ELECTRON-PHOTON TRANSPORT: ALWAYS SO GOOD AS WE THINK? EXPERIENCE WITH FLUKA

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ABSTRACT

Some Monte Carlo codes used to simulate electromagnetic showers have reached a reputation of high reliability. This has led many uncritical users to ignore important artefacts and to overlook limitations still present in the description of physical interactions. The effort to overcome some of such weak points in FLUKA is described, and remaining problems are discussed.

1. Introduction

The predictive power of Monte Carlo transport programs depends to a large extent on our knowledge of radiation interactions with matter. Electromagnetic (EM) shower codes, based on such a well-established theory as QED, are considered to attain the highest level of accuracy. Two of them in particular, EGS[1] and ETRAN-ITS[2,3] have gained a high reputation of reliability. EGS has been often referred to as *"the reference model"*[4], *"a recognized"*[5], *"international"*[6], *"world-wide"*[7], *"universal*[8] *standard"*, while ITS is the most requested EM transport code at the Radiation Shielding Information Center[9]. The authors of GEANT[10], the most popular Monte Carlo code among high-energy physicists, have used EGS to benchmark their EM transport[4], and an interface to EGS has been the solution of choice for many general code systems like LAHET[11], GHEISHA[12], CALOR[13], and HERMES[14].

This well deserved reputation, however, has generated a widespread and uncritical tendency to regard data calculated by EM Monte Carlo as fully equivalent to good experimental results. Yet, the authors themselves have given repeated warnings[1,15] about the limits of validity of their codes. Ignoring approximations and limitations still present even in the best EM transport codes may lead to serious drawbacks in some critical cases. It is the aim of this paper to present the experience on this matter accumulated during the recent evolution of the FLUKA program[16] from a traditional "black-box" interface with EGS to a new original model of electron-photon transport. The problems reviewed are of two types: those

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deriving from inadequate physics and those connected with technical artefacts due to the program structure or to common user practices.

Because the 1987 version of FLUKA relied for electron-photon transport on the officially distributed version of EGS4, many references will be made to that code, although several additions and corrections have been published in the meantime[17-19] aiming to improve some of the points raised in this paper. Such improvements, generally proposed in the form of macros or user-codes, are perhaps easy to implement in EGS when used in a stand-alone mode, but not in versions coupled to other programs. None of them seems to be available yet in any of the many high-energy Monte Carlo programs interfaced to EGS[11-14], neither in those based on a similar treatment of EM showers[10].

2. Step-length effects

The choice of electron step length and the calculation of the corresponding corrections have been recognized as a critical issue by several authors[20-22]. The problem is technical, being linked to the condensed history approximation generally adopted to represent the effect of many Coulomb interactions, but has also physical aspects which depend on the model chosen to describe multiple Coulomb scattering (MCS)[23,24].

In general, results may be strongly dependent on the electron step size, especially at low energies, at large scattering angles and when thin layers are present. There are several reasons:

- because of straggling, the effective length travelled by an electron in a transport step is longer than the distance between the two endpoints. The accuracy of the required path-length correction (PLC) generally decreases with increasing step length, especially in programs based on Fermi-Eyges theory[25].
- MCS models are applicable only if the step length is kept within well-defined energy and material-dependent limits.
- effective scattering angles and lateral displacements are correlated with step length and PLC (and with each other).
- the presence of magnetic fields and/or spatial boundaries affects all of the above in a complex way: scattering angles must be combined with magnetic deflections and electron steps must be truncated when crossing material interfaces. A tracking problem may also arise when an electron is backscattered just after crossing a boundary: in this case the deflection angle is rejected in ETRAN and ITS[26] and most EGS user-codes face the situation by discarding the electron.

To minimize unwanted effects, the most common solution is to set constraints to the step size, generally by imposing an upper limit to the fraction of energy lost per step. Too small steps, however, lead to long computing times and are incompatible with some MCS models. There is no obvious rule on how to "tune" the step length

in each possible case: and if "excellent reproduction" of the response has been reported even for a thin-layer calorimeter[21], that result was only possible by limiting the fractional energy loss per step to 1%, after systematical trials and comparison with experimental data available in advance.

A first improvement of step size dependence came with the introduction of the PRESTA algorithm[17] into EGS. PRESTA consists of three elements: a new PLC to replace the Fermi-Eyges correction, a lateral displacement algorithm and a special treatment of boundary crossing. The lateral displacement is obtained by sampling two deflection angles, at the beginning and at the end of each step, instead of one as in original EGS. However, GEANT and most EGS versions interfaced to general code systems still rely on Fermi-Eyges PLC, known to be overestimated even by large factors, probably because PRESTA relies on special geometrical information not provided by all geometry tracking packages. Anyway, quoting from the PRESTA authors themselves, *"PRESTA is not the final answer because it does not solve all step-size dependence problems, in particular, backscattering"*[20]. The reason given is that PRESTA uses an average PLC instead of sampling from a distribution and neglects the correlations between PLC and angular deflection. It can be added that, although PRESTA has proved successful in many cases, it forces Molière theory beyond its limits of validity, does not account for the energy dependence of the screening correction and offers only a partial solution of the boundary crossing problem.

Most of the mentioned step length difficulties, including those connected with magnetic fields, have been eliminated by a new multiple scattering model recently introduced in FLUKA[27], where it is applied to all charged particles. The PLC is rigorously calculated by analytical integration, strictly within the Molière range of validity. Sampling is performed in such a way that the PLC variance is also accounted for, thanks to a correlation algorithm involving the two angles required by step simulation (not necessarily coplanar as in PRESTA). The model includes spin-relativistic corrections, important in some special problems (backscattering) and the scattering suppression due to the finite size of nuclei. The two examples shown in Fig.1 and 2 illustrate the quality of FLUKA as a low-energy electron transport code. The power of the new MCS algorithm can be seen in the complete independence from step size and in the capability to simulate electron backscattering correctly, seldom found in Molière-based codes.

Boundary crossing in FLUKA is treated with extreme care, by a complex step adjustment based on two main tools. The first algorithm provides a smooth approach to the boundary by progressively shortening the step as the particle gets closer to it. The particle is forced to approach the boundary in such a way that eventually the distance from it in the direction of motion becomes comparable to the minimum step-length compatible with Molière theory. The second algorithm deals with step truncation at boundaries. When a proposed step crosses a boundary the deflection sampled at the beginning of the step is randomly tested against the ratio of probabilities of sampling such angle for the truncated and for the original step. If rejected the step is resampled without any initial lateral displacement and the final

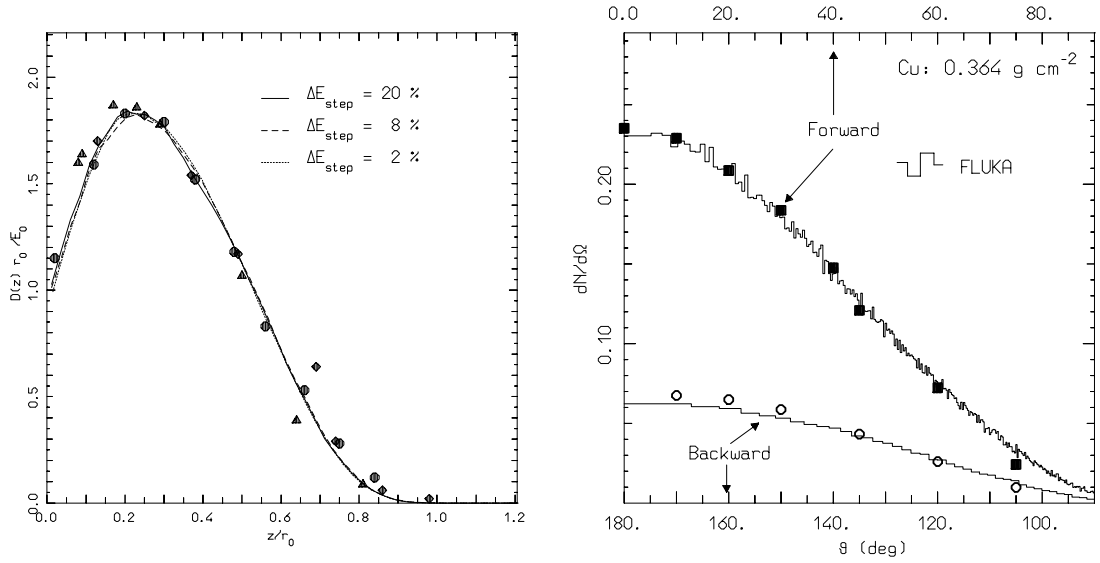

Figure 1: Low-energy electron experimental data (symbols) compared with FLUKA calculations. Left: Depth-dose profile for 0.5 MeV electrons incident on Al, with three different step sizes. Abscissae are in units of csda range. Right: Angular distributions of electrons transmitted or reflected from a Cu foil. For details see[27].

deflection is sampled accordingly from the proper distribution. By this scheme, only a few steps are performed without lateral deflection; and even for them the error introduced is negligible since their step-lengths are close to the Molière minimum. In this way Molière scattering is maintained as far as possible – always within its range of validity – providing an accurate PLC and a correct simulation of backscattering even near boundaries. The overall calculation may take slightly longer in thin-layer problems, where however no accurate result is possible otherwise. In all other cases the effect is more than compensated by a complete insensitivity to step size, which allows the use of large steps. An example of the FLUKA capability to reproduce thin-layer dose distributions with 20% energy loss per step is shown in the left part of Fig. 3.

3. Technical artefacts

3.1. Energy dependence of the electron cross-section

The need to simulate electron transport by a sequence of discrete steps can be the cause of other systematic errors. Generally, the next collision point is sampled evaluating the total cross-section at the beginning of the step, neglecting its energy dependence. Again of course, this error can be made as small as desired by reducing the length of the step, but with the already mentioned drawbacks. The error is not

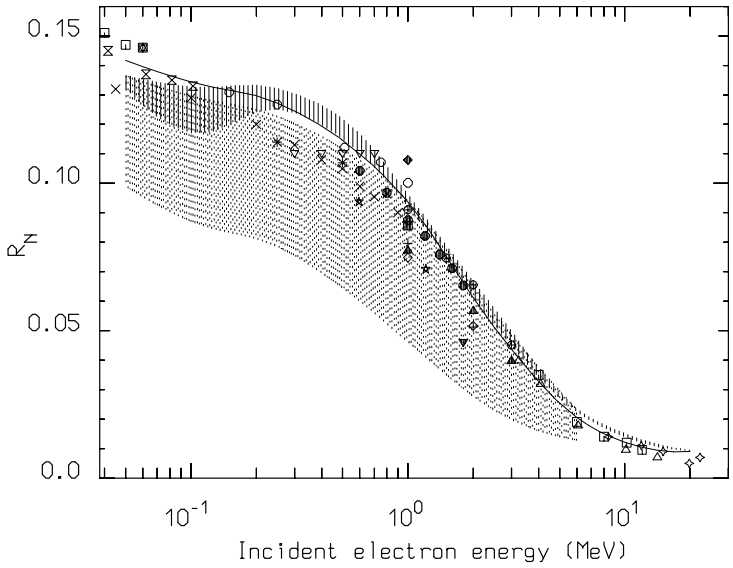

Figure 2: Number reflection coefficient R_N for electrons incident on aluminium foils. Symbols: experimental data. Solid line: FLUKA with spin-relativistic corrections. Dashed and dotted areas: variation band of FLUKA and EGS4 results for $\Delta E/E$ varying between 5 and 20% and 1 and 20% respectively. See[27] for details.

negligible: since at low energies the cross-section for δ-ray production is roughly inversely proportional to the electron energy, a 20% fractional energy loss per step would correspond to a similar variation in the cross-section.

This problem is solved in EGS by a rejection test: at the end of the step an actual collision occurs only with a probability equal to the ratio between the cross-section values at the two endpoints, otherwise the electron flight continues without interaction. Unfortunately, that approach gives correct results only when the cross-section is monotonically decreasing with decreasing energy. An approximate (although very complex) correction scheme, based on "optimized" pre-calculated correction factors, has been recently proposed[19] to overcome this difficulty: but an *exact* and much simpler solution is implemented in FLUKA. The *maximum* (instead of the *initial*) cross-section in the energy interval corresponding to the step is used to sample the interaction point. The cross-sections are interpolated from tables: since the maxima coincide with table points and only a few points are always concerned, the search is very fast and the rejection rate is low.

3.2. Energy cut-off

All EM Monte Carlo programs transport particles only above a certain predefined value of particle energy. When energy is degraded below cut-off, some non-physical approximation is applied which may affect the calculated results. In most cases, the residual particle energy is deposited at the endpoint of the last step and the particle history is terminated. Positrons are generally forced to annihilate.

Stopping particle histories below an energy cut-off excludes a whole region of phase space from the domain of Monte Carlo integration: similar situations arise also when defining the external spatial boundaries of the system considered, and when "discarding" particles which are thought to be irrelevant. The higher the cut-off, the more computer time is saved, but also the larger is the region excluded and the probability of biasing the integration. Physical judgment is needed to appreciate the effect of incorrect sampling in some phase space regions. This situation, common for weighted codes, is found in this case also in otherwise fully analog programs and is the cause of frequent errors made by inexperienced users. In FLUKA, to allow users to save CPU time without affecting the results, different cut-off values can be set in each region and for each type of particle.

It is a common error to underestimate how far particles could still travel at cut-off energy: 2 MeV electrons and 20 keV photons have a range (respectively a mean free path) of about 1 cm in water. In some thin-layer geometries such cut-off values would cause the particle energy to be deposited in the wrong layer. The difference (here a factor 100!) between the energy of a photon and that of an electron having a same "range of influence" is also worth noting: yet, setting the same cut-off for all particles is not an unusual practice.

But a more subtle deception is to be expected from positrons: the residual range at cut-off energy is not a good measure of their spatial reach, since even at extremely low energies they annihilate into 511 keV photons with mean free paths of several g/cm^2. For this reason, it is generally not recommended to set a photon cut-off larger than 511 keV, which would cause not only the residual kinetic energy, but twice the rest mass energy of stopped positrons to be deposited at one single point.

Another interesting artefact connected with positron annihilation has been noticed in EGS. Annihilation "at rest" is performed at the end of a step, after checking that energy has decreased below cut-off. Steps which would cross a boundary are truncated exactly on it: therefore more positrons are made to annihilate there than on any generic surface. Careful inspection may indeed reveal a non-physical clustering of 511 keV photons on boundaries. This odd feature, and the unpleasant dumping of residual electron energy at a single point, will be soon eliminated in FLUKA by "ranging out" electrons having reached cut-off, as it is already done for charged hadrons and muons: their energy will be distributed uniformly over their practical range and annihilation at rest will take place at the end of range. In particular, ranging out electrons will allow one to set higher cut-off energies and thus save computer time.

3.3. Scoring energy deposition in small volumes

It is important sometimes to calculate dose distributions with a high spatial resolution. For instance, the energy deposited in volumes of the order of 1 mm^3 must be known when predicting quenching of superconducting magnets. Most programs can only score energy deposition in regions defined for geometrical tracking. If a detailed dose pattern is required, a very large number of regions must be defined

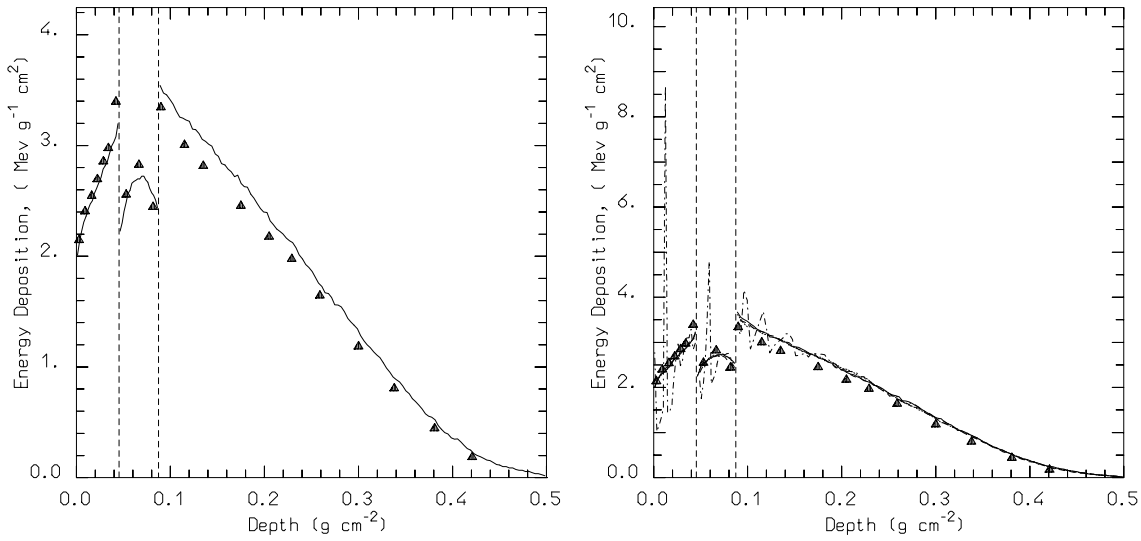

Figure 3: Energy deposition by 1 MeV electrons in an Al/Au/Al target. Left: Comparison of FLUKA distributed binning with experimental data (symbols). Right: Fluctuations appearing when depositing energy at step midpoint.

and tracking becomes very time expensive.

In some programs, like ITS and FLUKA, a general facility is provided to allow scoring of energy deposition in small volumes independently from geometry tracking. In ITS it is called *automatic subzoning* and, although independent from tracking, it is still related to the geometry regions (each region being subdivided in a number of equal subzones). In FLUKA it is referred to as *binning* and it is completely uncorrelated with geometry. Bin scoring is based on simple integer arithmetic and is extremely fast.

A problem arises if the bin dimensions are smaller than an electron step. The obvious solution to use steps shorter than the bin size was found to lead to unmanageable computing times in the 1987 version of FLUKA. Scoring at a point (the step endpoint in GEANT, the midpoint in FLUKA87, randomly chosen in ITS) produces large fluctuations between neighbouring bins. In FLUKA a new algorithm distributes the energy in proportion to the length of the bin chords traversed by the trajectory. The results converge much faster, as shown in the right part of Fig. 3. Something similar is suggested (but not implemented!) in the ITS manual[3], where the scheme is called "track-length apportioning".

4. Physics improvements

4.1. Photoelectric effect

At energies higher than the binding energy of the most tightly bound atomic electrons, the photon cross-sections are continuous and vary smoothly with atomic number; however, discontinuities exist at and below the K-edge (about 100 keV for the heaviest elements). In the standard version of EGS and in GEANT, photon cross sections of compounds are averaged over the whole range and in EGS even the energy of the K-edges is averaged, producing photoelectrons of incorrect energy and other non-physical effects. A correction to EGS has been described by Del Guerra et al.[18] but apparently it has not been implemented in any EGS-interfaced code. In FLUKA, interactions are sampled separately for each component element and for each edge higher than 1 keV. Fluorescence and Auger electron emission are simulated for all K and most L lines, including the angular distribution of fluorescent photons (fully relativistic theory of Von Sauter).

4.2. Bremsstrahlung

The Bethe-Heitler bremsstrahlung formulae, still used in most EM codes, are based on the Born approximation which cannot be applied to low-energy electrons and does not describe correctly the hardest part of the photon spectrum. In any case, the analytical formulae require several corrections. While the so-called DBMO[28] formulae including Coulomb corrections are implemented in most programs, the Elwert factor is not. In the screening corrections, based generally on the Thomas-Fermi statistical model, the old numerical values of Bethe have not always been replaced by the more modern evaluation of Tsai[29]. The Landau-Pomeranchuk-Migdal (LPM) suppression effect is considered by a few cosmic ray programs[30,31] and by GEANT, in which the Ter-Mikaelyan polarization effect is also included. Differences between electron and positron bremsstrahlung are generally ignored, although they are far from negligible below 50 MeV (for instance since the positron energy loss by radiation at 7 MeV in lead is about 20% smaller than that of electrons, strictly speaking the critical energy is different for the two particles). The photon angular distribution is in most cases replaced by a fixed polar angle approximation, adequate in problems where photon direction is dominated by electron multiple scattering, but not in low-density media. In the most recent version of GEANT, the angular distribution is approximated by an empirical analytical function uncorrelated with photon energy.

Very accurate electron-nucleus and electron-electron bremsstrahlung cross-sections, differential in photon energy, have been published in recent years by Seltzer and Berger[32] for all elements up to 10 GeV, and have been introduced in their ETRAN code. Those data were obtained at low energy by numerical phase-shift calculations, and above 50 MeV using the DBMO formulae with screening based on Hartree-Fock form factors and several corrections. In particular, a finite value

of the photon spectrum tip is provided.

A small subset of the new data is used in GEANT (6 elements out of 100, hydrogen not included), but only to derive a polynomial parametrization of the total cross-section. In FLUKA, where because of its accuracy and speed table look-up is systematically preferred to the computation of parametrized formulae, the full set of Seltzer and Berger cross-sections has been tabulated in extended form. The energy mesh has been concentrated, especially near the photon spectrum tip, and the maximum energy has been extended to 1 PeV taking into account the LPM and Ter-Mikaelyan effects. Positron bremsstrahlung is treated separately, using below 50 MeV the scaling function for the radiation integral given by Kim et al.[33] and differential cross-sections obtained by fitting proper analytical formulae to numerical results of Feng et al.[34]. The photon angular distribution is obtained sampling the emission angle from the double differential formula reported by Koch and Motz[35], fully correlated with the photon energy sampled from the Seltzer-Berger distributions.

But there is still room for improvement concerning bremsstrahlung. The deflection of the electron is systematically ignored in all EM codes. Another effect poorly treated is inelastic bremsstrahlung on orbital electrons. Although it gives a non negligible contribution to total photon production, especially in low-Z materials (about one half of the total in hydrogen!), all programs (including FLUKA) consider only one bremsstrahlung cross-section inclusive of electron-nucleus and electron-electron interactions. Using the DBMO formulae without the proper screening corrections would lead to wrong energy and angle distributions. The correct global photon spectrum due to both effects is obtained in ETRAN and FLUKA from the Seltzer and Berger distributions, but the angular distribution, assumed to be the same for both effects, can be incorrect at low energies. The recoil of the target electron is also neglected.

4.3. Pair production

The photon cross-sections used in most EM codes could be improved by replacing them with the extensive data base recently published by Cullen et al.[36] However, the old tabulations of Storm and Israel adopted by EGS and FLUKA or the more recent ones by Hubbell used in GEANT can still be considered quite accurate. The angular distribution of electron pairs is treated by several codes in a fixed angle approximation similar to that of bremsstrahlung. However, a common mistake is to adopt for the polar angle the expression $\Theta = m/E$, with m the electron mass energy and E the *photon* energy instead of the correct *electron* energy. A rather crude approximation used by EGS at photon energies lower than 2 MeV is to attribute the whole available energy to one single electron. Neither of these approximations is used in FLUKA, where angular and energy distributions are described in full detail. However triplets (pairs produced in photon interactions with orbital electrons), although included in the total cross-section, are still awaiting a correct formulation of the differential cross-section, presently available only for free

electrons.

4.4. Other effects

Due to lack of space only a non-exhaustive summary list will be given here of further possibilities to improve the physics of the most used EM codes. In some cases such improvements have been made in FLUKA, for instance by implementing the latest values of ionization potentials and density effect parameters by Sternheimer, Berger and Seltzer[37]; in other cases they are in preparation (inelastic Compton effect on bound electrons, already implemented in ITS[38]). Electron-induced fluorescence seems to have been implemented only in ETRAN. All codes treat hydrogenated materials in a very unsatisfactory way, in particular concerning triplet production, electron-electron bremsstrahlung and multiple Coulomb scattering: this is due mainly to the use of Thomas-Fermi form factors not applicable to atoms with only a few electrons. More effects deserve to be considered: the formulae for Bhabha and Møller scattering should be corrected for electron binding; positron annihilation, important for PET tomography applications, should be modified to account for single-photon annihilation and for the effect of electron motion on collinearity; the contribution of orbital electrons to multiple scattering should be taken into account more correctly below the threshold of δ-ray production.

5. Conclusions

The critical review of open problems presented in this paper should not be understood as a negative criticism of programs widely appreciated for their high quality, but rather as a reminder that the perfect Monte Carlo code does not, and will probably never, exist. In this view, the unanimous and insistent referring to some codes as "standards" does not serve progress well. New accelerator and detector technologies bring continuously new challenges and, as every Monte Carlo author knows well, no matter how accurate and complete a program might be some user will always be found to demand from it some unforeseen exotic performance. It is important that users be educated to be aware of the limitations of their favourite program, rather than trusting it blindly in every circumstance.

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