Challenges for Monte Carlo generators

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Abstract. This contribution lists challenges of Monte Carlo event generators for future lepton, especially linear colliders. A lot of the recent development benefits from the achievements at the Large Hadron Collider (LHC), but several aspects are unique for lepton colliders like beam simulation, polarization, electroweak higher order corrections and resummed QED corrections. We will describe the status of multi-purpose event generators and specialized codes and outline the challenges for these tools until such a collider starts data taking.

1 Introduction

Monte Carlo (MC) event generators for lepton colliders (both electron-positron and muon colliders, but also photon colliders) are not conceptually different than for hadron colliders. They simulate a hard scattering process in an order of perturbation theory as high as possible, however, they are dominated by QED and electroweak instead of QCD corrections, and hence theoretical uncertainties due to large scale variations are (almost) not present. Parton distribution function (PDF) uncertainties are either not present or can be perturbatively estimated. QCD parton showers and hadronization proceed in the same as at the LHC, however without multiple interactions and underlying event (though there are overlays from the bunch structures). In the following sections, we will discuss first discuss the simulation of beam spectra in Sec. 2, then hard matrix elements and the treatment of initial-state radiation in Sec. 3, parton showers, matching and hadronization are briefly reviewed in Sec. 4. The next Sec. 5 deals with specific processes that need a specialized treatment and sometimes specialized tools; in Sec. 6 we quickly discuss simulation of BSM processes, while in Sec. 7 we review phase space sampling, performance issues and parallelization, before we conclude.

This review is oriented along the lines of the ECFA Higgs-Top-Electroweak Factory studies, carried out 2022–2024, and the developments of MC generators there: according to this study, the focus here is on the the three multi-purpose multi-leg generators Madgraph5_aMC@NLO (MG5) [1], Sherpa [2, 3] and Whizard [4, 5], the two multi-purpose shower/hadronization programs Herwig [6, 7] and Pythia6/8 [8–10], and the specialized tools BabaYAGA [11], BHLumi/BHWide [12, 13], and KKMC [14]. An excellent overview is given in the input document for the US Snowmass Community Study [15]. Many interesting details on the simulation of the complete SM processes for ILC can be found in [16]. Details on the simulation can also be found in the conceptual or technical design reports of the electron-positron and muon colliders [17–23].

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2 Beam spectrum simulations

High-luminosity lepton colliders exhibit beamstrahlung, radiation from the bunch of electrons (or positrons) in the electromagnetic field of the approaching other colliding, highly collimated bunch. For synchrotrons, this effect is much less severe for the colliding bunches, and a Gaussian-shaped beam energy spread is mostly sufficient. Gaussian beam spreads are available in most Monte Carlos like e.g. KKMC, Pythia8, and Whizard. To cover a bit more features is possible by approximating the beam spectra by smeared delta-peak like structures with power-law tails, making the assumptions that the beam spectrum of the two lepton beams factorizes into two multiplicative components. This approach has been codified in the tool CIRCE1 [24] that was used for the simulations of the TESLA linear collider project. This approach is available in KKMC, MG5 [25], and Whizard, with slight variations in the parameterization. However, it has been shown that for ILC and drive-beam accelerators like CLIC, plasma accelerators like HALHF as well as photon colliders, such a parameterization is insufficient, as both the peak structure has a very complicated shape and also the tails do not exhibit simply a power-like behavior. Here, an MC generator based on a two-dimensional histogrammed fit to accelerator spectra simulated by tools like Guinea-Pig or Cain is used for the beam spectrum simulation within the event generator. Due to their limited statistics, a special smoothening has to be applied to avoid artifacts. Also the peaked parts of the spectra close to the full energy have to be special-cased in order to avoid unphysical beam energy spreads. This is realized in the CIRCE2 algorithm in the Whizard generator, where spectra for CEPC, CLIC, and ILC are available, while the FCC-ee spectra will be made available soon. Note that besides the e^+e^- components of the spectra, also the $e^+\gamma$, γe^- and $\gamma\gamma$ components are very important, especially for linear colliders ($\gamma\gamma$-induced backgrounds).

Further developments in the future comprise the first realistic spectra for plasma-driven accelerators like HALHF or energy-recovery LINACs (ERLs), the 3-dimensional structure of beam spectra, especially their dependence along the beam axis (e.g. using so-called copulas), and the use of advanced machine learning algorithms for the fitting of beam spectra from accelerator simulation tools.

3 Hard matrix elements and resummation of initial-state radiation

The structure of hard scattering amplitudes from the (multi-leg) matrix element generators are very similar to the corresponding LHC amplitudes. These are available at leading (LO) and next-to-leading order (NLO) fully automatized, and rely on recursive algorithms, cf. e.g. [26]. A comparison for multi-leg EW production processes at the LHC can be found e.g. in [27]. Obviously, compared to the LHC NLO QCD corrections are of minor importance as they do not lead to order-of-magnitude changes due to large scale variations. NLO electroweak (EW) corrections dominate due to phyics processes dominated by the EW resonance production. Examples for NLO QCD corrections to basically all important processes can be found in [1, 28–30], while examples for NLO EW corrections can be found in [31–33]. This has been made possible by the vast amounts of progress at the level of one-loop (matrix-element) providers like GoSam [34], MadLoop [1], Openloops [35, 36] and Recola [37], using the BLHA interface [38, 39]. Automated subtraction schemes like Catani-Seymour (CS) [40] and Frixions-Kunszt-Signer (FKS) [41, 42] take care of the numerical cancellation of infrared singularities in four spacetime dimensions where the MC integrations are performed. Generic subtraction schemes for at least QCD at the NNLO level are under active development.

The second major bottleneck to go to NNLO besides the automated NNLO subtraction, is the evaluation of two-loop master integrals which for EW processes at e.g. ILC or FCC-ee contains several different mass scales, and the frontier lies at 4- and 5-point functions with two different mass scales. First baby steps towards tools for simple processes like $e^+e^- \to ZH$ (on-shell) have started, but it will take a still many years until that is nearly as mature as for NLO. There is another bottleneck, which is unavoidable for fixed-order NLO or NNLO calculations, namely the appearance of negative-weight events which makes sending them to a (fast) detector simulation computationally extremely expensive. This is, of course, well-known from NLO and NNLO QCD MC simulations at the LHC, but plagues NLO QCD and NLO EW calculations at lepton colliders in the same way. This has been shown to apply especially to the top threshold simulation which will be described below in Sec. 5.

To achieve permil-level precision on total cross sections and differential distributions, the resummation of soft and collinear photon radiation in the initial state is mandatory. This has started from the soft-collinear resummation to all orders [43], with the inclusion of hard-collinear photons up to second [44] and third order [45]. In general, there are the two options to use either collinear factorization resumming collinear logarithms (at leading logarithmic (LL) [46] or next-to-leading logarithmic (NLL) accuracy [47–49]) or eikonal factorization resumming soft logarithms (also called YFS exponentiation [50–52]). In an ideal world, both types of logarithms have to be combined to achieve the highest possible precision. While there is an algorithmic procedure to improve YFS exponentation (which also can generate exclusive, though mostly soft, photons) by hard-collinear corrections, collinear factorization seems to be better suited for combination with higher fixed-order calculations of the hard process. Very likely, each of the methods has its own benefits and which is better suited for what processes needs to be studied in the future. For a nice summaries on these topics, cf. also [53, 54].

It should not be forgotten that the simulation of polarized processes (both in the initial state, but also in the final state for polarized event samples) is a must for the physics program of linear lepton colliders. The most general formalism here is based on spin-density matrices which allow arbitrary polarizations in the initial state, e.g. both longitudinal and transversal polarization of lepton beams.

4 Parton showers, matching, and hadronization

Parton showers resum large logarithms and provide exclusive multi-jet events; again, parton showers have profited tremendously from two decades of developments for LHC. This has driven the development of (final-state) showers that are accurate at NLL order, and hence include effects from color and spin correlations beyond the quasi-classical approximation of independent emissions. Examples of these are [55–58]. These showers are available for jet distributions at linear colliders and have been e.g. applied to hadronic Higgs events at future lepton colliders [59] or reapplied to LEP data [60]. For lepton colliders, QED showers, and for high-energy linear lepton colliders like ILC and CLIC also electroweak showers do become important. These are mostly realized as interleaved showers where the QED/EW suppression of emissions from quarks by a factor of α/α_s $1/15$ is dealt with by a combination of rejection and reweighting algorithms. For EW showers, the question of EW fragmentation of inclusive W/Z/H radiation into especially hadronic jets with jet masses around the EW resonances will become important. Techniques and algorithms to match fixed-order calculations to exclusive all-order showers have been developed for hadron colliders for LO (matrix element corrections in parton showers) to NLO – MC@NLO, POWHEG [61], CKKW(-L) – to NNLO (MiNNLOPS, UnLLOPS etc.) and even NNNLO, while consistently merging samples of exclusive jet multiplicities into inclusive multi-jet merged samples have been developed for the LHC. These techniques can be straightforwardly carried over to lepton colliders like ILC and CLIC. While the corresponding matching of photon emission (and lepton pairs) with (N)NLO EW corrections is in principle straightforward, the complete automation is still work in progress and will only be available in the future. A matching schemes at LO for matrix element and shower photons can be found in [62].

Hadronization is still based mostly on phenomenological models, either on Lund string fragmentation or the cluster hadronization paradigm. Machine-learning methods aim at simulating hadronization from trained real data event samples, which might result in realistic hadronic event generation, but, however, does not enhance our knowledge about the underlying QCD physics. There are speculations that samples of up to 200 ab^{-1} of very clean jet samples from e.g. FCC-ee might necessitate the development of new formalisms for our understanding of hadronization in order to understand the data.

5 Special processes and dedicated tools

There are several processes that exhibit special properties, (i) two-fermion production $e^+e^- \to f\bar{f}$, (ii) Bhabha scattering $e^+e^- \to e^+e^-$, two-photon production $e^+e^- \to \gamma\gamma$, (iii) photoproduction of low-p_T hadrons, (iv) the WW threshold, (v) the top threshold. The first two are important for high-precision luminometry, where linear colliders favor Bhabha scattering as the lumical and beam calorimeter allow to measure much more inclusive to very small angles. Matching the projected experimental precision of $10^{-4} - 10^{-5}$ theoretically is very challenging and needs a dedicated implementation of complete EW two-loop corrections and leading three-loop corrections together with resummation of all available soft and collinear logarithms. This has been achieved in dedicated tools like BabaYaga, BHLumi and BHWide. The photoproduction of low-p_T hadrons is one of the largest background processes especially in the central region and for high-energy versions like CLIC. Its simulation is based on fits to total cross section measurements from the CrystalBall experiment, while the hadronization for low effective center-of-mass energies is dominated by pion and kaon production. A special implementation exists e.g. in Whizard. For the WW threshold a very precise determination of the W mass necessitates the resummation of QED logarithms which can be added to a fixed-order calculation. More complicated is the top threshold where inclusive results are available at NNNLO NRQCD that will allow an extraction of the top mass from the threshold scan at the level of 30–50 MeV uncertainty. For the study of experimental acceptances and systematic uncertainties, this has to be included in an exclusive MC, which can be achieved at level of NLL matched to NLO NRQCD [63, 64]. Carrying this over to NNLL matched to NNLO would be desirable, but will be a major undertaking.

6 Simulation of beyond the Standard Model physics

Also the simulation of BSM processes builds upon 15 years of development for LHC BSM simulations, relying on Lagrangian-level tools like SARAH [65], LANHep [66] and FeynRules [67], that are connected to MC simulations via dedicated interfaces like e.g. in [68]. These tailor-made interfaces that have to be engineered for every pair of these tools with each MC generator. They have become redundant through the introduction of a python-syntax based meta-layer within the Universal Feynman Output (UFO) interface [69, 70]. For lepton colliders like the ILC and CLIC especially models with light EW particles like in extended Higgs sectors, axions and axion-like particles (ALPs), heavy neutral leptons etc. are very important. In addition, deviations of the SM are parameterized in terms of effective field theories like SMEFT or HEFT, which are available as well for such simulations. There are many attempts to carry these simulations over to NLO; for NLO QCD this is possible for most of these models as mandated to achieve a decent precision for LHC signal simulations; for NLO EW calculations this is much harder to achieve generically as proper renormalization schemes have to be available which can very likely never be fully automatized. Also colorful exotics are available, in direct production processes for the LHC or in terms of EFT operators for ILC/CLIC as they appear in Higgs portal and dark sector models. Details on their implementation based on the color-flow formalism can be found e.g. in [71, 72].

7 Phase space, parallelization and performance

Physics simulations are computationally costly, especially at NLO and NNLL. As lepton colliders like ILC and CLIC (or CEPC and FCC-ee) exhibit processes that are dominated by EW resonances, simulation usually is classified by the number of the fermions in the final state: $e^+e^-/e\gamma/\gamma\gamma \to 2f, 3f, 4f, 5f, 6f, 7f, 8f, \ldots$. These processes can become very costly with tens of thousands of phase space channels already at LO, but much more so at NLO. This already shows that phase spaces become much more complicated at lepton colliders with many intertwined electroweak production channels connected by (EW) gauge invariance compared to phase spaces dominated by soft-collinear QCD radiation phenomena at the LHC. Such processes need to be sampled in parallel and event generation needs to be treated parallelized as well. The latter is always trivially achievable as bundles of events can be generated on different nodes of large computer farms. There are straightforward algorithms for parallelized matrix element evaluation, e.g. parallelizing over the helicities of external particles (2^n for n external fermions) or the parallelization of color flows over different threads in hyper-threading. Phase space adaptation is much more complicated: not only need random number chains be independent on different nodes (as for event generation) but also correlations between different parts of the phase-space adaptation need to be taken into account. One example which shows speed-ups of 30–50 is the parallelization of multi-channel adaptive VEGAS-type phase space sampling using the message-imaging protocal (MPI) [73]. Also, the usage of GPUs for matrix-element evaluation as well as phase-space sampling shows interesting speed-ups, and there are attempts in all three multi-purpose generators MG5, Sherpa and Whizard [74–76]. Further interesting developments is the phase-space sampling using machine-learning techniques like invertible neural networks, normalizing flows or autoencoders, which is left out here for the sake of space.

8 Summary and outlook

MC generators for lepton colliders (electron-positron and muon colliders) build upon two decades of development for LHC: these have culminated in the automation of NLO QCD and NLO EW calculation for arbitrary multi-leg processes. While this is almost trivially carried over for NLO QCD, for NLO EW it is tremendously complicated due to the combination with the numerically demanding NLL QED PDFs. Future studies will show which processes and energies are in the regime of collinear radiation or of soft radiation which is simulated in the YFS formalism. Another future task is a universally applicable matching formalism between fixed-order and resummed calculations with exclusive radiation simulations and QED showers. This is mandated to achieve permil precision for both inclusive and exclusive predictions. Very high-energy lepton (especially muon) colliders might call for a full EW/SM collinear factorization using EW PDFs and corresponding EW fragmentation functions, which will be a very interesting field of research in the future. The inclusion of beam spectra are important for the full simulation of physics processes for the future experiments at lepton colliders. It has been shown that the most powerful is a two-dimensional histogrammed fit to beam spectra, that allows to properly describe synchrotrons like CEPC and FCC-ee, RF-based accelerators like ILC and C3, drive-beam accelerators like CLIC, plasma accelerators like HALHF and even photon colliders. Parton showers have matured in the LHC era, being available at NLL now, given access to non-trivial color and spin correlations, and will likely be carried to full NNLL in the future. Hadronization models might have to be rethought in an era with gigantic samples of very clean hadronic data from the Z pole. BSM simulations profit again from the LHC developments, and are available for multi-purpose MCs for almost arbitrary BSM models using Lagrangian-level tools connected to MCs via the UFO2 python layer. A challenge will be EW NLO corrections in arbitrary BSM models, as they always depend on the availability of appropriate renormalization schemes. There are several processes that need special treatment either because they are needed at a much higher theoretical precision than the rest or they are very delicate in terms of soft and collinear divergencies. These processes are very often described by dedicated tools, while sometimes multi-purpose generators contain specialized treatments of such processes. Examples are processes for luminometry, the WW and top threshold and photon-induced production of low-p_T hadrons. MC simulations have been understood as one of the computational bottlenecks of the data analysis at the LHC, and this still remains true at lepton colliders, especially at Tera-Z. Active areas of research are phase-space sampling improvements based on either adaptive multi-channel versions of VEGAS or machine-learning methods based on e.g. normalizing flows. Another very active field is the usage of heterogeneous computing where parts of the simulation remains on traditional CPU farms and parts are off-loaded to GPUs.

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