Numerical stability in hard and IR regions in OpenLoops2

> arXiv:1906.????? arXiv:1908.?????

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Introduction



 $\sigma \times B$ normalized to SM value

- ▶ 7 years since Higgs discovery
- Standard Model is very well consistent with LHC results
- No excesses observed with respect to the Standard Model
- Limited precision $\sim 20\%$ Expect NP at $\mathcal{O}(\delta_{\rm EW}) \sim 5\%$?

Introduction

Experiment future



Theory future

- ▶ Precision in SM predictions
 - Complete NLO for high multiplicities
 - ▶ NNLO QCD for $2 \rightarrow 2, 2 \rightarrow 3, ...$
- ▶ Precision in BSM predictions
 - ► UV complete models
 - ► SMEFT

Automation

Loops



Introduction

Computation of one-loop amplitudes (QCD & EW) is quite advanced

FeynArts / FormCalc	[Hahn et al]			
GoSam	Chiesa, Greiner, Heinrich, Jahn, Jones, Kerner, Luisoni			
	Mastrolia, Ossola, Peraro, Schlenk, Scyboz, Tramontano]			
NLOX	[Honeywell, Quackenbush, Reina, Reuschle]			
MadGraph5 aMC@NLO	Alwall, Frederix, Frixione, Hirschi, Maltoni,			
	Mattelaer, Shao, Stelzer, Torrielli, Zaro]			
NGluon	[Badger, Biedermann, Uwer, Yundin]			
OpenLoops	[Cascioli, Lindert, Maierhöfer, Pozzorini]			
BlackHat	[Bern, Dixon, Cordero, Höche, Ita, Kosower, Maitre, Ozeren]			
HELAC-NLO	[Bevilacqua,Czakon,Garzelli,van Hameren,Kardos,Papadopoulos,Pittau,Worek]			
Recola	[Actis, Denner, Hofer, Lang, Scharf, Uccirati]			

Used in many projects:

► Event generators

Complete NLO corrections available in:

- Sherpa arXiv:1712.07975
- MADGRAPH5_AMC@NLO arXiv:1804.10017

► In two-loop computations For the 1-loop part + real-virtual contributors e.g.: in MATRIX arXiv:1711.06631

We need *high-performance* one-loop providers that are *reliable* in *all phase-space*.

Content of this Talk

The OpenLoops2 algorithm

Numerical stability in the on-the-fly reduction

Performance and stability benchmarks

The OpenLoops2 algorithm

The OPENLOOPS tool-chain

▶ Fully automated framework for tree and one-loop amplitudes

 $\sum_{\rm colour/spin} \left|\mathcal{M}_0\right|^2, \quad \sum_{\rm colour/spin} 2{\rm Re}\left[\mathcal{M}_0^*\mathcal{M}_1\right], \quad \sum_{\rm colour/spin} \left|\mathcal{M}_1\right|^2, \ldots$

I Process generator:

Generation of (symbolic) amplitudes using FEYNARTS [Hahn] Transformation into recursive representation (OPENLOOPS algorithm)

II Process computation:

$$\mathcal{M}_1 = \sum_i \mathcal{N}_{i,\mu_1\dots} T_i^{\mu_1\dots} + \mathcal{M}_{\mathrm{CT}} + \mathcal{M}_{\mathrm{R}_2}$$

OPENLOOPS [Cascioli, Lindert, Maierhöfer, Pozzorini]: Computes coefficients and uses third-party tools for the reduction: COLLIER[Denner, Dittmaier, Hofer], CUTTOOLS[Ossola, Papadopoulos, Pittau], ONELOOP[van Hameren].

 OPENLOOPS2 [Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller]:
 Combines computation of coefficients and reduction for tree-loop, requires scalar integral providers (COLLIER, ONELOOP)

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OPENLOOPS2 for complete NLO computations

Ingredients for complete one-loop computations:

- ▶ Complete SM renormalization
 - ▶ $N_{\rm f}$ flavour scheme for $\alpha_{\rm s}$, $\alpha(0)$, $\alpha(M_{\rm Z})$, $G_{\rm F}$
 - On-shell renormalization
 - Complex-mass scheme [Denner, Dittmaier]

$$M_V^2 \to \mu_V^2 = M_i^2 - \mathrm{i}\Gamma_V M_V$$

• Complete set of R_2 [Pittau et al].

► Generation of full tower of orders $|\mathcal{M}_0|^2 \qquad \mathcal{O}\left(\alpha_{\rm s}^{n-1}\alpha^{m+1}\right) \qquad \mathcal{O}\left(\alpha_{\rm s}^n\alpha^m\right) \qquad \cdot$ Re $[\mathcal{M}_0^*\mathcal{M}_1] \qquad \mathcal{O}\left(\alpha_{\rm s}^{n-1}\alpha^{m+2}\right) \qquad \mathcal{O}\left(\alpha_{\rm s}^n\alpha^{m+1}\right) \qquad \mathcal{O}\left(\alpha_{\rm s}^{n+1}\alpha^m\right)$

OPENLOOPS2 publicly available (temporary link) https://openloops.hepforge.org

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Computation of One-Loop diagrams in OPENLOOPS

Cut colour-stripped loop-amplitudes can be written as

$$A_{1}^{(d)} = \int \mathrm{d}^{D}q \; \frac{\mathrm{Tr}\left[\mathcal{N}(q,h)\right]}{D_{0}D_{1}\dots D_{N-1}} = \underbrace{\begin{array}{c} \underbrace{\mathbf{w}_{N}}_{D_{n-1}} \underbrace{\mathbf{w}_{N}}_{D_{n}} \\ \underbrace{\mathbf{w}_{N}}_{D_{n}} \underbrace{\mathbf{w}_{N}}_{D_{n}} \end{array} \Rightarrow \underbrace{\begin{array}{c} \underbrace{\mathbf{w}_{N}}_{\beta_{N}} \underbrace{\mathbf{w}_{N}}_{\beta_{N}} \\ \underbrace{\mathbf{w}_{N}}_{D_{n}} \underbrace{\mathbf{w}_{N}}_{D_{n}} \end{array}$$
Numerator factorises into segments:

$$[\mathcal{N}(q,h)]_{\beta_0}^{\beta_N} = [S_1(q,h_1)]_{\beta_0}^{\beta_1} [S_2(q,h_2)]_{\beta_1}^{\beta_2} \dots [S_N(q,h_N)]_{\beta_{N-1}}^{\beta_N}$$

OPENLOOPS 1-loop recursion (dressing steps):

$$\mathcal{N}_{k}(q,\hat{h}_{n}) = \mathcal{N}_{k-1}(q,\hat{h}_{k-1}) \cdot S_{k}(q,h_{k})$$

$$= \underbrace{\underbrace{w_{1}}_{D_{1}} \underbrace{w_{2}}_{D_{2}} \underbrace{w_{k}}_{D_{k}} \underbrace{w_{k+1}}_{D_{k+1}} \underbrace{w_{N-1}}_{D_{N-1}} \underbrace{w_{N}}_{D_{N-1}}$$

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OPENLOOPS amplitude construction and reduction



Drawback/bottlenecks

- 1 Large structure growth prior to reduction (due to high rank)
- 2 Evaluation for each helicity configuration h

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On-the-fly operations in OPENLOOPS2

arXiv:1710.11452 [Buccioni, Pozzorini, Zoller '17]

1 On-the-fly helicity summation

Uses tree amplitude information in tree-loop interference

$$\mathcal{N}_k(q)
ightarrow \left(\sum_{ ext{col}} \mathcal{M}_0^* C^{(d)}
ight) \mathcal{N}_k(q)$$

and sums over external helicities after dressing steps. \Rightarrow No evaluation of one-loop helicity amplitudes

2 On-the-fly reduction

Reduce open loops by integrand and integral reduction identities \Rightarrow Avoids high rank objects at any stage in computation

Advantages

- ▶ Significant gain in CPU performance
- ▶ New algorithm which combines construction and reduction
- ▶ New systematic way to address numerical instabilities

On-the-fly reduction

Use reduction identities valid at integrand level [del Aguila, Pittau '05].

$$q^{\mu}q^{\nu} = A^{\mu\nu}_{-1} + A^{\mu\nu}_{0} D_{0} + \left(B^{\mu\nu}_{-1,\lambda} + \sum_{i=0}^{3} B^{\mu\nu}_{i,\lambda} D_{i}\right) q^{\lambda}, \qquad (\clubsuit)$$
$$D_{i} = (q+p_{i})^{2} - m_{i}^{2}$$

▶ Reduction identity follows from loop-momentum decomposition:

$$q^{\mu} = \sum_{i=1}^{4} c_i l_i^{\mu}, \quad l_i = l_i(p_1, p_2)$$

Integrand identity ♠ requires another *independent* momentum p₃
 A^{µν}_i, B^{µν}_i are constants depending on p₁, p₂, p₃

▶ p_1, p_2, p_3 can be chosen freely to cancel propagators D_i

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OPENLOOPS2 amplitude construction and reduction



On-the-fly reduction step

$$\frac{\mathcal{V}^{\mu\nu}q_{\mu}q_{\nu}}{D_{0}\dots D_{N-1}} = \frac{\mathcal{V}^{\mu}_{-1}q_{\mu} + \mathcal{V}_{-1}}{D_{0}\dots D_{N-1}} + \sum_{i=0}^{3} \frac{\mathcal{V}^{\mu}_{i}q_{\mu} + \mathcal{V}_{i}}{D_{0}\dots \mathcal{D}_{i}\dots D_{N-1}}$$

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On-the-fly reduction - technical details

Final integral reduction

- Reduce rank-2 2-point, rank-3 triangles and rank-1 boxes with integral level identities [del Aguila, Pittau '05].
- ▶ Reduce rank-0 and rank-1 N-point for N≥ 5 with OPP reduction [Ossola, Papadopoulos, Pittau '07].
- ▶ Use CollieR_[Denner, Dittmaier, Hofer '16] or ONELOOP_[van Hameren '10] for evaluation of scalar master integrals

Numerical stability in the on-the-fly reduction

Native implementation of the on-the-fly reduction Case study $gg \rightarrow t\bar{t}gg$



► Sample of 10⁶ hard events: $p_{\rm T} > 50 \,\text{GeV}, \,\Delta R_{ij} >= 0.5$ ► $\mathcal{M}_{qp} \,\text{CUTTOOLS}$ ► $\mathcal{A} = \frac{|\mathcal{M}_{\rm qp} - \mathcal{M}_{\rm dp}|}{|\mathcal{M}_{\rm qp} + \mathcal{M}_{\rm dp}|}$

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Comparison to other reduction methods

Case study $gg \to t\bar{t}gg$



- ▶ Large number of reduction methods available
- ▶ All algorithm suffer from (severe) numerical instabilities
- ▶ Necessity for a high-precision rescue system

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Approach to cure numerical instabilities

I Consider stability distributions for large samples

- Sample corresponding to size of **real-life applications**
- Estimate stability, e.g. by rescaling of dimension full parameter?
- ▶ Better: Derive stability from high-precision computation

II Construct stability correlator

• Capture *all* points in the tails of stability distributions

III Cure instability

- Avoid reduction steps with critical correlation
- Perform expansions
- ▶ ...

Sources of numerical instability in OFR

The on-the-fly reduction suffers from Gram determinant instabilities



- Severe numerical instabilities as $\Delta_{12} \to 0$
- ▶ Instabilities propagate $A_i/B_i \times A_i/B_i \times ... \sim \Delta_{12}^{-k}$ and amplify
- Moderate values of $1 \gg \frac{\Delta_{12}}{Q^2} \gg 0$ lead to numerical instabilities

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On-the-fly solution to (single) rank-2 GD instabilities

[Buccioni, Pozzorini, Zoller '17]

I Use freedom of on-the-fly reduction, choose i_1, i_2 such that $\sim \Delta_{i_1 i_2}$ maximal. Corresponds to propagator permutation

$$\frac{\mathcal{V}^{\mu\nu}q_{\mu}q_{\nu}}{D_0 D_1 D_2 D_3 \dots} \to \frac{\mathcal{V}^{\mu\nu}q_{\mu}q_{\nu}}{D_0 D_{i_1} D_{i_2} D_{i_3} \dots}, \quad i_1, i_2, i_3 \in [1, 2, 3]$$

 \Rightarrow Avoids small rank-2 GD up to triangle reduction \checkmark

II Only *t*-channel topology introduces numerical instabilities (hard region)



- ▶ Analytic solution instead of on-the-fly reduction
- Perform expansions in Δ_{12}

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Curing residual instabilities in the OFR

Goal: Cure residual instabilities in the tail

- ▶ Full control in hard region crucial for stability in IR regions
- ▶ Get rid of stability system which requires 2 fold evaluation

Obstacle: Clean QP Benchmarks

- On-the-fly reduction can operate in full QP ✓ (no double precision contamination)
- ► Truncation spoils rescaling tests Any-order expansions √

Any-order expansion



- ▶ Expansion to *arbitrary order*
- Analytic cancellation of Δ_{12} poles
- ► Multi-precision target accuracy (DP or QP)
- Efficient implementation for tensor integrals, allowing to reach ~ 1000 terms.
- ► All QCD cases implemented in library TRRED

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Conclusion rank-2 GD instabilities



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Beyond rank-2 GD instabilities

The local error estimation and propagation

• Each step in the OL2 algorithm has an (inherited) error

Local error sources

- $\label{eq:reduction} I \; \frac{\text{Reduction steps}}{\text{Estimated via reduction coefficients}}$
- II <u>Scalar integrals</u> Estimated using COLLIER (via mod. Cayley determinant)
- III <u>Reduction basis</u> Estimated via rank 3 Gram determinant
- $\Rightarrow \text{Propagate and combine to construct}\\ \textbf{global error estimation } \mathcal{E}$



On-the-fly trick to alleviate instabilities

Step I: Avoid error propagation

- ▶ Error propagation only in on-the-fly reduction
- ▶ New reduction: choose i_1, i_2, i_3 such that $\sim \Delta_{i_1 i_2}$ maximal and $\sim \Delta_{i_1 i_2 i_3}$ maximal \simeq propagator permutations + look ahead

$$\frac{\mathcal{V}^{\mu\nu}q_{\mu}q_{\nu}}{D_0 D_1 D_2 D_3 D_4 \dots} \to \frac{\mathcal{V}^{\mu\nu}q_{\mu}q_{\nu}}{D_0 D_{i_1} D_{i_2} D_{i_3} D_{i_4} \dots}, \quad i_1, i_2, i_3, i_4 \in [1, 2, 3, 4]$$

Step II: Cure remaining instabilities

 \blacktriangleright Expansion? \times

▶ Perform cancellation numerially in targeted way.

Hybrid precision mode

▶ Promote open loops \mathcal{N} with $\mathcal{E} > \mathcal{E}^{\text{thres}}$ to quad precision

$$\mathcal{N}
ightarrow \mathcal{N} = \begin{pmatrix} \mathcal{N}_{\mathrm{DP}} \\ \mathcal{N}_{\mathrm{QP}} \end{pmatrix}, \quad \mathrm{Upgrade}(\mathcal{N}) = \begin{pmatrix} 0 \\ \mathcal{N}_{\mathrm{QP}} + \mathcal{N}_{\mathrm{DP}} \end{pmatrix}$$

 \blacktriangleright Consecutive operations f performed in respective precision

$$\mathcal{N}_{\mathrm{out}} = f(\mathcal{N}_{\mathrm{in}}) \to \mathcal{N}_{\mathrm{out}} = \begin{pmatrix} f_{\mathrm{DP}}(\mathcal{N}_{\mathrm{DP}}) \\ f_{\mathrm{QP}}(\mathcal{N}_{\mathrm{QP}}) \end{pmatrix}$$

Cancellation takes places in QP in the last step

$$\operatorname{Result} = \left(\sum_{i} \mathcal{N}_{\mathrm{DP}}^{i} \mathrm{SI}_{\mathrm{DP}}^{i}\right) + \left(\sum_{i} \mathcal{N}_{\mathrm{QP}}^{i} \mathrm{SI}_{\mathrm{QP}}^{i}\right)$$

numerical cancellations in here



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New sources of instabilities in IR regions



New triggers/features encoded in hp_mode=2.

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Performance and stability benchmarks

Performance

processes @ NLO QCD	OL2[ms], hp_loopacc=8	OL2, hp_mode=0	OL2, hp_loopacc=11	OL1
$gg \rightarrow t\bar{t}$	0.96	1.0	1.01	1.32
$gg \rightarrow t\bar{t}g$	21.4	1.0	1.04	1.56
$gg \rightarrow t\bar{t}gg$	600	1.0	1.15	2.17
$gg \rightarrow t\bar{t}b\bar{b}$	95	1.0	1.18	2.05
$u\bar{u} \rightarrow t\bar{t}$	0.23	1.0	1.0	0.93
$u\bar{u} \rightarrow t\bar{t}g$	3.1	1.0	1.06	1.19
$u\bar{u} \rightarrow t\bar{t}gg$	73	1.0	1.16	1.45
$u\bar{u} \rightarrow t\bar{t}ggg$	2085	0.99	1.26	1.88
$d\bar{u} \rightarrow W^+g$	0.33	1.0	1.03	0.79
$d\bar{u} \rightarrow W^+ gg$	5.6	1.0	1.05	0.92
$d\bar{u} \rightarrow W^+ ggg$	134	0.99	1.16	1.28
$d \bar{u} ightarrow W^+ g g g g$	3760	0.98	1.14	1.41
$u\bar{u} \rightarrow W^+W^-$	0.19	1.0	1.0	1.19
$u \bar{u} \rightarrow W^+ W^- g$	6.7	1.0	1.16	1.24
$u \bar{u} ightarrow W^+ W^- g g$	154	0.99	1.19	1.63
$u \bar{u} ightarrow W^+ W^- g g g$	3660	0.98	1.17	2.18
processes @ NLO EW	OL2[ms], hp_loopacc=8	OL2, hp_mode=0	OL2, hp_loopacc=11	OL1
$d\bar{u} \rightarrow s\bar{c}h$	1.8	1.0	1.06	1.78
$u\bar{u} \rightarrow t\bar{t}h$	12.7	0.99	1.17	1.0
$d\bar{d} \rightarrow e^- \bar{\nu}_e \mu^+ \nu_\mu$	12.4	0.98	1.5	1.45
$u \bar{u} \rightarrow W^+ W^+ dd$	335	0.99	1.11	1.01

Table: Intel i7-4790K @ 4.00GHz. OL2[ms] is default hybrid precision mode ($h_{p_loopacc=8}$) given in milliseconds. Other columns display ratio t/t_{OL2} . OL1 with COLLIER run, but no stability system.

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IR phase-space point generation and performance

The soft and collinear events generated from hard underlying events

$$\begin{split} \xi_{\rm soft} &= E_{\rm soft}/Q \\ \xi_{\rm coll} &= \arccos\left(\frac{\boldsymbol{p}_i \cdot \boldsymbol{p}_j}{|\boldsymbol{p}_i||\boldsymbol{p}_j|}\right)^2 \end{split}$$

 \blacktriangleright E_{soft}: energy of a soft particle

 \blacktriangleright Q: the center of mass energy

▶ p_i, p_j : spacial momenta of collinear particles

The performance ranges between (*preliminary*)

•
$$t = \frac{t_{hp_mode=1}}{t_{hp_mode=0}} \approx 1.5 - 2.5$$

• $t = \frac{t_{hp_mode=2}}{t_{hp_mode=0}} \approx 3. - 7.$
For ξ values between 10^{-3} and 10^{-9} .

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Conclusion

- ▶ Release of OpenLoops2 featuring complete NLO corrections
 - New automated construction of one-loop amplitudes and reduction to scalar integrals
 - ▶ Major improvements in stability and performance
- ▶ Numerical instabilities addressed via:
 - Permutations/all-order expansions to cure single GD2 instabilities and avoid GD3 instabilities to the box reduction
 - Stable computation of invariants and use of analytic 2-point vertex functions to improve IR regions
 - Efficient hybrid precision mode to cure residual dominant numerical instabilities

Outlook

- NNLO subtraction tests with relaxed cutoffs to test deep IR cancellations
- \blacktriangleright Stability studies for $2 \rightarrow 4$ with one unresolved parton

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Backup slides

Any-order expansions - technical details

In the any-order expansions we define the functions

$$S_{0,n}(\delta,\ldots) := \sum_{m=n}^{\infty} \delta^{m-n} \left[\frac{1}{m!} \left(\frac{\partial}{\partial \delta} \right)^m S_0(\delta,\ldots) \right]_{\delta=0},$$

with S_0 being t-channel 2- and 3-point functions

•
$$B_0 (-p^2(1+\delta), m_0^2, m_1^2),$$

• $C_0 (-p^2, -p^2(1+\delta), 0, m_0^2, m_1^2, m_2^2):$
• $\sqrt{\Delta} = \frac{p^2}{2}\delta$

Deriving $S_{0,n}$ is a simple linear algebra task

$$C_0 = \frac{1}{p^2} \sum_{n=0}^{\infty} \delta^n C_n, \quad C_n = \int_0^1 \mathrm{d}y \ c_n,$$

 c_n is a rational number in y and by partial fraction:

$$c_n = \frac{P(y)}{Q(y)} = \sum_{j=1}^{n+1} \left[\frac{d_1(j,n)}{(y-y_1)^j} + \frac{d_2(j,n)}{(y-y_2)^j} \right]$$

. .

The direct reduction to scalar integrals yields

$$\begin{split} C^{\mu}\left(p_{1},p_{2},0,0,0\right)) &= \int \mathrm{d}^{D}q \, \frac{q^{\mu}}{D_{0}D_{1}D_{2}} = p_{1}^{\mu}C_{1} + (p_{1}-p_{2})^{\mu}C_{2},\\ C_{1} &= \frac{B_{0}(-p^{2}(1+\delta)) - B_{0}(-p^{2})}{p^{2}\delta} - C_{0}(-p^{2},-p^{2}(1+\delta)),\\ C_{2} &= -2\frac{B_{0}(-p^{2}) - B_{0}(-p^{2}(1+\delta))}{p^{2}\delta^{2}} \\ &+ \frac{B_{0}(-p^{2}(1+\delta)) - p^{2}C_{0}(-p^{2},-p^{2}(1+\delta))}{p^{2}\delta}, \end{split}$$

Any-order expansions yields

$$C_1 = \left[\frac{B_{0,1}}{p^2} - C_0\right], \quad C_2 = \frac{B_{0,1} + 2B_{0,2}}{p^2} - C_{0,1}, \quad (1)$$

- δ^n poles cancel, result numerically stable
- QCD/EW cases implemented in library TRRED as a multi-precision library (dp and qp)

Computation of tree-level diagrams OPENLOOPS

Amplitudes are decomposed into a colour basis

$$\mathcal{M} = \sum_{d} \mathcal{M}^{(d)}, \quad \mathcal{M}^{(d)} = C^{(d)} A^{(d)}$$

and recusion is applied to colour-stripped amplitudes:



Reconstruct subtrees via Berends-Giele-like recursion

$$\sigma_a \bullet w_a = \sigma_a \bullet w_b = w_a^{\alpha}(k_a, h_a) = \frac{X_{\beta\gamma}^{\alpha}(k_b, k_c)}{k_a^2 - m_a^2} w_b^{\beta}(k_b, h_b) w_c^{\gamma}(k_c, h_c)$$

▶ Recursion kernels derived from SM Lorentz structure

Subtrees recycled whenever possible

On-the-fly reduction - technical details

Reduction proliferates subtopologies



Efficient implementation requires merging: on-the-fly merging

