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Two-loop amplitude generation in OpenLoops

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in collaboration with

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RADCOR – LoopFest 2021

OpenLoops



OpenLoops is a fully automated numerical tool for the **tree and one-loop** computation of **hard scattering amplitudes** required in **Monte-Carlo simulations**

- $\bullet~$ Full $\rm NLO~QCD$ and $\rm NLO~EW$ corrections available
- Strong CPU performance and excellent numerical stability

Available from https://gitlab.com/openloops/OpenLoops.git or https://openloops.hepforge.org

Scattering probability densities in perturbation theory from sums of L-loop Feynman diagrams (L=0,1):

$$\mathcal{W}_{00} = \sum_{\text{hel col}} \sum |\mathcal{M}_0|^2, \qquad \mathcal{W}_{01} = \sum_{\text{hel col}} 2 \operatorname{Re} \Big[\mathcal{M}_0^* \mathcal{M}_1 \Big], \qquad \mathcal{W}_{11} = \sum_{\text{hel col}} \sum |\mathcal{M}_1|^2$$
$$\mathcal{M}_0 = \operatorname{Add}_{\text{Add}} + \operatorname{Add} + \operatorname{Add}_{\text{Add}} + \operatorname{Add}_{\text{Add}} + \operatorname{Add}_{\text{$$

Automation at NNLO highly desirable \rightarrow Goal: Two-loop OpenLoops

Outline

I. The OpenLoops algorithm at tree level and one loop

- II. Requirements for two-loop automation
- III. New algorithm to construct two-loop tensor coefficients in OpenLoops
- IV. Numerical stability
- V. Timings
- VI. Summary and Outlook

I. The OpenLoops algorithm at tree level

Tree-level amplitudes constructed recursively from sub-trees (starting from external lines)



 $+ \dots \rightarrow$ split into sub-trees

Numerical recursion step:



Highly efficient: Sub-trees constructed only once for multiple tree and loop diagrams

I. The OpenLoops algorithm at one loop

High complexity in loop diagram Γ due to analytical structure in loop momentum q



Factorisation into colour factor $\mathcal{C}_{1,\Gamma}$

and loop segments

$$S_i(\boldsymbol{q}) = \underbrace{w_i}_{\beta_{i-1} \underbrace{k_i}_{D_i}} = X_i^{\alpha}(k_i, p_i, \boldsymbol{q}) w_i^{\alpha}$$

Scalar propagators $D_i(\mathbf{q}) = (\mathbf{q} + p_i)^2 - m_i^2$

Universal building block \times sub-tree(s)

Open loop diagram at $D_0 \rightarrow$ **Dress chain of segments (open loop) recursively**:

$$\mathcal{N}_{k}(\boldsymbol{q}) = \prod_{i=1}^{k} S_{i}(\boldsymbol{q}) = \mathcal{N}_{k-1}(\boldsymbol{q})S_{k}(\boldsymbol{q}) = \underbrace{\begin{pmatrix} w_{1} & w_{2} & w_{k} & w_{k+1} & w_{N-1} & w_{N} \\ D_{1} & D_{2} & D_{k} & D_{k+1} & D_{N-1} & D_{0} \\ \hline & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & &$$

Completely generic and highly efficient algorithm

Implemented at the level of tensor integral coefficients $\mathcal{N}_{\mu_1...\mu_r}^{(k)}$

II. Requirements for NNLO automation



- $|\mathcal{M}_1|^2$, $\mathcal{W}_{NNLO}^{real-virtual}$, $\mathcal{W}_{NNLO}^{real-real}$ available in OpenLoops [Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, M.Z.]
- Amplitude of a two-loop diagram Γ :

$$\mathcal{M}_{2,\Gamma} = \underbrace{\mathcal{C}_{2,\Gamma}}_{\text{colour}} \quad \underbrace{\mathcal{C}_{2,\Gamma}}_{r_1=0} \underbrace{\mathcal{C}_{2,\Gamma}}_{r_2=0} \quad \underbrace{\mathcal{M}_{\mu_1\cdots\mu_{r_1}\nu_1\cdots\nu_{r_2}}}_{\text{tensor coefficient}} \quad \underbrace{\int \mathrm{d}^D q_1 \int \mathrm{d}^D q_2 \; \frac{q_1^{\mu_1}\cdots q_1^{\mu_{r_1}} q_2^{\nu_1}\cdots q_2^{\nu_{r_2}}}{\mathcal{D}(q_1,q_2)}}_{\text{tensor integral}}$$

- $\circ~$ Numerical construction of tensor coefficients in four dimensions \rightarrow this talk
- Restoration of (D-4)-dimensional numerator parts and renormalisation through UV and rational counterterms \rightarrow Hantian Zhang's talk on Friday
- Remaining tasks: Tensor integrals, treatment of IR divergences

III. New algorithm to construct two-loop tensor coefficients in OpenLoops

Amplitude of irreducible two-loop diagram Γ (1PI on amputation of all external subtrees):



Exploit factorisation of numerator $\mathcal{N}(q_1, q_2) = \prod_{i=1}^{3} \mathcal{N}^{(i)}(q_i) \prod_{j=0}^{1} \mathcal{V}_j(q_1, q_2)$

- Three chains, each depending on a single loop momentum q_i (i = 1, 2, 3)with chain numerators factorising into loop segments $\mathcal{N}^{(i)}(q_i) = S_0^{(i)}(q_i) \cdots S_{N_i-1}^{(i)}(q_i)$ \rightarrow Same structure as one-loop chain
- \bullet Two connecting vertices $\mathcal{V}_0, \mathcal{V}_1$
- Chain denominators $\mathcal{D}^{(i)}(q_i) = D_0^{(i)}(q_i) \cdots D_{N_i-1}^{(i)}(q_i)$ where $D_a^{(i)}(q_i) = (q_i + p_{ia})^2 m_{ia}^2$ (External momenta p_{ia} and masses m_{ia} along *i*-th chain)

Building blocks of two-loop amplitudes

Numerator $\mathcal{N}(\boldsymbol{q}_1, \boldsymbol{q}_2) = \begin{cases} 3 \\ \prod i=1 \end{cases} \left[\mathcal{N}^{(i)}(\boldsymbol{q}_i) \right]_{\beta_0^{(i)}}^{\beta_{N_i}^{(i)}} \right] \left[\mathcal{V}_0(\boldsymbol{q}_1, \boldsymbol{q}_2) \right]^{\beta_0^{(1)} \beta_0^{(2)} \beta_0^{(3)}} \left[\mathcal{V}_1(\boldsymbol{q}_1, \boldsymbol{q}_2) \right]_{\beta_{N_1}^{(1)} \beta_{N_2}^{(2)} \beta_{N_3}^{(3)}}$ can be constructed recursively, multiplying one chain segment or vertex \mathcal{V}_i per recursion step.

Observations:

- Chains have same complexity as one-loop chains
- Higher complexity in steps connecting V_j due to dependence on q_1, q_2 and three open Lorentz/spinor indices $\beta_k^{(i)}$
- Each chain segment or vertex V_j increases helicity d.o.f. by those of its external subtree(s) and the rank in a q_i by 0 or 1
- Number of independent tensor coefficients $\mathcal{N}_{\mu_1\cdots\mu_{r_1}\nu_1\cdots\nu_{r_2}}$ increases exponentially with ranks r_1, r_2 in q_1, q_2

<u>Naive algorithm</u>: Dress all chains first, then connect $\mathcal{V}_{0,1}$, interfer with Born and sum over helicities \rightarrow Would be inefficient due to expensive last steps



Number of tensor components				
$r_1 r_2$	0	1	2	3
0	1	5	15	35
1	5	25	75	175
2	15	75	225	525
3	35	175	525	1225
4	70	350	1050	2450
5	126	630	1890	4410

Connecting the building blocks of two-loop amplitudes

Final result: Helicity and colour-summed interference with Born $\mathcal{U}(q_1, q_2)$

$$=\sum_{h} 2\left(\sum_{col} \underbrace{\mathcal{M}_{0}^{*}(h)}_{\text{Born}} \underbrace{C_{2,\Gamma}}_{\text{colour}}\right) \left\{ \prod_{i=1}^{3} \underbrace{\left[\prod_{k=0}^{N_{i}-1} S_{k}^{(i)}(q_{i}, h_{k}^{(i)})\right]_{\beta_{0}^{(i)}}^{\beta_{N_{i}}^{(i)}}}_{\text{chain } \mathcal{N}^{(i)}(h^{(i)})} \right\} \underbrace{\left[\mathcal{V}_{0}(q_{1}, q_{2})\right]_{\beta_{0}^{(1)}\beta_{0}^{(2)}\beta_{0}^{(3)}}^{(3)} \left[\mathcal{V}_{1}(q_{1}, q_{2})\right]_{\beta_{N_{1}}^{(1)}\beta_{N_{2}}^{(2)}\beta_{N_{3}}^{(3)}}}_{\text{two-loop vertices}}$$
with segment helicities $h_{k}^{(i)} \rightarrow$ chain helicities $h^{(i)} = \underbrace{\sum_{k=0}^{N_{i}-1} h_{k}^{(i)}}_{k=0} \rightarrow$ global helicity $h = \underbrace{\sum_{i=1}^{3} h^{(i)}}_{i=1} h^{(i)}$
Algorithm will consist of N recursion steps:
$$\underbrace{\mathcal{N}_{n} = \mathcal{N}_{n-1} \cdot S_{n}, \quad (n = 1, \dots, N)}_{N_{1}}$$
with partially dressed numerators \mathcal{N}_{n} and building blocks $S_{n} \in \{S_{k}^{(i)}, \mathcal{V}_{j}, \mathcal{N}^{(i)}, \mathcal{M}_{0}^{*}C_{2,\Gamma}\}$.

CPU cost of step $n \sim$ number of multiplications

ightarrow dependent on structure of S_n and number of components of \mathcal{N}_n

= (number of tensor components in q_i) × (helicitiy d.o.f.) × 4^(number of open Lorentz/spinor indices)

\Rightarrow Most efficient algorithm found through cost simulation

of possible candidates for a wide range of QED and QCD Feynman diagrams

• Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type



Order of chains and of two-loop vertices $\mathcal{V}_0, \mathcal{V}_1$ has major impact on efficiency

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)



 $\mathcal{N}_{n}^{(3)}(\mathbf{q}_{3}, \hat{h}_{n}^{(3)}) = \mathcal{N}_{n-1}^{(3)}(\mathbf{q}_{3}, \hat{h}_{n-1}^{(3)}) \cdot S_{n}^{(3)}(\mathbf{q}_{3}, h_{n}^{(3)}) \qquad \text{with initial condition } \mathcal{N}_{-1}^{(3)} = \mathbb{1}$

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
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• Shortest chain \Rightarrow Low number of helicity d.o.f. $\hat{h}_n^{(3)} = \hat{h}_{n-1}^{(3)} + h_n^{(3)}$ and low rank in q_3 • Partial chains $\mathcal{N}_n^{(3)}$ computed only once for multiple diagrams

\Rightarrow Only a small number of low-complexity steps for the full process

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)
- Dress ${\cal U}^{(1)} \propto {\cal M}_0^* {\cal N}^{(1)}$ (longest chain)



$$\mathcal{U}_{n}^{(1)}(\boldsymbol{q}_{1},\check{\boldsymbol{h}}_{n}^{(1)}) = \sum_{\boldsymbol{h}_{n}^{(1)}} \mathcal{U}_{n-1}^{(1)}(\boldsymbol{q}_{1},\check{\boldsymbol{h}}_{n-1}^{(1)}) \cdot S_{n}^{(1)}(\boldsymbol{q}_{1},\boldsymbol{h}_{n}^{(1)}) \qquad \text{with} \quad \mathcal{U}_{-1}^{(1)}(\boldsymbol{h}) = 2 \Big(\sum_{\mathrm{col}} \underbrace{\mathcal{M}_{0}^{*}(\boldsymbol{h})}_{\mathrm{Born}} \underbrace{C_{2,\Gamma}}_{\mathrm{colour}}\Big)$$

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
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On-the-fly summation of segment helicities $h_n^{(1)}$

 \Rightarrow Partial chains depend on remaining helicities of the diagram $\check{h}_n^{(1)} = h - \sum_{k=1}^n h_k^{(1)}$

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)
- Dress ${\cal U}^{(1)} \propto {\cal M}_0^* {\cal N}^{(1)}$ (longest chain)



$$\mathcal{U}_{n}^{(1)}(q_{1}, \check{h}_{n}^{(1)}) = \sum_{\substack{h_{n}^{(1)}}} \mathcal{U}_{n-1}^{(1)}(q_{1}, \check{h}_{n-1}^{(1)}) \cdot S_{n}^{(1)}(q_{1}, h_{n}^{(1)}) \qquad \text{with} \quad \mathcal{U}_{-1}^{(1)}(h) = 2 \Big(\sum_{\text{col}} \underbrace{\mathcal{M}_{0}^{*}(h)}_{\text{Born}} \underbrace{C_{2,\Gamma}}_{\text{colour}}\Big)$$

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$$\mathcal{U}_{n}^{(1)}(q_{1},\check{h}_{n}^{(1)}) = \sum_{\substack{h_{n}^{(1)}\\ Born}} \mathcal{U}_{n-1}^{(1)}(q_{1},\check{h}_{n-1}^{(1)}) \cdot S_{n}^{(1)}(q_{1},h_{n}^{(1)}) \qquad \text{with} \quad \mathcal{U}_{-1}^{(1)}(h) = 2\left(\sum_{\text{col}} \underbrace{\mathcal{M}_{0}^{*}(h)}_{\text{Born}} \underbrace{C_{2,\Gamma}}_{\text{colour}}\right)$$

On-the-fly summation of segment helicities $h_n^{(1)}$

 \Rightarrow Partial chains depend on remaining helicities of the diagram $\check{h}_n^{(1)} = h - \sum_{k=1}^n h_k^{(1)}$

\Rightarrow Large portion of helicity d.o.f already summed over during dressing of longest chain

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)
- Dress ${\cal U}^{(1)} \propto {\cal M}_0^* {\cal N}^{(1)}$ (longest chain)
- \bullet Connect \mathcal{V}_1 with $\mathcal{U}^{(1)}$ and $\mathcal{N}^{(3)}$



$$\mathcal{V}(q_1, q_3, h^{(2)}) = \sum_{h^{(3)}} \mathcal{U}^{(1)}(q_1, h - h^{(1)}) \ \mathcal{N}^{(3)}(q_3, h^{(3)}) \ \mathcal{V}_1(q_1, q_3)$$

On-the-fly summation of chain helicity $h^{(3)}$ (and potential subtree helicity at \mathcal{V}_1) \Rightarrow Partial diagram depends on undressed chain helicity $h^{(2)}$

\Rightarrow Intermediate object depends on three open indices and two loop momenta

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)
- Dress ${\cal U}^{(1)} \propto {\cal M}_0^* {\cal N}^{(1)}$ (longest chain)
- ullet Connect \mathcal{V}_1 with $\mathcal{U}^{(1)}$ and $\mathcal{N}^{(3)}$
- Connect \mathcal{V}_0 and map $q_3 \rightarrow -(q_1+q_2)$



$$\mathcal{U}_{-1}^{(2)}(q_1, q_2, h^{(2)}) = \mathcal{Y}(q_1, q_3, h^{(2)}) \mathcal{V}_0(q_1, q_1) \Big|_{q_3 \to -(q_1 + q_2)}$$

 \circ Partial diagram depends on undressed chain helicity $h^{(2)}$ and two open indices

- Exploit analytical q_i -structure, e.g. dependence of maximal rank R_2 in q_2 on rank $r_1 \leq R_1$ in q_1 Example: $R_2(r_1 \leq 3) = 1$ and $R_2(r_1 = 4) = 0 \Rightarrow$ No simple $(R_1 = 4, R_2 = 1)$ array
- \Rightarrow Use this partial diagram as initial object for the last chain dressing

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)
- Dress ${\cal U}^{(1)} \propto {\cal M}_0^* {\cal N}^{(1)}$ (longest chain)
- \bullet Connect \mathcal{V}_1 with $\mathcal{U}^{(1)}$ and $\mathcal{N}^{(3)}$
- Connect \mathcal{V}_0 and map $q_3 \rightarrow -(q_1+q_2)$
- \bullet Connect segments of $\mathcal{N}^{(2)}$



$$\mathcal{U}_{n}^{(2)}(q_{1}, q_{2}, \tilde{h}_{n}^{(2)}) = \sum_{h_{n}^{(2)}} \mathcal{U}_{n-1}^{(2)}(q_{1}, q_{2}, \tilde{h}_{n-1}^{(2)}) S_{n}^{(2)}(q_{2}, h_{n}^{(2)})$$

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
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On-the-fly summation of segment helicities $\tilde{h}_n^{(2)} = \sum_{k=n+1}^{N_2-1} h_k^{(2)}$

 \Rightarrow Partial diagram depends only on helicities of remaining undressed segments

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)
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- \bullet Connect \mathcal{V}_1 with $\mathcal{U}^{(1)}$ and $\mathcal{N}^{(3)}$
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On-the-fly summation of segment helicities $\tilde{h}_n^{(2)} = \sum_{k=n+1}^{N_2-1} h_k^{(2)}$

 \Rightarrow Partial diagram depends only on helicities of remaining undressed segments

\Rightarrow Lowest complexity in helicities for steps with highest rank in loop momenta

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
- Dress $\mathcal{N}^{(3)}$ (shortest chain)
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- \bullet Connect \mathcal{V}_1 with $\mathcal{U}^{(1)}$ and $\mathcal{N}^{(3)}$
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- \bullet Connect segments of $\mathcal{N}^{(2)}$



Exploit diagram factorisation for full process:

 $\mathcal{U}_A + \mathcal{U}_B = \left(\mathcal{U}_{A,n} \cdot S_{n+1} \cdots S_N \right) + \left(\mathcal{U}_{B,n} \cdot S_{n+1} \cdots S_N \right) = \left(\mathcal{U}_{A,n} + \mathcal{U}_{B,n} \right) \cdot S_{n+1} \cdots S_N$

Merge partially dressed diagrams with same topology and subsequent recursion steps

- Sort chains by length: $N_1 \ge N_2 \ge N_3$ Choose order of $\mathcal{V}_0, \mathcal{V}_1$ by vertex type
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Merge partially dressed diagrams with same topology and subsequent recursion steps

Highly efficient and completely generic algorithm for two-loop tensor coefficients Fully implemented for QED and QCD corrections to the SM

IV. Numerical stability

Pseudo-tree test

- Cut diagram at two propagators
- Saturate indices with random wavefunctions e_1, \ldots, e_4
- Fixed values for loop momenta q_1, q_2



 \Rightarrow Compute with well-tested tree-level algorithm and with new two-loop algorithm

 \rightarrow contract coefficients $\mathcal{N}_{\mu_1\cdots\mu_{r_1}\nu_1\cdots\nu_{r_2}}$ with fixed-value tensor integrand $\frac{q_1^{\mu_1}\cdots q_1^{\mu_{r_1}}q_2^{\nu_1}\cdots q_2^{\nu_{r_2}}}{\mathcal{D}(q_1,q_2)}$

Test several processes in double and quadruple precision for 10^5 uniform random phase space points

Bulk of points has 14 - 16 digits agreement (all points 12 or more digits) in double precision \Rightarrow Implementation validated without computing two-loop tensor integrals

All points have more than 16 digits agreement in quad precision \Rightarrow **Quad precision calculation as benchmark**

IV. Numerical stability

Two-loop algorithm with fixed q_1, q_2 and pseudo wavefunctions e_1, \ldots, e_4 for 10^5 uniform random phase space points (psp). Numerical instability of double (dp) wrt quad precision (qp) calculation: $\mathcal{A} := \frac{|\mathcal{W}_{02}^{(dp)} - \mathcal{W}_{02}^{(qp)}|}{|\mathcal{W}_{02}^{(dp)}|, |\mathcal{W}_{02}^{(qp)}|)}$



Excellent numerical stability

⇒ Important for full calculation (tensor integral reduction will be main source of instabilities)

V. Timings for two-loop tensor coefficients





Strong CPU performance, comparable to real-virtual corrections in OpenLoops

VI. Summary and Outlook

Numerical calculation of two-loop tensor coefficients in the OpenLoops framework

- Exploit factorisation of diagrams
 - \rightarrow Highly efficient and completely generic recursive algorithm
- Fully implemented for NNLO QCD and NNLO QED corrections in the SM (irreducible and reducible two-loop diagrams)
- Excellent numerical precision
- Strong CPU performance ($\sim 150 \mu s$ per diagram and psp) due to
 - Efficient order of building blocks
 - Exploitation of analytical structure in loop momenta
 - On-the-fly helicity summation and diagram merging

Short-term and mid-term projects:

- Implementation of two-loop UV and rational counterterms
- Automation of all one-loop and two-loop ingredients in a single interface
- Tensor integral reduction and evaluation (in-house framework or external tool or mixture thereof)

Backup

Reducible two-loop diagrams

Amplitude of reducible diagram Γ_{red} (1-particle-reducible after amputation of external subtrees):



Two factorised one-loop diagrams connected by a tree-like bridge $P \Rightarrow$ Fully implemented