Numerical Multi-loop Computations: HJ and HH production at the LHC

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Outline

Motivation

Framework & the heavy top-quark limit

Gluon fusion

- (HJ) Higgs boson + jet production history
- (HH) Di-Higgs boson production history

NLO (2-loop) calculation including the full top-quark mass

Numerical multi-loop calculations

- Sector decomposition
- Quasi-Monte Carlo integration

Results & comparisons

HJ & HH

Motivation - Precision Higgs Physics

Higgs physics has transformed from discovery to precision study

Data are becoming more precise also for more differential observables

CMS 17: Search for boosted $H \rightarrow b\bar{b}$

 $p_T > 450 \text{ GeV}$

$$\sigma(H \to b\bar{b}) = 74 \pm 48(\text{stat})^{-10}_{+17}(\text{syst}) \text{ fb}$$





At moderate/large pT:

- Particles in the loop can be resolved
- May disentangle modified top quark Yukawa coupling from (BSM) point-like ggH coupling

Motivation - Higgs self-coupling

Standard Model Higgs Lagrangian:

$$\mathcal{L} \supset -V(\phi), \quad V(\Phi) = -\mu^2 (\Phi^{\dagger} \Phi) + \lambda (\Phi^{\dagger} \Phi)^2$$

EW symmetry breaking

$$V(H) = \frac{1}{2} m_H^2 H^2 + \frac{\lambda v H^3}{4} + \frac{\lambda}{4} H^4, \quad \begin{array}{l} \mu^2 = \lambda v^2 \\ m_H^2 = 2\lambda v^2 \end{array}$$
 SM: self-couplings
determined by m_H, v
Higgs pair production probes

triple-Higgs coupling



Higgs self-coupling not yet measured! Extremely challenging to measure at LHC due to $\mathcal{O}(fb)$ cross section and difficult backgrounds

Data & Constraints

HH extremely challenging to measure, combining $b\bar{b}b\bar{b}, b\bar{b}\tau^+\tau^-, b\bar{b}\gamma\gamma$ $\leq 6.7 \; \sigma_{
m SM}$ atlas-conf-2018-043 Several other promising ideas to obtain limits on λ_3 : **Electroweak corrections** 9 0000000 O_6 to single H production t (also VBF, VH) g $\infty \infty \infty \infty$ Gorbahn, Haisch 16; Bizoń, Gorbahn, Haisch, Zanderighi 16; Degrassi, Giardino, Maltoni, Pagani 16; Maltoni, Pagani, Shivaji, Zhao 17; Di Vita, Grojean, Panico, Riembau, Vantalon 17 Modification of precision EW observables (EW oblique corrections) S, TDegrassi, Fedele, Giardino 17; Kribs, Maier, Rzehak, Spannowsky, Waite 17;

Limits on λ_4 : from (partial) EW corrections to HH Bizon, Haisch, Rottoli 18; Borowka, Duhr, Maltoni, Pagani, Shivaji, Zhao 18

QCD Factorisation

Focus of this talk will be on the computation of higher order perturbative QCD corrections to HJ and HH production at the LHC

$$d\sigma = \int dx_a dx_b f(x_a) f(x_b) d\hat{\sigma}_{ab}(x_a, x_b) F_J + \mathcal{O}\left((\Lambda/Q)^m\right)$$
PDFs/ Input parameters Hard Scattering Non-perturbative Matrix Element effects ~ few % (Focus of this talk)

With $\alpha_s \sim 0.1$

Typically: NLO ~ 10% correction, NNLO ~ 1% correction

However, there are important exceptions:

- Higgs Boson production (NLO ~100%, NNLO ~10%, N3LO ~ 2%)
- New partonic channels can open (e.g. di-boson production)

and

• Distributions can be modified substantially (even if σ_{tot} is stable)

Heavy top quark limit

Heavy top quark limit (HTL): $m_T \to \infty$

Introduces effective tree-level coupling between Higgs and gluons Lowers the number of loops by 1



HTL valid for: $\sqrt{\hat{s}} \ll 2m_T$ HJ: Does not describe well high p_T region HH: $2m_H < \sqrt{\hat{s}}$

HJ Production History

1. LO (full m_T dependence)

Ellis, Hinchliffe, Soldate, van der Bij 87 Baur, Glover 89

2. NLO

Heavy Top Quark Limit

de Florian, Grazzini, Kunszt 99; Glosser, Schmidt 02; Ravindran, Smith, van Neerven 02

Approximate m_T dependence

Harlander, Neumann, Ozeren, Wiesemann 12; Neumann, Wiesemann 14; Buschmann, Goncalves, Kuttimalai, Schonherr, Krauss, Plehn 14; Frederix, Frixione, Vryonidou, Wiesemann 16; Neumann, Williams 16; Caola, Forte, Marzani, Muselliand, Vita 16; Braaten, Zhang, Zhang 17; Lindert, Kudashkin, Melnikov, Wever 18; Neumann 18;

Top quark/Bottom quark interference

(Lindert,) Melnikov, Tancredi, Wever 16, 17; Caola, Lindert, Melnikov, Monni, Tancredi, Wever 18

3. NNLO Heavy Top Quark Limit

Boughezal, Caola, Melnikov, Petriello, Schulze 13, 14; Chen, (Martinez,) Gehrmann, Glover, Jaquier 14, 16; Boughezal, Focke, Giele, Liu, Petriello 15; Bizon, Chen, Gehrmann-De Ridder, Gehrmann, Glover, Huss, Monni, Re, Rottoli, Torrielli 18

K≈1.2

K≈1.8





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HH Production History

1. LO (full m_T dependence) Glover, van der Bij 88

2. NLO

Heavy Top Quark Limit

Dawson, Dittmaier, Spira 98

Approximate m_T dependence

Grigo, Hoff, Melnikov, Steinhauser 13; Grigo, Hoff 14; Grigo, Hoff, Steinhauser 15; Maltoni, Vryonidou, Zaro 14;

3. NNLO Heavy Top Quark Limit

de Florian, Mazzitelli 13; Grigo, Melnikov, Steinhauser 14; Shao, Li, Li, Wang 13; de Florian, Mazzitelli 15; de Florian, Grazzini, Hanga, Kallweit, Lindert, Maierhöfer, Mazzitelli, Rathlev 16

Approximate m_T dependence

Grigo, Hoff, Steinhauser 15;

4. (Partial) N3LO Heavy Top Quark Limit Banerjee, Borowka, Dhani, Gehrmann, Ravindran 18





Calculation

The Goal

NLO QCD corrections to HJ/HH production with full top quark mass: \leq 7 propagator, 4-point, 2-loop diagrams, 4 mass scales (s, t, m_T, m_H)



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The Difficulty

What makes these processes so difficult to calculate?

One traditional method:

- 1. Decompose amplitude into form factors & construct projectors (**minutes**)
- 2. Generate Feynman diagrams (**seconds**)
- 3. Apply projectors & compute amplitude (hours/days)
- 4. Integral reduction (6+ months)
- 5. Compute master integrals (analytic: challenging, numeric: ~seconds/hours)
- 6. Generate events & compute (differential) cross-section

(analytic: seconds?, numeric: ~hours/days)

We applied this method (computing the integrals numerically) to both HH and HJ. Let us take a closer look at these steps for the case of HJ...

Form Factor Decomposition (HJ Gluon)

Expose tensor structure:
$$\mathcal{M} = \epsilon_{\mu}(p_{1})\epsilon_{\nu}(p_{2})\epsilon_{\tau}(p_{3})\mathcal{M}^{\mu\nu\tau}$$

Form Factors (Contain integrals)
 $\mathcal{M}_{physical}^{\mu\nu\tau} = F_{212}T_{212}^{\mu\nu\tau} + F_{332}T_{332}^{\mu\nu\tau} + F_{311}T_{311}^{\mu\nu\tau} + F_{312}T_{312}^{\mu\nu\tau}$
Choose tensor basis (constructed from external momenta & metric):
 $T_{212}^{\mu\nu\tau} = (s_{12}g^{\mu\nu} - 2p_{2}^{\mu}p_{1}^{\nu})(s_{23}p_{1}^{\tau} - s_{13}p_{2}^{\tau})/(2s_{13})$
 $T_{312}^{\mu\nu\tau} = (s_{13}g^{\nu\tau} - 2p_{3}^{\nu}p_{2}^{\tau})(s_{13}p_{2}^{\mu} - s_{12}p_{3}^{\mu})/(2s_{23})$
 $T_{311}^{\mu\nu\tau} = (s_{13}g^{\tau\mu} - 2p_{1}^{\tau}p_{3}^{\mu})(s_{12}p_{3}^{\nu} - s_{23}p_{1}^{\nu})/(2s_{23})$
 $T_{312}^{\mu\nu\tau} = \left(g^{\mu\nu}(s_{23}p_{1}^{\tau} - s_{13}p_{2}^{\tau}) + g^{\nu\tau}(s_{23}p_{2}^{\mu} - s_{12}p_{3}^{\mu}) + g^{\tau\mu}(s_{12}p_{3}^{\nu} - s_{23}p_{1}^{\nu}) + 2p_{3}^{\mu}p_{1}^{\nu}p_{2}^{\tau} - 2p_{2}^{\mu}p_{3}^{\nu}p_{1}^{\tau}\right)/2$
Build projectors P such that: $P_{\mu\nu\tau}^{212} \mathcal{M}^{\mu\nu\tau} = F_{212}$, etc...
With this choice form for term are series into a deploted by a calling a grave totic response to the series into a deploted by a calling a grave totic response totic respon

With this choice form factors are gauge invariant and related by cyclic permutations:

 $F_{311}(s_{23}, s_{12}, s_{13}) = F_{332}(s_{13}, s_{23}, s_{12}) = F_{212}(s_{12}, s_{13}, s_{23})$ $F_{312}(s_{23}, s_{12}, s_{13}) = F_{312}(s_{13}, s_{23}, s_{12}) = F_{312}(s_{12}, s_{13}, s_{23})$

Note: Need to generate code only for 2 form factors and use it to compute all In reality we generate code for all form factors and use this symmetry as a cross-check

Reduction (IBPs)

Integration by parts Identities: **Joop/external momentum** $\int \mathrm{d}^d p_i \frac{\partial}{\partial p_i^{\mu}} \left[q^{\mu} \mathbf{I}'(p_1, \dots, p_l; k_1, \dots, k_m) \right] = 0$

Produce linear relations between integrals Tkachov 81; Chetyrkin 81

Can perform e.g. Gaussian elimination on system of equations Relate integrals to a smaller set of Master integrals

Example:

$$I_{\alpha_1 \alpha_2 \alpha_3} = \int \frac{\mathrm{d}^d p}{i\pi^{d/2}} \frac{1}{D_1^{\alpha_1} D_2^{\alpha_2} D_3^{\alpha_3}}$$
$$k_1^2 = k_2^2 = 0, k_3^2 = s$$
$$D_1 = p^2$$
$$D_2 = (p+k_1)^2$$
$$D_3 = (p+k_1+k_2)^2$$

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^(d-4)
$$I_{111} - I_{102} - I_{201} = 0$$

 $sI_{102} + (d-3)I_{101} = 0$
 $sI_{201} + (d-3)I_{101} = 0$

$$\therefore I_{111} = \frac{-2(d-3)}{s(d-4)}I_{101}$$

HJ Integral Families



HJ Integral Families (II)

All 2-loop HJ integrals can be written in terms of 3 integral families:

	F1	F2	F3
D_1	$k_1^2 - m_T^2$	k_{2}^{2}	$k_1^2 - m_T^2$
D_2	$(k_1 + p_1)^2 - m_T^2$	$(k_2 + p_1)^2$	$(k_1 + p_1)^2 - m_T^2$
D_3	$(k_1 - p_2)^2 - m_T^2$	$(k_2 - p_2)^2$	$(k_1 - p_2 - p_3)^2 - m_T^2$
D_4	$(k_1 - p_2 - p_3)^2 - m_T^2$	$(k_2 - p_2 - p_3)^2$	$k_{2}^{2} - m_{T}^{2}$
D_5	$k_{2}^{2} - m_{T}^{2}$	$k_1^2 - m_T^2$	$(k_2 + p_1)^2 - m_T^2$
D_6	$(k_2 + p_1)^2 - m_T^2$	$(k_1 + p_1)^2 - m_T^2$	$(k_2 - p_3)^2 - m_T^2$
D_7	$(k_2 - p_2)^2 - m_T^2$	$(k_1 - p_2)^2 - m_T^2$	$(k_1 - k_2)^2$
D_8	$(k_2 - p_2 - p_3)^2 - m_T^2$	$(k_1 - p_2 - p_3)^2 - m_T^2$	$(k_1 - k_2 - p_2)^2$
D_9	$(k_1 - k_2)^2$	$(k_1 - k_2)^2 - m_T^2$	$(k_1 - k_2 - p_2 - p_3)^2$

Melnikov, Tancredi, Wever 16

Integrals written as:

$$I_{\alpha_1,\ldots,\alpha_9}^{F_j} = \int \mathrm{d}^d k_1 \int \mathrm{d}^d k_2 \frac{1}{D_1^{\alpha_1} \cdots D_9^{\alpha_9}}$$

HJ Integral Reduction

Full IBP reduction achieved with (modified) Reduze2 Chetyrkin, Tkachov 81; Laporta 01; von Manteuffel, Studerus 12

Unreduced Amplitude

- 3767 Integrals
- Up to 3 inverse propagators for 7-propagator integrals
- Up to 4 inverse propagators for factoring 6-propagator integrals

Reduced Amplitude

- 458 Integrals
- Up to 6 master integrals per sector, e.g:



Sector also known to be elliptic Frellesvig, Loops & Legs 2018

HJ Integral Reduction (II)

Reduze2 Modifications:

- Change order of solving system of equations, sort by number of unreduced integrals (prefer fewer)
- Specify list of required integrals, consider only equations containing these integrals
- Improve mechanism for pausing/resuming reductions

Reduction achieved using 2 different setups:

Symbolic mass dependence

Reduction directory size: **1.1 TB** Can include m_B, Γ_T setups: Current calculation uses only this result Fix mass ratio $\frac{m_H^2}{m_T^2} = \frac{12}{23} \rightarrow \begin{array}{c} m_H = 125 \text{ GeV} \\ m_T = 173.055 \text{ GeV} \end{array}$ Reduction directory size: 0.25 TB Can not include m_B, Γ_T

Finite Basis

Always possible to pick finite basis of integrals using:

- Dimension Shifts Tarasov 96; Lee 10
- Dots

Panzer 14; von Manteuffel, Panzer, Schabinger 15

Finding finite integrals and basis change implemented in Reduze2.1

Finite basis greatly improves numerical performance (but requires reduction of integrals with up to 2 inverse props and 2 dots)

	Finite Basis			Conventional			
	$(6-2\epsilon)$	201 s	2.34×10^{-4}	$(4-2\epsilon)$	384 s	8.12×10^{-4}	
Two-loop	$(6-2\epsilon)$	150 s	4.83×10^{-4}	$(4-2\epsilon)$	56538 s	1.67×10^{-2}	
EW-QCD	$(6-2\epsilon)$	280 s	1.00×10^{-3}	$(4-2\epsilon)$	214135 s	8.29×10^{-3}	
Drell-Yan	$(6-2\epsilon)$	294 s	1.21×10^{-3}	$(4-2\epsilon)$	3484378 s	30.9	_
von Manteuffel, Schabinger 17	$(4-2\epsilon)$ $(6-2\epsilon)$	91 s	3.76×10^{-4}	$(4-2\epsilon)$ $(4-2\epsilon)$ (s)	87 s	3.76×10^{-4}	
Sendoniger 17	$(0-2\epsilon)$ (s)	17 s	$5.15 imes 10^{-4}$	$(4-2\epsilon)$	20 s	$1.95 imes 10^{-4}$	← ^{Rel.} Err.
	$(0-2\epsilon)$ (s)	119 s	2.32×10^{-3}	$(4-2\epsilon)$ (s)	118 s	2.12×10^{-3}	
	Total/Max:	3995 s	5.84×10^{-3}	Total/Max:	5136862 s	30.9	1

Computing the integrals: numerical multi-loop computations

Analytic Results (so far)

 $(k_2+p_1)^2$

 $(k_2+p_1)^2(k_1-p_3)^2$

Planar integrals contributing to HJ at 2-loop are known analytically Bonciani, Del Duca, Frellesvig, Henn, Moriello, Smirnov 16; (See also Primo, Tancredi 16)

Most integrals:

- Canonical basis found
- \log, Li_2 up to weight 2
- 1-fold integrals at weights 3,4
- Alphabet with 3 variables, 49 letters, many square roots

Two sectors expressed in terms of $\boxed{}$ $(k_2+p_1)^2$ $(k_1-p_3)^2$

- 2- and 3-fold iterated integrals
- Elliptic kernel

Non-planar integrals not currently known analytically, but subject to ongoing work by other group(s) Bonciani, Del Duca, Frellesvig, Henn, Moriello, Smirnov, ...

Integration

Many methods to evaluate Feynman integrals

Here I will focus on the method of **Sector Decomposition**, a technique which enables dimensionally regulated parameter integrals to be integrated **numerically**

1) Feynman Parametrise integral and compute momentum integrals

$$G = (-1)^{N_{\nu}} \frac{\Gamma(N_{\nu} - LD/2)}{\prod_{j=1}^{N} \Gamma(\nu_j)} \int_0^\infty \prod_{j=1}^{N} \mathrm{d}x_j \ x_j^{\nu_j - 1} \delta(1 - \sum_{i=1}^{N} x_i) \frac{\mathcal{U}^{N_{\nu} - (L+1)D/2}(\vec{x})}{\mathcal{F}^{N_{\nu} - LD/2}(\vec{x}, s_{ij})}$$

Here \mathcal{U}, \mathcal{F} are 1st, 2nd Symanzik Polynomials

Have exchanged L D-dim. momentum integrals for N param. integrals

Sector Decomposition

2) After integrating out δ we are faced with integrals of the form:

$$G_{i} = \int_{0}^{1} \left(\prod_{j=1}^{N-1} \mathrm{d}x_{j} x_{j}^{\nu_{j}-1} \right) \frac{\mathcal{U}_{i}(\vec{x})^{\exp \mathcal{U}(\epsilon)}}{\mathcal{F}_{i}(\vec{x}, s_{ij})^{\exp \mathcal{F}(\epsilon)}} \xrightarrow{\mathsf{Powers depending on } \epsilon}_{\mathsf{Polynomials in F.P}}$$

Which may contain overlapping singularities which appear when several $x_j \rightarrow 0$ simultaneously (corresponding to UV/IR singularities) Sector decomposition maps each integral into integrals of the form:

$$G_{ik} = \int_0^1 \left(\prod_{j=1}^{N-1} \mathrm{d}x_j x_j^{a_j - b_j \epsilon} \right) \frac{\mathcal{U}_{ik}(\vec{x})^{\exp \mathcal{U}(\epsilon)}}{\mathcal{F}_{ik}(\vec{x}, s_{ij})^{\exp \mathcal{F}(\epsilon)}}$$

 $\mathcal{U}_{ik}(\vec{x}) = 1 + u(\vec{x})$ $\mathcal{F}_{ik}(\vec{x}) = -s_0 + f(\vec{x})$ $u(\vec{x}), f(\vec{x})$ Singularity structure can be read off $u(\vec{x}), f(\vec{x})$ have no constant term

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

Sector Decomposition (II)

One technique **Iterated Sector Decomposition** repeat: Binoth, Heinrich 00 $\int_{0}^{1} \mathrm{d}x_{1} \int_{0}^{1} \mathrm{d}x_{2} \frac{1}{(x_{1}+x_{2})^{2+\epsilon}} \quad \longleftarrow \text{ Overlapping singularity for } x_{1}, x_{2} \to 0$ $= \int_{0}^{1} \mathrm{d}x_{1} \int_{0}^{1} \mathrm{d}x_{2} \frac{1}{(x_{1} + x_{2})^{2+\epsilon}} (\theta(x_{1} - x_{2}) + \theta(x_{2} - x_{1}))$ $= \int_{0}^{1} \mathrm{d}x_{1} \int_{0}^{x_{1}} \mathrm{d}x_{2} \frac{1}{(x_{1} + x_{2})^{2+\epsilon}} + \int_{0}^{1} \mathrm{d}x_{2} \int_{0}^{x_{2}} \mathrm{d}x_{1} \frac{1}{(x_{1} + x_{2})^{2+\epsilon}}$ $= \int_{0}^{1} \mathrm{d}x_{1} \int_{0}^{1} \mathrm{d}t_{2} \frac{x_{1}}{(x_{1} + x_{1}t_{2})^{2+\epsilon}} + \int_{0}^{1} \mathrm{d}x_{2} \int_{0}^{1} \mathrm{d}t_{1} \frac{x_{2}}{(x_{2}t_{1} + x_{2})^{2+\epsilon}}$ $= \int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}t_2 \frac{x_1^{-1-\epsilon}}{(1+t_2)^{2+\epsilon}} + \int_0^1 \mathrm{d}x_2 \int_0^1 \mathrm{d}t_1 \frac{x_2^{-1-\epsilon}}{(t_1+1)^{2+\epsilon}} - \mathbf{Singularities factorised}$

If this procedure terminates depends on order of decomposition steps An alternative strategy **Geometric Sector Decomposition** always terminates; both strategies are implemented in pySecDec. Kaneko, Ueda 10; See also: Bogner, Weinzierl 08; Smirnov, Tentyukov 09

Sector Decomposition (III)

3) Expand in ϵ (simple case a = -1 "Logarithmic Divergence"):



By Definition: $g(0) \neq 0, g(0)$ finite

4) Numerically integrate

Key Point: Sector Decomposed integrals can be expanded in ϵ and numerically integrated

Numerical Integration

$$I[f] \equiv \int_{[0,1]^d} d\mathbf{x} \ f(\mathbf{x}) \quad \approx \quad Q[f] = \frac{1}{N} \sum_{i=1}^N w_i \ f(\mathbf{x}_i)$$

Goal: select points to minimise integration error $\varepsilon \equiv |I[f] - Q[f]|$

Monte Carlo:

Randomly select sampling points $\varepsilon\approx {\rm Var}[f]/\sqrt{N}, \quad \varepsilon\sim \mathcal{O}(N^{-1/2})$ Improves slowly with N

Quasi-Monte Carlo

Select points with low discrepancy D_N $\varepsilon \leq D_N \cdot V[f], \quad \varepsilon \sim \mathcal{O}(\log^d(N)/N)$ Poor performance for large d



Quasi-Monte Carlo (Rank 1 Lattices)

Quasi-Monte Carlo In a Weighted Function Space (QMC)

First application to sector-decomposed loop integrals: Li, Wang, Yan, Zhao 15 $\varepsilon \leq e_{\gamma} \cdot ||f||_{\gamma}, \quad \varepsilon \sim \mathcal{O}(N^{-1}) \text{ or better}$ $I[f] \approx \bar{Q}_{n,m}[f] \equiv \frac{1}{m} \sum_{k=0}^{m-1} Q_n^{(k)}[f], \quad Q_n^{(k)}[f] \equiv \frac{1}{n} \sum_{i=0}^{n-1} f\left(\left\{\frac{i\mathbf{z}}{n} + \mathbf{\Delta}_k\right\}\right)$ - Generating vec. \mathbf{Z} 0.8 Δ_k - Random shift vec. 0.6 {} - Fractional part \mathbf{Z} \overline{n} • 0.4 n - # Lattice points 0.2 0.2 0.0 **⊾** 0.0 m - # Random shifts 0.0 1.0 0.0 0.2 0.4 0.6 0.8 0.2 0.4 0.6 0.8 1.0

Unbiased error estimate computed using (10-50) random shifts

1 Shift

4 Shifts

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

. 2

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

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: $\phi(u) = 1 - |2u - 1|$



Scaling



High Performance Computing

Accuracy limited by number of function evaluations Can accelerate this using Graphics Processing Units (GPUs)



Note:

Plot made for old OpenCL implementation (new CUDA impl. similar)
 Performance gain highly dependent on integrand & hardware!

Variance Reduction

Can improve performance of numerical integrator by flattening integrand via a variable transformation y = p(x)

$$I = \int_0^1 dy \ f(y) = \int_0^1 dx \ p'(x) f(p(x)) \quad \text{s.t.} \quad p'(x) \propto |f(p(x))|^{-1}$$

VEGAS:

Assume integrand separable $f(\mathbf{x}) = g(x_1)g(x_2)\cdots g(x_d)$ Iteratively approximate p(x) with piecewise linear function **But:** Spoils smoothness of integrand (bad for QMC)

Alternative:

Choose a smooth function for p(x), for example:

$$p(x) = a_2 \cdot x \frac{a_0 - 1}{a_0 - x} + a_3 \cdot x \frac{a_1 - 1}{a_1 - x} + a_4 \cdot x + a_5 \cdot x^2 + \left(1 - \sum_{i=2}^5 a_i\right) \cdot x^3$$

Fit parameters a_i to inverse cumulative distribution function (CDF)

Variance Reduction (II)

 Pre-sample integrand
 In each dimension: fit inverse CDF
 Use fit as variable transformation, obtain flatter integrand without
 spoiling smoothness





Example: HJ Integral

Small *n*: ~ 3x improvement Large *n*: ~ 10x improvement

QMC Scaling preserved

pySecDec

pySecDec: a program to numerically evaluate dimensionally regulated parameter integrals (written in python, FORM & c++) Vermaseren 00; Kuipers, Ueda, Vermaseren 13; Ruijl, Ueda, Vermaseren 17

Code: https://github.com/mppmu/secdec/releases

Docs: https://secdec.readthedocs.io

Borowka, Heinrich, Jahn, SJ, Kerner, Schlenk, Zirke

Supports:

Contour deformation, Arbitrary loops/legs (within reason)

Soper 99; Binoth, Guillet, Heinrich, Pilon, Schubert 05; Nagy, Soper 06; Anastasiou, Beerli, Daleo 07; Beerli 08; Borowka, Carter, Heinrich 12; Borowka 14;

General parameter integrals (not just loop integrals)

Arbitrary number of regulators

Flexible numerators (contracted Lorentz vectors, inverse propagators)

Generates c++ Library (can be linked to your own program)

New: Quasi-Monte Carlo integration & CUDA GPU Support 1811.11720; Li, Wang, Yan, Zhao 15; Review: Dick, Kuo, Sloan 13; Putting it all together...

HJ Amplitude Structure

Write integrals with r propagators and s inverse propagators as

Arbitrary scale

$$I_{r,s}(\hat{s}, \hat{t}, m_h^2, m_t^2) = (M^2)^{-L\epsilon} (M^2)^{2L-r+s} I_{r,s} \left(\frac{\hat{s}}{M^2}, \frac{\hat{t}}{M^2}, \frac{m_h^2}{M^2}, \frac{m_t^2}{M^2}\right)$$

We renormalize strong coupling, a, in \overline{MS} scheme and top quark mass in OS scheme, each renormalized form factor can be written as:

$$F = a^{\frac{3}{2}} \left[F^{(1)} + a(\frac{n_g}{2} \delta Z_A + \frac{3}{2} \delta Z_a) F^{(1)} + a \delta m_t^2 F^{ct,(1)} + a F^{(2)} + O(a^2) \right]$$

$$F^{(1)} = \left(\frac{\mu_R^2}{M^2}\right)^{\epsilon} \left[b_0^{(1)} + b_1^{(1)} \epsilon + b_2^{(1)} \epsilon^2 + \mathcal{O}(\epsilon^3) \right] \quad \longleftarrow \text{ 1-loop}$$

$$F^{ct,(1)} = \left(\frac{\mu_R^2}{M^2}\right)^{\epsilon} \left[c_0^{(1)} + c_1^{(1)} \epsilon + \mathcal{O}(\epsilon^2) \right] \quad \longleftarrow \text{ Mass Counter-Terms}$$

$$F^{(2)} = \left(\frac{\mu_R^2}{M^2}\right)^{2\epsilon} \left[\frac{b_{-2}^{(2)}}{\epsilon^2} + \frac{b_{-1}^{(2)}}{\epsilon} + b_0^{(2)} + \mathcal{O}(\epsilon) \right] \quad \longleftarrow 2\text{-loop}$$

Scale variations do not require any re-computation of red terms

Amplitude Evaluation

Use Quasi-Monte Carlo (QMC) integration $\mathcal{O}(n^{-1})$ error scaling Li, Wang, Yan, Zhao 15; Review: Dick, Kuo, Sloan 13;

Implemented in OpenCL, evaluated on GPUs

Entire 2-loop amplitude evaluated with a single code

$$F = \sum_{i} \left(\sum_{j} C_{i,j} \epsilon^{j} \right) \left(\sum_{k} I_{i,k} \epsilon^{k} \right) = \epsilon^{-2} \left[C_{1,-2}^{(L)} I_{1,0}^{(L)} + \ldots \right]$$

coeff. integral
$$+ \epsilon^{-1} \left[C_{1,-1}^{(L)} I_{1,0}^{(L)} + \ldots \right] + \ldots$$

Dynamically set target precision for each sector, minimising time:

$$T = \sum_{i} t_{i} + \bar{\lambda} \left(\sigma^{2} - \sum_{i} \sigma_{i}^{2} \right), \quad \sigma_{i} \sim t_{i}^{-e}$$

- $\bar{\lambda}$ Lagrange multiplier
- σ precision goal
- σ_i error estimate

HJ Phase-Space & Real Radiation

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Real Radiation

For HJ Known analytically Del Duca, Kilgore, Oleari, Schmidt, Zeppenfeld 01

We use an upgraded GoSam setup: Cullen et al. 14

- Generate quadruple precision copy of the code
- Rescues unstable points on-the-fly with Ninja (quad)

Mastrolia, Mirabella, Peraro 12; Peraro 14

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• OneLoop for scalar integrals van Hameren 11

Implemented in POWHEG-BOX-V2, uses FKS subtraction Nason 04; Frixione, Nason Oleari 07; Alioli, Nason, Oleari, Re 10; Frixione, Kunszt, Signer 96

Virtual Phase Space

1. Apply VEGAS algorithm to LO matrix element 2. Using LO events generate unweighted events via accept/reject For HJ p_T distribution we include a reweighing factor to sample sufficiently also at large transverse momenta

Comparison of HJ and HH

	HJ production	HH production
#Form factors	4+2	2
Full reduction	\checkmark	only planar
(quasi-) finite basis	\checkmark	only planar
#Master integrals including crossings	458	327*
#Master integrals neglecting crossings	120	215*
#Integrals after sector decomposition and expansion in ϵ	22675	11244
Code size coefficients	~340 MB	~80 MB
Code size integrals	~330 MB	~580 MB
Compile time coefficients	~2 weeks	few days
Compile time integrals	~4 hours	~1-2 days
Time for linking the program	~3-4 days	few hours

Slide: Matthias Kerner, Radcor 2017

* HH non-planar not fully reduced

HJ Results

HJ Results: Total Cross Section

$$\begin{split} m_{H} &= 125 \text{ GeV}, \\ m_{T} &= \sqrt{23/12} \ m_{H} \approx 173.05 \text{ GeV} \\ p_{T,j} &> 30 \text{ GeV}, \text{ anti} - k_{T} \ R &= 0.4, \\ \mu &= \frac{H_{T}}{2} = \frac{1}{2} \left(\sqrt{m_{H}^{2} + p_{t,H}^{2}} + \sum_{i} |p_{t,i}| \right) \\ \texttt{PDF4LHC15_nlo_30_pdfas} \end{split}$$

Butterworth et al. 16; Dulat et al. 16; Harland-Lang et al. 15; Ball et al. 15 $d\sigma_{\rm NLO}^{\rm FT_{approx}} = \int d\phi_2 \left(d\sigma_B + \frac{d\sigma_B}{d\sigma_B^{\rm HEFT}} d\sigma_V^{\rm HEFT} \right)$ $+ \int d\phi_3 \ d\sigma_R$ FT_{approx}: Full Born & Reals Reweight virtuals event-by-event

Note: Non-negligible contribution from top-bottom interference known at NLO but not included here

(Lindert,) Melnikov, Tancredi, Wever 16, 17

HJ Results (II): Higgs Boson pT

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Confirm expected scaling of $d\sigma/dp_T^2$ in HEFT and full theory at NLO $\sim p_T^{-2}$ in HEFT Forte, Muselli 15; Caola, Forte, Marzani, Muselli, $\sim p_T^{-4}$ in full theory Vita 16;



LO Full

NLO Full

NLO FT_{approx}

 FT_{approx} predicts similar p_T distribution shape to full theory

Full theory predicts nearly flat K factor at large p_T

~8% increase in tail by including top quark mass dependence in virtuals

HJ Results (III): Different Scale Choices



With fixed scale ${\rm FT}_{\rm approx}$ has different shape to full theory (overestimates tail)

Note: K-factor only flat for dynamic scale choice, not for fixed scale

HJ Numerical Stability

Numerical evaluation of virtual amplitude:

- accuracy goal: 0.5% for each form factor
- wall-clock limit: 2d GPU-time (Tesla K20X GPU)

Thanks to MPCDF for compute resources



Accuracy reached for $|\mathcal{M}|^2$

- Better than per-mill for most points below $m_{hj} = 1.5 \text{ TeV}$
- Region $m_{hj} \ge 2 \text{ TeV}$ numerically challenging
- Forward region challenging

Run time per point:

- Minimum: 1.3h
- Median: 15h

MI Basis Change:

- Consider quasi-finite integrals (prefer finite integrals)
- Brute force combinations of masters, factor denominators and check that dimension factorises (achieved)
- Prefer simple denominator factors
- Prefer computing fewer orders in epsilon for each master
- Prefer simpler numerators (check number of terms/file size)

See: Matthias Kerner, Loops and Legs Proceedings 2018

Numerical Improvements:

- Improve modular arithmetic implementation (needed for larger lattices)
- Do not try to further evaluate integrals if rel. err. $< 10^{-14}$
- Adjust time spent integrating when iteration may exceed wall clock limit

HJ Numerical Stability (III)



Phase-space points significantly more stable:

- Good accuracy around top quark threshold
- Huge improvement in accuracy at larger invariant mass (2-3 TeV)
- Improvement in the forward region

Coefficient code size: 340 MB → 100 MB

Median runtime 15h \rightarrow <2h

HJ Results (IV): Higgs Boson pT



Recomputing unstable points improves fluctuations in tail Low fraction of points excluded 3/2004

HJ Expansion

Alternatively can consider Higgs boson & top quark masses as small Introduce variables:

$$\eta = -\frac{m_H^2}{4m_T^2}, \quad \kappa = -\frac{m_T^2}{s}, \quad z = \frac{m_T^2}{s}$$

Expand integrals to $\mathcal{O}(\eta^0\kappa^1)$ justified for $m_H^2, m_T^2 \ll |s| \sim |t| \sim |u|$, For example at large $\,p_T^2 = ut/s\,$

Kudashkin, Melnikov, Wever 17



Expanded 2-loop virtuals can be combined with full reals to predict Higgs boson p_T distribution above top threshold Lindert, Kudashkin, Melnikov, Wever 18; Neumann 18 $\frac{K^{\rm SM}}{K^{\rm HTL}} = 1.04 \dots 1.06$

Minor difference to full result, due to missing $\mathcal{O}(\eta^1)$ terms?

HH Results

HH Results (I): Invariant Mass



HH Results (II): pT either Higgs



HTL: Can poor approx. for larger $p_{T,h}$

Note: ambiguous how to rescale HTL reals by full LO born differentially

FTapp: Significantly better but still overestimating

Real radiation plays larger role for large $p_{T,h}$ (As hoped) Including full reals does improve over HTL in tails

Variation of the Higgs Self Coupling



Distributions: Can help to

distinguish between λ values

SM: Destructive interference between g_{hhh} and y_T^2 contrib.



Result has also been used in a full NLO QCD EFT analysis Buchalla, Capozi, Celis, Heinrich, Scyboz 18

HH Top Quark Mass Scheme Uncertainties

HH recently recomputed by another group (also using numerical methods)

Baglio, Campanario, Glaus, Mühlleitner, Spira, Streicher 18



Mutual agreement with our result Studied top quark mass scheme/scale uncertainties:

$$\frac{d\sigma(gg \rightarrow HH)}{dQ}\Big|_{Q=300 \text{ GeV}} = 0.0312(5)^{+9\%}_{-23\%} \text{ fb/GeV},$$

$$\frac{d\sigma(gg \rightarrow HH)}{dQ}\Big|_{Q=400 \text{ GeV}} = 0.1609(4)^{+7\%}_{-7\%} \text{ fb/GeV},$$

$$\frac{d\sigma(gg \rightarrow HH)}{dQ}\Big|_{Q=600 \text{ GeV}} = 0.03204(9)^{+0\%}_{-26\%} \text{ fb/GeV},$$

$$\frac{d\sigma(gg \rightarrow HH)}{dQ}\Big|_{Q=1200 \text{ GeV}} = 0.000435(4)^{+0\%}_{-30\%} \text{ fb/GeV},$$

$$\square$$

Large uncertainty obtained varying
scale of top quark mass (in $\overline{\text{MS}}$) by
factor 2 up/down

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HH: NNLO EFT Combined with NLO SM

Differential NNLO HTL + NLO SM

Top quark mass effects studied using 3 different approximations



Grazzini, Heinrich, SJ, Kallweit, Kerner, Lindert, Mazzitelli 18; (+NNLL) de Florian, Mazzitelli 18;

\sqrt{s}	$13 { m TeV}$	$14 { m TeV}$	$27 { m TeV}$	$100 { m TeV}$
NLO [fb]	$27.78^{+13.8\%}_{-12.8\%}$	$32.88^{+13.5\%}_{-12.5\%}$	$127.7^{+11.5\%}_{-10.4\%}$	$1147^{+10.7\%}_{-9.9\%}$
$\rm NLO_{FTapprox}$ [fb]	$28.91^{+15.0\%}_{-13.4\%}$	$34.25^{+14.7\%}_{-13.2\%}$	$134.1^{+12.7\%}_{-11.1\%}$	$1220{}^{+11.9\%}_{-10.6\%}$
$NNLO_{NLO-i}$ [fb]	$32.69^{+5.3\%}_{-7.7\%}$	$38.66^{+5.3\%}_{-7.7\%}$	$149.3^{+4.8\%}_{-6.7\%}$	$1337^{+4.1\%}_{-5.4\%}$
$NNLO_{B-proj}$ [fb]	$33.42^{+1.5\%}_{-4.8\%}$	$39.58^{+1.4\%}_{-4.7\%}$	$154.2^{+0.7\%}_{-3.8\%}$	$1406{}^{+0.5\%}_{-2.8\%}$
$NNLO_{FTapprox}$ [fb]	$31.05^{+2.2\%}_{-5.0\%}$	$36.69^{+2.1\%}_{-4.9\%}$	$139.9^{+1.3\%}_{-3.9\%}$	$1224 {}^{+0.9\%}_{-3.2\%}$
M_t unc. NNLO _{FTapprox}	$\pm 2.6\%$	$\pm 2.7\%$	$\pm 3.4\%$	$\pm 4.6\%$
$\rm NNLO_{FTapprox}/\rm NLO$	1.118	1.116	1.096	1.067

1) NNLO_{NLO-i}

Rescale NLO by $K_{NNLO} = NNLO_{HTL}/NLO_{HTL}$ 2) NNLO_{B-proj}

Project real radiation contributions to Born configurations, rescale by LO/LO_{HEFT}

3) NNLO_{FTapprox}

NNLO EFT correction rescaled for each multiplicity by:

$$\mathcal{R}(ij \to HH + X) = \frac{\mathcal{A}_{\text{Full}}^{\text{Born}}(ij \to HH + X)}{\mathcal{A}_{\text{HEFT}}^{(0)}(ij \to HH + X)}$$

HH Production via Expansions

Expansion about small $m_{H}^{2}, m_{T}^{2} \ll |s|, |t|$ can be applied to HH

Davies, Mishima, Steinhauser, Wellmann 18, 18;

Agreement between expanded integrals and numerical results (where expansion is valid)





Alternatively:

Expand only about small m_H^2 Larger range of validity, some integrals significantly more involved (Elliptic) Xu, Yang 18

HH Production via Expansions (II)

But, there is more than one way to skin a cat...

Produce a Padé approximation using: Large- m_T expansion + threshold expansion

Incorporate non-analytic threshold corrections into approximation

Method applicable to more processes: $gg \rightarrow H^{(*)}, HZ, ZZ$





Gröber, Maier, Rauh 17

Have: $p_T^2 + m_H^2 \leq \hat{s}/4$ Expand in: $p_T^2 + m_H^2$

Solve remaining dependence on \hat{s}, m_T

Invariant mass distribution agrees well with full (numerical) result up to ~900 GeV Bonciani, Degrassi, Giardino, Gröber 18

Conclusion

Higgs+Jet & Di-Higgs Production at the LHC

- Computed at NLO with full top quark mass dependence
- 2-loop virtual amplitude calculated numerically

Numerical Multi-loop Calculations

- Discussed basis choice which improves numerical performance
- Described sector decomposition procedure and pySecDec
- Public release of QMC integration code with CUDA GPU support

Future

- Complete study of HJ (more distributions, grid of results, combination with parton shower and NNLO HTL)
- Attack more multi-scale $2 \rightarrow 2$ processes and refine our technique

Thank you for listening!

Backup

Starting to look at other distributions...

Basis change improves numerical stability of invariant mass distribution



Note:

- Produced with fairly low statistics (817 points)
- No scale variations yet

BSM EFT

But: Just varying λ : one ``direction'' in EFT parameter space Parametrise **non-resonant** new physics with EFT (5 parameters):



Azatov, Contino, Panico, Son 15; Buchalla, Cata, Celis, Krause 15; (B.I. NLO HEFT) Gröber, Mühlleitner, Spira, Streicher 15; (B.I. NNLO HEFT) de Florian, Fabre, Mazzitelli 17; (Cluster analysis) Dall'Osso, Dorigo, Gottardo, Oliveira, Tosi, Goertz 15; + Carvalho, Manzano, Dorigo, Gouzevich 16; Kim, Sakaki, Son 18; (NLO) Buchalla, Capozi, Celis, Heinrich, Scyboz 18

HH Results: 100 TeV



Difference between full theory and HEFT more pronounced

Form Factor Decomposition (HJ Quark)

 p_1, α

 p_2, β

 p_3, μ

We compute $q\bar{q}gH$ and obtain other channels by crossing

Form Factors (Contain integrals) \mathbf{I} \mathbf{I} $\mathcal{M}^{\mu}_{\beta\alpha} = F_1 T^{\mu}_{1,\beta\alpha} + F_2 T^{\mu}_{2,\beta\alpha}$ Choose basis:

$$T_{1,\beta\alpha}^{\mu} = \left(\bar{v}_{\beta}(p_{2}) \not\!\!p_{3} u_{\alpha}(p_{1}) p_{1}^{\mu} - \bar{v}_{\beta}(p_{2}) \gamma^{\mu} u_{\alpha}(p_{1}) p_{1} \cdot p_{3} \right)$$
$$T_{2,\beta\alpha}^{\mu} = \left(\bar{v}_{\beta}(p_{2}) \not\!\!p_{3} u_{\alpha}(p_{1}) p_{2}^{\mu} - \bar{v}_{\beta}(p_{2}) \gamma^{\mu} u_{\alpha}(p_{1}) p_{2} \cdot p_{3} \right)$$

Build projectors P such that: $(P^1_{\alpha\beta})_{\mu}\mathcal{M}^{\mu}_{\beta\alpha} = F_1, \ (P^2_{\alpha\beta})_{\mu}\mathcal{M}^{\mu}_{\beta\alpha} = F_2$ Gehrmann, Glover, Jaquier, Koukoutsakis 11

NLO Showered Results

No Higgs decay or hadronization included Assume $\Gamma_h = 0$ (decay can be attached e.g. in narrow width approx.)

POWHEG-BOX



POWHEG-BOX/MG5 aMC@NLO



Shower has moderate impact on NLO accurate observables

Heinrich, SPJ, Kerner, Luisoni, Vryonidou 17

NLO accurate observables $(m_{hh}, p_T^h, p_T^{h_1}, p_T^{h_2})$ only moderately sensitive to matching procedure

NLO Showered Results (II)



Matching/shower has significant impact on LO accurate observables Can have large matching uncertainties

 $\langle \mathcal{O} \rangle = \int \left[\bar{B}(\phi_B) - B(\phi_B) \right] \frac{D(\phi_B, \phi_1)}{B(\phi_B)} \Theta(\mu_{\rm PS}^2 - t) \mathcal{O}(\phi_R) \, \mathrm{d}\phi_B \, \mathrm{d}\phi_1$ + $\int R(\phi_R) \mathcal{O}(\phi_R) \, \mathrm{d}\phi_R.$

Cancellation spoiled if:

- Large NLO corrections ($\bar{B} B$)
- Splitting kernels over Born (D/B) numerically large compared to real radiation
- Phase space accessible to the PS (depends on scale $\mu_{\rm PS}$ and PS evolution variable t)

NLO Showered Results (III)

Radial separation: $\Delta R^{hh} = \sqrt{(\eta_1 - \eta_2)^2 + (\Phi_1 - \Phi_2)^2}$

POWHEG

POWHEG/MG5_aMC@NLO

