Monte Carlo generators for future colliders

facilitating precision physics: challenges & research thrusts

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KET Future Collider Workshop

DESY Hamburg

29.11.2024

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung

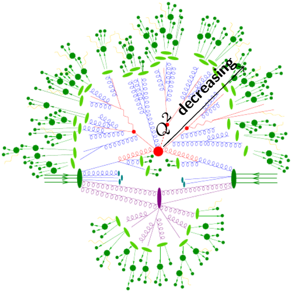
KISS

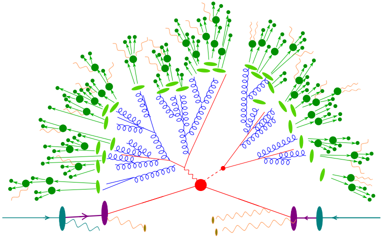
Funded by DFG Deutsche Forschungsgemeinschaft German Research Foundation

MCnet

Monte Carlo generators: setting the scene

- stochastic simulation of exclusive particle level events
  - ⇝ factorized approach to model event evolution (modularity/automation)
  - ⇝ hard process, QCD/QED radiation, underlying event, hadronization
- vital for realistic phenomenological and experimental analyses
  - ⇝ facilitate experiment planning, physics feasibility studies
- address breadth & depth of community needs & challenges
  - ⇝ ongoing experiments (pp/ee/HI) & future ee/pp/ep colliders
  - ⇝ from per-mil level EW physics to QCD at the 10 TeV scale





Monte Carlo generators: paradigms/challenges

- **precise & versatile** hard-process modelling
  - $\rightsquigarrow$ include higher-order QCD, EW and QED corrections, BSM physics
- **accurate** QCD parton showers & QED radiation
  - $\rightsquigarrow$ means to match/merge with higher-order matrix elements
- **quantifiable** systematics, comparable to experimental ones
  - $\rightsquigarrow$ perturbative & non-perturbative scales/parameters
  - $\rightsquigarrow$ plug-and-play alternative physics modules
- **resource efficient** delivery of high-statistics samples
  - $\rightsquigarrow$ incorporate recent machine learning developments
  - $\rightsquigarrow$ adapt to heterogeneous hardware systems (GPUs, HPC)

demands physics improvements & algorithmic developments

Physics improvements

illustrative examples

Future lepton collider: need for QED corrections

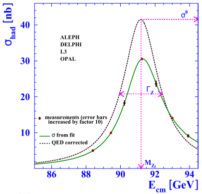
Electroweak Pseudo Observables at per-mil accuracy

- huge luminosity increase compared to LEP

  ↪ precision on EWPO will improve by factors up to 100

- need per-mil accurate cross sections and distributions

  ↪ account/correct for QED & EW higher orders



[Phys Rept 427 (2006) 257]

main QED developments needed

Observable	Source LEP	Err.{QED} LEP	Stat[Syst] FCC-ee	$\frac{\text{LEP}}{\text{FCC-ee}}$	main development to be done
M_Z [MeV]	Z linesh.	2.1{0.3}	0.005[0.1]	$3\times3^\star$	light fermion pairs
Γ_Z [MeV]	Z linesh.	2.1{0.2}	0.008[0.1]	$2\times3^\star$	fermion pairs
$R_l^Z \times 10^3$	$\sigma(M_Z)$	25{12}	0.06[1.0]	$12\times3^{\star\star}$	better FSR
σ^0_{had} [pb]	σ^0_{had}	37{25}	0.1[4.0]	$6\times3^\star$	better lumi MC
$N_\nu \times 10^3$	$\sigma(M_Z)$	8{6}	0.005[1.0]	$6\times3^{\star\star}$	CEEX in lumi MC
$N_\nu \times 10^3$	$Z\gamma$	150{60}	0.8[< 1]	$60\times3^{\star\star}$	$\mathcal{O}(\alpha^2)$ for $Z\gamma$
$\sin^2\theta_W^{eff} \times 10^5$	$A_{FB}^{lept.}$	53{28}	0.3[0.5]	$55\times3^{\star\star}$	h.o. and EWPOs
$\sin^2\theta_W^{eff} \times 10^5$	$\langle\mathcal{P}_\tau\rangle$,$A_{\text{FB}}^{pol,\tau}$	41{12}	0.6[< 0.6]	$20\times3^{\star\star}$	better τ decay MC
M_W [MeV]	mass rec.	33{6}	0.5[0.3]	$12\times3^{\star\star\star}$	QED at threshold
$A_{FB,\mu}^{M_Z\pm3.5\text{GeV}} \times 10^5$	$\frac{d\sigma}{d\cos\theta}$	2000{100}	1.0[0.3]	$100\times3^{\star\star\star}$	improved IFI

[Jadach, Skrzypek EPJC 79 (2019) 9]

- updates of precision luminosity Monte Carlo(s)

  ↪ low/wide angle Bhabha scattering (BHLUMI, BABAYAGA)

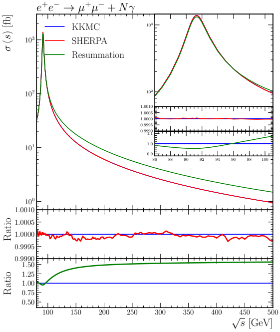
- QED initial- and final-state radiation

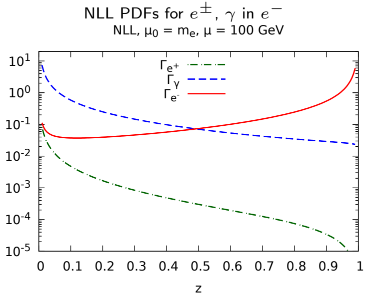
Dealing with QED initial-state radiation

(i) soft-photon resummation in YFS formalism with exact h.o.
  ↪ LEP era tools KKMC [Jadach et al.], recently SHERPA [Krauss et al.]

(ii) collinear structure functions & QED initial-state shower
  ↪ new NLL electron structure funcs [Bertone et al. JHEP 03 (2020) 135]
  ↪ steps towards MC@NLO$_{\mathrm{QED}}$ [Flower 2409.02203]

[Price et al. SciPost Phys 13 (2022) 2]



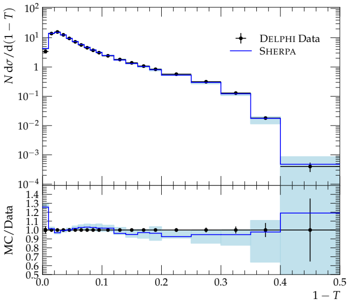


[Bertone et al. JHEP 03 (2020) 135]

Hadronic final states in direct & photoproduction

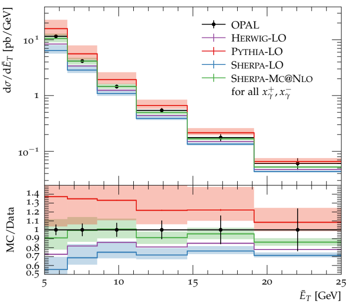
- precision tests of QCD in hadronic final states, e.g. α_s
- extraction of hadronic Higgs-boson decays
  - $\hookrightarrow$ (N)NLL accurate QCD showers [Salam et al., Plätzer et al., Reichelt et al.]
  - $\hookrightarrow$ scrutinize models for hadronisation (currently LEP data)
- sizeable photoproduction component, similar to pp collisions

hadronisation uncertainty thrust @ LEP



[Knobbe et al. JHEP 09 (2023) 160]

dijets in photoproduction @ LEP

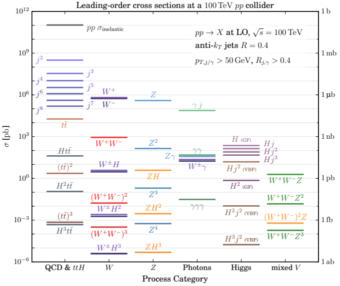


[Helenius et al. 2406.08026]

probing the SM in the multi-TeV regime

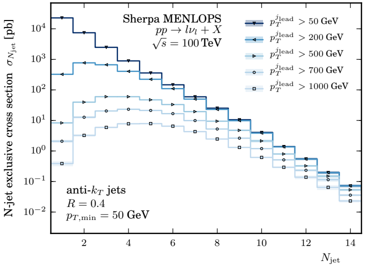
- enormous QCD production rates and jet multiplicities
- huge phase space for heavy states & extra radiation
  - $\hookrightarrow$ NNLO QCD for jet-associated channels, multi-leg NLO
  - $\hookrightarrow$ match/merge with QCD parton showers
- expect sizeable Underlying Event, Multiple Parton Scattering

SM cross sections @ 100 TeV



[Bothmann et al. PRD 94 (2016) 3]

exclusive jet multi W+jets @ 100 TeV

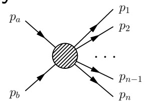


[Bothmann et al. PRD 94 (2016) 3]

high-energy enhancement of EW corrections

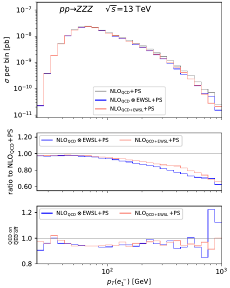
- large EW Sudakov logarithms in high-energy limit

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



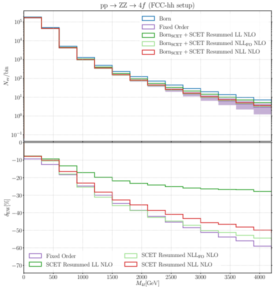
- current MC standard: NLL approximation to full NLO EW
  [Bothmann et al. '20 & '22] [Pagani, Zaro '22, Pagani et al. '23] [Lindert, Mai '23]
- towards NLL resummation in $\mathrm{SCET_{EW}}$ [Denner, Rode EPJC 84 (2024) 5]

leading lepton p_T in ZZZ @ 13 TeV



[Pagani et al. EPJC 84 (2024) 5, 514]

m_{4l} in ZZ @ 100 TeV

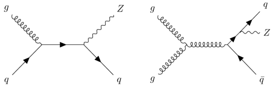


[Denner, Rode EPJC 84 (2024) 5, 542]

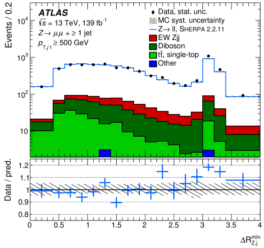
intra-jet EW boson radiation: the case for EW showers

- wide range of Vj kinematics

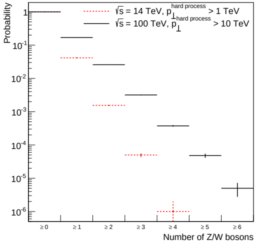
[ATLAS JHEP 06 (2023) 80]



  - ↪ multi-scale QCD problem
  - ↪ case for ME+PS simulations



- quasi-collinear if $p_{T,j} \gg M_V$
  - ↪ treat as EW shower emission
- mixed QCD/QED/EW evolution
  - ↪ competing emission probabilities
  - ↪ spin-correlations, flavour changes
- first steps in Pythia



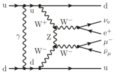
[Christiansen, Sjöstrand JHEP 04 (2014) 115]

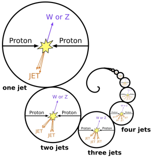
Algorithmic developments

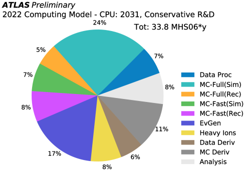
illustrative examples

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

$\hookrightarrow$ sustainable simulations on modern hardware

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

$\hookrightarrow$ 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]

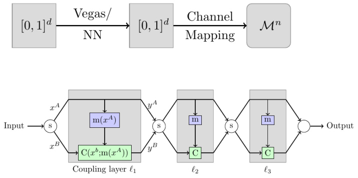
ML-assisted phase-space sampling

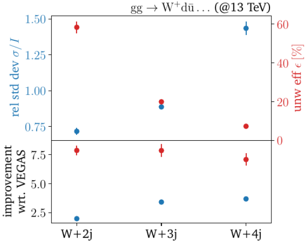
- MCEG use physics informed importance sampling
  - ⇝ aim to reduce event-weight variations (automation)
  - ⇝ adaptive multi-channel sampler: SHERPA, MG, WHIZARD
- **improve sampling efficiency through Normalizing Flows**
  - ⇝ bijective remapping of random numbers for channel maps

[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]

MADNIS

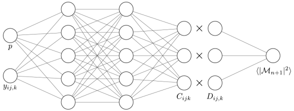


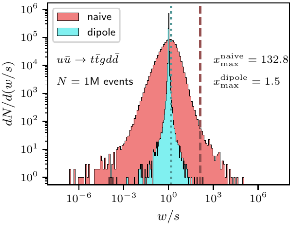


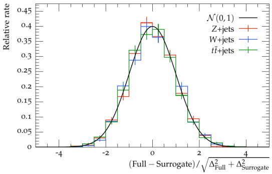
- ⇝ invertible *coupling layers* with tractable Jacobian
- ⇝ more expressive than standard VEGAS remapping

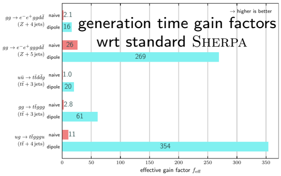
Unbiased unweighting algorithm employing NN emulators

- 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]









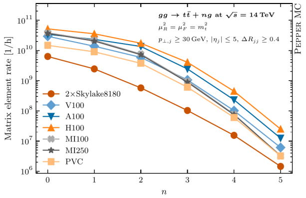
- alternative amplitude emulators for one-loop processes
  [Aylett-Bullock *et al.*, JHEP 8 (2021) 66] [Badger *et al.*, SciPost Phys. Core 6 (2023) 034]
  [Maître, Truong, JHEP 5 (2023) 159]

Novel algorithms: heterogeneous compute architectures

portability to different computing-hardware environments

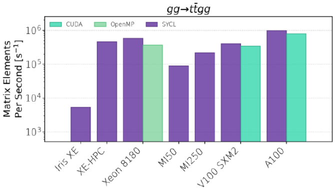
- off-load heavy computational components to GPU, i.e. HPC
  - $\hookrightarrow |\mathcal{M}|^2$ evaluation naturally parallel task
  - $\hookrightarrow$ natural habitat for AI applications
- currently pursued by SHERPA and MADGRAPH collabs

SHERPA/PEPPER event rate $t\bar{t} + ng$



[Bothmann et al. SciPost Phys 17 (2024) 081]

MADGRAPH on GPU, SIMD-CPU



[Hagenböck et al. EPJ Web Conf 295 (2024) 11013]

- achieve enormous hard-event simulation throughputs
- novel work flows & event formats [Bothmann et al. PRD 109 (2024) 1]
  - $\hookrightarrow$ need to adjust MC production software, e.g. Key4HEP

MC developer landscape

MC developer landscape

- Monte Carlo development historically largely centred in Europe
- MCnet Monte Carlo developer network
  $\hookrightarrow$ three EU funded training networks ('07-'22)
  $\hookrightarrow$ $\mathcal{O}(30)$ PhDs, $\mathcal{O}(100)$ short-term students, annual school
  $\hookrightarrow$ collaboration still active, organize annual MCnet school
- new CERN-LPCC working group, HEP Software Foundation
- strong involvement of German community (BMBF & DFG)

Herwig, Sherpa, Pythia
Whizard, MadGraph
Helac, PowHEG

LPCC
LHC Physics Centre at CERN

HSF
HEP Software Foundation

Theory expectations via Monte Carlo generators

- MCEG indispensable for the planning of future experiments
  $\hookrightarrow$ bridge gap between theoretical ideas & actual experiments
- strategic research programme at theo/exp/cs interfaces
  $\rightsquigarrow$ perturbative & non-perturbative methods, collider pheno
  $\rightsquigarrow$ innovative computational algorithms & software
- small but critically important developer community
  $\rightsquigarrow$ continued support and training opportunities needed

SciPost | SciPost Phys. 16, 130 (2024)

Event generators for high-energy physics experiments

Abstract

We provide an overview of the status of Monte-Carlo event generators for high-energy particle physics. Guided by the experimental needs and requirements, we highlight areas of active development, and opportunities for future improvements. Particular emphasis is given to physics models and algorithms that are employed across a variety of experiments. These common themes in event generator development lead to a more comprehensive understanding of physics at the highest energies and intensities, and allow models to be tested against a wealth of data that have been accumulated over the past decades. A cohesive approach to event generator development will allow these models to be further improved and systematic uncertainties to be reduced, directly contributing to future experimental success. Event generators are part of a much larger ecosystem of computational tools. They typically involve a number of unknown model parameters that must be tuned to experimental data, while maintaining the integrity of the underlying physics models. Making both these data, and the analyses with which they have been obtained accessible to future users is an essential aspect of open science and data preservation. It ensures the consistency of physics models across a variety of experiments.

SciPost | SciPost Phys. 14, 079 (2023)

Machine learning and LHC event generation

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Prepared for submission to JHEP

Initial state QED radiation aspects for future e^+e^- colliders

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