Next-to-leading order simulations with Sherpa+OpenLoops

Philipp Maierhöfer

Physik-Institut
Universität Zürich

Loops and Legs in Quantum Field Theory 2014

Weimar, 29 April 2014

In collaboration with
F. Cascioli, S. Höche, F. Krauss, N. Moretti, S. Pozzorini, M. Schönherr, and F. Siegert

Outline

1. The OpenLoops generator for one-loop matrix elements
2. $t\bar{t}b\bar{b}$ with massive bottom quarks matched to parton shower
3. Jet-merging of $t\bar{t} + 0, 1, 2$ jets

NLO in 2014

- Feasibility of $2 \to 4$ NLO QCD corrections is well established.
- Move from fixed order and proof of concept calculations to full simulations for experimental analyses.
- Develop tools of general applicability with focus on generic features rather than individual processes.
- Performance is crucial when NLO should become the default accuracy for LHC analyses.

Many more or less generic tools have been developed

Collier, CutTools, OneLOop, Samurai;
BlackHat, FormCalc, GoSam, HELAC-NLO, MadLoop, MCFM, NJet, OpenLoops, Recola, VBFNLO;
Herwig++, MadGraph/aMC@NLO, POWHEG, Pythia, Sherpa

OpenLoops algorithm for one-loop calculations

Numerical recursion for the tensor components of $\mathcal{N}_r^{\mu_1\dots\mu_r}$ in

$$\mathcal{A} = \int d^d q \, \frac{\mathcal{N}(q)}{D_0 \; D_1 \; \dots \; D_{N-1}} = \sum_{r=0}^{R} \mathcal{N}_r^{\mu_1\dots\mu_r} \cdot \int d^d q \, \frac{q_{\mu_1} \dots q_{\mu_r}}{D_0 \; D_1 \; \dots \; D_{N-1}},$$

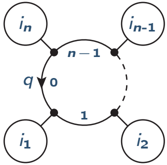
encoding the loop momentum dependence of the numerator.

- Diagrammatic, exploiting colour factorisation.
- Perform colour and helicity summation before reduction (also applicable to other methods).
- Works with both, tensor integral reduction [Melrose; Passarino, Veltman; Denner, Dittmaier; Binoth et al.; Fleischer, Riemann; & many others] and OPP reduction [Ossola, Papadopoulos, Pittau] in a straight forward way; with OpenLoops, OPP reduction becomes almost as fast as tensor integral reduction.

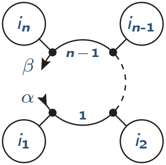
Inspired by van Hameren's ['09] work on multi-gluon amplitudes, where a Dyson-Schwinger-like recursion is used.

Recently also implemented in `MadLoop`.
Similar concept: `Recola`, closer to van Hameren's algorithm,
using current recursion + colour bookkeeping (see talk of S. Uccirati)

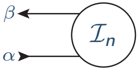
A one-loop diagram is an ordered set of trees i_k with wave functions $w^\delta(i_k)$, connected along the loop by vertices $X^\beta_{\gamma\delta}$.

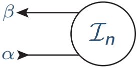


$\xrightarrow{\text{cut } D_0}$ $\mathcal{N}^\beta_\alpha(\mathcal{I}_n; q) =$

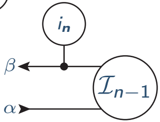


$\equiv$





$=$



$$\mathcal{N}^\beta_\alpha(\mathcal{I}_n; q) = X^\beta_{\gamma\delta}(q)\, \mathcal{N}^\gamma_\alpha(\mathcal{I}_{n-1}; q)\; w^\delta(i_n)$$

with the loop momentum q separated from the coefficients

$$\mathcal{N}^\beta_\alpha(\mathcal{I}_n; q) = \sum_{r=0}^{n} \mathcal{N}^\beta_{\mu_1\ldots\mu_r;\alpha}(\mathcal{I}_n)\, q^{\mu_1}\ldots q^{\mu_r}, \quad X^\beta_{\gamma\delta} = Y^\beta_{\gamma\delta} + q^\nu Z^\beta_{\nu;\gamma\delta}$$

Leads to the recursion formula for “open loops” polynomials $\mathcal{N}^\beta_{\mu_1\ldots\mu_r;\alpha}$:

$$\boxed{\mathcal{N}^\beta_{\mu_1\ldots\mu_r;\alpha}(\mathcal{I}_n) = \left[Y^\beta_{\gamma\delta}\, \mathcal{N}^\gamma_{\mu_1\ldots\mu_r;\alpha}(\mathcal{I}_{n-1}) + Z^\beta_{\mu_1;\gamma\delta}\, \mathcal{N}^\gamma_{\mu_2\ldots\mu_r;\alpha}(\mathcal{I}_{n-1})\right] w^\delta(i_n)}$$

OpenLoops: technical setup

- FeynArts [Hahn] to generate Feynman diagrams
- Mathematica to generate process specific Fortran code
- Process independent Fortran library
- Rational terms of type R_2 from couterterm-like Feynman rules
  [Draggiotis, Garzelli, Malamos, Papadopoulos, Pittau ‘09, ‘10; Shao, Zhang, Chao ‘11]
- QCD corrections to Standard Model processes,
  EW corrections to come

Tensor integral reduction with `Collier` [Denner, Dittmaier, Hofer], numerically stable thanks to expansions in small Gram determinants [Denner, Dittmaier] (see talk of L. Hofer).

Alternatively, OPP reduction with `CutTools` [Ossola, Papadopoulos, Pittau], or `Samurai` [Mastrolia, Ossola, Reiter, Tramontano], with scalar integrals from `OneLOop` [van Hameren].

Performance

process	diags	size/MB	time/ms
$u\bar{u} \to t\bar{t}$	11	0.1	0.27(0.16)
$u\bar{u} \to W^+W^-$	12	0.1	0.14
$u\bar{d} \to W^+g$	11	0.1	0.24
$u\bar{u} \to Zg$	34		0.75
$gg \to t\bar{t}$	44	0.2	1.6(0.7)
$u\bar{u} \to t\bar{t}g$	114	0.4	4.8(2.4)
$u\bar{u} \to W^+W^-g$	198	0.4	3.4
$u\bar{d} \to W^+gg$	144	0.5	4.0
$u\bar{u} \to Zgg$	408		17
$gg \to t\bar{t}g$	585	1.2	40(14)
$u\bar{u} \to t\bar{t}gg$	1507	3.6	134(101)
$u\bar{u} \to W^+W^-gg$	2129	2.5	89
$u\bar{d} \to W^+ggg$	1935	4.2	120
$u\bar{u} \to Zggg$	5274		524
$gg \to t\bar{t}gg$	8739	16	1460(530)

Measured on an i7-3770K (single thread) with gfortran 4.8 -O0, dynamic (ifort static ∼30% faster), tensor integral reduction with Collier.

Colour and helicity summed.

W/Z production includes leptonic decays and non-resonant contributions.

$t\bar{t}$ production numbers in brackets are for massless decays.

$2 \to 4$ runtime range: 10 ms (6 quarks) – 2 s (6 gluons)

Interfacing with Monte Carlo event generators

Sherpa version ≥ 2 contains an interface to OpenLoops

- Provides infrared subtraction, real radiation, phase space integration
- (S-)MC@NLO matching to the `Sherpa` parton shower and MEPS@NLO multi-jet merging [Höche, Krauss, Schönherr, Siegert '12, '13].
- Underlying event, hadronisation, ...

Interface to parton-level Monte Carlo by S. Kallweit (see talk).

Standard BLHA interface, developed for `Herwig++`.

Release plans

OpenLoops will be released as soon as `Collier` is public.
Depending on when this will happen, there may be an earlier release which uses `CutTools` instead, curing numerical instabilities with quadruple precision where needed.

A pre-release is already available to the Monte Carlo working groups of ATLAS and CMS.

Recent applications

- MEPS@NLO for $\ell\ell\nu\nu + 0, 1\,\mathrm{jets}$

  [Cascioli, Höche, Krauss, PM, Pozzorini, Siegert]
- LO merging for (loop-induced) $HH + 0, 1\,\mathrm{jets}$ [PM, Papaefstathiou]
- NLO $W^+W^-b\bar{b}$ with $m_b > 0$ [Cascioli, Kallweit, PM, Pozzorini]

  → talk by S. Kallweit
- MEPS@NLO $W^+W^-W^\pm + 0, 1\,\mathrm{jets}$

  [Höche, Krauss, Pozzorini, Schönherr, Thompson, Zapp]

NNLO (for real-virtual corrections):

- $Z\gamma$ [Grazzini, Kallweit, Rathlev, Torre]
- ZZ → talk by M. Grazzini
- $t\bar{t}$ [Abelof, Gehrmann-De Ridder, PM, Pozzorini]

  → talk by A. Gehrmann-De Ridder

This talk:

- MC@NLO for $t\bar{t}b\bar{b}$ with $m_b > 0$ [Cascioli, PM, Moretti, Pozzorini, Siegert]
- MEPS@NLO for $t\bar{t} + 0, 1, 2\,\mathrm{jets}$

  [Höche, Krauss, PM, Pozzorini, Schönherr, Siegert]

$t\bar{t}b\bar{b}$ with $m_b > 0$ matched to parton shower

MC@NLO matching for $t\bar{t}b\bar{b}$ with massive b quarks

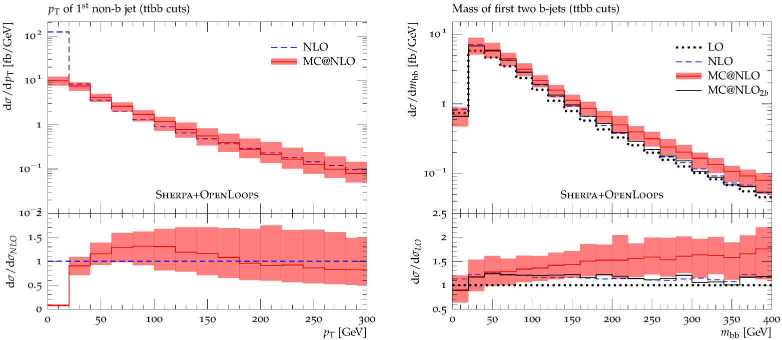
- Background to $t\bar{t}H(\to b\bar{b})$
- Signal/background $\sim 10\%$
- m_b regulates collinear singularities; NLO description of collimated $b\bar{b}$ pairs (otherwise only $t\bar{t}g$ + parton shower $g \to b\bar{b}$ splitting)

Setup

- Widely separated scales, adapt scale to b-jet p_T, inspired by CKKW:
  $\mu_R^4 = E_{T,t}E_{T,\bar{t}}E_{T,b}E_{T,\bar{b}}$
  $\to \alpha_s^4(\mu_R) = \alpha_s(E_{T,t})\alpha_s(E_{T,\bar{t}})\alpha_s(E_{T,b})\alpha_s(E_{T,\bar{b}})$
- Factorisation and resummation scale: $\mu_F = \mu_Q = \frac{1}{2}(E_{T,t} + E_{T,\bar{t}})$
- Analysis for stable top quarks, b-jets with $p_T > 25\,\text{GeV}$, $|\eta| < 2.5$, b-jet definition: at least one b-quark in the jet

Previous calculations with massless b quarks: [Bredenstein, Denner, Dittmaier, Pozzorini '08, '09, '10; Bevilacqua, Czakon, Papadopoulos, Pittau, Worek '09]
matched to parton shower: [Kardos, Trócsányi '13]

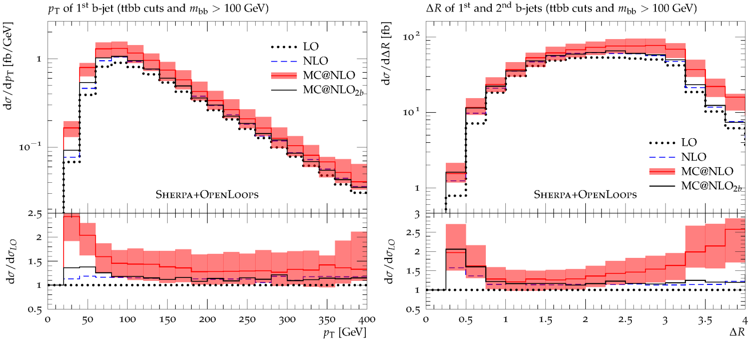
MC@NLO effects



Non-b-jet p_T: large Sudakov suppression below 50 GeV, due to strong QCD radiation from initial state gluons.

$>$ 30% MC@NLO effect in the Higgs signal region ($m_{b\bar{b}} > 100\,\mathrm{GeV}$) due to double collinear splittings. Exceeds the Higgs signal! Excess disappers when $g \to b\bar{b}$ shower splittings are disabled.

MC@NLO excess in the Higgs signal region

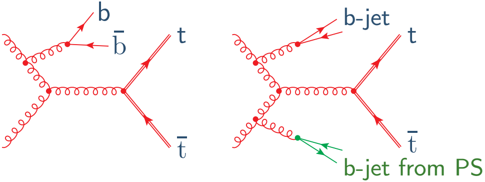


MC@NLO excess is located at small b-jet p_T
and large angular separation.

Fits the picture of attributing it to collinear double splittings:
strong enhancement of parent gluons at small p_T due to the
soft-collinear singularity related to radiation from initial state gluons.

Double collinear $g \to b\bar{b}$ splitting effect

The shower starting scale is set by the top-quark transverse energies
→ some b-quark pairs from the shower will have higher m_{bb}
than those from the matrix elements.



The second collinear splitting is described only at parton shower accuracy, originating from leading order $t\bar{t}b\bar{b}g(\to b\bar{b})$

In the picture of $t\bar{t} + \text{jets}$ merging:
$t\bar{t}gg/t\bar{t}b\bar{b}$ ratio grows at large m_{gg},
whereas the $g \to b\bar{b}$ splitting probability does not decrease.

Top quark pair prodction in association with jets

Top-quark pair production suffers from large scale uncertainties at leading order, growing rapidly with increasing jet multiplicity.

Many efforts in reducing the uncertainties:

- NLO fixed order $t\bar{t}jj$
  [Bredenstein, Denner, Dittmaier, Pozzorini '09, '10;
  Bevilacqua, Czakon, Papadopoulos, Worek '10, '11]
- NLO $t\bar{t}j$, showered
  [Kardos, Papadopoulos, Zoltan Trocsanyi '11; Alioli, Moch, Uwer '11]
- NLO $t\bar{t} + 0, 1j$ merged [Höche, Huang, Luisoni, Schoenherr, Winter '13]
- NNLO $t\bar{t}$ total cross section [Czakon, Fiedler, Mitov '13]

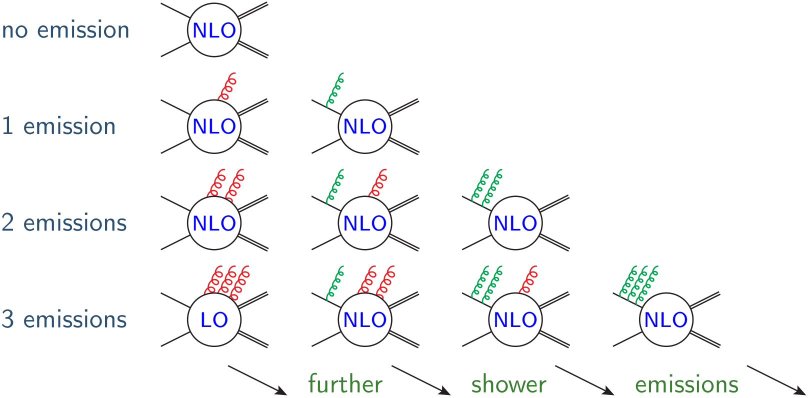
Especially to model backgrounds, a consistent description of different jet multiplicities is required → need jet merging

Currently experimentalists typically use

- NLO $t\bar{t}$ + parton shower
- LO merged $t\bar{t} + \mathrm{jets}$ with a k factor

Intermezzo: multi-jet merging

Core process and up to two hard jets described by NLO matrix elements.
Three hard jets described by LO matrix elements.
Soft and collinear emissions and all further emissions
described by the parton shower.



Intermezzo: multi-jet merging

Leading order matrix elements B_n (n jets), Observable O. Match to shower and use hard matrix element B_{n+1} for emission above scale Q_{cut}.

$$\langle O\rangle^{\mathrm{MEPS}} = \int \mathrm{d}\Phi_n B_n \Big[\Delta^{(\mathcal{K})}(t_0,\mu_Q^2) O_n + \int_{t_0}^{\mu_Q^2} \mathrm{d}\Phi_1 \Big(\mathcal{K}\,\Theta(Q_{\mathrm{cut}}-Q) + \frac{B_{n+1}}{B_n}\,\Theta(Q-Q_{\mathrm{cut}})\Big) \times \Delta^{(\mathcal{K})}(t_0,t_{n+1}) O_{n+1}\Big]$$

[Catani, Krauss, Kuhn, Webber ‘01; Lönnblad ‘02; Höche, Krauss, Schumann, Siegert ‘09; Hamilton, Richardson, Tully ‘09; Lönnblad, Prestel ‘12]

Parton shower starting scale μ_Q, IR cut-off t_0, splitting kernel $\mathcal{K}$, Sudakov form factor $\Delta^{(\mathcal{K})}(t,t') = \exp\big(-\int_t^{t'} \mathrm{d}\Phi_1 \mathcal{K}\big)$ (probability for no emission between t and t')

Generalisation to NLO → MEPS@NLO

[Höche, Krauss, Schönherr, Siegert ‘12; Gehrmann, Höche, Krauss, Schönherr, Siegert ‘13]

Remove contribution from the Sudakov form factor which is described by the matrix element to avoid double counting.

$t\bar{t} + 0, 1, 2j$ MEPS@NLO setup

Scale choice

- Scale for the $pp \to t\bar{t}$ core process:
  $1/\mu_{\mathrm{core}}^2 = 1/s + 1/(m_t^2 - t) + 1/(m_t^2 - u)$
  Used as factorisation scale μ_F and resummation scale μ_Q.
- The renormalisation scale for $pp \to t\bar{t} + n\,\mathrm{jets}$ is defined by $\alpha_s(\mu_R)^{2+n} = \alpha(\mu_{\mathrm{core}})^2 \prod \alpha_s(t_i)$.
- Merging scale $Q_{\mathrm{cut}} = 30\,\mathrm{GeV}$.

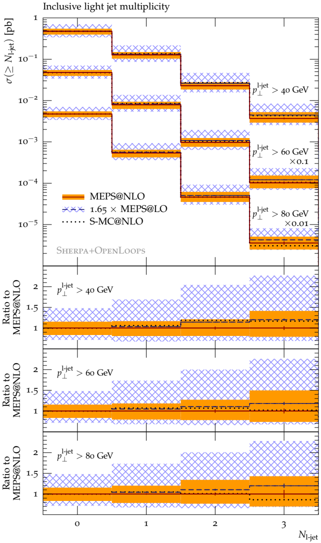
Uncertainty estimates

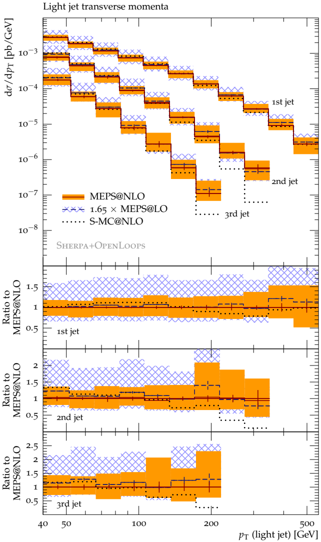
- Factor 2 variations of μ_R and μ_F, and factor $\sqrt{2}$ variation of μ_Q.
- Merging systematics: Q_{cut} varied between 20 GeV and 40 GeV.

Event selection based on

- Full top-quark decays, identify leptons with $p_T > 25\,\mathrm{GeV}$ and $|\eta| < 2.5$, and $E_T^{\mathrm{miss}} > 30\,\mathrm{GeV}$ due to neutrinos.
- Anti-k_t jets with $R = 0.4$.

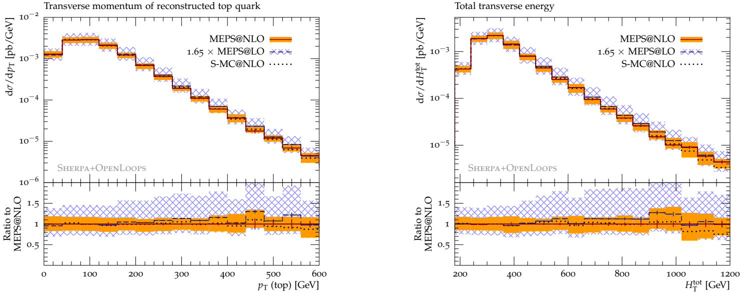
Light flavour jet multiplicity distributions for $p_T > 40, 60, 80$ GeV (left) and transverse momentum distributions for the first three light jets (right).





LO-like error for high p_T of the second jet: dominated by 3-jet topologies.

Top-quark transverse momentum (left) and total transverse Energy $H_T^{\rm tot} = \sum p_{T,\rm b-jet} + \sum p_{T,\rm l-jet} + \sum p_{T,\rm lep} + E_T^{\rm miss}$ (right) distributions.



→ relevant especially for new physics searches.

All in all, the shapes of the three different approximations agree quite well with a sizable deficit of S-MC@NLO in the high jet-p_T region.

MEPS@NLO reduces the uncertainties from typically 50-80% to 20-30% in the various distributions.

Merging scale variation yields uncertainties below 10%.

Summary

OpenLoops

- Automatic generator for one-loop matrix elements.
- Very fast and numerically stable (thanks to `Collier`), even for NNLO real-virtual corrections.

$t\bar{t}b\bar{b}$ with massive bottom quarks matched to parton shower

- Background to $t\bar{t}H(\to b\bar{b})$.
- Surprisingly large MC@NLO effects due to double collinear $g \to b\bar{b}$ splittings discovered. Parton shower matching is essential.

Jet-merging of $t\bar{t}+0,1,2$ jets

- Consistent description of individual jet multiplicities, crucial for applicability to experimental analyses. NLO+PS accuracy in 0, 1, 2 jet bins.
- Uncertainties reduced from $\mathcal{O}(50-100\%)$ to $\mathcal{O}(20-30\%)$, dominated by renormalisation scale variations.