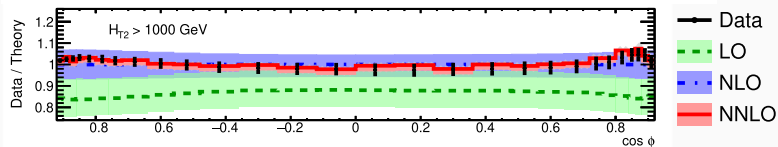
Evaluation of Feynman integrals: pentagon functions [Chicherin, VS '20]

Application in α_s measurement

Determination of the strong coupling constant from transverse energy—energy correlations in multijet events at $\sqrt{s} = 13$ TeV with the ATLAS detector

ATLAS Collaboration • Georges Aad (Marseille, CPPM) [Show All\(2916\)](#) (see also [Alvarez, Cantero, Czakon, Lorente, Mitov, Poncelet '23])

Jan 23, 2023



- Remarkable agreement between NNLO and data
- α_s measured at record scales
- Milestone for pQCD tool development

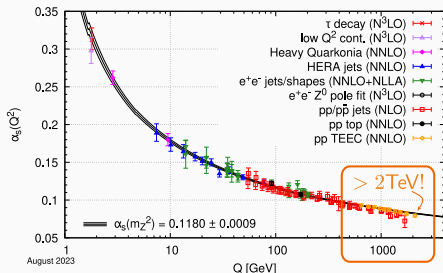
STRIPPER

[Czakon '11] [Czakon, Heymes '14]

Two-loop corrections

[Abreu, Febres Cordero, Ita, Page, VS '21]

[Chicherin, VS '20]



To be published in PDG 2024 review [arXiv:2312.14015]

Two-loop five-point amplitudes: one external mass

	Comment	Complete analytic results	Public code	Cross sections
$pp \rightarrow W b \bar{b}$	l.c.* , on-shell W	[1]		
$pp \rightarrow W(l\nu) b \bar{b}$	l.c., $m_b = 0$	[2, 3]	[10]	[3, 4, 7]
$pp \rightarrow W(l\nu) t \bar{t}$	l.c., $m_t = 0$	[2, 3]	[10]	[8]
$pp \rightarrow Z(l l) b \bar{b}$	l.c.* , $m_b = 0$	[2]	[10]	[9]
$pp \rightarrow W(l\nu) j j$	l.c.	[2]	[10]	
$pp \rightarrow Z(\bar{l} \bar{l}) j j$	l.c.*	[2]	[10]	
$pp \rightarrow W(l\nu) \gamma j$	l.c.*	[5]		
$pp \rightarrow H b \bar{b}$	l.c., $m_b = 0$	[6]		[Christian's talk]

[1] [Badger, Hartanto, Zoia '21]

[2] [Abreu, Febres Cordero, Ita, Klinkert, Page, VS '21]

[3] [Hartanto, Poncelet, Popescu, Zoia '22]

[4] [Hartanto, Poncelet, Popescu, Zoia '22]

[5] [Badger, Hartanto, Kryś, Zoia '22]

[6] [Badger, Hartanto, Kryś, Zoia '21]

[7] [Buonocore, Devoto, Grazzini, Kallweit, Mazzitelli, Rottoli, Savoini '22]

[8] [Buonocore, Devoto, Grazzini, Kallweit, Mazzitelli, Rottoli, Savoini '23]

[9] [Mazzitelli, VS, Wiesemann '24]

[10] [de Laurentis, Ita, Page, VS in preparation]

Evaluation of Feynman integrals: pentagon functions

[Chicherin, VS, Zoia '21] [Abreu, Chicherin, Ita, Page, VS, Tschernow, Zoia '23]

Two-loop five-point amplitudes: beyond one external mass

Comment

Complete
analytic results

Public code

Cross sections



[Image by DALL-E]

→ [Samuel's talk]

Two-loop five-point scattering: first results with masses in loops

No complete amplitudes or integral families known

Integrals

- Analytic study of integral families for $pp \rightarrow t\bar{t}j$ (l.c.)
[Badger, Becchetti, Chaubey, Marzucca '23] [Badger, Becchetti, Giraud, Zoia '24]
- Analytic study of integrals for $pp \rightarrow t\bar{t}H$ contribution with a light quark loop in l.c.
[Febres Cordero, Figueiredo, Kraus, Page, Reina '23]
- Numerical evaluation on a few points possible with AMFlow approach [Liu, Ma '21,'22]

Amplitudes

- Numerical evaluation of light and heavy quark loop contributions to $q\bar{q} \rightarrow t\bar{t}H$
[Agarwal, Heinrich, Jones, Kerner, Klein, Lang, Magerya, Olsson '24]

Warning: two-loop “mass-in-the-loop” frontier

⚠ With **massive particles in loops** analytic (mathematical) complexity may escalate abruptly and dramatically!

Underlying reason: integrals associated with nontrivial algebraic curves and surfaces (e.g. elliptic curves)

Example: $pp \rightarrow t\bar{t}$

- ✓ analytic results for $q\bar{q} \rightarrow t\bar{t}$ with top loops [Mandal, Mastrolia, Ronca, Bobadilla '22], evaluation “easy”
- ⚠ analytic results for $g\bar{g} \rightarrow t\bar{t}$ with top loops [Adams, Chaubey, Weinzierl '17,'18] [Badger, Chaubey, Hartanto, Marzucca '21], but **unclear how to evaluate efficiently** due to the presence of elliptic curves

But

- Cross sections computed with **numerical methods and interpolation grids** since long time ago [Czakon '08] [Bärnreuther, Czakon, Fiedler '13]
- Recent example: NLO corrections for $gg \rightarrow ZZ$ [Agarwal, Jones, Kerner, von Manteuffel '24]

Not discussed in this talk \rightarrow [Andreas's talk]

Dynamic scales

- Mandelstam invariants s_{ij} , off-shell legs p_i^2
- Monte Carlo integrals over phase space
$$\int d\Phi_n(s_{ij}, p_i^2) |\mathcal{A}_{2 \rightarrow n}(s_{ij}, p_i^2)|^2$$
- Need fast and robust numerical evaluation of $\mathcal{A}_{2 \rightarrow n}$ over phase space

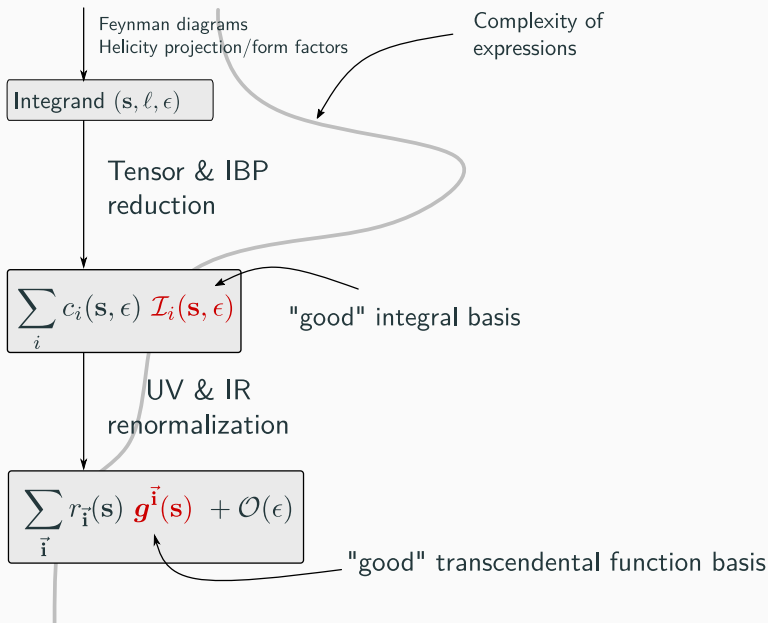
Fixed scales

- Particle (complex) masses, e.g. m_t, m_W
- Mathematical complexity can escalate very quickly
- With few dynamic scales can profit the most from numerical methods \oplus interpolation grids

In the following I mainly highlight dealing with many **dynamic scales**.

Analytic methods: selected highlights

Analytic multi-loop amplitude calculations



What is a “good” transcendental functions basis?

Analytic properties

- No hidden identities (basis)
- Analytic cancellation of UV and IR divergences (minimize regularization artifacts)
- Control over physics properties (amplitudeology friendly)
- Compact rational coefficients

Numerical evaluation

- Over whole physical phase space
- Fast (Monte-Carlo integration over large phase space)
- Stable

Analytic methods: selected highlights

Feynman integrals

Pure integrals and canonical differential equations

Pure Feynman integrals

[Henn '13]

$$d\vec{g} = \epsilon A \vec{g}$$

$$A = \sum_i d \log W_i(\mathbf{s}) A_i$$

Letters of symbol alphabet

Encode singularity structure
and branch cuts

Rational matrix

Pure integrals and canonical differential equations

Pure Feynman integrals

[Henn '13]

$$\begin{aligned} d\vec{g} &= \epsilon A \vec{g} \\ A &= \sum_i d \log W_i(\mathbf{s}) A_i \end{aligned}$$

Rational matrix

Letters of symbol alphabet

Encode singularity structure and branch cuts

⚠ Canonical DE very challenging to obtain for multi-scale integrals

Cutting edge examples:

# scales	# massive lines	Reference
6	0	[Abreu, Chicherin, Ita, Page, VS, Tschernow, Zoia '23]
7	0	[Jiang, Liu, Xu, Lin Yang '24] [Samuel's talk]
8	0	[Henn, Peraro, Xu, Zhang '21] [Henn, Matijašić, Miczajka, Peraro, Xu, Zhang '24]
6	≤ 1	[Badger, Becchetti, Chaubey, Marzucca '22]
6	≤ 2	[Badger, Becchetti, Giraudo, Zoia '24]
7	≤ 2	[Febres Cordero, Figueiredo, Kraus, Page, Reina '23]

beyond d log forms!

How to solve DE?

Pure Feynman
integrals



Canonical DE

$$d\vec{g} = \epsilon A \vec{g}$$
$$A = \sum_i d \log W_i(\mathbf{s}) A_i$$

How to solve DE?

Pure Feynman integrals

Canonical DE

$$d\vec{g} = \epsilon A \vec{g}$$
$$A = \sum_i d \log W_i(\mathbf{s}) A_i$$

Square roots

Multiple Polylogarithms
(MPLs, GPLs)



Map may **not** exist [Duhr, Brown '20]

Sometimes still possible

[Heller, von Manteuffel, Schabinger '19][Heller '21]

[Bonetti, Panzer, Smirnov, Tancredi '20]

[Kreer, Weinzierl '21][Duhr, Smirnov, Tancredi '21]

[Papadopoulos, Tommasini, Wever '15][Papadopoulos '14]

[Canko, Papadopoulos, Syrrakos '20]



but “good” representation
even more challenging

How to solve DE?

Pure Feynman integrals

Canonical DE

$$d\vec{g} = \epsilon A \vec{g}$$
$$A = \sum_i d \log W_i(\mathbf{s}) A_i$$

Semi-numerical DE solution
(local power-log series
expansions along a path)

DiffExp [Moriello '19] [Hidding '20]
AMFlow [Liu, Ma, Wang '17] [Liu, Ma '21]
SeaSyde [Armadillo, Bonciani, Devoto, Rana, Vicini '22]
[Hidding, Usovitsch '22]

- ✓ universal and easy to set up
- ✓ canonical DE not required
- ⚠ evaluation of integrals (no function basis)
 - hidden cancellations
 - prohibitive run times
 - stability over phase space?

Pentagon functions construction

[Abreu, Chicherin, Ita, Page, VS, Tschernow, Zoia '23]
(see also [Chicherin, VS '20] [Badger, Hartanto, Zoia '21] [Chicherin, VS, Zoia '21])

Pure Feynman
integrals

Canonical DE

$$d\vec{g} = \epsilon A \vec{g}$$
$$A = \sum_i d \log W_i(\mathbf{s}) A_i$$

weight = length = ϵ order

Chen iterated integrals [Chen '77]



$$\int_0^1 d \log W_n(t_n) \dots \int_0^{t_2} d \log W_1(t_1)$$

"Good" basis of functions

Use properties of iterated integrals
and simple linear algebra

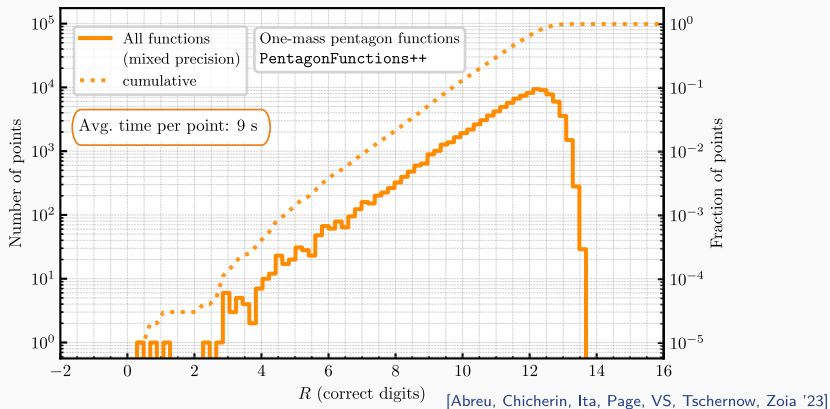
- ✓ complete
- ✓ non-redundant

Initial conditions
(AMFlow)

Efficient numerical evaluation

Control over analytic properties
 \implies optimized one-fold
integral representations

Example: one-mass pentagon functions



- Complete basis of two-loop transcendental functions for NNLO corrections for V_{jj}, H_{jj} , etc.
- Timing to evaluate all 1291 functions on one CPU
- Excellent numerical performance

The only viable method for $2 \rightarrow 3$ phenomenology so far!

Consider triphoton hadroproduction in NNLO QCD (l.c.)

[Chawdry, Czakon, Mitov, Poncelet '19]

using earlier incarnation of (planar) pentagon functions [Gehrmann, Henn, Lo Presti '18]

- Rationalized kinematics required due to precision loss
- Average time 17 minutes to typically get 2 digits
- Need interpolation grids (very challenging for many dynamic scales)

Consider triphoton hadroproduction in NNLO QCD (l.c.)

[Chawdry, Czakon, Mitov, Poncelet '19]

using earlier incarnation of (planar) pentagon functions [Gehrmann, Henn, Lo Presti '18]

- Rationalized kinematics required due to precision loss
- Average time 17 minutes to typically get 2 digits
- Need interpolation grids (very challenging for many dynamic scales)

[Abreu, Page, Pascual, VS '20]

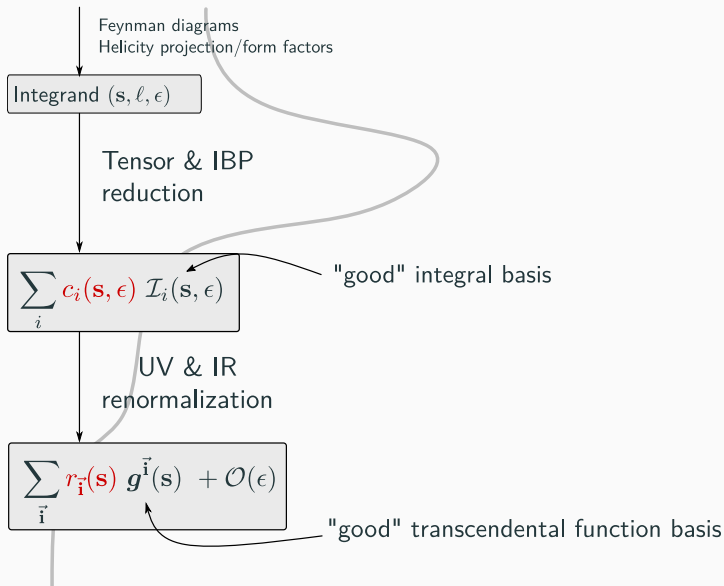
using “good” function basis [Chicherin, VS '20]

- Double precision sufficient
- 1 second to typically get 11 digits
- Same efficiency for full color !
[Abreu, de Laurentis, Ita, Klinkert, Page, VS '23]

Analytic methods: selected highlights

Rational coefficients

Rational coefficients



Main lesson

Rational coefficients $r_{\vec{i}}$ simple (given a good $g^{\vec{i}}$ function basis).

- Bypass intermediate expression swell by **exact numerical evaluations** over \mathbb{F}_p :
 $p < \text{machine integer} \implies$ **efficient**
- Reconstruct analytic expressions from numeric samples [von Manteuffel, Schabinger '14] [Peraro '16]
- Important bonus: **enables parallelization**

Analytics from (exact) numerics

Main lesson

Rational coefficients $r_{\vec{i}}$ simple (given a good $g^{\vec{i}}$ function basis).

- Bypass intermediate expression swell by **exact numerical evaluations** over \mathbb{F}_p :
 $p < \text{machine integer} \implies$ **efficient**
- Reconstruct analytic expressions from numeric samples [von Manteuffel, Schabinger '14] [Peraro '16]
- Important bonus: **enables parallelization**

Most powerful when applied to physical quantities (reconstruct finite remainders)



Caravel

[Abreu, Dormans, Febres Cordero,
Ita, Kraus, Page, Pascual, Ruf, VS '20]

FiniteFlow

[Peraro '19]

Less powerful, but also useful for IBP reduction only (reconstruct integral reduction rules)

LiteRed+FiniteFlow,
Kira+FireFly, FIRE6

numerous private codes
(e.g. Finred by A. von Manteuffel)

Remarks on integration-by-parts reduction

- Problem **conceptually solved** by Laporta's algorithm
- In practice, IBP equation systems remain **major bottleneck** in loop calculations
- No major breakthroughs, but **process specific optimizations** make the difference

Multiscale problems @ 2 loops

- Situation majorly improved by (exact) numerical frameworks
- Solving systems over \mathbb{F}_p (setting s, ϵ to integers) typically straightforward
- Eventually number of samples for reconstruction becomes the issue

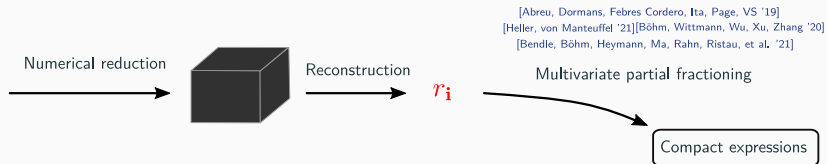
General observation

Avoiding generating identities that introduce auxiliary integrals (e.g. higher denominator powers [Gluz, Kadja, Kosower '11]) typically helpful.

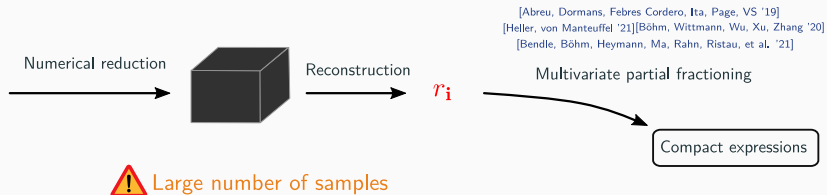
Public proof-of-principle implementation: NeatIBP [Wu, Boehm, Ma, Xu, Zhang '23].

Note: lots of experimentation and ideas in the literature not discussed here! [Andreas's talk]

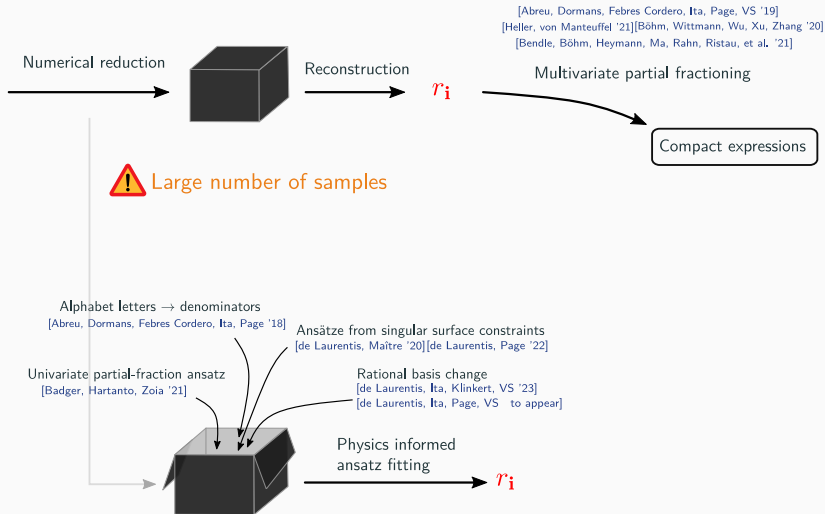
Analytics from numerics workflow



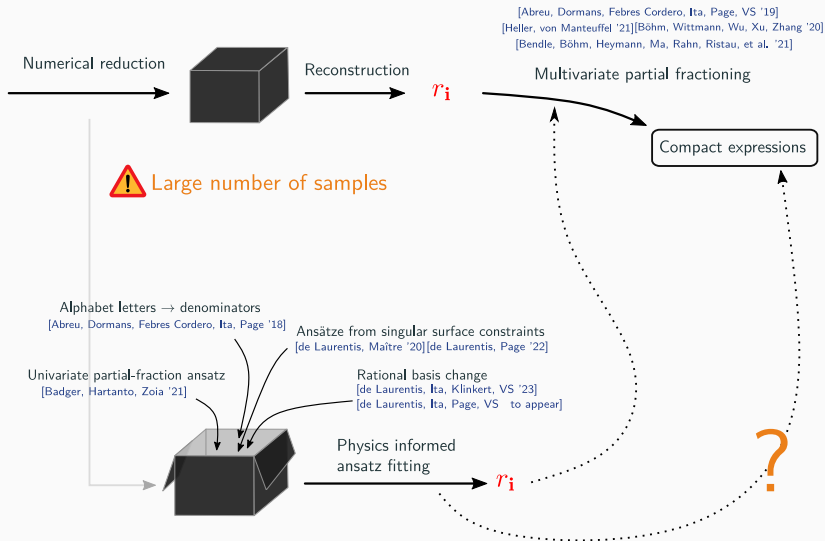
Analytics from numerics workflow



Analytics from numerics workflow



Analytics from numerics workflow



Rational basis change

[Abreu, Dormans, Febres Cordero, Ita, Page '18]

[de Laurentis, Ita, Klinkert, VS '23]

[de Laurentis, Ita, Page, VS to appear]

$$\sum_i r_i g_i \longrightarrow \sum_i r_i M_{ij} g_j \xrightarrow{\text{rational matrix}} \sum_i r'_i M'_{ij} g_j$$

$$r'_i = Q_{ij} r_j, \quad M'_{ij} = (Q^{-1})_{ik} M_{kj}$$

r_i generally has **spurious denominators**, which amplitudes not allowed to have

- exponent too high, e.g. $1/s_{23}^3$
- unphysical pole, e.g. $1/(s_{12} - s_{14})$

Idea: find transformations Q_{ij} to maximally cancel spurious denominators

- Can be done **before** full analytic reconstruction \Rightarrow **reduced number of samples**
- Positive impact on numerical stability expected

Example 1

Three-jet production (full color) [de Laurentis, Ita, Klinkert, VS '23].

(see also [Agarwal, Buccioni, Devoto, Gambuti, von Manteuffel, Tancredi '23]).

Numerical samples generated by CARAVEL.

- Reduction from 250k to 15k samples (reconstruct the latter)
- Rational basis (after additional massaging) printed in the paper, 4 pages

Example 2

Analytic results for Vjj production from [Abreu, Febres Cordero, Ita, Klinkert, Page, VS '21]

- Reconstructed analytic form that is hard to use (large numerical cancellations, large memory footprint)
- Multivariate partial fractioning fails due to complicated Gröbner basis
- With basis change 1.2Gb \rightarrow 25Mb [de Laurentis, Ita, Page, VS to appear]

Numerical methods

Mixed analytic-numerical

Light and heavy quark loop contributions to $q\bar{q} \rightarrow t\bar{t}H$

[Agarwal, Heinrich, Jones, Kerner, Klein, Lang, Magerya, Olsson '24]

(see also similar approach to Wjj production [Hartanto, Badger, Brønnum-Hansen, Peraro '19])

Amplitude reduction

- Numerical with rationalized kinematics, highly optimized systems of IBP equations.
- Impressive performance: **2 minutes on one CPU**.

Evaluation of integrals

- Basis optimized for sector decomposition (quasi-finite integrals [Andreas's talk]).
- Large numerical cancellations handled by Quasi-Monte-Carlo sampling (pySecDec).
- 5 minutes on a modern GPU.

Questions

- Scaling to more complex integrands (complete amplitudes)?
- Do high-dimensional interpolation grids work?
- Two-loop corrections expected small [Catani, Devoto, Grazzini, Kallweit, Mazzitelli, Savoini '22]
→ how many evaluations to validate approximations?

Idea

- **Universal IR structure** of **color-singlet** production
 \implies locally finite integrands (before loop integration).
 $q\bar{q} \rightarrow F$ [Anastasiou, Sterman, Venkata '22]
 $gg \rightarrow F$ [Anastasiou, Karlen, Sterman, Venkata '24]
- Simultaneous Monte-Carlo integration over **loops** and **phase-space**.
- No IBP reduction, no dedicated computations of Feynman integrals.

- E.g. applicable to $pp \rightarrow VVV$, which is challenging with current analytic methods.
- Proof-of-principle computation: closed-quark contributions for $q\bar{q} \rightarrow \gamma\gamma\gamma$
 [Matilde Vicini's talk @ Loops&Legs 2024]

Questions

- Scaling to more complex integrands (complete amplitudes)?
- Minkowski (or threshold) singularities?
- Easy to adapt standard cross section frameworks?

Conclusions & Outlook

Analytic

- ✓ Map to MPLs for $2 \rightarrow 2$, when possible.
- ✓ For $2 \rightarrow 3$ “pentagon functions” method, when possible.
- ⚠ **Biggest issue:** general class of functions not understood, even mathematically.
Pentagon functions beyond d logs?

(Semi-)numerical

Solving DEs by matching local series expansions, or numerical Monte-Carlo integration of optimized bases.

- ✓ Successfully sidestep analytic complexity with **few dynamic scales**.
- ✓ Less sensitive to analytic complexity, masses may actually help in practice.
- ✗ No function basis \implies analytic rational coefficients hard, large numerical cancellations
- ⚠ Too slow for many **dynamic scales**?

NNLO ~~r~~evolution

- Steady progress for $2 \rightarrow 3$ processes:
all massless complete, first result with external masses.
- Significant progress due to paradigm shift from symbolic computations to analytic reconstruction.
- Good grasp on analytic structure of Feynman integrals and associated function spaces has been essential.
- Multi-scale loop amplitudes remain major bottleneck, case by case computations.

NNLO ~~r~~evolution

- Steady progress for $2 \rightarrow 3$ processes:
all massless complete, first result with external masses.
- Significant progress due to paradigm shift from symbolic computations to analytic reconstruction.
- Good grasp on analytic structure of Feynman integrals and associated function spaces has been essential.
- Multi-scale loop amplitudes remain major bottleneck, case by case computations.

Outlook

- 5-point with massless loops (e.g. Hjj, VVj, VVV): feasible based on current methods.
- N^3 LO applications more challenging, potentially better analytic control will be needed.
- Massive loops, few dynamic scales: feasible with (semi-)numerical methods.
- Massive loops, many dynamic scales (e.g. $t\bar{t}j, t\bar{t}H, t\bar{t}W$):
requires major breakthroughs.
- Beyond 5-point: currently unimaginable (any relevant processes?).

Acknowledgments

This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme grant agreement 101019620 (ERC Advanced Grant TOPUP).



European Research Council

Established by the European Commission