METHODOLOGY OF PRECISION MONTE CARLO DEVELOPMENT — STASZEK JADACH IMPACT AS SEEN FROM MINE, 43 YEARS LONG PERSPECTIVE*

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I need to cover more than these 43 years! Staszek's achievements started before my time, that means before 1981. Some of these early steps were essential and hopefully his projects will continue to exist in the future. My aim is to collect the pivotal points of a lifetime research. Selection of these points was inevitable, moreover, some of them, which could be covered in an oral presentation, are not suitable for the printed version.

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1. Introduction

How to summarize life-long research activity of Staszek Jadach? I was hesitating how to cope with the task. Finally, I have decided that one should concentrate on research methods first, and also address main programs around which scientific work was organized. In the later sections, I will cover some of these points in more detail. The development of exclusive exponentiation, one of the breakthrough achievements by Staszek, was covered in Ward's talk [1] and I will not discuss those aspects here.

The main work aspects can be grouped in my opinion as follows:

- 1. Phase space and crude level Monte Carlo design.
- 2. Use of symmetries in phase-space parametrization and in matrix element ordering.
- 3. Matrix element preparation for use within numerical algorithms. Especially detailed recipes for factorization realization, or better say separation of amplitudes into parts.

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- 4. Design of programs and their development processes.
- 5. Parallel testing strategies of new features and older features, which may be degraded with new ones.
- 6. All aspects of user interaction, how can it help in collecting information on program usefulness and what priorities should define future work.
- 7. Choice of software tools, such as code managers algebraic algorithm useful in preparing matrix elements, configuration and makefile systems were of practical importance.
- 8. Of course, work on the projects required interaction with many other scientists, sometimes partners, sometimes competitors, but in many cases, the boundary between the two was opaque.

All these methods and work aspects were not pre-defined methodology elements. They appeared and could have been identified *a posteriori*. Nonetheless, they were present in all phenomenology activities. These research domain can be grouped around the computer programs. That is probably not an ideal choice but it is the best of what came to my mind.

- 1. FOWL [2] program Staszek mentioned many times. Was it the first source of his inspiration? That was before my time. I cannot add much.
- 2. To my knowledge, GENRAP is the first Staszek's published program [3]. It is for multi-particle final states and I may guess that many further projects development profited from this experience.
- 3. Mustraal [4] Monte Carlo for $e^+e^- \to \mu^+\mu^-$; 1(γ) process at LEP 1 energies.
- 4. KORALB [5] Monte Carlo for $e^+e^- \rightarrow l^+l^-$; $1(\gamma)$ at lower energies such as of Petra experiments. This program was the first to take into account τ -lepton pair production and its decay. Inevitably this required complete spin effects to be taken into account.
- 5. KORALZ [6] for $e^+e^- \rightarrow f\bar{f} 1(\gamma)$ (later $n\gamma$) at LEP 1 energies. It was the predecessor of KKMC, electroweak effects and Z boson exchange were carefully implemented, exponentiation was studied and validated but with respect to KORALB one step back was executed. Only longitudinal spin effects were taken into account.
- 6. KKMC [7] for $e^+e^- \to f\bar{f} n(\gamma)$ and for the center-of-mass energy range from several GeV to the one of FCC, is capable of taking into account complete spin effects.
- 7. BHLUMI [8] for luminosity, that is small angle $e^+e^- \rightarrow e^+e^- n(\gamma)$ process. It was of great importance to enable the measurement at 0.04% precision level, thus to control of all other cross-section measurements at LEP at that precision level as well.

- 8. Together with BHLUMI, the semianalytical calculation package for $e^+e^- \rightarrow e^+e^-$ was prepared and is also documented in [8]. This program provided BHLUMI tests with the alternative calculation of higher-order logarithmic corrections.
- 9. Similarly Oldbab [8] for $e^+e^- \rightarrow e^+e^- \ 1(\gamma)$ was instrumental in BH-LUMI tests with fixed, first-order matrix element simulations.
- 10. Bhwide [9] $e^+e^- \rightarrow e^+e^- n(\gamma)$ wide angles Bhabha scattering program.
- 11. Lesko [10] program for the $ep \rightarrow eX$ production at Hera.
- 12. TAUOLA [5] Monte Carlo program for τ lepton decays, this program was the offspring from KORALB and KORALZ projects¹.

Already from the above list, one can see that there is no clear separation between projects, some of them evolved from the independent ones into tests of the others. The opposite evolution direction took place sometimes as well. Inevitably the list is not complete. For example, the work on KORALZ, KKMC tests, which was as rich as for BHLUMI is dropped out from this list.

2. Projects

2.1. Phase space and Monte Carlo

For the precision predictions and integration over acceptance regions for realistic observables, Monte Carlo techniques are indispensable. This sounds trivial now, but it was not so. Still in 80s, only analytical results were considered to be of value, especially those of 1-dimensional functions which could be used for fitting. The Monte Carlo method was belonging to the peripheral experimental activity. This was to change slowly.

Exact phase-space generation and its explicit parametrization was one of the quality stamps² established by Staszek Jadach. All approximations were localized in matrix elements which were provided in explicit form, thus open for improvements. This was essential for the success of the method.

That opened the gate for solutions based on the Yennie–Frautchi–Suura re-organization of perturbative expansion, for this, see [1]. Into such designed programs, new physics effects can be easily injected, but what is more important, a systematic approach to ambiguities evaluation can be established.

¹ Program PHOTOS for radiative corrections in decays [11] represents offspring from TAUOLA, and for PHOTOS off-springs, the work on simulation of exotic new states like [12] can be classified. This is an example of how Staszek's work initialized other people's consecutive chain of projects. For sure, this is just an example.

² Advantages of semi-communist Poland of 70s: particular freedom in scientific work direction, long-term projects accepted.

Now, let me recall the KKMC Monte Carlo for $e^+e^- \rightarrow \tau^+\tau^-(n\gamma)$ process (with τ decays). This is because KKMC (together with its predecessor KORALZ) represent the rigorous implementation of "matrix element × full phase space" field theory calculation. The design consists of:

- Phase-space Monte Carlo simulator, the module producing "raw events" (including importance sampling for possible intermediate resonances, collinear and soft singularities)
- Library of Matrix Elements; input for "model weight"; this is complete independent module, see Fig. 1.



Fig.1. Structure of Matrix Element based Monte Carlo programs, the case of $\mathsf{KKMC}.$

- The solution was used extensively for LEP precision Monte Carlos.
- Earlier difficulties with the k_0 boundary could be overcome. The k_0 boundary earlier was necessary for the Monte Carlo implementation of fixed order field theory results. It was necessary to integrate soft photons configurations over some regions (limited by k_0) and the resulting function was summed with the virtual corrections to cancel infrared singularities. This was introducing technical bias or negative weight events. In practice, k_0 could not be set too small and that was bad for the detector response simulations.

2.2. Phase-space parametrization and Monte Carlo

The oldest phase-space Monte Carlo program Staszek was mentioning was FOWL [2] and it was referenced in GENRAP Staszek's early paper [3].

This work was important because experience with pre-samplers and multiparticle final states likely started there. Only few and indirectly accidentally achieved details are known to me. I have to rely on guesses from short scattered Staszek's comments. All that was happening before my time.

But let me recall some other aspects of phase-space generation. Careful, matrix element features adopted, choice of reference frames. We could offer ourselves to spend a lot of time on that, because there was no pressure on us from grant applications *etc*.

Let me mention now, two early papers, the first [13], with careful choice of phase-space parametrization matching perfectly the structure of matrix element enhancement³. To express details, I have provided a page from the old preprint in Fig. 2.



Fig. 2. Example of careful study of matrix element details. Useful for matching phase-space presamplers for matrix element peaks.

³ During my first trip to the West, in 1983, I was desperately digging into the inconsistency of that program run with benchmark print. Finally, I realized that the program code, which I had on magnetic tape, I brought from Cracow with me, was missing two lines. This was because the tape was written directly from the read of the punch card deck. What a waste of time and energy! Not really. Now I see that this was a blessing. I studied phase-space parametrization to the last details. Without that, miserable experience PHOTOS Monte Carlo would not be made.

The second paper [14] was about phase-space parametrization and choice of reference frames for the sake of spin degrees of freedom and interfaces between generator for intermediate τ -lepton pair state productions and then decays. In Fig. 3, a page from that paper is recalled. It is about the use of vector or spinor indices for the expression of intermediate quantum state configuration. That was an element of the attempt for the most compact, most intuitive expression. Without this experience, the work on applications like TauSpinner [15] would not be easy to start. In this work, the algebraic language SCHOONSHIP was used. With its help, long formulas could be controlled, but it was not possible to use them directly. The formulas, indispensable for tests, were difficult to shorten, and thus not very useful for intuition to build upon.

Lesson from Staszek:

The long 1000+ terms formula gives equally good results as the short one, so why waste time to get it shortened to few terms only? What a loss of time, many people were saying, computers are fast and soon will be even faster, I thought that way too. But in this work by hand, every detail had to be watched twice or more. I have profited till now from that.

The possibility was not exploited to the very end. I never got time to understand transformation of analytic (already short) functions for virtual corrections, in transition from massive fermions to ultra-relativistic regime. What could it bring for: factorizations, underlying events? What are the issues of many variables analytic functions? The change in Poland social environment prevented that. We had to work more efficiently for publications and reports, long-term investments could not be a priority anymore.

Lesson from Staszek:

- The use of vector or spinor indices is equivalent and in both cases formulas are short if proper frames are chosen.
- Formulas based on aggregated spinor degrees of freedom are slightly shorter.
- Vector degrees are easier for intuition and thus for optimal variables definitions.
- Spinor representation reappeared later [16], with Kleiss–Stirling spinor techniques it was a must. Generally, it is OK even inescapable, but unfriendly for intuition to build⁴.

⁴ Let me recall some keywords only for other, omitted here aspects: interferences, timeposition representation, visible in this representation partial cancellations, massive vs. massless calculations, precision counting beyond N^n .

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In the last formula the index i = 1, 2, 3 numbers the three components of \vec{w}_1 in the rest frame of the τ^+ lepton and the k = 1, 2, 3 numbers the axes in the rest system of the τ^- lepton. In both rest frames the third axis is the spin quantisation axis as in the definition of α_1 and α_2 and the first axis is defined to be perpendicular to the reaction plane i.e. along τ -vector. In (2.5) the absence of terms linear in w_k like $\sum_k R_{0k}^0 w_2^k$ and $\sum_k R_{i0}^0 w_1^i$ means that each τ^{\pm} separately is not polarized in the lowest order. There are, however, correlations between w_1 and w_2 which are controlled by the matrix R_{ik}^0 . We extend the matrix R_{ik}^0 to R_{ab}^0 with a, b = 0, 1, 2, 3 obtaining

$$R_{ab}^{0} = \begin{bmatrix} 1 + c^{2} + M^{2}s^{2}, & 0, & 0, & 0\\ 0, & -(1 - M^{2})s^{2}, & 0, & 0\\ 0, & 0, & (1 + M^{2})s^{2}, & 2Mcs\\ 0, & 0, & 2Mcs, & 1 + c^{2} - M^{2}s^{2} \end{bmatrix}.$$
 (2.6)

In order to calculate the matrix R_{ab}^0 as given by equation (2.6) directly from our spin amplitudes defined in Eq. (2.3), we have to translate the bispinor indices in the joint density matrix given by

$$\varrho^{0}_{\alpha_{1}\bar{\alpha}_{1}\alpha_{2}\bar{\alpha}_{2}} = \frac{1}{4} \sum_{\lambda_{1}\lambda_{2}} M^{0}_{\lambda_{1}\lambda_{2}\alpha_{1}\alpha_{2}} (M^{0}_{\lambda_{1}\lambda_{2}\bar{\alpha}_{1}\bar{\alpha}_{2}})^{*}$$
$$= \frac{1}{2} U^{2} \left[|\alpha_{+}\bar{\alpha}_{+}| + \alpha_{+}\bar{\alpha}_{+}c^{2} + M^{2}s^{2}\alpha_{-}\bar{\alpha}_{-} - \frac{i}{2} (\alpha_{+}\bar{\alpha}_{-} - \alpha_{-}\bar{\alpha}_{+})2Mcs \right]$$
(2.7)

into vector indices a and b, see (2.6). The answer may be read off from Eq. (2.4) by substituting in the operator $\Lambda_{\pm}(p, w)$ as polarisation vectors the three space-like vectors $\hat{e}_1 = (0, 1, 0, 0)$, $\hat{e}_2 = (0, 0, 1, 0)$ and $\hat{e}_3 = (0, 0, 0, 1)$ and comparing the results with the bispinor quantities $u(p, \alpha)\overline{u}(p, \overline{\alpha})$ in the τ rest frame, p = (M, 0, 0, 0), α being the spin projection onto $\overline{\hat{e}}_3$. The result is

$$\begin{split} \Lambda_{+}(p, \hat{e}_{1}) - \Lambda_{+}(p, 0) &= \tilde{\Lambda}_{+}(p, e_{1}) = u(p, +)\bar{u}(p, -) + u(p, -)\bar{u}(p, +), \\ \Lambda_{+}(p, \hat{e}_{2}) - \Lambda_{+}(p, 0) &= \tilde{\Lambda}_{+}(p, e_{2}) = iu(p, -)\bar{u}(p, +) - iu(p, +)\bar{u}(p, -), \\ \Lambda_{+}(p, \hat{e}_{3}) - \Lambda_{+}(p, 0) &= \tilde{\Lambda}_{+}(p, e_{3}) = u(p, +)\bar{u}(p, +) - u(p, -)\bar{u}(p, -), \end{split}$$
(2.8)

and in addition

$$\Lambda_+(p,0) = \tilde{\Lambda}_+(p,0) = u(p,+)\bar{u}(p,+) + u(p,-)\bar{u}(p,-).$$

Similarly Λ_{-} can be expressed in terms of $v(p, \alpha)\bar{v}(p, \bar{\alpha})$, see Appendix A. In practice, instead of employing directly the relations (2.8) to translate the sixteen elements of the joint density matrix in spinor notation into the sixteen elements of R_{ab} we rather introduce some sort of vocabulary which maps factors like $|\alpha_{+}\bar{\alpha}_{+}|$, $\alpha_{+}\bar{\alpha}_{+}$ etc. into elements of R_{ab} . For instance $\varrho_{\alpha_{1}\bar{\alpha}_{1}\alpha_{2}\bar{\alpha}_{2}} = \frac{1}{2}U^{2}|\alpha_{+}\alpha_{+}|$ yields the non-zero elements $R_{00} = 1$, $R_{11} = -1$, $R_{22} = 1$, $R_{33} = 1$; all other elements vanish. The complete set of the relations of this type is also

Fig. 3. Spin density matrix, vector or spinor degrees of freedom?

The reference frame trees, established in 80s, remain useful till now. The choices match the geometry of Lorentz group, its representations, and help to expose properties of field theory amplitudes. Not only of first order but of higher as well.

These reference frame trees were always in the background: (i) in design, (ii) in tests, (iii) in use for phenomenology, *e.g.* in the design of optimal variables for some physics quantities of particular interest.

The properties which are behind the choice of these reference frames break with $\mathcal{O}(\alpha^2)$ non-enhanced corrections. That is ~0.01% QED and ~1% level for QCD.

In KKMC different organization is used, it was imposed due to the Kleiss– Stirling spin amplitude techniques (on one side) and complexity of numerous cases for multi-particle final states (on the other). But previously accumulated experience was so much useful!

By now, implicitly I have addressed the following projects from the list: Mustraal, KORALB, TAUOLA, KORALZ, KKMC. Now, let me turn to another topic, work on phase-space and matrix element preparation.

Lesson from Staszek: they need to be dealt with together.

In the construction of Monte Carlo, properties of phase space and matrix elements are to be correlated. It is obvious that matrix elements represent forms on curved space (phase space can be understood as a tower of manifolds connected by triangulation-like relations induced by infrared singularity cancellations). But that is not all, one has to construct (if precision is at stake) a tower of theories/models. Let me recall some points, but without going into details:

- 1. Independently of event construction, step approximations need to be controlled in all details.
- 2. Only then, things can be improved in the following event construction steps and final ambiguities evaluated.
- 3. Solution of KKMC or BHLUMI generators was exploiting the fact that QED can be expanded starting from eikonal parts of matrix elements⁵.
- 4. At the eikonal level conformal symmetry is helpful both for matrix element and for phase-space representation.
- 5. Eikonal level QED can be solved to all orders and can be implemented into Monte Carlo generation as the crude level generator.

 $^{^{5}}$ Note the difference, I am not writing about eikonal approximation.

- 6. Up to the second order, it matches the structure of enhancements present in complete QED or even Standard Model processes (for many interesting processes at least).
- 7. Beyond that level, further effort on fundamental things including topological issues like manifold triangulation will be needed. Maybe mathematical theory of C-W complexes will be of help?

2.3. Testing strategies

For many years, people used to say, why do we need to control technicalities if we are missing a larger effect due to limited perturbation order. As seen from a short-time perspective, that is rather natural choice. It may be even inevitable if you work under pressure *e.g.* from the prospective of next post-doc applications to come. Staszek was following a different path. He was always devoted to details and that was beneficial for the later steps in his work.

Note that special strategies for systematic error control, with the help of correlated event samples were devised. For the KORALZ generator, it is described in [17] and for the W-pair production KandY-project, in [18].

Lesson from Staszek: control approximations as good as possible.

Luminosity calculations and the BHLUMI project was the field-theorybased Monte Carlo of the highest precision ever. It was one of the essential elements for OPAL and ALEPH luminosity measurements and their interpretation. The sub-permille precision level was reached.

2.4. User interaction

Luminosity and overall normalization of all cross section were essential for many important measurements, for example, number of neutrino species including heavy neutrinos, and for the Standard Model tests, including tests if its quantum effects were of importance.

When LEP experiments were about to start, it was expected that the precision of luminosity measurement will be about 2%. The demanded precision for luminosity Monte Carlo programs was about 0.5% only. Thanks to development on exponentiation, far better precision for theoretical predictions was possible. But why do devote one's time to project which may be of no need? Staszek first motivation was just that it was possible. Because of Staszek's previous achievements, a promise of precision delivery was convincing. Lumi detectors were constructed. First by ALEPH, later by OPAL. That was a **great success**, worth a long presentation in itself. Essential was users–authors interaction, and in particular, the resulting motivation.

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I will comment on how precision was evaluated. Luminosity quest for precision was fascinating and I will use it as an example. At the start, there was analytical (semi-analytical) calculation. Approximate acceptance did not require Monte Carlo. That was the case of luminosity many years before LEP too. But with time, it turned out that it was not true anymore. Some detector effects were implemented with the first-order Monte Carlo generators which we named **Oldbab**, for us it became part of the tests.

To avoid k_0 problems, some phase-space regions of bremsstrahlung photons were integrated over and results combined with virtual corrections. The price was systematic ambiguity. For the 2% precision level that was acceptable though. But with better detectors, in some regions (distinguishable by the detector), that would mean the locally negative cross section as k_0 had to be set low.

For theoretical calculations aiming at a fixed-order result, we could overcome that, with the help of introduction of negative weight events. Simulation had to be used for simplified observables only.

A combination of semi-analytical and fixed order calculations was useful. The use of correlated event samples was useful again, but it was awkward in use, flexibility for experimental application was not sufficient, precision was limited too.

Even once BHLUMI, luminosity Mote Carlo based on exponentiation was designed, these calculations and techniques based on correlated event samples, of fixed-order event generation and parallel generation based on the structure function approach (embedded in the Lumlog package) offered an essential test platform.

Numerous comparisons were collected. An approach based on three types of precision arose:

- 1. technical precision, should be at least 3 times better than statistical precision,
- 2. statistical precision, should be at least 3 times better than required physics precision,
- 3. physics precision

was finally established.

With all these works, Staszek and his collaborators and partners could provide the reliable tool-box, which was helpful to encourage work on lumi detectors. Finally, detectors were built. We can argue now what was first, the promise of precision for theory predictions or the start of work on detector work. This is not clear to me, in fact, it is not so important. But it offered an example of inter-inspiration for theory and detector efforts.

3. Summary

My presentation cannot be easily summarized. It is not rigorous and is missing essential to understand details. Instead, let me recall the last Staszek's demand for me: prepare the third-order QED (triple bremsstrahlung part) of matrix element in a form suitable for installation into a program like KKMC. The first step in that direction is already completed [19].

But this is the single step of a long journey. Further steps will include: double bremsstrahlung β_3 of YFS, with mixed real-virtual arts, contact interaction expansion for *t*-channel boson exchange.

One has to keep in mind — charged Higgs ghosts contributions to $e^+e^-\nu_e\bar{\nu}_e\gamma\gamma\gamma$ that complication, arose already at second order [20]. Then higher-order QCD corrections, running α_{QED} : both s- and t-channel; check if unitarity is not damaged by complex boson mass schemes beyond one-loop level. How to match fixed-order calculation results for matrix elements with the ones on exponentiation in its exclusive form?

Will differential geometry, topological expansion, triangulation theory, CW complexes, and resulting new formalism be needed? Conformal symmetry possibly not only for phase space and eikonal parts of ME, but its shadows for systematization of non-leading parts as well?

I was talking about aspects necessary for long-living projects developed like the ones of Staszek which have remained competitive for more than 4 decades now. How to convince community of future users and developers to follow? For children rising, one needs: father, mother, the whole village, and teachers too.

For Monte Carlo phenomenology projects, one needs to accumulate experience of:

- Mathematical, phase-space geometry side.
- Perturbative results represented in a useful form.
- Software development and test strategies, software organization.
- How to assure work stability.

It is important to realize (keep in mind projects like FCC) that so much better precision will be required then. New solutions will require thirdorder matrix elements in a form matching exclusive exponentiation. Only then, dominant higher than third-order parts of amplitudes can be included too. What about two-loop electroweak effects, complex masses *vs.* unitarity constraints? What about separating out QED from whole SM and what about parametric ambiguities?

Work with new contributors may be smooth for some time, but become challenging for long-term perspective like that of FCC. Educated/trained people choose other careers; often outside physics.

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In facing all these challenges, Staszek will be missing a lot! Let us do what we can for Staszek's work to continue into new horizons.

Therefore, send not to know For whom the bell tolls, It tolls for thee. John Donne 1572–1631

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