# Monte Carlo generators – recent advances

## physics improvements & algorithmic developments

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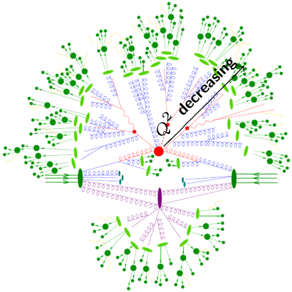
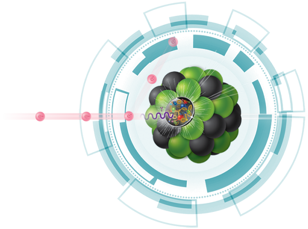
# Monte Carlo generators: setting the scene

- stochastic simulation of exclusive particle level events
  - ⇝ factorized approach to model event evolution (modularity)
  - ⇝ hard process, parton shower, underlying event, hadronization
- vital for realistic phenomenological and experimental analyses
  - ⇝ facilitate measurement planning, realization & interpretation
- address breadth & depth of community needs & challenges
  - ⇝ (HL-)LHC (pp and heavy ions), EIC, future ee/pp colliders



[https://www.bnl.gov/eic/]

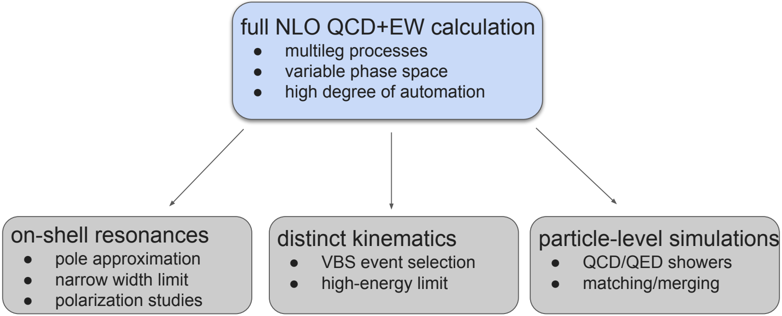
# Monte Carlo generators: requirements/challenges

- **precise & versatile** hard-process modelling
  - $\rightsquigarrow$ include QCD & EW corrections, polarizations, BSM processes
  - $\rightsquigarrow$ automated ME generators & IR subtractions, UFO [Darmé et al.]
  - $\rightsquigarrow$ dedicated loop-amplitude providers
- **accurate** QCD parton showers (Plätzer) & QED radiation
  - $\rightsquigarrow$ means to match/merge with matrix elements, formal accuracy
- **quantifiable** systematic uncertainties/variations
  - $\rightsquigarrow$ perturbative & non-perturbative scales/parameters
  - $\rightsquigarrow$ sophisticated on-the-fly reweighting approaches (multi-weight events)
- **resource efficiency**, adapt to new hardware (Bothmann)
  - $\rightsquigarrow$ incorporate recent machine learning developments
  - $\rightsquigarrow$ adapt to heterogeneous hardware systems (GPUs, HPC)

physics improvements & algorithmic developments

# Physics improvements

# Accounting for (dominant) electroweak corrections

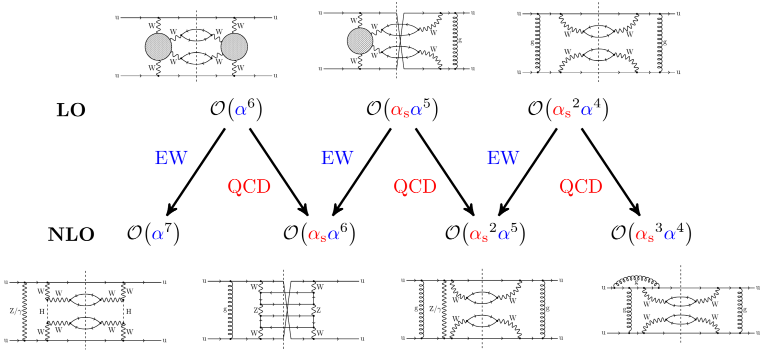



- generator frameworks to accomplish full calculations, e.g.
  MG5_aMC [Frederix *et al.*], PowHEG [Nason *et al.*], Sherpa [Bothmann *et al.*]
- EW one-loop and QED real-emission amplitudes needed, e.g.
  Recola [Denner *et al.*], OpenLoops [Pozzorini *et al.*]
- QED infrared subtraction terms (dipole/FKS)
  $\rightsquigarrow$ real weak-boson radiation excluded
- invoke QCD/QED showers for particle-level predictions
  Herwig [Bellm *et al.*], Pythia [Bierlich *et al.*], Sherpa

**state-of-the-art: full NLO calculation for $2 \rightarrow 6$ processes**

- full NLO QCD & EW corrections and QCD–EW interferences
  - $\rightsquigarrow$ crucial benchmark for approximation schemes used in MCs
  - $\rightsquigarrow$ see talk by Denner
- consider **like-sign $W$-boson scattering**: $pp \rightarrow e^+\nu_e\mu^+\nu_\mu jj$

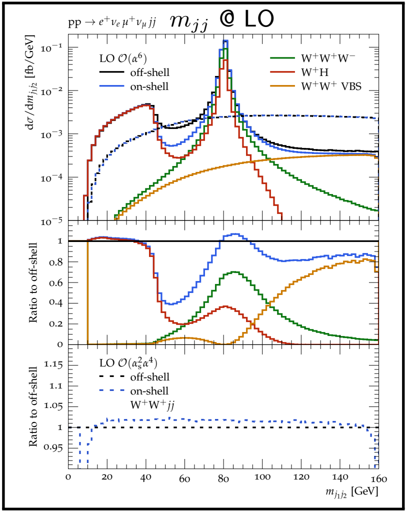
[Dittmaier et al. JHEP 11 (2023) 22] [Biedermann et al. JHEP 10 (2017) 124]

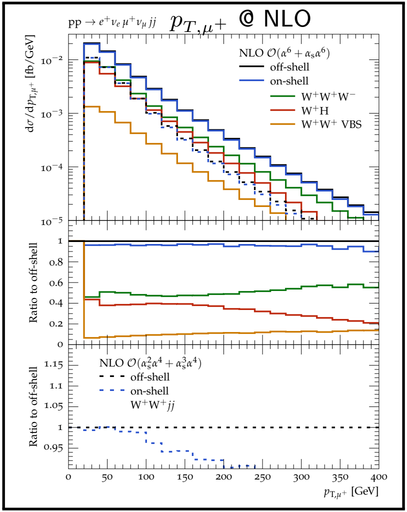


## state-of-the-art: triboson $pp \to e^+\nu_e\mu^+\nu_\mu jj$ at full NLO

[Denner, Pellen, Schönherr, S. JHEP **08** (2024) 043]

- full off-shell calc vs. incoherent sum of on-shell channels



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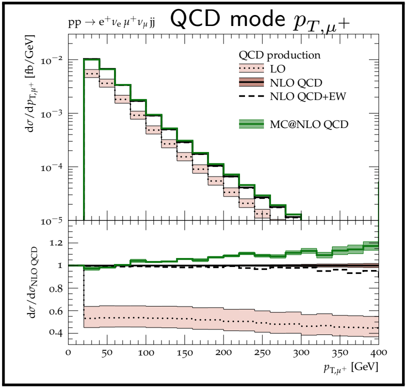
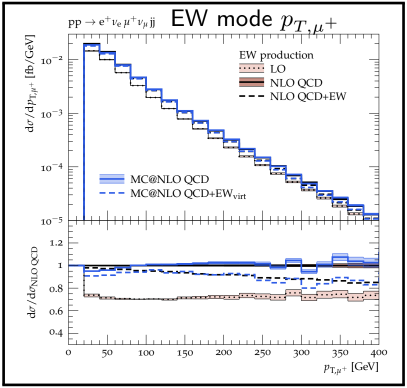
[Denner, Pellen, Schönherr, S. JHEP **08** (2024) 043]

- separate into EW $\mathcal{O}(\alpha^6)$ & QCD $\mathcal{O}(\alpha_s^2\alpha^4)$ production mode
- QCD corr via MC@NLO, EW mode split in $s/t$-channel piece
- EW corr to EW mode in the virtual approximation (EW$_{\text{virt}}$)

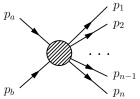


**universal high-energy enhancements**

- consider EW one-loop amplitudes in high-energy limit, where

$$s_{ij} \equiv (p_i + p_j)^2 \sim s \gg M_W^2 \quad \forall\, i, j$$




- amplitude factorization, dominance of scale-ratio logarithms

$$\mathcal{M}_1 \;\propto\; \mathcal{M}_0 \times \left(\delta^{\mathsf{DL}} + \delta^{\mathsf{SL}}\right)$$

$$\delta^{\mathsf{DL}} \sim \frac{\alpha}{4\pi} \log^2\left(\frac{|s_{ij}|}{M_W^2}\right) \qquad \delta^{\mathsf{SL}} \sim \frac{\alpha}{4\pi} \log\left(\frac{|s_{ij}|}{M_W^2}\right)$$

- algorithm to construct NLL EW corrections [Denner, Pozzorini '01]
- recent revisitations, refinements and new implementations

  SHERPA, MG5_aMC & OPENLOOPS

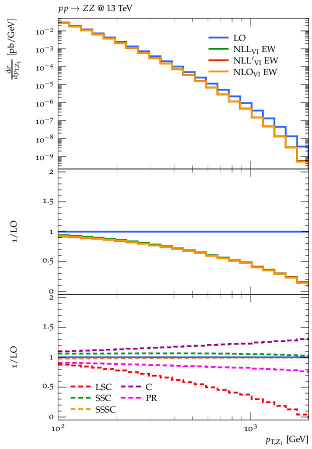
  [Bothmann, Napoletano '20, Bothmann et al. '22] [Pagani, Zaro '22, Pagani et al. '23] [Lindert, Mai '23]

# Taming the tails: EW Sudakov logarithms

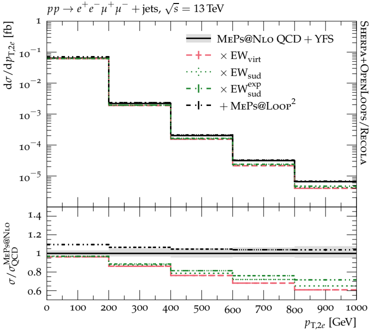
- extensive validation for OpenLoops [Lindert, Mai 2312.07927]
- comparison to $\text{NLO}_\text{VI}$ EW approximation [Kallweit et al. '15]

⇝ used in Sherpa MEPS@NLO approach [Bothmann et al. JHEP 06 (22) 131]

leading boson $p_T$ in $ZZ$ (OpenLoops)




MEPS@NLO $ZZ(\to 2e2\mu) + 0, 1j$ (Sherpa)




⇝ MG5_aMC Timea Vitos (Thu)

- NLL resummation in $\text{SCET}_\text{EW}$ [Denner, Rode EPJC 84 (2024) 5]

# Probing EWSB: vector-boson polarizations

**predicting vector-boson polarization fractions $f_{\text{pol}}$**

- consider decay of on-shell massive gauge boson $(m_{q/l} = 0)$
  $\rightsquigarrow$ use pole approximation, i.e. on-shell projection, or NWA

$$\mathcal{M}^{\text{tot}} \approx \sum_{\lambda=L,\pm} \mathcal{M}_\lambda^{\text{fac}} = \frac{i}{p^2 - M_V^2 + i\Gamma_V M_V} \sum_{\lambda=L,\pm} \mathcal{M}_\lambda^{\text{prod}}(\tilde{p}) \mathcal{M}_\lambda^{\text{dec}}(\tilde{p})$$

- consider inclusive & fiducial phase spaces
  $\rightsquigarrow$ residual interference contribution when fiducial cuts

$$|\mathcal{M}_{\text{res}}^{\text{tot}}|^2 = \sum_{\lambda=L,\pm} |\mathcal{M}_\lambda^{\text{fac}}|^2 + \sum_{\lambda\neq\lambda'} \mathcal{M}_\lambda^{\text{fac}} \mathcal{M}_{\lambda'}^{*\text{fac}}$$

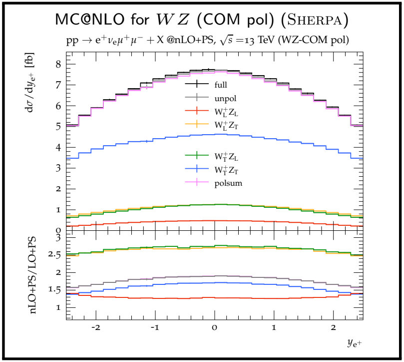
- seek for differential distributions with $\lambda = L$ enhancements
  $\rightsquigarrow$ for use in experimental template fits
  $\rightsquigarrow$ note, $f_{\text{pol}}$ frame dependent, e.g. lab or diboson rest frame

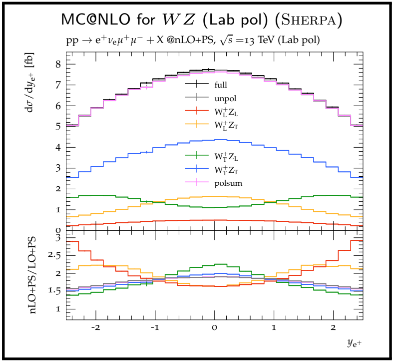
$\rightsquigarrow$ dedicated talk by Pellicciolі

## particle-level predictions for polarized gauge bosons

[Hoppe, Schönherr, Siegert JHEP 04 (2024), 001] [Pellicciloli, Zanderighi EPJC 84 (2024) 1]

- new implementations in SHERPA (NWA) & POWHEG (DPA)
- restrict to QCD corrections at (N)LO and QCD parton shower
- SHERPA utilizes its spin-correlated decay model [Höche et al. '15]
  - ⇝ event weights for different polarizations/frames on-the-fly
  - ⇝ (currently) assume virtual QCD amplitude as unpolarized

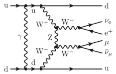


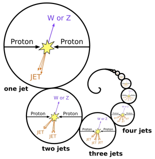



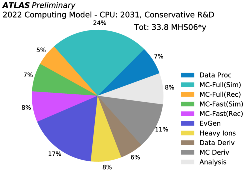
# Algorithmic developments

## Computational bottleneck: the hard event component

$$\sigma_{pp\to X_n} = \sum_{ab}\int \mathrm{d}x_a \mathrm{d}x_b\, \mathrm{d}\Phi_n\, f_a(x_a,\mu_F^2) f_b(x_b,\mu_F^2)\, |\mathcal{M}_{ab\to X_n}|^2\, \Theta_n(p_1,\ldots,p_n)$$






[CERN-LHCC-2022-005]

$\hookrightarrow$ $|\mathcal{M}|^2$ multi-modal, wildly fluctuating, expensive

$\hookrightarrow$ real- & virtual quantum corrections, IR subtractions

$\hookrightarrow$ Monte-Carlo phase-space sampling $[\dim[\Phi_n] = 3n-4]$

**main research thrusts** (towards HL-LHC)

$\hookrightarrow$ sustainable simulations on modern hardware

[Bothmann *et al.*] [Carrazza *et al.*] [Mattelaer *et al.*] (Bothmann)

$\hookrightarrow$ NN improved phase-space sampling

SHERPA [Janßen *et al.*], MADNIS [Heimel *et al.*]

$\hookrightarrow$ surrogate unweighting techniques

NN ME emulator [Danziger *et al.*]

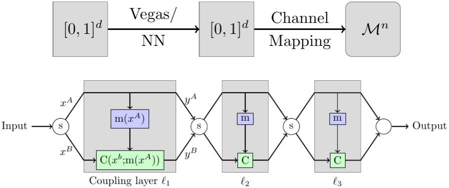
leading-color ME [Frederix, Vitos 2409.12128]

## ML-assisted phase-space sampling

- MCEG use physics informed importance sampling
  - ⇝ aim to reduce event-weight variations (automation)
  - ⇝ adaptive multi-channel sampler: SHERPA, MG, WHIZARD
- **improve sampling efficiency through Normalizing Flows**
  - ⇝ bijective remapping of random numbers for channel maps

    [Müller *et al.*, arXiv:1808.03856] [Bothmann *et al.*, SciPost Phys. 8 (2020) no.4, 069]

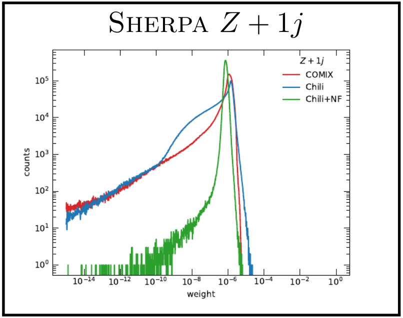
    [Gao *et al.*, PRD 101 (2020) no.7, 076002] [Heimel *et al.* SciPost Phys. 15 (2023) 141]

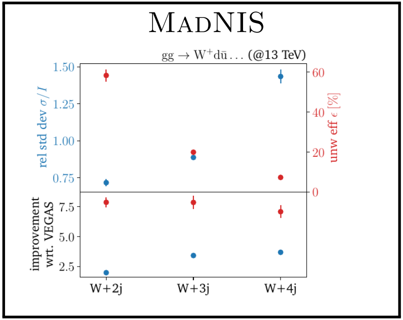



  - ⇝ invertible *coupling layers* with tractable Jacobian
  - ⇝ more expressive than standard VEGAS remapping

**ML-assisted phase-space sampling – closing in on production**

- implementation in SHERPA framework
  [Gao *et al.*, PRD 101 (2020) no.7, 076002] [Bothmann *et al.*, SciPost Phys. 15 (2023) 4]
- MADNIS multi-channel sampler for MADGRAPH
  [Heimel *et al.*, SciPost Phys. 15 (2023) 141 & 17 (2024) 23]



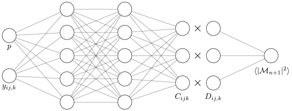



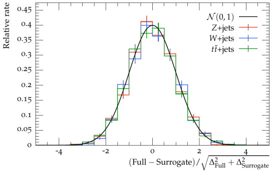

$\rightsquigarrow$ new powerful integration/sampling methods

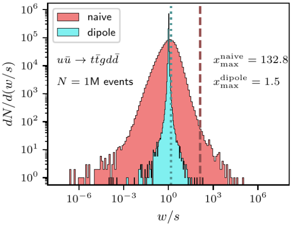
$\rightsquigarrow$ enormous potential for other applications, e.g. loop calcs
[Winterhalder *et al.*, SciPost Phys. 12 (2022) no.4, 129] [Jinno *et al.*, JHEP 7 (2023) 181]

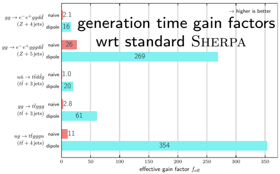
## Unbiased unweighting algorithm employing NN emulators

- QCD factorization-aware NN matrix-element emulator
  [Maître, Truong, JHEP 11 (2021) 66] [Janßen *et al.*, SciPost Phys. 15 (2023) 107]
- two-stage unweighting algorithm, correcting fast surrogate
  [Danziger *et al.*, SciPost Phys. 12 (2022) 164]




- alternative amplitude emulators for one-loop processes
  [Aylett-Bullock *et al.*, JHEP 8 (2021) 66] [Badger *et al.*, SciPost Phys. Core 6 (2023) 034]
  [Maître, Truong, JHEP 5 (2023) 159]

## Theory expectations via Monte Carlo event generators

- improved physics modelling capabilities
  - ⇝ (N)NLO QCD ME+PS (Zanoli, Napoletano)
  - ⇝ (approximate) inclusion of EW corrections (NLO, NLL)
  - ⇝ polarized vector bosons (Pellicciol)
  - ⇝ development of improved showers (Plätzer)
  - ⇝ better non-perturbative models (Gaunt, Lönnblad)
- innovative computational algorithms & software development
  - ⇝ ML-augmented event generation (Kuschick)
  - ⇝ clever reweighting methods [Ilten *et al.* 2308.13459] [Frederix, Vitos 2409.12128]
  - ⇝ massive parallelization: GPUs, HPC readiness (Bothmann)