HISTORICAL AND MATHEMATICAL ASPECTS OF ITERATIVE SOLUTIONS FOR MONTE CARLO SIMULATIONS* **

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(Received May 7, 2008)

Over the last 25 years Monte Carlo programs were being developed in Cracow in the group guided by Prof. Stanislaw Jadach. Many of those programs became standard in their application domains. In the following let us review some aspects of such projects which were probably at the foundation of their success. We will concentrate on mathematical aspects of their design and history of their construction. It is rather difficult to cover 25 years of the research in a single talk. That is why, I have organised my presentation around Monte Carlo `PHOTOS` but stressing its relation to other activities and projects often realized together with Prof. Jadach. Many of omitted aspects will find their way into other presentations collected in this volume. I will concentrate on issues related to phase-space parametrisation and spin amplitudes as used in our Monte Carlo programs such as `MUSTRAAL`, `TAUOLA` or `KKMC` and their similarities and differences with respect to solution used in `PHOTOS`.

PACS numbers: 11.15.Pg, 13.40.Ks, 12.38.Cy

1. Introduction

One of the essential steps in the construction of any algorithm for multi-particle final states is the appropriate analysis of the phase space parametrisation. In the `PHOTOS` Monte Carlo [1] for multi-photon production, an

* Presented at the Cracow Epiphany Conference on LHC Physics, Cracow, Poland, 4–6 January 2008.

** Supported in part by the EU grant MTKD-CT-2004-510126 in partnership with the CERN Physics Department, by RTN European Programme, MRTN-CT-2006-035505 (HEPTOOLS, Tools and Precision Calculations for Physics Discoveries at Colliders) and by the Polish Ministry of Scientific Research and Information Technology grant No 620/E-77/6.PRUE/DIE 188/ 2005–2008.

exact phase space parametrisation is embodied in an iterative algorithm, the details of which are best described in [2]. Control of the distributions and relative size of sub-samples for distinct numbers of final state particles requires a precise knowledge of the matrix elements including virtual corrections as well. In the KKMC Monte Carlo, the phase space generation is different, but the necessity to control matrix elements is also essential [3,4].

Iterative procedures for parts of amplitudes, which are at the foundation of exponentiation [4,5] and structure functions [6–10] were exploited for the sake of use in KKMC Monte Carlo. In particular the description of dominantly s-channel processes $e^+e^- \to \nu_e\bar{\nu}_e\gamma\gamma$ where, t-channel W-exchange diagrams with gauge boson couplings, contribute to matrix elements provide an interesting example [11]. These studies were motivated by practical reasons, but also pointed at quite astonishing properties of tree-level spin amplitudes, namely that they can be separated into gauge invariant parts in a semi-automated way, easy to apply in the Kleiss–Stirling methods [12,13].

One could ask the question whether similar techniques can be used in QCD, whether they are of any practical use, and in fact to which degree they were already included in previous publications. These questions will be discussed elsewhere [14,15]. We will not elaborate on these points requiring good understanding of factorisation in QCD. Instead let us point to old, but important for me Ref. [16], where properties of factorisation for cross section, visualise themselves in a fully differential environment, even though only for QED and at first order of perturbation expansion. For the sake of caution, let us mention the existence of limitations in such strategies, if applied to parton shower applications beyond NLO [17].

Our presentation is organised as follows. In Section 2 we will discuss different aspects of phase space parametrisation, as used in PHOTOS Monte Carlo and how it compares to other programs. Discussion of approximations necessary to construct crude distributions is started in Section 2. Presentation of the form of first order cross section, matrix elements and approximations which were essential for construction of the first version of the program is given in Section 3. With all material collected, we will point in Section 4 to mathematical properties of elements used in the project, which actually made it possible, even though their documentation was never of high priority until now. The summary in Section 5 closes the paper.

2. Phase space

It is of no surprise that phase space must play a central role in preparation of the algorithm of any Monte Carlo based on predictions originating from field theory. That is direct consequence of Quantum Mechanics, basic formula for cross section consists of phase space element, matrix element

squared and the flux factor. Over many years we were stressing, in a multitude of talks and papers that the control of the eventual approximations is essential. Let me recall here one of such S. Jadach's plots, see Fig. 1. At that time it was an achievement [3, 18]. It required enormous amount of work to prepare such an organisation of the phase space that would be exact, cover complete multibody phase space, and capable to manage highly peaked distributions of complex structure due to collinear and soft singularities.

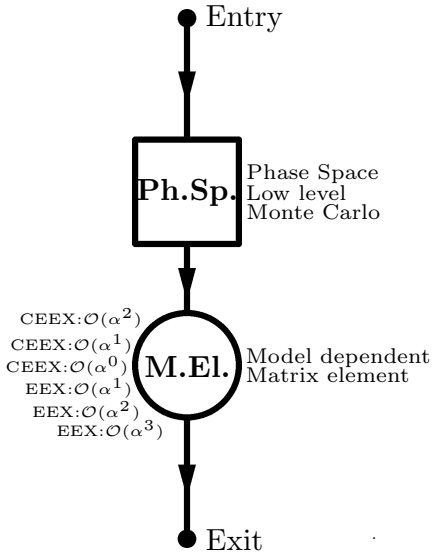

Fig. 1. Phase space plot for the KKMC and KORALZ Monte Carlo programs.

As these programs are discussed elsewhere in the proceedings, let us follow here the phase space organisation of another program originating from S. Jadach group, that is `PHOTOS` Monte Carlo[1]. It is also capable of covering multibody phase space distributions without any approximation, but contrary to `KKMC/KORALZ` solutions conformal symmetry of the eikonal approximation is not used. Thanks to that, this solution is closer to iterative solution used in QCD parton showers, but is still relatively simple to explain and formalise.

Let us start with the explicit expression for the parametrisation of an $n+1$ body phase space in decay of the object of four-momentum P ($P^2 = M^2$), as used in `PHOTOS` Monte Carlo. As our aim is to define iterative relations, let us denote the four momenta of the first n decay products as k_i ($i = 1, n$) and the last $n+1$ decay product as k_{n+1}. In our case the $n+1$-th

[1] The most detailed description of the program [1, 19], can be found in recent Ref. [2].

particle will always be the real and massless photon[2]. In the later steps of our construction the masslessnes of photons and properties of QED matrix elements will be used.

In the following, notation from Refs. [20, 21] will be used. We will not rely on any particular results of these papers. We only point to other, similar options for the exact n-body phase space parametrisations, which are also in use.

The Lorentz invariant phase space is defined as follows:

$$\begin{aligned} d\mathrm{Lips}_{n+1}(P) &= \frac{d^3k_1}{2k_1^0(2\pi)^3}\cdots\frac{d^3k_n}{2k_n^0(2\pi)^3}\frac{d^3k_{n+1}}{2k_{n+1}^0(2\pi)^3} \\ &\quad\times(2\pi)^4\delta^4\Big(P-k_{n+1}-\sum_{i=1}^{n}k_i\Big) \\ &= d^4p\delta^4(P-p-k_{n+1})\frac{d^3k_{n+1}}{2k_{n+1}^0(2\pi)^3}\frac{d^3k_1}{2k_1^0(2\pi)^3}\cdots\frac{d^3k_n}{2k_n^0(2\pi)^3} \\ &\quad\times(2\pi)^4\delta^4\Big(p-\sum_{i=1}^{n}k_i\Big) \\ &= d^4p\delta^4(P-p-k_{n+1})\frac{d^3k_{n+1}}{2k_{n+1}^0(2\pi)^3}d\mathrm{Lips}_n(p\to k_1\ \ldots\ k_n), \end{aligned} \tag{1}$$

where extra integration variables: four components of p (compensated with $\delta^4\big(p-\sum_1^n k_i\big)$) is introduced. If further, $M_{1\ldots n}$ (compensated with $\delta\big(p^2-M_{1\ldots n}^2\big)$) is introduced, the element of the phase space takes the form:

$$\begin{aligned} d\mathrm{Lips}_{n+1}(P) &= \frac{dM_{1\ldots n}^2}{(2\pi)}d\mathrm{Lips}_2(P\to p\ k_{n+1})\times d\mathrm{Lips}_n(p\to k_1\ldots k_n) \\ &= dM_{1\ldots n}^2\left[d\cos\hat{\theta}d\hat{\phi}\frac{1}{8(2\pi)^3}\frac{\lambda^{\frac{1}{2}}(M^2,M_{1\ldots n}^2,m_{n+1}^2)}{M^2}\right] \\ &\quad\times d\mathrm{Lips}_n(p\to k_1\ldots k_n). \end{aligned} \tag{2}$$

The part of the phase space Jacobian corresponding to integration over the direction and energy of the last particle (or equivalently invariant mass $M_{1\ldots n}$ of the remaining system of $1\ldots n$ particles) is explicitly given. We will use later in the formulas $m_i^2=k_i^2$, and analogously $M_{i\ldots n}$, defining invariant masses of $k_i\ldots k_n$ systems. The integration over the angles $\hat{\theta}$ and $\hat{\phi}$ is defined in the P rest-frame. The integration over the invariant mass, $M_{1\ldots n}$,

[2] However the construction does not rely on a photon to be massless. In principle it can be applied to define other phase space relations, for example the emission of an extra massive pion or emission of a pair of heavy particles.

is limited by phase space boundaries. Anybody familiar with the phase space parametrisation as used in FOWL [22], TAUOLA [21], or many other programs will find the above explanation quite standard[3].

The question of choice of axes with respect to which angles are defined, and order in kinematical construction, is less trivial. The choice for the particular option stems from necessity to presample collinear singularities. It is rather well known that the choice of the reference directions for the parametrisation of the unit sphere is free, and can be used to advantage. We will use related, but somewhat different freedom of choice. Instead of variables $\hat{\theta}$ $\hat{\phi}$ defining orientation of k_{n+1} in P rest-frame we will use angles θ_1 ϕ_1 orienting k_1 (also in P rest-frame). The Jacobian for this reparametrisation of unit sphere equals unity.

Formula (2) can be iterated and provide a parametrisation of the phase space with an arbitrary number of final state particles. In such a case, the question of orientation of the frames used to define the angles and the order of $M_{i...n}$ integrations (consequently, the choice of limits for $M_{i...n}$ integration), becomes particularly rich. Our choice is defined in Ref. [1]. We will not elaborate on this point here.

If the invariant mass $M_{1...n}$ is replaced with the photon energy defined in the P rest-frame, k_γ, then the phase space formula can be written as:

$$d\mathrm{Lips}_{n+1}(P) \;=\; \left[k_\gamma dk_\gamma d\cos\hat{\theta} d\hat{\phi}\frac{1}{2(2\pi)^3}\right] \times d\mathrm{Lips}_n(p \to k_1 \dots k_n)\,. \quad (3)$$

If we had l photons accompanying n other particles, then the factor in square brackets is iterated. The statistical factor $\frac{1}{l!}$ would complete the form of the phase space parametrisation, similar to the exponent. The last formula, supplemented with definition of frames with respect to which angles are defined is used to define the full kinematic configuration of the event. From angles and energies (k_{γ_i}) of photons and also angles, energies and masses of other decay products, four-momenta of all final state particles can be constructed.

If in formula (3) instead of $d\mathrm{Lips}_n(p \to k_1 \dots k_n)$ one would use $d\mathrm{Lips}_n(P \to k_1 \dots k_n)$ the *tangent space* would be obtained. Then k_{n+1} photon does not affect other particles' momenta at all, and thus has no boundaries on energy or direction. If this formula was iterated then all such photons would be independent from one another as well[4]. Energy and

[3] The parametrisations of such a type, use properties of the Lorentz group in an explicit manner, in particular measure, representations and their products. That is why, they are useful, for event building Monte Carlo programs in phase space constructions based on boosts and rotations.

[4] Expression (3) would be slightly more complicated if instead of photons a massive particle was added.

momentum constraints on the photon(s) are introduced with the relation between tangent and real $n+1$-body phase space. The formula defining one step in the iteration reads as follows[5]:

$$
\begin{aligned}
&d\mathrm{Lips}_{n+1}(P \to k_1 \dots k_n, k_{n+1}) = d\mathrm{Lips}_n^{+1\ \mathrm{tangent}} \times W_n^{n+1},\\
&d\mathrm{Lips}_n^{+1\ \mathrm{tangent}} = dk_\gamma d\cos\theta d\phi \times d\mathrm{Lips}_n(P \to \bar{k}_1 \dots \bar{k}_n),\\
&\{k_1, \dots, k_{n+1}\} = \boldsymbol{T}\big(k_\gamma, \theta, \phi, \{\bar{k}_1, \dots, \bar{k}_n\}\big).
\end{aligned}
\tag{4}
$$

The W_n^{n+1} depends on details of $\boldsymbol{T}$, and will be thus given later in formula (10). To justify (4), we have to convolute formula (2) for $\mathrm{Lips}_{n+1}(P \to k_1 \dots k_n, k_{n+1})$ with itself (for $\mathrm{Lips}_n(p \to k_1 \dots k_n)$):

$$
\begin{aligned}
\mathrm{Lips}_{n+1}(P \to k_1 \dots k_n, k_{n+1}) &= \frac{dM^2_{1\dots n}}{2\pi}\mathrm{Lips}_2(P \to k_{n+1}p)\\
&\quad \times \mathrm{Lips}_n(p \to k_1 \dots k_n)\,,\\
\mathrm{Lips}_n(p \to k_1 \dots k_n) &= \frac{dM^2_{2\dots n}}{2\pi}\mathrm{Lips}_2(p \to k_1 p')\\
&\quad \times \mathrm{Lips}_{n-1}(p' \to k_2 \dots k_n)
\end{aligned}
\tag{5}
$$

and use it also for $\mathrm{Lips}_n(P \to \bar{k}_1 \dots \bar{k}_n)$:

$$
\mathrm{Lips}_n(P \to \bar{k}_1 \dots \bar{k}_n) = \frac{dM^2_{2\dots n}}{2\pi}\mathrm{Lips}_2(P \to \bar{k}_1 \bar{p}') \times \mathrm{Lips}_{n-1}(\bar{p}' \to \bar{k}_2 \dots \bar{k}_n)\,. \tag{6}
$$

Note that our tangent space of variables $dk_\gamma d\cos\theta d\phi$ is unbounded from above and the limit is introduced by W_n^{n+1} which is set to zero for the configurations outside the phase space. In principle, we should distinguish between variables like $M_{2\dots n}$ for invariant mass of $k_2 \dots k_n$ and $\bar{M}_{2\dots n}$ for invariant mass of $\bar{k}_2 \dots \bar{k}_n$, but in our choice for G_n, G_{n+1} below, $M_{2\dots n} = \bar{M}_{2\dots n}$ and $M_{1\dots n}$ is defined anyway for the $n+1$-body phase space only.

We direct the reader to Refs. [1,19] for an alternative presentation. Let us remark that formula (4) is quite general, many options, motivated by the properties of the matrix elements, can be introduced. Generally the transformation T may differ from the choice to choice quite a lot. The most straightforward choice can be based on any n and $n+1$ body phase space parametrisations using invariant masses and angles (*e.g.* exactly as in `TAUOLA` [21] formulas 11 to 13).

[5] The $\{\bar{k}_1, \dots, \bar{k}_n\}$ can be identified with the event before the radiation of k_γ is introduced.

If

$$G_n \,:\, M^2_{2\ldots n}, \theta_1, \phi_1, M^2_{3\ldots n}, \theta_2, \phi_2, \ldots, \theta_{n-1}, \phi_{n-1} \to \bar{k}_1 \ldots \bar{k}_n \tag{7}$$

and

$$G_{n+1} \,:\, k_\gamma, \theta, \phi, M^2_{2\ldots n}, \theta_1, \phi_1, M^2_{3\ldots n}, \theta_2, \phi_2, \ldots, \theta_{n-1}, \phi_{n-1} \to k_1 \ldots k_n, k_{n+1} \tag{8}$$

then

$$\boldsymbol{T} = G_{n+1}(k_\gamma, \theta, \phi, G_n^{-1}(\bar{k}_1, \ldots, \bar{k}_n))\,. \tag{9}$$

The ratio of the Jacobians (factors $\lambda^{1/2}$ like in formula (2), *etc.*) form the factor W_n^{n+1}, which in our case is rather simple,

$$W_n^{n+1} = k_\gamma \frac{1}{2(2\pi)^3} \times \frac{\lambda^{1/2}(1, m_1^2/M^2_{1\ldots n}, M^2_{2\ldots n}/M^2_{1\ldots n})}{\lambda^{1/2}(1, m_1^2/M^2, M^2_{2\ldots n}/M^2)}\,, \tag{10}$$

because of choice for G, as explained in the Appendix of Ref. [2]. Note that $k_\gamma = \frac{M^2 - M^2_{1\ldots n}}{2M}$. There are additional benefits from such a choice. In all relations $\bar{k}_2 = Lk_2$, $\ldots$, $\bar{k}_n = Lk_n$ and $\bar{p}' = Lp'$ common Lorentz transformation L is used. Transformation L is defined by $k_1, \bar{k}_1, \bar{p}', p'$ and P; internal relations between four vectors $k_2 \ldots k_n$, $(\bar{k}_2 \ldots \bar{k}_n)$ are not needed.

Formula (4) can be realized algorithmically in the following way:

1. For any point in n-body phase space (earlier generated event), described for example with the explicit configuration of four vectors $\bar{k}_1 \ldots \bar{k}_n$, coordinate variables can be calculated, using formula (7).

2. Photon variables can be generated according to Eq. (4). The weight W_n^{n+1} has to be also attributed.

3. Variables obtained in this way from the old configuration and the one of a photon can be used to construct the new kinematical configuration for the $n+1$-body final state. The phase space weight, which is zero for configurations outside phase space boundaries, can be calculated at this point from (4), (10) and finally combined with the matrix element.

Here we have chosen two sub-groups of particles. The first one consisted of particle 1 alone, and the second, of particles 2 to n combined together. Obviously in the case of 2-body decays, there is not much choice when construction of the first photon is performed.

By iteration, we can generalise formula (4) to the case of l photons and we write:

$$d\mathrm{Lips}_{n+l}(P \to k_1 \dots k_n, k_{n+1} \dots k_{n+l}) = \frac{1}{l!}\prod_{i=1}^{l}\left[dk_{\gamma_i} d\cos\theta_{\gamma_i} d\phi_{\gamma_i} W_{n+i-1}^{n+i}\right]$$
$$\times d\mathrm{Lips}_n(P \to \bar{k}_1 \dots \bar{k}_n),$$
$$\{k_1, \dots, k_{n+l}\} = \boldsymbol{T}\big(k_{\gamma_l}, \theta_{\gamma_l}, \phi_{\gamma_l}, \boldsymbol{T}\big(\dots, \boldsymbol{T}\big(k_{\gamma_1}, \theta_{\gamma_1}, \phi_{\gamma_1}, \{\bar{k}_1, \dots, \bar{k}_n\}\big)\dots\big)\,. \tag{11}$$

In this formula we can easily localise the *tangent space* for the multiple photon configuration. In this space, each photon is independent from other particles' momenta. Note that it is also possible to fix upper boundary on k_{γ_i} arbitrary high. Photons are independent one from another as well. Correlations appear later, thanks to iterated transformation $\boldsymbol{T}$. The factors W_{n+i-1}^{n+i} are calculated when constraints on each consecutive photon are introduced; the previously constructed ones are included in the $n+i-1$ system[6].

Of course, for the tangent space to be useful, the choice of the definition of $\boldsymbol{T}$ must be restricted at least by the condition $\{k_1, \cdots k_n\} \to \{\bar{k}_1, \cdots \bar{k}_n\}$ if all $k_{\gamma_i} \to 0$.[7]

It is important to realize that one has to choose matrix elements on the tangent space to complete the construction used in PHOTOS. The number and energies of photons will be generated on the tangent space first. Regularisation of (at least) soft singularity must be defined. Rejection, and event construction, is performed with the help of formula (4) for each consecutive photon. It diminishes photon multiplicity with respect to the one defined for the tangent space. Of course, as rejection implements changes in phase space density, a matrix element (with virtual corrections) of the physical space can be introduced as well.

The treatment of the phase space presented here lies at the heart of the construction of PHOTOS kinematics, and was used since its beginning. It exhausts the case when there is only one charged particle in final state. For multiple charged particle final states new complication appear, because all collinear configurations need simultaneous attention, and not only the one along k_1 direction. A presampler with multichannel generation is needed. In our case we follow the same method as explained in Ref. [21].

[6] Configurations of k_{γ_i} which can not be resolved are reduced to the ones with that photon dropped out.

[7] In fact, further constraints have to be fulfilled to enable presampling for the collinear singularities. Note that variables $k_{\gamma_m}, \theta_{\gamma_m}, \phi_{\gamma_m}$ are used at a time of the m-th step of iteration only, and are not needed elsewhere in construction of the physical phase space; the same is true for invariants and angles $M^2_{2\dots n}, \theta_1, \phi_1, \dots, \theta_{n-1}, \phi_{n-1} \to \bar{k}_1 \dots \bar{k}_n$ of (7), (8), which are also redefined at each step of the iteration.

Let us now sum the above expression over l. If we add arbitrary factors $f(k_{\gamma_i}, \theta_{\gamma_i}, \phi_{\gamma_i})$ and sum over l we obtain:

$$\begin{aligned}
&\sum_{l=0} \exp(-F) \frac{1}{l!} \prod_{i=1}^{l} f(k_{\gamma_i}, \theta_{\gamma_i}, \phi_{\gamma_i}) d\mathrm{Lips}_{n+l}(P \to k_1 \dots k_n, k_{n+1} \dots k_{n+l}) \\
&= \sum_{l=0} \exp(-F) \frac{1}{l!} \prod_{i=1}^{l} \left[f(k_{\gamma_i}, \theta_{\gamma_i}, \phi_{\gamma_i}) dk_{\gamma_i} d\cos\theta_{\gamma_i} d\phi_{\gamma_i} W_{n+i-1}^{n+i} \right] \\
&\times d\mathrm{Lips}_n(P \to \bar{k}_1 \dots \bar{k}_n) \,, \\
&\{k_1, \dots, k_{n+l}\} = \boldsymbol{T}\big(k_{\gamma_l}, \theta_{\gamma_l}, \phi_{\gamma_l}, \boldsymbol{T}\big(\dots, \boldsymbol{T}\big(k_{\gamma_1}, \theta_{\gamma_1}, \phi_{\gamma_1}, \{\bar{k}_1, \dots, \bar{k}_n\}\big) \dots\big) \,, \\
&F = \int_{k_{\min}}^{k_{\max}} dk_\gamma d\cos\theta_\gamma d\phi_\gamma f(k_\gamma, \theta_\gamma, \phi_\gamma) \,. \qquad (12)
\end{aligned}$$

Some parts of r.h.s. taken alone, give crude distribution over tangent space (orthogonal set of variables k_i, θ_i, ϕ_i). Factors f must be integrable over this tangent space and regulators of singularities must be introduced. We may simply request that

$$\sigma_{\text{tangent}} = 1 = \sum_{l=0} \exp(-F) \frac{1}{l!} \prod_{i=1}^{l} \left[f(k_{\gamma_i}, \theta_{\gamma_i}, \phi_{\gamma_i}) dk_{\gamma_i} d\cos\theta_{\gamma_i} d\phi_{\gamma_i} \right]$$

and that sum rule originating from perturbative approach (Kinoshita–Lee–Nauenberg theorem) can be used to control virtual corrections; both for tangent and later also final distributions.

At this point we already have Monte Carlo solution of `PHOTOS` phase space. In reality, for that solution to work, real emission and virtual corrections need to be calculated and their factorisation properties must be understood. That is why, choice of f is free only in principle, in practice it must be synchronised with those results for the sake of program efficiency. In case of final state QED bremsstrahlung it is rather simple, eventual complications due to QED corrections to rates are of no major consequences [23] for the program construction. Non leading corrections appear only.

Note that this formula is very close to other ones, used in other programs or calculations. For example, formal solution [9, 10] of evolution equation reads

$$D(x, \beta_{\text{ch}}) = \delta(1-x) + \beta_{\text{ch}} P(x) + \frac{1}{2!} \beta_{\text{ch}}^2 \{P \times P\}(x) + \frac{1}{3!} \beta_{\text{ch}}^3 \{P \times P \times P\}(x) + \dots \,, \qquad (13)$$

where

$$P(x) \;=\; \delta(1-x)\left(\ln\varepsilon+\frac{3}{4}\right)+\Theta(1-x-\varepsilon)\frac{1}{x}\,\frac{1+x^2}{1-x}$$

and

$$\{P\times P\}(x) \;=\; \int\limits_0^1 dx_1 \int\limits_0^1 dx_2\delta(x-x_1x_2)P(x_1)P(x_2)\,.$$

One can easily observe, that in the LL contributing regions, the phase space Jacobians as used in PHOTOS trivialise [1] and lead directly to this solution. In 1994, this solution was truncated to second order. It was indeed profitable that solutions for similar problems were available in Cracow at that time. Let us give one example [24]. In this first, on multiphoton Monte Carlos, paper written in 1987 by S. Jadach formula (3.1) is basically the same as tangent space of multi-photon PHOTOS (and not much different from $D(x,\beta_{\rm ch})$ discussed just above):

$$\begin{aligned}\sigma(K) \;=\; &\exp\left(\frac{2\alpha}{\pi}\left(\ln\frac{s}{m^2}-1\right)\ln\frac{k_s}{E}+\frac{\alpha}{\pi}\ln\frac{s}{m^2}\right)\\ &\times\sum_{n=0}\frac{1}{n!}\prod_{m=1}^{n}\int_{k_s<k_m<K}\frac{d^3k_m}{k_m}\tilde{S}(k_1)\ldots\tilde{S}(k_n)\tilde{\beta}_0\,. \qquad (14)\end{aligned}$$

The difference appears in projection from this tangent space to the physical one. Classical solution as proposed by Jadach, use conformal symmetry, projection from eikonal (tangent) to physical space is performed in one step. In PHOTOS eikonal symmetry is not used. Iterative projection is used instead, it is somewhat similar to the one introduced in TAUOLA [25] for radiative corrections in leptonic tau decays. Analogies to solutions used in QCD parton shower algorithms can be found.

Very important aspect of all these solutions is that the structure of singularities is the same in tangent and final physical space.

3. Matrix elements

It is out of the question, that detailed analysis of MUSTRAAL Monte Carlo [16], which was a consequence of accidental error in copying source code from punch cards to tape, was essential for the design of PHOTOS program. At that time (1983) I was forced to study MUSTRAAL line after line. Not only the two missing lines[8] of code were found, but I have studied the matrix

[8] Punch card reader glued them together at the last time they were ever to be read?

element and crude distributions in all possible details. This unintentionally collected experience combined with importance of QED radiative corrections in phenomenology of leptonic Z couplings at the time of preparation for first measurements of τ polarisation at LEP was few years later a starting point for PHOTOS.

Let us recall the properties of the $Z \to l^+l^-\gamma$ matrix element as studied by me at that early time and also the approximate matrix element, which was and still is used in PHOTOS.

Let us write the explicit form of the real-photon matrix element (separated from the phase space Jacobians), for the $e^+e^- \to Z^0/\gamma^* \to \mu^+\mu^-(\gamma)$ process and as used in the standard version of PHOTOS (published in [1,19]):

$$
\begin{aligned}
X_f^{\rm PHOTOS} &= \frac{Q'^2\alpha(1-\Delta)}{4\pi^2 s} s^2 \\
&\times \Bigg\{ \frac{1}{k'_+ + k'_-}\frac{1}{k'_-}\left[\left(1+(1-x_k)^2\right) \frac{d\sigma_{\rm B}}{d\Omega}\left(s, \frac{s(1-\cos\Theta_+)}{2}, \frac{s(1+\cos\Theta_+)}{2}\right)\right] \\
&\times \frac{(1+\beta\cos\Theta_\gamma)}{2} \\
&+ \frac{1}{k'_+ + k'_-}\frac{1}{k'_+}\left[\left(1+(1-x_k)^2\right) \frac{d\sigma_{\rm B}}{d\Omega}\left(s, \frac{s(1-\cos\Theta_-)}{2}, \frac{s(1+\cos\Theta_-)}{2}\right)\right] \\
&\times \frac{(1-\beta\cos\Theta_\gamma)}{2} \Bigg\}, \qquad (15)
\end{aligned}
$$

where:

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

For its calculation (with respect to the 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 notation from Refs. [16,23]. This expression is to be compared with the exact one, taken from Ref. [16]:

$$
\begin{aligned}
X_f &= \frac{Q'^2\alpha(1-\Delta)}{4\pi^2 s} s^2 \Bigg\{ \frac{1}{(k'_+ + k'_-)}\frac{1}{k'_-}\left[\frac{d\sigma_{\rm B}}{d\Omega}(s,t,u') + \frac{d\sigma_{\rm B}}{d\Omega}(s,t',u)\right] \\
&\quad + \frac{1}{(k'_+ + k'_-)}\frac{1}{k'_+}\left[\frac{d\sigma_{\rm B}}{d\Omega}(s,t,u') + \frac{d\sigma_{\rm B}}{d\Omega}(s,t',u)\right]\Bigg\}. \qquad (16)
\end{aligned}
$$

The resulting weight is rather simple, and reads:

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

$$WT_2 = \frac{\frac{d\sigma_{\rm B}}{d\Omega}(s,t,u') + \frac{d\sigma_{\rm B}}{d\Omega}(s,t',u)}{\left[(1+(1-x_k)^2)\frac{d\sigma_{\rm B}}{d\Omega}\left(s,\frac{s(1-\cos\Theta_-)}{2},\frac{s(1+\cos\Theta_-)}{2}\right)\right]\frac{(1-\beta\cos\Theta_\gamma)}{2}\left(1+\frac{3}{4}\frac{\alpha}{\pi}\right)}. \quad (17)$$

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 stress on the event record: the details of the process of the Z production 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 $q\bar{q} \to ngZ/\gamma^*; Z/\gamma^* \to \mu^+\mu^-$ into the event record.

The NLO solution for PHOTOS, as presented in Ref. [23], would therefore be feasible with some universal, *standard* event record, nonetheless difficult due to practical issues of interfacing. One should ask the question, what is the price related to the approximation as implemented in public version of PHOTOS. The results for this standard and NLO improved PHOTOS are collected in figures 2 and 3. As one can see, improvement due to the use of exact first order matrix elements is unquestionable. On the other hand,

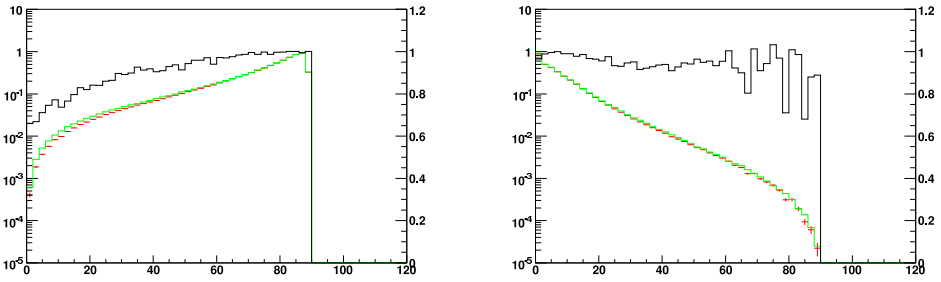

Fig. 2. The comparison [23] of the standard PHOTOS (with multiple photon emission) and the KKMC generator (with second-order matrix-element and exponentiation). In the left frame the invariant mass of the $\mu^+\mu^-$ pair; SDP= 0.00918. In the right frame the invariant mass of the $\gamma\gamma$ pair; SDP=0.00268. The fraction of events with two hard photons was 1.2659 ± 0.0011% for KORALZ and 1.2952 ± 0.0011% for PHOTOS. For the definition of shape difference parameter (SDP) see [26].

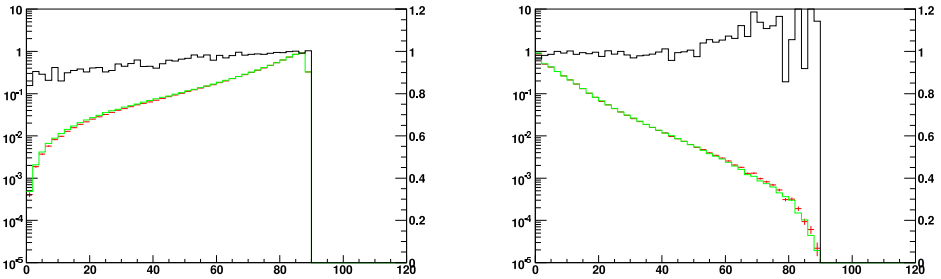

Fig. 3. The comparisons [23] of the improved PHOTOS (with multiple photon emission) and the KKMC generator (with second order matrix element and exponentiation). In the left frame the invariant mass of the $\mu^+\mu^-$ pair; SDP= 0.00142. In the right frame the invariant mass of the $\gamma\gamma$; SDP=0.00293. The fraction of events with two hard photons was 1.2659 ± 0.0011% for KORALZ and 1.2868 ± 0.0011% for PHOTOS. For the definition of shape difference parameter (SDP) see [26].

the standard, easier to use, version seem to be sufficient in practically all phenomenological applications as well. For the time being the problem of the optimal choice remains rather academic.

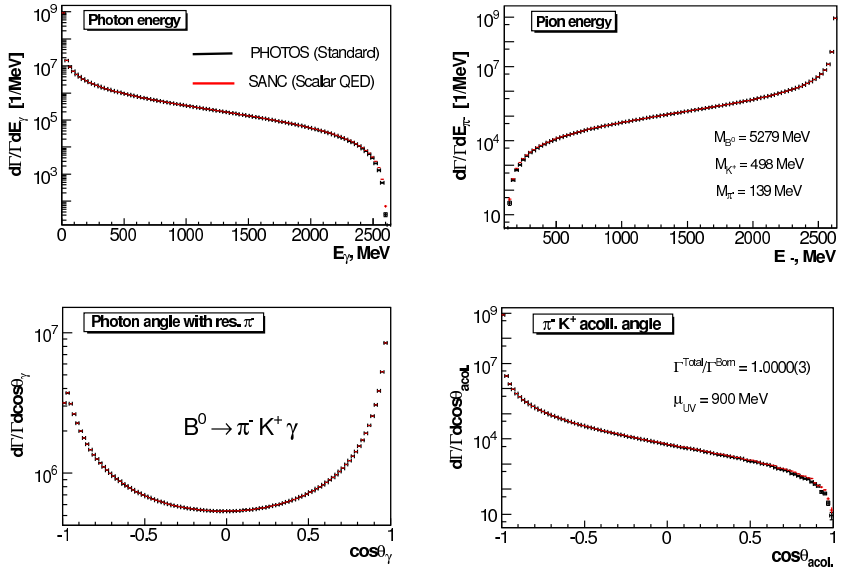

Fig. 4. Results [2] from PHOTOS, standard version, and SANC for $B^0 \to \pi^- K^+(\gamma)$ decay are superimposed on the consecutive plots. Standard distributions, as defined in the text and logarithmic scales are used. The distributions from the two programs overlap almost completely. Samples of 10^9 events were used. The ultraviolet scale, $\mu_{\rm UV}$, was chosen to leave total decay width unchanged by QED.

In Ref. [2], 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 4, 5 and 6 the implementation of the exact (but scalar-QED only) kernel brings a minuscule improvement in the agreement between PHOTOS and the reference exact simulation of SANC [27]. 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 price paid for improvement 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 standard one.

This high precision as documented in Figs. 5 and 6 is elusive: the dependencies on the production process may appear if form-factors (originating from some unspecified here models) which have to be fitted to the data.

From the technical side, one can interpret this excellent agreement as a strong test of numerical performance of the program. The necessary studies of the exact parametrisation 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. [2].

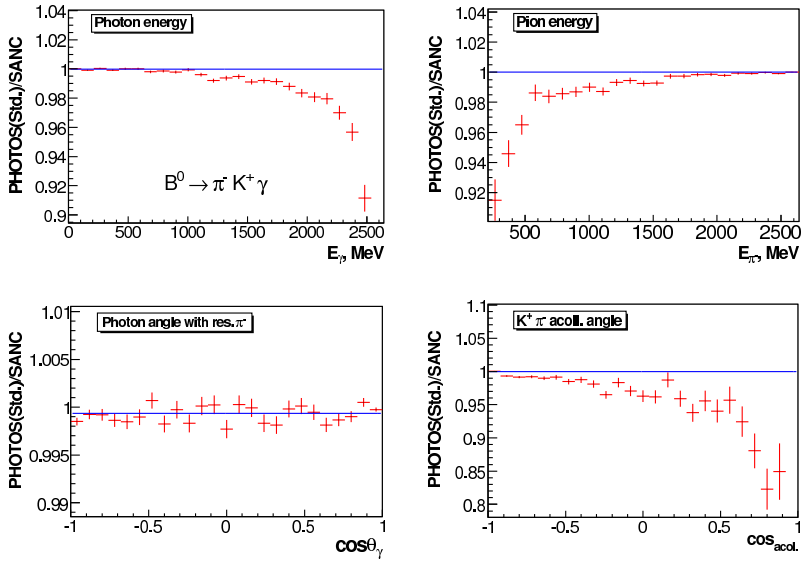

Fig. 5. Results [2] from PHOTOS, standard version, and SANC for ratios of the $B^0 \to \pi^- K^+(\gamma)$ distributions are presented. Differences between PHOTOS and SANC are small, but are clearly visible now.

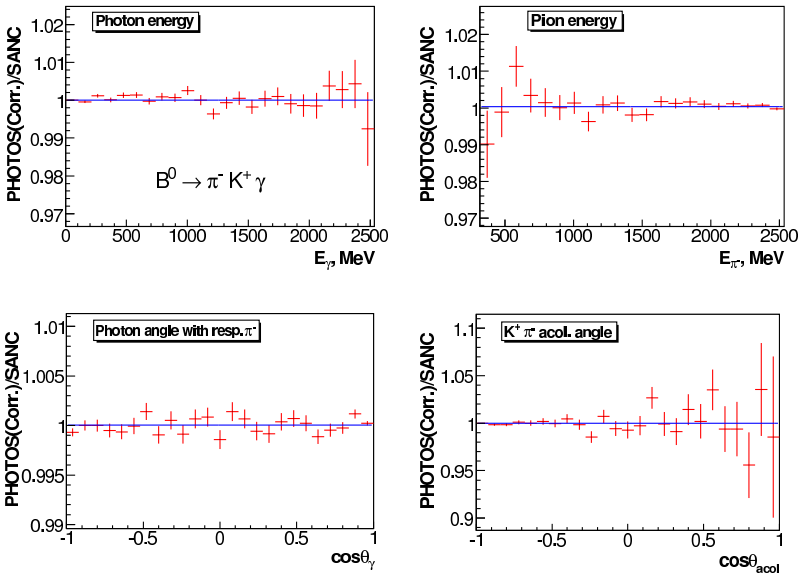

Fig. 6. Results [2] from PHOTOS with the exact matrix element, and SANC for ratios of the $B^0 \to \pi^- K^+(\gamma)$ distributions. Differences between PHOTOS and SANC are below statistical error for samples of 10^9 events.

4. Mathematical aspects of the solution

One can ask if there is anything substantial in common in all these solutions presented in Section 2, and whether systematisation with the help of mathematical language is worth an effort. Indeed, at the time of writing the first versions of the programs, which are now in a wide use, such considerations were of low priority. In fact to a good reason: they were expected to slow progress and bring little.

At present, when multitude of different solutions is available and technical complexity of details dominates over main principles of construction such effort may be well motivated and bring useful results.

Let us look at Fig. 7 where points, curved lines and surfaces on this heuristic plot represent consecutive manifolds of phase spaces for n, $n+1$, $n+2$ particles. Note that the dimensionality of manifolds is in principle counted by number of particles times dimension of Lorentz group representation, minus overall energy-momentum and orientation constraints. Curvature appears as an ultimate expansion parameter. The crude level distribution is also defined for phase spaces of n, $n+1$, $n+2$ particles but as energy momentum constraint affects only first n particles, the further ones constitute flat Cartesian sub-space. One step of the iterative projections as presented in Section 2 is symbolically presented in Fig. 8.

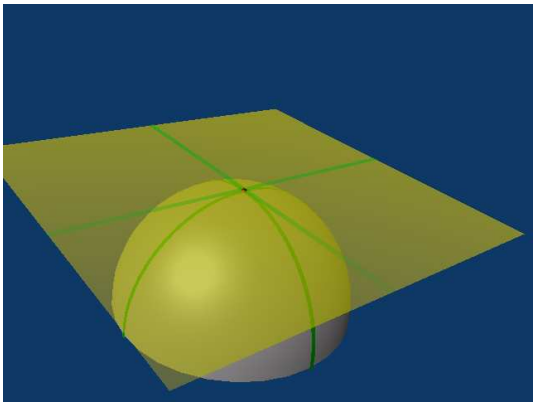

Fig. 7. Symbolic representation of phase space with up to two extra particles. Curved surface represent actual phase space and the flat one tangent space. The thin bands represent configurations where only one extra particle is added. Point in the center configuration of the Born level. It is implicitly assumed that particles of soft momenta do not provide much difference with respect to configurations when they are absent. That is why symbolically such configuration seem to coincide.

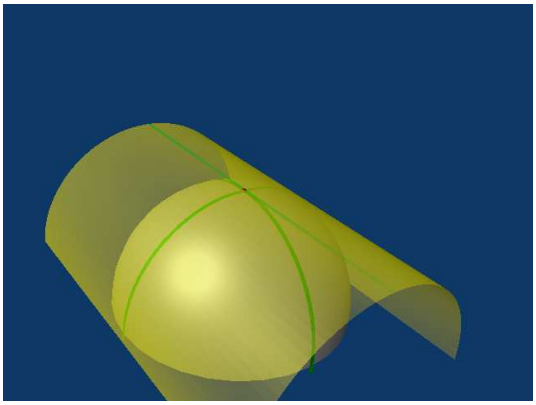

Fig. 8. As in Fig. 7 this plot symbolically reprints phase space with up to two extra particles. Curved surface represent actual phase space and the cylindric one the tangent space, where projection of kinematical constraint of one of its dimensions was already executed.

Case of QED and exponentiation of multiple photon radiation is rather simple, we do not need to worry about topological structure which is the same for the final (physical) phase space of multiphoton configuration and for the tangent space (constructed from eikonal phase space and matrix elements). The projection from tangent space to the real one is trivial

(at least from the point of view of topological properties). In the case of QCD we may expect complications, on the other hand, hadronisation models simplify the task anyway as they enforce separation of colour in the specific way. On the other hand it may be unhelpful for the discussion of the systematic errors.

There is another mathematical concept which is worth mentioning. Thanks to infrared sensitive regions of $n+1$ body phase space we obtain, in a natural way, a triangulation line for this $n+1$ body phase space manifold. In fact, structure of such induced triangulation needs to be (topologically) the same for tangent and physical space, the projections must match these triangulations. One can realize that the language of CW complexes (known in theory of homotopy groups) may be useful to systematise the description and to separate it into easier to digest parts.

Finally, let us point to nice relation between `PHOTOS` algorithm for single (and fixed order) bremsstrahlung on one side and for the multibremsstrahlung cases. The relation is a consequence of the properties of the tangent spaces. It can be seen from formal expansion of Poissonian distribution into sum of binomial ones. In the following formula we identify coefficients of binomial and Poissonian distributions: $p=\lambda$, $q=1-p$. Powers of p denote distinct multiplicities.

$$\begin{aligned}
\exp(-\lambda)\sum_{n=0}\frac{1}{n!}\,p^n\,|_1 &= 1(p+q)^1\\
\exp(-\lambda)\sum_{n=0}\frac{1}{n!}\,p^n\,|_2 &= \frac{1}{2}(p+q)^0+\frac{1}{2}(p+q)^2\\
\exp(-\lambda)\sum_{n=0}\frac{1}{n!}\,p^n\,|_3 &= \frac{2}{6}(p+q)^0+\frac{3}{6}(p+q)^1+\frac{1}{6}(p+q)^3\\
\exp(-\lambda)\sum_{n=0}\frac{1}{n!}\,p^n\,|_4 &= \frac{9}{24}(p+q)^0+\frac{8}{24}(p+q)^1\\
&\quad +\frac{6}{24}(p+q)^2+\frac{1}{24}(p+q)^4\,. \qquad (18)
\end{aligned}$$

These somewhat unexpected numerical constants, just ratios of natural numbers, provide trivial example of expansion of one set of special functions into another one. The consecutive lines of formula (18) correspond to expansion at, respectively, $1^{\rm st}$, $2^{\rm nd}$, $3^{\rm rd}$ and $4^{\rm th}$ orders.

5. Summary

In this talk we have presented some principles used in Monte Carlo construction. It was a perfect occasion to look into history of projects, often common with Prof. Jadach's. For that purpose illuminating mathematical aspects of the constructions seemed to be useful. They were one of the cornerstones in achieving quality and robustness of the results. In the presented talk we have concentrated on phase space and its possible description with the help of iterative Monte Carlo methods. Of course, main motivation of such a systematisation is to search for prototypes of algorithms to be applied *e.g.* in QCD. Work on matrix elements was only marginally mentioned here. It is only starting, but some results could have been already presented now, see talk by André van Hameren. For more, I am afraid, we need to wait for some time, even though some promising results are already available [28,29]. The next anniversary Epiphany conference, ten years from now, will hopefully bring some nice summary on that development.

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