Proceedings of the Eleventh EGS4 Users' Meeting in Japan, KEK Proceedings 2003-15, p.9-16

A FAST AND ACCURATE SAMPLING OF MOLIÈRE DISTRIBUTION BY DIVIDING THE SCATTERING CROSS SECTION

K. Okei[†] **and T. Nakatsuka**[‡]
[†]*Okayama University, Okayama 700-8530, Japan*
[‡]*Okayama Shoka University, Okayama 700-8601, Japan*

Abstract

A sampling method for multiple Coulomb scattering is presented. The method is constructed by dividing the scattering cross section and exploiting the central limit theorem. If we use the screened Rutherford cross section with the small angle approximation, our method yields Molière distribution, however, it can be implemented as simple as, and as fast as Gaussian approximation methods. It is found that a simple correction make the method applicable to the case where particle pathlength is very small, that is, the expected total number of deflections is down to about five. A correction for taking constant energy loss into account is also presented.

1 Introduction

Many cosmic ray experiments need Monte Carlo simulations to analyze their data. Because the simulations usually deal with a huge number of particles or a great distance of transport, the simulations must be able to run very fast. Thus, efficient charged particle transport algorithms are required.

We have been developing a method for sampling multiple Coulomb scattering [1, 2, 3, 4]. The method is constructed by dividing the scattering cross section into the moderate scattering and the large angle scattering. Many small angle deflections less than the dividing angle are expected to form Gaussian distribution, whereas the large scattering is directly sampled from the scattering cross section. Our method can yield Molière distribution [5, 6, 7], however, it doesn't require auxiliary numerical tables which are in general used for Molière distribution sampling. Therefore, it can be implemented as simple as, and as fast as Gaussian approximation methods.

Since no approximation is made for the sampling of the large angle scattering, the validity of our method depends on the Gaussian approximation for the moderate scattering only. Hence we will begin by considering the goodness of the Gaussian approximation.

2 The Central Limit Theorem and Small Angle Deflections

If we have N independent random variables X_i $(i = 1, \ldots, N)$, each from a distribution with mean μ_i and variance σ_i^2, the distribution of the sum $S = \sum X_i$ will have a mean $\sum \mu_i$ and variance $\sum \sigma_i^2$. The central limt theorem [8] says that as $N \to \infty$,

$$\left(S - \sum_{i=1}^{N} \mu_i \right) \Bigg/ \sqrt{\sum_{i=1}^{N} \sigma_i^2} \to \mathrm{N}(0, 1). \tag{1}$$

This theorem is very powerful since it does not specify the distribution of X_i except for their means and variances. This means that the resulting angular distribution from a large number of small angle deflections will be Gaussian despite the shape of single scattering cross section $f(\chi)$. In this paper, we use the screened Rutherford cross section with the small angle approximation,

$$f(\chi) = \frac{2\chi_c^2}{(\chi^2 + \chi_a^2)^2} \tag{2}$$

where χ_a and χ_c are defined in [5, 6, 7].

Dividing the cross section at $\chi_{\rm D}$, we have the expected numbers of moderate and large scattering, $n_{\rm M}$ and $n_{\rm L}$,

$$n_{\rm M} = \int_0^{\chi_{\rm D}} 2\pi\chi f(\chi) d\chi \tag{3}$$

$$n_{\rm L} = \int_{\chi_{\rm D}}^{\infty} 2\pi\chi f(\chi) d\chi \tag{4}$$

and variance of moderate scattering,

$$\sigma^2 = \int_0^{\chi_{\rm D}} 2\pi\chi^3 f(\chi) d\chi. \tag{5}$$

The selection of $\chi_{\rm D}$ is crucial since small $\chi_{\rm D}$ makes the Gaussian approximation better but $n_{\rm L}$ larger and vice versa. (Sampling with larger $n_{\rm L}$ requires longer time.) The dividing angle should vary with the expected number of deflections, that is, the energy of scattered particle and the thickness of material traversed. Balancing the sampling accuracy and speed, we have selected $\sqrt{\chi_c^2 - \chi_a^2} \sim \chi_c$ to be the dividing angle $\chi_{\rm D}$. Then $n_{\rm L}$ is always unity and the sampling speed would be fast enough. Hence we can focus on the goodness of Gaussian approximation for moderate scattering.

One measure of how close to Gaussian a distribution is, is given by the measures of skewness and kurtosis. (For Gaussian, these are zero.) The symmetry of scattering cross section makes the coefficient of skewness be always zero and we use the coefficient of kurtosis γ_2.

The projected distribution of the central part of single scattering cross section can be written as

$$p(x) \propto \int_0^{\sqrt{\chi_{\rm D}^2 - x^2}} \frac{1}{x^2 + y^2 + \chi_a^2}\, dy$$
$$= \frac{\sqrt{\chi_{\rm D}^2 - x^2}}{(x^2+\chi_a^2)(\chi_{\rm D}^2 + \chi_a^2)} + \frac{1}{(x^2+\chi_a^2)^{\frac{3}{2}}} \arctan\left(\sqrt{\frac{\chi_{\rm D}^2 - x^2}{x^2+\chi_a^2}}\right) \tag{6}$$

where x and y are plane angles and $\chi^2 = x^2 + y^2$. For simplisity, we used $p(x)$ for calculating γ_2.

Figure 1 shows the coefficient of kurtosis calculated for $\chi_{\rm D} = \sqrt{\chi_c^2 - \chi_a^2}$ as a function of the expected total number of deflections $n = n_{\rm M} + n_{\rm L} = n_{\rm M} + 1$. The solid curve shows the result numerically calculated with the cumulant K_4 [8]. A Monte Carlo method is also used for checking the calculation and the result is shown by the solid circles. It can be seen that $|\gamma_2| < 0.1$ for $n \geq 3$. Since γ_2 for the well known simple Gaussian random number generator which uses 12 uniform random numbers is -0.1, it can be said that the Gaussian approximation for moderate scattering with the dividing angle of $\sqrt{\chi_c^2 - \chi_a^2}$ is good enough for practical purposes. For example, figure 2 shows the distributions after many small deflections for the case 100 MeV electrons traversed iron of thickness, 2×10^{-4}, 8×10^{-4} and 3.2×10^{-3}, obtained from direct Monte Carlo simulations with the screened Rutherford cross section. The curves in the figure show corresponding Gaussian distributions for comparison and the agreement is very well except for the region where dominated by the large angle deflections in the final multiple scattering distribution. For comparison, the same distributions as figure 2 but obtained for $\chi_{\rm D} = \chi_{\rm B}$ [4] are shown in figure 3. In this case, though $n_{\rm L} < 1$, the distributions are deviated from Gaussian distributions.

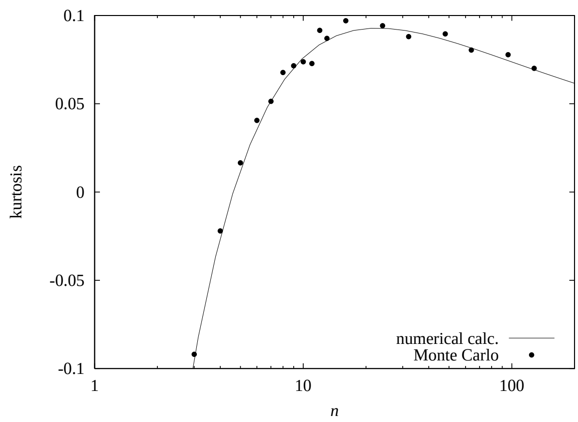

Figure 1: The coefficient of kurtosis calculated for $\chi_{\rm D} = \sqrt{\chi_c^2 - \chi_a^2}$ as a function of the expected total number of deflections n.

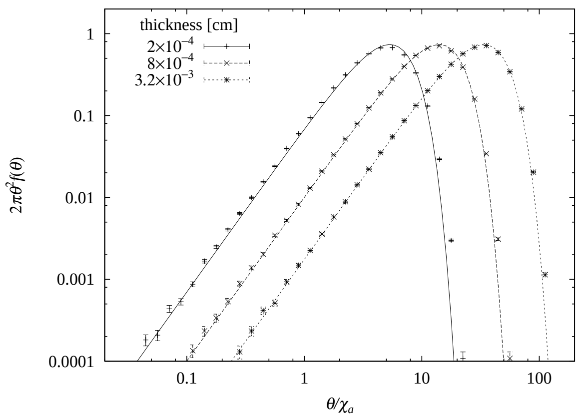

Figure 2: The distribution after many small deflections for the case 100 MeV electrons traversed iron of thickness, 2×10^{-4}, 8×10^{-4} and 3.2×10^{-3}. The points with error bars show the results from direct Monte Carlo simulations and the curves show corresponding Gaussian.

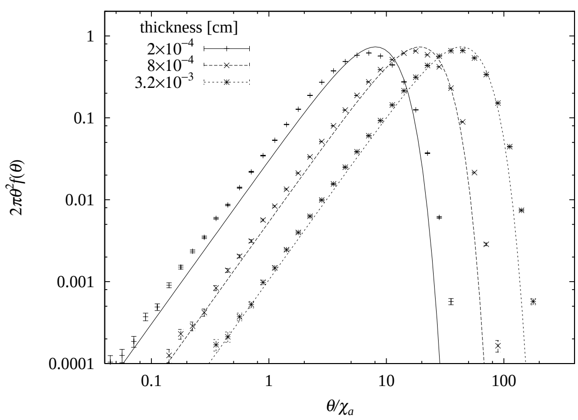

Figure 3: Same as figure 2 but for $\chi_{\rm D} = \chi_{\rm B}$.

3 The Sampling Procedure

Here we describe the procedure for sampling the deflection polar azimuthal angle θ, ϕ due to multiple Coulomb scattering:

1. Calculate χ_c, χ_a and $n = \chi_c^2/\chi_a^2$ (see for example refs. [9, 10]).
2. Using the single scattering cross section, equation (2), and according to equation (5), calculate the variance of the central Gaussian distribution,

$$\sigma^2 = \chi_c^2 \left[\ln(n) - \frac{n-1}{n} \right]. \tag{7}$$

3. Sample θ and ϕ due to the moderate scattering with Gaussian and uniform random number generators.
4. Sample n_{L} from the Poisson distribution which has the mean value of one.
5. If $n_{\mathrm{L}} > 0$, sample the large angle deflections directly from the single scattering cross section.

None of these sampling steps reqires special numerical tables calculated from Moliére theory. Therefore, a very simple and intuitive implementation is possible.

4 Results and Discussion

Figure 4 shows multiple scattering angular distributions for 100 MeV electrons in iron and $n = 10^2, 10^3, 10^4$ and 10^5 (corresponding thicknesses traversed are $1.27 \times 10^{-3}, 1.27 \times 10^{-2}, 1.27 \times 10^{-1}$ and 1.27 cm respectively). It can be seen that our results agree with Molière's theory very well. The same distributions as figure 4 but for $n = 5, 20$ and 10^2 are shown in figure 5. In this figure, results from direct Monte Carlo simulations with the single scattering cross section are also plotted. For the case $n = 5$, there is descrepancy between our multiple scattering sampling and the direct simulation where the distribution is dominated by the moderate scattering.

4.1 Small Path Length Correction

Although the descrepancy at very short path lengths is much smaller than the one between Molière's theory and the direct simulation and would be negligible in many cosmic ray applications, here we discuss a correction to the sampling procedure discribed above.

As a path length becomes smaller, n_{M} becomes smaller and the fluctuation of the number of small deflections becomes significant. This causes the descrepancy since equation (5) does not take the fluctuation into account. Therefore, we correct the σ^2 calculation at procedure 2. as

i. Sample n_{P} from the Poisson distribution which has the mean value of n_{M}.

ii. If $n_{\mathrm{P}} > 0$, calculate

$$\sigma^2 = \frac{n_{\mathrm{P}}}{n_{\mathrm{M}}} \chi_c^2 \left[\ln(n) - \frac{n-1}{n} \right]. \tag{8}$$

Now, σ^2 is a random variable and the fluctuation can be simulated. Figure 6 and 7 compares the distribution from the corrected procedure and the direct simulation for $n = 5$. It can be seen that the correction works very well.

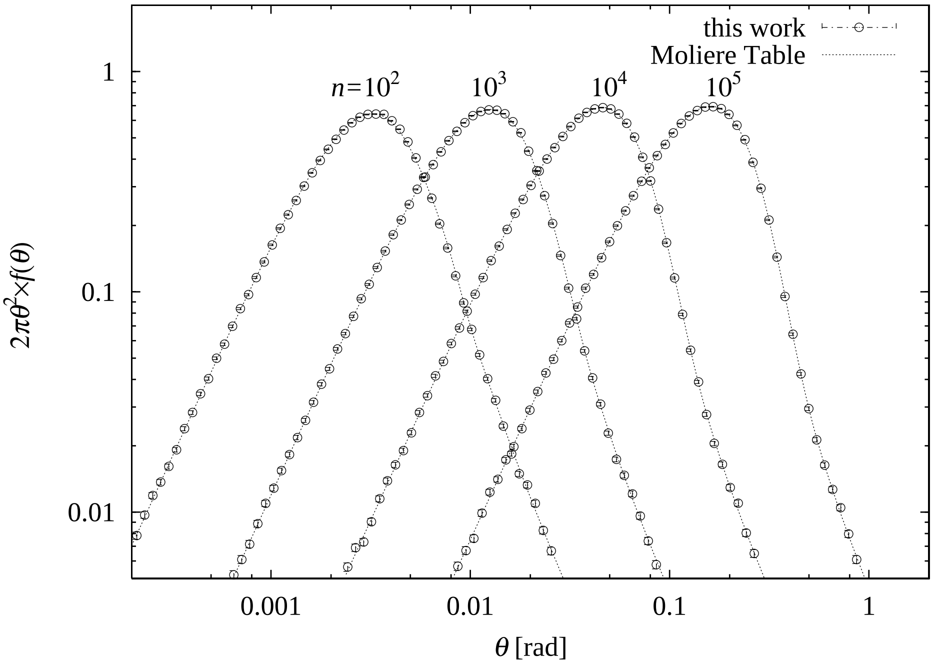

Figure 4: Multiple scattering angular distributions for 100 MeV electrons in iron for $n = 10^2, 10^3, 10^4$ and 10^5, open circle: this work, dotted curve: Molière theory.

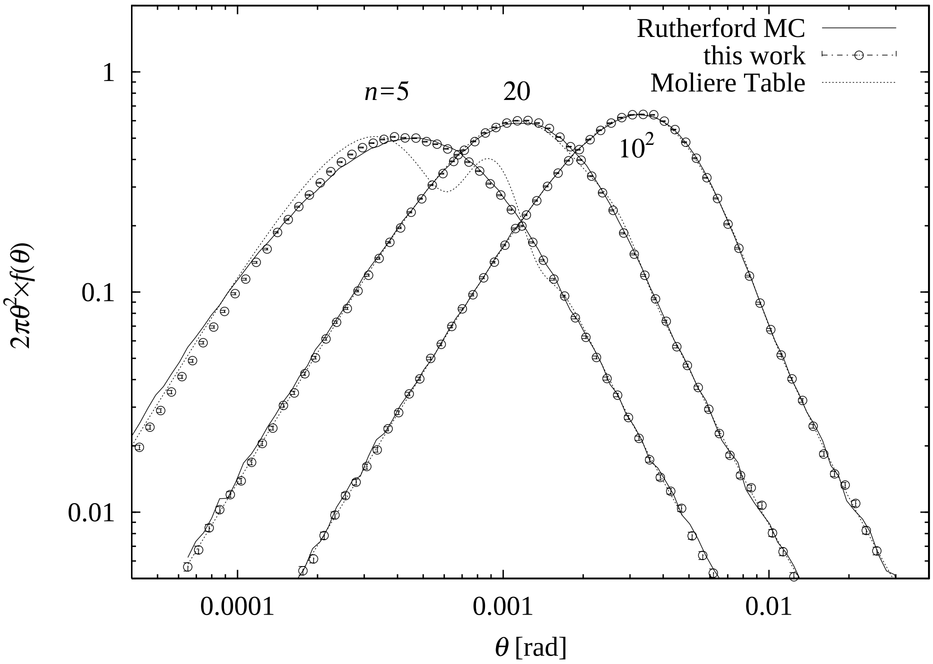

Figure 5: Same as figure 4 but for $n = 5, 20$ and 10^2. The solid curves show results from direct Monte Carlo simulations with the screened Rutherford cross section.

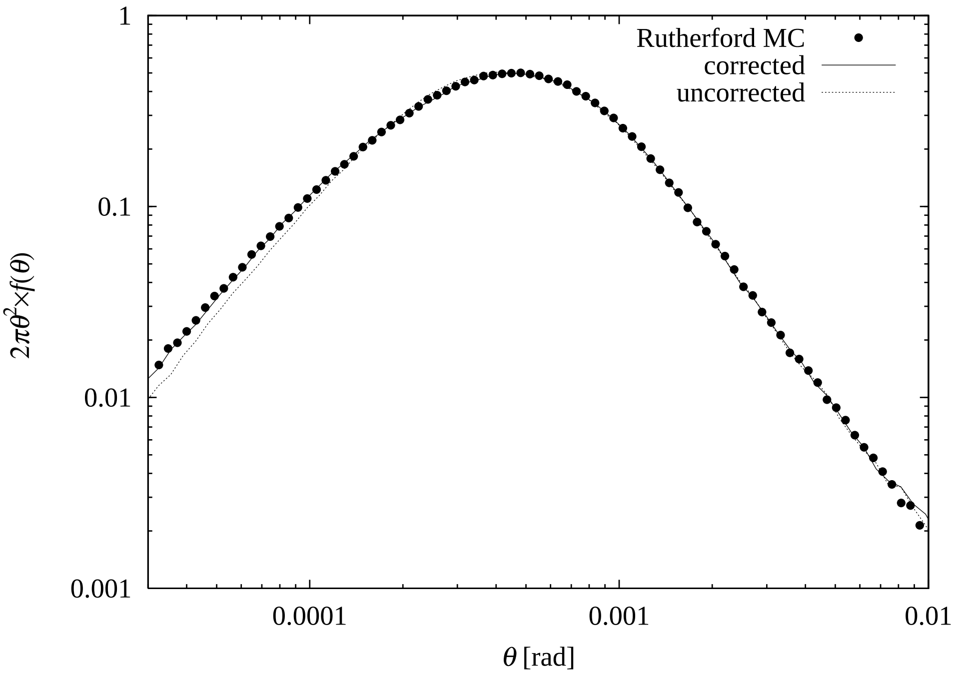

Figure 6: Multiple scattering angular distributions for 100 MeV electrons in iron for $n = 5$, solid circle: direct simulation, solid curve: corrected procedure, dotted curve: uncorrected procedure.

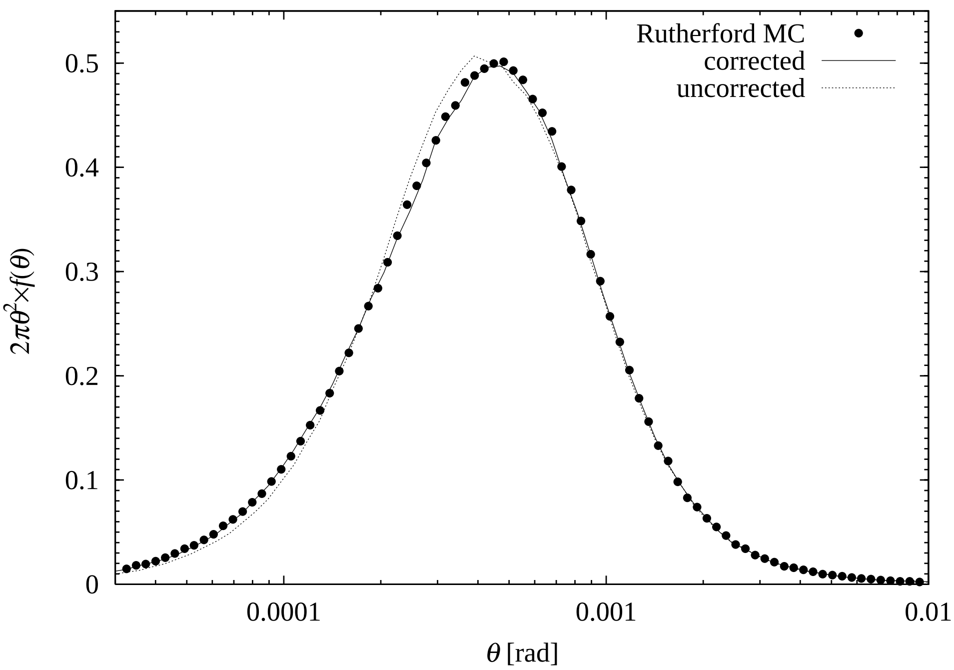

Figure 7: Same as figure 6 but ordinate in linear scale.

4.2 Large Path Length Correction

Finally, we describe the correction for the large pathlength cases where particle energy loss is not negligible. If a particle of mass m and energy E_0 traverses material of thickness t and loses its energy at a constant rate of ε, we replace χ_c with

$$\chi_c' = \chi_c \sqrt{\frac{E_0}{E}} \tag{9}$$

and the variance of the central Gaussian distribution is calculated as

$$\sigma^2 = {\chi_c'}^2 \left[\ln(n) - 1 + \left(\frac{E_0 + E}{E_0 - E} \right) \ln \left(\frac{E}{E_0} \right) + 2 \right], \tag{10}$$

where $E = E_0 - \varepsilon t$ and we assumed that $E \gg mc^2$.

Figure 8 shows multiple scattering angular distributions for muons in water for the case, $E_0 =$ 100 GeV, t = 450 m, ε = 2 MeV/cm and E = 10 GeV. The distribution from Monte Carlo samplings by one large step of 450 m agrees well with the result from samplings by many small steps. The agreement means that the maximum step length for high energy muon transport is not limited by multiple scattering.

The solid curve in figure 8 shows the distribution obtained from analytical calculation [11, 12] for comparison. This possibility of direct comparison with the analytical solution is one of advantages our sampling method has.

Although equation (10) is applicable to relativistic particles only, this large path length correction would play significant roll for speeding up high energy cosmic ray simulations.

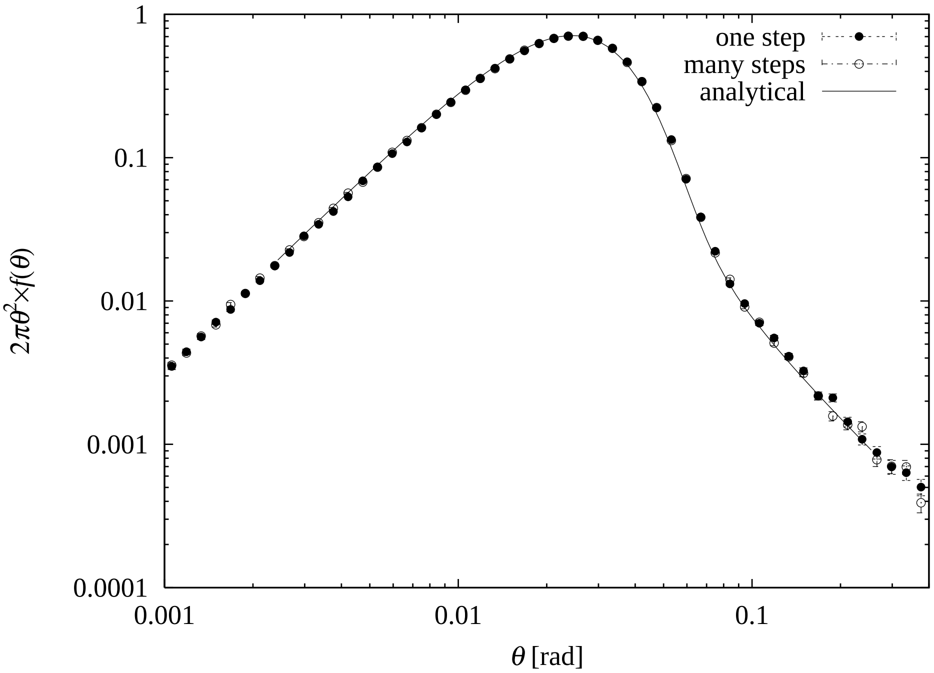

Figure 8: Multiple scattering angular distributions for 100 GeV muons after traversed 450 m of water. Closed circle: Monte Carlo samplings by step length of 450 m. Open circle: Monte Carlo samplings by many small steps. Solid curve: analytical calculation [11, 12].

5 Conclusion

A method for sampling multiple Coulomb scattering is presented. It is found that our sampling method yields same distributions as Molière's theory at usual path lengths. At very small path lengths, our method gives better results than Molière's theory, but slightly different from the direct simulations with the screened Rutherford cross section. A procedure to correct the small descrepancy is suggested.

Since our method can be implemented quite simply and intuitively, it is easily optimized for a particular CPU or incorporated into a transport code of particular application. Furthermore, the method can take account of a constant energy loss process. Hence, our method would speed up high energy charged particle transport simulations.

From what has been said, we conclude that our sampling method is useful for many cosmic ray applications.

References

[1] T. Nakatsuka, Proc. 28th International Cosmic Ray Conferance **3**, 1491(2003).

[2] T. Nakatsuka and K. Okei, Proc. 28th International Cosmic Ray Conferance **3**, 1495(2003).

[3] K. Okei and T. Nakatsuka, Proc. 28th International Cosmic Ray Conferance **3**, 1499(2003).

[4] T. Nakatsuka and K. Okei, in this Proceedings.

[5] G. Molière, Z. Naturforsch. **2a**, 133(1947).

[6] G. Molière, Z. Naturforsch. **3a**, 78(1948).

[7] H.A. Bethe, Phys. Rev. **89**, 1256(1953).

[8] W.T. Eadie et al., Statistical Methods In Experimental Physics, North-Hollnad Publishing Company (1971).

[9] W.R. Nelson, D.W.O. Rogers and H. Hirayama, The EGS4 Code System, Stanford Linear Accelrator report SLAC-265 (1985).

[10] GEANT Detector Description and Simulation Tool, CERN Program Library Long Writeup, PHYS325 (1993).

[11] T. Nakatsuka, Proc. 26th International Cosmic Ray Conferance **1**, 486(1999).

[12] T. Nakatsuka and J. Nishimura, Proc. 27th International Cosmic Ray Conferance **1**, 286(2001).