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ASSOCIATED PROJECTS TO PRECISION MONTE CARLO PROJECTS*

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I cover usually omitted essentials from more than 43 years of my own experience in the domain of precision Monte Carlo programs development. I was not working alone, my work was a continuation of earlier efforts. For example, Stanisław Jadach's achievements before 1981 were essential. I was working with him and B.F.L. Ward over most of these years. Also, monumental projects of Bryan Lynn, Robin Stuart, Dima Bardin, and Wolfgang Hollik in the domain of precision physics need to be mentioned, because they affected my work. This is a challenging call for me! Usually, we were publishing our own projects, and the following incomplete lists of methodology domains and projects were left aside in references, appendices, and private notes: *(i)* phase space: symmetries, *(ii)* matrix element preparation → factorizations, *(iii)* program and development process design, *(iv)* testing strategies, *(v)* user interaction, *(vi)* software tools, *(vii)* partners and competitors. The work started on the basis of previous efforts which can be listed following names of the programs: *(i)* FOWL, *(ii)* GENRAP, *(iii)* Mustraal, *(iv)* Koralb, *(v)* Lesko, *(vi)* TAUOLA, *(vii)* KORALZ, *(viii)* LUMLOG, *(ix)* OLDBAB, *(x)* BHLUMI, *(xi)* BHWIDE, and *(xii)* KKMC. I will focus on some of these points. Others, hopefully, are sufficiently well covered in other papers. In particular, I do not need to cover exponentiation, see contribution to the proceedings by W. Placzek and talk of B.F.L. Ward. Developments took years and did not follow a straight line; that is why there are inevitable simplifications and biases in my presentation. Also, a review of the essential literature could not be completed.

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1. Introduction

One of the aims of high-energy physics experiments is to confront measurements of interesting observables with field theory predictions. Agreements mean *precision tests* of theory and/or measurements of *coupling constants, masses*, *etc.* Disagreement points to *New Physics*. What is needed to

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perform such a program in the case of accelerator measurements, especially in cases when precision is essential? I need to address the lifetime effort of several people and only as a starting point, because I want to point the direction for future work. There are too many aspects to be covered in my article.

Experiments (even of *pp* collisions) best measure directions of muons, then of electrons, then energies of muons, later of electrons. Jets are measured less precisely. From the experimental side, one needs to adopt acceptance details, often irregular and direction-dependent. Detectors consist of rectangular (even worse nearly rectangular and of vague edges) cells forming a lattice or better to say kind of 3 dimensional web. In this web, there are dead zones (due to cables). The detector response in the barrel and forward regions differs somewhat. Sometimes, parts of detectors are faulty, and this makes even more irregular shapes of acceptance domain.

That, as we have seen in the past, does not bring big complications if precision requirements are not very high. At the 1% precision level, things look fine. The complications arise at the 0.3% precision level. The methods of lesser precision become complicated, but are still possible to use. Things change if the precision level of 0.1% or better is demanded. These are essential preconditions from the experimental side, and they define what is needed from the theory community. That are the lessons from the past.

I cannot cover details of the projects nor provide even a partly completed list of publications. Let me address interested reader to references in [1–5] for the main projects. Typically, each one is involving many man-year efforts. I will rely on achievements and LEP I era observations [6], where in some cases, precision better than 0.1% in comparison of data with theory predictions was achieved. Now I will underline the importance of efforts not directly on the phenomenology programs used by the experiments in theory–data comparisons, but other projects developed independently earlier. More than often, their results needed adaptation and, often painful and complicated interactions with users. Hopefully, that experience will be useful for work on the future 0.01% precision regime of experiments such as at FCC, where precision at least *one order of magnitude* better than that at LEP is expected.

Precision predictions require managing **conflicting requirements**. *The most important are those from experiments,* because massive human and financial efforts are involved. That is why I have mentioned that at the start. Can phenomenology work ease these burdens? Break no-go limitations? For high precision or for rare processes where background tails play an important role, nothing is easy ...

2. From the past

Theoretical calculations, due to ultraviolet infinities, tend/must be organized keeping in mind renormalization. That is understandable; that is the way to deal with it. That implies that usually mass corrections (thus phase-space details too) are added later, sometimes at a lower perturbation level.

What does it mean? What are the challenges and pressure on solutions, that must include details from theory and experiments simultaneously? This is not always necessary. For example, fitting functions (analytic or semi-analytic) with idealized acceptance are essential, even now, in the Machine Learning (ML) world.

Intermediate detail level tools are helpful and will remain so in the future. I was advocating such solutions too [7] (and at the end, this failed). **Advantage:** For simplified acceptance with dressed leptons, *etc.*, mass corrections are less important and, in general, higher-order results are easier to get and incorporate.
Disadvantage: Detector acceptance details have to be calculated/simulated separately.

I am advocating the necessity of the approach where all details of experimental acceptance and theory predictions can be evaluated together. But we have also used incomplete phase-space solutions which worked well and smoothly down to the 0.5 % precision level. Let me list them now: a good example was a first-order, matrix element based simulation, combined with a statistically correlated leading log based simulation with collinear photons only: OLDBAB+LUMLOG. The semi-analytical approaches like that of Refs. [8, 9] were useful. But later at 0.3 %, 0.1%, 0.043% levels, they gave way to more refined tools (but remained as essential tests [10]). Another example is KandY [11] correlated simulations of 4-fermion final states with initial-state exponentiation KORALW for all tree diagrams, and YFSWW3 for initial- and final-state radiation with only double resonant diagrams for the hard interaction. An idea is rather a trivial application of the Taylor expansion. Replacing $(1+A+B)^2 \to (1+A)^2+(1+B)^2-1$ can work well in many conditions. One has to define A and B carefully:

A — effects of all tree-level diagrams with respect to double resonant ones (initial-state exclusive exponentiation of QED only);

B — effects of exclusive exponentiation for initial- and final-state QED effects but for hard interaction of double resonant diagrams only.

These were also essential steps of work on Monte Carlos, and in many cases, enough, even if it brings *massive difficulties for the experimental users.*

Final, precision solutions were based on simulations with all details of phase space and higher-order induced kinematical configurations included, and cutting-edge theoretical effects included. On the other side, fitting functions to evaluate the impact of theory variations were used as well. The demands were not easy to follow. At LEP I, simulation had to take care of configurations *with explicit 3 bremsstrahlung photons*. For FCC, this will probably require *5 photons*. Such configurations are essential to understand effects due to the detectors' cell structure, but their inclusion complicates the implementation of other theory effects. That points to an important work domain, how to match calculations of distinct perturbation order.

In the future, precision requirements will bring more complications. One of the necessary steps will include the need to simultaneously include new processes such as production of 4-fermion, 6-fermion (or jets) final states (of intermediate states such as WW, ZZ, ZH, or tt).

Many solutions will be working smoothly at the 0.5% level and will also open the gate to new applications as benchmarks. But finally, no compromise on phase-space details can be assumed. As KandY was a step forward with respect to solutions such as OLDBAB+LUMLOG, or Mustraal+YFS2 installed in earlier version of KORALZ, this will have to give way to solutions such as KKMC, BHLUMI with fitting functions for idealized but matching simplified kinematics.

In the following, let us look at 2-fermion production such as $e^+e^- \to l\bar{l}$ or Bhabha scattering. In these cases, high precision was achieved in comparisons between experiments and theory. There were several steps of the effort. Separation of SM results into one of QED and hard-interaction effects, effectively of genuine weak effects and vacuum polarization, including some strong interaction loop effects. Also New Physics can often be treated as part of the hard interactions. Logically, that was the first step, enabling treatment of QED separately. For QED, eikonal parts of amplitudes for the process of multi-photon production $\beta_0 \times \int \ldots$ plus corrections where one of $\int$ in the product was replaced by β_1 or the pair by β_2 were necessary to be available perturbatively. That is the essence of the YFS way for the reordering of the QED perturbation expansion. Already at the zero-th order, kinematical configurations with arbitrary large number of photons and all over the phase space become available. Gauge invariant sectors: initial-state, final-state, and their interference (for Bhabha upper line, lower line and interference) could be established and treated separately. Note that interference effects (real and virtual) can be added at later steps by re-weighting (with bounded from above weights). For the interference, contributions for $\beta_0, \beta_1, and \beta_2$ appear later. I have omitted the topic of QED loops. They follow a similar pattern. Instead now, let us turn to foundation of event generation algorithms.

Part of QED consisting of eikonal terms for initial- and final-state bremsstrahlung can be solved to all orders, results represent a **functional** exponent. That includes an algorithm for complete phase space (number of explicit photons is one of the generation variables too), which could be constructed on the basis of incomplete, but known exactly and analytically, amplitudes.

Why the algorithm was possible? This is due to the *conformal symmetry* of eikonal factors and the phase space of massless photons. That created the basis of an algorithm where initial-state photons, invariant mass of intermediate state, and final-state photons could be generated independently. Firstly, independently generated photons could be constrained to phase-space limits using scale symmetry.

One should mention a minor difficulty. To match into the formulae virtual corrections, one has to have an algorithm to deal with photon candidates of energies (after re-scaling) below the lower limit for generation. The lower limit of photon energy can be arbitrarily low, but should be the same for all photons to enable matching with virtual corrections and their infrared singularities. Fortunately, for that regime, eikonal parts of amplitudes are enough.

Once events are generated with the algorithm based on eikonal parts, with re-weighting, we can introduce matrix elements of QED: β_1, β_2. That looks simple, but it is not always so. For ν_e production and β_2 contribution, one has to add charged Higgs ghost exchange Feynman diagrams. Is it still QED when emissions from charged Ws must be taken into account?

Now let us turn our attention to non-QED parts of the amplitudes. The cancellation of singularities requires QED contributions to be organized before adding hard interactions in the form of form-factors to be introduced for couplings, otherwise gauge invariance would be ruined. That worked fabulously well at the 0.1% precision level and Center of Mass System (CMS) energies below 205 GeV. But already at slightly higher 212 GeV CMS energy, picture started to change.

A huge effort on genuine weak corrections was needed, even at the one-loop level of LEP I times. Lots of discussions accompanied, on so-called star couplings, and at the end on electroweak form factors used to parameterize improved Born. Analytic and anti-analytic constraints of field theory need to be preserved. This was proven to work well at the 0.1% precision level. No compromises were needed. Anti-analytic features, optical theorem, Cutkosky rules, were broken only at $\mathcal{O}(\alpha^2) \sim 10^{-4}$. This may not be enough for the FCC regime. One may need to revisit and extend this massive effort on perturbation expansions re-ordering, before Monte Carlo implementation can be completed.

2.1. From the past, summary . . .

Even at the LEP precision level, the eikonal part of QED was needed at least to *the third order.* Thanks to re-ordering of the perturbation expansion, one-loop genuine weak effects were sufficient. For FCC, that will probably mean two-loop genuine weak plus third order QED and may mean 5th order for the eikonal in its part? We have some hints on how to start work for the 0.01% precision level, see *e.g.* [12] but the question is how to keep projects ongoing, with expertise to be passed to new contributors and let it be extended.

One should not forget the usefulness of older style solutions such as OLDBAB+LUMLOG or KORALZ(YFS2)+Mustraal(FSR) which offered a gateway to the framework of NLL-NNLL picture of some ambiguities evaluation. In every case, observable-dependent evaluation of ambiguities must be in numbers. Only that is meaningful for measurement–theory comparisons. In fact, it was succesful for the 0.3% precision level and even somewhat beyond. It became, with precision, rapidly very laborious and thus not very convenient (to say the least) for the experimental users, who had many other things to keep in mind.

2.2. Technicality hint from the KKMC project

My intention was not to talk about internal elements of KKMC because this is supposed to be covered in other talks. Nonetheless, before I will comment on some requirements for the future, I need to mention one essential step: from vector indices to spinor indices. KKMC works not only on spin amplitudes, to enable reduction of the number of terms, because interferences can be calculated directly from squares of the sum of complex interfering contributions (true for real emissions). Vector objects residing in the Feynman diagram (like $\not{k}$) are represented as the outer product of spinors. That is due to the Kleiss–Stirling spin amplitude language. That was an achievement of the CALKUL Collaboration [13]. Lots of repetitions in calculations could be avoided. It was advantageous and reduced the size of the code for formulas a lot. It enabled useful tests, also for partial results. One should not ignore that, from spin amplitudes, density matrices for τ-pairs can be calculated safely and accurately from first principles, in the presence of an arbitrary number of photons. Also, the spin amplitudes level was helpful in the definitions of β_i terms for the Yennie–Frautchi–Suura exponentiation and to exploit it fully.

3. Toward the future

For the precision level $\sim 0.01\%$ two-loop electroweak corrections will probably be needed. Also, the third-order QED correction and possibly up to 5^{th} order of dominant eikonal parts of QED, because that means configurations of 5, to be generated including detector response, photons. For that purpose, two-loop electroweak corrections need to have the form with separated, QED and remaining genuine weak parts, and already at the amplitude levels. Only then, results can be matched with QED at a higher, that is, third order. On the other side, two-loop electroweak corrections will impose new pressure on how, also necessary for precision, higher than second-order QCD corrections can be introduced. This is also true about the part of non-perturbative QCD effects taken from low energy $e^+e^- \to$ hadrons data. In contrast to what was the case at LEP I, for two electroweak loops, higher-order QED-QCD needs to be added not only for s-channel or t-channel exchanges but for both of them *simultaneously*. Then, one may need to review details of complex mass schemes. Solutions proposed by R. Stuart and later by A. Denner, to preserve constraints of the optical theorem and Cutkosky rules need to remain valid with the first offending terms at the $\mathcal{O}(\alpha^3)$ level.

At the 0.01% precision level, corrections due to 4-fermion production (and corresponding virtual corrections) will be needed in full. All that complicates the framework for the calculation and implementation of bremsstrahlung amplitudes. In particular, effects of interferences (which are sensitive to delicate cancellations between virtual and real corrections) and finally crude level generation will need revisiting. For that purpose, the mathematical language of tangent spaces and CW-complexes may be helpful. CW-complexes may be helpful to systematize the matching of collinear/soft sub-spaces. That was already used in the case of PHOTOS Monte Carlo.

If s-channel and t-channel exchanges contribute simultaneously in a sizable manner, the use of contact interaction and expansion with respect to contact interaction may be helpful. The inspiring example [14] for ν_e may be hopeful in the future as well. One should not forget the questions of tests. *It is so easy* to make the code work 'nearly correctly'. New tests may be needed, because one may need to introduce many adaptations which may make automatic algebraic manipulations not straightforward to use.

This may result in many of the calculations not being used as off-the-shelf segments. That is why there is a quite broad spectrum of necessary tests to prepare. Such tests, as in the past, will sometimes coincide with phenomenological projects. Big pressure comes from the need to identify the QED part of complete electroweak calculations.

Lots of new testing techniques, theoretical calculations to provide benchmarks and numerical results to evaluate the reliability of physics parts will be needed. That means long-term projects. Also from the software side, using physics input, development of algorithms and tests will be needed. For the computer software engineer perspective, see [15, 16]. We should not forget about the manpower and expertise of all subdomains to survive. One needs to keep the following in mind: How does one identify the requested parts of amplitudes? How does one explore properties of the Lorentz group, its sub-groups and corresponding layers? How does one treat extended theories and their symmetries? Subtracting at the cross-section level was found to be useful at the one-loop level, but what about higher orders? How does one then avoid negative weight events? In this, beware of detector granularities and details.

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