NLO Physics Simulation with Whizard

Wolfgang Kilian
with slides from Pia Bredt

CPPS, University of Siegen

CEPC 23, Nanjing, Oct 24, 2023

The Whizard MC generator

1999 WHIZARD 1 + 2007 Whizard 2

- Hard-interaction physics at high-energy colliders (LHC, ILC, . . .)
- Tree-level ME code generated&linked on-the-fly by O'Mega
- Universal multi-channel integrator VAMP
- Cross sections, distributions, event streams (HepMC, LCIO, . . .)
- Full polarization support
- Beam spectra/ISR/PDF, shower/hadronization (PYTHIA), etc.
- SM and BSM models

Applications:

ILC/CLIC samples for physics studies
Signal and background processes for LHC analyses
Future collider studies (muon collider, photon collider, etc.)

2021 Whizard 3 (this talk)

- MPI/OpenMP, UFO, improvements/updates, NLO (full SM)

Matrix Elements for Hard Processes (LO)

`O'Mega:`

automated perturbative helicity-amplitude calculation for multi-leg processes with interfering resonances [hep-ph/0102195]

- avoid redundant common subexpressions altogether: no Feynman-graph expansion ⇒ factorial growth of # terms reduced to power law
- color-flow formalism (phantom 9th gluon) [JHEP 10 (2012) 022]

Matrix Elements for Hard Processes (NLO)

EW + QCD at NLO

- Virtual matrix elements: One-Loop Provider (GoSam, Recola, OpenLoops, etc.)

  One-loop amplitudes = NLO in any gauge/Yukawa/Higgs coupling, UV-renormalized

- Real-radiation matrix elements: O'Mega or also OLP

IR and collinear cancellation against massless radiation is (slightly) non-local in phase space

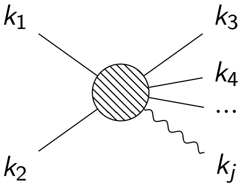
$\Rightarrow$ Subtraction algorithm (e.g. Catani-Seymour or Frixione-Kunszt-Signer)

FKS subtraction for soft/collinear cancellation

$$\sigma_{\text{NLO}} = \underbrace{\int d\Phi_n \mathcal{B}}_{\text{Born}} + \underbrace{\int d\Phi_{n+1} \mathcal{R}}_{\text{div. real}} + \underbrace{\int d\Phi_n \mathcal{V}}_{\text{div. virtual}} = \text{finite}$$

For observables **exclusive** in kinematic properties:

$$\sigma_{\text{NLO}} = \int d\Phi_n \mathcal{B} + \int \underbrace{d\Phi_{n+1} \left[\mathcal{R} - d\sigma_S\right]}_{\text{finite by construction}} + \underbrace{\int d\Phi_n \mathcal{V} + \int d\Phi_n d\sigma_{S,\text{int}}}_{\text{IR poles cancelled analyt.}}$$



‘j’ radiated with several different emitters $\Rightarrow$ Subtract singularities related to QED splittings systematically

Divide phase space into disjoint regions with **at most one** soft and/or collinear singularity.

$\Rightarrow$ kinematical weight factors related to pairs (i, j)

LHC: on-shell heavy bosons at NLO EW

Cross-validation of WHIZARD and MUNICH/MATRIX orig. ref. [Kallweit *et. al.*: 1412.5157]

process $pp \to$	MUNICH$_{(CS)}$ +OpenLoops $\sigma^{\text{tot}}_{\text{NLO}}$ [fb]	WHIZARD +OpenLoops $\sigma^{\text{tot}}_{\text{NLO}}$ [fb]	δ [%]	dev [%]	$\sigma^{\text{sig}}_{\text{NLO}}$
ZZ	$1.05729(1) \cdot 10^{4}$	$1.05729(11) \cdot 10^{4}$	-4.20	0.0001	0.01
W^+Z	$1.71505(2) \cdot 10^{4}$	$1.71507(2) \cdot 10^{4}$	-0.15	0.001	0.88
W^-Z	$1.08576(1) \cdot 10^{4}$	$1.08574(1) \cdot 10^{4}$	$+0.07$	0.001	0.90
W^+W^-	$7.93106(7) \cdot 10^{4}$	$7.93087(21) \cdot 10^{4}$	$+4.55$	0.002	0.89
ZH	$6.18523(6) \cdot 10^{2}$	$6.18533(6) \cdot 10^{2}$	-5.29	0.002	1.17
W^+H	$7.18070(7) \cdot 10^{2}$	$7.18072(9) \cdot 10^{2}$	-2.31	0.0003	0.18
W^-H	$4.59289(4) \cdot 10^{2}$	$4.59299(5) \cdot 10^{2}$	-2.15	0.002	1.62
ZZZ	$9.7429(2) \cdot 10^{0}$	$9.7417(11) \cdot 10^{0}$	-9.47	0.012	1.01
W^+W^-Z	$1.08288(2) \cdot 10^{2}$	$1.08293(10) \cdot 10^{2}$	$+7.67$	0.004	0.45
W^+ZZ	$2.0188(4) \cdot 10^{1}$	$2.0188(23) \cdot 10^{1}$	$+1.58$	0.0001	0.01
W^-ZZ	$1.09844(2) \cdot 10^{1}$	$1.09838(12) \cdot 10^{1}$	$+3.09$	0.006	0.51
$W^+W^-W^+$	$8.7979(2) \cdot 10^{1}$	$8.7991(15) \cdot 10^{1}$	$+6.18$	0.014	0.79
$W^+W^-W^-$	$4.9447(1) \cdot 10^{1}$	$4.9441(2) \cdot 10^{1}$	$+7.13$	0.013	2.52
ZZH	$1.91607(2) \cdot 10^{0}$	$1.91614(18) \cdot 10^{0}$	-8.78	0.004	0.39
W^+ZH	$2.48068(2) \cdot 10^{0}$	$2.48095(28) \cdot 10^{0}$	$+1.64$	0.011	0.96
W^-ZH	$1.34001(1) \cdot 10^{0}$	$1.34016(15) \cdot 10^{0}$	$+2.51$	0.011	1.02
W^+W^-H	$9.7012(2) \cdot 10^{0}$	$9.700(2) \cdot 10^{0}$	$+9.83$	0.014	0.75
ZHH	$2.39350(2) \cdot 10^{-1}$	$2.39337(32) \cdot 10^{-1}$	-11.06	0.005	0.41
W^+HH	$2.44794(2) \cdot 10^{-1}$	$2.44776(24) \cdot 10^{-1}$	-12.04	0.007	0.74
W^-HH	$1.33525(1) \cdot 10^{-1}$	$1.33471(19) \cdot 10^{-1}$	-11.53	0.041	2.80

LHC setup (Run II) $\delta \equiv \frac{\sigma^{\text{tot}}_{\text{NLO}} - \sigma^{\text{tot}}_{\text{LO}}}{\sigma^{\text{tot}}_{\text{LO}}}$ dev $\equiv \frac{|\sigma^{\text{tot}}_{\text{WHIZARD}} - \sigma^{\text{tot}}_{\text{MUNICH}}|}{\sigma^{\text{tot}}_{\text{WHIZARD}}}$ $\sigma^{\text{sig}} \equiv \frac{|\sigma^{\text{tot}}_{\text{WHIZARD}} - \sigma^{\text{tot}}_{\text{MUNICH}}|}{\sqrt{\Delta^2_{\text{err,WHIZARD}} + \Delta^2_{\text{err,MUNICH}}}}$

Multi-boson processes at a muon collider at NLO EW

[PB, W. Kilian, J. Reuter, P. Stienemeier, 2208.09438] WHIZARD+RECOLA, G_μ scheme, $m_\mu = 0.1056\ldots$ GeV

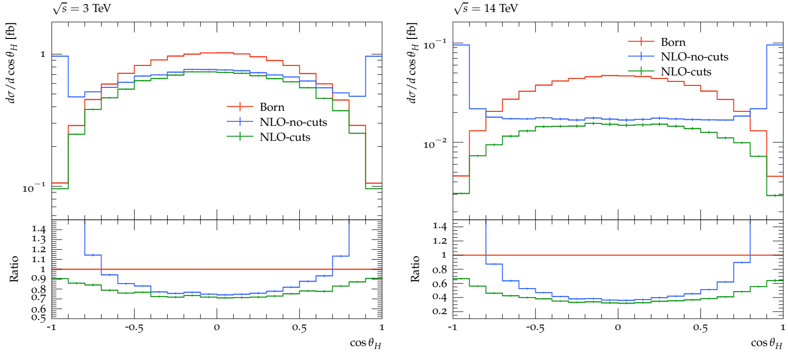
$\mu^+\mu^- \to X, \sqrt{s} = 3$ TeV	$\sigma^{\text{incl}}_{\text{LO}}$ [fb]	δ_{EW} [%]	δ_{ISR} [%]
W^+W^-	$4.6591(2) \cdot 10^2$	$+4.0(2)$	$+13.82(4)$
ZZ	$2.5988(1) \cdot 10^1$	$+2.19(6)$	$+15.71(4)$
HZ	$1.3719(1) \cdot 10^0$	$-1.51(4)$	$+30.24(3)$
W^+W^-Z	$3.330(2) \cdot 10^1$	$-22.9(2)$	$+2.90(9)$
W^+W^-H	$1.1253(5) \cdot 10^0$	$-20.5(2)$	$+7.10(8)$
ZZZ	$3.598(2) \cdot 10^{-1}$	$-25.5(3)$	$+5.24(8)$
HZZ	$8.199(4) \cdot 10^{-2}$	$-19.6(3)$	$+8.39(8)$
HHZ	$3.277(1) \cdot 10^{-2}$	$-25.2(1)$	$+7.58(7)$
$W^+W^-W^+W^-$	$1.484(1) \cdot 10^0$	$-33.1(4)$	$-1.3(1)$
W^+W^-ZZ	$1.209(1) \cdot 10^0$	$-42.2(6)$	$-1.8(1)$
W^+W^-HZ	$8.754(8) \cdot 10^{-2}$	$-30.9(5)$	$-0.1(1)$
W^+W^-HH	$1.058(1) \cdot 10^{-2}$	$-38.1(4)$	$+1.7(1)$
$ZZZZ$	$3.114(2) \cdot 10^{-3}$	$-42.2(2)$	$+0.8(1)$
$HZZZ$	$2.693(2) \cdot 10^{-3}$	$-34.4(2)$	$+1.4(1)$
$HHZZ$	$9.828(7) \cdot 10^{-4}$	$-36.5(2)$	$+2.2(1)$
$HHHZ$	$1.568(1) \cdot 10^{-4}$	$-25.7(2)$	$+5.7(1)$

with $\delta_{\text{EW}} = \sigma^{\text{incl}}_{\text{NLO}}/\sigma^{\text{incl}}_{\text{LO}} - 1$ and $\delta_{\text{ISR}} = \sigma^{\text{incl}}_{\text{LO,LL-ISR}}/\sigma^{\text{incl}}_{\text{LO}} - 1$

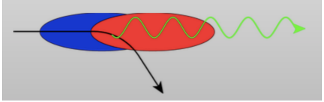
Multi-boson processes at a muon collider at NLO EW

[PB, W. Kilian, J. Reuter, P. Stienemeier, 2208.09438]

Fixed order differential distributions: $d\sigma(\mu^+\mu^- \to HZ)/d\cos\theta_H$



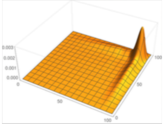
Beam Properties (e^+e^-)



Beamstrahlung

- Detailed simulation of machine and interaction region (GuineaPig)
  $\Rightarrow$ to be repeated for each parameter set
- Circular colliders: beamstrahlung $\Rightarrow$ beam-energy spread
- Fit to beam-simulation data
  - parameterized spectra (Circe1)
  - beam-event generator (Circe2)

https://whizard.hepforge.org/circe.html



- Beamstrahlung interfaced with MCGenerator
  - Whizard: integrated in e^+e^- physics simulation framework
  - Others: Circe2 available as plug-in module

CEPC Items

NLO (full EW + QCD) for e^+e^-

- Matrix elements: available (GoSam, Recola, OpenLoops), as in $\mu^+\mu^-$
- NLO structure functions for (massless) electrons [Frixione, et al.]:
  - implemented, working on complete numerical stability (near $x = 1$)
  - to be validated (ILD, etc.)
- PowHeg matching and Pythia8 $\Rightarrow$ full NLO events

And...

- Beam simulation data to be established
- NNLO: future developments

Conclusions and Outlook

- Whizard is a viable tool for physics studies and analyses at HEP experiments: LHC, Belle II, ILC/CLIC/FCC/CEPC, MuCol, . . .
- Any SM (NLO) and BSM processes can be handled, limited mainly by external programs and CPU time
- Specific support for e^+e^- to be improved to full SM NLO (and SMEFT,. . .)

The WHIZARD 3 Team

U Siegen: WK, Pia Bredt, Nils Kreher, Tobias Striegl

DESY: Jürgen Reuter, Krzysztof Mękała
(S. Brass, B. Chokoufe, V. Rothe, P. Stienemeier, C. Weiss)

U Würzburg: Thorsten Ohl

U Warsaw (exp.): Filip Żarnecki

Links

- Reference: WK/Ohl/Reuter, EPJ C71 (2011) 1742
- WHIZARD Portal: `https://whizard.hepforge.org/`
- Launchpad Page: `https://launchpad.net/whizard`
- gitlab repo: `https://gitlab.tp.nt.uni-siegen.de/whizard/public`

BACKUP

Technical Remarks

Language: `Fortran` (2018, object-oriented/modular) with `O'Caml`

Development: `gitlab` with automated test suite and CI

Installation: `configure && make && make install`

Numerics: Support for extended and quadruple precision (if needed)

Running: Options

1. Stand-alone with input script: `whizard` ⟨*input*⟩`.sin` (optional workspace transfer for cluster operation)
2. As a library, callable from: `Fortran`, `C`, `C++`, `Python`

BSM: Predefined (many models) and UFO (everything else)

Script: SINDARIN (input, parameters, cuts, workflow, result aggregation, output control, . . .)

Parallel: OpenMP (multi-core), MPI (HPC cluster)

Hadron collisions at NLO EW

- QED FKS subtraction terms:

$$d\sigma_{S,\text{coll}} \sim \alpha \underbrace{\hat{P}^{\mu\nu}_{E\to(i,j),\text{QED}}\mathcal{B}^{(E)}_{\mu\nu}}_{\text{pol. AP kernel}\,\times\,\text{spin-corr.}} \qquad d\sigma_{S,\text{soft}} \sim \alpha \sum_{k,l=1}^{n} \underbrace{\frac{\bar{k}_k\cdot\bar{k}_l}{(\bar{k}_k\cdot\hat{k}_j)(\bar{k}_l\cdot\hat{k}_j)}\mathcal{B}_{kl}}_{\text{eikonal}\,\times\,\text{charge-corr.}}$$

- EW schemes & photons entering at Born level (e. g. $pp \to W^+W^-$)

$Q^2_\gamma \to 0$	$Q^2_\gamma \sim$ EW scale
on-shell photons no γ splittings	*off-shell* photons $\gamma^* \to f\bar{f}$
$\alpha(0)$	$\alpha\vert_{G_\mu},\ \alpha(M_Z)$
$\left[\frac{\delta\alpha(0)}{\alpha(0)} + \delta Z_{AA}\right]_{\text{light}} = 0$	$\left[\frac{\delta\alpha(M_Z)}{\alpha(M_Z)} + \delta Z_{AA}\right]_{\text{light}} + \delta Z_{\gamma,\text{PDF}}$ $\to$ finite overall photon factor $\neq 0$

with photon virtuality Q^2_γ

Hadron collisions at NLO EW

IR-safety conditions:

- photon recombination with charged leptons – 'dressed' leptons
- jet clustering including photon – 'democratic' jets

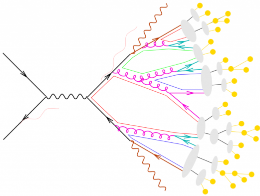
Pure electroweak pp processes with off-shell vector bosons

LHC setup (Run II): $\sqrt{s} = 13$ TeV $\quad \mu_R = \mu_F = \frac{1}{2}\sum_i \sqrt{p_{T,i}^2 + m_i^2}$ EW scheme: G_μ CMS

PDF set: `LUXqed_plus_PDF4LHC15_nnlo_100` cuts from ref. [1804.10017]

process $pp \to$	α^m	`MG5_aMC@NLO`[1804.10017] $\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	`WHIZARD+OpenLoops` $\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	`WHIZARD+OpenLoops` δ [%]	$\sigma^{\text{sig}}_{\text{NLO}}$
$e^+\nu_e$	α^2	$5.2005(8) \cdot 10^3$	$5.1994(4) \cdot 10^3$	-0.73	1.24
e^+e^-	α^2	$7.498(1) \cdot 10^2$	$7.498(1) \cdot 10^2$	-0.50	0.004
$e^+\nu_e\mu^-\bar{\nu}_\mu$	α^4	$5.2794(9) \cdot 10^{-1}$	$5.2816(9) \cdot 10^{-1}$	$+3.69$	1.69
$e^+e^-\mu^+\mu^-$	α^4	$1.2083(3) \cdot 10^{-2}$	$1.2078(3) \cdot 10^{-2}$	-5.25	1.26
$He^+\nu_e$	α^3	$6.4740(17) \cdot 10^{-2}$	$6.4763(6) \cdot 10^{-2}$	-4.04	1.24
He^+e^-	α^3	$1.3699(2) \cdot 10^{-2}$	$1.3699(1) \cdot 10^{-2}$	-5.86	0.32
Hjj	α^3	$2.7058(4) \cdot 10^0$	$2.7056(6) \cdot 10^0$	-4.23	0.27
tj	α^2	$1.0540(1) \cdot 10^2$	$1.0538(1) \cdot 10^2$	-0.72	0.74

Final-state effects



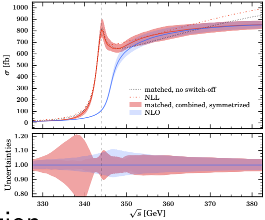
- Jets: integrated `FastJet` interface
- Polarized decays (e.g., W, Z, H, t) as alternative to full matrix elements
- Tau decays via TAOLA
- Resonance selection for shower initialization
- Parton shower + hadronization: PYTHIA6 (integrated)
- Parton shower + hadronization: Pythia 8 (interface or via event file)
- Event file formats: ILC-like (legacy, LCIO/Key4HEP) and LHC-like (legacy, LHE, HepMC)

Polarization in Whizard

- Lazy method for simulation: merge distinct event samples with 100% $\pm$left/right polarization
- "Classical" polarization: project on helicities and postprocess particles with definite helicity
- "Quantum" method: polarization via initial-state and final-state density matrices, allows for arbitrary polarization fraction, spin rotation, polarized decays, etc.
  $\Rightarrow$ supported in Whizard since v1
- Polarization of outgoing particles: depend on event-file formats

$\Rightarrow$ NLO: polarization support relies on spin-correlated squared matrix element output

Specific Processes



$e^+e^- \to t\bar{t}$ (and $t\bar{t}H$)

- tt on-shell multi-loop / threshold resummation
- off-shell NLO MC + threshold resummation: Whizard

Soft Background

- $\gamma\gamma \to$ hadrons
  $\Rightarrow$ SLAC code based on Chen, Barklow, Peskin, PRD49 (1994)