Modern Particle Physics Event Generation with WHIZARD

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Abstract. We describe the multi-purpose Monte-Carlo event generator WHIZARD for the simulation of high-energy particle physics experiments. Besides the presentation of the general features of the program like SM physics, BSM physics, and QCD effects, special emphasis will be given to the support of the most accurate simulation of the collider environments at hadron colliders and especially at future linear lepton colliders. On the more technical side, the very recent code refactoring towards a completely object-oriented software package to improve maintainability, flexibility and code development will be discussed. Finally, we present ongoing work and future plans regarding higher-order corrections, more general model support including the setup to search for new physics in vector boson scattering at the LHC, as well as several lines of performance improvements.

1. Introduction

WHIZARD [1] is a general event generator for all kinds of scattering and decay processes at highenergy hadron and lepton colliders.

The default matrix element generator of WHIZARD is O'Mega [2]. This latter subpackage provides matrix elements for multi-leg tree-level processes, using the helicity formalism. The high-dimensional phase-space integrations are performed by the multi-channel Monte-Carlo integrator VAMP [3]. Its algorithm is adaptive both between and within channels, and thus computes accurate phase-space integrals and efficiently generates weighted and unweighted event samples.

The WHIZARD core acts as a connector of these different components. The core contains the algorithm for multi-channel phase-space parameterization and mapping, provides the user interface, and also interfaces external programs (e.g., parton distributions, event formats, hadronization), the routines for writing and reading event files, and modules for parton shower and jet physics. Further modules allow for the for numerical analyses and visualization of event samples.

In order to be able to describe realistic ILC and CLIC environments, WHIZARD contains a dedicated package for beam-spectrum simulation, CIRCE [4]. As an alternative, GuineaPig

beam-event samples can be fed into WHIZARD using CIRCE2.

2. Program Overview

WHIZARD – initiated along the lines of the TESLA design study [5] to provide improved simulations for electroweak processes at lepton colliders – has developed into a universal generator for partonic events at all types of present and future (lepton and hadron) colliders.

With the new millenium, the implementation of QCD color flows finalized the support for the full Standard Model (SM), and parton distributions, different event samples and an ever enlarging list of models beyond the SM (BSM) came up. Here, we should mention particularly the implementation of the MSSM and several variations thereof, like the NMSSM [6]. For this purpose, the SUSY Les Houches Accord (SLHA) [7, 8, 9] has been provided in order to interface SUSY spectrum generators. WHIZARD has been used for a plethora of both theoretical and experimental studies for TESLA and the ILC as well as the LHC. The SLAC event database for Linear Collider events has been generated with the package.

To meet the enormous technical demands of event simulations in the LHC and ILC era, the core of the program has been thoroughly rewritten in 2007-2010, which gave rise to the WHIZARD 2 release series.

The rigid input files of the early versions have been replaced in WHIZARD 2 by input commands within the domain-specific language SINDARIN. Besides a simplification and unification of the input inside the user interface, the user gets the full power of a programming language at hand. With the help of SINDARIN, cuts, analyses, interfaces, process collection, parameter scans and many more things can be defined.

By means of external packages like SARAH [10] or FeynRules [11], interfaced to WHIZARD [12], new physics models can easily be added. Inside WHIZARD, complete quantum-mechanical correlations are kept using a generic density-matrix formalism. In addition, the program is endowed with its own parton-shower module [13] as an alternative to showering being performed externally. Exact matrix elements can be matched to the shower by means of the MLM scheme, while other merging and matching schemes are planned for the near future.

WHIZARD 2 is written in Fortran2003 that is supported in modern Fortran compilers. Backwards compatibility is kept until version 4.7.4 of gfortran. The matrix element generator O'Mega is written in the functional programming language OCaml, for which complete packages exist for all major platforms. The current WHIZARD production version is 2.2.2 (as of October 2014), while the next release, 2.2.3, is planned for end of November. The complete package is thoroughly tested and can be installed on all recent Linux and MAC OS systems.

3. Technical Details

The standard installation of WHIZARD is foreseen centrally on a machine, but it can of course also be installed locally in a user directory. It uses the standard toolchain of automake, autoconf, and libtool. The program is located at the HepForge server [14]. Downloads are available either as tagged versions (.tar.gz format), or as a development version from the public svn repository. The package conforms to the standard installation procedure, using the usual configure – make – make install chain and the optional make check and make installcheck steps for additional safety checks.

Event generation and simulation projects of the users can then be set up in arbitrary directories without any predefined structure. For this purpose, a single command whizard exists, calling a single SINDARIN command file as input. Alternative modes of using WHIZARD exist, namely an interactive mode, or linking it as a subroutine library that is interoperable with C, C++ or any other C-compatible language (e.g., Python). The package generates and processes matrix element codes on-the-fly as dynamically linked libraries. There is also a statically linked mode for the work e.g. on batch clusters.

According to the modern object-oriented programming paradigm, there should be a clear separation between abstract type declarations and specific implementations. This is reflected in the modern Fortran standard, and hence WHIZARD 2 is broken down into these building blocks. There has been a major refactoring of the code between versions 2.1 and 2.2 (which is still partially ongoing) along these lines. The consequent separation of interface from implementation greatly improves the maintainability and enhances the possibilities for future module replacements, reimplementations, and extensions enormously. This is now realized in most parts of the core code like the process structure, matrix element calculation methods, beam structure, integration methods, decays, the phase space and the shower. For parallelization, WHIZARD 2 uses OpenMP. This is especially used in a new high-performance virtual machine and will be made available in the upcoming version 2.2.3. An MPI implementation is foreseen for the nearer future.

Quality assignment for WHIZARD is provided at first by using the svn version control at HepForge. Secondly, a continuous integration system runs all commits automatically through a chain of several hundreds of unit and function tests. Bugs and feature requests are steered by means of HepForge's tracking system.

4. Physics

The main method for matrix elements inside WHIZARD is provided by the matrix element generator O'Mega [2] which is able to generate complete tree-level matrix elements with multiple external legs (successful tests on standard hardware have involved up to 15 external particles). O'Mega is based on a recursive algorithm that reuses *all* common subexpressions and replaces the forest of all tree diagrams by the equivalent directed acyclical graph (DAG). It is able to provide the complete color correlations of QCD matrix elements, using the color-flow formalism with phantom U(1) particles [15] as an efficient way to generate colorized DAGs that can be evaluated exactly or be projected onto color-flow amplitudes.

WHIZARD now supports processes to consist of several different components, e.g. for inclusive production samples using process containers or to combine NLO subtraction terms with real emission and virtual matrix elements. Also available are flavor sums which are however technically different, as masses have to be equal to commonly use the same phase space. Within the SINDARIN steering language this feature is easily available for the user with an appropriate syntax for inclusive processes and a detailed specification of decay chains. The latter will be refined in upcoming versions. Exact spin and color correlations are kept using the internal density-matrix formalism inside WHIZARD.

WHIZARD 2 can not only process complete matrix elements, but also generate decay chains and cascades. They consist of arbitrarily chosen elementary processes to be integrated each separately, but concatenated for the event generation. The default option is to take full spin correlation among intermediate states into account. There is also an option to restrict to classical spin correlations (only diagonal entries in the spin-density matrix), or to even switch off spin correlations completely in order to test the importance of spin correlations. WHIZARD can also set up decays and branching fractions for chosen physics models automatically.

Arbitrary factorization and renormalization scale settings (affecting QCD) can be used in WHIZARD 2 using the same syntax expressions as the one for cuts or analyses. Furthermore, since version WHIZARD 2.2 there is the possibility to reweight existing event samples, generated either internally or read from file, when changing the setup of the original process, e.g. parameters in the hard matrix elements, the event scale, the chosen structure functions, or the QCD parton shower.

5. Linear Collider Simulation

WHIZARD is an event generator for all kinds of high-energy colliders, but a particular focus has always been its vast support for a realistic lepton collider environment. A description as accurate as possible of the beam properties is manadatory for studies and analyses, given the required level of precision at ILC and CLIC.

WHIZARD incorporates the CIRCE1 [4] package that parameterizes the beams of an e^+e^- collider and provides an event generator for factorized beam spectra. Adapting this generator (or, alternatively, the parameterized spectrum directly), WHIZARD can integrate and simulate any e^+e^- process with a realistic beam description. As an upgrade to previous versions, WHIZARD 2.2 ships with beam spectra that correspond to the current ILC design parameters. To account for cases where such a factorized form is insufficient, WHIZARD can alternatively read beam-event files as they are produced by GuineaPig. From version 2.2.3, the CIRCE2 package inside WHIZARD now directly interfaces GuineaPig(++) and allows for the use of correlated lepton collider beam spectra with their steeply rising peaks where a power-law parameterization is insufficient.

Lepton-collider processes are not only influenced by beamstrahlung, but also strongly affected by electromagnetic initial-state radiation (ISR). WHIZARD uses a standard structure-function formalism that resums the corrections from infrared (leading) and collinear (3rd order) radiation to implement ISR. It takes ISR into account both in kinematics and dynamics, if requested.

WHIZARD enables the user to specify arbitrary beam polarizations, ranging from unpolarized, left- or right-handed circular or transversal polarization to arbitrary spin-density matrices. The polarization and polarization fractions are specified for both beams independently. The user can also define asymmetric beam setups and a crossing angle, which will be taken into account in the kinematics setup.

Photons as initial particles are available in various incarnations: on-shell, radiated from e^{\pm} (effective photon approximation), or beamstrahlung photons generated by CIRCE1. A photoncollider option that uses the CIRCE2 beam description is also available but no longer maintained, due to the lack of current ILC or CLIC photon-collider mode beam parameters and simulations of the corresponding beam-beam interactions.

For cuts, reweighting and internal analysis, WHIZARD employs its dedicated language SINDARIN that allows for computing a wide range of event-specific and generic observables.

WHIZARD supports various event output formats, including the traditional HEPEVT format and its derivatives, StdHEP, LHEF, HepMC, and others. A direct interface to LCIO is planned.

6. QCD

For a precise calculation of exclusive processes, a program needs fine control over QCD corrections. Regarding real radiation, the multi-leg capability of WHIZARD allows to include high orders of the QCD coupling. Collinear and soft radiation in exclusive events is affected by large logarithms, which are conveniently resummed in the semi-classical approach of a parton shower algorithm.

Using standard event formats and suitable cuts, WHIZARD allows for attaching an external parton-shower generator. WHIZARD 2 furthermore contains an internal showering module in two different incarnations: a k_T ordered shower along the lines of the Pythia shower [16], and an analytic parton shower, which keeps the complete shower history and allows to reweight it [13]. There is support for combining exact matrix elements and QCD radiation from the parton shower using the MLM matching prescription. These modules are foreseen to receive a more detailed validation, tuning and further improvements after the 2.2 release.

Beyond the parton shower, hadronization and hadronic decays are not performed by WHIZARD internally, but can be applied to the generated partonic event samples via the Pythia 6 package [16] which is attached to the WHIZARD distribution, or using e.g. LHE event samples that are then fed into a external (shower and) hadronization package.

A high-luminosity linear collider will be capable of a high-precision scan of the top-quark pairproduction threshold [17]. To match this on the theoretical side, one needs to resum logarithms of the top velocity $\sim \alpha_s \ln v$ as well as gluon Coulomb potential terms $\sim \alpha_s/v$ in a non-relativistic approach and to relate this to the relativistic matrix elements in the continuum. There is an ongoing project for including these effects in WHIZARD 2 which will make the theoretical calculation available in the simulation of exclusive events. As a first step, the next-to-leadinglogarithmic approximation matched to next-to-leading-order matrix elements has already been implemented and will be included in the upcoming release 2.2.3 [18].

7. Status of next-to-leading order calculations

WHIZARD 2 with O'Mega matrix elements is an event generator of tree-level processes. There have been several projects that extended it to next-to-leading order, including loop corrections and proper infrared-collinear subtraction. Ref. [19, 20] describes the extension of WHIZARD 1 to a positive-definite NLO event generator for the electroweak pair production of charginos in the MSSM, including full electroweak SUSY corrections matched to the photon initial and final state radiation. Independently, Ref. [21, 22] implemented the QCD NLO correction with subtraction for a particular LHC process. Along these lines, the Binoth Les Houches Accord (BLHA) interface [23, 24] has been implemented for reading and writing contract files with one-loop programs (OLP), and has been validated.

Building upon the new data structures of WHIZARD 2.2, an implementation of automatic NLO QCD corrections is currently being developed.

WHIZARD is being extended to calculate cross sections at next-to-leading order in α_s . For this purpose, we have implemented the FKS subtraction scheme [25], which relies on a partition of the phase space into disjoint regions. Using this scheme, WHIZARD computes the real-subtracted and virtual-subtracted part of the cross section.

The virtual amplitude is calculated using GoSam [26], which can be interfaced very easily with WHIZARD using the BLHA conventions [23].

For the real amplitude, standard O'Mega matrix elements are used. The subtraction terms require color- and spin-correlated Born matrix elements. However, the treatment of the latter has not been adressed yet, because spin-correlated matrix elements are only non-zero if at least one external particle is a gluon. For the color-correlated Born matrix element we use the usual Born matrix element multiplied with C_F , which is suited for 2-jet cross sections. These parts of the calculation will be fully generalized soon, also using GoSam.

The implementation has been tested using the analytically known R-ratio for 2-jet production in lepton collisions. WHIZARD correctly reproduces the result $\sigma_{\rm NLO} = (1 + \alpha_s/\pi) \sigma_{\rm LO}$. It has also been tested for the processes $e\nu_e \rightarrow q\bar{q}'Z$ and $e^+e^- \rightarrow q\bar{q}'l\nu_l$ and has been validated for those processes.

The calculation of NLO-QCD cross sections will be an experimental feature of Release 2.2.3 and at least supports processes including two colored particles in the final state.

8. Physics models

As a generator of hard matrix elements, WHIZARD has to support various particle species and interactions. The allowed spin representations for particles are 0, 1, 2 (bosons) and 1/2, 3/2 (fermions), all massive or massless, both Dirac and Majorana spinors, optionally colored (triplet or octet). The WHIZARD libraries support all Lorentz structures for interactions in the models described below. A completely general framework supporting all possible Lorentz structures is under construction.

BSM Models Beyond the SM and its QCD and QED subsets, WHIZARD supports the minimal supersymmetric Standard Model (MSSM) with different variants and extensions. These include

models with gravitinos [27, 28, 29] and the NMSSM [6] (see also [30]).

Among models with strongly interacting sectors WHIZARD includes Little Higgs models in different incarnations, with and without discrete symmetries, cf. [31, 32, 33, 34, 35, 36].

WHIZARD has also been used for studying more exotic models such as the noncommutative SM [37, 38, 39] (not included in the official release). It further supports the completely general two-Higgs doublet model (2HDM), as well as generic models containing a Z' state, and extradimensional models like Universal Extra Dimensions (UED). A more detailed list can be found in the WHIZARD documentation [14].

Effective Theories As an alternative tool for studying deviations from the SM, WHIZARD contains SM extensions with anomalous couplings, expressible as coefficients of higher-dimensional operators in an effective theory. Several models in WHIZARD's library define either anomalous triple and quartic gauge boson couplings, which have been used for studies at LCs [40, 41] or at LHC [42, 43]. Anomalous top-quark couplings are also supported [44, 45].

Recent interest in the physics of high-energy vector-boson scattering has triggered the development and addition of simplified models for strong interactions and compositeness (SSC) [43]. In addition to generic new degrees of freedom, they implement a unitarization procedure that is required for extrapolating into the energy range that will become accessible at ILC and, in particular, at CLIC.

9. Conclusion and Outlook

WHIZARD is a versatile and user-friendly tool for both SM and BSM physics at all possible highenergy colliders. In these proceedings, we report the recent progress in the technical development of the program as well as new physics features. Two main points to be mentioned are the special focus on lepton-collider beam spectra, which involves a detailed account of correlated beam spectra, arbitrary polarization and interfaces to the machine simulation. Future development will be devoted to a better description of QED radiation from both the initial and final states at lepton colliders and their proper matching to hard matrix elements. The second topic is the progress in the automation of QCD higher-order processes by interfacing external one-loop programs through the BLHA interface, the automatic generation of subtraction terms for softcollinear singularities in the real emission as well as the virtual part and an automatic phase-space integration of the different components by using the method of FKS regions.

Further plans for new features include the support for more general Lorentz and color structures in models, a more convenient model interface, power-counting of coupling constants in the matrix element, further refinements in the beam description, and many technical improvements.

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