

INTRODUCING A SEMI-GAUSSIAN MIXTURE MODEL FOR SIMULATING MULTIPLE COULOMB SCATTERING IN RF-TRACK

B. Stechauner^{*1}, A. Latina, D. Schulte, CERN, 1211 Geneva 23, Switzerland

R. Frühwirth¹, J. Schieck¹, Institute of High Energy Physics, 1050 Vienna, Austria

¹also at TU Wien, 1040 Vienna, Austria

Abstract

Within the context of a design study of a LINAC for ionization cooling, this paper presents the result of incorporating a scattering model in RF-Track (v2.1) for charged particles heavier than electrons. This inclusion enables simulations for applications like ionization cooling channels for muon colliders. Within RF-Track, a novel semi-Gaussian mixture model has been introduced to describe the deflection of charged particles in material. This innovative model comprises a Gaussian core and a non-Gaussian tail function to account for the effects of single hard scattering. To validate the accuracy of our results, we conducted a benchmarking comparison against other particle tracking codes, with the outcomes demonstrating a high level of agreement.

INTRODUCTION

Charged particle deflection in matter, known as multiple Coulomb scattering (MCS), is crucial in various fields in physics. While simulating all particles interacting multiple times with the material nuclei is time-consuming, scattering probability models like G. Molière's framework [1], refined by others [2, 3], offer efficient approximations. Despite its non-Gaussian nature, MCS is often treated as a Gaussian core with non-Gaussian tails resulting from single scatterings. This phenomenon is crucial in the development of multi-TeV muon colliders [4], where technologies like ionization cooling [5] are essential for reducing the muon beam's phase space and achieving high luminosities. Precise modeling of ionization cooling requires an accurate understanding of MCS events. In this study we describe enhancement of the RF-Track program [6] by integrating a fast MCS model, thereby bolstering RF-Track's capabilities in designing final cooling lattices for muon colliders [7]. It achieves this by leveraging a semi-Gaussian mixture model parameterized with the Bethe-Wentzel deflection width. We begin this paper with a swift but essential theoretical and historical overview of single scattering approaches and continue with the description of the fast semi-Gaussian algorithm. Lastly, we benchmark our results from RF-Track with similar tracking programs and interpret our results in the conclusion.

SCATTERING THEORY

Single Scattering

The single scattering can be described by quantum electrodynamics. In this context, if a charged particle passes close enough to the Coulomb field of a nucleus, both to exchange virtual force carriers, which are mostly photons. This quantum interaction changes the direction of the moving particle, which is the actual scattering process. Such an elastic process is described by the Rutherford differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{Z^2 \Xi}{\theta^4}, \quad \text{with } \Xi = \left(\frac{2z\alpha}{\beta p} \right)^2. \quad (1)$$

In Eq. (1) (natural units are used), Z is the nuclear charge number, while z is the charge number of the deflected particle. Additionally, in Eq. (1), Sommerfeld's fine structure constant is $\alpha \approx 1/137$, c is the speed of light, and βp is the Lorentz factor multiplied by the momentum of the scattered particle.

Quantitative Approach of MCS

The first idea of MCS came from B. Rossi and K. Greisen [8]. In their work they assumed a MCS probability density function composed of Eq. (1) and the number of atoms per unit area $N_A \rho ds / A$ in a slab of material with thickness ds , where N_A is the Avogadro number, ρ and A are the density and the atomic mass of the material. They expressed the MCS variance per unit path length as

$$\frac{d\langle \theta^2 \rangle}{ds} = \int_{\theta_{\min}}^{\theta_{\max}} \theta^2 \frac{d\sigma}{d\Omega} \frac{N_A}{A} \rho d\Omega, \quad (2)$$

where $d\Omega \approx \theta d\theta d\phi$ can be used in the small-angle approximation. The angular cut-offs in Eq. (2) are

$$\theta_{\min} = \frac{2.66 \cdot 10^{-6} Z^{1/3}}{p [\text{GeV}/c]}, \quad \theta_{\max} = \frac{0.14}{A^{1/3} p [\text{GeV}/c]}, \quad (3)$$

and come from the Thomas-Fermi model [9].

Later, V. Highland [10] compared in his work Eq. (2) with the modified Molière theory from H. Bethe [2] and found inconsistencies for lower Z materials. He adjusted Eq. (2) with a fitting parameter and an additional logarithmic term. G. Lynch and O. Dahl [11] fine-tuned Highland's idea and found the final analytical expression

$$\sqrt{\langle \theta^2 \rangle} = \frac{13.6 [\text{MeV}]}{\beta p c} z \sqrt{\frac{s}{L_R}} \left[1 + 0.038 \ln \left(\frac{s}{L_R} \right) \right], \quad (4)$$

* bernd.stechauner@cern.ch

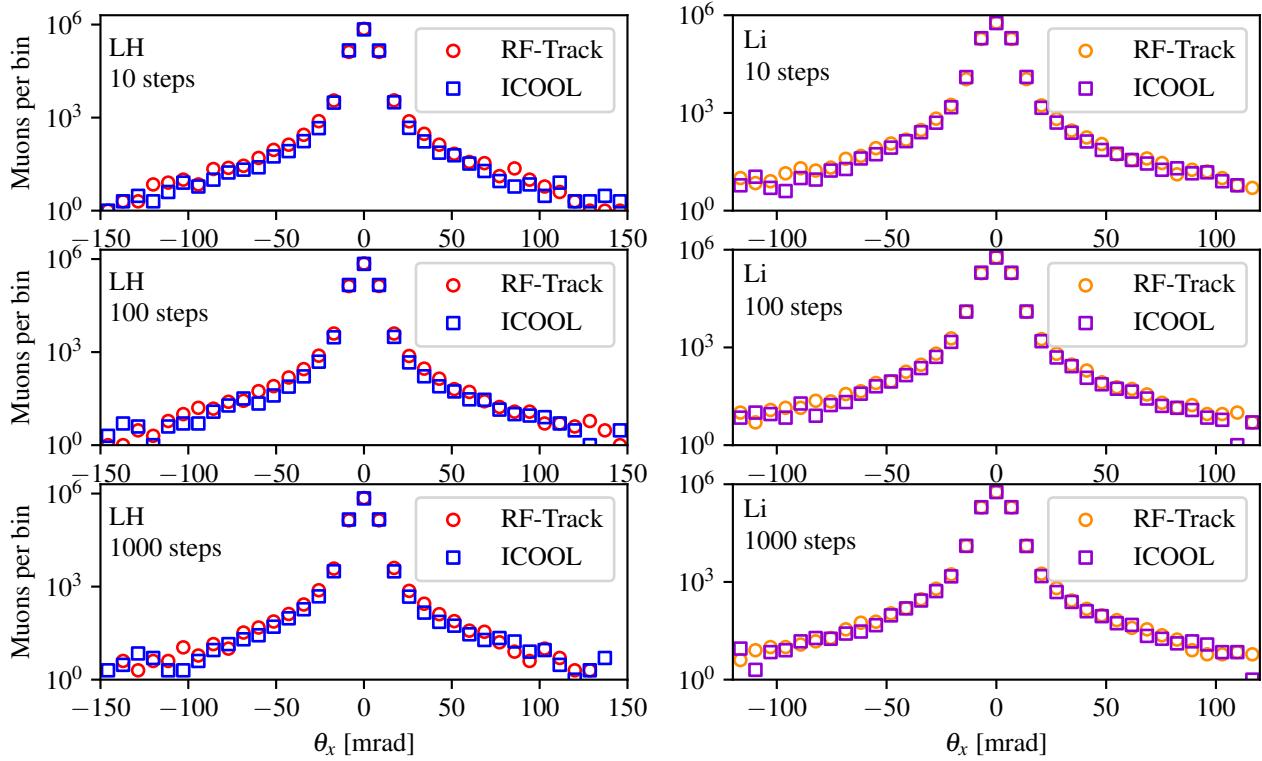


Figure 1: A 100 MeV pencil beam with 10^6 muons is simulated with RF-Track and ICOOL traveling through liquid hydrogen and lithium. The sample thickness is 1% of the material's radiation length. We vary the integration steps in the simulations and demonstrate that the long-range MCS tails of RF-Track's semi-Gaussian mixture models do not disappear.

with an accuracy of 11% for $10^{-3} < s/L_R < 10^2$, with L_R as the radiation length. Eq. (4) gives a quick analytical estimation of 98% of the central distribution and is also quoted in [12].

Nevertheless, for tracking simulations, Eq. (4) cannot be used due to the non-additive behavior of the logarithmic term. Our first attempt was to ignore the logarithmic term of Eq. (4) and compare the standard deviation of the scattered muons for lithium and beryllium and found good agreements with similar tracking codes [13]. However, we found significant overestimations with liquid hydrogen, which was our primary material of interest for ionization cooling simulations. Therefore, we searched for a better estimation than Eq. (4) and found the following.

Bethe-Wentzel Scattering

The Rutherford differential cross section in Eq. (1) can be modified by including the minimum cut-off angle $\theta^{-4} \rightarrow (\theta^2 + \theta_{\min}^2)^{-2}$ from Eq. (3) in order to avoid singularities and introducing scattering with constituent electrons by changing Z^2 to $Z(Z+1)$ [2, 14]. The MCS variance per unit length can be separated into a nuclear and an electronic component [15], including the modifications from above, which leads to

$$\frac{d\langle\theta^2\rangle}{ds} = \int_{\theta_{\min}}^{\theta_{\max}} \frac{Z^2 \theta^2 \Xi d\Omega}{(\theta^2 + \theta_{\min}^2)^2} + \int_{\theta_{\min}^e}^{\theta_{\max}^e} \frac{Z \theta^2 \Xi d\Omega}{(\theta^2 + \theta_{\min}^2)^2}. \quad (5)$$

The integration limits in the second term of Eq. (5) are

$$\theta_{\min}^e = \arccos \frac{p^2 c^2 - I(m_e c^2 + E)}{pc \sqrt{(E - I)^2 - m^2 c^4}}, \quad \theta_{\max}^e \approx \frac{m_e}{m}, \quad (6)$$

where E stands for the total energy, m symbolizes the mass, m_e is the electron mass, and I represents the ionization energy of the material [15].

THE SEMI-GAUSSIAN MIXTURE MODEL

The semi-Gaussian mixture model is a suitable option for particle tracking models in material [16]. In the semi-Gaussian mixture model, the core of the MCS is a Gaussian, while the long-range tails follow the distribution of the single scattering function of Eq. (1). There exists also a Gaussian tail description [17], but this is not considered in this study.

Tracking Code Overview

To generate a random scattering angle θ , two inverse cumulative distribution functions

$$\theta = \begin{cases} \sigma \sqrt{-2 \ln u}, & \text{if } v > \varepsilon, \\ ab \sqrt{\frac{1-u}{ub^2 + a^2}}, & \text{if } v < \varepsilon, \end{cases} \quad (7)$$

are necessary, where the function above describes the generator for the Gaussian core and the equation below characterizes the one for the long-range tails (all variables are

defined in the following.) In Eq. (7), u and v are independent and stochastic variables with a uniform distribution in the interval $[0, 1]$. The variables $(\sigma, a, b, \varepsilon)$ in Eq. (7) were estimated using the methods provided in [18]. They depend on the penetrating particle and on the material properties. For a given material thickness ds and particle velocity, two specific functions have to be introduced, which are

$$n = Z^{0.1} \ln \bar{N}, \quad \text{with} \quad \bar{N} \approx \frac{2.215 \cdot 10^4 \cdot Z^{\frac{4}{3}}}{\beta^2 A} ds. \quad (8)$$

The Gaussian core variance in Eq. (7) is given by

$$\sigma^2 = 0.1827 + 0.01803 \cdot n + 0.0005782 \cdot n^2. \quad (9)$$

The tail parameter is calculated as

$$a = 0.2822 + 0.09828 \cdot n - 0.01355 \cdot n^2 + 0.001330 \cdot n^3 - 4.590 \cdot 10^{-5} \cdot n^4. \quad (10)$$

The third parameter of the single scattering distribution is expressed as

$$b = \frac{\theta_{\max}}{\theta_{\min}} \sqrt{\bar{N} \left(\ln \frac{\theta_{\max}}{\theta_{\min}} - 0.5 \right)}. \quad (11)$$

After calculating a , b and σ , we get the tail weight factor

$$\varepsilon = \frac{1 - \sigma^2}{a^2 (\ln(a/b) - 0.5) - \sigma^2}, \quad (12)$$

that controls whether the scattered particle contributes to the core or to the tail of the distribution. The projected angles in x and y direction are perpendicular to the longitudinal particle propagation s and are connected via the azimuth angle ϕ ,

$$\theta_x = \theta \cos \phi, \quad \theta_y = \theta \sin \phi, \quad (13)$$

where ϕ follows a uniform distribution in the range $[0, 2\pi]$. These two angles are uncorrelated but not independent. The total variance of the generated angles from Eq. (7) is equal to one and has to be parameterized with Eq. (5).

RESULTS

The sum of a large number of random variables, regardless of their individual distribution, tends towards a normal distribution, which is known as the central limit theorem. Since the semi-Gaussian mixture model is not a normal distribution, we must clarify that the scattering distributions' tails remain after multiple tracking steps. Therefore, we analyzed the muon deflections while varying the computational step size in RF-Track in simulations of liquid hydrogen and lithium, each with a thickness of 1% of their radiation length and compared the distributions with ICOOL (v331.1) [19]. In both programs, we penetrated the samples with a 100 MeV pencil beam of 10^6 muons and repeated these simulations with 10^1 , 10^2 , and 10^3 tracking steps. In Fig. 1, both tracking patterns in RF-Track and ICOOL show very good agreement,

and the shape of RF-Track's semi-Gaussian model remains independent from the tracking steps.

Further, we checked the dependency of the standard deviation with the material thickness to test the Bethe-Wentzel parameterization with the semi-Gauss mixture. We used a 100 MeV pencil beam of 10^5 muons and tracked it through a liquid hydrogen target. We propagated the muon beam in RF-Track, ICOOL, and G4Beamline (v3.08) [20] and analyzed the angular deflections at different sample thicknesses. The benchmarking results between RF-Track and the other codes can be seen in Fig. 2. We observe that the semi-Gaussian mixture model together with Bethe-Wentzel parametrization shows a high degree of agreement with ICOOL and G4Beamline.

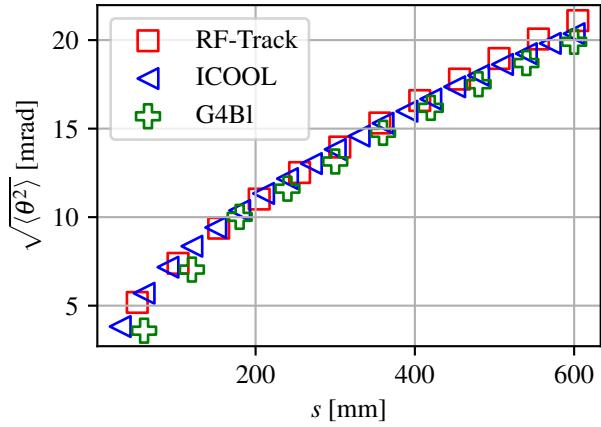


Figure 2: We compare the standard deviation of the scattering distribution at different liquid hydrogen lengths s with ICOOL, RF-Track and G4Beamline and find a high degree of agreement.

CONCLUSION

We proposed a semi-Gaussian mixture model for MCS in RF-Track and parameterized it with the Bethe-Wentzel cross section. We demonstrated that the long-range scattering tails remain at a high number of integration steps and saw good agreements with similar ICOOL simulations. We found excellent benchmarking results of the MCS standard deviated angles of RF-Track with ICOOL and G4Beamline. The novel scattering model in RF-Track can be used for any particles heavier than muons.

ACKNOWLEDGEMENT

Funded by the European Union (EU). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the EU or European Research Executive Agency (REA). Neither the EU nor the REA can be held responsible for them. Special thanks must be given to A. Salzburger from CERN, who gave very valuable suggestions during the code implementation.

REFERENCES

[1] G. Molière, “Theorie der Streuung schneller geladener Teilchen I. Einzelstreuung am abgeschirmten Coulomb-Feld”, *Zeitschrift für Naturforschung A*, vol. 2, no. 3, pp. 133–145, Mar. 1947. doi:10.1515/zna-1947-0302

[2] H. A. Bethe, “Molière’s Theory of Multiple Scattering”, *Phys. Rev.*, vol. 89, no. 6, pp. 1256–1266, Mar. 1953. doi:10.1103/PhysRev.89.1256

[3] W. T. Scott, “The Theory of Small-Angle Multiple Scattering of Fast Charged Particles”, *Rev. Mod. Phys.*, vol. 35, no. 2, pp. 231–313, Apr. 1963. doi:10.1103/revmodphys.35.231

[4] C. Accettura *et al.*, “Towards a muon collider”, *The European Physical Journal C*, vol. 83, no. 9, p. 864, Sep. 2023. doi:10.1140/epjc/s10052-023-11889-x

[5] D. Neuffer, “Principles and applications of muon cooling”, in *Proc. of the third LAMPF II workshop*, Los Alamos, 1983.

[6] A. Latina, *RF-Track Reference Manual*, CERN, Geneva, 2020, <https://gitlab.cern.ch/rf-track>

[7] E. Fol, “Final cooling lattice”, *IMCC and MuCol annual meeting 2024*, CERN, Geneva, 2024, <https://indico.cern.ch/event/1325963>

[8] B. Rossi and K. Greisen, “Cosmic-Ray Theory”, *Rev. Mod. Phys.*, vol. 13, no. 4, pp. 240–309, Oct. 1941. doi:10.1103/revmodphys.13.240

[9] J.D. Jackson, *Classical Electrodynamics*, New York: Wiley, 1998.

[10] V. L. Highland, “Some practical remarks on multiple scattering”, *Nucl. Instrum. Methods*, vol. 129, no. 2, pp. 497–499, Nov. 1975. doi:10.1016/0029-554x(75)90743-0

[11] G. R. Lynch and O. I. Dahl, “Approximations to multiple Coulomb scattering”, *Nucl. Instrum. Methods Phys. Res., Sect. B*, vol. 58, no. 1, pp. 6–10, May 1991. doi:10.1016/0168-583x(91)95671-y

[12] R. L. Workman *et al.*, “Review of Particle Physics”, *Prog. Theor. Exp. Phys.*, vol. 2022, no. 8, pp. 549–564, Aug. 2022. doi:10.1093/ptep/ptac097

[13] B. Stechauner, E. Fol, A. Latina, C. Rogers, D. Schulte, and J. Schieck, “Comparison of tracking codes for beam-matter interaction”, in *Proc. IPAC’23*, Venice, Italy, May 2023, pp. 921–924. doi:10.18429/JACoW-IPAC2023-MOPL165

[14] G. Wentzel, “Zwei Bemerkungen über die Zerstreuung körpukularer Strahlen als Beugungsscheinung”, *Zeitschrift für Physik*, vol. 40, no. 8, pp. 590–593, Aug. 1926. doi:10.1007/bf01390457

[15] T. Carlisle, “Step IV of the Muon Ionization Cooling Experiment (MICE) and the multiple scattering of muons”, *PhD thesis*, 2013.

[16] R. Frühwirth and M. Liendl, “Mixture models of multiple scattering: computation and simulation”, *Comput. Phys. Commun.*, vol. 141, no. 2, pp. 230–246, Nov. 2001. doi:10.1016/s0010-4655(01)00403-9

[17] R. Frühwirth and M. Regler, “On the quantitative modelling of core and tails of multiple scattering by Gaussian mixtures”, *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 456, no. 3, pp. 369–389, Jan. 2001. doi:10.1016/s0168-9002(00)00589-1

[18] R. Frühwirth and M. Regler, “Modelling of multiple scattering distributions by mixture models”, in *Conference proceedings of Advanced Monte Carlo for Radiation Physics, Particle Transport Simulations and Applications*, Lisbon, 2001, pp. 571–576.

[19] R. C. Fernow, “ICOOL: a simulation code for ionization cooling of muon beams”, in *Proc. PAC’99*, New York, 1999, pp. 3020–3022. doi:10.1109/PAC.1999.792132

[20] T.J. Roberts, “G4beamline simulation program for matter-dominated beamline”, in *Proc. PAC’07*, Albuquerque, 2007, pp. 3468–3470. doi:10.1109/PAC.2007.4440461