

(Facilitating) Precision Physics at the LHC

Spotlight on Monte Carlo event generators

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GEFÖRDERT VOM



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für Bildung
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FSP ATLAS
Erforschung von
Universum und Materie



KISS

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The HEP trinity

Theory

relativistic QFT

quantum \rightsquigarrow non-deterministic

reference Standard Model \mathcal{L}_{SM}

hypothetical New Physics \mathcal{L}_{BSM}

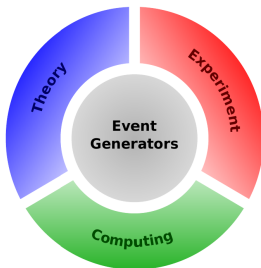
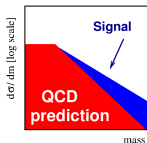
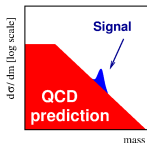
Experiment

multi-component detector

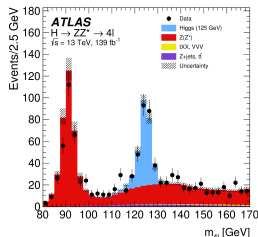
ATLAS, CMS, LHCb, ALICE, ...

reconstruction of events

operation, degrading, upgrades



[ATLAS EPJC 80 (2020) 942]



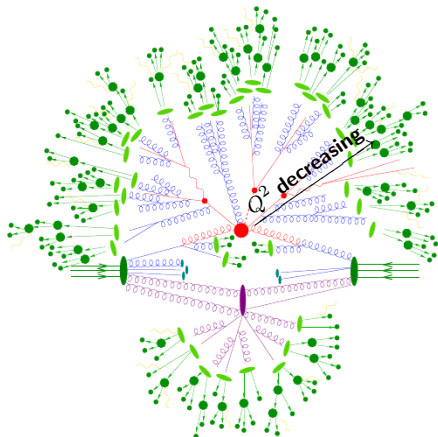
Simulation – emulating nature

particle-level event generation (theory)

detector-response simulation (experiment)

Monte Carlo Event Generators: the bigger picture

- perturbative methods
 - **Hard interaction**
exact matrix elements $|\mathcal{M}|^2$
LO, NLO, NNLO – QCD, NLO – EW
 - **Radiative corrections**
parton showers in the initial and final state
resummation of soft-collinear logs: LL, NLL
- non-perturbative models
 - **Multiple Interactions**
beyond factorization: modelling
 - **Hadronization**
parton-hadron transition
 - **Hadron Decays**
phase space or effective theories



German contributions to

- ↪ HERWIG [Gieseke], SHERPA [Siegert, S.]
- ↪ POWHEG [Jäger, Zanderighi]
- ↪ WHIZARD [Killian, Ohl, Reuter]
- ↪ **new** MADGRAPH [Plehn]

LHC exp. papers[†] MCEG citations

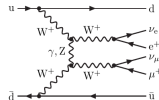
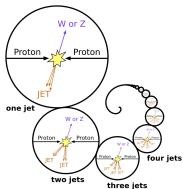
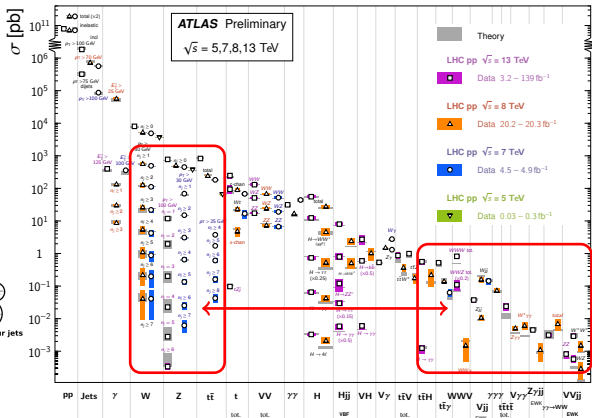
MCEG	ATLAS	CMS
SHERPA	60%	6%
HERWIG	36%	12%
MADGRAPH	55%	64%

[†] journal publ. since 2015 (A: ≈ 800 , C: ≈ 900)

Scrutinizing the Standard Model: physics challenges

Standard Model Production Cross Section Measurements

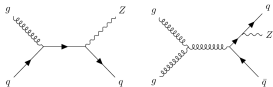
Status: February 2022



- rare & subtle electroweak signal processes
- multi-scale, high-multiplicity QCD backgrounds

Precision predictions meet precision experiments: $V+jets$

- wide range of kinematics



↪ multi-scale QCD problem

- omnipresent background

↪ huge samples required

↪ speed & efficiency essential

- case for ME+PS simulations

SHERPA-2.2.11

$pp \rightarrow l^+l^- + 0, 1, 2j @ \text{NLO} + 3, 4, 5j @ \text{LO}$

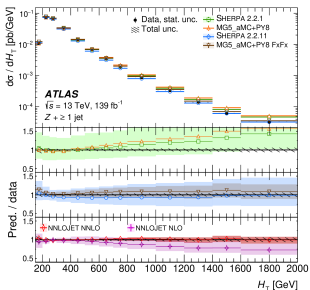
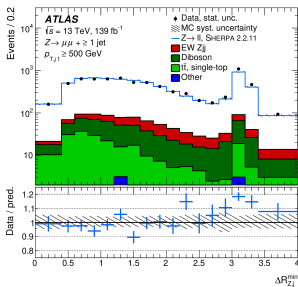
MG5_aMC+Pythia8 FxFx

$pp \rightarrow l^+l^- + 0, 1, 2, 3j @ \text{NLO}$

- Zj at NNLO QCD

[Gehrmann *et al.*, PRL 117 (2016) 022001]

[ATLAS JHEP 06 (2023) 80]

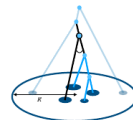
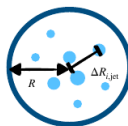


Precision predictions meet precision experiments: jets

Looking inside jets [Reichelt *et al.*, JHEP 7 (2021) 76 & JHEP 3 (2022) 131]

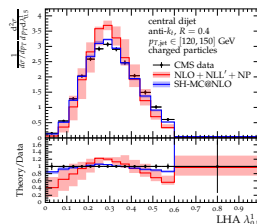
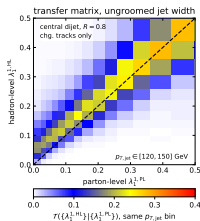
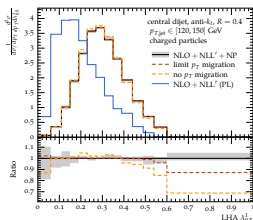
- analyse substructure of QCD jets in dijets & Z +jet at LHC
 - \rightsquigarrow probe intra-jet radiation pattern: tool to tag quark/gluon
 - \rightsquigarrow analytic resummed calculations within SHERPA framework

$$\lambda_{\alpha}^{\kappa} \equiv \sum_{i \in \text{jet}} \left(\frac{p_{T,i}}{p_{T,\text{jet}}} \right)^{\kappa} \left(\frac{\Delta R_{i,\text{jet}}}{R} \right)^{\alpha}$$



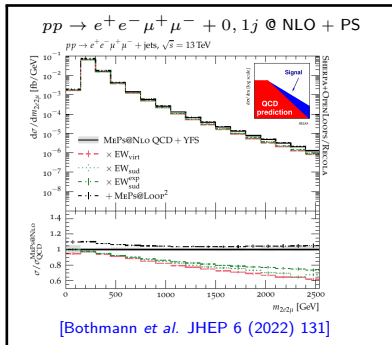
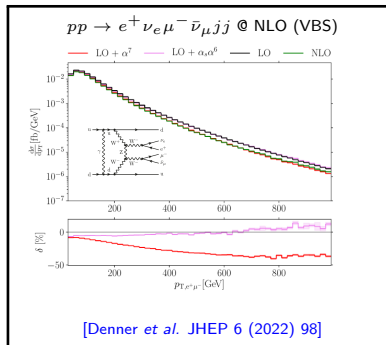
- NLO+NLL'+NP predictions to target CMS measurement

[Tumasyan *et al.* [CMS], JHEP 01 (2022), 188]



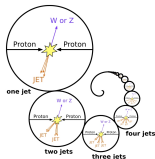
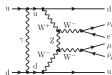
Account for (dominant) electroweak corrections

- naive power counting $\mathcal{O}(\alpha_s^2) \sim \mathcal{O}(\alpha_{EW})$
- automation of NLO EW & NLO SM calcs
 - \rightsquigarrow MEs e.g. RECOLA [Denner *et al.*] or OPENLOOPS [Pozzorini *et al.*]
- logarithmic enhancement in tails [Denner, Pozzorini, EPJC 18 (2001) 461]
 - \rightsquigarrow EW Sudakov logarithms within SHERPA & MG5_aMC [Bothmann, Napoletano, EPJC 80 (2020) 11] [Pagani, Zaro, JHEP 2 (2022) 161]

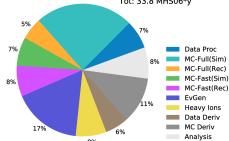


Computational bottleneck: the hard event component

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



ATLAS Preliminary
2022 Computing Model - CPU: 2031, Conservative R&D
Tot: 33.8 MHS06*yr



[CERN-LHCC-2022-005]

- ↪ $|\mathcal{M}|^2$ multi-modal, wildly fluctuating, expensive
- ↪ real- & virtual quantum corrections, IR subtractions
- ↪ Monte-Carlo phase space sampling [$\dim[\Phi_n] = 3n - 4$]

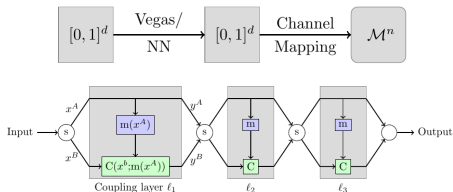
main research thrusts (towards HL-LHC)

- ↪ sustainable simulations on modern hardware (GPU)
[Bothmann *et al.*] [Carrazza *et al.*] [Mattelaer *et al.*]
- ↪ application of machine learning (ML), e.g.
ML sampling algorithms, NN surrogate unweighting



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

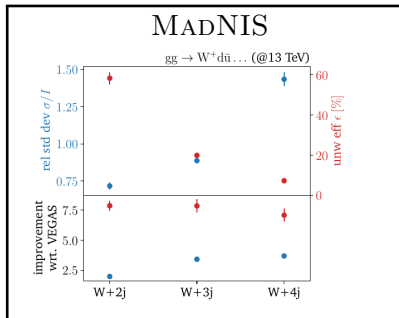
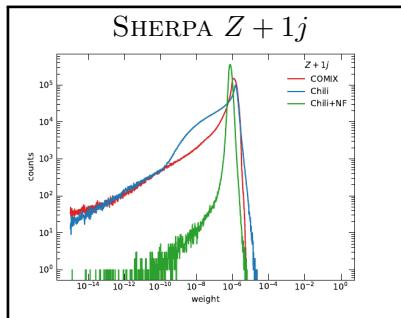
ML-assisted phase space sampling – closing in on production

- 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 & 2311.01548]



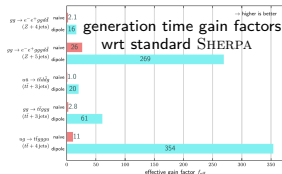
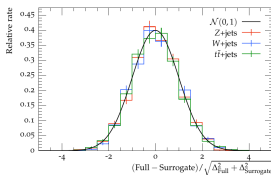
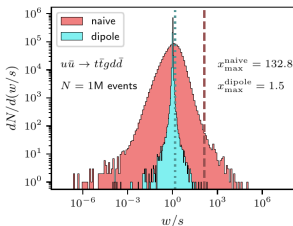
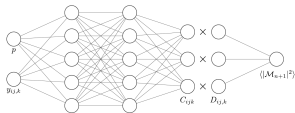
~> powerful integration/sampling method

~> 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 factorisation-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, with (approx) NLO EW corrections
 - ↪ polarised vector bosons [Zanderighi et al. 2311.10346] [Hoppe et al. 2310.14803]
 - ↪ development of improved showers (NLL accuracy)
 - ↪ better non-perturbative models [Gieseke et al.]
- innovative computational algorithms & software development
 - ↪ unbiased ML-augmented event generation for production
 - ↪ novel tuning and model calibration methods
 - ↪ massive parallelisation: GPUs, NHR compute centers
 - ↪ collaboration with other communities, e.g. KAT, KHuK, ...

Submitted to the US Community Study
on the Future of Particle Physics (Snowmass 2021)

Event Generators for High-Energy Physics Experiments

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 explored 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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