NLO (+PS) predictions with a multi-purpose event generator

Beyond Flavor Physics

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Collaborative Research Center TRR 257

Particle Physics Phenomenology after the Higgs Discovery

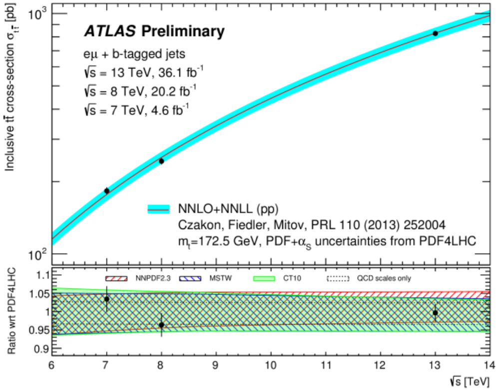
Outline

- Top quark pair production at the LHC
  – NLO+PS predictions with `WHIZARD`
- Higgs phenomenology at the LHC
  – VBF+HH production at NLO QCD in HEFT
- Future collider simulations with `WHIZARD`
  – NLO corrections in the SM and beyond

Top quark pair production at the LHC

Relevance of top quark production in physics

- Precise measurements and predictions of $t\bar{t}$ production rates yield
  - precise SM tests
- new physics potential: Top as the heaviest particle in the SM
  - strongest coupling to the Higgs sector
  - relation to vacuum stability
  - understand EWSB, how does mass arise?
- Top quark decays before hadronizing
  - direct observation of its properties (spin, mass, ...)
  - direct determination of $|V_{tb}|$ (without assuming unitarity)



[ATLAS Collaboration (Cern)]

Top quark pair production at the LHC

LHC precision wishlist for top-quark associated processes [Les Houches 2023]:

process	known	desired
$pp \to t\bar{t}$	$\mathrm{NNLO_{QCD}} + \mathrm{NLO_{EW}}$ (w/o decays) $\mathrm{NLO_{QCD}} + \mathrm{NLO_{EW}}$ (off-shell) $\mathrm{NNLO_{QCD}}$ (w/ decays)	$\mathrm{N^3LO_{QCD}}$
$pp \to t\bar{t} + j$	$\mathrm{NLO_{QCD}}$ (off-shell effects) $\mathrm{NLO_{EW}}$ (w/o decays)	$\mathrm{NNLO_{QCD}} + \mathrm{NLO_{EW}}$ (w decays)
$pp \to t\bar{t} + 2j$	$\mathrm{NLO_{QCD}}$ (w/o decays)	$\mathrm{NLO_{QCD}} + \mathrm{NLO_{EW}}$ (w decays)
$pp \to t\bar{t} + V'$	$\mathrm{NLO_{QCD}} + \mathrm{NLO_{EW}}$ (w decays)	$\mathrm{NNLO_{QCD}} + \mathrm{NLO_{EW}}$ (w decays)
$pp \to t\bar{t} + \gamma$	$\mathrm{NLO_{QCD}}$ (off-shell)	
$pp \to t\bar{t} + Z$	$\mathrm{NLO_{QCD}} + \mathrm{NLO_{EW}}$ (off-shell)	
$pp \to t\bar{t} + W$	$\mathrm{NLO_{QCD}} + \mathrm{NLO_{EW}}$ (off-shell)	
$pp \to t/\bar{t}$	$\mathrm{NNLO_{QCD}}$*(w decays) $\mathrm{NLO_{EW}}$ (w/o decays)	$\mathrm{NNLO_{QCD}} + \mathrm{NLO_{EW}}$ (w decays)
$pp \to tZj$	$\mathrm{NLO_{QCD}} + \mathrm{NLO_{EW}}$ (off shell)	$\mathrm{NNLO_{QCD}} + \mathrm{NLO_{EW}}$ (w/o decays)
$pp \to t\bar{t}t\bar{t}$	$\mathrm{NLO_{QCD}}$ (w decay) $\mathrm{NLO_{EW}}$ (w/o decays)	$\mathrm{NLO_{QCD}} + \mathrm{NLO_{EW}}$ (off-shell) $\mathrm{NNLO_{QCD}}$

Table 5: Precision wish list: top quark final states. $\mathrm{NNLO_{QCD}}^*$ means a calculation using the structure function approximation. $V' = W, Z, \gamma$.

Many contributions from our CRC, e.g. recent ones for $t\bar{t}\gamma$ [Stremmer, Worek: 2403.03796, 2411.02196]

Exclusive top quark pair production at the LHC

However, for fully exclusive **offshell** $t\bar{t} + (W/Z/\gamma/H)$ production N(N)LO **matched** and **showered** results are rare ...

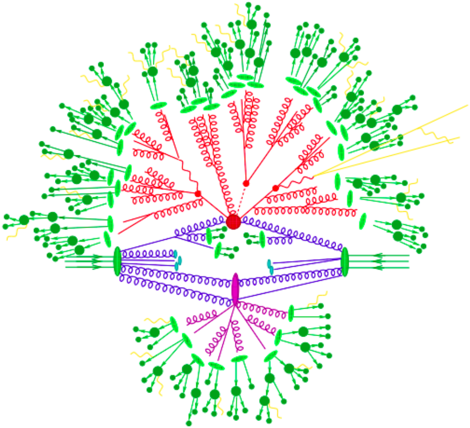
$\rightarrow$ **event** generation needed for a 1:1 comparison with data! (Malgorzata's talk)

Technical challenges:

- 6 and more final states; $e^-\nu_e\mu^+\nu_\mu b\bar{b} + X$
- complicated phase space (small top width)
- many ingredients: hard MEs, subtraction, matching, parton shower, hadronization, ...

Simulating physics at the LHC

Essential tool for physics simulation at the LHC $\rightarrow$ Monte-Carlo event generators



hard collision,
parton shower,
hadronization&decay,
secondary hard scattering event,
soft photon radiation
[1411.4085]

$\rightarrow$ higher order predictions require matching to parton showers!

WHIZARD

What is WHIZARD?

Multi-purpose event generator for cross sections and differential distributions of **arbitrary processes** at HEP experiments (LHC, Belle II, ILC/CLIC/FCC/CEPC, MuCol, ...)

recent version: `v3.1.5`
team: **Wolfgang Kilian, Thorsten Ohl, Jürgen Reuter**
PB, Marius Höfer, Maximilian Löschner, Nils Kreher, Krzysztof Mękała, Tobias Striegl
webpage: `https://whizard.hepforge.org/`
support: `https://launchpad.net/whizard`
email contact: `whizard@desy.de`

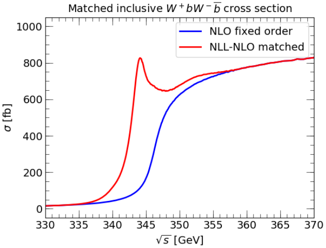
- physics models: SM, internal (hard-coded) BSM and UFO models
- phase-space integrator: VAMP (VEGAS AMPlified),VAMP2 incl. MPI parallelization
- matrix elements: tree-level ME generator O'Mega, interface to OLPs OpenLoops, RECOLA and GoSam

$\texttt{WHIZARD}$ a tool for NLO simulations at the LHC?

- very generic ansatz; any process can be simulated ‘out-of-the-box’
- very well validated **automated** NLO QCD/EW framework (checks for about 50 processes at fNLO)
  + automated Powheg matching (validation for $pp \to e^+e^-$ and $e^+e^- \to t\bar{t}j$)

Specifically for the top-threshold: (Jürgen’s talk)

- already available code for simulation of $e^+e^- \to W^+bW^-\bar{b}$ production at NLO QCD with NLL top threshold-resummation in NRQCD [Bach *et. al.*: 1712.02220]
  - can be extended to pp processes



Validation for offshell top quark pair production at the LHC

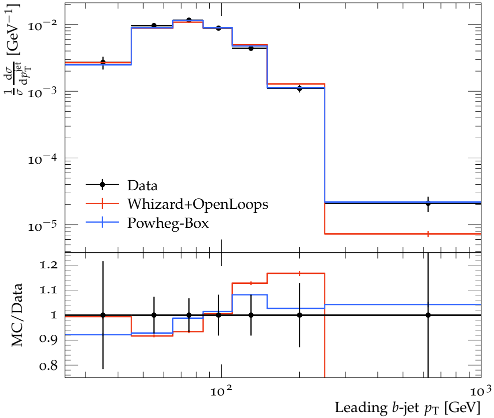
`WHIZARD` compared to `Powheg-Box bb4l` wrt. $pp \to e^- \nu_e \mu^+ \nu_\mu b\bar{b}$ at NLO QCD matched and showered

- **both**:
  - full matrix element (incl. non-resonant diagrams beyond $t\bar{t}$ and Wt),
  - resonance-aware FKS subtraction (accurate and efficient NLO phase space sampling despite small widths of resonances)
  - Powheg matching method, `Pythia8` for parton showering, `OpenLoops` for 1-loop amplitudes
- `bb4l`: process specific improvements (multiple radiation scheme, ...)
- `Whizard`: focus on automated framework, simulation of offshell $t\bar{t} + (Z/W/\gamma/H)$ production possible with same code $\to$ more exp. input needed!

Validation for offshell top quark pair production at the LHC

Current status:

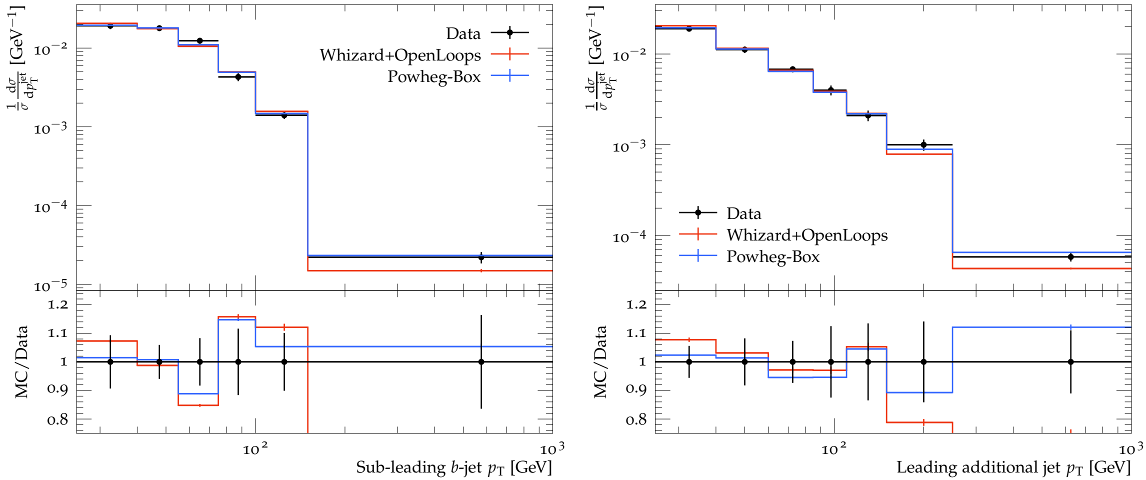
Recent checks of differential distributions of $pp \to e^- \nu_e \mu^+ \nu_\mu b\bar{b}$ at NLO QCD matched and showered with `WHIZARD` compared to `Powheg-Box bb4l` (with thanks to Katharina Voß)



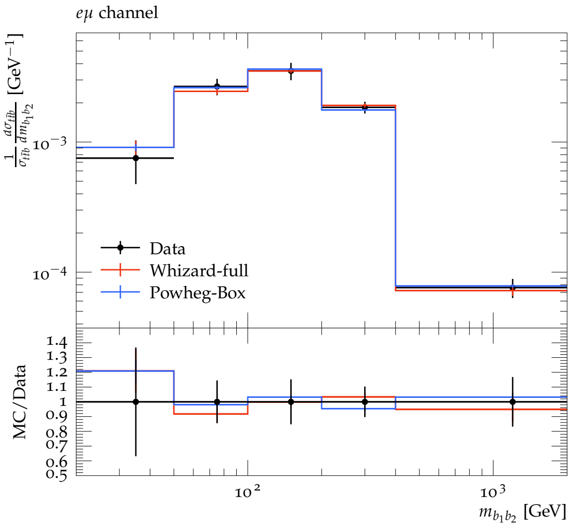
ATLAS_2017_I1495243

Measurement of jet activity produced in top-quark events with an electron, a muon and two b-tagged jets in the final state in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

Validation for offshell top quark pair production at the LHC



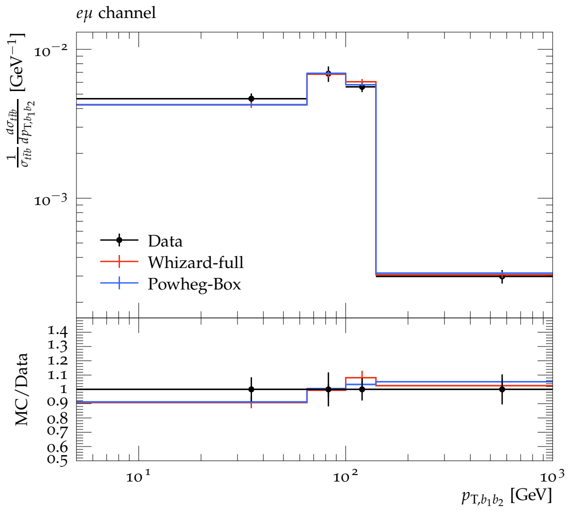
Validation for offshell top quark pair production at the LHC

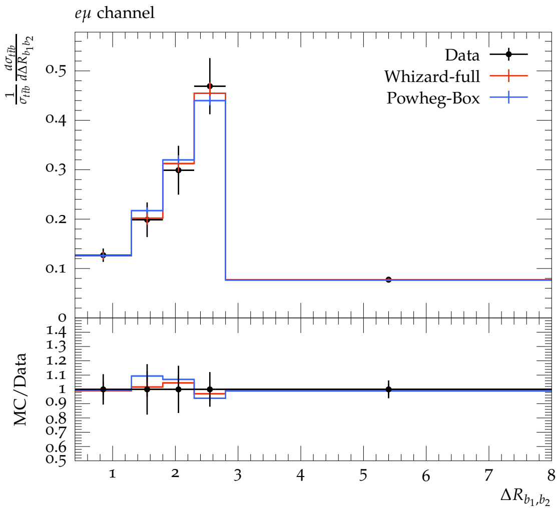


ATLAS_2018_I1705857

Measurements of inclusive and differential fiducial cross-sections of $t\bar{t}$ production with additional heavy-flavour jets in proton–proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

Validation for offshell top quark pair production at the LHC





Associated top quark pair production at the LHC with complete NLO SM corrections

Cross-validation for $pp \to t\bar{t}(+W^\pm/Z/H)$ and $pp \to l^+l^-b\bar{b}$ with complete NLO SM corrections with `MATRIX` orig. ref. [Kallweit *et. al.*: 1412.5157] using `OpenLoops`

$\to$ Example for cross-check for all leading and sub-leading contributions in $t\bar{t}H$ production

		σ^{tot} [fb]		σ^{sig}	*rel. deviation*
$pp \to t\bar{t}H$	$\alpha_s^m\alpha^n$	`MUNICH+OpenLoops`	`WHIZARD+OpenLoops`		
LO_{21}	$\alpha_s^2\alpha$	$3.44865(1)\cdot 10^2$	$3.4487(1)\cdot 10^2$	0.76	0.003%
LO_{12}	$\alpha_s\alpha^2$	$1.40208(2)\cdot 10^0$	$1.4022(1)\cdot 10^0$	1.44	0.011%
LO_{03}	α^3	$2.42709(1)\cdot 10^0$	$2.4274(2)\cdot 10^0$	2.07	0.011%
NLO_{31}	$\alpha_s^3\alpha$	$9.9656(4)\cdot 10^1$	$9.968(4)\cdot 10^1$	0.62	0.023%
NLO_{22}	$\alpha_s^2\alpha^2$	$6.209(1)\cdot 10^0$	$6.208(2)\cdot 10^0$	0.20	0.009%
NLO_{13}	$\alpha_s\alpha^3$	$1.7238(2)\cdot 10^0$	$1.7232(5)\cdot 10^0$	1.24	0.040%
NLO_{04}	α^4	$1.5053(3)\cdot 10^{-1}$	$1.5060(7)\cdot 10^{-1}$	1.00	0.048%

In `WHIZARD`

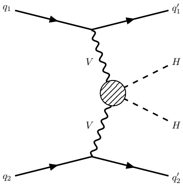
- full NLO SM corrections for heavy quark pair production validated
- future project: extend POWHEG matching to NLO EW $\to$ goal: include NLO EW corr. in parton showered results

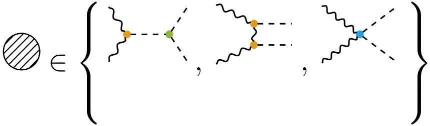
Higgs phenomenology at the LHC

[Braun, PB, Heinrich, Höfer, 2502.09132]

Many questions left open about the Higgs sector ... how to constrain it using LHC measurements?

- multi-Higgs couplings very suppressed
- Higgs boson pairs e. g. in gg fusion or VBF processes
- VBF clean wrt. QCD background, however $\sigma_{VBF} \sim 1.7$ fb $\sim 5\%$ of σ_{ggF}





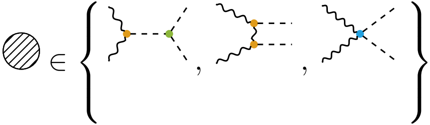
- g_{HHH} and g_{HHVV}, exp. constraints rather loose $\rightarrow$ BSM effects
- sensitive to $g_{HHVV} - g_{HVV}^2$ $\rightarrow$ linked to unitarity, SMEFT vs. HEFT [Kilian *et. al.*:1808.05534, 2101.12537]

Higgs phenomenology at the LHC

In HEFT $\rightarrow$ non-linear realisation of the Higgs sector; NP in anomalous Higgs couplings?

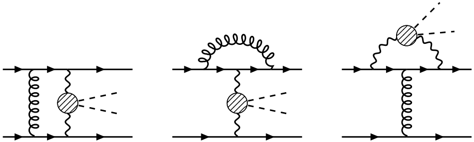
For VBF-HH in HEFT at LO ($d_\chi = 2$) we have ...

$$\mathcal{L}_{\text{eff}} \supset \left(2c_V \frac{h}{v} + c_{2V}\frac{h^2}{v^2}\right)\left(m_W^2 W_\mu^+ W^{-\mu} + \frac{1}{2} m_Z^2 Z_\mu Z^\mu\right) + c_\lambda \frac{m_h^2}{2v} h^3 \,.$$

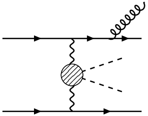


Higher precision: At NLO QCD ...

virtual:



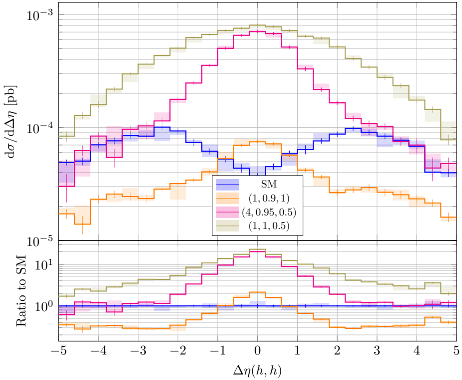
real:



Double Higgs Production in Vector Boson Fusion at NLO QCD in HEFT

- no VBF-approximation (only t-channel) but **all channels** included (t-, u- and s-channel)

di-Higgs pseudorapidity separation distribution at NLO:



different scenarios (c_λ, c_V, c_{2V})
in SM: (1, 1, 1)

shape changes significantly!

Higgs phenomenology at the LHC

In the course of this pheno study ...

- extension of the `WHIZARD+GoSam` interface to work fully flexible with any UFO model – at LO and NLO

$\rightarrow$ potential to be used for more precision pheno studies applying EFTs (independent of process or collider)

Future collider simulations with WHIZARD

Next future collider most likely an e^+e^- machine (European Strategy Update), e. g. ILC/CLIC/FCC/CEPC . . .
also the multi-TeV muon collider concept got a lot of attention recently

$\rightarrow$ EW and Higgs parameters could be measured to a high accuracy (compared to LHC)

- higher order EW corrections essential for theoretical predictions
  - `WHIZARD` framework provides automated NLO EW corrections; for ISR at lepton colliders use massive initial states (IR subtraction only in soft limit)
  - `WHIZARD+Recola2` interface for BSM loops (validated)

Multi-boson processes at a muon collider at NLO EW

[PB, W. Kilian, J. Reuter, P. Stienemeier; JHEP 12 (2022)]

WHIZARD+RECOLA, G_μ scheme, $m_\mu = 0.1056...$ GeV

$\mu^+\mu^- \to X, \sqrt{s} = 3$ TeV	$\sigma_{\mathrm{LO}}^{\mathrm{incl}}$ [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 $\delta_{\mathrm{EW}} = \sigma_{\mathrm{NLO}}^{\mathrm{incl}}/\sigma_{\mathrm{LO}}^{\mathrm{incl}} - 1$ (NLO EW corr.) and $\delta_{\mathrm{ISR}} = \sigma_{\mathrm{LO,LL\text{-}ISR}}^{\mathrm{incl}}/\sigma_{\mathrm{LO}}^{\mathrm{incl}} - 1$ (LL QED ISR corr.)

Summary

- Comparisons of `WHIZARD` with `bb4l` and data for $pp \to e^- \nu_e \mu^+ \nu_\mu b\bar{b}$ at $\sqrt{s} = 13$ TeV
  - `WHIZARD`s results show agreement within uncertainties for a large set of observables; still more technical understanding and improvement needed
  - due to automation $\to$ stress-test `WHIZARD` with offshell $t\bar{t} + (W/Z/\gamma/H)$ studies
- Possibilities to study processes at NLO applying EFTs with the new developments in the `WHIZARD-Gosam` framework
- Future lepton collider studies require higher order QED and EW corrections in theory predictions $\to$ `WHIZARD` technically suited for such calculations

Back-Up

1. FKS subtraction scheme
2. Fixed-order masive approximation for lepton collisions at NLO EW
3. Complex-mass scheme at NLO
4. NLL EW $\mu^+\mu^- \to HZ$ Sudakov factor
5. `WHIZARD` features

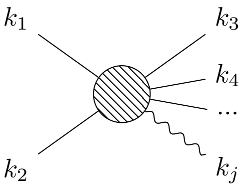
Backup: NLO framework in WHIZARD

(contributors: PB, B. C.-Nejad, W. Kilian, J. Reuter, V. Rothe, P. Stienemeier, C. Weiss)

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

Need 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 IR splittings systematically!

Frixione-Kunszt-Signer (FKS) subtraction

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

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

Backup: NLO framework in `WHIZARD`

(contributors: PB, B. C.-Nejad, W. Kilian, J. Reuter, V. Rothe, P. Stienemeier, C. Weiss)

FKS subtraction per α_r region

$$\mathcal{R} = \sum_{\alpha_r} \mathcal{R}_{\alpha_r} = \sum_{\alpha_r} \mathcal{S}_{\alpha_r} \mathcal{R} \qquad \text{for } \mathcal{I}_{\alpha_r} = (i,j) \in P_{\text{FKS}}(f_r)$$

works in conjunction with POWHEG matching scheme

$$d\sigma_{\text{NLO}} = \bar{\mathcal{B}}(\Phi_n) \left(\Delta(p_{T,\min}) + \Delta(k_T(\Phi_{n+1})) \frac{\mathcal{R}(\Phi_{n+1})}{\mathcal{B}(\Phi_n)} d\Phi_{\text{rad}} \right) d\Phi_n$$

using a *modified* Sudakov form factor

$$\Delta(\Phi_n, p_T) = \exp\left[- \int \frac{\mathcal{R}(\Phi_{n+1})}{\mathcal{B}(\Phi_n)} \theta\left(k_T(\Phi_{n+1}) - p_T\right) d\Phi_{\text{rad}} \right]$$

$$\Delta^{f_{\mathcal{B}}}(\Phi_n, p_T) = \prod_{\alpha_r \in \{\alpha_r | f_{\mathcal{B}}\}} \Delta^{f_{\mathcal{B}}}_{\alpha_r}(\Phi_n, p_T)$$

Backup: NLO framework in WHIZARD: NLO EW

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

process $pp \to$	MUNICH$_{\text{(CS)}}$ +OpenLoops $\sigma^{\text{tot}}_{\text{NLO}}$ [fb]	WHIZARD +OpenLoops $\sigma^{\text{tot}}_{\text{NLO}}$ [fb]	δ [%]	dev [%]	σ^{sig}
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), $\delta \equiv (\sigma^{\text{tot}}_{\text{NLO}} - \sigma^{\text{tot}}_{\text{LO}})/\sigma^{\text{tot}}_{\text{LO}}$, dev $\equiv |\sigma^{\text{tot}}_{\texttt{WHIZARD}} - \sigma^{\text{tot}}_{\texttt{MUNICH}}|/\sigma^{\text{tot}}_{\texttt{WHIZARD}}$

Backup: NLO framework in WHIZARD: NLO EW

Pure electroweak pp processes with off-shell vector bosons

process $pp \to$	α^m	MG5_aMC@NLO [1804.10017] $\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	WHIZARD+OpenLoops $\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	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

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]

Backup: NLO framework in WHIZARD: NLO EW and mixed

Cross-validation with MUNICH/MATRIX using OpenLoops for $pp \to t\bar{t}$ and $pp \to t\bar{t} + W^{\pm}/Z/H$ with complete NLO SM corrections, e. g.

$pp \to t\bar{t}W^+$	$\alpha_s^n \alpha^m$	σ^{tot} [fb] MUNICH$_{(\text{CS})}$	σ^{tot} [fb] WHIZARD	σ^{sig} / *dev* MUNICH$_{(\text{CS})}$-WHIZARD
LO$_{21}$	$\alpha_s^2\alpha$	$2.411403(1) \cdot 10^2$	$2.4114(1) \cdot 10^2$	0.72 / 0.003%
LO$_{12}$	$\alpha_s\alpha^2$	0.000	0.000	0.00 / 0.000%
LO$_{03}$	α^3	$2.31909(1) \cdot 10^0$	$2.3193(1) \cdot 10^0$	1.76 / 0.009%
δNLO$_{31}$	$\alpha_s^3\alpha$	$1.18993(2) \cdot 10^2$	$1.1905(5) \cdot 10^2$	1.06 / 0.048%
δNLO$_{22}$	$\alpha_s^2\alpha^2$	$-1.09511(9) \cdot 10^1$	$-1.0947(3) \cdot 10^1$	1.13 / 0.035%
δNLO$_{13}$	$\alpha_s\alpha^3$	$2.93251(3) \cdot 10^1$	$2.9334(8) \cdot 10^1$	1.14 / 0.030%
δNLO$_{04}$	α^4	$5.759(3) \cdot 10^{-2}$	$5.756(4) \cdot 10^{-2}$	0.58 / 0.049%

Non-negligible and even enhanced EW effects for α_s subleading contributions at NLO!

($pp \to b\bar{b}X$ in validation progress)

Backup: NLO framework in WHIZARD: NLO EW and mixed

Comparison with MG5_aMC@NLO for $pp \to e^+\nu_e j$ and $pp \to e^+e^-j$ at NLO EW

process	$\alpha_s^n\alpha^m$	MG5_aMC@NLO		WHIZARD+OpenLoops			σ^{sig}
$pp \to Xj$		$\sigma^{\text{tot}}_{\text{LO}}$ [pb]	$\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	$\sigma^{\text{tot}}_{\text{LO}}$ [pb]	$\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	δ [%]	LO/NLO
$e^+\nu_e j$	$\alpha_s\alpha^2$	914.81(6)	904.75(8)	914.74(7)	904.59(7)	-1.11	0.8/1.5
e^+e^-j	$\alpha_s\alpha^2$	150.59(1)	149.09(2)	150.59(1)	149.08(2)	-1.00	0.05/0.4

LHC-setup (Run II), cuts with photon recombination **and** jet clustering

II) Application of NLO EW corrections to multi-boson processes at a future muon collider

Back-Up: FKS subtraction scheme

FKS parametrisation:

For $2 \to n$ processes: integrands parametrised by

Φ_n for $\mathcal{B}$, $\mathcal{V}$, $d\sigma_{S,\text{int}}$ and $\Phi_{n+1} = (\Phi_n, \Phi_{\text{rad}})$ for $\mathcal{R}$, $d\sigma_S$

$$\text{FKS variables:} \quad \Phi_{\text{rad}} \to \{\xi, y, \phi\}$$

$$d\Phi_{n+1} = d\Phi_{\text{rad}} d\Phi_n = \underbrace{\mathcal{J}(\xi, y, \phi)}_{\text{Jacobian}} d\xi dy d\phi d\Phi_n$$

with $\xi \equiv 2E_{\text{rad}}/\sqrt{s}$, $y \equiv \cos\theta_{ij}$ and ϕ: angle difference in transversal plane

$$\text{collinear limit:} \quad y \to 1$$
$$\text{soft limit:} \quad \xi \to 0$$

Back-Up: FKS subtraction scheme

IR cancellation:

- Define:

$$\mathcal{R}_{(i,j)} = \mathcal{S}_{(i,j)}\mathcal{R}$$

  with $\mathcal{S}_{(i,j)}$ depending on the kinematics of (i,j), $\sum_{i,j}\mathcal{S}_{(i,j)} = 1$ and $\lim_{y\to 1}\mathcal{S}_{(i,j)} = 1$, $\lim_{\xi\to 0}\mathcal{S}_{(i,j)} = \mathcal{S}^{\text{soft}}_{(i,j)}$
  Subtraction:

$$\tilde{\mathcal{R}}(\xi, y) \equiv (1-y)\xi^2\mathcal{R}(\xi, y)$$

$$\frac{\hat{\tilde{\mathcal{R}}}_{(i,j)}(\xi, y)}{\xi^2(1-y)} = \frac{1}{\xi^2(1-y)}\left(\tilde{\mathcal{R}}_{(i,j)}(\xi, y) - \underbrace{\tilde{\mathcal{R}}_{(i,j)}(0, y)}_{\text{soft}} - \underbrace{\tilde{\mathcal{R}}_{(i,j)}(\xi, 1)}_{\text{collinear}} + \underbrace{\tilde{\mathcal{R}}_{(i,j)}(0, 1)}_{\text{soft-collinear}}\right)$$

- Subtraction "events" get Born phase-space configuration
  $\Rightarrow$ Mind IR-safe observables for event generation!

$$\lim_{p_i \| p_j} O_{n+1}(p_1, \ldots, p_i, \ldots, p_j, \ldots, p_{n+1}) = O_n(p_1, \ldots, p_{ij}, \ldots, p_n)$$

$$\lim_{p_i \to 0} O_{n+1}(p_1, \ldots, p_j, \ldots, p_{n+1}) = O_n(p_1, \ldots, p_{j-1}, p_{j+1}, \ldots, p_n)$$

Back-Up: FKS subtraction scheme

Subtraction terms: For split. partons $\bar{\mathcal{I}}_i \to \mathcal{I}_i\mathcal{I}_j$ and $k_i^2 = 0$ for emitting parton $\mathcal{I}_i$ after splitting

- collinear limit: unreg. polarised splitting functions $\times$ spin-correlated ME^2

$$\lim_{y\to 1} \tilde{\mathcal{R}}_{(i,j)}(\xi, y) \simeq \tilde{\mathcal{R}}_{(i,j)}(\xi, 1) = \lim_{y\to 1} \frac{8\pi\alpha_s(1-y)\xi^2}{\bar{k}_i^2} \hat{P}^{\mu\nu}_{\bar{\mathcal{I}}_i\to\mathcal{I}_i\mathcal{I}_j,\mathrm{QCD}}(z, k_\perp)\mathcal{B}^{(i)}_{\mu\nu}$$

$$\text{For } \bar{\mathcal{I}}_i = g, \quad \mathcal{B}^{(i)}_{\mu\nu} = N_B \sum_{\{m\},s_i,s_i'} \mathcal{M}_n(\{m\}, s_i)\mathcal{M}_n^\dagger(\{m\}, s_i')(\epsilon_{s_i})^*_\mu(\epsilon_{s_i'})_\nu$$

with $\{m\}$ colour, spins of Born conf. and s_i the spin of emitting gluon

- soft limit: eikonal $\times$ color- or charge-correlated Born ME^2

$$\lim_{\xi\to 0} \tilde{\mathcal{R}}_{(i,j)}(\xi, y) \simeq \tilde{\mathcal{R}}_{(i,j)}(0, y) = 4\pi\alpha_s(1-y) \sum_{k,l=1}^{n} \frac{\bar{k}_k \cdot \bar{k}_l}{(\bar{k}_k \cdot \hat{k}_j)(\bar{k}_l \cdot \hat{k}_j)} \mathcal{B}_{kl}$$

$$\mathcal{B}_{kl} = -|\mathcal{M}^n_{kl}|^2 = \langle \mathcal{M}^n | \mathbf{T}_k \cdot \mathbf{T}_l | \mathcal{M}^n \rangle$$

with $\mathcal{I}_j = g$ the radiated parton and $\mathbf{T}_k$ the colour charge operator

$$\boxed{\text{QCD} \to \text{QED: } \{g, \alpha_s, \hat{P}^{\mu\nu}_{\bar{\mathcal{I}}_i\to\mathcal{I}_i\mathcal{I}_j,\mathrm{QCD}}, \mathbf{T}_k\} \longrightarrow \{\gamma, \alpha, \hat{P}^{\mu\nu}_{\bar{\mathcal{I}}_i\to\mathcal{I}_i\mathcal{I}_j,\mathrm{QED}}, \mathbf{Q}_k\}}$$

Back-Up: FKS subtraction scheme

Regularisation by integrated subtraction terms:

From dimensional regularisation with $d = 4 - 2\varepsilon$ and expansions in ε

$\xi^{-1-2\varepsilon} = -\frac{1}{2\varepsilon}\delta(\xi) + \left(\frac{1}{\xi}\right)_+ - 2\varepsilon\left(\frac{\log\xi}{\xi}\right)_+ = -\frac{1}{2\varepsilon}\delta(\xi) + \mathcal{P}_+(\xi)$ and

$(1-y)^{-1-\varepsilon} = -\frac{2^{-\varepsilon}}{\varepsilon}\delta(1-y) + \left(\frac{1}{1-y}\right)_+ - \varepsilon\left(\frac{\log(1-y)}{1-y}\right)_+$ we get

$$\begin{aligned}
\int d\Phi_{\mathrm{rad}}\mathcal{R} &= \int d\Phi_{\mathrm{rad}}(\xi,y)\frac{\tilde{\mathcal{R}}(\xi,y)}{\xi^2(1-y)} \\
&= \frac{s^{1-\varepsilon}}{(4\pi)^{3-2\varepsilon}}\int d\Omega^{(2-2\varepsilon)}\int_{-1}^{1} dy(1-y)^{-1-\varepsilon}\int_0^{\xi_{\max}} d\xi\xi^{-1-2\varepsilon}\tilde{\mathcal{R}}(\xi,y) \\
&= \underbrace{\frac{I^{(2)}_{\text{soft-coll}}}{\varepsilon^2} + \frac{I^{(1)}_{\text{soft}}}{\varepsilon} + +I^{(0)}_{\text{soft}}}_{①} + \underbrace{\frac{I^{(1)}_{\text{coll}}}{\varepsilon} + I^{(0)}_{\text{coll}}}_{②} + \int \underbrace{d\Phi_{\mathrm{rad}}\hat{\mathcal{R}}}_{③} + \mathcal{O}(\varepsilon)
\end{aligned}$$

with plus-distributions $\int_{-1}^{1} dy\left(\frac{g(y)}{1-y}\right)_+ f(y) = \int_{-1}^{1} dy g(y)\frac{f(y)-f(1)}{1-y}$

① soft (and soft-collinear) limit: $\sim -\frac{1}{2\varepsilon}\int dy(1-y)^{-1-\varepsilon}\int d\xi\delta(\xi)\tilde{\mathcal{R}}(\xi,y)$

② collinear limit: $\sim -\frac{2^{-\varepsilon}}{\varepsilon}\int d\xi\mathcal{P}_+(\xi)\int dy\delta(1-y)\tilde{\mathcal{R}}(\xi,y)$

③ subtracted Real: $d\phi dy d\xi\frac{\mathcal{J}(\xi,y,\phi)}{\xi}\left(\frac{1}{\xi}\right)_+\left(\frac{1}{1-y}\right)_+\tilde{\mathcal{R}}(\xi,y)$

Back-Up: Lepton collisions at NLO EW

Fixed-order massive approximation for NLO cross sections:

- IS leptons considered as massive $\Rightarrow$ no collinear counterterms needed
- lepton mass dependencies kept explicit in matrix elements
- NLO phase-space construction with on-shell projection: radiated momentum according to FKS parametrisation; IS momenta fixed; boost of Born FS into recoiling system

Checks with `MCSANCee`, e. g.

$e^+e^- \to HZ$	`MCSANCee`[Sadykov,2020]		`WHIZARD+RECOLA`			σ^{sig}
$\sqrt{s}$ [GeV]	$\sigma^{\text{tot}}_{\text{LO}}$ [fb]	$\sigma^{\text{tot}}_{\text{NLO}}$ [fb]	$\sigma^{\text{tot}}_{\text{LO}}$ [fb]	$\sigma^{\text{tot}}_{\text{NLO}}$ [fb]	δ_{EW} [%]	LO/NLO
250	225.59(1)	206.77(1)	225.60(1)	207.0(1)	−8.25	0.4/2.1
500	53.74(1)	62.42(1)	53.74(3)	62.41(2)	+16.14	0.2/0.3
1000	12.05(1)	14.56(1)	12.0549(6)	14.57(1)	+20.84	0.5/0.5

$e^+e^- \to \mu^+\mu^-$	`MCSANCee`[2206.09469]		`WHIZARD+RECOLA`			σ^{sig}
$\sqrt{s}$ [GeV]	$\sigma^{\text{tot}}_{\text{LO}}$ [pb]	$\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	$\sigma^{\text{tot}}_{\text{LO}}$ [pb]	$\sigma^{\text{tot}}_{\text{NLO}}$ [pb]	δ_{EW} [%]	LO/NLO
5	2978.6(1)	3434.2(1)	2978.7(1)	3433.5(3)	+15.27	0.3/2.2
7	1519.6(1)	1773.8(1)	1519.605(4)	1773.1(2)	+16.68	0.05/3.0

$\alpha(0)$ scheme, $m_e = 0.5109...$ MeV

Back-Up: Electron PDFs for lepton collisions

At LO-LL:

Parametrisation of beam energy fractions in mapping variables $p_1, p_2 \in [0,1]$

$$x_1 = p_1^{p2} \qquad\qquad x_2 = p_1^{1-p2}$$

For random numbers $r_1, r_2 \in [0,1]$

$$p_1 = 1 - (1-r_1)^{1/\epsilon} = 1 - \bar{r}_1^{1/\epsilon}$$

$$p_2 = \begin{cases} 1 - (2r_2)^{1/\epsilon}/2, & u > 0 \\ (2r_2)^{1/\epsilon}/2, & u < 0 \\ 1/2, & u = 0 \end{cases} \qquad\qquad u = 2r_2 - 1.$$

$\Rightarrow$ for small ϵ mapping enhanced at the endpoints $p_1 \to 1$, $p_2 \to 1$ and $p_2 \to 0$

$\Rightarrow$ Jacobian factors '$(1-r_1)^{1/\epsilon - 1} \log p_1$' which **flattens** the integrand in the region $p_1 \to 1$, i. e. $x \to 1$ (where $\lim_{x\to 1} \Gamma_e(x) \to \infty$)

At NLO-NLL:

Rescaling of the PDF arguments for real-emission and collinear subtraction terms (and ISR remnant of collinear subtraction) – beam energy fraction differs before and after radiation

FKS phase-space construction: From Born to real configurations

Ratio of the rescaled over the unrescaled PDFs:

$$\lim_{x'\to 1} \frac{\Gamma(x')}{\Gamma(x)} = \lim_{x\to 1-\delta x} \frac{\Gamma(x+\delta x)}{\Gamma(x)} \to \infty \qquad \Rightarrow \text{ additional mapping for } \delta x$$

Back-Up: Electron PDFs for lepton collisions

Remnant of the subtraction of collinear ISR singularities in integrated form (DGLAP remnant):
The momentum dependence of the PDFs rescales as

$$\Gamma(x_j, \mu) \longrightarrow \Gamma(x_j/z_j, \mu)$$

with $x_j \leq x_j/z_j < 1$ and emitter $j \in \{1, 2\}$
Mapping of the random variable $r_z \in [0, 1]$ defining

$$p_z = 1 - (1 - r_z)^{1/\epsilon}$$

Condition $[0, 1] \longmapsto [x_j, 1]$ mapping $p_z \longrightarrow z_j$ we can find the parametrisation

$$z_j = 1 - p_z(1 - \log p_z)(1 - x_j)$$

Overall Jacobian per emitter

$$f_{\mathrm{DGLAP,j}} = f_{p_z} f_{z_j} = \frac{1}{\epsilon}(1 - r_z)^{1/\epsilon - 1}(1 - x_j) \log p_z$$

Back-Up: Electron PDFs for lepton collisions

For the real component the momentum dependencies of the PDFs rescale as

$$\Gamma(x_1,\mu) \longrightarrow \Gamma(x_1',\mu) = \Gamma\left(\frac{x_1}{\sqrt{1-\xi}}\sqrt{\frac{2-\xi(1-y)}{2-\xi(1+y)}}\right)$$

$$\Gamma(x_2,\mu) \longrightarrow \Gamma(x_2',\mu) = \Gamma\left(\frac{x_2}{\sqrt{1-\xi}}\sqrt{\frac{2-\xi(1+y)}{2-\xi(1-y)}}\right)$$

Mapping for $\{x_1, x_2, x_1', x_2'\}$ instead of $\{x_1, x_2, \xi, y\}$!
Conditions

$$x_1 \leq x_1' < 1 \qquad\qquad x_2 \leq x_2' < 1$$

Construct $\hat{p}_j \in [0,1]$ from random numbers $\hat{r}_j \in [0,1]$ as

$$\hat{p}_j = 1 - (1-\hat{r}_j)^{1/\epsilon}$$

Define rescaled variables with mapping

$$x_j' = 1 - \hat{p}_j(1-\log\hat{p}_j)(1-x_j) \qquad\qquad j = 1,2$$

leads to Jacobians

$$f_{x',j} = \frac{1}{\epsilon}(1-\hat{r}_j)^{1/\epsilon-1}(1-x_j)\log\hat{p}_j$$

Back-Up: Electron PDFs for lepton collisions

Define auxiliary quantities

$$A \equiv \frac{x_1 x_2'}{x_2 x_1'} = \frac{2-\xi(1+y)}{2-\xi(1-y)} \qquad B \equiv \frac{x_1 x_2}{x_1' x_2'} = 1-\xi$$

such that ξ and y can be derived, yielding

$$\xi = 1 - B \qquad y = \left(\frac{1+B}{1-B}\right)\left(\frac{1-A}{1+A}\right) \quad .$$

Considering

$$d\xi dy = \mathcal{J}_1(A,B)\; dAdB = \mathcal{J}_1(A,B)\mathcal{J}_2(x_1', x_2')\; dx_1' dx_1'$$

with

$$\mathcal{J}_1(A,B) = 2\left(\frac{1+B}{1-B}\right)\frac{1}{(1+A)^2} \qquad \mathcal{J}_2(x_1', x_2') = 2\frac{x_1^2}{x_1'^3 x_2'}$$

we get the final Jacobian factor for ξ and y parametrised in random numbers $\hat{r}_{1/2}$,

$$f_{\text{real},j} = \mathcal{J}_1(A,B)\mathcal{J}_2(x_1', x_2') f_{x',1} f_{x',2} \quad .$$

Back-Up: Complex-mass scheme at NLO

Renormalised self-energy:

$$\hat{\Sigma}^i(p^2) = \Sigma^i(p^2) - \delta M_i^2$$

Complex location of the pole $p^2 = \mu_i^2$ of propagator: $\mu_i^2 - M_{0,i}^2 + \Sigma(\mu_i^2) = 0 \quad \Rightarrow \hat{\Sigma}^i(\mu_i^2)$ vanishes

$\Rightarrow$ renormalised masses $M_i^2 = M_{0,i}^2 - \delta M_i^2$ fixed at this pole due to OS condition $\delta M_i^2 = \Sigma(p^2)|_{p^2=\mu_i^2}$

Complex-mass scheme requires calculating self-energies for complex squared momenta!

Solutions:

- analytic continuation of the self-energies in the complex momentum variable to the unphysical Riemann sheet (`MadLoop`)[Frederix *et. al.*, 1804.10017]
- expansion of self-energies around real arguments such that one-loop accuracy is retained (`OpenLoops`, `Recola`) [Denner *et. al.*, 0505042]
  - 2-point integrals with $p^2 = \mu_i^2 = M_i^2 - i\Gamma_i M_i$ can be obtained through first-order expansion in Γ_i/M_i around $p^2 = M_i^2$

Back-Up: NLL EW $\mu^+\mu^- \to HZ$ Sudakov factor

Using the abbreviations for double and single logarithmic factors

$$L(s, M_W^2) = \frac{\alpha}{4\pi} \log^2 \frac{s}{M_W^2} \qquad\qquad l(s, M_W^2) = \frac{\alpha}{4\pi} \log \frac{s}{M_W^2}$$

For $s \gg M_W$, leading logarithmic, angular-independent, terms (from exchange of soft-collinear gauge bosons between pairs of external legs)

$$\Lambda_{l,\lambda}^{\kappa} = A_{\lambda}^{\kappa}\, L(s, M_W^2) + B_{\lambda}^{\kappa}\, \log \frac{M_Z^2}{M_W^2} l(s, M_W^2) + C_{\lambda}$$

with $\lambda = T, L$ the transverse and longitudinal polarisation of the Z boson, and $\kappa = L, R$ the muon initial state chirality

$$\begin{aligned} A_T^{\kappa} &= -\frac{1}{2}\left[2C_{\mu^\kappa}^{\mathrm{EW}} + C_{\Phi}^{\mathrm{EW}} + C_{ZZ}^{\mathrm{EW}}\right] & A_L^{\kappa} &= -\left[C_{\mu^\kappa}^{\mathrm{EW}} + C_{\Phi}^{\mathrm{EW}}\right] \\ B_T^{\kappa} &= 2(I_{\mu_\kappa}^Z)^2 + (I_H^Z)^2 & B_L^{\kappa} &= 2\left[(I_{\mu_\kappa}^Z)^2 + (I_H^Z)^2\right] \\ C_T &= \delta_H^{LSC,h} & C_L &= \delta_H^{LSC,h} + \delta_\chi^{LSC,h} \quad . \end{aligned}$$

Back-Up: NLL EW $\mu^+\mu^- \to HZ$ Sudakov factor

Subleading, angular-dependent, terms due to $W^\pm$ boson exchange between initial- and final-state legs

$$\Lambda^{\kappa}_{\theta,\lambda} = -\delta_{\kappa L} \frac{D_\lambda}{I^Z_{\mu_\kappa}}\, l(s, M_W^2) \left[\log \frac{|t|}{s} + \log \frac{|u|}{s}\right]$$

Mandelstam variables t and u approximated in the high-energy limit

$$t = \ (p_{\mu^+} - p_H)^2 \sim -\frac{s}{2}(1 - \cos\theta_H) \qquad u = \ (p_{\mu^+} - p_Z)^2 \sim -\frac{s}{2}(1 + \cos\theta_H)$$

Back-Up: NLL EW $\mu^+\mu^- \to HZ$ Sudakov factor

Estimation for the unpolarised approximation factor:

- Born amplitudes for transverse polarized Z bosons are suppressed by M_Z^2/s

$$\Lambda_\lambda^\kappa \mathcal{M}_0^{\mu_\kappa^+\mu_\kappa^- \to HZ_\lambda} \xrightarrow{s \gg M_W^2} \delta_{\lambda L} \Lambda_\lambda^\kappa \mathcal{M}_0^{\mu_\kappa^+\mu_\kappa^- \to HZ_\lambda} \tag{1}$$

- Chirality and helicity of the muon coincide in the ultrarelativistic limit (two helicity configurations $(+,-)$ and $(-,+)$ remaining, equivalent to chiralities $\kappa = L, R$). Spin-averaging yields

$$\Lambda_{\text{est}}^{\text{unpol}} = \frac{\sum_\kappa \Lambda_L^\kappa |\mathcal{M}_0^{\mu_\kappa^+\mu_\kappa^- \to HZ_L}|^2}{|\mathcal{M}_0^{\mu^+\mu^- \to HZ_L}|^2} \tag{2}$$

Back-Up: WHIZARD features

WHIZARD provides

- phase space evaluation with VAMP2 [Braß *et. al.*: 1811.09711]:
  - twofold self-adaptive multi-channel parametrization
  - OpenMP and MPI for parallelization ⇒ speedup of factor $\mathcal{O}(100)$
- matching to parton showers: POWHEG scheme
- showering and hadronization: PYTHIA6 shipped with WHIZARD, interface between WHIZARD and PYTHIA8
- event formats: LHE, HepMC2/3, Stdhep, LCIO, ...
- special support for lepton collider processes:

beamstrahlung	CIRCE1/CIRCE2 [CPC 101 (1997) 269]
bremsstrahlung	LL resummation via ISR and EPA functions
beam polarization	inclusion for a user-defineable setup