

ON THE ROLE OF THE PRECISION MONTE CARLO GENERATORS IN FUTURE ELECTRON COLLIDERS* **

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In this note, we argue that in the future electron–positron colliders with up to two orders higher event rates, the role of the Standard Model precision calculations in the data analysis performed using Monte Carlo (MC) event generators will be dominant, much more important than in the past LEP era experiments. This will require designing, constructing and testing an entirely new class of the precision Monte Carlo event generators for all important processes such as production and decay of the Z and Higgs boson, W pairs and the Bhabha process. We are going to outline challenges on the way to construction of these new MC tools and foresee possible lines of technical developments which will be necessary.

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1. Introduction

In the FCC-ee, the most ambitious of the future electron–positron colliders [1], thanks to very high luminosity, the experimental precision will be higher than in the past experiments by up to two orders of magnitude. It is therefore quite urgent to think already now what will be needed for full exploitation of the future data at this precision level. In particular, we are going to cover in this note the new increased role of the Precision Monte Carlo simulation in constructing the so-called pseudo-observables, encapsulating the essence of the future experimental data.

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In the celebrated global fits of the SM or SM + higher-order operators, we see pseudo-observables such as $\sin^2 \theta_{\text{eff}}$, masses, couplings, which are essentially “tree level” and are extracted from data using the mapping:

$$\text{DATA} \longleftrightarrow \text{Born}(x_i) \otimes \text{QED}.$$

This technique of electro-weak pseudo-observables x_i (EWPOs) was coined up while analysing data at LEP experiments. It is not obvious at all whether this technique will work in the future e^+e^- colliders with the precision much higher than that at LEP — simply because it involves many approximations and simplifications which may turn unrealistic at higher precision of the electron colliders. More precise experimental data in their multi-dimensional space may expose a much richer structure which cannot be cast into the primitive $\text{Born}(x_i) \otimes \text{QED}$ template of the LEP algorithms. This LEP EWPO technique is described in a detail in Ref. [2] by Bardin, Grunewald and Passarino, where it was proven that it is barely compatible with the LEP data precision, but not beyond. Already in their case, in order to describe data, it was necessary to include imaginary parts in the Z coupling constants taken from the SM. They are formally of $\mathcal{O}(\alpha^1)$ but, luckily again, at “tree level”. Similarly, it is not excluded that in the future electron colliders, we shall be forced to replace $\text{Born}(x_i) \otimes \text{QED}$ with $|M_{\text{EW}}^{(1)}(x_i)|^2 \otimes \text{QED}$, thus removing from the data the complete $\mathcal{O}(\alpha^1)$ SM electroweak corrections in $M_{\text{EW}}^{(1)}(x_i)$, in addition to higher-order QED effects, while extracting pseudo-observable x_i from experimental data.

In the LEP data analysis, Monte Carlo event generators were used mainly for removing detector effects on the way from data to “tree-level” effective Born spin amplitudes. Extracting EWPOs from “rounded” data and removing QED effects were done using semianalytic non-MC codes ZFITTER [3] and TOPAZ0 [4], the same which were also used to calculate $\mathcal{O}(\alpha^1)$ EW corrections and fitting parameters of the SM to LEP experiment’s data. However, it has to be stressed that the procedure of extracting EWPOs and fitting of the parameters of the SM to LEP experiment’s data was well separated. EWPOs were extracted from data in a separate procedure, in a maximally model-independent way and they were truly representing (parametrizing) data without any assumptions concerning the validity of the SM. Fitting SM parameters was then done not to original real data but to EWPOs. The role of EWPOs was to provide a very *convenient bridge* between raw data and the SM or any extension of the SM. It would be very desirable to preserve this role of the bridge between data and theory in the future extensions of the EWPOs.

As already said, the role of the MC event generators in the LEP scheme of EWPOs was limited to removing or simplifying effects of the experimental cut-offs and detector inefficiencies. Semianalytic codes such as ZFITTER and TOAPZ0 can cope only with very simple kinematical cut-offs. At the precision better than that at LEP, the control over cut-offs will become critical, especially for higher-order QED effects and semi-analytical codes will be eliminated almost completely due to their inability to deal with them. Their sole, albeit very important role will continue in testing Monte Carlo programs in the case of absent or very simple cut-offs *i.e.* providing useful benchmarks. In order to better understand the future increased role of the MC generators in the future schemes of the EWPOs, let us first recall briefly the main points in the LEP scheme of EWPOs.

2. LEP scheme of EWPOs

EWPOs scheme used in LEP was described in detail in Refs. [2, 5]. Let us summarize its main points using the effective EW mixing angle as an example. In the very essence, this angle parametrizes the ratio of the vector-to-axial coupling constant of the Z boson extracted directly in a model-independent way from the experimental data, typically for the $e^+e^- \rightarrow f\bar{f}$ process. Obviously, it is not any SM parameter, validity of the SM is not assumed — it represents solely experimental data. This EWPO is denoted as $\sin^2 \theta_{\text{eff}}^f$, underlying its dependence on the fermion type f , as lepton universality is not assumed. How $\sin^2 \theta_{\text{eff}}^f$ is extracted from the data? It is described very precisely in Ref. [5]. First, the effective Born spin amplitudes including complex coupling constants of the Z boson to fermion f are defined in Eq. (1.34) and denoted as $\mathcal{G}_{Vf,Af}$. The $\sin^2 \theta_{\text{eff}}^f$ pseudo-observable is defined through the relation

$$\frac{g_{Vf}}{g_{Af}} = 1 - \frac{2Q_f}{T_{3f}} \sin^2 \theta_{\text{eff}}^f,$$

where the real parts of the Z couplings $g_{Vf} = \Re(\mathcal{G}_{Vf,Af})$ do enter. Since the small imaginary part of the couplings is difficult to extract from data, it is taken from the SM, at the tree level. The effective Born spin amplitudes are used to fit experimental data on the experimental observables: charge asymmetries $A_{\text{FB}}^{e,\mu,\tau}(s_i)$, total cross sections $\sigma^{h,e,\mu,\tau}(s_i)$, τ spin asymmetry $P_\tau(s_i)$ and more, all of them measured in several center-of-mass square energies s_i . The $\sin^2 \theta_{\text{eff}}^f$ and other EWPOs are parameters in the effective Born spin amplitudes and their values are fitted to all available data. They are independent of s_i . Trivial detector effects and some cut-off effects were already removed from the above experimental observables before fitting to

data. On the other hand, the remaining QED cut-off-dependent effects were at LEP taken into account in the process of the above fitting procedure of experimental observables using effective Born spin amplitudes with an embedded EWPOs like $\sin^2 \theta_{\text{eff}}^f$ and other such as M_Z , Γ_{ff} , σ_{had}^0 *etc.* However, let us stress that $\sin^2 \theta_{\text{eff}}^f$ and many other EWPOs are in a sense “secondary”, because they are calculated from g_{Vf} *after* the fitting of g_{Vf} has been done. Also, the naming g_{Vf} themselves as EWPOs seems misleading — they should be better named as EW pseudo-parameters (EWPPs) of the effective Born. Fitting of the SM parameters in the LEP scheme was done to EWPOs instead of fitting directly to experimental data. In Ref. [2], it was proven that the above LEP scheme is compatible with the precision of the combined data of all four LEP experiments.

In Ref. [6], it was summarized what kind of precision we may expect to reach at the high luminosity future electron collider. The most demanding will be future experiments at the proposed e^+e^- circular collider FCC-ee, see Refs. [7, 8]. For instance, according to Ref. [6] the theoretical control of the SM prediction for the charge asymmetry A_{FB}^μ near Z pole will have to be improved by a factor up to 300. That means that $\sim 0.1\%$ effects, which could be neglected at LEP and listed in the systematic error budget, at FCC-ee will have to be controlled with two-digit precision! For other EWPOs, the improvement factor of 10–150 will be needed. It is therefore quite obvious that the extension of the LEP EWPO scheme to the FCC-ee has to be quite fundamental. It is even not guaranteed that it can be successfully re-invented.

3. Possible future scheme of EWPOs

The above LEP scheme of extracting EWPOs from experimental data, including possible future extensions, is depicted in Fig. 1. Let us focus on the possible future extensions and improvements, which most likely will be necessary in the future electron colliders. The first step (A)→(B) of removing detector inefficiencies and simplifying cut-offs in principle will remain the same as in the LEP scheme. At this stage (B), all QED effects are still present in data. (In the terminology of Refs. [2, 5] data transformed in this way are called “realistic observables”).

The next step (B)→(C) of extracting EWPOs from data in the LEP version was realized using non-MC programs like ZFITTER and TOPAZ0. Due to up to two orders better precision of the future electron colliders (especially at Tera- Z option of FCC-ee), this step will have to be executed using precision MC event generators because semi-analytical non-MC programs cannot take into account realistic cut-off effects with sufficient precision. This is probably the main point to be kept in mind. In the following, we shall try to elaborate on the necessary improvements in the MC programs

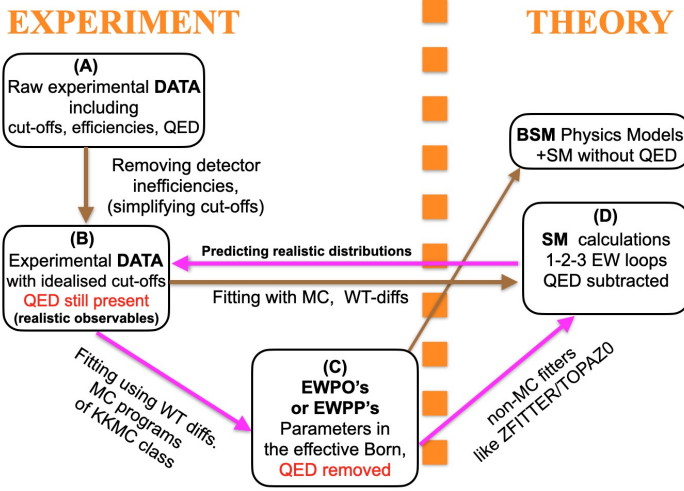


Fig. 1. Scheme of extracting EWPOs/EWPPs from experimental data.

such that they are up to the needs of this new role. As already said, it might be necessary to remove in this (B)→(C) step not only QED effects but also the complete or a well-defined dominant subset of the $\mathcal{O}(\alpha^1)$ pure EW corrections.

Fitting SM model parameters, or SM + its extensions, to EWPOs in the next step (C)→(D) will be able to be done using non-MC programs, such as ZFITTER and TOPAZ0 with higher-order EW corrections.

In the above scheme, the clear and very useful separation of experimental details and of the theory is kept with the help of EWPOs, similarly as in the original LEP version. This always comes with some loss of the information embedded in the data. How big is the bias due to the use of the intermediate data representation in the form of EWPOs was determined in the LEP scheme by means of the circular cross-check (B)→(C)→(D)→(B), see Refs. [2, 5]. The same cross-check should be used in the new scheme proposed here.

4. The ultimate precision Monte Carlo event generators for the future electron colliders

In the following, we will be trying to formulate the specification for the ultimate precision Monte Carlo event generators for the future electron colliders, having in mind the needs of the upgrade of EWPO scheme along the lines outlined in the previous section. We are going to focus on the needs of the physics near the Z pole in the high luminosity circular colliders such as FCC-ee [7] or CEPC [9]. Let us refer to such a future MC which fulfills these specifications as an “ultimate MC” (UMC).

For the fermion pair production $e^+ + e^- \rightarrow f\bar{f}$, $f = \mu, \tau$, quarks, we are in a unique position, because of the existence of the KKMC Monte Carlo program [10, 11], which can provide calculations with the precision far beyond what was needed at LEP, albeit still not high enough for the most ambitious goals of the future electron colliders. Nevertheless, KKMC can be treated as a first step in the direction of a UMC and a starting point for the future developments. In fact, KKMC was already used in several studies of the SM predictions which go substantially beyond the precision and the state-of-the-art of the LEP era. In Ref. [12], a new study of the QED effects in the charge asymmetry near the Z resonance using calculations of KKMC has pushed the precision estimates (missing higher orders) down to $\delta A_{\text{FB}} \simeq 0.01\%$. In another Ref. [13], it was shown how to exploit high-precision results from KKMC for the process $e^+e^- \rightarrow \nu\nu\Gamma$, in order to extract the coupling constant of the Z to the electron neutrino. This coupling is known from the LEP experiments with a big uncertainty.

Two classes of the problems are to be addressed on the way to the UMC specification, technical and physics.

A notorious technical problem with the use of the MC as a precision calculation tool is that changing input parameters may require a new MC run, which may take a very long CPU time. This could be the problem preventing from the use of a UMC in the fitting procedure of the construction/extraction of the EW pseudo-observables from experimental data.

The solution is however well known: UMC must be armed with the functionality of recalculating its matrix element with modified input parameters in a very short time, such that the technique of the MC weight differences could be used. With this technique, one could correct the results of a long CPU time run performing only an additional very short CPU time run, which calculates and uses MC weight differences to calculate the corresponding correction. These MC weight differences will be very tiny, because variations of the SM input parameter variation will be at the per-mile level. The above goes also well with the ongoing effort of parametrising/interpolating multi-loop EW corrections beyond the first order in terms of the input parameters and kinematical variables. This effort will be necessary in any practical calculations of the pure EW corrections beyond first order, because they are/will be very costly in terms of CPU time as well! This kind of technique was already tested in the KKMC program.

Better physics in the UMC means first of all improvements in the QED and SM matrix elements. The present version of KKMC is already armed with the best type of the QED matrix element available — the so-called coherent exclusive exponentiation (CEEX) scheme. In this unique scheme, soft photon resummation is done at the amplitude level. CEEX is the best candidate for the QED matrix element in the future UMC. Let us compare

it with other types of the QED matrix elements used for QED and QCD in other MC programs, omitting older outdated solutions not featuring any kind of soft and/or collinear resummation.

The most popular group of the QED matrix element solutions in the MC programs is based on strictly collinear parton distribution functions (PDFs) for the initial-state radiation (ISR) from the incoming $e^\pm$ beams. LO formulas for the ISR PDFs are available analytically at any higher order. This technique is convenient and useful only for very inclusive observables like total cross section. For charge asymmetry, it is already problematic. Matching with the NLO calculations to the hard process is possible but messy. A correct soft limit is available only in the inclusive form. Among many examples of the program using this technique are: LUMLOG, ALIBABA, SABSPV, RACONWW, ZFITTER, TOPAZ0, KKsem, KKfoam, WHIZARD and more, see, for instance, Refs. [14–17] for more details.

The so-called parton shower technique is the main collinear resummation technique in the QCD Monte Carlos, but it is rarely used in the QED applications. Its problems are the same as in QCD: lack of NLO evolution, factorisation scheme dependence, kinks and gaps in the angular distributions in the soft limit, messy algorithms of matching with the NLO hard process, approximate treatment of the Lorentz-invariant phase space. In principle, the resummation of collinear mass logs to infinite order is there, but in practice, it not so easy to implement — it needs backward evolution based on predefined PDFs. In QED applications, the only successful implementation is in the BABAYAGA program for the Bhabha process [18].

The most successful class of the QED matrix elements in the MCs is based on the Yennie–Fratschi–Suura [19] soft photon resummation (exponentiation) in the exclusive form, as invented in Refs. [20, 21]. It features the soft photon limit for both real or virtual photons to infinite order and the exact Lorentz-invariant Phase Space (LIPS) treatment. It provides also a well-defined scheme of including non-soft real and virtual corrections at any order. The resummation of collinear mass logs is truncated in this technique to finite order, but contrary to QCD, this is not the problem due to the smallness of the QED coupling constant. There are two variants of this technique: the older one nicknamed exclusive exponentiation (EEX) of Ref. [21] and more powerful CEEX variant defined in Refs. [10, 22]. The EEX may turn out in certain applications to be simpler algebraically, but it is not very handy for calculating spin effects and interference effects. It was implemented in the MC programs YFS2, YFS3 in KORALZ YFS3WW, BH-WIDE programs, see Refs. [14–16, 23], and was recently also implemented in Sherpa [24]. The CEEX-style QED matrix element amplitudes are perfectly well suited for spin polarised photon emitters. They are well suited for the narrow resonances such as Z , W and automatically accounts for the interfer-

ences between initial and final states. It allows for an easy and transparent separation of the QED and pure EW corrections. We are going to elaborate more on this important point in the following. The only implementation of CEEX is present in the KKMC program. Note also that it was generalised recently to include resummation of the soft photon emissions from the narrow charged resonances [25] like W boson, but this new scheme is not yet implemented.

Summarizing, the best candidate for the QED matrix element type in the future UMCs is CEEX, or any of its further improvements or developments.

5. Separating and recombining non-soft pure EW and QED corrections

The transparent systematic methodology of separating and/or recombining non-soft pure EW, on the one hand, and of the QED corrections, on the other hand, is of paramount importance in any future EW+QED Standard Model calculation beyond the 1st order. This is so because QED corrections are much bigger, hence they have to be calculated at the 1–2 orders higher level than the pure EW corrections. For instance, in the LEP era, QED corrections were soft-resummed to infinite order, adding non-soft QED typically up to $\mathcal{O}(\alpha^2)$, while the complete EW corrections were implemented up to $\mathcal{O}(\alpha^1)$. In the future Tera-Z/Giga-Z data analysis, the non-soft QED corrections will have to be calculated typically up to $\mathcal{O}(\alpha^4)$, with non-soft EW corrections up to $\mathcal{O}(\alpha^2)$. This is why the following issue has been recently risen quite often: is there any systematic and practical scheme of calculating these two classes of corrections separately and recombining them, without violating gauge invariance, IR cancellations *etc.*?

Fortunately, the CEEX matrix elements of KKMC offer a good workable example of such a scheme already tested up to QED $\mathcal{O}(\alpha^2)$, and easily extendable to higher orders. The Monte Carlo implementation is the key part of this methodology.

Let us briefly summarize on the CEEX solution for the above problem following Sect. (2.7) in [26] using notation of Refs. [10, 11]. The total cross section for the process $e^-(p_a) + e^+(p_b) \rightarrow f(p_c) + f(p_d) + \Gamma(k_1), \dots, \Gamma(k_n)$ reads as follows:

$$\sigma^{(r)} = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\tau_n(p, k_j) e^{2\alpha \Re B_4(p_a, \dots, p_d)} \frac{1}{4} \sum_{\text{spin}} \left| \mathfrak{M}_n^{(r)}(p, k_1, k_2, \dots, k_n) \right|^2, \quad (5.1)$$

where, for instance, the $\mathcal{O}(\alpha^2)$ CEEX spin amplitudes have the following structure:

$$\mathfrak{M}_n^{(2)}(p, k_j) = \prod_{s=1}^n \mathfrak{s}(k_s) \left\{ \hat{\beta}_0^{(2)}(p) + \sum_{j=1}^n \frac{\hat{\beta}_1^{(2)}(p, k_j)}{\mathfrak{s}(k_j)} + \sum_{j_1 < j_2} \frac{\hat{\beta}_2^{(2)}(p, k_{j_1}, k_{j_2})}{\mathfrak{s}(k_{j_1})\mathfrak{s}(k_{j_2})} \right\}, \quad (5.2)$$

where $\mathfrak{s}(k)$ are soft photon emission factors and the subtracted amplitudes $\hat{\beta}_j^{(2)}$ are

$$\hat{\beta}_0^{(2)}(p) = \mathfrak{M}_0^{(2)}(p) = \left[e^{-\alpha B_4(p)} \mathcal{M}_0^{(2)}(p) \right] \Big|_{\mathcal{O}(\alpha^2)}. \quad (5.3)$$

Here, $\mathcal{M}_0^{(2)}(p_a, \dots, p_d)$ represent Born-like spin amplitudes corrected up to 2-loops, derived directly from Feynman diagrams. In this IR-finite object, the QED non-IR corrections are complete to $\mathcal{O}(\alpha^2)$, while EW corrections are truncated in the present version of KKMC to 1-loop $\mathcal{O}(\alpha^1)$.

The 1-loop EW corrections to the $2 \rightarrow 3$ process would enter into

$$\begin{aligned} \hat{\beta}_1^{(2)}(p, k_1) &= \mathfrak{M}_1^{(2)}(p, k_1) - \hat{\beta}_0^{(1)}(p) \mathfrak{s}(p, k_1), \\ \mathfrak{M}_1^{(2)}(p, k_1) &= \left[e^{-\alpha B_4(p)} \mathcal{M}_1^{(2)}(p, k_1) \right] \Big|_{\mathcal{O}(\alpha^2)}. \end{aligned} \quad (5.4)$$

In the present KKMC implementation, 1-loop complete QED corrections are included in $\hat{\beta}_1^{(2)}$. The genuine complete one-loop EW corrections are not yet included in this object¹.

Last but not least, the CEEX scheme easily accommodates resummation of big logs $\ln(I/M)$ in the vicinity of narrow resonances, which are instrumental for screening initial final QED interferences. For the real emissions, this requires coherent summation over partitions of all photons among initial- and final-state emitters, and adding an extra term in the exponential virtual form factor, see Refs. [10, 11] for details.

Finally, practical advice for anybody calculating multi-loop corrections in the SM: better avoid the Bloch–Nordsieck [27] method of killing IR singularities in the EW+QED loop integrals. Instead, subtract IR parts as early as possible! This is because in the MC with the soft resummation, the IR cancellations are a built-in feature and have been already done for you.

6. Conclusions and summary

Staying again with the KKMC program as a prototype of the ultimate precision MC for the future high luminosity electron colliders, let us briefly summarize the ongoing improvements and development of KKMC and the

¹ They are not yet available in the literature.

front of the future innovations which must follow. Note that the development of KKMC was recently split into two separate branches KKM_{Cee} for the future electron colliders and KKM_{Chh} [28] for LHC and other hadron colliders.

The completed and *ongoing developments* in KKMC includes

- (a) The upgrade of the DIZET electroweak library [29] and hadronic VP routines (done, see Ref. [30]).
- (b) The upgrade of TAUOLA library to the level of Ref. [31] (done).
- (c) Cleanup and posting on the web next improved version, also f77 version with enriched C++ interface (done, <https://github.com/KrakowHEPSoft>).
- (d) The provisions for recalculating matrix elements with modified input EW parameters, like for example $\alpha_{\text{QED}}(M_Z)$, for fitting SM parameters using MC (started, see Ref. [12]).
- (e) The translation of the source code from FORTRAN 77 to C++ (done, to be published).
- (f) The LHEF interface to PYTHIA and Herwig programs for hadronization of the final state (done).

For the Bhabha process, most of the above list is also valid². For the W -pair production, the planing for the future high-precision MC is partly outlined in Refs. [6, 25]. Specification of the precision MC for the HZ process is left beyond the scope for this note, but most likely has a lot in common with the above examples.

What are the most urgent *innovation fronts* in the development of KKM_{Cee} for the future electron colliders?

- (a) The upgrade of CEEX matrix element including LO $\mathcal{O}(\alpha^3)$.
- (b) A better Monte Carlo algorithm for phase space with very hard photons. Phase-space generation in KKMC for extremely hard photons is inefficient.
- (c) Novel ideas for better incorporation of the collinear resummation within soft photon resummation, especially at the amplitude level (CEEX), main problems seem to be loops.
- (d) Alternative methods of calculating spin amplitudes in CEEX, some other method instead of Kleiss–Stirling for massive spinors?
- (e) Subtraction of the IR part from (gauge-invariant) sets of the multi-loop diagrams at the loop integrand level.

² In fact, it will make sense in the future to unite KKMC with programs for the Bhabha process.

- (f) Fitting EWPOs to data using high statistics “MC templates”, weight differences, machine learning *etc.*
- (g) Effective methods of parametrising the virtual (loop) correction to be used in the matrix element in the MC generators.
- (h) Soft photon emission resummation from the unstable charged particles like the W boson. The outline is already there [32] but the implementation will be nontrivial.

Based on the experience from the LEP era Monte Carlo development process, one may also point out more general strategy issues:

- (a) The “monopoly” of a single MC for a given process/observable should be avoided. The best would be (at least) two MCs of similar high quality developed independently by two groups of authors. An example of duo-poly: YFSWW3 + RACONWW, examples of monopoly: KKMC, BHLUMI, BHWIDE, see LEP workshop proceedings [14, 15, 23].
- (b) Upgrade of the LEP legacy MCs is a good but limited strategy. For improvement in precision by a factor of 50–150, one needs definitely new innovative projects.
- (c) The division of MCs into “general purpose” class covering hundreds of processes, background, BSM, good for fast simulation of the detectors, on the one hand, and of the “high precision” MCs specialising for a single or small subset of observables/processes, on the other hand, was and always will be the most optimal and economic approach.

LEP experience shows that developing a good quality MC costs many years of hard work and bright ideas. It should be planned and pursued well in advance of the start of the experiments. LEP was lucky that this activity has started already almost a decade before its start, at the beginning of 1980s.

Summarizing, the LEP era has seen the development of the precision MC event generators tailored for just one process/measurement. KKMC is the most sophisticated LEP legacy MC program for the $e^+e^- \rightarrow 2f$ process and is being maintained and further developed. Legacy MCs will help, but at the precision two orders higher, developing new much better innovative projects for future electron collider experiments is mandatory. We are at the very beginning of this process.

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