Complete NLO QCD Corrections to Z-boson Pair Production in Gluon-Fusion

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Agarwal, Kerner, von Manteuffel [2011.12325, 2404.05684]

+ Heinrich, Jahn, Langer, Magerya, Olsson, Põldaru, Schlenk, Villa [2108.10807, 2305.19768]





Outline

Motivation

Calculating the Massive 2-loop Amplitude

- Amplitude generation
- Integral reduction
- Numerical calculation of Feynman integrals

Results

- $gg \rightarrow ZZ$ @ NLO via massive quark loops
- $gg \rightarrow ZZ @$ NLO massless + massive quark loops

Outlook

Collider Precision



$$d\sigma = \int dx_a dx_b f_a(x_a) f_b(x_b) d\hat{\sigma}_{ab}(x_a, x_b) F_J + \mathcal{O}\left((\Lambda/Q)^m\right)$$
Parton Distribution Hard Scattering Non-perturbative Functions (PDFs) Matrix Element effects ~ few %

Perturbation Theory



Motivation: ZZ Production





Overview of $pp \rightarrow ZZ$



The $gg \rightarrow ZZ$ channel contributes to $pp \rightarrow ZZ$ starting at NNLO in QCD

However due the large gluon-gluon luminosity at the LHC:

Contributes significantly to the total cross section (5-10%)

Accounts for 60% of NNLO corrections

Expected to have very large 2-loop contribution

Motivation

Why calculate Z boson pair production via gluon-fusion?

Precision measurements

Background to Higgs production through gluon fusion CMS 18; ATLAS 20;

Higgs width

Provides indirect constraints on Higgs width via off-shell Higgs production ATLAS 18; CMS 19;

BSM Searches

Searches for heavy diboson resonances decaying to 4 lepton final states ATLAS 20; CMS 23;

Anomalous couplings

Provides constraints on anomalous $t\overline{t}Z$ & triple gauge couplings ATLAS 23

Higgs Width

Channel opens @ NNLO for $pp \rightarrow ZZ$, interferes with $pp \rightarrow H \rightarrow ZZ$ @ LO



ATLAS
$$\Gamma_H = 4.5^{+3.3}_{-2.5}$$
 MeV

CMS
$$\Gamma_H = 3.2^{+2.4}_{-1.7}$$
 MeV
CERN-EP-2021-272

Strong destructive interference with Higgs amplitude probes unitarizing behaviour of the Higgs

Off-shell measurements can provide model-dependent indirect constraints on Higgs properties (e.g. width)

$$\sigma_{gg \to H \to ZZ}^{\text{on-shell}} \sim \frac{g_{ggF}^2 g_{HZZ}^2}{m_H \Gamma_H}$$
$$\sigma_{gg \to H \to ZZ}^{\text{off-shell}} \sim \frac{g_{ggF}^2 g_{HZZ}^2}{m_{ZZ}^2}$$

Kauer, Passarino 12; Caola, Melnikov 13; Campbell, Ellis, Williams 14; (See also: Englert, Spannowsky 14)

Anomalous Couplings

vector ~
$$v_t \gamma_\mu$$
 axial-vector ~ $a_t \gamma_\mu \gamma_5$
 $\mathcal{V}_{\mu}^{Vf\bar{f}} = i \frac{e}{2\sin\theta_W \cos\theta_W} \gamma_\mu \left(v_t + a_t \gamma_5\right)$

For $m_q \neq 0$ production of longitudinally polarised ZZ via $gg \rightarrow ZZ$ can probe axial-vector coupling ($a_t = 1/2$ in SM)

$$\mathcal{M}_{\pm\pm00} \sim \frac{m_t^2}{m_Z^2} \left(a_t^2 - \frac{1}{4} \right) \left[\ln^2 \left(\frac{s}{m_t^2} \right) - 2i\pi \ln \left(\frac{s}{m_t^2} \right) \right]$$

Complements measurements of $t\bar{t}Z, tZj$





Calculation: $gg \rightarrow ZZ$



Known Amplitudes for $gg \rightarrow ZZ$

Full leading order (loop induced)

Glover, van der Bij 89

NLO (massless quark loop contribution)

von Manteuffel, Tancredi 15

NLO expansion around large top quark mass

Melnikov, Dowling 15; Caola, Dowling, Melnikov, Röntsch, Tancredi 16

+ Padé approx Campbell, Ellis, Czakon, Kirchner 16

+ Threshold (Higgs int.) Gröber, Maier, Rauh 19

NLO expansion around small top quark mass

Davies, Mishima, Steinhauser, Wellmann 20

NLO amplitudes (massive quark loop) obtained via sector decomposition or series solutions of differential equations Agarwal, SJ, von Manteuffel 20; Brønnum-Hansen, Wang 21

NLO amplitudes small- p_T + small top quark mass Degrassi, Gröber, Vitti 24







Virtual Amplitudes



Decomposition

Tensor structure $\mathcal{M} = \mathcal{M}_{\mu\nu\rho\sigma} \epsilon_1^{\mu}(p_1) \epsilon_2^{\nu}(p_2) \epsilon_3^{*\rho}(p_3) \epsilon_4^{*\sigma}(p_4)$

- \rightarrow 138 parity-even tensor structures
- + transversality $\epsilon_1(p_1).p_1 = 0, \epsilon_2(p_2).p_2 = 0$
- + gauge fixing $\epsilon_1(p_1).p_2 = 0, \epsilon_2(p_2).p_1 = 0, \epsilon_3(p_3).p_3 = 0, \epsilon_4(p_4).p_4 = 0$
- \rightarrow 20 tensor structures remain
- + Bose symmetry 9 indep. + 11 related by crossing

$$g \stackrel{\mu}{\longrightarrow} p_1^{\mu} \qquad p_3^{\rho} \stackrel{\mu}{\longrightarrow} Z$$

$$\mathcal{M}^{\mu\nu\rho\sigma}(p_1, p_2, p_3, p_4) = \sum_{i=1}^{20} A_i(s, t, m_t^2, m_Z^2) T_i^{\mu\nu\rho\sigma}$$

$$\begin{split} T_{1}^{\rho\sigma\mu\nu} &= g^{\mu\nu}g^{\rho\sigma} & T_{2}^{\rho\sigma\mu\nu} = g^{\mu\rho}g^{\nu\sigma} & T_{3}^{\rho\sigma\mu\nu} = g^{\mu\sigma}g^{\nu\rho} & T_{4}^{\rho\sigma\mu\nu} = p_{1}^{\rho}p_{1}^{\sigma}g^{\mu\nu} \\ T_{5}^{\rho\sigma\mu\nu} &= p_{1}^{\rho}p_{2}^{\sigma}g^{\mu\nu} & T_{6}^{\rho\sigma\mu\nu} = p_{1}^{\sigma}p_{2}^{\rho}g^{\mu\nu} & T_{7}^{\rho\sigma\mu\nu} = p_{2}^{\rho}p_{2}^{\sigma}g^{\mu\nu} & T_{8}^{\rho\sigma\mu\nu} = p_{1}^{\sigma}p_{3}^{\nu}g^{\mu\rho} \\ T_{9}^{\rho\sigma\mu\nu} &= p_{2}^{\sigma}p_{3}^{\nu}g^{\mu\rho} & T_{10}^{\rho\sigma\mu\nu} = p_{1}^{\rho}p_{3}^{\nu}g^{\mu\sigma} & T_{11}^{\rho\sigma\mu\nu} = p_{2}^{\rho}p_{3}^{\nu}g^{\mu\sigma} & T_{12}^{\rho\sigma\mu\nu} = p_{1}^{\sigma}p_{3}^{\mu}g^{\nu\rho} \\ T_{13}^{\rho\sigma\mu\nu} &= p_{2}^{\sigma}p_{3}^{\mu}g^{\nu\rho} & T_{14}^{\rho\sigma\mu\nu} = p_{1}^{\rho}p_{3}^{\mu}g^{\nu\sigma} & T_{15}^{\rho\sigma\mu\nu} = p_{2}^{\rho}p_{3}^{\mu}g^{\nu\sigma} & T_{16}^{\rho\sigma\mu\nu} = p_{3}^{\mu}p_{3}^{\nu}g^{\rho\sigma} \\ T_{17}^{\rho\sigma\mu\nu} &= p_{1}^{\rho}p_{1}^{\sigma}p_{3}^{\mu}p_{3}^{\nu} & T_{18}^{\rho\sigma\mu\nu} = p_{1}^{\rho}p_{2}^{\sigma}p_{3}^{\mu}p_{3}^{\nu} & T_{19}^{\rho\sigma\mu\nu} = p_{2}^{\rho}p_{1}^{\sigma}p_{3}^{\mu}p_{3}^{\nu} & T_{20}^{\rho\sigma\mu\nu} = p_{2}^{\rho}p_{2}^{\sigma}p_{3}^{\mu}p_{3}^{\nu} \end{split}$$

von Manteuffel, Tancredi 15

Our task is now to compute the 20 scalar form factors $A_i(s, t, m_t^2, m_Z^2)$

Dimensional Regularisation & γ_5





In dim. reg. ($d = 4 - 2\epsilon$) we can't retain all properties of γ_5 in $d \neq 4$ dimensions

Larin Scheme

Sacrifice anti-commuting property of γ_5

$$J^{5}_{\mu} = Z_{5,ns} J^{5}_{\mu,B} = Z_{5,ns} \left[\frac{i}{3!} \epsilon_{\mu\nu\rho\sigma} \bar{\psi} \gamma^{\nu} \gamma^{\rho} \gamma^{\sigma} \bar{\psi} \right]$$
$$P^{5} = Z_{5,p} P^{5}_{B} = Z_{5,p} \left[\frac{i}{4!} \epsilon_{\mu\nu\rho\sigma} \bar{\psi} \gamma^{\mu} \gamma^{\nu} \gamma^{\rho} \gamma^{\sigma} \bar{\psi} \right]$$

Fix Ward identities/ABJ anomaly:

$$Z_{5,ns} = 1 + \alpha_s(-4C_F) + \dots$$

$$Z_{5,p} = 1 + \alpha_s(-8C_F) + \dots$$

Larin, Vermaseren 91; Larin 93

Kreimer Scheme

Retain $\{\gamma_5, \gamma^{\mu}\} = 0$, but, sacrifice cyclicity of traces involving γ_5

Define `reading point' and carefully manipulate all traces

Kreimer 90; Korner, Kreimer, Schilcher 92

Diagrams



von Manteuffel, Tancredi 15

Class A_l Z bosons couple to same massless fermion line



Agarwal, SPJ, von Manteuffel 20

Class A_h Z bosons couple to same massive fermion line



Class B Z bosons couple to different fermion lines



Djouadi, Spira, Zerwas 91

Class C Z bosons couple to Higgs boson

Campbell, Ellis, Czakon, Kirchner 16

15

Diagrams



von Manteuffel, Tancredi 15







Class B Z bosons couple to different fermion lines



Class C Z bosons couple to Higgs boson

Djouadi, Spira, Zerwas 91

Campbell, Ellis, Czakon, Kirchner 16

Diagrams: $gg \rightarrow ZZ$

Class A_h



Most challenging piece Contains a total of 29247 scalar \rightarrow 264 master Feynman Integrals

Basis choice

Choice of master integral basis is **very** important for size/performance of amplitude

Basis Choice:

1) Select finite integrals ^{Bern,} Again

Bern, Dixon, Kosower 92; Panzer 14; von Manteuffel, Panzer, Schabinger 14; Agarwal, SPJ, von Manteuffel 20

2) Require *d*- and kinematic dependence of denominators factorises Smirnov, Smirnov 20; $\frac{N(s,t,d)}{D(s,t,d)}I + \ldots \rightarrow \frac{N'(s,t,d)}{D'_{1}(d)D'_{2}(s,t)}I' + \ldots$

Avoid monstrosities like: $D(s,t,d) = \begin{array}{c} 1250 - 500 \, d - 9000 \, t + 3600 \, d \, t + 16200 \, t^2 - 6480 \, d \, t^2 \\ -4050 \, s + 1575 \, d \, s + 19440 \, s \, t - 8100 \, d \, s \, t - 52488 \, s \, t^2 \\ +20412 \, d \, s \, t^2 - 29160 \, s^2 \, t + 11664 \, d \, s^2 \, t \end{array} \xrightarrow{d \to 4} \begin{array}{c} -125 + 375 \, s + 900 \, t - 2160 \, s \, t \\ +2916 \, s^2 \, t - 1620 \, t^2 + 4860 \, s \, t^2 \\ +2916 \, s^2 \, t - 1620 \, t^2 + 4860 \, s \, t^2 \end{array}$ They increase expr. size and introduce spurious singularities in the amplitude

Finite Integrals

Not all finite integrals are created equal

Can take vastly different times to numerically integrate (will discuss this shortly)



Can algorithmically construct finite linear combinations

Agarwal, SPJ, von Manteuffel 20 See also: Gambuti, Kosower, Novichkov, Tancredi 23

Baikov Representation

Scalar integrals can be written as Baikov 96

$$I = \mathcal{N} \int dz_1 \dots dz_N \, \frac{1}{\prod_{i=1}^N \, z_i^{\nu_i}} \, P^{\frac{d-L-E-1}{2}}$$

IBPs become

$$0 = \int dz_1 \dots dz_N \sum_{i=1}^N \frac{\partial}{\partial z_i} \left(f_i \frac{1}{\prod_{i=1}^N z_i^{\nu_i}} P^{\frac{d-L-E-1}{2}} \right)$$

$$0 = \int dz_1 \dots dz_N \sum_{i=1}^N \left(\frac{\partial f_i}{\partial z_i} + \frac{d-L-E-1}{2P} f_i \frac{\partial P}{\partial z_i} - \nu_i \frac{f_i}{z_i} \right) \frac{1}{\prod_{i=1}^N z_i^{\nu_i}} P^{\frac{d-L-E-1}{2}}$$

Dimension shift Dots (doubled propagators)

IBPs generate dim shifted & dotted integrals \rightarrow huge linear system to solve

Impose `Syzygy' Constraints

$$\begin{pmatrix} \sum_{i=1}^{N} f_i \frac{\partial P}{\partial z_i} \end{pmatrix} + f_{N+1} P = 0 \qquad \rightarrow \text{No dimension shift} \qquad \begin{array}{l} \text{Larsen, Zhang 15;} \\ \text{Abreu, Febres Cordero, Ita, Page, Zeng 17;} \\ \text{Boehm, Georgoudis, Larsen, Schoenemann,} \\ T_{i} \sim z_i \qquad \rightarrow \text{No doubled props.} \end{cases}$$

Reduction

IBP system now contains $\mathcal{O}(10^5)$ equations (was $\mathcal{O}(10^8)$ before syzygy constraints) Still need tools to actually solve this system of equations...

FinRed +	Syzygy Solver
von Mantueffel	Agarwal, von Mantueffel

Input Integrals: ~29000 integrals After symmetry: ~1500 integrals Master Integrals: 264 integrals Time: $\mathcal{O}(\text{months})$ on cluster Output IBP Tables: $\mathcal{O}(200 \text{ GB})$

Toolchain relies extensively on the use of finite fields

See e.g: von Mantueffel, Schabinger 14; Peraro 16

Even with these tools, still too difficult to obtain fully symbolic amplitudes! Fix mass ratio: $m_z^2/m_t^2 = 5/18$

Substituting in Amplitude

Now need to substitute O(200 GB) expression into a complicated amplitude... Yields intermediate expressions of O(1 TB)

Multivariate partial fractioning

- 1. Employ multivariate partial fractioning
- Pak 11; Abreu, Dormans, Febres Cordero, Ita, Page, Sotnikov 19; Böhm, Wittman, Wu, Xu, Zhang 20; Bendle, Böhm, Heymann, Ma, Rahn, Ristau, Wittmann, Wu, Zhang 21; Heller, von Manteuffel 21;
- 2. Partial fraction in d to separate the poles

3. Expand about
$$d = 4 - 2\epsilon$$

$$\frac{1}{(-1+d)(-3+d)^2(-4+d)(-7+2d)} = (\frac{1}{3} + \frac{2\epsilon}{9})(1+2\epsilon)^2(\frac{-1}{2\epsilon})(1+4\epsilon) \sim 16 \text{ terms}$$

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

Reduces coefficients of amplitude to <1 MB per coefficient For one of the hardest coefficients:

 $\{deg(num, s) + deg(den, s), deg(num, t) + deg(den, t), deg(num, d) + deg(den, d)\} = \{107, 117, 38\}$ $\{deg(num, s) + deg(den, s), deg(num, t) + deg(den, t), deg(num, d) + deg(den, d)\} = \{20, 15, 9\}$

Intermezzo: Computing Feynman Integrals



Computing Feynman Integrals

Feynman integrals can be difficult to compute analytically

Various methods to approximate/evaluate them numerically

Numerical differential equations

Series solutions of differential equations (AMFlow, DiffExp, Seasyde) Taylor expansion in Feynman parameters (TayInt)

Numerical Mellin-Barnes (MB, Ambre)

Tropical sampling (Feyntrop)

Numerical Loop-Tree Duality (cLTD, Lotty)

Sector decomposition (Sector_decomposition, FIESTA, pySecDec)

ODE/PDE

Series Solutions

~Monte Carlo Integration

pySecDec

pySecDec: a program for numerically evaluating dimensionally regulated parameter integrals on CPU or GPU



Latest Version:

Improved: Method of Regions Improved: Amplitude Evaluation + disteval Integrator

+ Median QMC Rules

Heinrich, SPJ, Kerner, Magerya, Olsson, Schlenk 23

python3 -m pip install --user --upgrade pySecDec

Well known in the QCD community, often used for checking master integrals

Used to compute two-loop amplitudes for $pp \rightarrow \{HH, HJ, \gamma\gamma, ZH, ZZ, t\bar{t}H\}$

Borowka, Greiner, Heinrich, SPJ, Kerner, Schlenk, Schubert, Zirke 16; SPJ, Kerner, Luisoni 18; Chen, Heinrich, Jahn, SPJ, Kerner, Schlenk, Yokoya 19; Chen, Heinrich, SPJ, Matthias Kerner, Klappert, Schlenk 20; Agarwal, SPJ, von Manteuffel 20; Agarwal, Heinrich, SPJ, Kerner, Klein, Lang, Magerya, Olsson 24

Sector Decomposition in a Nutshell

Can exchange loop integrals for integrals over Feynman parameters

$$I \sim \int \mathrm{d}^{d} k_{1} \dots \mathrm{d}^{d} k_{l} \frac{1}{\prod_{i=1}^{N} (q_{i} - m_{i})^{\nu_{i}}} \leftrightarrow I \sim \int_{\mathbb{R}^{N+1}_{>0}} \left[\mathrm{d}\boldsymbol{x} \right] \boldsymbol{x}^{\nu} \frac{[\mathcal{U}(\boldsymbol{x})]^{N-(L+1)D/2}}{[\mathcal{F}(\boldsymbol{x}, \mathbf{s}) - i\delta]^{N-LD/2}} \,\delta(1 - H(\boldsymbol{x}))$$

$$\mathcal{U}, \mathcal{F} \text{ are polynomials in FP } \boldsymbol{x}$$

Singularities

- 1. UV/IR singularities when some $\{x\} \rightarrow 0$ simultaneously \implies Sector Decomposition
- 2. Thresholds when \mathscr{F} vanishes inside integration region $\implies i\delta$

Sector decomposition

Find a local change of coordinates for each singularity that factorises it (blow-up)

Hepp 66; Roth, Denner 96; Binoth, Heinrich 00; Heinrich 08

Sector Decomposition in a Nutshell

$$I \sim \int_{\mathbb{R}_{>0}^{N}} \left[d\mathbf{x} \right] \mathbf{x}^{\nu} \left(c_{i} \mathbf{x}^{\mathbf{r}_{i}} \right)^{t}$$
$$\mathcal{N}(I) = \text{convHull}(\mathbf{r}_{1}, \mathbf{r}_{2}, \ldots) = \bigcap_{f \in F} \left\{ \mathbf{m} \in \mathbb{R}^{N} \mid \langle \mathbf{m}, \mathbf{n}_{f} \rangle + a_{f} \ge 0 \right\}$$

Normal vectors incident to each extremal vertex define a local change of variables* Kaneko, Ueda 10

$$\begin{aligned} x_i &= \prod_{f \in S_j} y_f^{\langle \mathbf{n}_f, \mathbf{e}_i \rangle} \\ I &\sim \sum_{\sigma \in \Delta_{\mathcal{N}}^T} |\sigma| \int_0^1 \left[\mathrm{d} \mathbf{y}_f \right] \prod_{f \in \sigma} y_f^{\langle \mathbf{n}_f, \nu \rangle - ta_f} \left(c_i \prod_{f \in \sigma} y_f^{\langle \mathbf{n}_f, \mathbf{r}_i \rangle + a_f} \right)^t \\ & \overline{\text{Singularities}} \quad \overline{\text{Finite}} \end{aligned}$$

*If $|S_i| > N$, need triangulation to define variables (simplicial normal cones $\sigma \in \Delta_{\mathcal{N}}^T$)

Sector Decomposition in a Nutshell



For each vertex make the local change of variables

e.g.
$$\mathbf{r}_1: x_1 = y_1^{-1}y_3^1, x_2 = y_1^0y_3^1, \mathbf{r}_2: x_1 = y_1^{-1}y_2^0, x_2 = y_1^0y_2^{-1}, \mathbf{r}_3: x_1 = y_2^0y_3^1, x_2 = y_2^{-1}y_3^1$$

$$I = -\Gamma(-1+2\varepsilon) (m^2)^{1-2\varepsilon} \int_0^1 dy_1 dy_2 dy_3 \frac{y_1^{-\varepsilon} y_2^{-\varepsilon} y_3^{-1+\varepsilon}}{(y_1+y_2+y_3)^{2-\varepsilon}} [\delta(1-y_2) + \delta(1-y_3) + \delta(1-y_1)]$$

Schlenk 2016

Performance Improvements

v1.5: Adaptive sampling of sectors, automatic contour def. adjustment

v1.5.6: Optimisations in integrand code

v1.6: New Quasi-Monte Carlo integrator ``Disteval"

Faster implementation of old integrator ``IntLib"
CPU & GPU: fusion of integration/integrand code (less modular arithmetic)
CPU: better utilisation via SIMD instructions (AVX2, FMA)
GPU: sum result on GPU, less synchronisation
Parse amplitude coefficients w/GiNaC (supports e.g. partial fractioned input)
Workers can run on remote machines (via ssh)

Does it help?

Performance Improvements





Vitaly Magerya (Radcor 2023)

Profiling

m	$d = 6 - 2\varepsilon$	10 ⁻² 10 ⁻³ 10 ⁻⁴ 10 ⁻⁴ 10 ⁻⁵ 10 ⁻⁶ 10 ⁻⁷ 10 ⁻⁸	~ <i>t</i> ~ <i>i.</i> ₆	1 Integra	10 ² ation time [secon	Diste	eval Qmc, GPU b Qmc, GPU 10 ⁴
Integra	tor \Accuracy	10 ⁻³	10^{-4}	10 ⁻⁵	10 ⁻⁶	10 ⁻⁷	10 ⁻⁸
GPU	DISTEVAL	4.2 s	6.3 s	27 s	1.5 m	17 m	54 m
	IntLib	22.0 s	22.0 s	110 s	6.7 m	50 m	263 m
	Speedup	5.2	5.2	4.1	5.6	3.0	4.9
CPU	DISTEVAL	5.1 s	14 s	1.6 m	8.3 m	57 m	4.7 h
	IntLib	20.8 s	86 s	14.2 m	62.2 m	480 m	43.1 h
	Speedup	4.1	6.1	8.7	7.5	8.4	9.2

[GPU: NVidia A100 40GB; CPU: AMD Epyc 7F32 with 32 threads]

Vitaly Magerya (Radcor 2023)

Profiling

pySecDec Disteval integration times for 3-loop sel	lf-energy integrals: ³
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Relative precision		10 ⁻³	10^{-4}	10 ⁻⁵	10 ⁻⁶	10 ⁻⁷	10 ⁻⁸
m_Z m_W m_Z	GPU	15s	20s	40s	200s	13m	50m
	CPU	10s	50s	400s	4000s	180m	1200m
m_t m_t m_Z	GPU	18s	19s	30s	20s	1.2m	2m
m_t m_t m_t m_t	CPU	5s	14s	60s	50s	12m	16m
m _Z m _t m _Z	GPU	6s	11s	12s	30s	3m	24m
m _W m _t	CPU	5s	10s	50s	800s	60m	800m

[Same diagrams as in Dubovyk, Usovitsch, Grzanka '21]

In short: seconds to minutes per integral to achieve practical precision.

[GPU: NVidia A100 40GB; CPU: AMD Epyc 7F32 with 32 threads]

Vitaly Magerya (Radcor 2023)

Quasi-Monte Carlo

Li, Wang, Yan, Zhao 15; de Doncker, Almulihi, Yuasa 17, 18; de Doncker, Almulihi 17; Kato, de Doncker, Ishikawa, Yuasa 18

$$Q_n^{(k)}[f] \equiv \frac{1}{n} \sum_{i=0}^{n-1} f\left(\left\{\frac{i\mathbf{z}}{n} + \mathbf{\Delta}_k\right\}\right) \qquad I[f] \approx \bar{Q}_{n,m}[f] \equiv \frac{1}{m} \sum_{k=0}^{m-1} Q_n^{(k)}[f],$$

- {} Fractional part Δ_k Random shift vector
- ${\boldsymbol{z}}$ Generating vector

Previously:

Precompute **z** with (CBC) construction

Guarantee error ~ $1/n^{\alpha}$ if $\delta_x^{(\alpha)}I(\mathbf{x})$ is squareintegrable and periodic Dick, Kuo, Sloan 13

CBC needs $\mathcal{O}(n)$ bytes memory $n \leq 4.10^{10}$ @ 2TB Can encounter ``unlucky'' lattices



Quasi-Monte Carlo: Unlucky Lattices



Good: Asymptotic error scaling $\sim 1/n^{1.5}$

Bad: Huge drop in precision for some "unlucky" lattices Not consistent across integrands

Quasi-Monte Carlo: Unlucky Lattices



Good: Asymptotic error scaling $\sim 1/n^{1.5}$

Bad: Huge drop in precision for some "unlucky" lattices Not consistent across integrands

Median Lattice Rules

Instead:

Compute \mathbf{z} on-the-fly

- 1. Choose *R* random $z \in \text{Uniform}(0; N-1)$
- 2. Estimate integral on each lattice

3. Choose lattice with median integral value

If $\delta_x^{(\alpha)} I(\mathbf{x})$ is square-integrable and periodic Integration error: $C(\alpha, \varepsilon)/(\rho n)^{\alpha-\epsilon}$ With probability: $1 - \rho^{R+1/2}/4$ $\forall 0 < \varepsilon \& 0 < \rho < 1$

Goda, L'Ecuyer 22



Some Future Developments

Computing integrals with leading Landau singularities inside the integration domain

w/ Gardi, Herzog, Ma (WIP)

Impossible \rightarrow Possible to compute

 p_2 p_4 p_1 p_3

 $I = \epsilon^{-4} \left[8.3400403920\mathbf{28} - 52.35987755983\mathbf{47}i \right] + \mathcal{O}\left(\epsilon^{-3}\right)$ $I^{\text{ana.}} = \epsilon^{-4} \left[8.34004039223768 - 52.35987755984493i \right] + \mathcal{O}\left(\epsilon^{-3}\right)$

Avoiding contour deformation even in the Minkowski/physical regime

w/ Olsson, Stone (WIP)

Speedup ~100-1000x for some cases



Results

Checks

Uncovered bug in nvcc

(fixed in current version)

This calculation was **complicated**, before we do anything we should check it:

Symmetries between form factors (and helicity amplitudes)

Crossing relations

Pole cancellation (UV and IR)

Alternate finite basis (checks definition of our finite integrals, basis change to finite integrals, and their numerical evaluation)

Different γ_5 schemes (Kreimer/Larin scheme)

Large top-mass and small top-mass expansions in the relevant regions

Our amplitudes agree with the later calculations using series solutions and with the small- p_T expansion in the relevant region

Brønnum-Hansen, Wang 21; Degrassi, Gröber, Vitti 24

NLO QCD Corrections



Gosam (cross-checked with MadGraph and OpenLoops)

Virtual ($d\sigma^V$) and Real ($d\sigma^R$) parts not separately finite for $\epsilon \to 0$ 1) UV renormalize: α_s in $\overline{\text{MS}}$ & top quark mass in OS scheme 2) IR structure well known @ NLO subtract divergences from V add them back to R

q_T -scheme:

$$\mathcal{A}_{i}^{(0),\text{fin}} = \mathcal{A}_{i}^{(0),\text{UV}},$$

 $\mathcal{A}_{i}^{(1),\text{UV}} - I_{1}\mathcal{A}_{i}^{(0),\text{UV}},$

$$I_{1} = I_{1}^{\text{soft}} + I_{1}^{\text{coll}},$$

$$I_{1}^{\text{soft}} = -\frac{e^{\epsilon \gamma_{E}}}{\Gamma(1-\epsilon)} \left(\frac{\mu_{R}^{2}}{s}\right)^{\epsilon} \left(\frac{1}{\epsilon^{2}} + \frac{i\pi}{\epsilon}\right) 2C_{A},$$

$$I_{1}^{\text{coll}} = -\frac{\beta_{0}}{\epsilon} \left(\frac{\mu_{R}^{2}}{s}\right)^{\epsilon}.$$

Catani, Cieri, de Florian, Ferrera, Grazzini 14

Amplitudes

First present results for the Born and Born-Virtual interference helicity amplitudes

Expand the helicity amplitudes in α_S

$$\mathscr{M}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{fin} = \left(\frac{\alpha_s}{2\pi}\right)\mathscr{M}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{(1)} + \left(\frac{\alpha_s}{2\pi}\right)^2 \mathscr{M}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{(2)} + \dots$$

Compute the square/interference

$$\mathcal{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{(1)} = |\mathcal{M}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{(1)}|^2,$$

$$\mathcal{V}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{(2)} = 2 \operatorname{Re} \left(\mathcal{M}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{*(1)} \mathcal{M}_{\lambda_1\lambda_2\lambda_3\lambda_4}^{(2)} \right)$$

We also define

$$\mathscr{V}_{\lambda_{3}\lambda_{4}}^{(i)} = \frac{1}{4} \sum_{\lambda_{1},\lambda_{2}} \mathscr{V}_{\lambda_{1}\lambda_{2}\lambda_{3}\lambda_{4}}^{(i)} \text{ and } \mathscr{V}^{(i)} = \sum_{\lambda_{3},\lambda_{4}} \mathscr{V}_{\lambda_{3}\lambda_{4}}^{(i)}$$

 $2 \rightarrow 2$ amplitude depends on two kinematic variables (after fixing masses)

Choose:

$$s = (p_1 + p_2)^2$$

 θ_z - angle in c.o.m frame between p_1 -axis and p_3



Comparison to Expansion



Expanded results from: Davies, Mishima, Steinhauser, Wellmann 20

Expansion can be improved by fitting Padé approximants & conformal mapping, have not compared to these approaches Campbell, Ellis, Czakon, Kirchner 16; Davies, Mishima, Schönwald, Steinhauser 23

Scheme Dependence

Can change the subtraction scheme of our finite virtuals with shifts \propto Born

 $A_i^{(1),\text{fin},C} = A_i^{(1),\text{fin}} + \Delta I_C A_i^{(0),\text{fin}}$

$$\Delta \mathbf{I}_{\rm C} = -\frac{1}{2}\pi^2 C_A + i\pi\beta_0,$$

$$\Delta \mathbf{I}_{\rm CS} = -i\pi C_A \left(\frac{1}{\epsilon} + \ln\left(\frac{\mu_R^2}{s}\right)\right) - \frac{\pi^2 C_A}{3} + \beta_0 + k_g$$

This significantly impacts the level of agreement of the full virtual vs expansions



Observation: quality of an approximation depends strongly on the scheme

Top-Quark Only NLO QCD Corrections

We find that the NLO corrections considering only massive quarks are not small!

Size of virtual contribution varies between different schemes (NLO result is independent of scheme)

→ Some schemes are better when virtual phase-space statistics limited

Approximation obtained by applying the massless K-factor to the massive born ~agrees within scale uncertainty



Agarwal, SPJ, Kerner, von Manteuffel 24

We also have the complete **Class A+B+C** NLO QCD corrections implemented, Let's examine the interference patterns



Observe the unitarizing behaviour of the massive & Higgs-mediated amplitudes Above ~ $2m_t$ significant destructive interference between A_h and C, LO and NLO Putting it all together: complete NLO corrections are indeed large, K-factor ~ 1.7

NLO corrections reduce the scale uncertainties significantly

 $\sigma_{\rm LO} = 1316^{+23.0\%}_{-18.0\%} \,\text{fb}$ $\sigma_{\rm NLO} = 2275(12)^{+14.0\%}_{-12.0\%} \,\text{fb}$

Approximation obtained by applying the massless Kfactor to the massive born agrees well within the scale uncertainty, also for the invariant mass distribution



Agarwal, SPJ, Kerner, von Manteuffel 24

Conclusion

Z-boson Pair Production in Gluon-Fusion

NLO corrections are indeed very significant, also for massive amplitudes (~100% enhancement) Size of finite remainder depends strongly on subtraction scheme Approx. based on rescaling the massive Born by massless K-factor quite good for unpol. cross-section Huge cancellations between Higgs and top-quark contributions, sensitive to exact SM couplings Potential to examine p_T , longitudinal cross-section, anomalous couplings at NLO...

Sector Decomposition

New disteval integrator: ~3-10x faster than old intlib Median lattice rules provide lattices of unlimited size, smaller fluctuations in error Can now accept GiNaC compatible coefficient input Work in progress: potential to avoid contour deformation in some cases provides huge speedups

Thank you for listening!

Backup

Periodizing Transforms

Sector decomposed functions are typically continuous and smooth but not periodic Functions can be periodized by a suitable change of variables: $\mathbf{x} = \phi(\mathbf{u})$

$$I[f] \equiv \int_{[0,1]^d} d\mathbf{x} \ f(\mathbf{x}) = \int_{[0,1]^d} d\mathbf{u} \ \omega_d(\mathbf{u}) f(\phi(\mathbf{u}))$$

$$\phi(\mathbf{u}) = (\phi(u_1), \dots, \phi(u_d)), \quad \omega_d(\mathbf{u}) = \prod_{j=1}^d \omega(u_j) \quad \text{and} \quad \omega(u) = \phi'(u)$$

Korobov transform: $\omega(u) = 6u(1-u), \quad \phi(u) = 3u^2 - 2u^3$ Sidi transform: $\omega(u) = \pi/2 \sin(\pi u), \quad \phi(u) = 1/2(1 - \cos \pi t)$ Baker transform: $\phi(u) = 1 - |2u - 1|$



Weighted Function Spaces

Review: Dick, Kuo, Sloan 13

Assign weights $\gamma_{\mathfrak{u}}$ to each subset of dimension $\mathfrak{u} \subseteq \{1, \ldots, d\}$

Sobolev Space

Functions with square integrable first derivatives

Korobov Space

Periodic functions which are α times differentiable in each variable

Generating vector **z** precomputed for a **fixed** number of lattice points, chosen to minimise worst-case error Nuyens 07

Interesting Example



$$= \int_0^\infty \mathrm{d}x_0 \dots \mathrm{d}x_7 \frac{\mathcal{U}(\mathbf{x})^{4\epsilon}}{\mathcal{F}(\mathbf{x};\mathbf{s})^{2+3\epsilon}} \delta(1-x_7)$$

 $\mathcal{U}(\alpha) = \alpha_0 \alpha_2 \alpha_4 + \alpha_0 \alpha_2 \alpha_5 + \alpha_0 \alpha_2 \alpha_6 + (29 \text{ terms})$

$$\begin{aligned} \mathscr{F}(\boldsymbol{\alpha};\mathbf{s}) &= -s_{12} \left(\alpha_1 \alpha_4 - \alpha_0 \alpha_5 \right) \left(\alpha_3 \alpha_6 - \alpha_2 \alpha_7 \right) - s_{13} \left(\alpha_1 \alpha_2 - \alpha_0 \alpha_3 \right) \left(\alpha_5 \alpha_6 - \alpha_4 \alpha_7 \right), \\ \\ \frac{\partial \mathscr{F}(\boldsymbol{\alpha};\mathbf{s})}{\partial \alpha_0} &= s_{12} \alpha_5 (\alpha_3 \alpha_6 - \alpha_2 \alpha_7) + s_{13} \alpha_3 (\alpha_5 \alpha_6 - \alpha_4 \alpha_7), \\ \\ \vdots \\ \frac{\partial \mathscr{F}(\boldsymbol{\alpha};\mathbf{s})}{\partial \alpha_7} &= s_{12} \alpha_2 (\alpha_1 \alpha_4 - \alpha_0 \alpha_5) + s_{13} \alpha_4 (\alpha_1 \alpha_2 - \alpha_0 \alpha_3) \end{aligned}$$

Can have a leading Landau singularity with generic kinematics (arbitrary s_{12}, s_{13}) when each factor of \mathcal{F} vanishes!

Resolution

1) Rescale parameters to *linearise* singular surfaces

$$\mathcal{F}(\boldsymbol{\alpha}; \mathbf{s}) = -s_{12} \left(\alpha_1 \alpha_4 - \alpha_0 \alpha_5 \right) \left(\alpha_3 \alpha_6 - \alpha_2 \alpha_7 \right) - s_{13} \left(\alpha_1 \alpha_2 - \alpha_0 \alpha_3 \right) \left(\alpha_5 \alpha_6 - \alpha_4 \alpha_7 \right)$$
$$\alpha_0 \to \alpha_0 \alpha_1, \ \alpha_2 \to \alpha_2 \alpha_3, \ \alpha_4 \to \alpha_4 \alpha_5, \ \alpha_6 \to \alpha_6 \alpha_7$$
$$\mathcal{F}(\boldsymbol{\alpha}; \mathbf{s}) = \alpha_1 \alpha_3 \alpha_5 \alpha_7 \left[-s_{12} (\alpha_4 - \alpha_0) (\alpha_6 - \alpha_2) - s_{13} (\alpha_2 - \alpha_0) (\alpha_6 - \alpha_4) \right]$$

2) Split the integral by imposing $\alpha_i \ge \alpha_j \ge \alpha_k \ge \alpha_l$

$$\begin{aligned} \alpha_0 &\to \alpha_0 + \alpha_2 + \alpha_4 + \alpha_6, \\ \alpha_2 &\to \alpha_2 + \alpha_4 + \alpha_6, \\ \alpha_4 &\to \alpha_4 + \alpha_6, \\ \alpha_6 &\to \alpha_6 \end{aligned} + perms$$

$$\mathcal{F}_{1}(\boldsymbol{\alpha}; \mathbf{s}) = \alpha_{1}\alpha_{3}\alpha_{5}\alpha_{7} \left[-s_{12}(\alpha_{0} + \alpha_{2})(\alpha_{2} + \alpha_{4}) - s_{13}(\alpha_{0})(\alpha_{4}) \right]$$

$$\mathcal{F}_{2}(\boldsymbol{\alpha}; \mathbf{s}) = \alpha_{1}\alpha_{3}\alpha_{5}\alpha_{7} \left[-s_{12}(\alpha_{2})(\alpha_{0} + \alpha_{2} + \alpha_{6}) + s_{13}(\alpha_{0})(\alpha_{6}) \right]$$

$$\vdots$$

$$\mathcal{F}_{24}(\boldsymbol{\alpha}; \mathbf{s}) = \alpha_{1}\alpha_{3}\alpha_{5}\alpha_{7} \left[-s_{12}(\alpha_{2} + \alpha_{4})(\alpha_{4} + \alpha_{6}) - s_{13}(\alpha_{2})(\alpha_{6}) \right]$$

All coefficients of s_{12}, s_{13} now have definite sign

NoCD: Avoiding Contour Deformation

Idea:

1. Construct transformations of the Feynman parameters which map the zeroes of the \mathcal{F} -polynomial to the boundary of integration



Figure: Thomas Stone

NoCD: Avoiding Contour Deformation

Idea:

2. For transformations which make \mathscr{F} non-positive extract an overall minus sign (using the $i\delta$ prescription to generate the physically correct imaginary part)

3. Stitch together the resulting integrals

$$I = \sum_{n_{+}=1}^{N_{+}} I_{n_{+}}^{+} + (-1 - i\delta)^{-(\nu - LD/2)} \sum_{n_{-}=1}^{N_{-}} I_{n_{-}}^{-}$$

The individual integrals $\{I_{n_+}^+, I_{n_-}^-\}$ have manifestly non-negative integrands \implies no contour deformation, trivial analytic continuation, faster to integrate

NoCD: Example 3

For s > -t > 0, two of the 6 independent integrals require contour deformation:

$$\mathcal{F}_{3} = x_{1}x_{3}x_{5}x_{7} \left[-sx_{0}x_{2} + |t| \left(x_{0} + x_{4} \right) \left(x_{2} + x_{4} \right) \right]$$
$$\mathcal{F}_{5} = x_{1}x_{3}x_{5}x_{7} \left[sx_{6} \left(x_{0} + x_{2} + x_{6} \right) - |t| \left(x_{0} + x_{6} \right) \left(x_{2} + x_{6} \right) \right]$$

Can express each of these in terms of 4 manifestly non-negative integrands

Putting the pieces together for the full integral:

$$I = \sum_{n_{+}=1}^{8} I_{n_{+}}^{+} + (-1 - i\delta)^{-2 - 3\varepsilon} \sum_{n_{-}=1}^{4} I_{n_{-}}^{-}$$

Verified result numerically against known analytic result

Henn, Mistlberger, Smirnov, Wasser 20; Bargiela, Caola, von Manteuffel, Tancredi 21

NoCD: Example 3

Can now obtain results numerically ($s_{12} = 1, s_{13} = -1/5$)

$$\begin{split} I_3 &= \epsilon^{-4} \left[(18.5195704502 - 15.707988011i) \pm (5.897 \cdot 10^{-5} + 5.897 \cdot 10^{-5}i) \right] + \dots \\ I_3^{\text{NoCD}} &= \epsilon^{-4} \left[(18.51948920208488 - 15.70796326794897i) \pm (4.032 \cdot 10^{-11} + 4.592 \cdot 10^{-11}i) \right] + \dots \\ I_5 &= \epsilon^{-4} \left[(12.7432949988 - 23.561968275i) \pm (1.605 \cdot 10^{-5} + 1.415 \cdot 10^{-5}i) \right] + \dots \\ I_5^{\text{NoCD}} &= \epsilon^{-4} \left[(12.74326269721394 - 23.5619449018131i) \pm (4.125 \cdot 10^{-11} + 6.919 \cdot 10^{-11}i) \right] + \dots \end{split}$$

Full result after a few minutes integration with pySecDec:

$$I = \epsilon^{-4} \left[8.34055 - 52.3608i \right] + \mathcal{O} \left(\epsilon^{-3} \right)$$
$$I^{\text{NoCD}} = \epsilon^{-4} \left[8.340040392028 - 52.3598775598347i \right] + \mathcal{O} \left(\epsilon^{-3} \right)$$
$$I^{\text{analytic}} = \epsilon^{-4} \left[8.34004039223768 - 52.35987755984493i \right] + \mathcal{O} \left(\epsilon^{-3} \right)$$

Numerics are much, much faster and more stable