Modern calculation techniques for multi-scale loop amplitudes

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Precision calculations for future e^+e^- colliders: targets and tools,
CERN

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Outline

1. Introduction

2. Loops & legs: state of the art

3. Recent developments on the multi-scale frontier

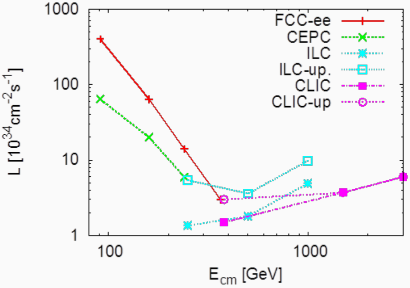
4. Towards $e^+e^- \to 4j$ @ NNLO QCD

5. Discussion

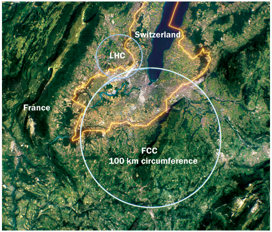
Introduction

Precision at future e^+e^- colliders

[1910.11775]



- Measure EW & Higgs observables, α_s to unprecedented precision
- Discovery via precision: search anomalous deviations from SM
- Sub-percent uncertainties
- Theoretical input crucial



Fixed order partonic cross sections

Collinear factorization:

$$d\sigma(p_1, p_2) = \int \mathrm{d}x_1\, \mathrm{d}x_2\, f_{e^+}(x_1, \mu, m) f_{e^-}(x_2, \mu, m)\, \mathrm{d}\hat{\sigma}(x_1 p_1, x_2 p_2, \mu) \quad \oplus \text{ QED/QCD PS}$$

Intrinsic uncertainty

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

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

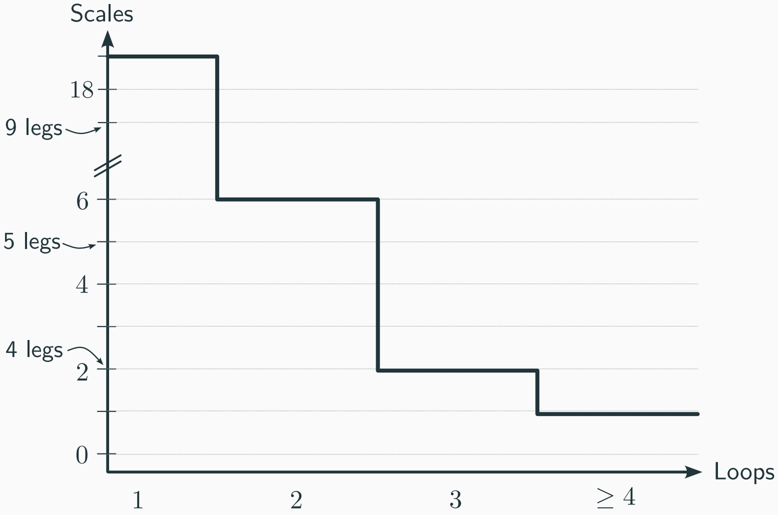
$$\int_{\Phi_{F+2}} \mathrm{d}\sigma_{\mathsf{RR}} + \int_{\Phi_{F+1}} \mathrm{d}\sigma_{\mathsf{RV}} + \int_{\Phi_F} \mathrm{d}\sigma_{\mathsf{VV}}$$

IR divergences

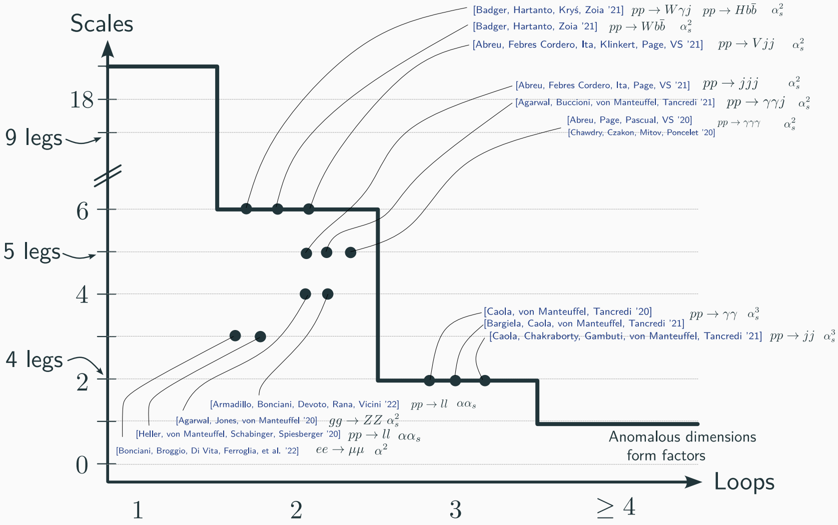
Multi-loop amplitudes

Loops & legs: state of the art

Loops&legs: state of the art

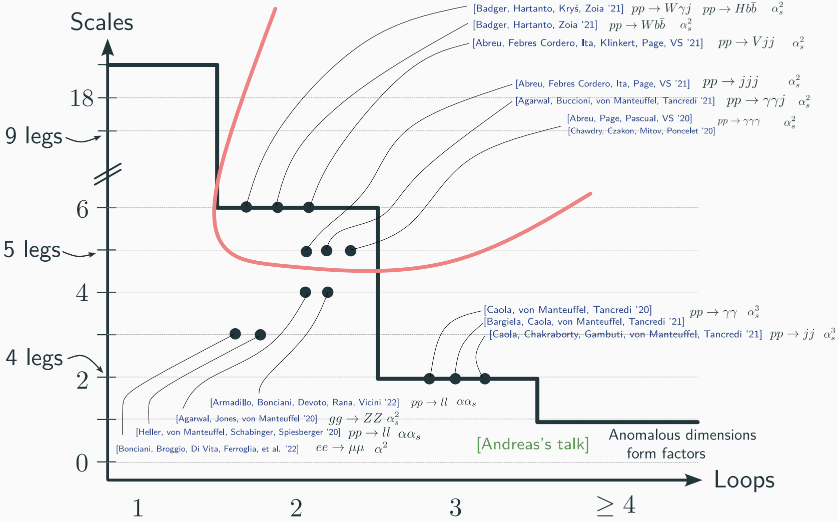


Loops&legs: state of the art



Warning: a biased selection of references!

Loops&legs: state of the art



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Dynamic and fixed scales

Dynamic scales

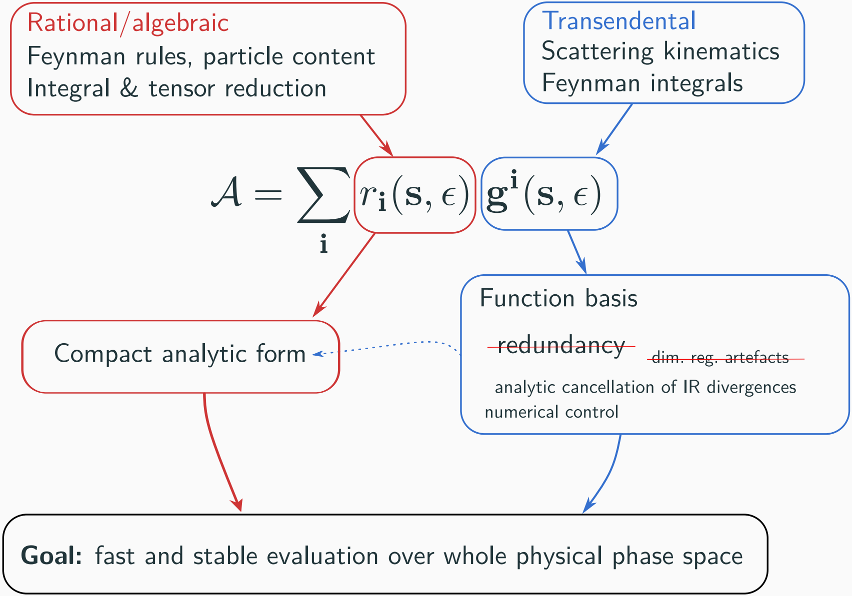
- Mandelstam invariants s_{ij}, off-shell legs p_i^2
- Monte Carlo integrals over phase space $\int \mathrm{d}\Phi_n\,(s_{ij}, p_i^2)\big|\mathcal{A}_{2\to n}(s_{ij}, p_i^2)\big|^2$
- Need fast and robust numerical evaluation of $\mathcal{A}_{2\to n}$ over phase space

Fixed scales

- Particle (complex) masses, e.g. m_t, m_W
- Mathematical complexity can escalate very quickly [see Stefan's talk]
- With few dynamic scales can profit the most from numerical methods [see talks by Vitalii, Janusz, Martijn, Xiao]

Recent developments on the multi-scale frontier

Structure of analytic loop amplitudes



Recent developments on the multi-scale frontier

Transcendental part

Feynman integrals: the canonical way

Feynman integrals

Initial conditions
physics, limits, PSLQ

Canonical DE [Henn '13]

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

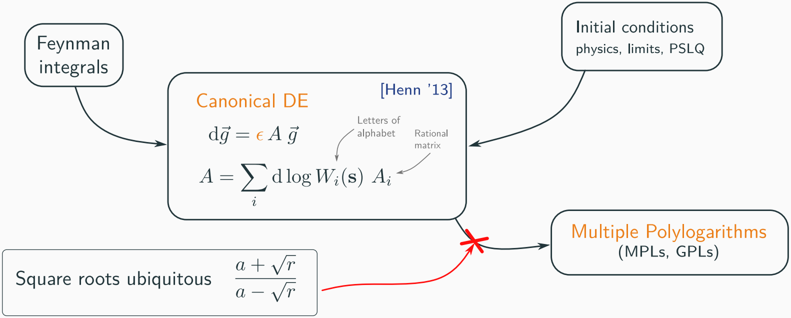
$$A = \sum_i \mathrm{d}\log W_i(\mathbf{s})\; A_i$$

Letters of alphabet

Rational matrix

Multiple Polylogarithms
(MPLs, GPLs)

Feynman integrals: the canonical way



Feynman integrals: the canonical way

Feynman integrals

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Multiple Polylogarithms
(MPLs, GPLs)

Square roots ubiquitous $\dfrac{a+\sqrt{r}}{a-\sqrt{r}}$

Workarounds

Ansatz fitting, parametric integration
[Heller, von Manteuffel, Schabinger '19][Heller '21]
[Bonetti, Panzer, Smirnov, Tancredi '20]
[Kreer, Weinzierl '21][Duhr, Smirnov, Tancredi '21]

Simplified DE
[Papadopoulos, Tommasini, Wever '15] [Papadopoulos '14]
[Canko, Papadopoulos, Syrrakos '20]

⚠ Finding good representation in physical regions very difficult

[Papadopoulos, Tommasini, Wever '15] [Gehrmann, Henn, Lo Presti '18]
[Canko, Papadopoulos, Syrrakos '20] [Duhr, Smirnov, Tancredi '21]

- proliferation of spurious branch cuts
- analytic continuation
- explosion of number of MPLs

Special function basis construction

[Chicherin, VS, Zoia '21] (see also [Chicherin, VS '20] [Badger, Hartanto, Zoia '21])

Feynman integrals

Canonical DE

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

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

Initial conditions
physics, limits, PSLQ

Special function basis construction

[Chicherin, VS, Zoia '21] (see also [Chicherin, VS '20] [Badger, Hartanto, Zoia '21])

Feynman integrals

Initial conditions
physics, limits, PSLQ

Canonical DE

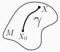
$$\mathrm{d}\vec{g} = \epsilon\, A\, \vec{g}$$

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

weight = length = ϵ order

Chen iterated integrals [Chen '77]

$$[W_1, \ldots, W_n]_\gamma =$$



$$\int_0^1 \mathrm{d}\log W_n(t_n)\ \ldots\ \int_0^{t_2} \mathrm{d}\log W_n(t_1)$$

Vector subspace, weight-graded

$$\mathbf{G} = \bigoplus_w \mathbf{G}^{(w)}$$

+ shuffle product

$$\mathbf{G}^{w_1} \times \mathbf{G}^{(w_2)} \mapsto \mathbf{G}^{(w_1+w_2)}$$

$$[W_1, \ldots, W_r]_\gamma [W_{r+1}, \ldots, W_n]_\gamma = \sum_{\mathbf{i} \in \text{shuffles}} [W_{i_1}, \ldots, W_{i_n}]_\gamma$$

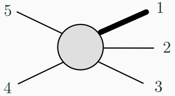
Basis in $\mathbf{G}^{(w)}$ mod products

- ✓ complete
- ✓ non-redundant
- ✓ amplitudeology friendly

Example: two-loop five-point one-mass integrals

One-mass kinematics

e.g. $pp \to Vjj$, $e^+e^- \to 4j$

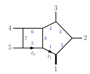


$p_1^2,\ s_{12},\ s_{23},\ s_{34},\ s_{45},\ s_{15}$

Example: two-loop five-point one-mass integrals

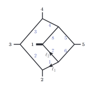
Canonical DE

Planar



[Abreu, Ita, Moriello, Page, Tschernow, Zeng '20]

Hexa-box



[Abreu, Ita, Page, Tschernow '21]

GPL results

[Papadopoulos, Tommasini, Wever '15]
[Canko, Papadopoulos, Syrrakos '20] [Syrrakos '20]
[Kardos, Papadopoulos, Smirnov, Syrrakos, Wever '22]

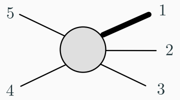
Function basis (planar)

[Badger, Hartanto, Zoia '21] color-ordered, numerical evaluation

[Chicherin, VS, Zoia '21]

One-mass kinematics

e.g. $pp \to Vjj$, $e^+e^- \to 4j$



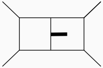
$p_1^2, \; s_{12}, \; s_{23}, \; s_{34}, \; s_{45}, \; s_{15}$

Semi-numerical DE solution

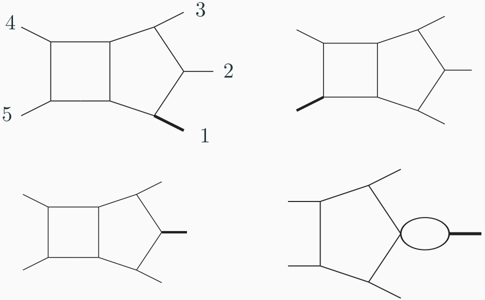
`DiffExp` [Moriello '19] [Hidding '20]
`AMFLow` [Liu, Ma, Wang '17] [Liu, Ma '21]

Initial values, validation, small scale sampling

Missing:
W.I.P.



Example: planar function basis



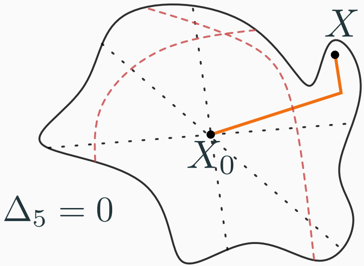
$+ 24$ permutations $\{p_2, p_3, p_4, p_5\}$

1417 master integrals →

Weight	# functions
1	11
2	25
3	145
4	675

Weights 1 and 2

Well-defined combinations of $\log$, Li_2 functions



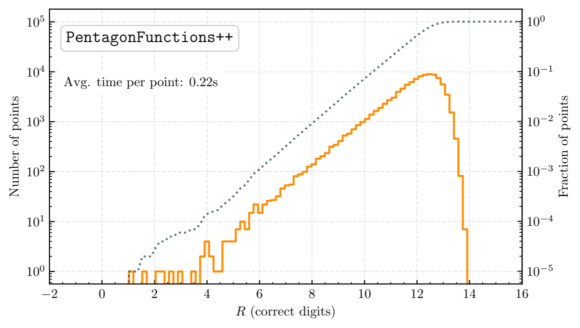
Weights 3 and 4

- Numerical one-fold integration [Caron-Huot, Henn '14] of analytic integrands
  $\Longrightarrow$ exponential convergence [Takahasi, Mori '73]
- No crossing of physical thresholds $\Longrightarrow$ no analytic continuation needed
- Dedicated series expansions around spurious singularities

Numerical performance

All functions: any one mass planar five-point amplitude in all "crossings"

Sample over physical phase space



(vs. quad precision targets) [Chicherin, VS, Zoia '21]

Available as a C++ library `PentagonFunctions++`

`https://gitlab.com/pentagon-functions/PentagonFunctions-cpp`

(also `Mathematica` interface)

So far the only method to get to $2 \to 3$ cross sections!

[Czakon, Mitov, Poncelet '21] [Chen, Gehrmann, Glover, Huss, Marcoli '21] [Chawdry, Czakon, Mitov, Poncelet '21] [Kallweit, VS, Wiesemann '20] [Badger, Gehrmann, Marcoli, Moodie '21] [Hartanto, Poncelet, Popescu, Zoia '22]

Recent developments on the multi-scale frontier

Rational coefficients

Rational coefficients: algebraic complexity

Integrand $\sum_i \frac{m_i(\mathbf{s},\epsilon;\,\ell)}{\prod_j \rho_{i,j}}$

Tensor & IBP reduction

$\sum_i c_i(\mathbf{s},\epsilon)\;\mathcal{I}_i$ ← pure MIs

UV & IR renormalization

$\sum_{\vec{\mathbf{i}}} r_{\vec{\mathbf{i}}}(\mathbf{s})\;\boldsymbol{g}^{\vec{\mathbf{i}}}(\mathrm{s}) \;+\mathcal{O}(\epsilon)$ ← functions basis

Key bottleneck
intermediate expression swell

Central lesson

- Coefficients $r_{\vec{\mathbf{i}}}$ simple
- Bypass complexity with exact numerics (finite fields)
- Reconstruct analytic form from numerical samples

[von Manteuffel, Schabinger '14] [Peraro '16]

FiniteFlow [Peraro '19]
[Badger, Brønnum-Hansen, Hartanto, Peraro '18]
[Badger, Chicherin, Gehrmann, Heinrich, Henn, Peraro, Wasser, Zhang, Zoia '19]

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

Kira+FireFly [Klappert, Lange, Maierhöfer, Usovitsch '20]
FIRE6 [Smirnov, Chukharev '19]

Better construction of IBP identities

[Gluza, Kadja, Kosower '11] [Ita '15] [Larsen, Zhang '15]
[Georgoudis, Larsen, Zhang '16] [Böhm, Georgoudis, Larsen, Schulze, Zhang '17]
[Agarwal, Jones, von Manteuffel '20] [Guan, Liu, Ma '19]

Numerical unitarity: universal ansatz

Build ansatz for integrand of full amplitude:

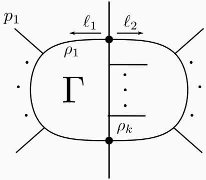
$$\mathcal{A}(\ell_l) = \sum_{\Gamma} \sum_{i \in M_\Gamma \cup S_\Gamma} c_{\Gamma,i} \frac{m_{\Gamma,i}(\ell_l)}{\prod_j \rho_{\Gamma,j}}$$

Master terms

coefficients of master integrals

Surface terms

vanish upon loop integration



Generalization of one-loop unitarity methods:

[Bern, Dixon, Kosower, Dunbar '94, '95] [Britto, Feng, Cachazo '05] [Ossola, Papadopoulos, Pittau '07] [Ellis, Giele, Kunszt '08] [Giele, Kunszt, Melnikov '08]

Related work

[Badger, Frellesvig, Zhang '12] [Zhang '12] [Mastrolia, Mirabella, Ossola, Peraro '13] [Ita '15] [Mastrolia, Peraro, Primo '16] [Abreu, Febres Cordero, Ita, Jaquier, Page, Zeng '17]

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Master terms
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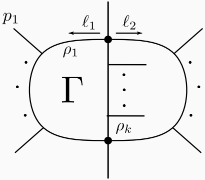


Surface terms produced from unitarity-compatible IBPs [Gluza, Kadja, Kosower '11]:

$$\int \left(\prod_l \mathrm{d}^D \ell_l \right) \sum_l \frac{\partial}{\partial \ell_l^\nu} \left(\frac{u_l^\nu \; m(\ell_l)}{\prod_{j \in P_\Gamma} \rho_j} \right) = 0, \qquad u_l^\nu \frac{\partial}{\partial \ell_l^\nu} \rho_j = f_j \rho_j$$

Generating vectors u_l^ν from computational algebraic geometry (e.g. with `Singular`) [Ita '15] [Larsen, Zhang '15] [Georgoudis, Larsen, Zhang '16] [Abreu, Febres Cordero, Ita, Page, Zeng '17] [Böhm, Georgoudis, Larsen, Schulze, Zhang '17]

- Targeted set of identities for each Γ
- Eliminate linear dependencies with on-shell conditions $\rho_j = 0, \; j \in P_\Gamma$ imposed
- No need to invert IBP systems at this stage

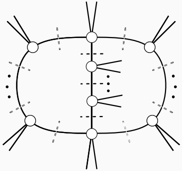
Numerical unitarity: cut equations

Obtain coefficients $c_{\Gamma,i}$ from linear systems of cut equations:

$$\lim_{\ell_l \to \ell_l^\Gamma} \left(\mathcal{A}(\ell_l) \prod_j \rho_j \right) = \sum_i c_{\Gamma,i}\, m_{\Gamma,i} \quad + \quad \text{topologies with more propagators (from previous steps)}$$

on-shell limit for Γ

|| Unitarity $\to$ factorization into product of trees



Solve cut equations numerically

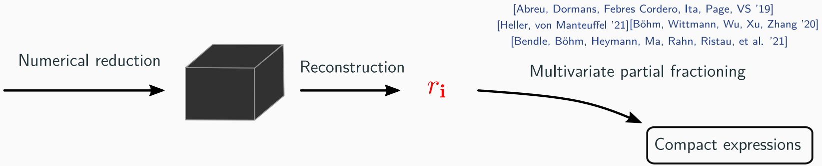
- ✓ analytic integrand or individual Feynman diagrams not needed
- ✓ numerical IBP reduction included
- ✓ suitable for floating point and finite fields

Implemented in C++ library CARAVEL

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

Caravel

Analytic results from finite-field evaluations



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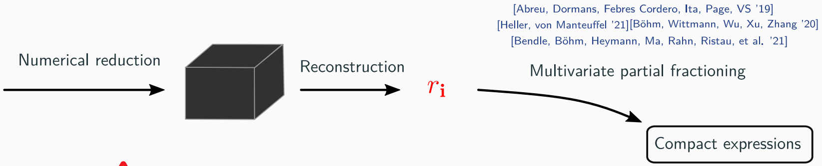
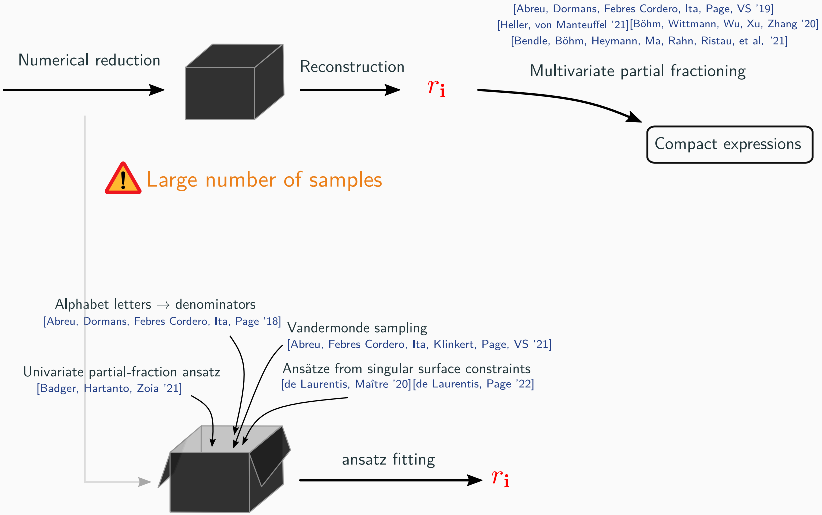


Large number of samples

Analytic results from finite-field evaluations



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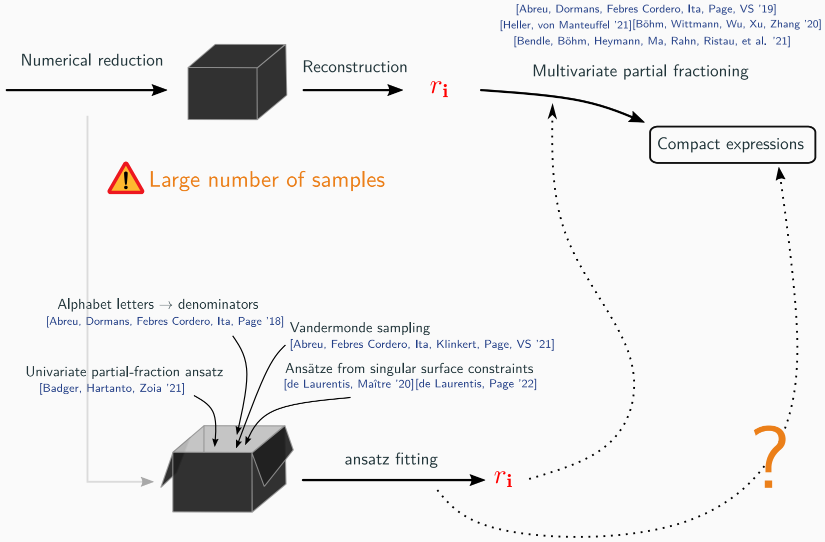
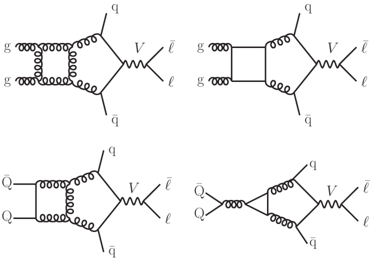


Towards $e^+e^- \to 4j$ @ NNLO QCD

Two-loop amplitudes for Vjj production at hadron colliders

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

$$pp \to Vjj, \quad V = W, Z/\gamma^*$$
$$\hookrightarrow \ell\bar{\ell}$$



Helicity amplitudes

$$\mathcal{M}\left(\bar{q}^+_{p_1}, \mathrm{g}^{h_2}_{p_2}, \mathrm{g}^{h_3}_{p_3}, q^-_{p_4}; \bar{\ell}^+_{p_5}, \ell^-_{p_6}\right)$$

$$\mathcal{M}\left(\bar{q}^+_{p_1}, Q^h_{p_2}, \bar{Q}^{-h}_{p_3}, q^-_{p_4}; \bar{\ell}^+_{p_5}, \ell^-_{p_6}\right)$$

- $N_c \to \infty$, $N_f \sim N_c$, 5FNS, no top loops

$$\mathcal{M}_\kappa = \mathcal{M}^{(0)}_\kappa \left(1 + \frac{\alpha_s}{2\pi}\tilde{\mathcal{M}}^{(1)}_\kappa + \left(\frac{\alpha_s}{2\pi}\right)^2 \tilde{\mathcal{M}}^{(2)}_\kappa + \ldots\right), \qquad \text{for } \kappa = \mathrm{g}, Q$$

$$\mathcal{M}^{(k)}_{\mathrm{g}} \xrightarrow{\text{L.C.}} \left(\frac{N_c}{2}\right)^k \sum_{\sigma \in S_2} \left(T^{a_{\sigma(3)}} T^{a_{\sigma(2)}}\right)^{\bar{i}_1}_{i_4} \sum_{j=0}^{k} \left(\frac{N_f}{N_c}\right)^j \mathcal{A}^{(k)[j]}_{\mathrm{g}}$$

$$\mathcal{M}^{(k)}_{q} \xrightarrow{\text{L.C.}} \left(\frac{N_c}{2}\right)^k \delta^{\bar{i}_1}_{i_2} \delta^{\bar{i}_3}_{i_4} \sum_{j=0}^{k} \left(\frac{N_f}{N_c}\right)^j \mathcal{A}^{(k)[j]}_{q}$$

Numerical benchmark
[Hartanto, Badger, Brønnum-Hansen, Peraro '19]

Analytic reconstruction

Numerical reduction (in $\mathbb{F}_p$) to finite remainders expressed in basis of pentagon functions [Chicherin, VS, Zoia '21]

$$\mathcal{R}^{(2)} = \mathcal{A}^{(2)} - \mathbf{I}^{(1)}\mathcal{A}^{(1)} - \mathbf{I}^{(2)}\mathcal{A}^{(0)} = \sum_{\vec{\mathbf{i}}} r_{\vec{\mathbf{i}}}(\vec{s})\, \boldsymbol{g}^{\vec{\mathbf{i}}}$$

with Caravel.

Black-box reconstruction too hard: would require 10^7 samples, each few minutes!

- Denominators are letters of the alphabet,

$$r_i = \frac{n_i}{\prod_{j=1}^{37} W_j^{q_{ij}}}, \qquad \left(\text{recall:} \quad \mathrm{d}\vec{g} = \epsilon \left(\sum_i \mathrm{d}\log W_i\, A_i\right)\vec{g}\right)$$

$\implies$ exponents q_{ij} from univariate reconstruction

- Reconstruct in one variable s_{23} $\rightarrow$ partial fraction $\rightarrow$ dense ansatz for polynomials in remaining variables

- Maximal ansatz size 500k, exploit special structure of Vandermonde matrix to invert in $\mathcal{O}(N^2)$

Analytic results available at `http://www.hep.fsu.edu/~ffebres/W4partons`

From $pp \to Vjj$ to $e^+e^- \to 4j$

Analytic results for 6-point helicity amplitudes in the form

$$\mathcal{R} = \sum_{\vec{\mathbf{i}}} r_{\vec{\mathbf{i}}}(\vec{s})\ \boldsymbol{g}^{\vec{\mathbf{i}}}(\vec{s})$$

alternatively we know the vector current

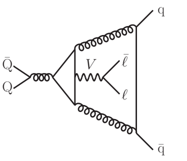
$$\mathcal{R}^\mu = \sum_{\vec{\mathbf{i}}} r^\mu_{\vec{\mathbf{i}}}(\vec{s})\ \boldsymbol{g}^{\vec{\mathbf{i}}}(\vec{s}), \qquad \mathcal{R}^\mu J_\mu, \quad J_\mu = \frac{\kappa}{s_{56} - M_v^2 + \mathrm{i}\,\Gamma_v M_v} \bar{u}(p_6)\gamma_\mu v(p_5)$$

Crossing from scattering to decay kinematics

- Attach appropriate lepton current; permutations, charge/parity conjugation of $r^\mu_{\vec{\mathbf{i}}}(\vec{s})$ trivial
- Special function basis constructed for scattering kinematics $2 \to 3$.
  Need to redo the construction [Chicherin, VS, Zoia '21] for decay kinematics $1 \to 4$.

Nonplanar contributions

- All subleading in N_c not included, likely suppressed
- Contribution proportional to $\sum_f Q_f$ not small?



Summary

- Loop amplitudes remain major bottleneck in precision of theoretical predictions
- Future e^+e^- colliders will benefit from advances in calculation techniques for the LHC
- Two-loop QCD corrections for $2 \to 3$ processes, mixed QCDxEW corrections for $2 \to 2$ are becoming a reality

Main lessons

- Multiscale calculations require new techniques and ideas
- Large final-state phase space $\implies$ loop amplitudes must evaluate fast
- Good grasp on analytic structure of Feynman integrals and associated function spaces has been essential
- Judicious combination of analytic and numerical methods fruitful

Discussion

Analytic vs numerical methods: rational

Analytic reconstruction from samples in $\mathbb{F}_p$

- Best bet so far: framework for educated guess work, we hope to get much better at it!
- Also useful for deriving DEs for Feynman integrals
- Can we handle even more scales comfortably?
- Special function basis needed

Fully numerical?

- Numerical (floating point) amplitude reduction is in principle possible right now (e.g. `Caravel`)
- But: slow due to severe numerical instabilities in integral reduction, cancellations between Feynman integrals $\implies$ high intermediate precision needed
- Can developments by [Lang, Pozzorini, Schär, Zhang, Zoller] (OpenLoops@2loops) help with this? [see Max's talk]

Analytic vs numerical methods: Feynman integrals

Analytic

- ✓ MPLs successful for $2 \to 2$, also with masses, when possible
- ✓ For $2 \to 3$ up to two loops "pentagon functions" method, when possible
- ? Biggest issue: general class of functions not understood, even mathematically [see Stefan's talk]

(Semi-)numerical

Solutions of DEs by matching local series expansions [see talks by Martijn, Xiao]

- ✓ Successfully sidestep analytic complexity with few dynamic scales
- ✓ Even very difficult multi-scale integrals integrals can be tackled [Liu, Ma '21]
- ? Still too slow for many dynamic scales?

To the shopping list

Basically there

- $e^+e^- \to 4j$, α_s^2 (also as a $4f$ background)

Still difficult, but imaginable with incremental progress

- $e^+e^- \to 3j$, α_s^3 (do we need $\alpha_s\alpha$?)
- $e^+e^- \to 5j$, α_s^2
- $e^+e^- \to QQj$, α_s^2, massive b

Terrifying

α^2 corrections to five-point functions

- $e^+e^- \to \nu\nu H$
- $e^+e^- \to l^+l^- H$

A break-through in understanding of elliptic Feynman integrals might be required

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