On the treatment of energy straggling in track following

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Abstract

A treatment of the error propagation due to energy loss during particle tracking is given, in view of applications in track following codes. Both ionization energy loss and bremsstrahlung are considered. Some results in typical model detectors are given.

Key words: Energy loss; Charged particle tracks; Track following codes

1. Introduction

With the words "track following", one usually intends two main tasks:

a) to transport the track parameters (particle momentum, position and direction) from one point to another in the apparatus, forward and backward. The forward part can be obtained by simply using the Monte Carlo (MC) codes with the fluctuations switched off. For the backward tracking (with increasing momentum) only minor modifications of the MC codes are usually required;

b) to propagate the errors on the track parameters together with the mean values. This is usually obtained by calculating, step by step, the 5×5 error or covariance matrix of the track [1]. The detailed formulae, that are rather complicated and have been implemented during many years in the specific codes [2, 5], only recently have been published [3].

The main tasks of track following are the merging of tracks from different detectors during pattern recognition and track fitting, and the realization of the prediction step in global track fitting methods as the Kalman or other filters [7, 8].

Preprint submitted to Nuclear Instruments and Methods B *December 24, 2010*

The Monte Carlo and track fitting tasks have been treated jointly by the CERN community in the nineties. The famous GEANT3 program was used for the point a), that is for the determination of the track mean values. For the point b), the routines for the calculation and the transport of the error matrix, written by the CERN EMC collaboration [2], were interfaced with the structure, giving rise to a FORTRAN package called GEANE [7].

The great advantage of this structure is that the track following is automatically obtained *with the same geometry banks of the Monte Carlo*, without the necessity to write *ad hoc* codes.

The old GEANT3-GEANE chain can be used also in modern software platforms, for example in a Virtual Monte Carlo framework [6]. A similar tool is available also in the GEANT4 framework, as the code GEANT4E developed by the CMS Collaboration [19].

In this paper we describe a new and general treatment of the error propagation of the energy loss in track following. This could be immediately implemented in the GEANE and GEANT4E codes, that at present consider only heavy particles and thick absorbers. We consider mainly the $1/p$ variable, which is the energy dependent variable of the covariance matrix in most of track propagation algorithms.

The results are complementary to the analyses made previously for track fitting algorithms and codes [25, 26, 27].

2. Energy loss fluctuations by ionization

The fluctuations in ionization for one particle of charge z, mass m, velocity β, are characterized by the parameter κ,

$$\kappa = \frac{\xi}{E_{\rm max}} \ , \tag{1}$$

which is proportional to the ratio of mean energy loss to the maximum allowed energy transfer $E_{\rm max}$ in a single collision with an atomic electron:

$$E_{\rm max} = \frac{2m_e\beta^2\gamma^2}{1+2\gamma m_e/m+(m_e/m)^2} \ , \tag{2}$$

where $\gamma = 1/\sqrt{1-\beta^2} = E/m$ and m_e is the electron mass. The parameter ξ comes from the Rutherford scattering cross section and is defined as [14]:

$$\xi = 153.4\frac{z^2 Z}{\beta^2 A}\,\rho d \quad ({\rm keV}) \ , \tag{3}$$

where ρ, d, Z and A are the density (g/cm^3), thickness, atomic and mass number of the medium.

The parameter κ takes into account both the projectile energy and the geometrical thickness of the absorber; it defines univocally the absorber characteristics, that is the straggling conditions [18], that we define as follows:

a) heavy absorbers: $\kappa > 10$ and the distribution is Gaussian;

b) moderate absorbers: $0.01 < \kappa < 10$. The distribution follows the function of Vavilov [18], that tends smoothly to the Gaussian by increasing the thickness;

c) thin absorbers: $\kappa < 0.01$. When the number of collisions $N_c > 50$, the distribution follows the Landau function [18];

d) very thin absorbers: $N_c < 50$ (the condition $\kappa \ll 0.01$ is implicitly fulfilled). There are no universal straggling functions, but only approximated models [17]. This situation usually occurs in gaseous detectors at GeV energies.

For the cases a) and b) the straggling problem has a definite solution, both in simulation and in track following, because the general theory of the moments of the energy straggling distribution, based on the transport equation [12], shows that the energy variance is given by:

$$\sigma^2(E) = \frac{\xi^2}{\kappa}(1-\beta^2/2) = \xi\, E_{\rm max}(1-\beta^2/2)\ . \tag{4}$$

Then, taking into account the energy-momentum equation

$$E^2 = p^2 + m^2 \quad \rightarrow \quad \frac{\rm dp}{\rm dE} = \frac{E}{p} = \frac{1}{\beta}\ ,$$

and the error transformation

$$\begin{aligned} \sigma^2(1/p) &= \left[\frac{\rm d}{\rm dp}\left(\frac{1}{p}\right)\right]^2 \sigma^2(p) \\ &= \frac{1}{p^4}\,\sigma^2(p) = \frac{E^2}{p^6}\,\sigma^2(E) \end{aligned} \tag{5}$$

we obtain the variance of $1/p$. Concerning the cases c) and d), for thin and

$\lambda_{\max}$	α	Mean	σ_λ
11.1	0.90	1.61	2.83
22.4	0.95	2.40	4.23
110.0	0.99	4.19	10.16
200.0	0.995	4.82	13.88
256.0	0.996	5.08	15.76
339.0	0.997	5.37	18.19
507.0	0.998	5.78	22.33
1007.0	0.999	6.48	31.59

Table 1: Result of the integration $\alpha = \int_{\lambda_{\min}}^{\lambda_{\max}} f(\lambda)\,\mathrm{d}\lambda$ of the Landau distribution from $\lambda_{\min} \simeq -3.5$ to $\lambda_{\max}$ of the table. The mean and the standard deviation of the truncated distribution are also shown. We recall that the mean and the variance of the full Landau distribution are infinite, only the cumulative can be calculated.

very thin absorbers, we note that a rigorous solution exists for the simulation but not for the track following. Indeed, whereas in the simulation the sampling and the tracking of the δ-electrons reproduces correctly some rare effects in the detectors or the noise characteristics, in track following the long tail of the energy lost by the particle, due to the δ-electron emission, makes the energy straggling variance infinite (for the Landau distribution [1, 16]) or so big (in very thin absorber models [17]) that the uncertainty in the track momentum could be meaningless, because these fluctuations refer to "enormous" energy losses occurring with very low probability.

Since an universally accepted solution of this problem at present does not exists, we use some approximations based on truncated distributions.

For the Landau case we use the same method of the simulation codes GEANT3 and GEANT4 [18, 19]. We consider the Landau variable

$$\lambda = \frac{E - \langle E \rangle}{\xi} - (1-\gamma) - \beta^2 - \ln\kappa \; , \tag{6}$$

where E is the particle energy, $\gamma = 0.57725$ is the Euler's constant, and we cut the Landau distribution to a $\lambda_{\max}$ value so that, if only values $\lambda < \lambda_{\max}$ are accepted, the average value of the distribution is:

$$\langle \lambda \rangle = -(1-\gamma) - \beta^2 - \ln\kappa \; . \tag{7}$$

In tis way the average of the λ fluctuations remains consistent with the energy loss mean value $\langle E \rangle$. A parametric fit to the universal Landau distribution gives for $\lambda_{\max}$ the following formula [18, 19]:

$$\begin{aligned}\lambda_{\max} &= 0.60715 + 1.1934\,\langle\lambda\rangle + \\ &\quad (0.67794 + 0.052382\,\langle\lambda\rangle)\exp(0.94753 + 0.74442\,\langle\lambda\rangle)\ ,\end{aligned} \tag{8}$$

To find an effective variance to be used in track following, we use an interpolation formula of the values of tab 1. Then, from eq. (6), for the Landau case we assume:

$$\sigma(E) = \xi\,\sigma_\lambda\ . \tag{9}$$

For example, for $\alpha = 0.95$ we have, from tab. 1, $\sigma(E) = 4.23\,\xi$.

In the case of very thin absorbers, the difficulty is due to the non existence of a straggling density in a closed analytical form [17]. In this case we decided to use a variance value obtained from the Urban model [20], which is one of the models used to sample the energy lost by the particle in very thin absorbers both in GEANT3 and GEANT4 [18, 19].

The Urban model is based on the empirical definition of excitation and ionization macroscopic cross sections, defined as follows [20]:

- excitation macroscopic cross sections Σ_1 and Σ_2:

  $$\Sigma_i = C\frac{f_i}{E_i}\frac{\ln(2m\beta^2\gamma^2/e_i) - \beta^2}{\ln(2m\beta^2\gamma^2/I) - \beta^2}(1-r)\ ,\quad i = 1, 2$$

  where:

  $$I = 16\,Z^{0.9}\ (\mathrm{eV})\ ,\quad f_2 = \begin{cases} 0 \ \mathrm{if} Z \le 2 \\ 2/Z \ \mathrm{if} Z > 2 \end{cases}\ ,$$

  $$e_2 = 10\,Z^2\ (\mathrm{eV})\ ,\quad e_1 = \left(\frac{I}{e_2^{f_2}}\right)^{1/f_1}\ ,$$

  $$f_1 = 1 - f_2\ ,\quad r = 0.4\ ,\quad C = \frac{\langle E\rangle}{\Delta x}\ ,$$

  and $\langle E\rangle \equiv (\mathrm{d}E/\mathrm{d}x)\cdot\Delta x$ is the energy lost in the absorber of thickness Δx. The parameter r is the fraction of the ionization over the excitation and is usually set around 0.4.

- ionization macroscopic cross section Σ_3:

  $$\Sigma_3 = C\,\frac{E_{\max}}{I(E_{\max} + I)\ln((E_{\max} + I)/I)}\,r$$

- number of total collisions N_c:

$$N_c = (\Sigma_1 + \Sigma_2 + \Sigma_3)\Delta x = N_1 + N_2 + N_3 \ . \tag{10}$$

- total energy lost:

$$\begin{aligned} E &= (\Sigma_1 e_1 + \Sigma_2 e_2 + \Sigma_3 E_3)\Delta x \\ &= N_1 e_1 + N_2 e_2 + N_3 E_3 \ , \end{aligned} \tag{11}$$

where e_1 and e_2 are the two fixed excitation energies of the model and E_3 is the energy lost by δ-electron emission. This is a stochastic quantity that follows approximately the distribution [20]:

$$\begin{aligned} E_3 \sim g(E) &= \frac{I(E_{\max} + I)}{E_{\max}} \frac{1}{E^2} \ , \\ & \quad I < E < E_{\max} + I \ . \end{aligned} \tag{12}$$

In GEANT3 and GEANT4 the energy E is obtained by eq. (11) by sampling N_1, N_2 and N_3 from the Poisson distribution and E_3 from $g(E)$. Therefore, the sampling of the excitation energy is

$$E_e = N_1 e_1 + N_2 e_2 \ , \tag{13}$$

with e_1 and e_2 are constant and N_1, N_2 are sample from the Poisson distribution.

The delta ray ionization energy is sampled by inversion of the cumulative function of the distribution of eq. (12):

$$E_3 = \sum_{j=1}^{N_3} \frac{I}{1 - R_j(E_{\max}/(E_{\max} + I))} \ , \tag{14}$$

where R_j is a random number uniformly distributed in $[0, 1]$. The Urban model gives good results when compared with more detailed calculations with a photoionization absorption model [20], which gives results in good agreement with the experimental data [21].

We checked the Urban model with a direct simulation in a 1 cm thick 90% Ar-10%$CO2$ gas mixture at NTP. We sample from the exponential distribution the point where an electron cluster is generated. Then the number of electrons in the cluster is sampled. After 1 cm, we have the number of free

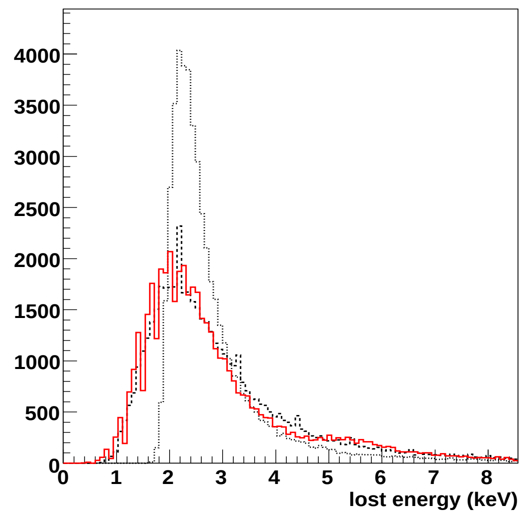

Figure 1: Energy loss of 1 GeV pion traversing a 1cm of 90% *Ar* 10% CO2 gas mixutre at NTP. Solid line: Urban distribution; dashed line: specific simulation model; dotted line: Landau distribution,

electrons generated. By knowing the mean value of the energy spent per free electron (to create a ion pair), the overall energy loss of the projectile on the whole path can be calculated. The number of clusters/cm is taken from ref. [24] (25 for *Ar* and 35.5 for CO2), whereas the cluster size distribution is taken from [22] for *Ar* and from [23] for CO2. The mean energy lost per ion pair is assumed to be 27 eV for *Ar* and 33.5 eV for CO2 [24]. We compared the Urban model and the simulation for a variety of projectiles and energies (see for example fig. 1) and found that the Urban model reproduces well the energy loss in very thin absorbers.

The Urban distribution has finite mean and variance, which includes (unlikely) strong fluctuations: for example, for 1 GeV pions in a 1 cm thick *Ar* layer, we have $\langle E \rangle \simeq 2.7$ keV, $E_{\max} \simeq 66$ MeV and a standard deviation of about 80 keV due to the δ-electron tail. We find now the expression of this standard deviation, as a function of a truncation parameter δ, which is the fraction of the area considered of the δ-ray energy distribution. We can write:

$$\frac{I(E_{\max}+I)}{E\max}\int_I^{E_\delta}\frac{1}{E^2}\,\mathrm{d}E = \frac{(E_{\max}+I)}{E_{\max}}\frac{E_\delta - I}{E_\delta} = \delta\ ,$$

hence:

$$E_\delta = \frac{I}{1 - \delta\, E_{\mathrm{max}}/(E_{\mathrm{max}} + I)} \ . \tag{15}$$

When $\delta = 1$, the whole distribution is considered, including fully the δ-electron tail and $E_\delta = E_{\mathrm{max}} + I$, in agreement with (12).

The mean and variance of the δ-ray energy distribution are:

$$\begin{aligned}
\langle E_3 \rangle &= \frac{I(E_{\mathrm{max}} + I)}{E_{\mathrm{max}}} \int_I^{E_\delta} \frac{1}{E}\, \mathrm{d}E \\
&= \frac{I(E_{\mathrm{max}} + I)}{E_{\mathrm{max}}} \ln\left(\frac{E_\delta}{I}\right) \ , \\
\left\langle E_3^2 \right\rangle &= \frac{I(E_{\mathrm{max}} + I)}{E_{\mathrm{max}}} \int_I^{E_\delta} \mathrm{d}E \\
&= \frac{I(E_{\mathrm{max}} + I)}{E_{\mathrm{max}}} (E_\delta - I) \ , \\
\sigma^2[E_3] &= < E_3^2 > - < E_3 >^2 \ .
\end{aligned} \tag{16}$$

To find the variance of the Urban distribution, to be used in track following, we have to apply the error propagation to eq. (11), where a random sum is present. If N_1, N_2, N_3 are Poisson variables and E_3 is a random variable which follows the δ-ray energy distribution, we obtain:

$$\begin{aligned}
\sigma_\lambda^2(E) &= \langle N_1 \rangle\, e_1^2 + \langle N_2 \rangle\, e_2^2 + \langle N_3 \rangle \langle E_3 \rangle^2 \\
&\quad + \sigma^2[E_3] \langle N_3 \rangle
\end{aligned} \tag{17}$$

where the last two terms come from the variance of a random sum of random variables X_i, when the upper index N follows the Poisson distribution [4]:

$$\sigma^2 \left[\sum_i^N X_i \right] = \langle X \rangle^2 \langle N \rangle + \sigma^2[X] \langle N \rangle \ .$$

The variance of eq. (17) depends of the cut parameter δ. We decided to use, for $\kappa \simeq 0.01$ and $N_c \simeq 50$ (see eq. (10)), a δ value that gives the same variance of the truncated Landau distribution. This matching, for the absorbers and thicknesses that we have tried, is assured when $\delta \simeq 0.9999$. This value, although very near to the unity, corresponds to a non negnligible cut of the long δ-ray tail of the Urban distribution. For example, for 1 GeV

absorber	energy (GeV)	Heitler equation μ	σ	GEANT3 μ	σ	GEANT4 μ	σ
10 cm Ar	0.5	0.4995	0.0097	0.4995	0.0097	0.4995	0.0105
10 cm Ar	1.0	0.9991	0.0194	0.9991	0.0198	0.9991	0.0203
1 cm Al	0.5	0.447	0.098	0.444	0.100	0.444	0.098
1 cm Al	1.0	0.894	0.195	0.891	0.203	0.891	0.201
1 cm Al	10	9.01	1.95	8.96	2.04	8.95	2.06

Table 2: comparison between the mean energy μ and standard deviation σ (MeV) from the the GEANT3 and GEANT4 simulated distributions relative to 10^5 electrons and from the Heitler formula after passing some absorbers.

pions on a 1cm thick Ar layer, we have $\sigma_\delta = 80$ keV for $\delta = 1$ and $\sigma_\delta = 15$ keV for $\delta = 0.9999$.

In summary, our method calculates the $1/p$ variance of eq. (5) with a variance $\sigma^2(E)$ due to the ionization energy loss calculated as follows:

a) for big and moderate absorbers when $\kappa > 0.01$, the variance $\sigma^2(E)$ is given by eq. (4) (old GEANE method);

b) for thin absorbers, $\kappa < 0.01$, when the number of collisions from eq. (10) is $N_c > 50$, $\sigma^2(E)$ is given by eq. (9);

c) for very thin absorbers, when $\kappa < 0.01$ and $N_c < 50$, the variance $\sigma^2(E)$ is given by eq. (17).

3. Energy loss fluctuations by bremsstrahlung

The energy loss by bremsstrahlung becomes the dominant process for electrons above the critical energy $E_c \simeq 800/Z$ MeV and for muons in dense media above 10 GeV.

The radiative energy loss straggling distribution for the energy E of a particle of incident energy E_0 on an absorber of thickness x, was first deduced by Heitler [28], using an approximate expression for the bremsstrahlung cross section:

$$f(E) = \frac{1}{E_0 \Gamma(l)} \left(\ln \frac{E_0}{E} \right)^{l-1} \quad , \quad l = \frac{x}{X_0 \ln 2} \ , \tag{18}$$

where X_0 is the radiation length of the absorber and Γ is the gamma function.

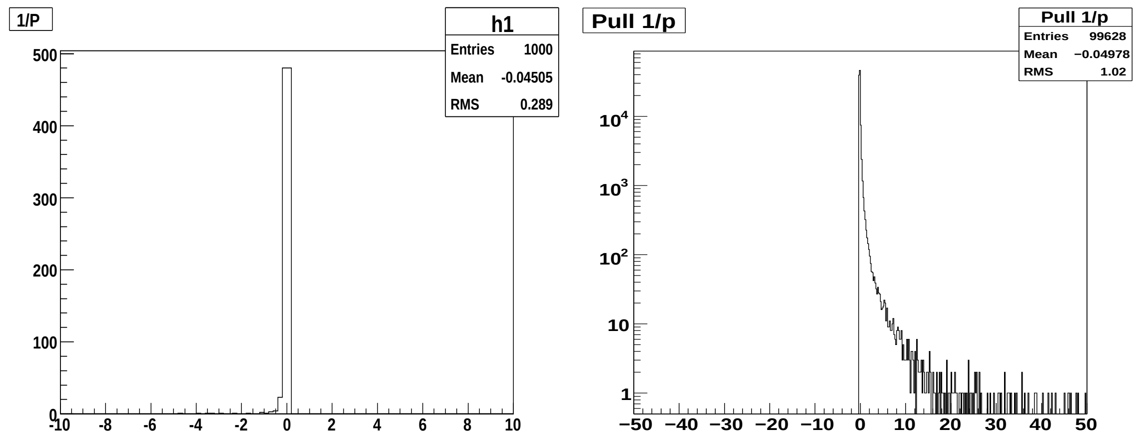

Figure 2: Pull distribution $\Delta(1/p)/\sigma$ for 1 GeV muons after passing through 22 straw tube layers. Left: Standard GEANE result (RMS$\simeq$ 0.3 in the displayed window); right: result after the modification with $\delta = 0.9999$ (see the text). The region between the vertical lines has RMS= 1.03.

From eq. (18) one deduces that, if $Z = E/E_0$, $-\ln Z$ is Γ-distributed and that the first two moments and the variance are given by [27, 25]:

$$\langle E \rangle = E_0 \frac{1}{2^l} , \qquad \langle E^2 \rangle = E_0^2 \frac{1}{3^l} \tag{19}$$

$$\sigma^2[E] = \langle E^2 \rangle - \langle E \rangle^2 = E_0^2 \left(\frac{1}{3^l} - \frac{1}{4^l} \right) . \tag{20}$$

The Heitler distribution (18) gives surprisingly good results when compared with the full treatments of the bremsstrahlung energy loss as in the simulation programs GEANT3 [18] and GEANT4 [19] (see tab.2). We note also that the difference between positrons and electrons is not taken into account by eq. (18). However, in most cases this effect is less than 1%.

In conclusion, the bremsstrahlung process can be adequately modeled with the very forward peaked, highly asymmetric and long tailed distribution of eq (18). It can also be approximated with Gaussian mixtures to be used in track fitting algorithms [26]. Regarding the track following, the existence of a finite variance for the energy in principle allows the analytical treatment of the error propagation of the track parameters. However, the track following is usually done in term of the $1/p$ variable instead of E. Neglecting the electron mass, this means the use of the $1/E$ variable. Unfortunately, it is easy to

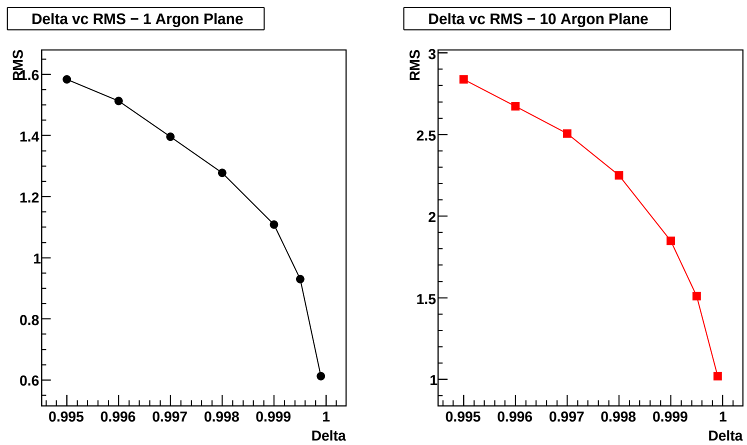

Figure 3: Values of the standard deviations of the $1/p$ pull variable as a function of the truncation parameter δ from eq. (15), for 1 Gev pions traversing a 1 mm thick Al absorbers.

see, from the distribution (18), that this variable has no finite moments: even $\langle E^{-1}\rangle$ does not exist.

To overcome this problem, we decided to assign to $1/E$ an uncertainty interval

$$\begin{aligned} \sigma[1/E] &= 0.5\,[1/E_2, 1/E_1]\ , \qquad \text{where} \\ E_2 &= \mathrm{Min}(E_0, \langle E\rangle + \sigma[E])\ , \\ E_1 &= \begin{cases} \langle E\rangle - \sigma[E] & \text{if} \quad E_2 = \langle E\rangle + \sigma[E] \\ E_0 - 2\sigma[E] & \text{if} \quad E_2 = E_0 \end{cases} \quad . \end{aligned} \tag{21}$$

The standard deviation $\sigma[E]$ comes from eq. (20). In this way the probability corresponding to the uncertainty interval of E is the same also for the uncertainty of $1/E$. We found also empirically that this "standard deviation" $\sigma[1/E]$ can be approximated within 15% for any energy and absorber thickness with an equation similar to (5):

$$\sigma^2[1/E] \simeq 1.44\,\frac{1}{\langle E\rangle^4}\,\sigma^2[E]\ , \tag{22}$$

where the approximation $p \simeq E$ has been used.

The treatment used here is only approximated. Indeed, the shape of the bremsstrahlung energy loss distribution is far from gaussian, so that its use in the Kalman filter is not correct. The standard treatment is in this case to

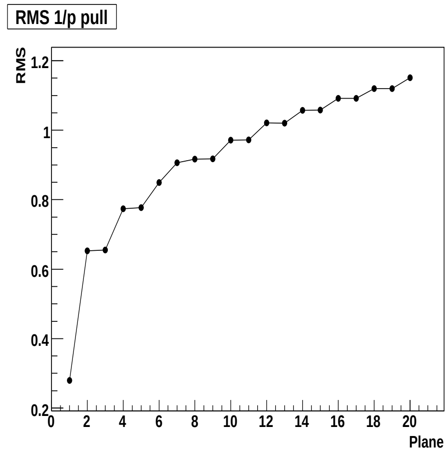

Figure 4: Values of the standard deviations of the $1/p$ pull variable with truncation parameter $\delta = 0.9999$ from eq. (15), as a function of the number of the traversed layers. The data refer to 1 Gev pions traversing layers formed by a 1 mm thick Al (Landau distribution) and a 1 cm thick Ar gas (Urban distribution) absorbers at NTP.

approximate the distribution as the sum of (at least two) Gaussians, to model the sharp peak and the flat background. The method is called Gaussian Sum Filter (GSF) [1, 27, 25, 26]. It must be implemented in our software in the next future.

4. Results and conclusions

To check the effects of our modifications to the energy straggling in track following, we used the chain GEANT/GEANE (version 3.21) for simulation and tracking. The default formula for the energy straggling in GEANE is given by eq. (4).

For a given quantity x, the results are mainly reported in terms of the pull distribution $(x_{\rm MC} - \langle x \rangle)/\sigma[x]$, where $\langle x \rangle$ and $\sigma[x]$ are given by the track following code.

Firstly, we consider the case of ionization enegy loss in very thin absorbers. The pull histograms of $1/p$ in the case of 9 Ar layers 1 cm thick traversed by 1 GeV pions are shown in fig. 1. The uncertainties in energy straggling are from eq. (4) and from eq. (17). Clearly, the σ from the Urban distribution gives a better result.

In fig. 3 we explore systematically the behaviour of the σ of the $1/p$ pull variable with the truncation parameter δ of the Urban distribution. One sees

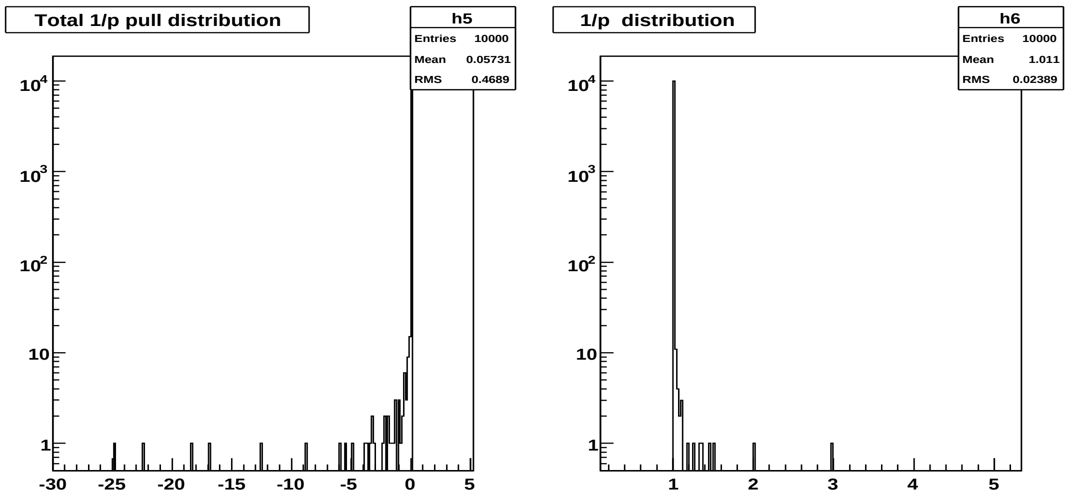

Figure 5: Pull distributons of E (left) and $1/p$ (right) variables with σ from eqs. (20, 22) for 1 Gev electrons traversing a 10 mm thick Al layer.

that values $\delta > 0.995$ give resonable results.

In fig 3 we consider the momentum of 1 GeV pions after a 1 mm thick Al absorber (Landau distribution) and after a very thin absorber formed by a 10 cm Ar gas layer at NTP (Urban distribution). The results show that the value $\delta = 0.9999$, that assures a good matching between the Landau and Urban distributions, give a resonable pull distribution, which remains stable during the tracking.

Finally, we check the behaviour of track following for electrons taking into account the bremsstrahlung energy loss. In fig. 5 the shape of E and $1/p$ distributions for 1 GeV electrons on 10 cm Ar gas at NTP are reported, obtained using eqs. (20, 22). The result show that the uncertainty due to bremsstrahlung is reproduced reasonably well, in spite of the long tailed shape of the distribution.

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