

PHOTOS Monte Carlo and its theoretical accuracy

Z. Wąs^{a,b}, P. Golonka^a, G. Nanava^{c,d}

^a CERN, 1211 Geneva 23, Switzerland

^b Institute of Nuclear Physics, PAN, Kraków, ul. Radzikowskiego 152, Poland

^c Universitaet Bonn, Physiklisches Institut, Nussallee 12, 53115 Bonn, Germany

^d On leave from IHEP, TSU, Tbilisi, Georgia

Because of properties of QED, the bremsstrahlung corrections to decays of particles or resonances can be calculated, with a good precision, separately from other effects. Thanks to the widespread use of *event records* such calculations can be embodied into a separate module of Monte Carlo simulation chains, as used in High Energy Experiments of today. The PHOTOS Monte Carlo program is used for this purpose since nearly 20 years now. In the following talk let us review the main ideas and constraints which shaped the program version of today and enabled it widespread use. Finally, we will underline importance of aspects related to reliability of program results: event record contents and implementation of channel specific matrix elements.

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1. Introduction

In the construction of complex modular simulation systems, as the one used in High Energy Physics, the question of dividing the system to functional parts is essential. In the modular approach, the problem can be divided into parts, and each part can be addressed by different researchers or teams. However, such approach is only possible if the mathematical structure of the problem have certain algebraic properties.

In practice, the module-based work model is often an idealization: creating scientific software can not be separated from the research itself. As a consequence, the architecture of programs needs to be modified at various steps of projects development, for example to accommodate more precise models.

Another class of difficulties in the development of a simulation segment arise from the constraints, imposed by other segments of the large project, namely in the definition of data structures and interfaces.

Finally, the demands of the end-users, their expertise in handling simulation blocks (which is often limited) and understanding the conceptual models used are of critical importance.

These types of difficulties are quite universal for

any complex, scientific problem. In the following let us concentrate on a relatively simple model (yet already quite sophisticated) for the simulation of QED radiative corrections in decays, and the corresponding simulation package PHOTOS [1,2,3,4]. We believe that presented “development drama” can be of interest not only to the readers interested in QED bremsstrahlung, but also in general case. In this respect our presentation can be understood as a summary and invitation to reading [5]. With respect to previous [6] longer version of the presentation let us point on the particular property of the simulation of decays and in particular necessary in that step radiative corrections. Functionality of such modules in some cases can be attributed to the physics of hard processes but in the other ones to the periferic ones, often to be used to measure spin states of the decaying particles. In the second case lower energy experiments provide invaluable framework necessary to evaluate systematic error for high energy applications. Finally such simulation modules need to match (directly or with the help of tests) the ones of low energy e^+e^- experiments.

Our contribution is organized as follows. We start with the presentation of the PHOTOS algorithm in section 2. We highlight the role of the event record in

program's construction. We will also specify those properties of event record that are necessary for the program precision.

Section 3 is devoted to the description of recent years' developments in the PHOTOS algorithm, which lead to the improvement of its performance, but at the same time introduced more strict constraint on the event record used as a data source. We will present our efforts in preventing the complications for other users of data structures.

During the years of project's evolution special techniques devoted to detect and resolve various types of difficulties related to event record(s) were developed. Section 4 will be devoted to their presentation. Internal instrumentation utilities of PHOTOS: debugging subroutine PHLUPA and kinematic rounding error correction subroutine PHCORK will be discussed. Then, MC-TESTER [7] will be briefly presented. Finally, we will justify the need to duplicate the event information which is originally stored in a standard event record HEPEVT.

Section 5 will be devoted to the discussion of the issues related to event record standardization. The question of porting the algorithm to C++ - the process technically completed in 1999 - [8] will be covered in that section as well. We will stress the important, yet often ignored, aspect of event record construction: the structure must not only be convenient and flexible from the software engineer point of view, its contents must also be clear, from the point of view of involved physics models, to the end-users processing the data produced by Monte Carlo event generators. This is particularly important if extensions of the standards are to be not only proposed but also used.

The summary, Section 6, closes the paper.

2. Basic design of PHOTOS

Already at an early step of preparation for the τ -lepton polarization measurement at LEP1 it became evident [9], that bremsstrahlung corrections in τ decays are necessary for proper modeling of theoretical predictions for measurement of the Z boson couplings using τ -polarization. For that purpose, special routine RADCOR was designed. With certain probability it was replacing the decay products of τ simulated using TAUOLA [10] by the ones with an extra photon added. This action was performed in a strict environment of

the explicit list of momentum four-vectors and in the rest-frame of τ . In fact, the parameter defining the actual decay mode of τ was also passed into RADCOR, identifying the physical process.

The τ decay products, modified in such way, were passed into the TAUOLA interface to KORALZ [11], which was the Monte Carlo program for τ pair production at LEP1 energies.

This awkward, yet useful, design was only tailored for a single application, and was missing the documentation. The limits of its reliability were not explored at all. Indeed, the fact that it could properly simulate the leading-log parts of the first-order corrections was enough. The issues of dependence on the choice of the gauge were not risen, nor were the question of the phase-space coverage.

However, this exercise provided an important observation: to simulate the dominant part of QED corrections it is sufficient to search through the full event structure, identify the branchings corresponding to elementary decays of some particles, extract the information describing all decay products, and apply a routine such as RADCOR. In the early 90's and late 80's the HEPEVT event record was providing the complete environment that could allow for extension in use of RADCOR routine. The first version of PHOTOS [1] was created. Its design relied heavily on the assumption that the HEPEVT event record hosts a tree-like structure and that all pointers to decay products (daughter pointers) and origins (mother pointers) are defined and consistent. At each decay splitting the energy-momentum conservation was supposed to be fulfilled exactly, even if only with a single-precision computer arithmetics level.

The PHOTOS generator gained popularity, and in the documentation of its 1994 version [2] a multitude of tests were presented for physical processes for which the theoretical predictions were available. The corrections for double bremsstrahlung were added as well. Further development was stalled due to limited interest in improvements, expressed by experimental users.

3. Toward high precision in PHOTOS

Already in [2] it was found, that if the algorithm for the single-photon generation is properly iterated, the leading corrections of the double-photon emis-

sions can be incorporated as well. In [3] this iterative solution was extended to multiple-photon emission and the tests for leptonic Z decays have shown that this solution reproduce the results for the final-state bremsstrahlung of the KKMC Monte Carlo program [12] with amazing precision. Few years earlier, other tests and extensions important for Higgs or W decays were introduced also [13]. The good performance of the program was related to other improvements, introduced at that time and valid for all decays. For example the implementation became exact in the soft-photon limit. These improvements, however, are of limited importance from the point of view of software organization of PHOTOS interface with other packages.

Let us now concentrate on another class of corrections, discussed in refs. [4,14] and corresponding to the implementation of the exact, first-order matrix-element kernel in bremsstrahlung correction generation for $Z \rightarrow l^+l^-$ and $B \rightarrow K(\pi)K(\pi)$ decays. In the latter case, all possible combinations of charges and the replacement of π with K were used.

Let us start with the presentation of the numerical results of the test for $Z \rightarrow \mu^+\mu^-$ decays taken from ref. [4].

For that purpose we have to analyze the plots giving largest discrepancies between PHOTOS (run with standard options) and KKMC (run with second order matrix element and exponentiation). The plots presenting the invariant mass of the $\mu^+\mu^-$ pair and the invariant mass of the two hardest photons for the events with at least two photons of energies above 1 GeV in the rest frame of the Z are convenient for that purpose. The rates for the event samples predicted by the two programs are given in the figure's caption. The agreement between KKMC and PHOTOS is better than 0.1 % (if calculated with respect to the total Z decay rate), yet the differences are still visible from the results of simulations with 10^8 events. If, as in figure 2, the complete NLO kernel is activated in PHOTOS, the differences get reduced by about a factor of 50! This is rather interesting result of ref. [4].

At this point it is important to realize what is the price to pay for such improvement. Certainly, it is not the computer time - it remains small and the samples of order of 10^9 could easily be simulated overnight (PHOTOS is in fact significantly faster than KKMC). To answer this question one has to recall the formula for

the final Monte Carlo weight in PHOTOS.

Let us write (separated from the phase-space Jacobians) the explicit form of the real-photon matrix element, as used in the standard version of PHOTOS (as published in [1,2]) for the $e^+e^- \rightarrow Z^0/\gamma^* \rightarrow \mu^+\mu^- (\gamma)$ process:

$$X_f^{\text{PHOTOS}} = \frac{Q^2 \alpha (1-\Delta)}{4\pi^2 s} s^2 \frac{1}{k'_+ k'_-} (1 + (1-x_k)^2) \left\{ \begin{aligned} & \frac{1}{k'_-} \left[\frac{d\sigma_B}{d\Omega} \left(s, \frac{s(1-\cos\Theta_+)}{2}, \frac{s(1+\cos\Theta_+)}{2} \right) \right] \frac{(1+\beta\cos\Theta_\gamma)}{2} \\ & + \frac{1}{k'_+} \left[\frac{d\sigma_B}{d\Omega} \left(s, \frac{s(1-\cos\Theta_-)}{2}, \frac{s(1+\cos\Theta_-)}{2} \right) \right] \frac{(1-\beta\cos\Theta_\gamma)}{2} \end{aligned} \right\}$$

where $\Theta_+ = \angle(p_+, q_+)$, $\Theta_- = \angle(p_-, q_-)$,

$\Theta_\gamma = \angle(\gamma, \mu^-)$ is defined in (μ^+, μ^-) -pair rest frame.

For its calculation (with respect to Born cross-section) it is enough to know the four momenta of the Z and its decay products. In the presented formulae we follow the notations from refs. [4,15]. This expression is to be compared with the exact one, taken from ref. [15]:

$$X_f = \frac{Q^2 \alpha (1-\Delta)}{4\pi^2 s} s^2 \left\{ \begin{aligned} & \frac{1}{(k'_+ + k'_-)} \frac{1}{k'_-} \left[\frac{d\sigma_B}{d\Omega}(s, t, u') + \frac{d\sigma_B}{d\Omega}(s, t', u) \right] \\ & + \frac{1}{(k'_+ + k'_-)} \frac{1}{k'_+} \left[\frac{d\sigma_B}{d\Omega}(s, t, u') + \frac{d\sigma_B}{d\Omega}(s, t', u) \right] \end{aligned} \right\}.$$

The resulting weight is rather simple, and reads:

$$WT_1 = \frac{\frac{d\sigma_B}{d\Omega}(s, t, u') + \frac{d\sigma_B}{d\Omega}(s, t', u)}{\left[(1+(1-x_k)^2) \frac{d\sigma_B}{d\Omega} \left(s, \frac{s(1-\cos\Theta_+)}{2}, \frac{s(1+\cos\Theta_+)}{2} \right) \right] \frac{(1+\beta\cos\Theta_\gamma)}{2} \left(1 + \frac{3}{4} \frac{\alpha}{\pi} \right)},$$

$$WT_2 = \frac{\frac{d\sigma_B}{d\Omega}(s, t, u') + \frac{d\sigma_B}{d\Omega}(s, t', u)}{\left[(1+(1-x_k)^2) \frac{d\sigma_B}{d\Omega} \left(s, \frac{s(1-\cos\Theta_-)}{2}, \frac{s(1+\cos\Theta_-)}{2} \right) \right] \frac{(1-\beta\cos\Theta_\gamma)}{2} \left(1 + \frac{3}{4} \frac{\alpha}{\pi} \right)}.$$

For its calculation the numerical value of the electroweak couplings of Z to fermions, as well as information on the state from which the Z was produced is nonetheless necessary. This seemingly trivial requirement puts new requirements on the event record: the details of the process of the Z productions need to be coded in the event record, then correctly deciphered by PHOTOS to calculate the process-dependent

weight. From our experience this requirement of PHOTOS may be difficult to accept by other users of event records. The authors of event generators often choose their own conventions in encoding the details of hard process such as $q\bar{q} \rightarrow n g Z/\gamma^*; Z/\gamma^* \rightarrow \mu^+ \mu^-$ into the event record.

The NLO solution for PHOTOS would therefore be feasible with some universal, *standard* event record, nonetheless difficult due to practical issues of interfacing. However, the NLO precision in PHOTOS for today and tomorrow experiments is most likely not required. For the time being the problem remain rather academic. That is why we recommend the users to remain with the program version as distributed since October 2005. Only the users interested in special tests and in particular incorporation of decay channel dependent electromagnetic formfactors are advocated to incorporate further optional changes. In such a case even larger care on event record content is required.

In ref [14], we presented similar modifications in the PHOTOS kernel for the decay of B mesons into a pair of scalars. The implementation of the exact (scalar-QED only) kernel brings a minuscule improvement in the agreement between PHOTOS and the reference exact simulation of SANC [16]. In this case both: SANC and PHOTOS are used to simulate single photon emission (There exists no reference simulation with which the multi-photon version of PHOTOS could be compared.).

The way to play with form-factors, originating from phenomenological models, and fits to the experimental data is open now.

4. PHOTOS debugging tools

During the years of PHOTOS development, various software-related problems needed to be faced by its authors. The majority of the workload (and actual lines of code) needed to be devoted to the treatment of the data stored in a “standard” HEPEVT event record.

In an ideal situation, if all rules of the HEPEVT standard definition were respected, PHOTOS would easily identify the branching points (particle decays with charged products) in the decay tree, extract the required data, then eventually append the generated photons (if any) as additional decay products. It would also traverse the decay tree to identify all pos-

sible places where QED corrections might need to be generated. Initially, the algorithms employed in PHOTOS assumed that the data structure is consistent, with all pointers (to “mothers” and “daughters”) set up correctly. An acyclic tree of $1 \rightarrow n$ (or exceptionally $2 \rightarrow n$) processes could have easily been navigated using standard algorithms.

However, the rigidity of the HEPEVT standard, and the lack of possibility of extending it in a consistent way forced the authors of event generators to overload the meaning of the elements of the HEPEVT data structure. Certainly, one could consider having bi-directional relations (i.e. mothers pointing to daughters, and daughters pointing to mothers) as redundancy, and the place where additional information (such as spin or colour flow) may be stored instead. The meaning of the pointers become generator-specific and the navigation in such data structure could not be performed by a generic algorithm. Pandora’s box of event-record problems has been opened, hurting mainly the coordinators of the large experimental simulation chains.

The pointers in the HEPEVT structure were not the only element that became non-standard. Due to evolving needs of physics models (such as bigger number of particles being simulated, or precision), HEPEVT data structure has been modified to store single- or double-precision data, with various array sizes. Dubious matching of the HEPEVT layout between simulation blocks became yet more complicated.

To alleviate the problem with varying precision and layout of HEPEVT, PHOTOS has been equipped with a set of debugging and data-interpretation facilities. Firstly, it was modified to work on a local copy of the event record (the layout of which followed the “well-behaved” HEPEVT standard), and have a set of functions that would transfer the data between whatever external variant of HEPEVT data structure, and the internal storage. Secondly, a set of sanity-checking and pointer-reconstructing procedures were applied during the transfer of the data between the external event record and the internal one. Finally, a debugging function PHLUPA was provided. It prints out the data as interpreted/modified by PHOTOS routines, at different steps of event construction.

Because of the specifics of the PHOTOS algorithm, namely massive search and modification of the com-

plete event tree, PHOTOS itself has become a debugging tool for large simulation chains in the experimental collaborations. Strengthened with its debugging tools, it helped to identify many problems related to event grammatic.

This class of problems will remain with C++ applications as well. The origin of the difficulty is physics. On theoretical side authors of main Monte Carlo programs explore different options on storing information on the process generation, on the other, experimental users prefer to rely only on the information, which can be obtained from the measurement.

To be able to explore, in such conditions, the potential of the PHOTOS algorithm, and to make the debugging of the event record data easier, a tool: MC-TESTER [7] originally developed for tests of TAUOLA was adopted. It performs comparison tests of distributions of invariant masses produced by two, or more, (versions of) event generators. In semi-automatic way (thus eliminating the risk of accidental programmatic error) it extract the data from event records filled by an event generators: it identifies the decay modes of a given particle, and for every mode it builds the histograms of invariant masses of all combinations of decay products.

5. Challenges of event record

On reading the paper, one could get an impression that the communication between the modules of the simulation tree is a challenging, yet standard, goal, which could be realized in any modern, or even not so modern software environment. Our discussion in the previous chapters pointed to possible constraints and requirements in the organization of such data structure imposed by relatively modest application PHOTOS, if its precision requirements would need to be increased beyond certain level.

One can ask the question why the C++ implementation of PHOTOS did not meet so far as much attention as its seemingly obsolete FORTRAN version. On a first sight the answer is simple: there was until recently no commonly agreed standard for the event record data structure in C++ accepted by the dominant part of the community. Recently, it seems that the HepMC [17] structure is gaining popularity in the LHC applications.

From the past experience of HEPEVT standard, one

could postulate that a viable event record could be seen as a system of parallel trees, the nodes of each being bound with correspondence relations spanning across the layers. Each individual tree should be easy to investigate or modify by program such as PHOTOS, or the detector simulation software.

For MC-TESTER to be effective in comparing the results generated by various Monte Carlo simulators, it was essential to provide access to various standards (or: flavors) of event record data structures. Similarly to PHOTOS, MC-TESTER performs exhaustive search and data extraction from event record, it however doesn't need to modify the contents of the event record. Typical data that needed to be extracted was the mother-daughter relationships (including finding out the non-decaying final-state particles in the cascade decay), and determining the properties (four-momenta, and type) for involved particles. To separate MC-TESTER from problems related to event record processing, the HEPEventLib abstraction layer was created

At the technical layer, HEPEventLib does nothing more than interpretation of the data stored in various event record standards, and providing these data in a consistent form to the main program, hence hiding all dependencies and data-translation operations. The data is provided by abstract object representing a particle, a list of particles and an event. As no modification is performed on the structure of the event record, the properties visible in a "particle" object may be mapped directly to the corresponding data in the underlying event record. Thanks to that feature, particle's properties (such as four-momenta, but not the mother-daughter attributions) might even be modified from within HEPEventLib's abstract view, and the changes would be propagated to the actual event record in a consistent way.

At the bottom of the HEPEventLib there are implementations of the HEPEventLib abstraction to concrete event record types, of FORTRAN or C++ applications. New "backends" for any (future) event record may be implemented as needed - MC-TESTER will automatically profit from the new standard with no need of adding a single line of code in it.

6. Summary

In the present talk we have reviewed the basic properties of theoretical (QED) and software environment which is at foundation of design and performance of PHOTOS Monte Carlo program for simulation of QED bremsstrahlung corrections in decays of resonances and particles encoded in different type of event records used in simulations of High Energy physics. Special emphasis was on the points important for evaluation of systematic errors.

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