PHOTOS Monte Carlo for precision simulation of QED in decays - History and properties of the project

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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. We will concentrate specially on conflicting requirements originating from the properties of QED matrix elements on one side and degrading (evolving) with time standards of event record(s). These issues, quite common in other modular software applications, become more and more difficult to handle as precision requirements become higher.

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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 − 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].

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 basic precision level, that is essentially as PHOTOS design in years 1991-1994.

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 discusses. Then, MC-TESTER [6] 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 - [7] 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 [8], that bremsstrahlung corrections in τ decays are necessary for proper modelling 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 [9] 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 [10], 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. This assumption was behind other projects realized by Bob van Eijk at that times, as well, see eg. [11]. 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 intersest in improvements, expressed by experimental users. Numerical problems blocked development as well. It was only almost 10 years later, when the origins of theses problems were identified and corrected [3], since then, significant improvements could be introduced into the program.
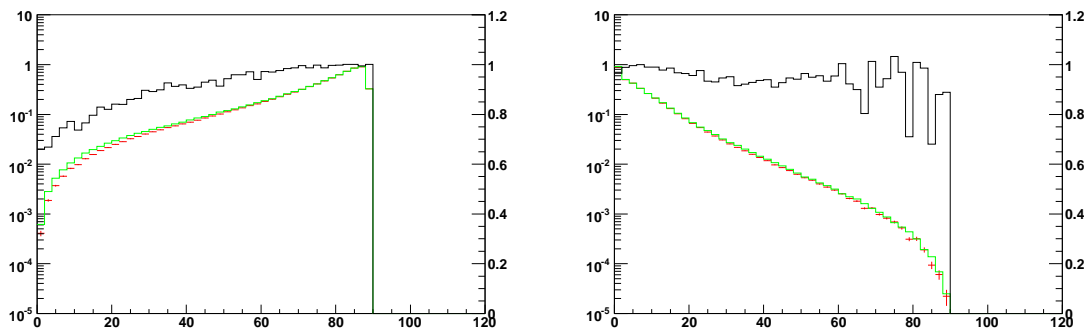
Figure 1: The comparison [4] of the standard PHOTOS (with multiple photon emission) and the KKMC generator (with second-order matrix-element and exponentiation). In the left frame the invariant mass of the $\mu^+\mu^-$ pair; SDP= 0.00918. In the right frame the invariant mass of the $\gamma\gamma$ pair; SDP=0.00268. The fraction of events with two hard photons was $1.2659 \pm 0.0011\%$ for KORALZ and $1.2952 \pm 0.0011\%$ for PHOTOS.

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 emissions 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 $Z \to l^+l^-$ and $B \to K(\pi)K(\pi)$ 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 $Z \to \mu^+\mu^-$ decays.

In the first figure we show the comparison of the two plots giving largest discrepancies between PHOTOS (run with standard options) and KKMC (run with second order matrix element and exponentiation). The plots present 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*. The rates for the event samples predicted by the two programs are given in the figure's caption. As one can see 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 indeed interesting results of ref. [4].
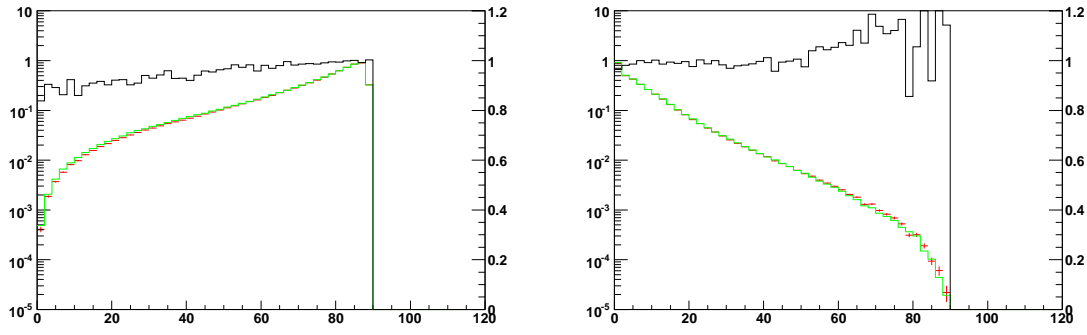
Figure 2:　The comparisons [4] of the improved PHOTOS (with multiple photon emission) and the KKMC generator (with second order matrix element and exponentiation). In the left frame the invariant mass of the $\mu^+\mu^-$ pair; SDP= 0.00142. In the right frame the invariant mass of the $\gamma\gamma$; SDP=0.00293. The fraction of events with two hard photons was $1.2659 \pm 0.0011\%$ for KORALZ and $1.2868 \pm 0.0011\%$ for PHOTOS.

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 $e^+e^- \to Z^0/\gamma^* \to \mu^+\mu^-(\gamma)$ process:

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

$$
\begin{aligned}
\text{where}: \quad & \Theta_+ = \angle(p_+, q_+), \ \Theta_- = \angle(p_-, q_-), \\
& \Theta_\gamma = \angle(\gamma, \mu^-) \text{ is defined in } (\mu^+, \mu^-)\text{-pair rest frame.}
\end{aligned}
\tag{1}
$$

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]:

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

The resulting weight is rather simple, and reads:

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

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

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 $q^-q \rightarrow ngZ/\mathring{\gamma}; Z/\gamma^* \rightarrow \mu^+\mu^-$ 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, as can be seen from the figures, the NLO precision in PHOTOS for today and tomorrow experiments is most likely not required. For the time being the problem remain rather academic.

In ref [14], we presented similar modifications in the PHOTOS kernel for the decay of *B* mesons into a pair of scalars. As one can see from the comparison of plots in figures 3, 4 and 5 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.).

For the NLO kernel in PHOTOS the results are indistinguishable from those of SANC, even at statistical level of 10^9 events. In this case, the technical price seems to be zero, as there is no need for extra information to be pumped from the event record to the calculation of the PHOTOS weight. Actually, the exact kernel is even simpler than the one used so far.

However, this gain may be elusive: the dependencies on the production process may appear if form-factors (originating from some unspecified here models) are fitted to the data.

From the practical side, one can interpret this excellent agreement as a strong test of numerical performance of the program. The necessary studies of the exact parametrization of the phase space used in PHOTOS, which will also be important for future version of PHOTOS, are described in detail in the journal version of ref. [14].

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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.
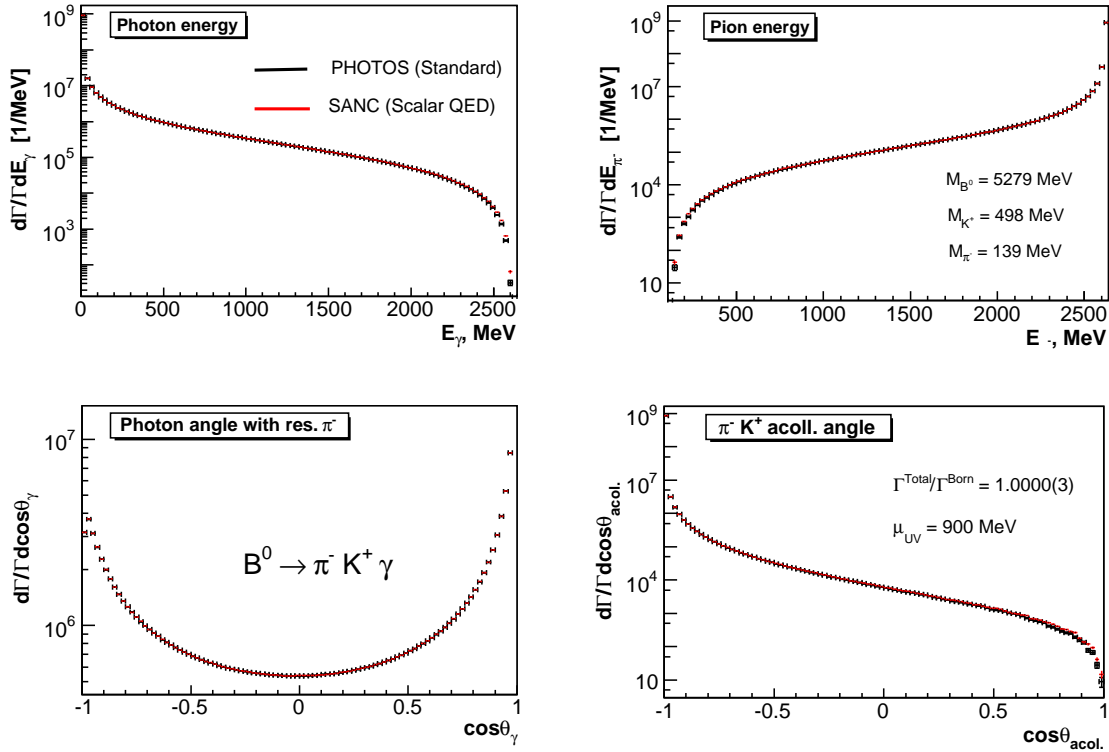
Figure 3: Results [14] from PHOTOS, standard version, and SANC for $B^0 \rightarrow \pi^- K^+ (\gamma)$ decay are superimposed on the consecutive plots. Standard distributions, as defined in the text and logarithmic scales are used. The distributions from the two programs overlap almost completely. Samples of 10^9 events were used. The ultraviolet scale, μ_{UV}, was chosen to leave total decay width unchanged by QED.

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 possible 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 rigidness 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.
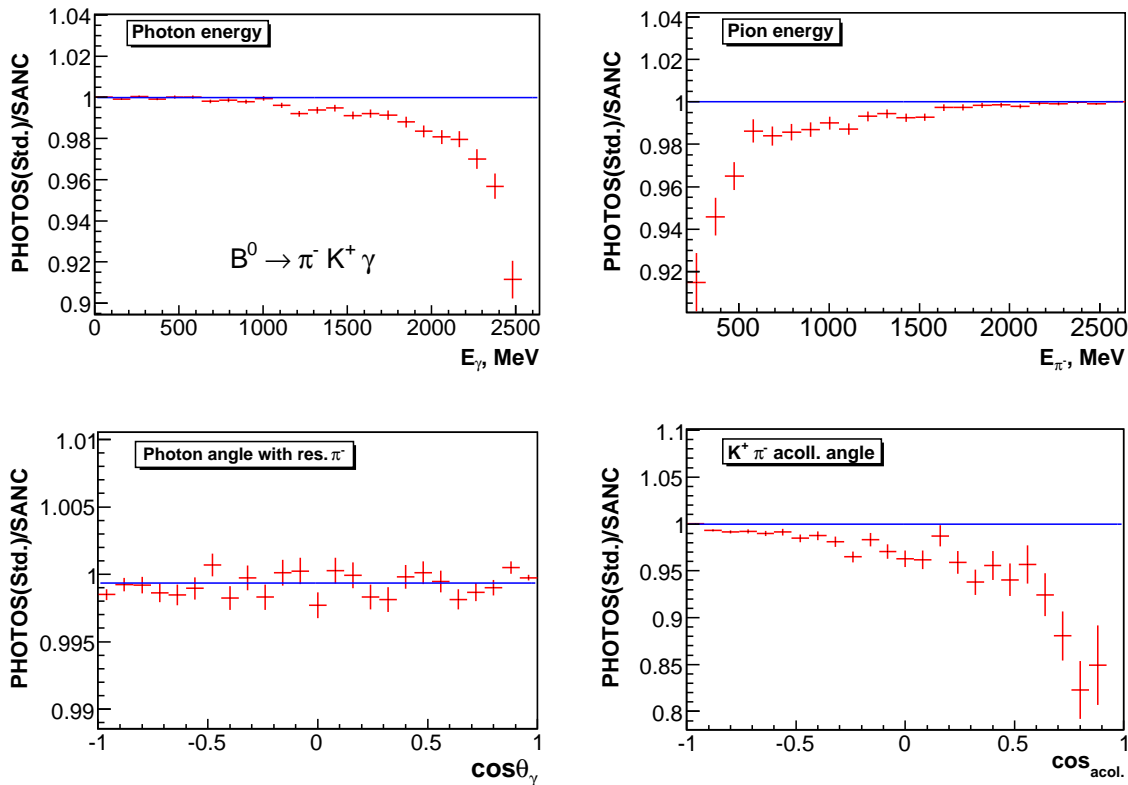
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Figure 4: Results [14] from PHOTOS, standard version, and SANC for ratios of the $B^0 \to \pi^- K^+ (\gamma)$ distributions are presented. Differences between PHOTOS and SANC are small, but are clearly visible now

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 complete event tree, PHOTOS itself has became 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.
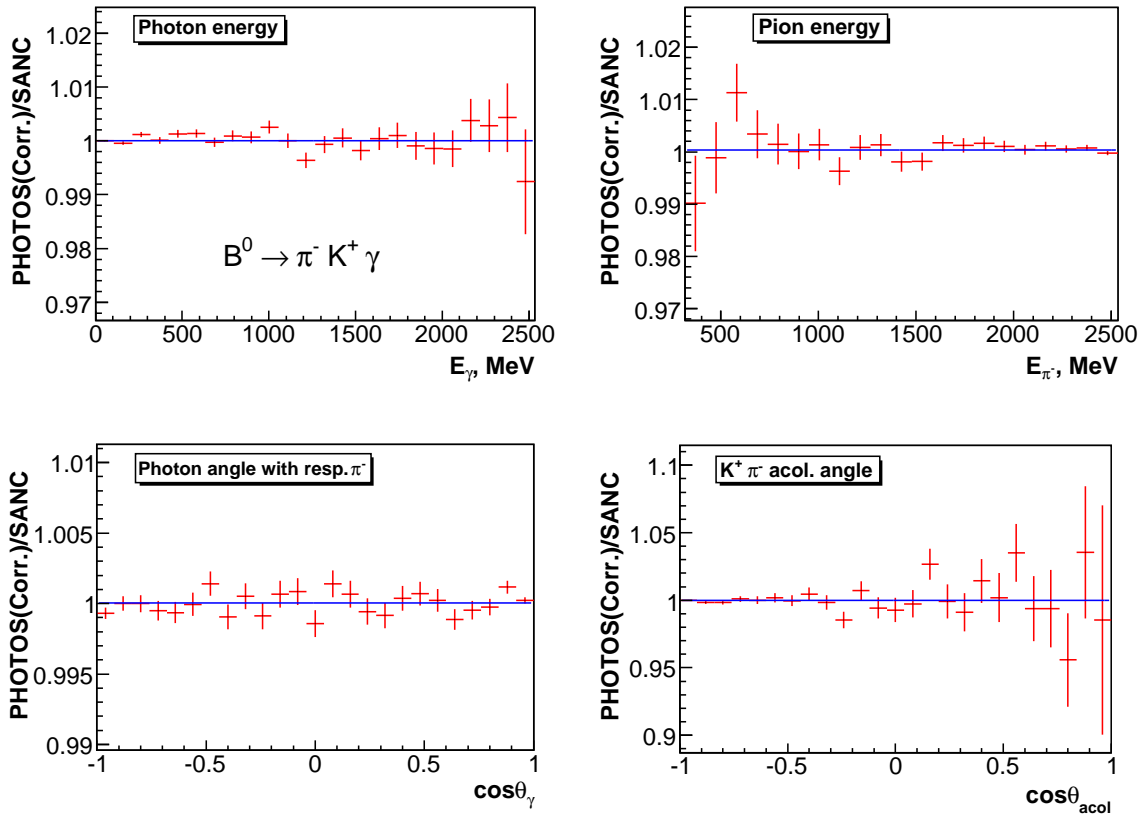
Figure 5: Results [14] from PHOTOS with the exact matrix element, and SANC for ratios of the $B^0 \rightarrow \pi^- K^+(\gamma)$ distributions. Differences between PHOTOS and SANC are below statistical error for samples of 10^9 events.

The numerical stability of PHOTOS was, for many years, a problem faced by its users (and authors). As the energy ranges, to which it was applied, were raising towards the ones of the LHC, the problems became more and more severe. Again, the event record data, filled by other generators, was often the main culprit of these instabilities. PHOTOS requires that the Energy-Momentum conservation in a decay process is absolutely respected, and with a numerical high precision, otherwise the boost operations performed between the laboratory rest-frame and the rest-frame of highly energetic particles cannot be calculated. To deal with the problem of insufficient precision of the energy-momentum conservation in the event data, the PHCORK routine was added to PHOTOS. It verified (and corrected) the kinematics of particles being processed by PHOTOS, so that the four-momenta of children sum up to the four-momentum of the mother particle, and the $E^2 - p^2 = m^2$ invariant was preserved for all of particles. From physical point of view, this latter relation contain ambiguity: for wide resonances (particles the mass of which has wide spectrum) one might speak about "off-mass-shell" particles, for which the mass doesn't need to match this equation... A few modes of operation of PHCORK were prepared to deal with various scenarios, and interpret the data correctly.

To be able to explore the potential of the PHOTOS algorithm, and to make the debugging of the

event record data easier, a tool: `MC-TESTER` 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. After the data from two runs of `MC-TESTER` - instrumented generator is completed, the data collected by `MC-TESTER` in the runs is compared, and presented in a visual form of plots. For each plot, corresponding distributions from the two runs are plotted, and the ratio of the distribution is overimposed, giving an overview of discrepancies between the corresponding distribution. A "Shape Difference Parameter" (SDP) is also calculated, to quantify these differences. All the plots, with the values of the SDP and branching ratios for all identified decay channels are presented in an easy to navigate, printable "booklet".

The results of the `MC-TESTER` - based comparisons of `PHOTOS` with high-precision Monte Carlo generators (for processes such as leptonic Z decays) were actually the motivation to improve the precision of `PHOTOS`.

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 FORTAN 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, as shown in Fig.6, 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.

We believe that the universal event record of the future should be kept independent of the theorist applications, or - better - from any direct applications. That has been the case for the `JETSET/PYTHIA` family of programs, which had their internal event structure, and a translation routine allowing to transfer the data from/to the universal `HEPEVT`. The authors of `PHOTOS` have also realized the advantages of such approach.

In the last part of this Section let us show our approach to the event record problem as used in our `MC-TESTER` tool.

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
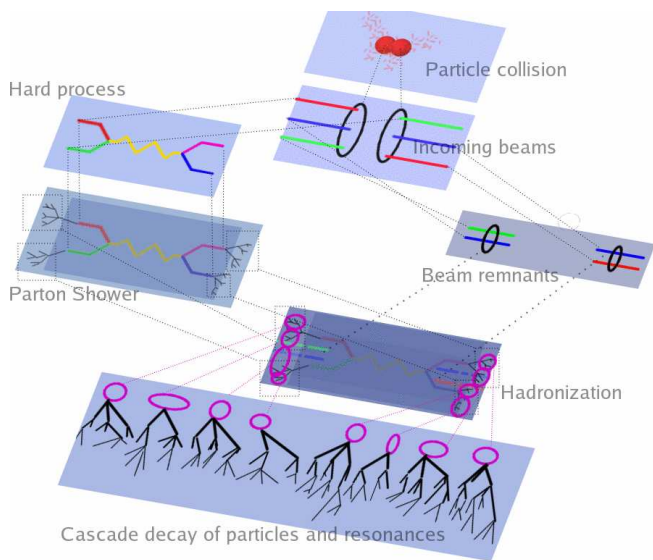
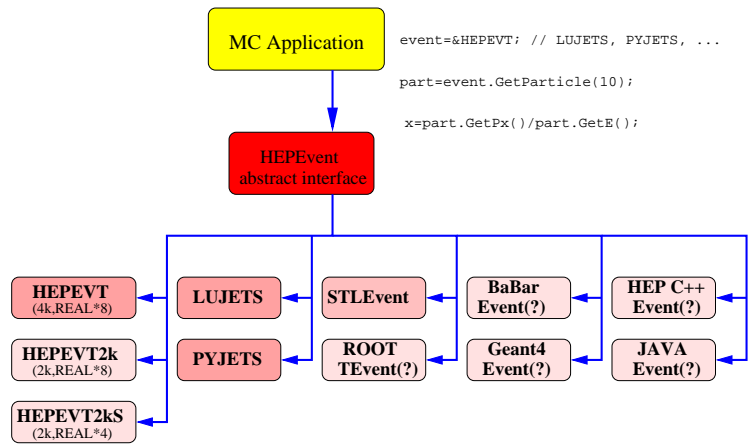**Figure 6:** Event Record as inter-linked layers of trees.

Figure 7: The concept of the HEPEventLib interface.

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 (see Fig. 7).

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

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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, such as `HEPEVT`, `LUJETS`, `PYJETS`, and `HERWIG`-specific version of `HEPEVT`. 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.

The use of HEPEventLib is currently limited to the `MC-TESTER` project. However, it may also be used by any other project, without introducing any dependencies on `MC-TESTER`. We believe that similar "screening" (or "interpreter") approach, for separating-out the dependencies on the external event record from the main code of simulation may provide substantial simplification of the code. It also interplays in a natural way with the approach of having an "external event record" for data-exchange with other simulation modules and "private event record" to keep the state of the simulation while a new event is being generated.

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. This presentation may be of interest not only for the program users (present and future ones) involved in experimental data analysis and organizing software for such analysis, but also for people interested in similar software organization problems appearing in other applications and their matching with software environment.

Acknowledgments

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