

Multi-Scale 2-Loop Amplitudes

Matthias Kerner (KIT)

Aachen – 2. March 2023

Annual Meeting of the CRC TRR 257



Introduction

Timeline of NNLO calculations for hadronic collisions



Introduction

Timeline of NNLO calculations for hadronic collisions



Fast progress for $2 \rightarrow 2$ processes with massless legs

Introduction

The NNLO revolution was partly caused by the observation, that Differential Equations can usually be brought into canonical form [Henn 13]

 $\partial_{x_i} \vec{I}(\vec{x}) = \epsilon A_i(\vec{x}) \vec{I}(\vec{x})$

 \rightarrow DEQ can be solved order-by-order in ε

→ Solution in terms of iterated integrals for massless integrals: mostly HPLs/GPLs resp. PolyLogs

However, with massive propagators, the calculation can quickly become complicated



Outline of the Talk

Multi-Scale 2-Loop Amplitudes

scales = # indep. Mandelstam invariants
 + # indep. masses

- Introduction
- The standard (analytic) approach
 - application to massless 2 \rightarrow 3 processes
- $2 \rightarrow 2$ processes with massive internal legs
 - heavy top limit
 - series expansions
 - numerical methods
 - new ideas
- Common issues
 - expression swell
 - mass-scheme uncertainties
- Conclusion

Disclaimer:

The focus of this talk is on an overview of the methods used, not on the presentation of all calculations

The Standard Approach to Multi-Loop Calculations

 Identify possible tensor structures using (gauge/permutation) symmetries, e.g. for HH production

 [']
 ^t
 ^t

New ideas: direct calculation of polarized amplitudes L. Chen 19; Peraro, Tancredi 19,20

$$\mathcal{M}^{\mu\nu} = A_1(s, t, m_H^2, m_t^2, D) T_1^{\mu\nu} + A_2(s, t, m_H^2, m_t^2, D) T_2^{\mu\nu} T_2^{\mu\nu} + \frac{1}{p_j^2} \int_{\mathcal{T}_j^{\mu\nu}}^{p_1 + p_2} \frac{p_1 \cdot p_2}{p_1 + p_2} \left\{ m_H^2 p_1^{\nu} p_2^{\mu} - 2(p_1 \cdot p_3) p_3^{\nu} p_2^{\mu} - 2(p_2 \cdot p_3) p_3^{\nu} p_1^{\mu} + 2(p_1 \cdot p_2) p_3^{\nu} p_3^{\mu} \right\}$$
Construct projectors $P^{\mu\nu}$ such that

2. Calculate the form factors using projectors

$$P_1^{\mu\nu}\mathcal{M}_{\mu\nu} = A_1(s,t,m_H^2,m_t^2,D) \qquad P_2^{\mu\nu}\mathcal{M}_{\mu\nu} = A_2(s,t,m_H^2,m_t^2,D)$$

 \rightarrow all Lorentz indices are contracted L-loop N-propagator integrals written as

$$I(\{\nu_i\}) = \int \prod_{l \le L} d^d l_l \frac{\prod_{i > N} D_i (q_i^2 - m_i^2)^{-\nu_i}}{\prod_{i \le N} D_i (q_i^2 - m_i^2)^{\nu_i}} \qquad \nu_i \in \mathbb{Z}$$

3. IBP reduction [Chetyrkin, Tkachov; Laporta]

$$\int d^{d}p_{i} \frac{\partial}{\partial p_{i}^{\mu}} \left[q^{\mu} \mathbf{I}'(p_{1}, \dots, p_{l}; k_{1}, \dots, k_{m}) \right] = 0$$

$$q: \text{ loop or external momentum}$$

$$\rightarrow \text{ employ linear relations} \quad express to reduce all loop integrals to minimal set of independent integrals integrals to minimal set of independent integrals i$$

The Standard Approach to Multi-Loop Calculations

4. Differentiate master integrals wrt. kin. invariants $x_j \rightarrow$ system of differential equations (DEQs)

$$\frac{\partial \vec{I}(\vec{x},\epsilon)}{\partial x_j} = A_{x_j}(\vec{x},\epsilon)\vec{I}(\vec{x},\epsilon)$$

5. Find transformation U to canonical basis, such that

$$I'(\vec{x},\epsilon) = U(\vec{x},\epsilon)I(\vec{x},\epsilon) \qquad \qquad \frac{\partial \vec{I'}(\vec{x},\epsilon)}{\partial x_j} = \epsilon A'_x(\vec{x})\vec{I'}(\vec{x},\epsilon)$$

For multi-scale problems, this often introduces square roots or elliptic functions into the system of DEQs

can sometimes be removed by variable change, e.g. $\sqrt{s(s-4)}$

$$\overline{m} \xrightarrow[s \to -m \frac{(1-x)^2}{x}]{} m \frac{1-x^2}{x}$$

6. Solve DEQs order by order in ε ,

integration constants can be fixed, e.g. known integral result in specific limits (easier to calculate)

The integration is straightforward in terms of GPLs, if A'_{x} contains only simple poles

$$G(z_1, \dots, z_n; y) = \int_0^y \frac{dx}{x - z_1} G(z_2, \dots, z_n; x) \qquad \qquad G(; x) = 1$$

The z_i are called letters

7

Massless $2 \rightarrow 3$ scattering

Gehrmann, Henn, Presti 18 Chicherin, Gehrmann, Henn, Wasser, Zhang, Zoia 18 Chicherin, Sotnikov 20



scales: 5 independent Mandelstam invariants + parity-odd invariant $\epsilon_5 = tr \left[\gamma_5 \not\!\!\!/ _1 \not\!\!\!/ _2 \not\!\!\!/ _3 \not\!\!\!/ _4 \right]$

Letter	v notation	momentum notation	cylic
W_1	v_1	$2p_1 \cdot p_2$	+ cyclic (4)
W_6	$v_3 + v_4$	$2p_4 \cdot (p_3 + p_5)$	+ cyclic (4)
W_{11}	$v_1 - v_4$	$2p_3 \cdot (p_4 + p_5)$	+ cyclic (4)
W_{16}	$v_4 - v_1 - v_2$	$2p_1 \cdot p_3$	+ cyclic (4)
W_{21}	$v_3 + v_4 - v_1 - v_2$	$2p_3 \cdot (p_1 + p_4)$	+ cyclic (4)
W_{26}	$\frac{v_1v_2 - v_2v_3 + v_3v_4 - v_1v_5 - v_4v_5 - \sqrt{\Delta}}{v_1v_2 - v_2v_3 + v_3v_4 - v_1v_5 - v_4v_5 + \sqrt{\Delta}}$	$\frac{\mathrm{tr}[(1-\gamma_5)\not\!\!p_4\not\!\!p_5\not\!\!p_1\not\!\!p_2]}{\mathrm{tr}[(1+\gamma_5)\not\!\!p_4\not\!\!p_5\not\!\!p_1\not\!\!p_2]}$	+ cyclic (4)
W_{31}	$\sqrt{\Delta}$	$\mathrm{tr}[\gamma_5 \not\!\!p_1 \not\!\!p_2 \not\!\!p_3 \not\!\!p_4]$	

many different letters, but integration in terms of polylogarithms possible

Planar integrals with one off-shell leg are also known [Canko, Papadopoulos, Syrrakos 20]



Applications:

- **yyy**. [Chawdhry, Czakon, Mitov, Poncelet] [Kallweit, Sotnikov, Wieseman] [Abreu, Page, Pascual, Sotnikov]
- ɣɣj [Agarwal, Buccioni, von Manteuffel, Tancredi]
 [Chawdhry, Czakon, Mitov, Poncelet]
 [Badger, Gehrmann, Marcoli, Mood]
- jjj [Abreu, Cordero, Ita, Page, Sotnikov]
- Wyj [Badger, Hartanto, Kryś, Zoia]
- Wbb [Badger, Hartanto, Zoia]
 - [Hartanto, Poncelet, Popescu, Zoia]

$2 \rightarrow 2$ scattering with massive propagators

Representative example: NLO QCD corrections to Higgs + Jet production

- Involves elliptic integrals
- Many square roots, cannot be rationalized simultaneously



(semi-)analytic result for planar integrals: [Bonciani, Del Duca, Frellesvig, Henn, Moriello, Smirnov 16]

- weight 2 contributions written in terms of Li₂ for polylogarithmic sectors
- weight 3&4 and elliptic contributions via integration (over elliptic kernel)
- \rightarrow analytic continuation & physics application not straightforward

First full calculations of NLO HJ production:

- Using HE expansion [Lindert, Kudashkin, Melnikov, Wever 18]
- Using sector decomposition [Jones, Luisoni, MK 18]
- Using DiffExp [Frellesvig, Hidding, Maestri, Moriello, Salvatori 19; Bonciani, Del Duca, Frellesvig, Hidding, Hirschi, Moriello, Salvatori, Somogyi, Tramontano 22]

This process also contributes to H production at NNLO [Czakon, Harlander, Klappert, Niggetiedt 21]

Analytic integration often not first choice for massive integrals

Nevertheless, lots of progress on elliptic integrals:

Abreu, Adams, Beccetti, Bezuglov, Bogner, Bourjaily, Broedel, Chaubey, Duhr, Dulat, Frellesvig, Laporta, Müller, Onishchenko, Ozcelik, Primo, Remiddi, Schweitzer, Tancredi, Veretin, Walden, Weinzierl

Heavy Top Limit



Further improvement: m_t -dependence in reals: FT_{approx}

Many integrals have been calculated as Series Expansions in various limits \rightarrow simpler integrals The expansion can be performed using expansion by regions [Beneke, Smirnov 98] using the tool asy [Pak, Smirnov; Jantzen, Smirnov, Smirnov]

Example HH production: • HTL $(m_t \to \infty)$ [Grigo, Hoff, Melnikov, Steinhauser 13, 15; Degrassi, Giardino, Gröber 16] • High Energy $(m_t \to 0)$ [Davies, Mishima, Steinhauser, Wellmann 18]





$$\mathcal{V}_{\text{fin}}^{N} = \frac{a_0 + a_1 x + \ldots + a_n x^n}{1 + b_1 x + \ldots + b_m x^m} \equiv [n/m](x)$$



Integrals typically depend on multiple scales

e.g. $gg \rightarrow ZH$ in HE region:

 $m_Z, m_H < m_t \ll s, t$

expansion around small masses up to m_Z^4, m_H^4, m_t^{32}

Davies, Mishima, Steinhauser 20; Chen, Davies, Heinrich, Jones, MK, Mishima, Schlenk, Steinhauser 22



Many more results using m_t -expansions:

- HH: Grigo, Hoff, Steinhauser; Davies, Herren, Mishima, Steinhauser; Degrassi, Giardino, Gröber
- HJ: Harlander, Neumann, Ozeren, Wiesemann; Neumann, Wiesemann; Kudashkin, Melnikov, Wever
- ZZ: Davies, Mishima, Steinhauser, Wellmann; Gröber, Rauh
- ZH: Hasselhuhn, Luthe, Steinhauser; Davies, Mishima, Steinhauser; Degrassi, Gröber, Vitti, Zhao

Different method using expansions:

- Expand in masses of external particles •
- Solve remaining integrals with full m_t dependence ٠



Further results based on expansions for HH production



Combine large mass expansion with Padé ansatz and threshold logarithms



Works well below and at top-quark pair threshold

ZH production: combination of HE and p_T expansion [Bellafronte, Degrassi, Giardino, Gröber, Vitti]

Sector Decomposition

Numerical evaluation of loop integrals with pySecDec

[Borowka, Heinrich, Jahn, Jones, MK, Langer, Magerya, Olsson, Põldaru, Schlenk, Villa]

• Sector decomposition [Binoth, Heinrich 00] factorizes overlapping singularities

• Subtraction of poles & expansion in $m{\epsilon}$

• Contour deformation [Soper 00; Binoth et.al. 05, $\frac{1}{(x_{1}-x_{2})^{2+\varepsilon}} = \begin{bmatrix} \theta(x_{1}-x_{2})^{2}+\theta(x_{2}-x_{1}) \end{bmatrix}$ • $f(x_{1}-x_{2})^{2+\varepsilon} = \begin{bmatrix} \theta(x_{1}-x_{2})^{2}+\theta(x_{2}-x_{1}) \end{bmatrix}$ • $f(x_{2}-x_{1})^{2}$ • $f(x_{2}-x_{1})^{2$ Available at github.com/gudrunhe/secdec

New in version 1.5:

- expansion by regions
- evaluation of linear combinations of integrals, with automated optimization of sampling points per sector, minimizing

$$T = \sum_{\substack{\text{integral } i \\ \sigma_i = \text{ error estimate (including coefficients in amplitude) \\ \lambda = \text{ Lagrange multiplier}} \sigma_i = c_i \cdot t_i^{-e}$$

- automated reduction of contour-def. parameter
- automatically adjusts FORM settings

pySecDec integral libraries can be directly linked to amplitude code

$$= -\frac{1}{\varepsilon} g(0,\varepsilon) + \int_0^1 \mathrm{d}x \, x^{-1-\varepsilon} \left(g(x,\varepsilon) - g(0,\varepsilon) \right)$$

pySecDec – Quasi-Monte Carlo

Our preferred integration algorithm is a Quasi-Monte Carlo using rank-1 shifted lattice rule Review: Dick, Kuo, Sloan 13 First application to loop integrals: Li, Wang, Yan, Zhao 15

Integrator available at github.com/mppmu/qmc [Borowka, Heinrich, Jahn, Jones, MK, Schlenk]

Processes calculated using (py-)SecDec with QMC:

- HH [Borowka, Greiner, Heinrich, Jones, MK, Schlenk, Schubert, Zirke 16]
- HJ [Jones, MK, Luisoni 18]
- AA [Chen, Heinrich, Jahn, Jones, MK, Schlenk, Yokoya 19]

ZH [Chen, Heinrich, Jones, MK, Klappert, Schlenk 20] ZZ [Agarwal, Jones, Manteuffel 20]

pySecDec – Work in Progress

Vitaly Magerya, L&L `22

Coming soon:

pySecDec v1.6 \rightarrow significant speed improvements

Performance improvements by pySEcDEc version

Time to integrate $\xrightarrow{m_Z}$ $\xrightarrow{m_W}$ $\xrightarrow{m_Z}$ to

to 7 digits of precision with pySecDec + QMC:

Speedup sources:

- * v1.5: adaptive sampling, automatic contour deformation adjustment;
- * *dev*: separation of real and complex variables in the integrand code;
- * *wip*: simlification of the integrand code, vectorization on CPU (AVX2).

The latest release is fast; the next release will be faster.

Auxiliary Mass Flow

$$I \propto \lim_{\eta \to 0^+} \int \prod_{l=1}^{L} d^{d} k_{i} \prod_{i=1}^{N} \frac{1}{[q_{i}^{2} - (m_{i}^{2} - i\eta)]^{\nu_{i}}}$$

Idea:

• Solve DEQ in $x \propto -i\eta$

 $\partial_x I = MI$

- Start from boundary point $x = -i\infty$ \rightarrow (massive vacuum graphs) × (massless graphs)
- Transfer to x=0 using power-log expansions

Public Implementation: AMFlow [Liu, Ma 22]

Full amplitudes evaluated using this method: $gg \rightarrow WW$, $gg \rightarrow ZZ$ [Brønnum-Hansen, Wang 21] can achieve 15-20 digits precision in ~1h CPU time Liu, Ma, Wang 17; Liu, Ma, Tao et.al. 20; Liu, Ma 22 Brønnum-Hansen, Wang 21

arlsruhe Institute of Technology

Expand *I* around **boundary** in variable $y = x^{-1} = 0$:

$$\boldsymbol{I} = \sum_{j}^{M} e^{j} \sum_{k}^{N} \sum_{l} \boldsymbol{c}_{jkl} y^{k} \ln^{l} y + \dots$$

Evaluate and expand around regular points:

$$m{I} = \sum_{j}^{M} \epsilon^{j} \sum_{k=0}^{N} m{c}_{jk} x'^{k} + \dots$$

Series Expansion Along Path – DiffExp & SeaSyde

Moriello 19 General Idea: Solve DEQs along path $\gamma(t): t \mapsto \{x_1(t), \ldots, x_m(t)\},\$ $\vec{x}(t_a) = \vec{a}, \ \vec{x}(t_b) = \vec{b}$ see also Lee, Smirnov, Smirnov 17 $\frac{\partial}{\partial t}\vec{f}(t,\epsilon) = \mathbf{A}_t(t,\epsilon)\vec{f}(t,\epsilon) \qquad \mathbf{A}_t(t,\epsilon) = \sum_{i=1}^m \mathbf{A}_{x_i}(t,\epsilon)\frac{\partial x_i(t)}{\partial t}$ $\vec{f}(\vec{a})$ known Series expansion near singular/regular points: $\vec{f}_{\text{sing}}^{(i)}(t) = \sum_{i=0}^{\infty} \sum_{j=0}^{N_i} \vec{c}^{(i,j_1,j_2,j_3)}(t-\tau)^{w_{j_1}+j_2} \log (t-\tau)^{j_3} \qquad \vec{f}_{\text{reg}}^{(i)}(t) = \sum_{j=0}^{\infty} \vec{c}^{(i,j)}(t-\tau)^{j_3}$ $j_1 \in S_i \ j_2 = 0 \ j_3 = 0$ 2 public implementations: SeaSyde DiffExp [Hidding 20] [Armadillo, Bonciani, Devoto, Rana, Vicini 22] transform 1 variable at a time works for real parameters choose path avoiding branch cuts arbitrary path also works with complex masses specify $i\delta$ -prescription for each physical singularity, ٠ cross threshold by expanding in singular points e. g. $\sqrt{4m^2 - s - i\delta}$ 2 3 5 Expansion 1 0 $\frac{100}{100}$ -0.5 Expansion 2 $P_{
m singular}$ _ P_{below} P_{regular} P_{mid} Pabove -1.0 Analytical Continuation -2-2Threshold $^{-3+}_{-3}$ -1.5 -3-22 -2 -12 3 0 -2.0 150 50 int Physics application: -50-150

> 2L mixed QCD-EW corrections to NC DY

0 50

100 150200

Vs

250 - 1.0

int

250

Physics application: NLO QCD (2L) corrections to HJ Bonciani, Del Duca, Frellesvig, Henn, Hidding, Maestri, Moriello, Salvatori, Smirnov 19; Frellesvig, Hidding, Maestri, Moriello, Salvatori 19

Iterative Application of Feynman's trick

Feynman's trick $D_1 = -(k+p)^2 + m_1^2$, $D_2 = -(k+q)^2 + m_2^2 \longrightarrow xD_1 + (1-x)D_2 = -(k+P)^2 + M^2$

can be used to combine pairs of propagators into one propagator with generalized kinematics. This procedure can be applied iteratively:

Integration split into multiple, simpler 1-dimensional problems \rightarrow computationally efficient

Computational Challenge: Expression Swell

The size of the expressions can become huge, with reduction tables of size O(1TB)

- \rightarrow it can be beneficial to $~\bullet~$ fix mass ratios during reduction
 - or perform numerical reduction for each phase-space point

Strategies to avoid Expression Swell:

- Finite-field methods
 - FiniteFlow [Peraro]
 - Firefly [J. Klappert, Klein, Lange]
 New tool for faster evaluation of numerical samples: Ratracer [V. Magerya]

• Syzygy Equations

Gluza, Kajda, Kosower 10; Schabinger 11; Lee 14; Ita 15; Larsen, Zhang 15; Bitoun, Bogner, Klausen, Panzer 17; Manteuffel, Panzer, Schabinger 20; Agarwal, Jones, Manteuffel 20;

- good basis of master integrals, with d-dependence factorizing from kinematic dependence in denominators of reduction and possibly additional properties Usovitsch 20; Smirnov, Smirnov 20; see also MK Radcor `19 proc.
- direct projection to physical amplitudes typically simpler; avoid evanescent tensor structures L. Chen 19; Peraro, Tancredi 19,20

Interesting new development:

Direct construction of reduction coefficients using Intersection Numbers

In contrast to Laporta's algorithm, no need for full reduction tables

Mizera 17; Mastrolia Mizera 18; Frellesvig, Gasparotto, Laporta, Mandal, Mastrolia, Mattiazzi, Mizera 19,20; Abreu, Britto, Duhr, Gardi, Matthew 19; Weinzierl 20; Caron-Huot, Pokraka 21; Chen, Jiang, Ma, Xu, Yang 22; Chestnov, Gasparotto, Mandal, Mastrolia, Matsubara-Heo, Munch, Takayama 22

Renormalization Scheme Uncertainties

Amplitude with massive internal particles depends on mass-renormalization scheme \rightarrow additional uncertainty can be estimated by comparing OS and \overline{MS} results

Renormalization Scheme Uncertainties

Scheme uncertainties of similar size also for other processes:

HJ production (using DiffExp approach) Bonciani, Del Duca, Frellesvig, Hidding, Hirschi, Moriello, Salvatori, Somogyi, Tramontano 22

ZH production (using SecDec & HE expansion) Chen, Davies, Heinrich, Jones, MK, Mishima, Schlenk, Steinhauser 22

Scheme uncertainty typically reduced by factor of ~2 going from LO to NLO, but still O(20-50%) at large \sqrt{s} , p_T

Renormalization Scheme Uncertainties

Leading HE contributions in gg \rightarrow HH and gg \rightarrow ZH production

HH

 $A_i^{(0)} \sim m_t^2 f_i(s, t)$ $A_i^{(1)} \sim 6C_F A_i^{(0)} \log\left[\frac{m_t^2}{s}\right]$

LO: m_t^2 from y_t^2 NLO: leading $\log(m_t^2)$ from mass c.t. converting to \overline{MS} gives $\log(\mu_t^2/s)$ motivating scale choice of $\mu_t^2 = s$ $gg \rightarrow HH$

$$A_i^{\text{fin}} = a_s A_i^{(0),\text{fin}} + a_s^2 A_i^{(1),\text{fin}} + \mathcal{O}(a_s^3)$$

MS

ZH

$$A_i^{(0)} \sim m_t^2 f_i(s,t) \log^2 \left[\frac{m_t^2}{s}\right] ,$$

$$A_i^{(1)} \sim \frac{(C_A - C_F)}{6} A_i^{(0)} \log^2 \left[\frac{m_t^2}{s}\right] .$$

LO: one m_t from y_t NLO: leading $\log(m_t^2)$ not coming from mass c.t. $\log(m_t^2)$

 \rightarrow The leading contributions seem to have different origins for the 2 processes

Open questions:

- Can the origin of these logarithms be understood and predicted for higher orders?
- Does this result in a preferred mass-renormalization scheme?
- Can these uncertainties be reduced w/o calculating the next order?

For H production, these logarithms were also studied in [Liu, Modi, Penin 22]

 $\log \left[\mu_t^2 / s \right]$

Conclusions

- Fully analytical methods remain challenging for multi-scale processes
- Powerful alternatives to analytic calculations:
 - Series Expansions in Kinematics
 - Sector Decomposition
 - Solve DEQs via series expansions
- Mass renormalization important source of uncertainty

Conclusions

- Fully analytical methods remain challenging for multi-scale processes
- Powerful alternatives to analytic calculations:
 - Series Expansions in Kinematics
 - Sector Decomposition
 - Solve DEQs via series expansions
- Mass renormalization important source of uncertainty

Thank you for your attention!