JOINT INSTITUTE FOR NUCLEAR RESEARCH
The Laboratory of Radiation Biology

FINAL REPORT ON THE INTEREST PROGRAMME

Validation extension of Geant4-DNA physics for accurate modeling of accelerated charged particle interactions in biological media

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Contents

Abstract

Ion components in Galactic and Solar cosmic rays cause various radiation effects and health risks for astronauts during space missions. Reliable Monte Carlo simulations, like those performed with the Geant4 toolkit, are essential for accurately modeling ion transport and interactions at nanometer scales within the space radiation environment. Geant4 is widely utilized in space and medical applications, including hadrontherapy and heavy-ion irradiation studies.

Recent Geant4 physics models for ion transport have undergone significant updates and validation. This work presents a continuation of the validation that was started in the "START" JINR internship program. In particular, this validation has a unique comparison with the physics list that is based on our dynamic charge approach - G4EmDNAPhysics_option8.

Introduction

Currently, humanity is actively planning and implementing numerous space missions, particularly manned flights. These missions pose various risks, ranging from single-event upsets (SEUs) in electronics to severe radiation effects on the human body. The primary source of these risks is cosmic radiation. A key question arises: how exactly does cosmic radiation affect biological systems?

Cosmic radiation consists of approximately 85% protons, 10% alpha particles, and 4–5% heavier ions, with the remaining 1% composed of electrons and positrons. However, this study focuses on electrons. While this may seem counterintuitive given their insignificant contribution to the primary cosmic radiation flux, the justification lies in the physics of interaction.

Specifically, we are interested not in electrons of cosmic origin (primary radiation), but in delta-electrons (secondary radiation). These are generated when ions traverse a medium—particularly water, which constitutes the main chemical component of human cells (60–80% of the total cell mass).

Biological systems are inherently complex, and there is currently no complete theory representing the effects of ionizing radiation on biological structures through a full set of analytical expressions. For this reason, the Geant4 software package is employed to investigate the effects of delta-electrons on an aqueous medium.

Geant4 (***Ge****ometry* ***an****d* ***t****racking*) is a software toolkit based on the Monte Carlo method, enabling the simulation of particles passing through matter. This package is utilized in a wide range of scientific tasks. At the Joint Institute for Nuclear Research (JINR), it is actively used and developed; for instance, it is employed to simulate the SPD detector at the NICA accelerator using the GeoModel library. It is also used to model the effects of ionizing radiation on biological structures at various organizational levels at the Laboratory of Radiation Biology (LRB) [1–3, 5], under whose auspices this work was conducted.

Within the framework of this study, two primary objectives are established:

1. (Sci.) Validation of the cluster size distribution for protons, deuterons, alpha particles, lithium isotopes, and carbon ions using the Geant4 software package version 11.4 (cand01).

2. (Ill.) Visualization of the transverse track structure.

The second objective is characterized as illustrative (or educational) because, while it offers no scientific novelty, it provides essential visual support for the forthcoming scientific article.

I Cluster size distribution

Problem Statement

The radial dose distribution is defined as the dependence of the energy deposited in a cylindrical shell, normalized to the mass of that shell (dose), on the radius of the shell.

This distribution allows for the estimation of the energy contribution of delta-electrons in the vicinity of an incident ion track. Essentially, it helps to characterize the radius of damage caused by a specific particle with a given energy in the context of human radiation safety.

To provide such estimates, a tool capable of performing these simulations is required. The Geant4 software package, introduced earlier, serves as a potential candidate. However, before its application, validation of the physical models implemented in Geant4 is essential. More specifically, the validation of the *physics lists* is required.

Physics Lists in Geant4

Geant4 provides the capability to simulate various processes, including particle transport, electromagnetic and hadronic interactions, decay, and optical phenomena. For any given task, a specific set of particles and processes, described by a collection of models, must be selected. Such a combination is referred to as a *physics list*.

In the context of this study, the focus is on electromagnetic physics lists, as they enable the modeling of ionization processes, which are the source of delta-electrons.

Among the available electromagnetic physics lists, the following five are investigated in this work: EM Standard Option 4 and DNA Options 2, 4, 6, and 8. This selection is based on the following reasons:

1. To confirm the necessity of developing DNA physics lists: standard physics lists (e.g., EM Standard Option 4) are currently not adapted to model ionization losses at low energies and small spatial scales.

2. To evaluate and compare the simulation quality offered by different DNA physics lists.

The distinction between the proposed physics lists lies not only in the different models and applicable particles but also in the fundamental approach upon which the EM Standard and DNA lists are based. EM Standard physics lists are developed based on the Condensed History approach, whereas DNA physics lists rely on the Detailed Track Structure approach. Let us examine the content of these physics lists in greater detail.

The models used in EM Standard physics lists are presented in Table 1. The models used in DNA physics lists (for options 2, 4, and 8) are presented in Table 2.

Thus, each physics list possesses unique features defined by its set of models. Two physics lists are of particular interest: DNA Option 6 and DNA Option 8[1].

[1]Based on the Rudd Dynamic model.

Model	Particle	Based on data
G4BetheBlochModel	default high-energy model for heavy particles	–
G4LindhardSorensenModel	used for ions Z > 2	ICRU73 & ICRU90
G4BraggModel	for protons, backup for all ions, effective charge for ions	ICRU90 & PSTAR
G4BraggIonModel	for alpha particles	ICRU90 & ASTAR

Table 1 – Models in the EM Standard physics list

Energy	Particle		
	Protons	Alpha-type	Other Ions
$E < 0.5$ MeV/amu	*Rudd model*	*Rudd model*	
$0.5 < E < 100$ MeV/amu	*Born model*		
$100 < E < 300$ MeV/amu	*RPWA model*		
$E > 300$ MeV/amu	*Standard models*		

Table 2 – Models in DNA physics lists (2, 4, 8)

Interest in the first case arises because the models used in this configuration are specifically designed for electron modeling. The second case is notable for its novelty: it employs a new concept in Geant4 modeling—*dynamic charge*—which will be tested for protons and alpha particles[2].

Validation

During the internship at the START program, a study of the physical quantity known as the *Radial dose distribution* was conducted. In the framework of the current work, a different quantity is of interest—the *Ionisation cluster size distribution*.

The essence of this quantity is as follows: a certain target volume is defined, and the number of ionizations (secondary, tertiary, etc.) occurring within it is counted.

A water-filled cylinder with dimensions characteristic of DNA is considered as such a target volume: specifically, the distance between adjacent DNA strands (2.3 nm) and one full DNA turn (3.4 nm).

In fact, the Geant4 software package already contains an application capable of calculating this value, but it is restricted to a nitrogen medium and a limited number of physics lists. In the application developed for this work, the medium was changed from nitrogen to water, and the physics list can be specified via a macro file. Most importantly, the visualization of the resulting plots was modified to match the style established during the START program: two blocks containing the main plot and the deviations, with the root mean square error (RMSE) indicated in the legend. Let us now analyze the obtained plots in order of increasing mass number[3]: proton, deuteron, alpha particle, lithium-6 isotope, lithium-7 isotope, and carbon-12 isotope.

The first case is the proton (hydrogen nucleus) with an energy of $E = 20$ MeV. This case is particularly interesting because the dynamic charge concept is currently developed only for protons and alpha particles. Similar to the results from the START internship, the standard physics list shows a significant deviation from experimental values almost everywhere. This deviation is comparatively larger than in the

[2] As of version 11.4 (cand08), the *dynamic charge* concept has been implemented only for protons and alpha particles.
[3] Experimental data for all ions, except carbon, were taken from [6].

cases of the DNA physics lists. The smallest deviation is observed for G4EmDNAPhysics_option6, which corresponds to an RMSE = 0.5672.

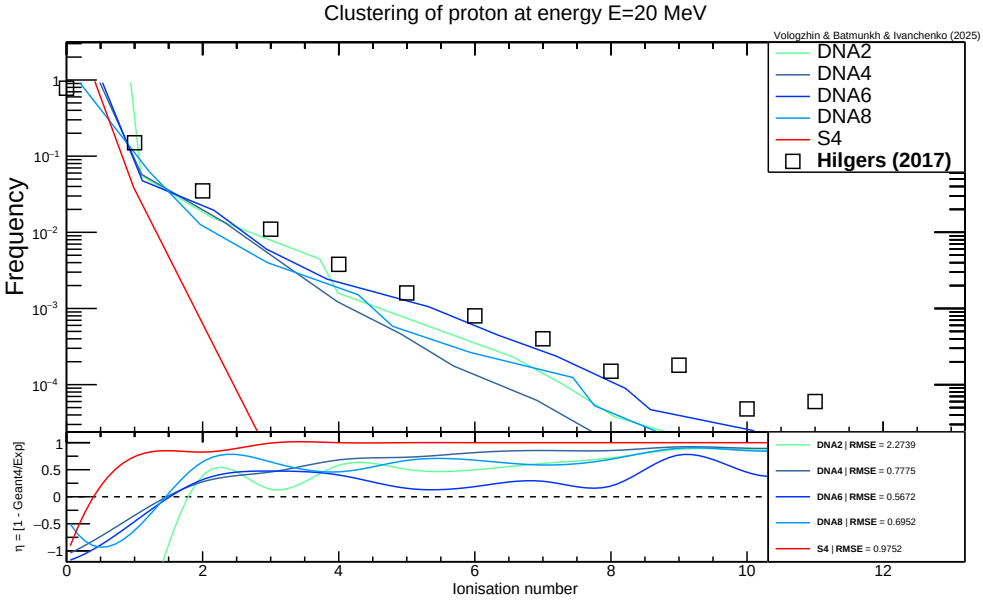

Figure 1 – Ionization cluster size distribution for a proton with energy $E = 20$ MeV

The deuteron (a hydrogen isotope with one neutron) with an energy of $E = 16$ MeV shows a more significant deviation from experimental values. G4EmStandard_option4 continues to exhibit similar behavior, while the remaining DNA physics lists deviate by an order of magnitude; however, Option 8 shows the lowest RMSE. This behavior raises questions, as the plot visually suggests that DNA Option 6 is closer to the experimental points[4].

[4]Presumably, this discrepancy is caused by the histogram plotting method, where a random point within the bin width is selected rather than the bin center.

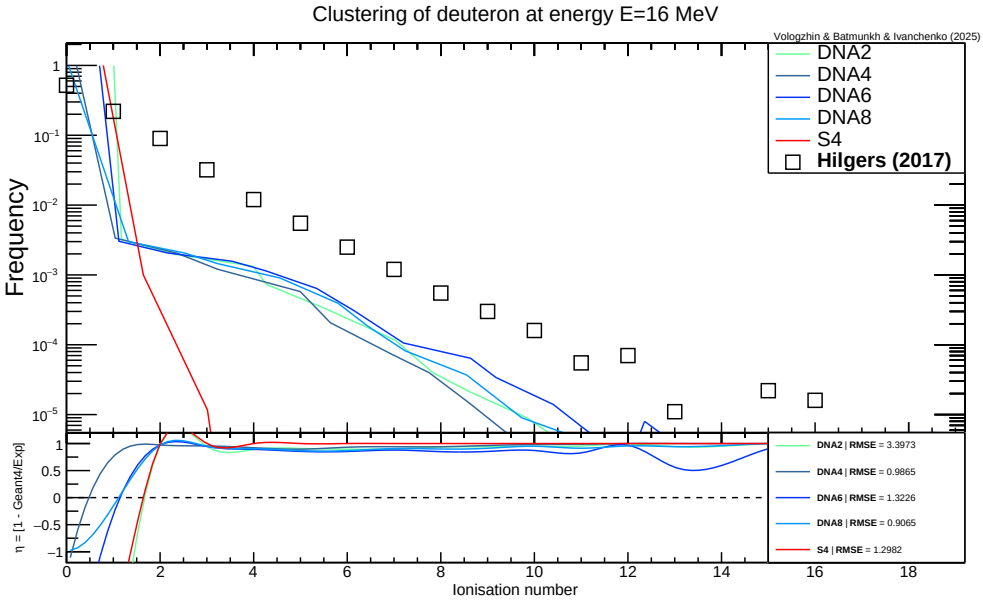

Figure 2 – Ionization cluster size distribution for a deuteron with energy $E = 15$ MeV

Another interesting case is the alpha particle at an energy of $E = 4$ MeV. It is notable for the presence of dynamic charge in the case of G4EmDNAPhysics_option8. As can be seen from the plot, this physics list lies close to the experimental points; however, G4EmDNAPhysics_option6, formed by CPA100 models for electrons, shows better agreement with the experimental data, possessing a lower RMSE.

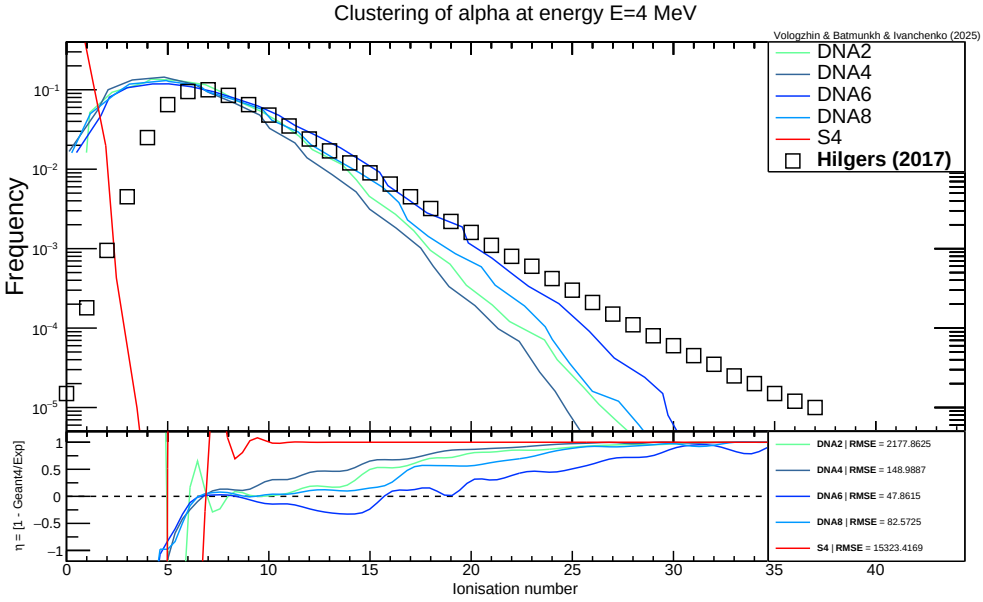

Figure 3 – Ionization cluster size distribution for alpha particles with energy $E = 4$ MeV

A similar picture can be observed for both the Lithium-6 isotope ($E = 48$ MeV) and the Lithium-7 isotope ($E = 26.7$ MeV). The significant difference from the previous cases is that the maximum has shifted substantially toward lower values relative to the experimental maximum. Physically, this implies that, on

average, Geant4 simulates fewer ionizations than occur in the experiment, with large numbers of ionizations being a rarity.

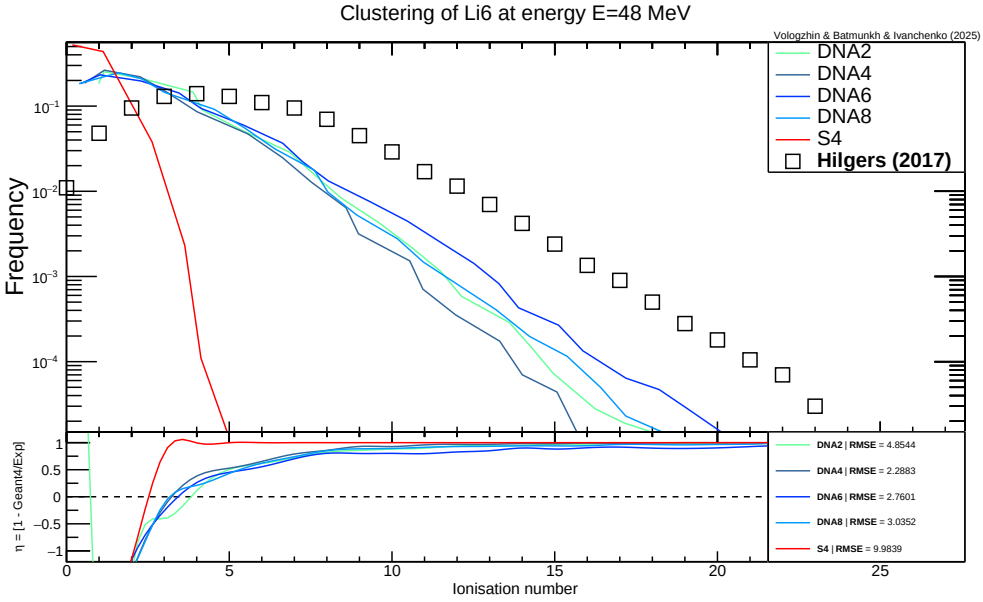

Figure 4 – Ionization cluster size distribution for the lithium-6 isotope with energy $E = 48$ MeV

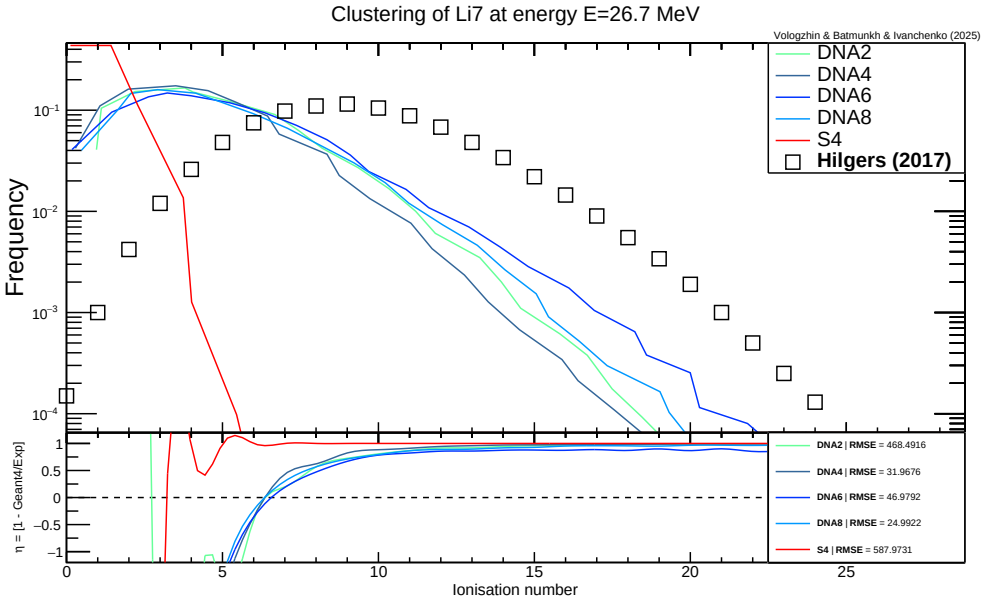

Figure 5 – Ionization cluster size distribution for the lithium-7 isotope with energy $E = 26.7$ MeV

The final case is carbon nuclei ^{12}C at an energy of $E = 88$ MeV[5]. We can observe that the picture has aligned again: the maximum has almost returned to its previous position, and G4EmDNAPhysics_option6 qualitatively almost completely reproduces the shape of the experimental curve, with a root mean square

[5]Experimental data taken from [7].

error of $RMSE = 0.7133$. However, the G4EmStandardPhysics_option4 case remains entirely unsuitable for calculating the cluster size distribution.

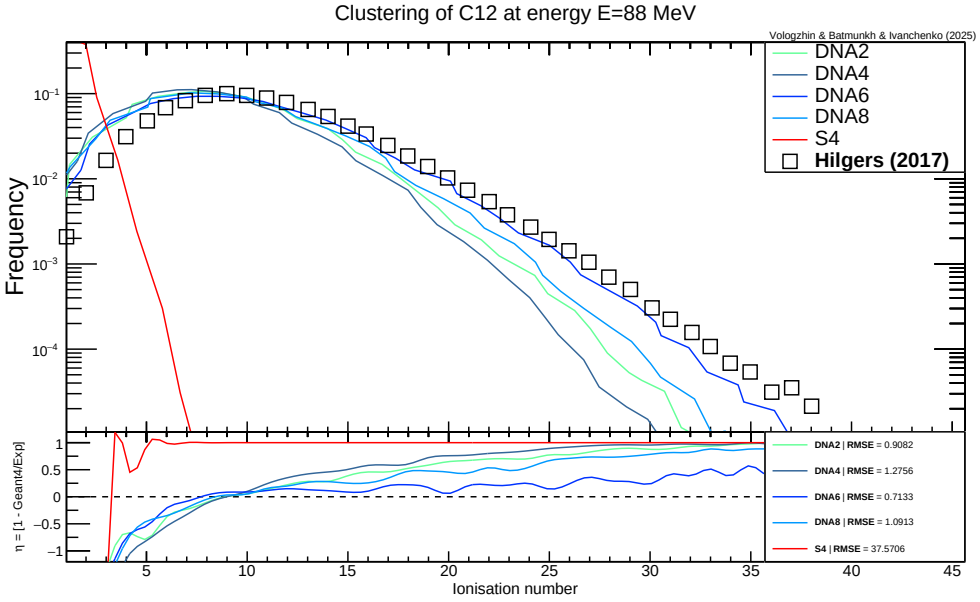

Figure 6 – Ionization cluster size distribution for the carbon-12 isotope with energy $E = 88$ MeV

II Transverse track structure

The investigation of the impact of radiation fields on organisms requires an understanding not only of the dynamics of the primary particle passing through the medium but also of the secondary particles [4] generated during its passage through biological tissue. This interest stems from the complex nature of DNA damage. A conventional classification distinguishes two types of damage: physical and chemical.

Physical damage arises when there is sufficient energy deposition within a specific volume characteristic of DNA, such as the vicinity of a nucleotide or the sugar-phosphate backbone.

Chemical damage, in turn, is caused by the interaction of chemical species formed during water radiolysis with the DNA molecule.

Visualizing such phenomena is challenging without illustrative examples; in an educational context, visualization serves as an auxiliary tool that accelerates the assimilation of information.

Since this study focuses on physical lists rather than chemical ones, a visualization of the transverse track structure of an incident ion has been developed, as shown in Fig.7.

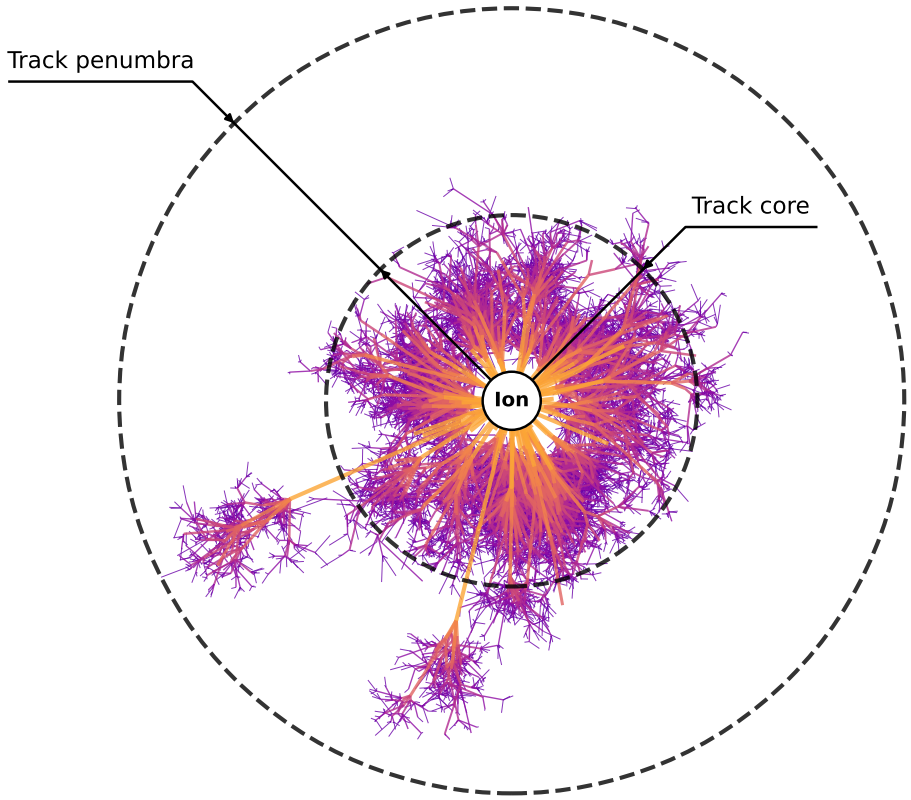

Figure 7 – The transverse structure of the ion track: the gradient from orange to purple represents generations of delta-electrons (orange — secondary electrons, brown — tertiary electrons, etc.)

In this figure, two distinct regions can be observed: the track core and the track penumbra. The former is the region with the highest ionization density, while the latter consists of rare events that influence the transverse range of the ionizing radiation but do not contribute significantly to the total dose. The color palette represents the generational hierarchy: orange lines correspond to secondary electrons, slightly darker

shades indicate tertiary electrons, and so on. The line thickness represents the track length of an electron of a specific generation.

The illustration was generated using the Python programming language and the Matplotlib library. To produce this image, a uniform distribution (for angles) and an exponential distribution (for secondary particle track lengths) were employed. For the corresponding source code, please contact the author.

The presented illustration will be utilized in the author's future scientific work.

Conclusion

Over the course of the six-week INTEREST internship at the Laboratory of Radiation Biology, the following results were obtained:

1. Validation of the Ionization Cluster Size Distribution (ICSD) within the Geant4 version 11.4 (cand01) framework for the following ions and corresponding energies: proton ($E = 20$ MeV), deuteron ($E = 16$ MeV), alpha particle ($E = 4$ MeV), ^{6}Li ($E = 48$ MeV), ^{7}Li ($E = 26.7$ MeV), and ^{12}C ($E = 88$ MeV). The physics lists considered were: EM Standard Option 4 and DNA Options 2, 4, 6, and 8.

2. It was established that the EM Standard physics list is entirely unsuitable for estimating the number of ionizations within volumes characteristic of DNA dimensions.

3. It was determined that among the DNA physics lists, G4EmDNAPhysics_option6 is the most suitable for calculating ICSD. This suggests that electron-induced ionizations make a dominant contribution to the total ionization count, as G4EmDNAPhysics_option6 is specifically designed for electron transport modeling based on the CPA100 models.

4. DNA physics lists demonstrate good agreement with experimental data regarding ICSD for protons and comparatively heavier ions, such as ^{12}C. However, significant discrepancies are observed for intermediate ions and isotopes (e.g., deuterons).

5. An illustrative visualization of the transverse track structure of an incident ion was generated using the Matplotlib library.

The obtained results will be incorporated into a forthcoming validation article in *Medical Physics*, which will include findings from both the INTEREST internship and the previous START internship.

We emphasize the importance of this internship, as it fostered collaboration between researchers at the Laboratory of Radiation Biology (LRB) JINR and the Laboratory of High Energy Physics Data Analysis (LHEPDA) TSU to study the effects of cosmic radiation on biological structures.

The intern plans to continue collaborating with the scientific supervisor of this project within the framework of the INTEREST program.

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