NLO QCD effects in the fully off-shell process $e^+e^- \to b\bar{b}l\nu l\nu$ with WHIZARD

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in collaboration with

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LoopFest XV, University at Buffalo, Amherst, August 16th

Overview

1. The WHIZARD event generator at NLO
2. Fully off-shell top decay

The WHIZARD Event Generator

WHIZARD 2.3.0 - July 21st 2016 (`http://whizard.hepforge.org`)
Multi-purpose event generator for lepton and hadron colliders.

Modular structure:

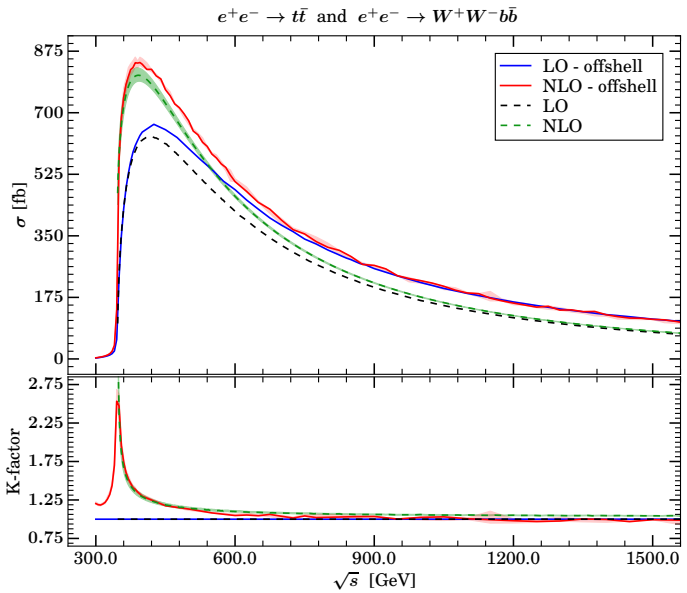
- O'MEGA: Matrix element generator
- VAMP: Adaptive multi-channel Monte Carlo integrator
- CIRCE: Simulation tool for lepton collider beam spectra
- SINDARIN: Script language for simulation and analysis
- Lepton beam ISR and polarization

EPJ C71 (2011) 1742, [arXiv:0708.4233], `whizard@desy.de`

WHIZARD at next-to-leading-order

Easy-to-use simulation tool desired which matches experimental accuracy.
WHIZARD+NLO is in beta state.
First working focus on QCD corrections.

```
 alpha_power = 2
alphas_power = 0
process eett = e1, E1 => t, T
{ nlo_calculation = "Full" }
```



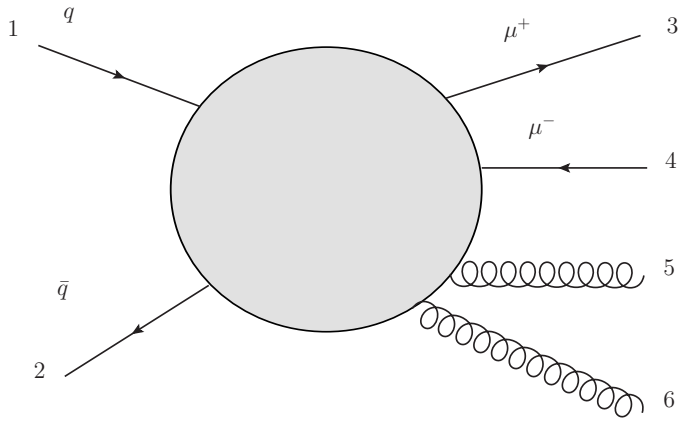
Supported One-Loop-Providers:

- GoSam [G. Cullen et.al.]
- OpenLoops [F. Cascioli et.al.]
- RECOLA [A. Denner et.al.] (→ Talk by J.N. Lang)

FKS subtraction (Frixione/Kunszt/Signer)

Numerically cancel divergencies separately in real and virtual contribution:

$$d\sigma^{\mathsf{NLO}} = \underbrace{\int_{n+1} \left(d\sigma^{\mathsf{R}} - d\sigma^{\mathsf{S}}\right)}_{\text{finite}} + \underbrace{\int_{n+1} d\sigma^{\mathsf{S}} + \int_{n} d\sigma^{\mathsf{V}}}_{\text{finite}}$$



- Find all singular tuples

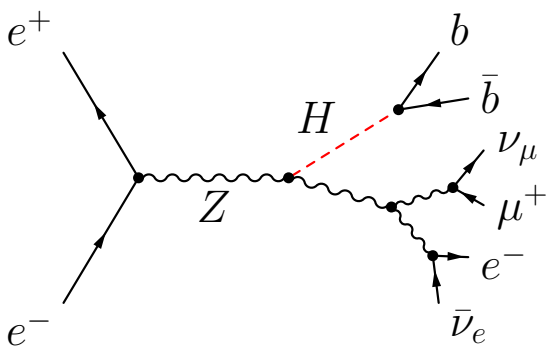
$$\mathcal{I} = \{(1,5),(1,6),(2,5),(2,6),(5,6)\}$$

- Partition phase space into singular regions

$$1 = \sum_{\alpha \in \mathcal{I}} S_\alpha(\Phi)$$

- $\mathcal{R} \to \mathcal{R} S_\alpha$, for each $\alpha \in \mathcal{I}$.

Resonance-aware FKS subtraction [Ježo/Nason, 1509.09071]



Very narrow resonance, e.g. $\Gamma_H = \mathcal{O}(100MeV)$.

- $D_H^{\text{Born}} = \left[\left(\bar{p}_{bb}^2 - m_H^2\right)^2 + m_H^2\Gamma_H^2\right]^{-1}$,
- $D_H^{\text{Real}} = \left[\left(p_{bbg}^2 - m_H^2\right)^2 + m_H^2\Gamma_H^2\right]^{-1}$

Parameterize deviation from resonance:
$p_{bbg}^2 = \bar{p}_{bb}^2 + \Delta_{bbg}^2$

Divergence close to resonance: $\frac{D_H^{\text{Born}}}{D_H^{\text{Real}}} \overset{\bar{p}_{bb}^2 \to m_H^2}{=} 1 + \frac{\Delta_{bbg}^4}{m_H^2\Gamma_H^2}$

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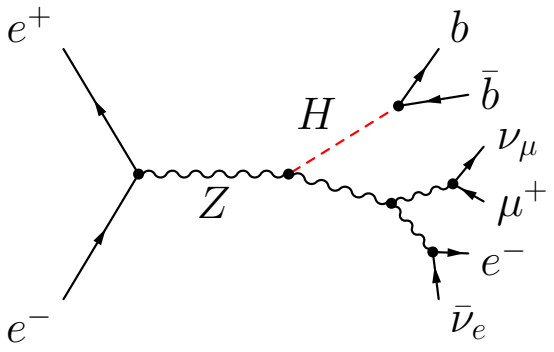

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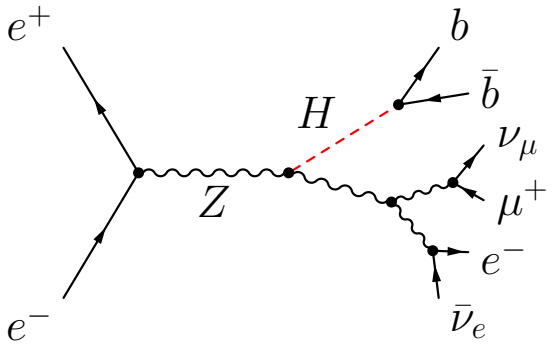
Solution: Fix $\Delta_{bbg} = 0$. The real phase space is constructed in such a way that the invariant mass of the resonance system including the radiated particle (gluon) is conserved.

Resonance-aware FKS subtraction [Ježo/Nason, 1509.09071]



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WHIZARD Example: $e^+e^- \to \mu^+\mu^- b\bar{b}$ ($Z \to b\bar{b}$ and $H \to b\bar{b}$).

It	Calls	Integral[fb]	Error[fb]	Err[%]	Acc	Eff[%]	Chi2	N[It]
1	11988	2.2175098E+00	4.41E-01	19.87	21.75*	1.92		
2	11960	1.1077441E+01	6.73E+00	60.74	66.42	0.58		
3	11946	3.4101393E+00	9.97E-01	29.24	31.96*	0.59		
4	11925	3.3646085E+00	7.55E-01	22.45	24.51*	0.42		
5	11901	2.2647497E+00	2.70E-01	11.91	13.00*	0.81		
5	59720	2.4046466E+00	2.15E-01	8.93	21.83	0.81	1.19	5

Standard FKS

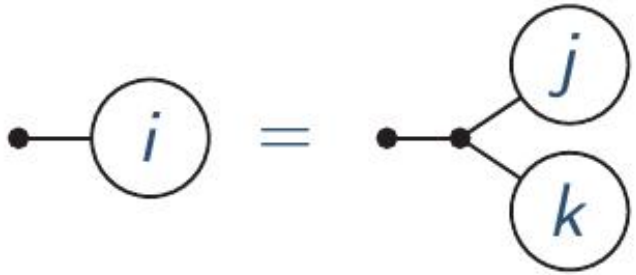
It	Calls	Integral[fb]	Error[fb]	Err[%]	Acc	Eff[%]	Chi2	N[It]
1	11988	2.8839926E+00	1.00E-01	3.48	3.81*	7.18		
2	11960	3.0292088E+00	5.23E-02	1.73	1.89*	11.44		
3	11932	2.9856296E+00	4.36E-02	1.46	1.59*	15.18		
4	11911	2.9943992E+00	4.23E-02	1.41	1.54*	13.84		
5	11887	3.0283492E+00	4.08E-02	1.35	1.47*	16.24		
5	59678	3.0025429E+00	2.16E-02	0.72	1.75	16.24	0.56	5

Resonance-aware FKS

OpenLoops [Cascioli, Maierhöfer, Pozzorini, arXiv:1111.5206]

Tree-level recursion:

Connect wave functions w^α with vertices and propagators:

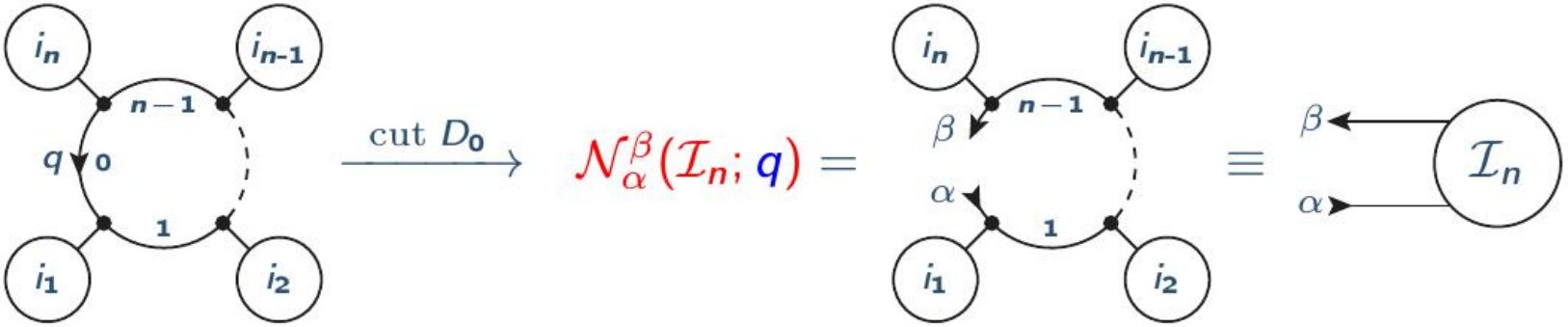


$$w^\beta(i) = \frac{X^\beta_{\gamma\delta}}{p_i^2 - m_i^2} w^\gamma(j) w^\delta(k)$$

$X^\beta_{\gamma\delta}$: Interaction vertex of i, j and k.

From loops to tree-level diagrams:

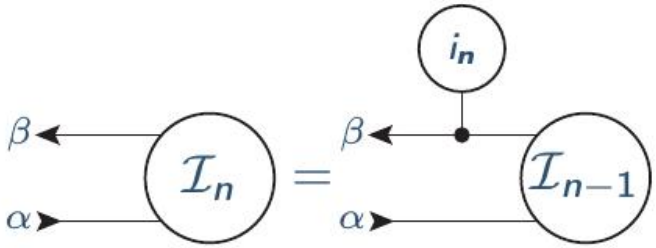
Separate amplitude into tree-like numerator function and tensor integrals:



Recover numerator: $\mathcal{N} = \mathcal{N}^\alpha_\alpha$

OpenLoops [Cascioli, Maierhöfer, Pozzorini, arXiv:1111.5206]

Recursion of cut diagrams:



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

- **Standard OPP:** Recursion requires fixed loop momentum q. Sample a large set of q values $\rightarrow$ high CPU cost.
- **OpenLoops:** $\mathcal{N}$ is a polynomial in q. $\rightarrow$ Recursion relations for polynomial coefficients.

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

OpenLoops coefficients

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

OpenLoops [Cascioli, Maierhöfer, Pozzorini, arXiv:1111.5206]

- Works with both tensor integrals and OPP reduction
  - tensor integral reduction: `Collier` ($\rightarrow$ Talk by L. Hofer)
  - OPP reduction: `CutTools` and `OneLoop`
- By 1-2 orders of magnitude faster than original OPP based algorithms due to cheap multiple evaluation of the numerator function.
- OpenLoops libraries are dynamically linked to WHIZARD during run-time. The interface works with the BLHA standard. Contract files are automatically written by WHIZARD .
- Dedicated process libraries for lepton collisions are present in the `public` process repository of OpenLoops.

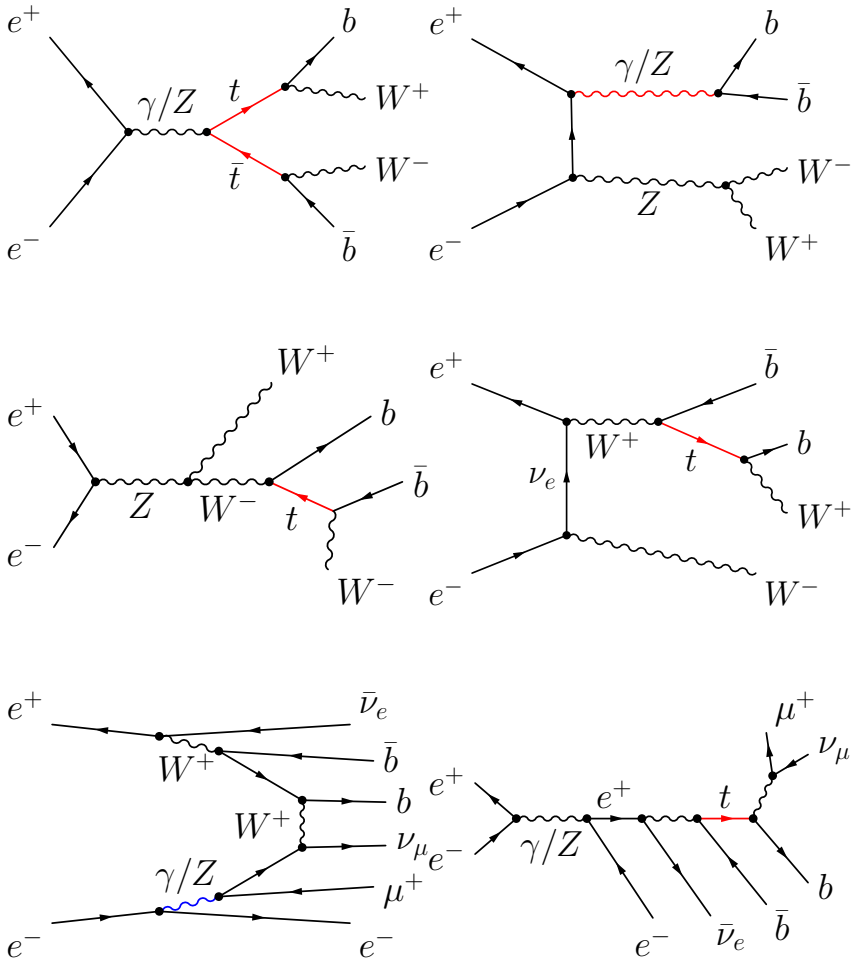
Overview

1. The WHIZARD event generator at NLO
2. Fully off-shell top decay

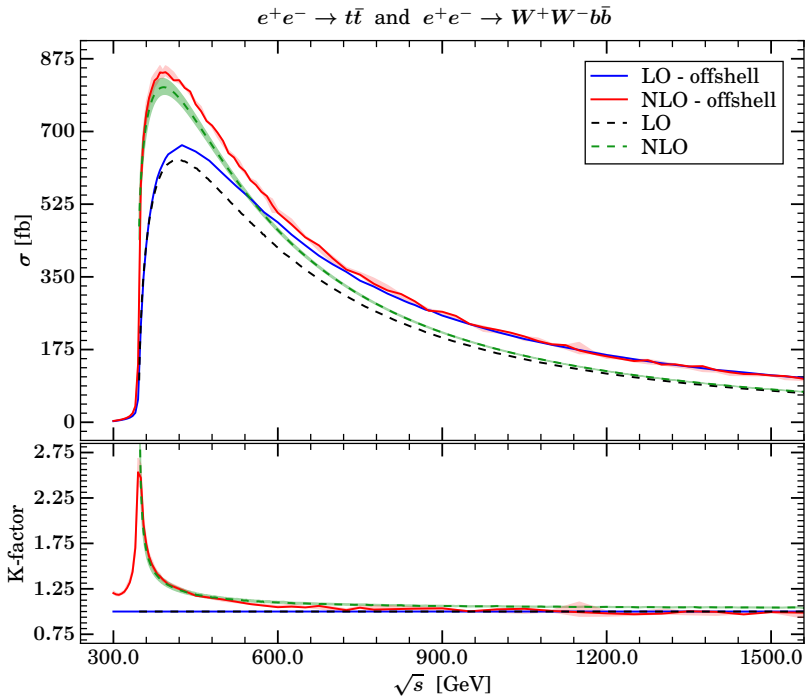
$e^+e^- \to bW^+\bar{b}W^-$ and $e^+e^- \to b\bar{b}e^-\bar{\nu}_e\mu^+\nu_\mu$: Overview

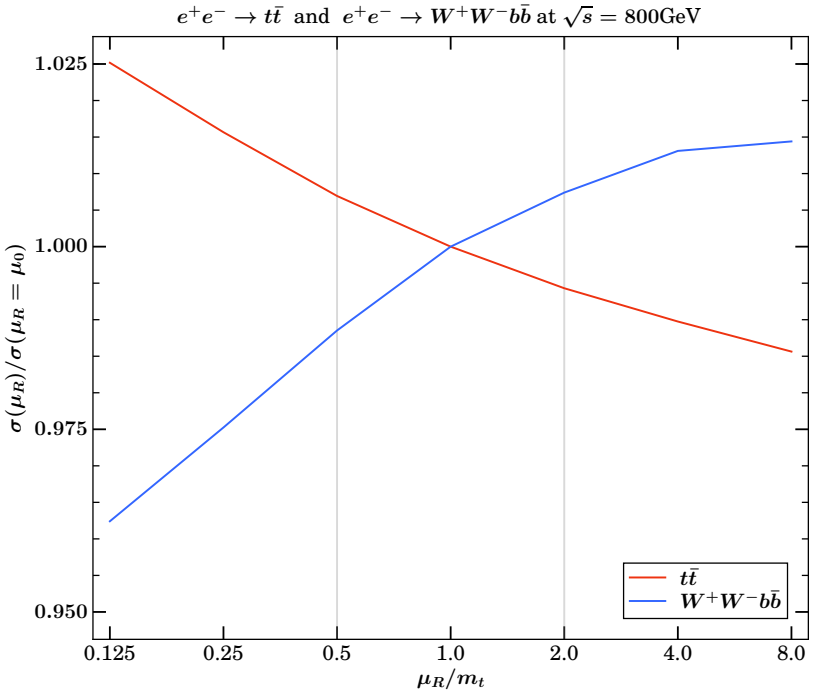
- Beyond NWA: Single-resonant and non-resonant background and interference contributions.
- Also include off-shell leptonic W-decays. No additional complexity concerning subtraction.
- Treatment of Z- and H-resonances using resonance-aware FKS subtraction shows a significant improvement.
- Phase-space cut:

$$\sqrt{\left(k_{e^-}^{\text{in}} - k_{e^-}^{\text{out}}\right)^2} > 20\,\text{GeV}$$



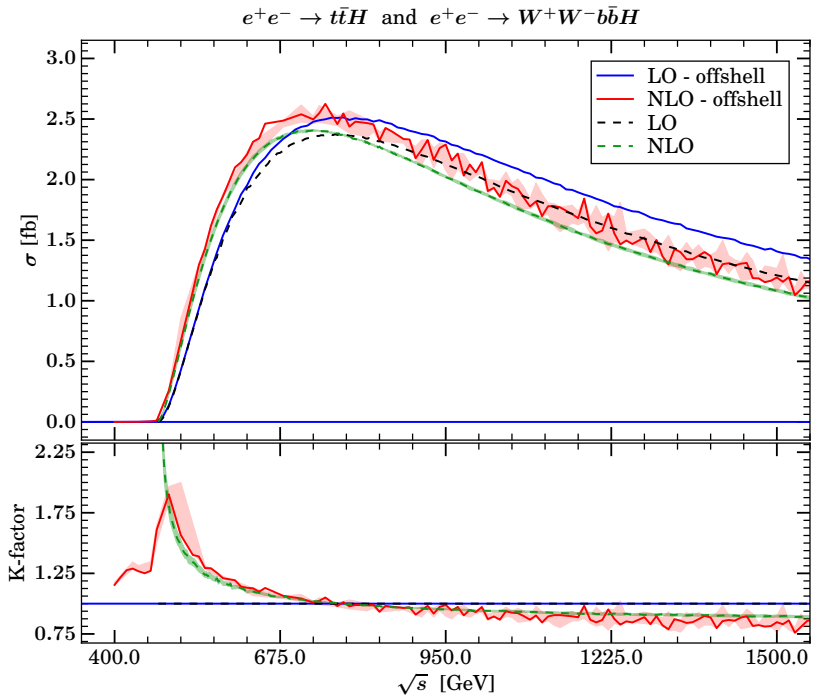
Total cross section & Scales - $e^+e^- \to t(W^+b)\bar{t}(W^-\bar{b})$

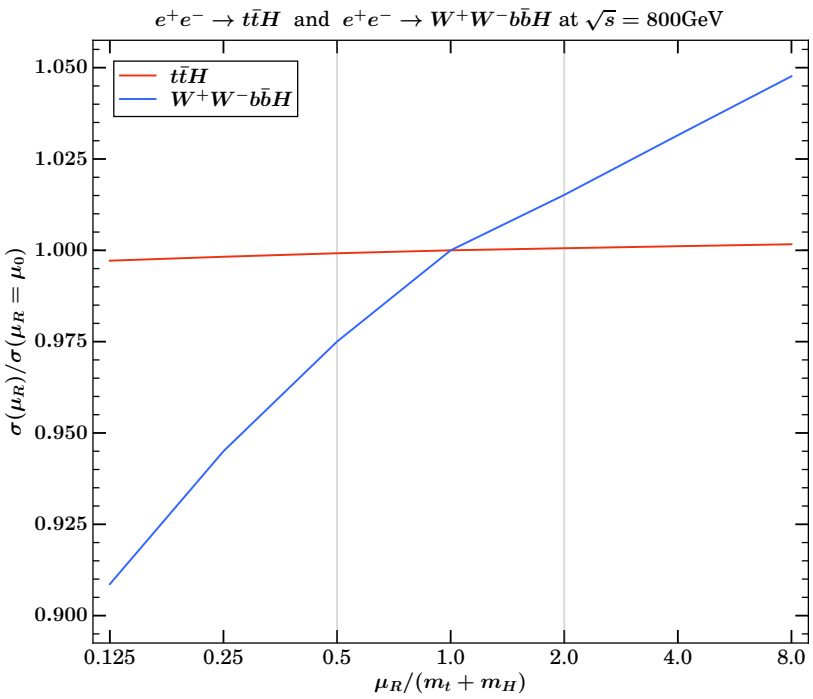




- Large corrections ($K \sim 2.5$) around $\sqrt{s} = 2m_t$ due to non-relativistic threshold enhancements.
- NLO QCD corrections turn negative around $\sqrt{s} = 850\,\mathrm{GeV}$, reaching up to -20%. $\to$ Negative contributions from background diagrams.
- Scale variations have opposite slope, corresponding to the same background effects.

Total cross section & Scales - $e^+e^- \to t(W^+b)\bar{t}(W^-\bar{b})H$

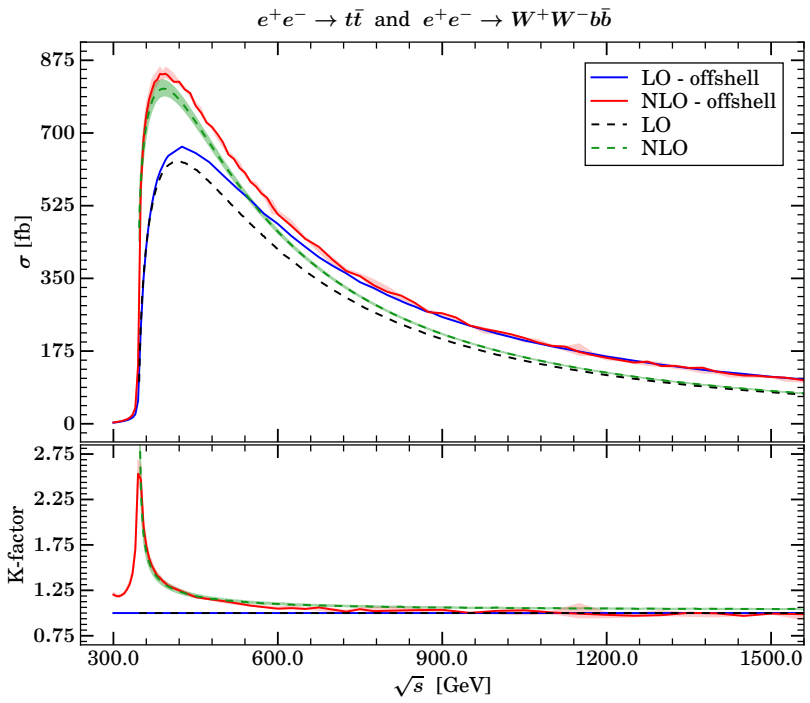


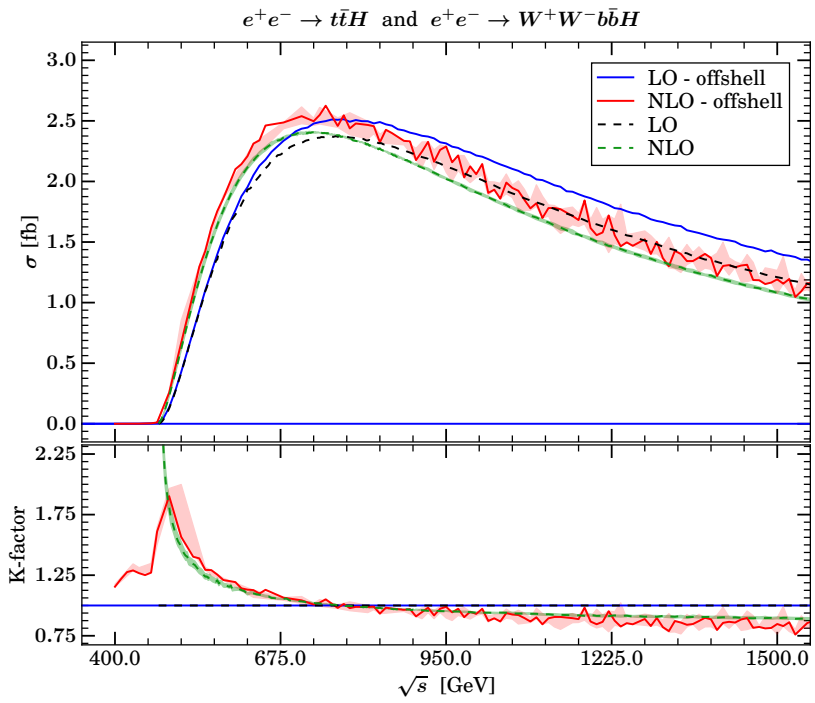


- Qualitatively same results.
- Total cross section two orders of magnitude smaller, with a maximum at about $\sqrt{s} = 800\,\mathrm{GeV}$.

$\to$ Focus study on $\sqrt{s} = 800\,\mathrm{GeV}$.

Complexity





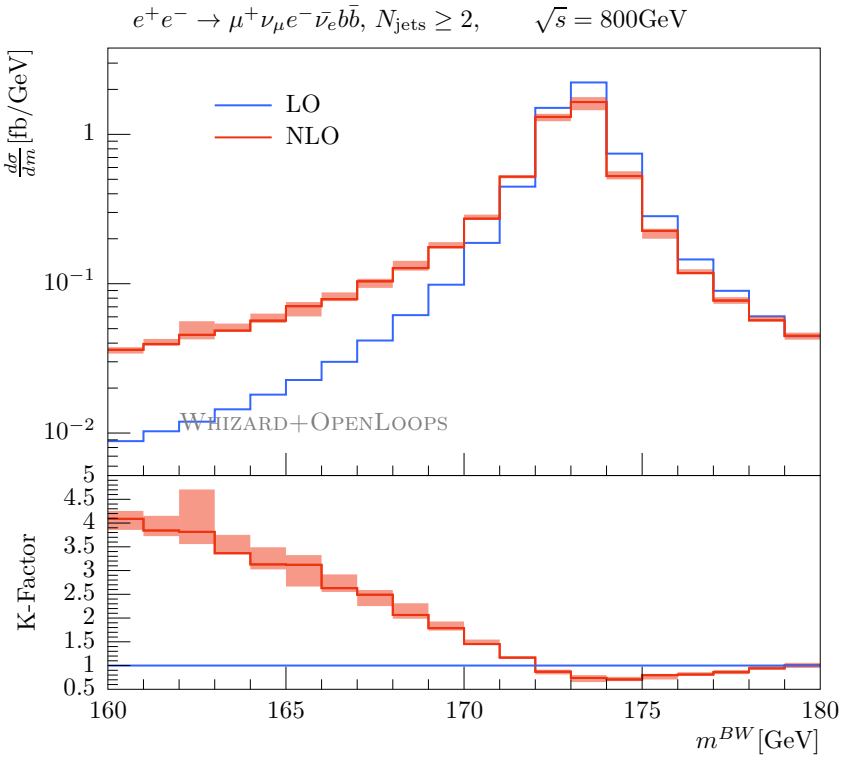
$e^+e^- \to$	$n_{\text{loop}}^{\text{diags}}$	$n_{\text{prop.}}^{\text{max}}$	n_{hel}
$t\bar{t}$	2	3	16
$bW^+\bar{b}W^-$	157	5	144
$b\bar{b}\bar{\nu}_e e^-\nu_\mu\mu^+$	830	5	16

$e^+e^- \to$	$n_{\text{loop}}^{\text{diags}}$	$n_{\text{prop.}}^{\text{max}}$	n_{hel}
$t\bar{t}H$	17	4	16
$bW^+\bar{b}W^-H$	1548	6	144
$b\bar{b}\bar{\nu}_e e^-\nu_\mu\mu^+H$	7436	6	16

Top-quark invariant mass

- NLO QCD corrections negative at and above the peak because the invariant mass is lowered by gluon emissions.
- Huge K-factors due to opening up of the gluon radiation phase space.
- Overall picture strongly depends on the jet parameters (here: generalized k_{T}-algorithm with $R = 0.4$ and $p = -1$).
- Only slight difference to the on-shell-W spectrum.

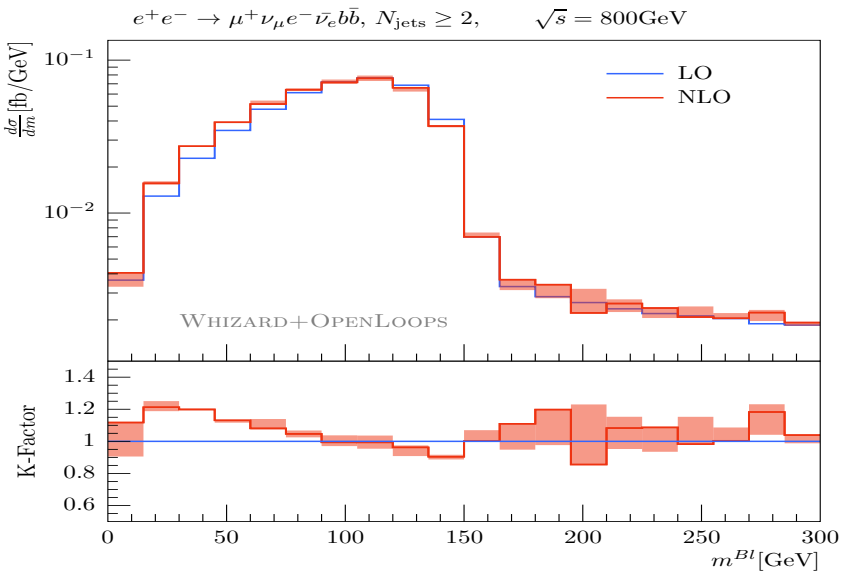
m^{BW}: Invariant mass of correctly associated b-jet and $l\nu$.



Top-quark invariant mass

- Top-quark mass peak completely erased.
- m_t nevertheless accessible via

$$m_t^2 = m_W^2 + \frac{2\langle m_{lj_b}^2 \rangle}{1 - \langle \cos\theta_{lj_b} \rangle}$$



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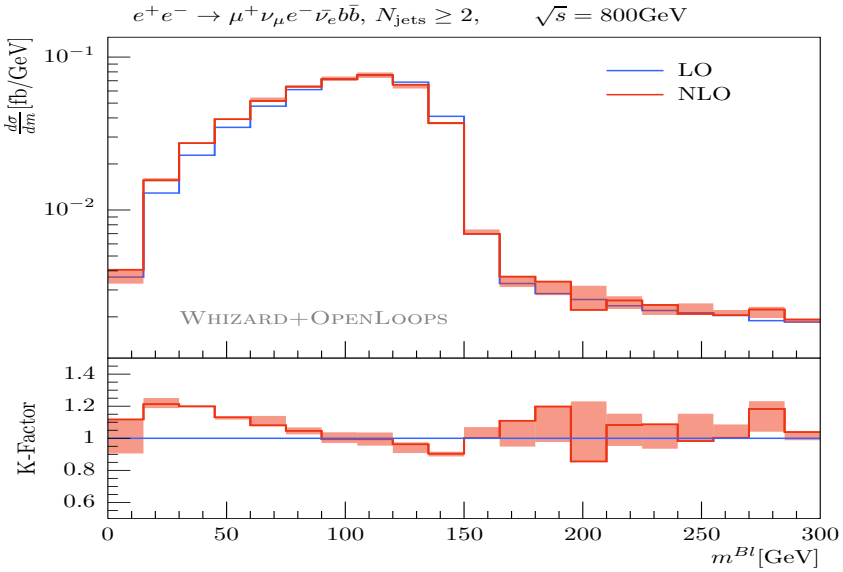
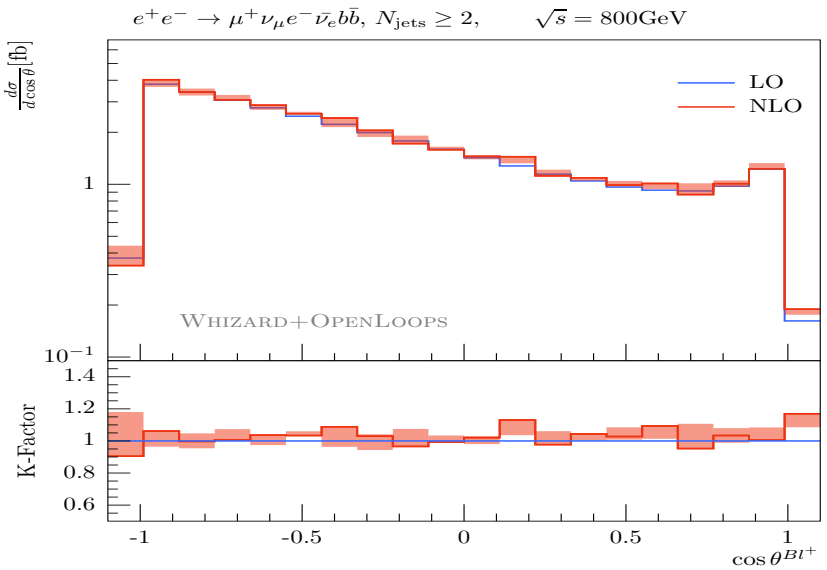
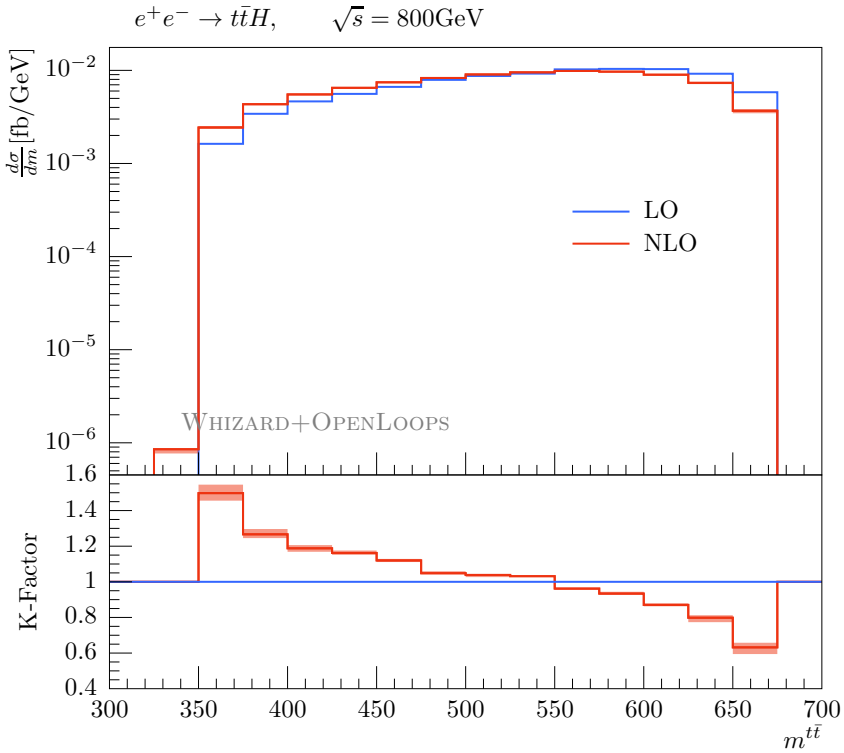
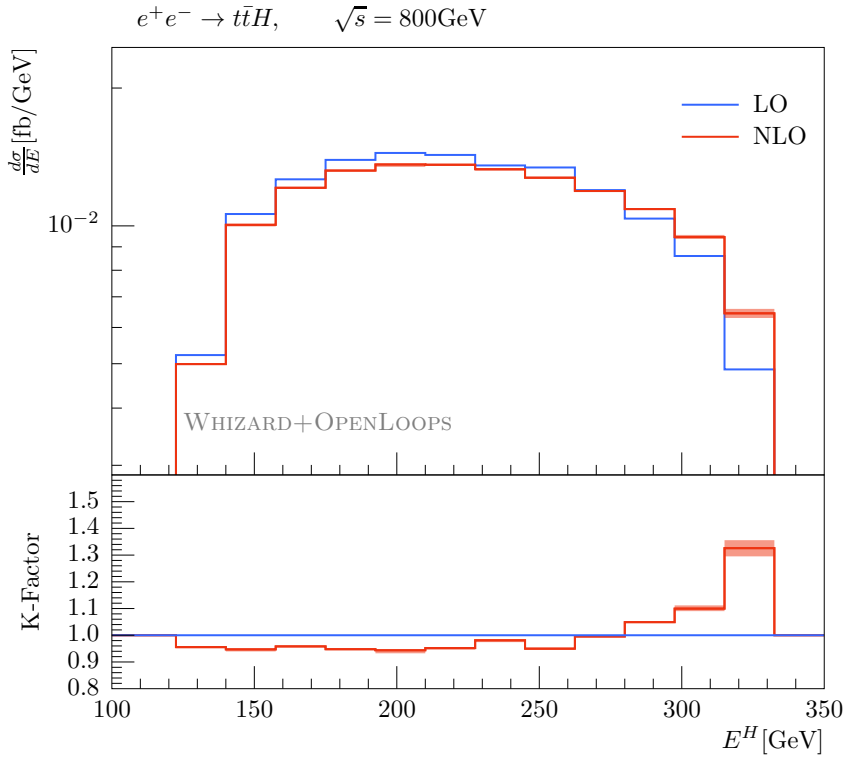
- NLO QCD corrections to $m_{lj_b}^2$ sizeable at the edges ($\mathcal{O}(10\%)$), angular distribution shifted by small global K-factor.





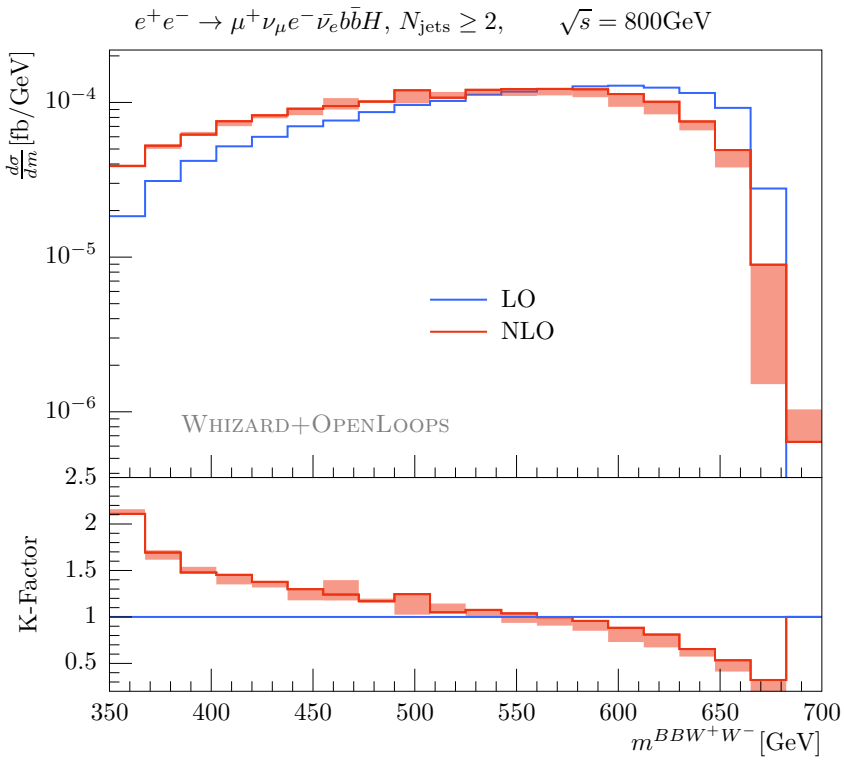
Higgs-associated top-pair production

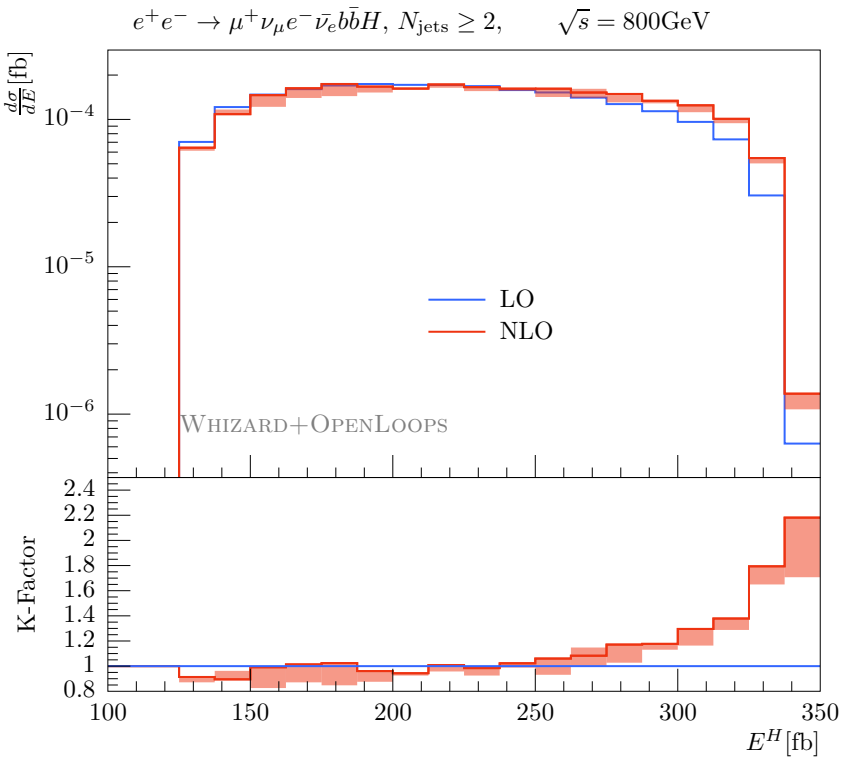




- E_H and m_{tt} are related: $E_H = \frac{1}{2\sqrt{s}}\left(s + M_H^2 - m_{tt}^2\right)$
  $\to$ Threshold effects visible in E_H spectrum.
- E_H completely indepent of jet clustering, but m_{tt} is affected by hard gluon radiation
  $\to$ K-factor correspondence invalid for small E_H.

Higgs-associated top-pair production including decays

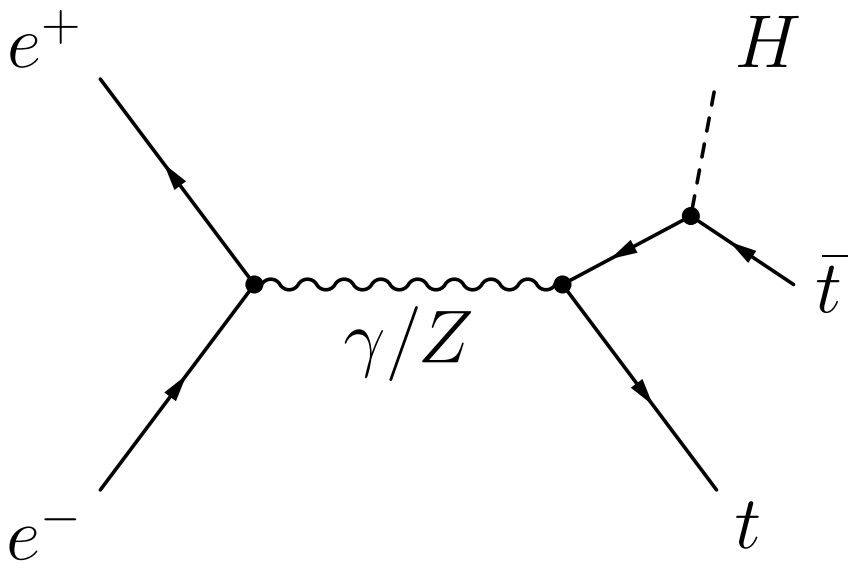


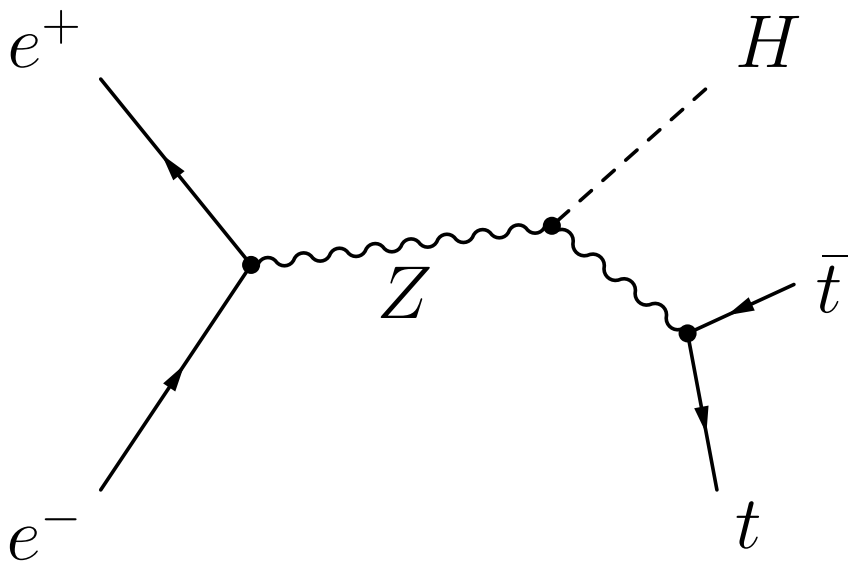


- Real radiation further increases the K-factor at the edges.
- K-factor correspondence is same as in the on-shell distributions.

Yukawa Coupling

y_t: Largest coupling of a fermion to the Higgs boson and possible window to new physics.



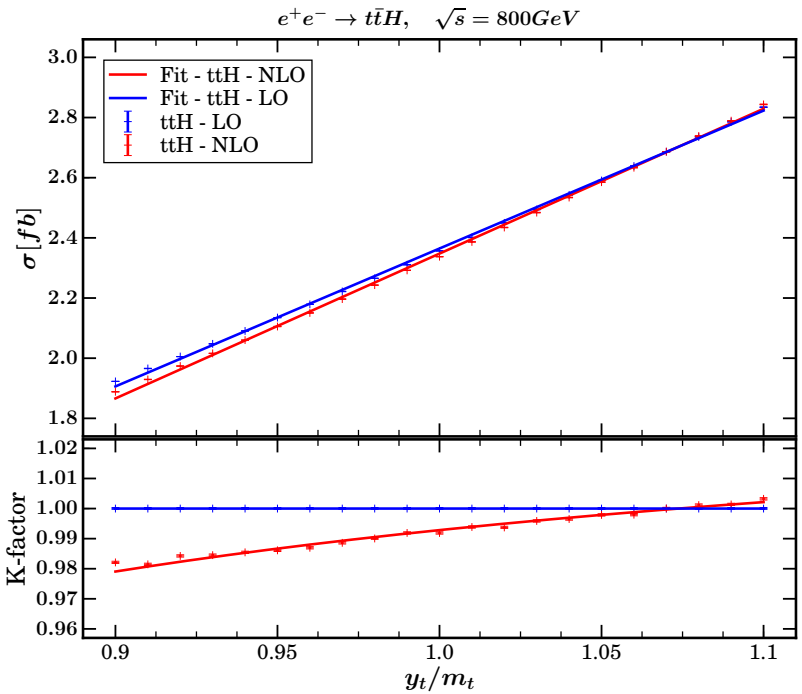


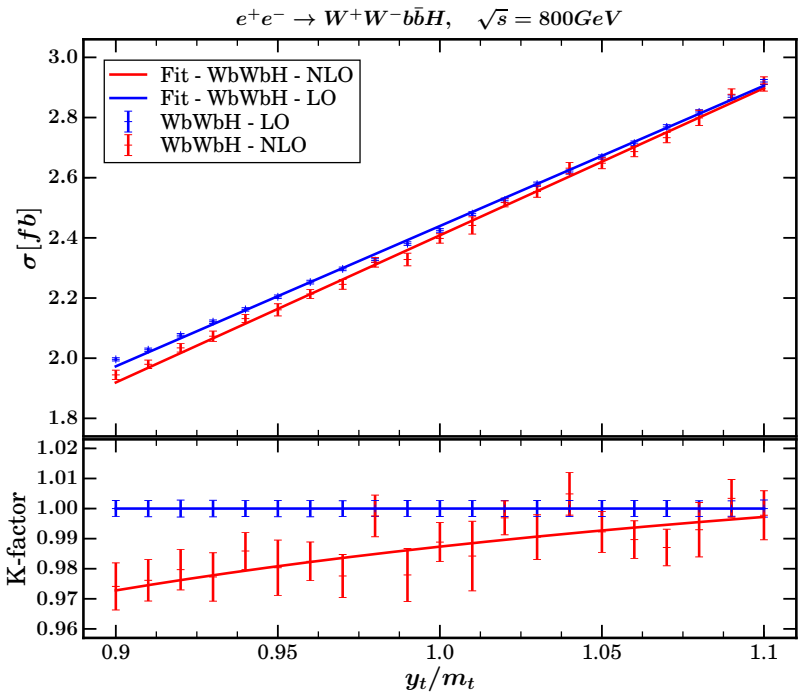
$$\frac{\Delta y_t}{y_t} = \kappa \frac{\Delta \sigma}{\sigma},$$

Pure signal: $\sigma \propto y_t^2 \rightarrow \kappa = 0.5$.
Interference and off-shell background diagrams shift κ away from this value.

Yukawa Coupling

y_t: Largest coupling of a fermion to the Higgs boson and possible window to new physics.





$$\frac{\Delta y_t}{y_t} = \kappa \frac{\Delta \sigma}{\sigma},$$

κ	ttH	$W^+W^-b\bar{b}H$
LO	0.514 ± 0.0002	0.520 ± 0.001
NLO	0.485 ± 0.0002	0.497 ± 0.002
Corr.	-5.64%	-6.52%

Beam Polarization

WHIZARD+NLO allows for the simple inclusion of beam polarization effects into NLO QCD calculations (same syntax as at LO).
It is easily verified that beam polarization has no effect on K-factors, as is expected for colorless initial states.

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

		$\sqrt{s} = 800\,\mathrm{GeV}$			$\sqrt{s} = 1500\,\mathrm{GeV}$		
$P(e^-)$	$P(e^+)$	$\sigma^{\mathrm{LO}}[\mathrm{fb}]$	$\sigma^{\mathrm{NLO}}[\mathrm{fb}]$	K-factor	$\sigma^{\mathrm{LO}}[\mathrm{fb}]$	$\sigma^{\mathrm{NLO}}[\mathrm{fb}]$	K-factor
0%	0%	2.358	2.337	0.991	1.210	1.064	0.879
-80%	0%	1.583	1.571	0.992	1.576	1.381	0.876
+80%	0%	1.584	1.571	0.992	0.843	0.746	0.885
-80%	30%	3.988	3.950	0.990	2.003	1.757	0.877
-80%	60%	4.840	4.795	0.991	2.429	2.128	0.876
80%	-30%	1.860	1.846	0.992	0.996	0.879	0.883
80%	-60%	2.134	2.120	0.993	1.148	1.018	0.886

Conclusion & Outlook

Software:

- WHIZARD 2.3 is an event generator for collider experiments
- Easy-to-use automated NLO QCD corrections for lepton colliders.
- Modular usage of matrix-element generators (O'MEGA, OPENLOOPS, ...)
- Several points not mentioned in this talk: NLO+PS matching (Powheg), NLO QCD at hadron colliders, top threshold resummation and matching to continuum, NLO decays, ...

Physics:

- Soft & collinear emissions can successfully be treated with a resonance-aware FKS subtraction approach.
- Problem not mentioned in this talk: Double resonances.
- Off-shell effects in combination with NLO corrections are sizeable for various observables and should be taken into account in experimental studies at lepton colliders.

Overview

3 Backup slides

Input parameters & Complex mass scheme

Massive particles:
$m_Z = 91.1876\,\mathrm{GeV}, \quad m_W = 80.385\,\mathrm{GeV}$
$m_b = 4.2\,\mathrm{GeV}, \quad m_t = 173.2\,\mathrm{GeV}$
$m_H = 125\,\mathrm{GeV}$

Particle Widths:
$\Gamma_Z^{\mathrm{LO}} = 2.4409\,\mathrm{GeV}, \quad \Gamma_Z^{\mathrm{NLO}} = 2.5060\,\mathrm{GeV}$
$\Gamma_W^{\mathrm{LO}} = 2.0454\,\mathrm{GeV}, \quad \Gamma_W^{\mathrm{NLO}} = 2.0978\,\mathrm{GeV}$

Gauge Boson Widths:
$\Gamma_Z^{\mathrm{LO}} = 2.4409\,\mathrm{GeV}, \quad \Gamma_Z^{\mathrm{NLO}} = 2.5060\,\mathrm{GeV}$
$\Gamma_W^{\mathrm{LO}} = 2.0454\,\mathrm{GeV}, \quad \Gamma_W^{\mathrm{NLO}} = 2.0978\,\mathrm{GeV}$

Top Quark Widths:
$\Gamma_{t\to Wb}^{\mathrm{LO}} = 1.4986\,\mathrm{GeV}, \quad \Gamma_{t\to Wb}^{\mathrm{NLO}} = 1.3681\,\mathrm{GeV}$
$\Gamma_{t\to ffb}^{\mathrm{LO}} = 1.4757\,\mathrm{GeV}, \quad \Gamma_{t\to ffb}^{\mathrm{NLO}} = 1.3475\,\mathrm{GeV}$

Complex Mass Scheme

Restores gauge-invariance for unstable particles and allows for proper renormalization.
All masses are treated complex:

$$\mu_i^2 = M_i^2 - i\Gamma_i M_i, \quad i = W, Z, t, H$$

Complex Weinberg angles:

$$s_w^2 = 1 - c_w^2 = 1 - \frac{\mu_W^2}{\mu_Z^2}$$

Electromagnetic coupling:

$$\alpha_e = \frac{\sqrt{2}}{\pi} G_\mu \left|\mu_W^2 s_w^2\right|$$

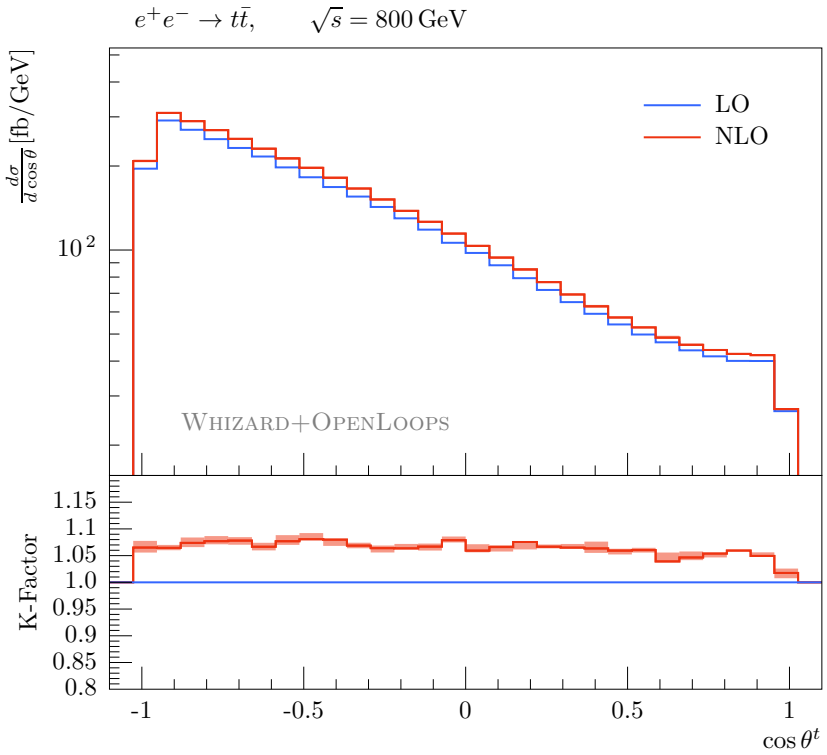
SINDARIN

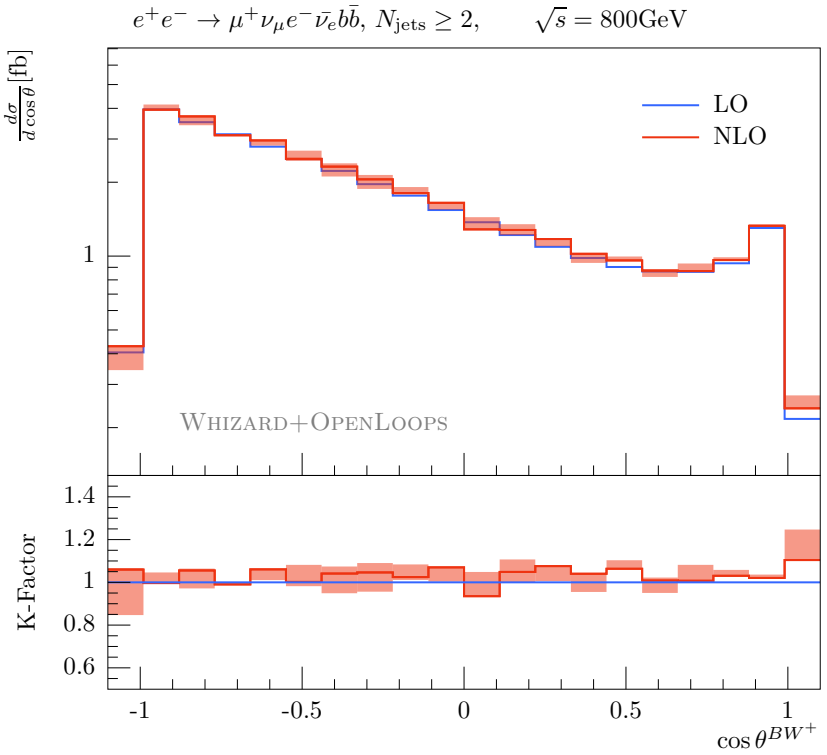
Zprime.sin

```
 model = Zprime

alias pr = u:d:s:c:gl:U:D:S:C
alias lepton = e1:E1
process zp_drell_yan = pr, pr => e1, E1

# Define model parameters mZH = 1500 GeV
wZH = 50 GeV
ms = 0
mc = 0

cuts = all Pt >= 50 GeV [lepton]
and all -2.5 <= Eta <= 2.5 [e1:E1]
and all M >= 800 GeV [e1,E1]

scale = 1500 GeV

sqrts = 14 TeV
beams = p,p => pdf_builtin
integrate (zp_drell_yan) {iterations = 3:10000:''gw'',6:20000}

sample_format = hepmc
simulate (zp_drell_yan) {checkpoint = 5000, n_events = 10000}
```

Top forward-backward asymmetry

$$A_{\mathrm{FB}} = \frac{\sigma(\cos\theta_t > 0) - \sigma(\cos\theta_t < 0)}{\sigma(\cos\theta_t > 0) + \sigma(\cos\theta_t < 0)}$$





Top forward-backward asymmetry

$$A_{\mathrm{FB}} = \frac{\sigma(\cos\theta_t > 0) - \sigma(\cos\theta_t < 0)}{\sigma(\cos\theta_t > 0) + \sigma(\cos\theta_t < 0)}$$

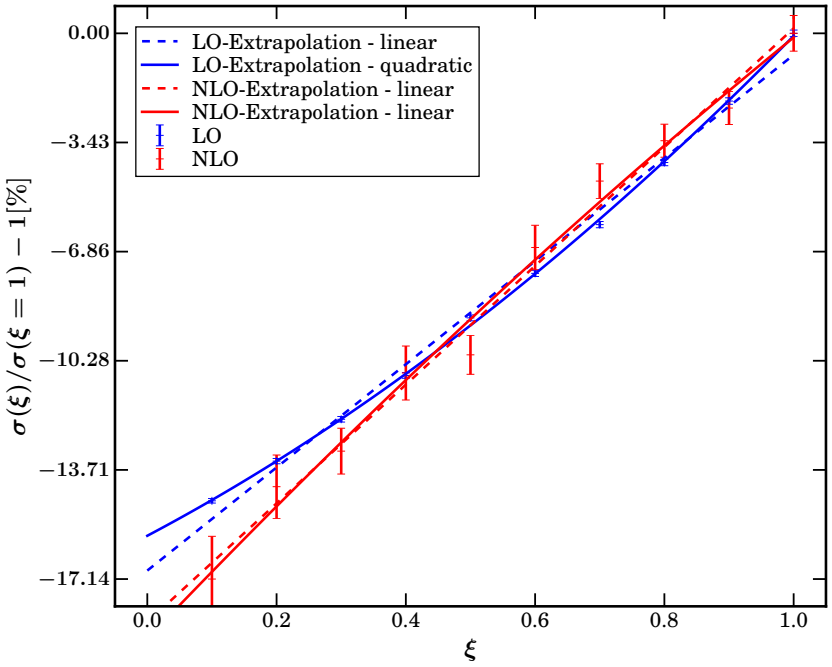
	$e^+e^- \to$	A_{FB}^{LO}	A_{FB}^{NLO}	K^{NLO}
A_{FB}	$t\bar{t}$	-0.59(3)	-0.59(8)	1.00
	$bW^+\bar{b}W^-$	-0.48(4)	-0.4(7)	0.98
	$\mu^+e^-\nu_\mu\bar{\nu}_e b\bar{b}$	-0.500(5)	-0.49(4)	0.98
	$\mu^+e^-\nu_\mu\bar{\nu}_e b\bar{b}$, without neutrinos	-0.48(5)	-0.48(0)	0.99
$\bar{A}_{FB}$	$t\bar{t}$	0.47(6)	0.47(8)	1.00
	$bW^+\bar{b}W^-$	0.36(7)	0.3(7)	1.00
	$\mu^+e^-\nu_\mu\bar{\nu}_e b\bar{b}$	0.326(7)	0.32(6)	0.99
	$\mu^+e^-\nu_\mu\bar{\nu}_e b\bar{b}$, without neutrinos	0.265(6)	0.26(0)	0.98

Off-shell effects more relevant than NLO effects!

Off-shell effects on inclusive cross sections

Narrow-width approximation follows from

$$\lim_{(M\Gamma)\to 0} \frac{1}{(q^2 - M^2)^2 + (M\Gamma)^2} = \delta\left(q^2 - M^2\right) \frac{\pi}{M\Gamma},$$



- The plot shows the numerical limit by varying $\xi = \Gamma/\Gamma_t$ in $\sigma(\xi) = \sigma \cdot \xi^2$.
- In the continuum, finite top width effects can strongly affect the inclusive cross section.
- Already at LO significantly larger effects than at hadron colliders.

Resonance-aware FKS subtraction: Soft mismatch component

In this approach, the $\mathcal{S}_\alpha$ functions are evaluated in the corresponing resonance's rest frame. $\rightarrow \sum_\alpha \mathcal{S}_\alpha \neq 1$!
Restore introducing the the soft mismatch:

$$R^{\text{mism}}_{\alpha_r} = \int d\Phi_B \int_0^\infty d\xi \int_{-1}^1 dy \int_0^{2\pi} d\phi \frac{s\xi}{(4\pi)^3} \left(\mathcal{R}^{soft}_{\alpha_r} \left[e^{-\frac{2k\cdot k_{\text{res}}}{k^2_{\text{res}}}} - e^{-\xi} \right] - \frac{32\pi\alpha_s C_F}{s\xi^2} \mathcal{B} \left[e^{-\frac{\bar{k}_{\text{em}}\cdot k_{\text{res}}}{k^2_{\text{res}}} \frac{k^0}{\bar{k}^0_{\text{em}}}} - e^{-\xi} \right] (1-\cos\theta)^{-1} \right).$$

- Essentially real-like kinematics, but $\xi \in [0, \infty)$. Requires separate integration.
- Automatically computed by WHIZARD if resonance-aware FKS is desired.

Cross-checks

We performed in-depth cross-chechs of WHIZARD with other Monte-Carlo generators.

σ[fb]	WHIZARD	SHERPA	MUNICH[S. Kallweit, in preparation]
$t\bar{t}$	271.16	271.15	271.37
$W^+W^-b\bar{b}$	320.98 $\pm$ 1.42	323.40 $\pm$ 0.34	323.80 $\pm$ 0.42