Automated NLO QCD Corrections with WHIZARD

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We briefly discuss the current status of NLO QCD automation in the Monte Carlo event generator WHIZARD. The functionality is presented for the explicit study of off-shell top quark production with associated backgrounds at a lepton collider.

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1. The WHIZARD Event Generator

WHIZARD [1] is a multi-purpose event generator for in principle arbitrary processes at hadron and lepton colliders. It is especially suited for lepton collider physics due to its generic treatment of beam-spectra and initial-state photon radiation. Moreover, the simulation and analysis can be very conveniently performed using the built-in script language SINDARIN.

WHIZARD is written in Fortran2003. Its structure is strictly object-oriented, so that a modular structure enables the convenient interface to numerous other programs. The main sub-components of WHIZARD are O’ Mega [2], VAMP [3] and CIRCE [4]:

O’Mega provides multi-leg tree-level matrix elements using the helicity formalism. VAMP is used for Monte-Carlo integration and grid sampling. It is a multi-channel version of usual adaptive integration methods. The CIRCE packages create and evaluate lepton beam spectra.

Scattering amplitudes and color factors are factorized in WHIZARD. Color factors are evaluated using the color-flow formalism [5].

WHIZARD can be used for event generation on parton level as well as for the subsequent shower simulation. For this purpose, it has its own analytical parton shower [6] as well as a built-in interface to Pythia6 [7]. An automated interface to Pythia8 [8] or HERWIG++ [9] is not yet present, but planned.

The list of external packages that can be linked to WHIZARD covers the most commonly used high-energy physics simulation and analysis tools, such as FastJet [10], LHAPDF [11] or HepMC [12]. For next-to-leading order studies, GoSam [13] or OpenLoops [14] can be used to compute virtual loop matrix elements.

Though WHIZARD spearheaded many BSM phenomenological studies [15–20] we will focus here on automation of SM QCD NLO corrections.

2. Automated NLO Calculation with WHIZARD

Next-to-leading order (NLO) calculations have become standard for the prediction of most observables during the last decade. Substantial progress has been made in the automation of loop matrix-element computation as well as in NLO parton shower matching [21,22]. At the LHC, NLO simulations are routinely employed.

Computer programs in this field cover a range from dedicated, single-purpose codes to automated multi-purpose event generators. In the latter category, NLO support has so far been achieved by Madgraph [23] and Sherpa [24].

With the ILC approaching its possible approval phase, ILC studies become more specific [25], thereby increasing the need for easy to use NLO programs increases. Here, we want to combine the expertise of WHIZARD in the field of lepton collisions with the improved accuracy of NLO predictions.

There have been earlier works on NLO QED extensions to WHIZARD for certain supersymmetric processes [26, 27] as well as on NLO QCD corrections for $pp \rightarrow b\bar{b}b\bar{b}$ [28, 29] using Catani-Seymour subtraction. However, the fully generic NLO framework is a recent development.
2.1 Subtraction schemes

The main task about an automated NLO framework is to treat the UV- and IR-divergences which come along with loop matrix elements and real-emission amplitudes. Whereas UV-divergences can be absorbed via renormalization into the physical quantities of the underlying field theory, IR-divergences only cancel in the sum of real and virtual matrix elements, as stated by the KLN theorem [30, 31]. However, this requires the choice of a regularization scheme, e.g. a lower cutoff parameter like gluon masses, or, most commonly, dimensional regularization. The latter method makes divergences explicit by extending the number of integration dimensions to an arbitrary (complex) number different from the four physical ones.

Subtraction schemes are a different approach especially suited for numerical calculations. Additional subtraction terms \( C \), which reproduce the singularities of the real and virtual matrix elements, are added to the NLO cross section, such that

\[
d_{\sigma}^{\text{NLO}} = d_{\sigma}^{\text{LO}} + \int_{n+1}^{n+1} \left(d_{\sigma}^{R} - d_{\sigma}^{S}\right) + \int_{n+1}^{n+1} d_{\sigma}^{S} + \int_{n}^{n} d_{\sigma}^{V}.
\]

The explicit form of \( C \) is arbitrary. Several approaches have been developed, the most popular ones being the Catani-Seymour scheme [32] and the FKS (Frixione-Kunszt-Signer) scheme [33, 34], described below. Catani-Seymour subtraction has been the standard method for the last two decades, due to the fact that it can be used with any phase space generator. Thus, it is especially suited for process-specific event generators and is also widely used in this context. However, the FKS scheme has increased in popularity over last ten years and is also used by WHIZARD. Other programs with their own FKS-implementation are MG5_amC@NLO, HERWIG++, HELAC-NLO [35] and the POWHEG-BOX [36]. All of them are automated or semi-automated event generators, which allow for the coherent use of a single phase space generator, suited for FKS. Also, the number of CS dipoles grows larger than the number of FKS regions. Moreover, it is known that the Catani-Seymour procedure requires an increased complexity when NLO parton shower matching, e.g. with the POWHEG method, is performed [37].

2.2 BLHA interface

WHIZARD with O’Mega matrix elements can only generate tree-level processes. External programs can be interfaced to WHIZARD, so-called One-Loop Providers (OLPs), to obtain virtual matrix elements. To standardize the interface between OLP and Monte-Carlo program, the Binnoth Les Houches Accord (BLHA) [38, 39] has been developed. It specifies standards for the communication files between OLP and the Monte-Carlo program and also explicitly prescribes the functions with which the OLP program can be called, mostly to compute matrix elements.

WHIZARD has a generic BLHA-interface. This means that OLPs which comply with the BLHA standards can be linked to the main program with only minor programming effort. For a working interface, WHIZARD will produce an .olp-file, which contains general information about the process, e.g. the type of correction (QCD or electroweak) or the desired regularisation scheme, as well as the involved flavor structures and the corresponding amplitude types (tree, color-correlated tree,
spin-correlated tree and loop). The One-Loop Provider then reads in the .olp-file and, if successful, will provide the necessary libraries, which can be linked to WHIZARD. It also generates a contract(.olc)-file, which in turn is read by WHIZARD. The .olc-file contains information about the interfaces to the BLHA-library.

Up to now, WHIZARD has working BLHA interfaces for two programs, GoSam and OpenLoops. GoSam is an OLP creating explicit analytical code based on Feynman diagrams using QGraf [40] and FORM [41]. This makes GoSam a very flexible program, suited for SM as well as for BSM processes. Virtual diagrams are evaluated using D-dimensional reduction [42] or tensorial reconstruction [43].

On the other hand, OpenLoops uses recursion relations to compute matrix elements. The desired process libraries have to be installed from the OpenLoops-repository. This introduces the drawback that only these pre-compiled libraries can be used. However, this is made up for by the increased speed of the program, which is mainly due to the faster matrix-element evaluation, but also because the user does not have to compile the libraries by himself as is the case with GoSam.

3. Top Quark off-shell Production and Associated Background

In this section, we present a phenomenological study of the process $e^+e^- \rightarrow W^+W^-b\bar{b}$ at next-to-leading order QCD for a future lepton collider. A comprehensive study of this process for hadron colliders is given in [44].

This signature is dominated by top-quark pair production and the subsequent decay $t \rightarrow bW$, but also contains the process $e^+e^- \rightarrow HZ$, which yields the same final state for the subsequent decays $H \rightarrow b\bar{b}$ and $Z \rightarrow W^+W^-$. Both processes have never been measured at a lepton collider. However, future lepton colliders will definitely have the necessary center-of-mass energy and luminosity. Especially the ILC is designed to also operate at the top-production threshold. Thus, a detailed study of top-quark properties will be possible.

A first numerical approach to this process was made by Ref. [45], focusing on Higgs mass effects using a cut-off regularization specialized on this process. However, we were not able to reproduce both their LO- and NLO-results with WHIZARD as well as with MG5_amC@NLO.

We present the preliminary results for the total cross section at next-to-leading order as well as fixed-order NLO event shapes for selected observables. Our calculation was performed with the release version 2.2.7 of WHIZARD, using the standard NLO-setup. The loop matrix elements are obtained from OpenLoops.

For our setup, we use $m_h = 4.7$ GeV and $m_t = 172$ GeV. The renormalization scale is chosen as $\mu_R = m_t$. We set $\alpha^{-1}_c = 132.160$ and $\alpha_s(M_Z) = 0.118$. All amplitudes are computed using the top-quark width at NLO for massive b-quarks, as computed in [46]. The LO cross section, accordingly, is obtained using the well-known LO value for $\Gamma_t$. This yields $\Gamma_t^{NLO} = 1.409$ GeV and $\Gamma_t^{LO} = 1.538$ GeV.

Figure 1 shows the total cross section for the process $e^+e^- \rightarrow W^+W^-b\bar{b}$ at leading and next-to-leading order. For comparison, also the result for on-shell $t\bar{t}$-production is displayed. It can be seen that the simple assumption $\Gamma_{\text{offshell}}/\Gamma_{\text{onshell}} \approx BR(t \rightarrow bW) \approx 1$ cannot be applied everywhere due to background contributions. We see that the NLO curves display the same behaviour. However, the intersection of both curves is at higher values of $\sqrt{s}$, and the difference between on-shell and
off-shell results is not as distinct after this intersection as it is in the LO-case. The K-factor close
to the $t\bar{t}$-threshold can go up to almost 3. This large value is due to non-relativistic top quarks that
can form a quasi-bound state via the exchange of Coulomb gluons. This leads to a contribution of
large logarithms which have to be treated with resummation [47, 48].

Figure 2 displays several observables obtained from a simulated LO and NLO event sample. The
LO sample contains 500K unweighted events. The NLO event sample consists of 45M weighted
events. Of these, 15M have Born kinematics and their associated weight is $B + V - \sum \alpha C_\alpha$. Each
singular region $\alpha$ gets associated with a real-emission event with weight $R_\alpha$, thus giving the additional 30M events in the NLO sample.

The event samples are stored in the HepMC-format. We have used a variant of the anti-$k_t$
algorithm [49] with $\Delta R = 1$ to cluster jets, in this case b-quarks and gluons with $E > 1$ GeV, and re-
quired at least two jets to be present after clustering. The analysis was performed with Rivet [50].
In the $t\bar{t}$-production channel, the $bW$-pairs originate from the decay of the individual top quarks, so
there is a clear resonance at $m_t = 172$ GeV. We see that this resonance is not affected significantly
by NLO corrections. However, outside the resonance region, background contributions increase.
We observe a similar enhancement in the other observables.

It must be noted that the events displayed in Figure 2 have not been processed further with a parton
shower algorithm. However, this will lead to unphysical results because double-counting occurs.
To circumvent this, WHIZARD has its own implementation of the Powheg method, which is pre-
sented in [51].
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4. Summary and Outlook

We have shown that WHIZARD is capable of performing full NLO QCD calculations in an automated way. For this purpose, WHIZARD uses the FKS subtraction scheme. External BLHA one-loop providers can be used, primarily for the computation of loop amplitudes, but also for the evaluation of tree-level diagrams. The latter is useful to filter leading-order diagrams if GoSam is used.

We have presented phenomenological results for the specific example of off-shell top quark pair production with its associated backgrounds. We observe that NLO corrections can become large in certain distributions even if the correction to the total cross section is small.

Next-to-leading order simulations in WHIZARD are still an experimental feature and not fully validated. Additionally, the focus of the development is on NLO QCD corrections for lepton collisions. Hadron collisions involve additional initial-state corrections and corrections to parton density functions. This feature will be supported once the support for lepton collisions in WHIZARD is complete.
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