



Track - a Monte Carlo computer code to assist design of scattering and collimating systems for proton therapy beams

Miloslav Rajčan¹, Mária Pavlovič²

¹Flerov Laboratory of Nuclear Reactions, The Joint Institute for Nuclear Research, 141980, Dubna, Moscow Region, Russia; on leave from The Slovak University of Technology, ²The Slovak University of Technology, Faculty of Electrical Engineering and Information Technology, Department of Nuclear Physics and Technology, Ilkovičova 3, SK-812 19, Bratislava, The Slovak Republic

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Summary

Purpose: Heavy charged particle therapy beams need to be modified before entering the target in order to deliver the prescribed spatial dose distribution. Small and medium lateral treatment fields are usually formed by a system of scatterers and collimators. A design goal is to minimize the beam-losses in the vicinity of the patient in order to reduce the patient's irradiation by secondary particles while keeping a homogeneous dose distribution over the treatment field.

Materials and methods: Track - a Monte Carlo code to calculate beam profiles on the target after passing through a system of scatterers and collimators has been developed. A physical model used in the code is presented. Its approximations and restrictions are discussed.

Results: Results of simulations are compared with experimental data. Validity of the current physical model is discussed.

Conclusions: The results are in a good agreement with experimental data.

Key words: proton therapy, Molière theory, Monte Carlo, multiple scattering.

Track - Monte Carlo kod komputerowy wspomagający zaplanowanie systemów rozpraszających i kolimujących dla terapii protonowej

Streszczenie

Cel: Wiązki ciężkich cząstek naładowanych wymagają modyfikacji zanim dostaną się do targetu w celu podania przepisanej dawki przestrzennej. Małe i średniej wielkości boczne pola do naświetlania tworzone są zazwyczaj przez system rozpraszaczy i kolimatorów. Celem projektu jest zminimalizowanie strat wiązki w pobliżu pacjenta, aby zmniejszyć naświetlenie pacjenta przez wtórne cząstki, a równocześnie utrzymać jednorodny rozkład dawki w polu naświetlania.

Materiał i metody: Opracowano Track, kod typu Monte Carlo, dla obliczenia profili wiązek na targacie po przejściu przez system rozpraszaczy i kolimatorów. Przedstawiono fizyczny model stosowany w kodzie. Przedyskutowano również ograniczenia i przybliżenia nałożone na kod.

Wyniki: Wyniki symulacyjne porównano z danymi doświadczalnymi. Omówiono poprawność obecnego modelu fizycznego.

Wnioski: Wyniki pozostają w zgodzie z danymi doświadczalnymi.

Słowa kluczowe: terapia protonowa, teoria Molière, Monte Carlo, rozproszenie wielokrotne.

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Introduction

The paper is destined for radiation therapy specialists who use innovative treatment techniques with charged par-

ticle beams as well as for experts who design the technical (beam-shaping) part of proton therapy facilities.

Proton and ion beams have favourable physical and biological properties in their use in radiotherapy [1]. However,

covering real tumour volumes by a homogeneous dose requires essential modification of some of their physical parameters, namely the residual range in the patient's body (i.e. the initial beam energy) and the lateral size of the beam. One possibility to spread the beam laterally is to increase the beam divergence by scattering and to use an appropriate system of drift spaces and collimators. Scattering takes place in one or several scatterers typically in the form of thin foils from a suitable material. In this paper a system of scatterers, collimators and drift spaces will be referred to as a *scattering system*. Scattering systems were historically first used to get desirable treatment fields [2,3]. Various modifications such as single-scattering or double-scattering systems have been developed. Scattering systems are mostly used for proton therapy of small and medium-size tumours. A typical application is proton therapy of the eye [4]. For larger treatment fields or spreading of the beams of heavier ions, active scanning is more efficient [5,6,7,8].

Scattering systems must be designed in a custom-tailored way taking into account specific properties of the incoming beam and the required output beam parameters. That is why it is necessary to have a design tool in order to predict the output beam parameters under different configuration of the scattering system and different input beam parameters. Our design goal is to optimize the scattering system to reduce the number of particles stopped at the collimator in front of the patient while keeping the flat beam-profile on the target. The reduction in the number of particles hitting this collimator leads to a lower extra dose delivered to the patient by secondary particles during the treatment as well as to a lower activation of the patient-specific hardware [9]. A dedicated computer code Track has been developed for this particular purpose.

Track is a Monte Carlo code that simulates a passage of a charged particle beam through a scattering system. It helps to calculate a beam profile and a beam emittance diagram at a specified position of the system. In addition, it calculates beam-losses on individual components, such as, collimators and the vacuum-pipe. The Monte Carlo technique is used rather frequently for this type of problems [10] and various codes are available. However, universal codes such as GEANT (GEometry ANd Tracking) [11], TRIM (TRansport of Ions in Matter) [12] etc. usually require longer computing time, because they can calculate many other physical quantities that are irrelevant with respect to our specific problem. Track combines the Monte Carlo approach with the well-established Molière theory of multiple Coulomb scattering, which leads to savings in computing time without considerably compromising the accuracy of the results.

This paper presents a physical model implemented in Track. Preliminary results of Track are compared with experimental data and the validity of the model is discussed.

Material and methods

The scattering system is represented in Track as a sequence of the following elements: an input beam, a scattering foil, a drift space, a collimator and a target. The number of elements is not limited. Each element is given its physical parameters that are written into an input file. The input file has an ASCII-text format, which allows easy and fast modification to be made of the system configuration.

Input beam

The input beam is given by its emittance diagram [13]. The user specifies the beam emittance, the maximum beam-size and the maximum beam-divergence. The program calculates corresponding Twiss parameters to get the shape of the emittance diagram. The emittance diagram is randomly filled in by a default number of particles with the Gaussian beam profile. The user specifies the number of particles at the end of the system (on the target) rather than the input number of particles. The simulation is repeated until the required number of particles on the target has been reached. Each cycle starts with the same default number of particles, but their distribution inside the emittance diagram is random, i.e. it may vary from cycle to cycle. This approach guarantees reasonable particle statistics on the target, as well as easy comparison of results. Horizontal and vertical emittances need not necessarily be identical. That is why, transport of non-symmetric beams can also be investigated [14,15,16].

Scattering foil

The action of the scattering foil is simulated using the Molière theory of multiple Coulomb scattering. Due to the multiple Coulomb scattering, particles are deflected with respect to their original direction through a spatial angle θ , as illustrated in Figure 1. Molière has found a probability distribution function for θ [17]:

$$F(\theta, t) = \frac{1}{2\pi} \frac{1}{2\theta_M^2} \left[2e^{-\nu^2} + \frac{1}{B} F^{(1)}(\nu) + \frac{1}{B^2} F^{(2)}(\nu) + \dots \right] \quad (1)$$

where t is the thickness of the scatterer, θ_M is the so-called characteristic scattering angle, ν is a reduced angle variable, B is a reduced thickness of the scatterer and $F^{(1)}(\nu)$, $F^{(2)}(\nu)$ are the terms of distribution function expansion.

The reduced angle variable ν is defined as:

$$\nu = \frac{\theta}{\sqrt{2}\theta_M} \quad (2)$$

The reduced scattering thickness B is defined as a root of:

$$B - \ln B = b \quad (3)$$

where b is the natural logarithm of the effective number of scattering collisions calculated in [17,18].

The extension terms $F^{(1)}(\nu)$, $F^{(2)}(\nu)$ are given by:

$$F^{(n)}(\nu) = \frac{1}{n!} \int_0^\infty \eta d\eta J_0(\nu\eta) \exp(-\eta^2/4) \left(\frac{\eta^2}{4} \ln \frac{\eta^2}{4} \right)^n \quad (4)$$

where $J_0(V\eta)$ is a Bessel function:

$$J_0(\nu\eta) = \sum_{k=0}^{\infty} (-1)^k \frac{\left(\frac{1}{4} (\nu\eta)^2 \right)^k}{(k!)^2} \quad (5)$$

It is possible to approximate the probability distribution function (1) by a two dimensional Gaussian distribution [18]:

$$f(\theta) = \frac{1}{2\pi\theta_0^2} \exp\left(-\frac{1}{2}\left(\frac{\theta}{\theta_0}\right)^2\right) \quad (6)$$

where θ_0 can be calculated from the Highland formula [19]

$$\theta_0 = \frac{14.1 \text{ MeV}}{pv} z \sqrt{\frac{t}{L_R} \left[1 + \frac{1}{9} \log_{10} \left(\frac{t}{L_R} \right) \right]} \quad (7)$$

where L_R is the radiation length of the scatterer, t is the depth of the scatterer, pv is the particle energy in **MeV** and z is the particle charge-state.

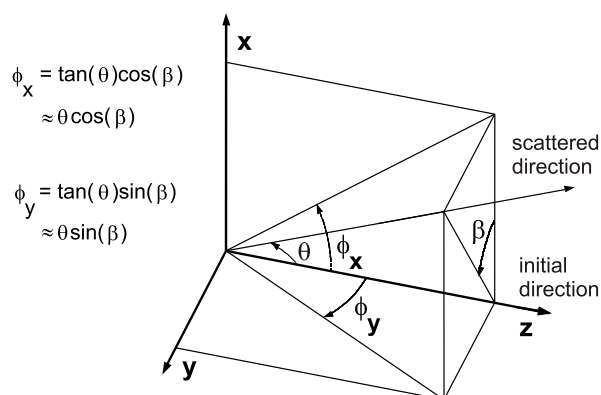


Figure 1. View of the polar and azimuthal angle θ β and projected angles ϕ_x , ϕ_y .

The Track program can use either the Molière probability distribution (1) or its Gaussian approximation (6). Differences between these two distributions are discussed in [18]. The scatterer in the input file is described by an attribute that instructs the program which probability distribution should be applied. In the case of the Molière probability distribution, the user specifies the atomic number, mass number and thickness of the scatterer and the particle kinetic energy. From these quantities, the Molière characteristic scattering angle θ_M is calculated. The present version of the program traces proton beam only. The energy loss in the scatterer is not yet included in the program. However, a reasonable approximation is to specify just the geometric mean of the initial and final kinetic energy, where the initial and final

kinetic energies are taken at the entrance to and exit from the scatterer, respectively. These energies can be calculated by other codes, like TRIM [12]. The condition of the maximum scatterer thickness (one slab) in this approximation is at $(\text{thickness} / R) \leq 0.2$, where R is the range of the proton entering the same material as the scatterer at the initial energy [18]. In the case of Gaussian probability distribution, the user specifies directly the Highland characteristic scattering angle θ_0 [7].

Using the so called invertible cumulative distribution function technique [10], a scattering angle θ is set to each particle following the above mentioned probability distributions. Horizontal and vertical projections of the scattering angle are added to the particle divergence in the horizontal and vertical emittance diagram, respectively. As an example, the action of a 100 μm aluminum scattering foil on a 72 MeV proton input beam with the emittance of 5 mm x 5 mrad waist is illustrated. Figure 2 shows the emittance diagram immediately in front of the scattering foil. Figure 3 shows the emittance diagram of the same beam after the scattering. Apparently, the particle positions are not changed, whereas the particle angles change due to the contribution of the scattering. The overall beam divergence increases. The plots show only 5.000 particles out of 1.000.000 traced by the program.

Drift space

A drift space represents a part of the scattering system where particles move in vacuum and no other external forces are present. The particle coordinates are transformed as:

$$\begin{aligned} x_{\text{new}} &= x_{\text{old}} + x'_{\text{old}} L, & x'_{\text{new}} &= x'_{\text{old}}, \\ y_{\text{new}} &= y_{\text{old}} + y'_{\text{old}} L, & y'_{\text{new}} &= y'_{\text{old}}, \end{aligned} \quad (8)$$

where L is the length of the drift space, x_{new} , y_{new} , x'_{new} , y'_{new} are particle coordinates at the end of the drift space, and

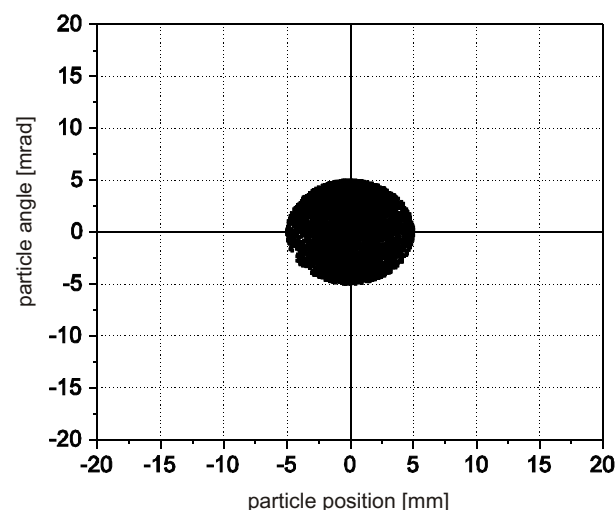


Figure 2. Emittance diagram of the initial beam.

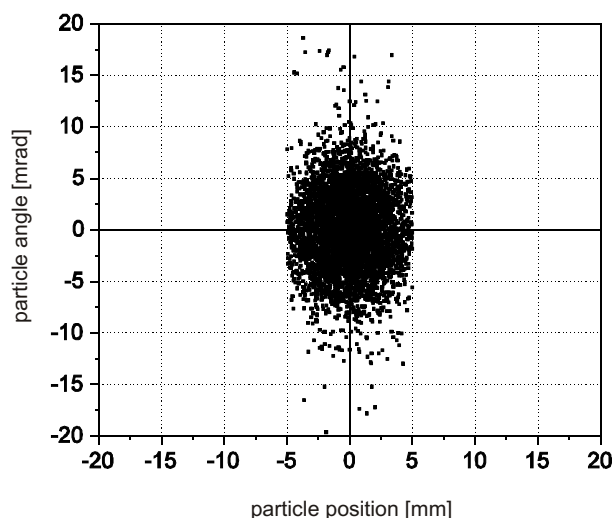


Figure 3. Emittance diagram of the scattered beam.

x_{old} , y_{old} , x'_{old} , y'_{old} are the particle coordinates at the beginning of the drift space.

Figure 4 illustrates the above input beam at the end of 1 m drift space downstream the aluminum scattering foil. Just in contrast to the action of the scattering foil, the particle angles remain constant in the drift space, and the particle positions change proportionally to the angle. If there is any material in the drift space such as air, water, etc., it is recommended to cut it into reasonable short pieces and to place equivalent scattering foils in order to account for scattering.

The drift space is characterized by its lengths and aperture. Because the aperture has the same effect as a collimator, it is modelled in the program as two identical collimators at the entrance to and the exit from the drift space.

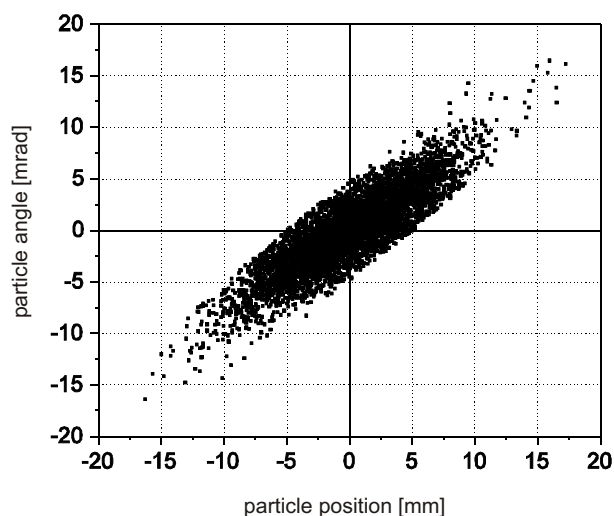


Figure 4. Emittance diagram of the scattered beam after having passed 1 m of drift space.

Collimator

A collimator is defined by its length L and aperture D . At the entrance to the collimator, the program identifies particles outside the aperture. The criterion is:

$$x^2 + y^2 \geq D^2 / 4 \quad (9)$$

where x and y are particle coordinates.

These particles are discarded from the beam. The remaining particles are transported to the end of the collimator according to transformation [8], and the same criterion [9] is applied. This approach automatically also discards the particles that would hit the collimator in-between its entrance and exit. The program stores the number of lost particles in order to evaluate the beam losses through the whole scattering system. Figure 5 shows the action of a collimator ($D=10$ mm, $L=300$ mm) on the above beam (Figure 4).

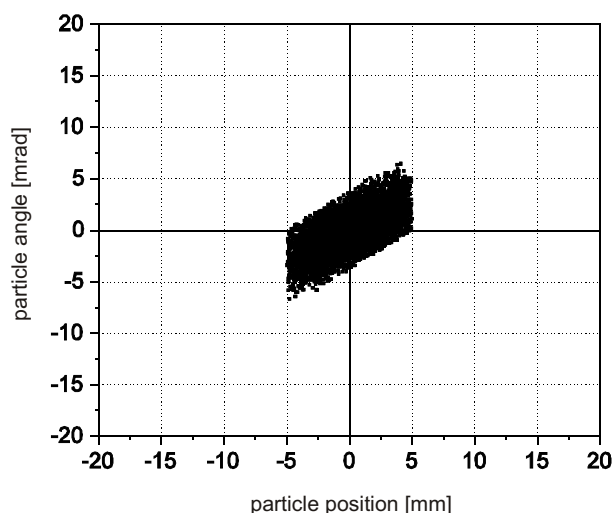


Figure 5. Emittance diagram at the end of the collimator.

Target

A target is the position where the output beam parameters are calculated. This position is specified by the user. The program calculates the final horizontal and vertical emittance diagrams on the target and keeps the information about beam losses on the collimators. Horizontal and vertical beam profiles can be calculated from the emittance diagrams.

Special features

The program makes it possible to model scattering foils and collimators with complex geometry. The scattering foils may have holes in the centre. This feature is provided to simulate scattering on the walls of the collimator. The collima-

tors may also have holes in the centre that may contain cylindrical beam stoppers. This feature is provided to design a multiple scattering system.

Results and discussion

The Track combines the Monte Carlo technique with the analytical Molière theory (or its approximation by the Highland formula). This leads to considerable savings in computing time compared to a pure Monte Carlo approach. At the present stage of code development, it was necessary to verify the correctness and to assess the accuracy of its physical model and mathematical approach. For this purpose, special test calculations were run and the results were compared with the published experimental data [18]. In addition, dedicated experiments were performed at the Joint Institute for Nuclear Research (JINR) in Dubna.

After this verification, the code was successfully applied to calculate and optimize the beam transport through the scattering system for the proton therapy of the eye. This system is currently being designed for the Cyclotron Centre of the Slovak Republic. The optimization was related to the thickness of the scatterers, lengths and apertures of the collimators and positions of these elements. Beam profiles obtained by Track can be converted into dose distributions over the treatment field. This option is under development and will become an integrated part of the code in the future.

Comparison with the published experimental data

The theory of multiple scattering was discussed and verified experimentally with 158.6 MeV proton beam by Gottschalk [18]. We simulated these experiments with Track

Table 1. Comparison between published experimental data and simulated data on multiple scattering of a 158.6 MeV proton beam. D_θ represents the relative deviation between experimental and simulated data, $D_\theta = (\theta_{0\text{sim}} / \theta_{0\text{exp}} - 1) \cdot 100\%$. Accuracy of the first two columns values was taken from [18].

Pb, Z = 82, A = 207.19			
thickness g / cm ²	experiment θ_0 [mrad]	simulation θ_0 [mrad]	D_θ [%]
0.086	4.300	4.4	2.3
0.454	11.185	11.4	1.9
1.823	24.003	24.6	2.5
4.491	39.768	41.2	3.6
Cu, Z = 29, A = 63.546			
thickness g / cm ²	experiment θ_0 [mrad]	simulation θ_0 [mrad]	D_θ [%]
0.114	3.483	3.6	3.4
0.453	7.462	7.7	3.2
1.450	14.327	14.5	1.2
4.456	28.247	27.9	-1.2
Al, Z = 13, A = 26.982			
thickness g / cm ²	experiment θ_0 [mrad]	simulation θ_0 [mrad]	D_θ [%]
0.216	3.534	3.6	1.9
0.871	7.670	7.8	1.7
2.1729	13.104	13.1	0.0
3.3500	16.258	16.7	2.7
Be, Z = 4, A = 9.012			
thickness g / cm ²	experiment θ_0 [mrad]	simulation θ_0 [mrad]	D_θ [%]
0.644	3.743	3.7	-1.1
1.220	5.209	5.3	1.7
2.412	7.640	7.8	2.1
4.758	11.821	11.6	-1.9

for Be, Al, Cu, Pb scatterers of various thicknesses. Each scatterer in the simulation was represented by one slab. To prevent error in the calculation, the scatterers maximum thickness was observed, as shown above (sec. 2.2). The Highland scattering angle θ_h was determined from the beam profiles simulated by Track and compared with the Highland angles obtained from the experimentally measured beam profiles. The results are collected in *Table 1*.

The Molière scattering angle θ_M was calculated analytically and compared with experimentally obtained data. A similar trend of accuracy has been observed.

Comparison with dedicated experiments

Scattering experiments were performed on a 175 MeV proton beam obtained from the synchrocyclotron at Dzhelapov Laboratory of Nuclear Problems, the JINR in Dubna. The experimental set-up is shown in *Figure 6*. The simulations started at the position where the input beam parameters

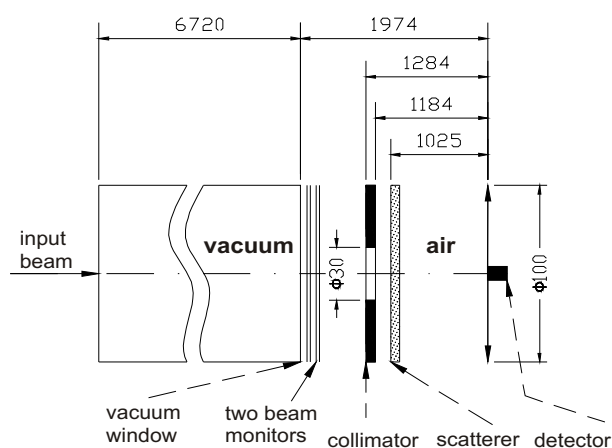


Figure 6. Schematic view of the experimental set-up.

(emittance diagrams) were measured. The beam passed through a vacuum window, two multi-wire beam-profile monitors and a 30 mm diameter collimator. A set of scattering foils from different materials (lead and LUCITE) and thicknesses (from 0.1 to 3.16 g/cm²) was inserted into the beam. The beam profile was measured by a silicon diode detector 102.5 cm downstream the scattering foils.

The Molière distribution was used in the case of lead, and the Highland distribution in the case of LUCITE. The measured and simulated beam profiles were fitted by Gaussian distribution and their standard deviations σ_{exp} and σ_{sim} were compared. The results are listed in *Table 2*. It can be seen that simulation underestimates the experiment approximately by 5.5%. There are several possible causes for this discrepancy. First of them is that real emittance diagrams may differ from the elliptical shape, which means that the input beam parameters assumed by the model may not correspond exactly to reality. The second one is neglecting the scattering from the inner wall of the collimator. This effect is not yet included in our model. Scattering action of the multi-wire profilometer and monitor chamber foils is also difficult to describe precisely.

Conclusion

A dedicated computer code Track has been described in the paper. It provides a suitable tool for the design of complex scattering systems for proton therapy beams. The validity of its physical model was verified by comparison with experimental data. The combination of the Monte Carlo technique with the analytical Molière (Highland) theory was proved to be a correct approach for fast simulation of multiple Coulomb scattering. Computing time is considerably shorter compared to the pure Monte Carlo approach while satisfactory accuracy is still preserved.

Table 2. Comparison between our experimental and simulated data of multiple scattering on lead and LUCITE with a 175 MeV proton beam. Standard deviations of measured and simulated beam profiles are compared.

Pb			
thickness g / cm ²	experiment σ [mm]	simulation σ [mm]	D_σ [%]
0.1	12.9	12.3	-4.7
0.2	13.8	13.0	-5.8
0.3	14.7	13.9	-5.4
0.4	15.6	14.7	-5.8
0.5	16.4	15.6	-4.9
LUCITE			
thickness g / cm ²	experiment σ [mm]	simulation σ [mm]	D_σ [%]
1.57	13.6	12.9	-5.1
3.16	15.7	15.3	-2.5

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