

Mareen Hoppe TUD University of Technology

RECENT DEVELOPMENTS IN MONTE CARLO EVENT GENERATORS







TECHNISCHE UNIVERSITÄT DRESDEN



INSTITUTE OF NUCLEAR AND PARTICLE PHYSICS



LHCP 2024 Boston, June 7 2024

MONTE-CARLO EVENTGENERATORS

... are essential for all branches of HEP:

- Collider experiments
- Neutrino physics ...

 provide fully realistic SM & BSM predictions usable by experiments to
 design analyses & detectors
 predict backgrounds
 unfold detector effects
 compare with theory predictions







Here: focus on most common event generators for LHC physics

[1]



















[3]

đ

MONTE-CARLO EVENTGENERATORS

Factorization of QCD

$$\sigma_{p_1p_2 \to X} = \sum_{i,j \in \{q,g\}} \int \mathrm{d}x_1 \mathrm{d}x_2 \underbrace{f_{p_1,i}(x_1,\mu_F^2) f_{p_2,j}(x_2,\mu_F^2)}_{\text{long distance}} \underbrace{\hat{\sigma}_{ij \to X}(x_1x_2,\mu_F^2)}_{\text{short di$$

Modular structure of event generators

Short distance interactions

Long distance interactions

Hard process

Parton shower

QED radiation

Hadronization

Hadron decays

Multiple interactions



C F. Siegert

HARD PROCESS

State of the art

• Automated NLO QCD & approximate NLO EW

Current challenges Precision • Speed / Efficiency



Fully differential NNLO matching N3LO matching

Polarized XS





POLARIZED CROSS SECTIONS FOR VECTOR BOSON PRODUCTION

- Probe for the electroweak gauge sector & electroweak symmetry breaking
- Measurement strategy: fully exclusive polarized XS from MC as fitting templates
- Established generators: PHANTOM & MadGraph5 @LO+PS
- **NEW:** Extension of SHERPA & POWHEG:
 - SHERPA: nLO+PS for arbitrary VB production processes [МН, М. Schönherr & F. Siegert 2023]
 - POWHEG: NLO+PS for inclusive diboson production [G. pelliccioli & G. Zanderighi 2023]



WZ production



More details? <u>MH Fri 11:36 AM</u>



[A. Ballestrero et al. 2008, 2017]

[D. Buarque Franzosi et al. 2020, M. Javurkova et al. 2024]

[G. Pelliccioli & G. Zanderighi 2023]

state	NLOPS	nLO+PS 37	$\frac{\text{nLO}+\text{PS}}{\text{NLOPS}} - 1$
full off-shell	34.04(5)	33.80(4)	-0.7%
unpolarised	33.30(5)	33.46(3)	+0.5%
$\mathbf{L}\mathbf{L}$	1.892(3)	1.902(2)	+0.5%
LT	5.140(7)	5.241(4)	+1.9%
TL	4.888(6)	5.002(4)	+2.3%
TT	21.16(3)	21.10(2)	-0.3%
interference	0.217	0.215	-0.9%

NLO QCD polarization effects strongly dominated by real corrections!

SIMPLER ALGORITHMS FOR MATRIX **ELEMENT GENERATION**

Chirality flow formalism

- Introduced in [A. Lifson, C. Reuschle & M. Sjodahl 2020], []. Alnefjord et al. 2020]
- -> Lorentz structure analogue to color flow picture
 - Recently extended to one-loop calculations [A. Lifson, S. plätzer & M. Sjodahl 2023]
 - Proof-of-concept in MadGraph5@NLO for QED: improvement up to factor 10 in $\,{
 m e}^+{
 m e}^ightarrow{
 m n}\gamma$ [A. Lifson, M. Sjodahl & Z. Wettersten 2022]
 - Most recent: implementation for QCD [E. Boman et al. 2023]
 - Performance improvements due to: simplified Lorentz structures gauge based Feynman/chirality-flow diagram removal due to clever choice of reference momenta / spin axes









$$\sigma^{\mu,\dotlphaeta}ar\sigma_{\mu,lpha\doteta}=2\delta^{\dotlpha}{}_{\doteta}\delta_{lpha}{}^{eta}$$

EVENTGENERATION ON MODERN ARCHITECTURES

- Current event generation codes written for traditional CPU+RAM model
- Computing architectures designed for data parallelism increasingly standard in data centers
- Improvements of at least one order of magnitude expected [E. Bothmann et al. 2021]

PEPPER

[E. Bothmann et al. 2023]

- Parallelized LO parton-level event generator in C++
- Color-summed Berends-Giele recursion, CHILI phasespace integration method [E. Bothmann et al. 2023]
- CUDA/kokkos for GPU portability, CPU parallization via MPI parallel performance







Madgraphs_aMC@NLO on GPUS

Process	Matrix elm	Total	Momenta+unweight	Matrix elm
$qq \rightarrow t\bar{t}qq$	Fortran	108.10± 0.27s	6.27± 0.41s	101.84± 0.14s
55 55	C++ AVX2	$31.08 \pm 0.01s$	$6.88 \pm 0.01 s$	$24.20 \pm 0.02 s$
		$3.48\pm 0.01\times$	$0.91\pm~0.06\times$	$4.21 \pm 0.01 \times$
	Cuda Tesla A100	$5.32 \pm 0.03s$ $20.32 \pm 0.13 \times$	$4.67 \pm 0.02s$ $1.34 \pm 0.09 \times$	$0.66 \pm 0.02 s$ 155.4 $\pm 2.7 \times$







[A.Valassi et al, 2023; S. Hageböck et al. 2023; Z. Wettersten et al. 2023]

• madgraph4gpu plugin: LO C++ MadGraph based on helicity amplitudes on GPUs & SIMDs -> GPU: ME-calculation, event re- & unweighting • Code generator for CUDA, SYCL output & for vectorized code using AVX2 extension for SIMDs

ML-ASSISTED EVENTGENERATION

Improving phase space sampling and unweighting efficiency

- <u>Problem</u>: VEGAS decreasing performance for complex final states / higher orders - bad unweighting efficiency
- Idea: ML for faster importance sampling & improved unweighting efficiency
- Much interest in last years: Generative Adversarial Networks, Normalizing & autoregressive Flows ... []. Bendavid 2017, M.D. Klimek & M. Perelstein 2020, C. Gao et al. 2020, S. Pina-Otey et al. 2020, B. Stienen & R. Verheyen 2020, M. Backes et al. 2020, E. Bothmann et al. 2021, ...]

Surrogate unweighting in SHERPA









MadNIS [T. Heimel et al. 2022, 2023]

Neural importance sampling



phase space mapping with Normalizing flows



State of the art

- LL accurate shower @ leading color
- Different types:
 - o dipole/antenna showers e.g. in SHERPA (default CS, Dire), HERWIG 7, PYTHIA 8 (default CS, Vincia, Dire)
 - angular-ordered shower in HERWIG 7

Good enough?



Good description of many observables Other observables with significant discrepancies between data & shower models / shower models it selves Influences many analyses e.g. via jet energy scale calibration







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Current challenges

- Improve underlying approximations:
 - NLL & NNLL accuracy
 - NLO showers
 - beyond leading color
 - NLL accurate NLO, NNLO & N3LO matching
 - quantum interference effects, spin correlations
 - new approaches: quantum computers, amplitude evolution ...
- Faster algorithms

uc parton shower for simulating QCD radiation at hadron colliders and Introduction to the PanScales framework, version 0.1 from an implementation in the event generator SHERPA. ALARIC provides Melissa van Beekveld¹, Mrinal Dasgupta², Basem Kamal El-Menoufi^{2,3}, Silvia Ferrario quantify certain systematic uncertainties which cannot be eliminated by Ravasio⁴, Keith Hamilton⁵, Jack Helliwell⁶, Alexander Karlberg⁴, Rok Medves⁶, Pier ower with analytic resummation. In particular, it allows to study recoil Francesco Monni⁴, Gavin P. Salam^{6,7}, Ludovic Scyboz^{3,6}, Alba Soto-Ontoso⁴, Gregory and collinear limits without the need to change the evolution variable or Soyez⁸, Rob Verheyen⁵ e assess the performance of ALARIC in Drell-Yan lepton pair and QCD jet he first multi-jet merging for the new algorithm.

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FERMILAB-PUB-24-0178-T, IPPP/24/20, MCNET-24-07

The Alaric parton shower for hadron colliders

Stefan Höche,¹ Frank Krauss,² and Daniel Reichelt²

¹Fermi National Accelerator Laboratory, Batavia, IL, 60510, USA ²Institute for Particle Physics Phenomenology, Durham University, Durham DH1 3LE, UK

A partitioned dipole-antenna shower with improved transverse recoil

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ABSTRACT: The implementation of a new final-state parton-shower algorithm in the PY-THIA event generator is described. The shower algorithm, dubbed APOLLO, combines cent ral aspects of the VINCIA antenna shower with the global transverse-recoil scheme of the ALARIC framework in order to achieve formal consistency with next-to-leading logarithmic (NLL) resummation. The shower algorithm is constructed in such a way that it facilitates a straightforward combination with fixed-order calculations. As an explicit proof of concept a general scheme for matrix-element corrections (MECs) and two separate multiplicative next-to-leading order (NLO) matching schemes are outlined. It is argued that both match ing schemes retain the logarithmic accuracy of the shower. The improved modelling of radiation is examined by contrasting the new algorithm with existing leading-logarithmic parton showers in Pythia.

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8 Rudolf Peierls Centre for Tl

Further NLL showers

Deductor [Z. Nagy & D. E. Soper 2020]

Manchester-Vienna []. R. Forshaw, J. Holguin & S. Plätzer 2020] Herwig 7 (angular ordered shower) [G. Bewick et al. 2019, 2021]

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LOGARITHMIC ACCURACY IN **PARTON SHOWERS**

• Parton showers connect hard-process high-energy scales O(TeV) & hadronization regimes O(1GeV)

During evolution large logarithms $L = \log Q / \Lambda$ appear

All-order resummation of large logarithms?

- + controlled formal accuracy, systematically extendable
- only one or few observables, for simple processes
- no exclusive events

analytical resummation should reproduce

for rIRC observables

• Criteria for NLL accurate parton showers @ leading color [M. Dasgupta et al. 2018, 2020] • standard dipole showers only LL accurate [M. Dasgupta et al. 2018] main problem: kinematic mapping





[A. Banfi, G.P. Salam & G. Zanderighi 2005]

- + very exclusive
- + non-perturbative effects easily accessible
- formal accuracy bad or unknown

parton showers

A LOGARITOR A LOGARITHMICALLY ACCURATE RESUMMATION IN C++ [F. Herren et al. 2022]

- Shower based on Catani-Seymour dipols
- Partial fractioning of eikonal [s. Catani & М. Н. Seymour 1997]
- full phase space coverage
- New global recoil scheme
 - <u>analytical</u> proof of NLL accuracy
- Evolution variable

ISR $t^{(n)} = 2E_j^2 (1 - \cos \theta_j^{\ i}) = v (1 - z) 2\tilde{p}_i \tilde{K}$

Inclusion of

 $W_{ik,j} = \bar{W}^i_{ik,j} + \bar{W}^k_{ki,j} ,$

 $t^{(K)} = 2E_j^2 \left(1 - \cos \theta_j^{\ i}\right) = \frac{v}{1 - v} \left(1 - z\right) 2\tilde{p}_i \tilde{K}$ FSR

• massive quark effects [B. Assi & S. Höche 2023] initial state radiation & LO multi-jet merging

Next steps to become "competitive" for LHC

- Spin correlations
- Sub-leading color
- effects

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- Implementation of NLO matching, merging
- Matching to light-flavor PDFs
- Beyond: NLO splitting kernels, Alaric@NNLL



APOLLO Antenna Partitioning Overcomes Logarithmically Limiting Obstacles [C. T. Preuss 2024]

- Antenna shower VINCIA with global recoil scheme from ALARIC
- Partitioned dipole antenna functions

$$P_{qg}(p_{i}, p_{j}, p_{k}; n_{j}) = \frac{1}{s_{ij}} \left[\frac{2s_{ik}(p_{i}n_{j})}{s_{jk}(p_{i}n_{j}) + s_{ij}(p_{k}n_{j})} + \frac{s_{jk}}{s_{ijk}} \right],$$

$$P_{gg}(p_{i}, p_{j}, p_{k}; n_{j}) = \frac{1}{s_{ij}} \left[\frac{2s_{ik}(p_{i}n_{j})}{s_{jk}(p_{i}n_{j}) + s_{ij}(p_{k}n_{j})} + \frac{s_{jk}s_{ik}}{s_{ijk}^{2}} \right]$$

$$K^{\mu} = -\sum_{k \in FS} p_{k}^{\mu} = \sum_{k \in IS} p_{k}^{\mu}$$

- Matrix element corrections in PS implemented
- Two multiplicative NLO matching schemes developed

Next steps to become "competitive" for LHC

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Differences to ALARIC

Evolution variable

 $t = (1-z)s_{ij} = z(1-z)2\tilde{p}_{ij}\tilde{K}$

PANSCALES SHOWERS

[<u>M. van Beekveld et al. 2022]</u>

Hadron collider PanGlobal showers

- Antenna showers
- Evolution observable v: $0 \leq eta_{PS} < 1$
- Recoil ||: conserved locally
- Recoil __: conserved globally

Hadron collider PanLocal showers

- Antenna & dipole showers
- Evolution observable v: $0 < eta_{PS} < 1$
- Dipole-local recoil
 - o dipole variant: emitter takes transverse recoil
 - antenna: transverse recoil
 shared by emitter & spectator

Included:

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sub-leading color effects IK. Hamilton et al. 2020, M. van Beekveld et al. 2022]
 soft & collinear spin correlations IA. Karlberg, et al. 2021, K. Hamilton et al. 2021, M. van Beekveld et al. 2022]
 first steps towards matching & NNLL accuracy IK. Hamilton et al. 2023 [M. van Beekveld et al. 2024]
 Published in PANSCALES framework IM. van Beekveld et al. 2023]
 interface to PYTHIA 8
 tests of logarithmic accuracy
 opportunity to implement & test own showers



VBF: pp->hjj

HADRONIZATION MODELLING



State of the art

- Actual connection from "pure theory" to measurable quantities
- No derivation from first principles
- ---> Based on phenomenological models
- --> Model parameters need to be tuned on data
 - Common models
 - cluster hadronization: SHERPA, HERWIG 7
 - string fragmentation: PYTHIA 8

why important?

- Many perturbative improvements: soft physics likely become limitation for more & more LHC measurements e.g. [M. Johnson & D. Maitre 2017], [M. Freytsis et al. 2018], [S. Argyropoulos & T. Sjöstrand 2014]
- High expected luminosity at FCC-ee @ Z-pole
- predictions surely limited by non-perturbative effects







C A. Siódmok



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Current challenges

- Improve existing string & cluster models
- Add / better understand new effects: colour reconnection, hadron spin, hadron rescattering, Bose-Einstein effects, rope hadronization ...
- Alternative models / application of ML methods
- Better tuning on more data (more than LEP)

More discussions also: J. Altmann Wed 11:18 AM & A.Beraudo Wed 2:18 PM









C A. Siódmok





BARYON CORRELATIONS



 Baryon correlations badly modeled in pp collisions (e+e- / meson correlation in pp 🖌) • QCDCR model for color reconnection additional baryon production mechanism, but less correlation improvement for opposite-sign pairs Hadronic rescattering & toy model for suppression of baryon production close to gluon kinks improves modelling for same-sign pairs aggravates model for opposite-sign pairs

Newer ALICE measurements: M. van Leeuwen Mon 9:30 AM









at QCD@LHC 202.



ML FOR HADRONIZATION

- Proof-of-principle studies: parts of cluster- / string fragmentation replaced with ML models
 - HERWIG: cluster decay by Generative Adversarial Network (GAN) model [A. Ghosh et al. 2022]
 - PYTHIA 8: string break by Conditional sliced-Wasserstein autoencoders [P. 1(ten et al. 2022]



- Training access to cluster/string-hadron assignments
 More recently: GAN model fitted on observable features []. Chan et al. 2023]
 currently restricted on clusters created from pre-confined
 - partons, pions in FS
 - -> Inclusion of hadron flavor in HadML v1 []. Chan et al. 2023]

permutation invariance



$$D_E(x) = F\left(\frac{1}{n}\sum_{i=1}^n \Phi(h_i, \omega_{D_\Phi}),\right)$$

Discriminator Deep Hadron kinematics



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CONCLUSION

H7

A lot of ONGOING WORK in ALL PARTS of









to reach

NEEDs of the HL-LHC & beyond!



More details?

Snowmass 2021 Event

<u>Generators report</u>

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thank you for your for your attention!

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Current challenges Precision • Speed / Efficiency

Fully differential NNLO matching

N3LO matching

Polarized XS





Impact beyond Particle physics

2071-2095 (RCP8.5)

"SIMPLE" OPTIMIZATIONS CAN HELP MUCH

Improved new event format [E.Bothmann et al. 2023]

- New event format LHEH5
 - allow for scalability of event production over many MPI ranks
 - optimize, extend to NLO QCD new format proposed in [S.Höche, S.Prestel & H.Schulz 2019]
- Large performance improvements:
 - consolidation of HDF5 data sets
 - collective I/O
 - stat calls to master rank limited





LHEHS event format LHE-like data format based on HDF5-HighFive

- LHE information collected in HDF5 data sets
- Established LHEF: based on XML
- HDF5: database-kind computing model

• rigid, but efficient in parallel workflows

Similar simple optimizations : Faster LHAPDF + simplified pilot runs ~ 40x speed up [E. Bothmann et al. 2022]



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[ALICE CERN-EP-2016-322]



Baryon correlations badly modeled in pp collisions
(e+e- / meson correlation in pp)
Modes of baryon production in string models:

diquark model
popcorn model

 Gluon participation (gluon kink) important for angular correlation











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[L. Lönnblad & H. Shah 2023] • Baryon correlations badly modeled in pp collisions (e+e- / meson correlation in pp) Modes of baryon production in string models: diquark model popcorn model • Gluon participation (gluon kink) important for angular correlation • QCDCR model for color reconnection additional baryon production mechanism, but less correlation improvement for opposite-sign pairs









HERWIG Proc at QCD@LHC 202.