



Original Article

Developing an approach for fast estimation of range of ion in interaction with material using the Geant4 toolkit in combination with the neural network

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ABSTRACT

Precise modelling of the interaction of ions with materials is important for many applications including material characterization, ion implantation in devices, thermonuclear fusion, hadron therapy, secondary particle production (e.g. neutron), etc. In this study, a new approach using the Geant4 toolkit in combination with the Bayesian regularization (BR) learning algorithm of the feed-forward neural network (FFNN) is developed to estimate the range of ions in materials accurately and quickly. The different incident ions at different energies are interacted with the target materials. The Geant4 is utilized to model the interactions and to calculate the range of the ions. Afterward, the appropriate architecture of the FFNN-BR with the relevant input features is utilized to learn the modelled ranges and to estimate the new ranges for the new cases. The notable achievements of the proposed approach are: 1- The range of ions in different materials is given as quickly as possible and the time required for estimating the ranges can be neglected (i.e. less than 0.01 s by a typical personal computer). 2- The proposed approach can generalize its ability for estimating the new untrained cases. 3- There is no need for a pre-made lookup table for the estimation of the range values.

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1. Introduction

The interaction of ions with matter is important from the viewpoint of many applications [1] including material characterization, ion implantation in devices, thermonuclear fusion, hadron therapy, secondary particle production (e.g. neutron), etc.

The energy loss of ion during its transition in the material which is due to elastic/inelastic collisions is given by Eq. (1) [2,3].

$$\frac{dE}{dr} = \left(\frac{dE}{dr}\right)_{nuclear} + \left(\frac{dE}{dr}\right)_{electronic} + \left(\frac{dE}{dr}\right)_{radiation} \quad (1)$$

where, dE/dr is energy loss per unit length of ion along its trajectory, E is the energy of ion, and r is ion displacement. The energy loss due to the radiation (i.e. bremsstrahlung and Cherenkov) is very small and can be neglected. At low energies, scattering (i.e. Rutherford scattering [4]) of the ion by the nuclear potential of the target

material is the reason of energy loss. The main mechanism of energy loss, at higher energies, is the inelastic interaction of incident ion with the electrons of material causing ionization/excitation of the target material atoms.

Up to now, different studies for modelling of ions interaction with matter have been done. Examples are calculating stopping power and range values of some human tissues [5], modelling of neutron emission from the neutron generator [6], calculation of stopping power ratio for proton therapy [7], and calculating the distribution of deposited energy for simulation of ultra-fast detection of proton and alpha particles [8].

In this study, a new approach based on the combination of the Geant4 toolkit [9] and the feed-forward neural network with the Bayesian regularization learning algorithm (FFNN-BR) is developed to estimate the values of ion ranges in the materials accurately and quickly. The developed approach using the Geant4 toolkit is able to calculate the range of ions without any specific restriction on its extension for new ions/energies/targets. The use of the FFNN-BR is to speed up the calculations. In this study, we intend to train the neural network only for ions with energies less than 2 MeV. First, this cut-off energy is considered to examine the efficiency of the

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proposed approach without need for the deep neural networks (DNNs). Increasing the interaction energy increases the number of patterns for training, which as a result, the network variables and the number of layers should be increased to avoid underfitting. Eq. (2) shows this criterion. Where, N_p is the number of training patterns, N_V is the number network variables, N_W and N_B are the number of weights and biases, respectively, N_F is the number of input features, N_{L1} , N_{L2} , N_{Lf} , and N_O are the number of neurons in hidden layer 1, hidden layer 2, final hidden layer, and output layer, respectively. Since the main purpose of this paper is to develop a method for calculating range of ions using the Geant4 and to accelerate computations with the neural network, the purpose is not to emphasize the capability of the DNNs. The further development of the proposed approach to cover the full range of energies/ions/targets that require DNNs will be presented in the next work. Secondly, many prevalent applications utilize low energy ions and some defined models in *PhysicsList* of Geant4 (e.g., *G4Bragg* model) are different for energies above 2 MeV.

$$\begin{aligned} N_p &\cong N_V = N_W + N_B \\ N_W &= N_F \times N_{L1} + N_{L1} \times N_{L2} + \dots + N_{Lf} \times N_O \\ N_B &= N_{L1} + N_{L2} + \dots + N_{Lf} + N_O \end{aligned} \quad (2)$$

Outline of the present work is as follows. In Section 2, the modelling of ions tracking in the materials using the Geant4 toolkit is explained. The utilized neural network is explained in Section 3. The proposed approach is illustrated in Section 4. The estimation results of the ions range using the proposed approach is discussed in Section 5. Section 6 gives the conclusion.

2. The modelling details of ions interaction with matter using the Geant4 toolkit

The Geant4 ver10.1 is used to model the ion interaction with matter. *PhysicsList* is an object in the Geant4 toolkit which collects the particles, interactions, and secondary production threshold needed for the simulation. An inherited class from *G4UserPhysicsList* should be created in which the required processes and models for the simulation are selected. In this study, the *emstandard_opt4* constructor which uses the most accurate models for low energy particles is employed. In this constructor, *Urban* and *WntzelVI* models are applied to model multiple scattering of ions and protons, respectively. Moreover, the nuclear stopping phenomena is considered using *ICRU49* based models. For proton and alpha ionization, the *Bragg Ionization* model is utilized. The *ICRU73* based *G4IonParametrisedLoss* is for ionization modelling of ions heavier than Helium. However, in this study, this model is applied for simulation of deuterons transport in the target and as will be shown in the results, it shows good accuracy. The *G4IonFluctuations* model including the fluctuation of ions in matter is also applied. The *G4UserTrackingAction* class functions are used to calculate the track length at each event. The final location of particles at each event is stored on the x -axis as the range of it. The mean of the range value is calculated using 10^5 events. In addition, in order to compare the calculated values of different particles range more accurately, the *G4SteppingAction* class functions are utilized at each step. Since the aim of this study is modelling of the interaction of low energy ions with matter, the inelastic, bremsstrahlung, and pair production are not considered in the modelling.

In the performed modelling, the target geometry is considered to be a 2 mm cube whose dimensions are far beyond the range of low-energy ions. The ions are defined as a point source in the center of the geometry with momentum on the x -axis direction.

3. The utilized neural network for learning of ions range in the materials

The FFNN is one of the best-known supervised neural networks which is widely used in detection, identification, clustering, parameters regression, and values estimation [10,11]. In the FFNN, training data are fed forward and are propagated backward to change the weights and biases and to construct the mapping function between input data and their related outputs. In order to have an efficient FFNN, three main characteristics including the selected features, the appropriate architecture of the network, and the learning algorithm should be addressed carefully.

The relevant features increase the effectiveness and the accuracy of estimation and decrease the computational cost [12,13]. In this study, the atomic mass number of incident ions, the energy of incident ions, and the density of the target material are used as the input features of the FFNN. It is important to mention, features such as ionization energy, chemical composition, etc. may be helpful for the estimation of the range values. In fact, there are many different filter/wrapper/embedded and ensemble techniques for features selection [14,15]. In addition, the DNN will also be needed to cover the full range of energies/ions/targets. However, in this study, the goal is to show the ability of the combination of the FFNN-BR and the Geant4 toolkit for accurate and fast estimation of the ion ranges in the materials. The development of a DNN with all relevant features which is the objective of commercial softwares/computer codes is out of the scope of this paper.

The number of hidden layers, the number of neurons, and the distribution of neurons in hidden layers make the architecture of the FFNN [16,17]. It is important to mention that there is no analytical or deterministic method to obtain the most efficient architecture and the heuristic techniques are employed to find the appropriate one [18–20]. In this study, according to the universal approximation theorem and because of the slow convergence rate of neural networks with more than one hidden layer, a single hidden layer neural network is used [21].

The learning algorithm of the FFNN is the third most important characteristic. The gradient descent (GD) as the well-known learning algorithm of the FFNN is given by Eq. (3). Where, CF is the cost function given by Eq. (4), w is connecting weight of two neurons of different layers, and α is the learning rate [16]. In Eq. (4), TV_i and OV_i are the target value and the output value for i -th input pattern. The slow convergence and overfitting are the main challenges of the GD.

$$w^{new} = w^{old} + \alpha \frac{\partial CF}{\partial w} \quad (3)$$

$$CF = \sum_i (TV_i - OV_i)^2 \quad (4)$$

In the Bayesian regularization (BR) learning algorithm, the CF is redefined to overcome overfitting [22]. The CF of the BR is given by Eq. (5) in which the weights are distributed according to the Gaussian function and are updated by the Bayes' rule which are given by Eq. (6).

$$CF_{BR} = \beta \sum_i (TV_i - OV_i)^2 + \gamma \sum_j w_j^2 \quad (5)$$

$$P(w|ID, \beta, \gamma) = \frac{P(ID|w, \beta)P(w|\gamma)}{\sum P(ID|w, \beta)P(w|\gamma)\Delta w} \quad (6)$$

where, P is probability function, ID is the input-target data set, β and

γ are positive variables which are given by Eq. (7) and Eq. (8), respectively.

$$\gamma = \frac{NP}{2 \sum_j w_j^2 (w^{MAP})} \tag{7}$$

$$\beta = \frac{TS - NP}{2 \sum_i (TV_i - OV_i)^2 (w^{MAP})} \tag{8}$$

where MAP is maximum a posteriori, TS and NP are the number of total samples and the network parameters, respectively [23]. The schematic view of the applied FFNN-BR is presented in Fig. 1.

4. The proposed approach

The proposed approach for estimating the ion ranges in the matter using the combination of the Geant4 and the FFNN-BR is illustrated in Fig. 2 performing its function according to the following steps:

- 1 Modelling of the ion interaction with matter by the Geant4,
- 2 Calculation of ion ranges using the Geant4,
- 3 Training of the FFNN-BR using the selected features and the calculated ion ranges,
- 4 Test of the FFNN-BR using the new values of the selected features,

The estimated results by the FFNN-BR for each ion are compared with the calculated results by the Geant4 using the average mean relative error (AMRE) and the cumulative distribution function (CDF) which are given by Eq. (9) and Eq. (10), respectively.

$$AMRE = \frac{\sum_{E_i=E_1}^{E_n} \frac{|\text{Estimated by FFNN-BR}(E_i) - \text{Calculated by Reference}(E_i)|}{|\text{Calculated by Reference}(E_i)|}}{K} \tag{9}$$

where, E_i is the interaction energy of the incident ion with the target matter and K is the number of estimations. In other words,

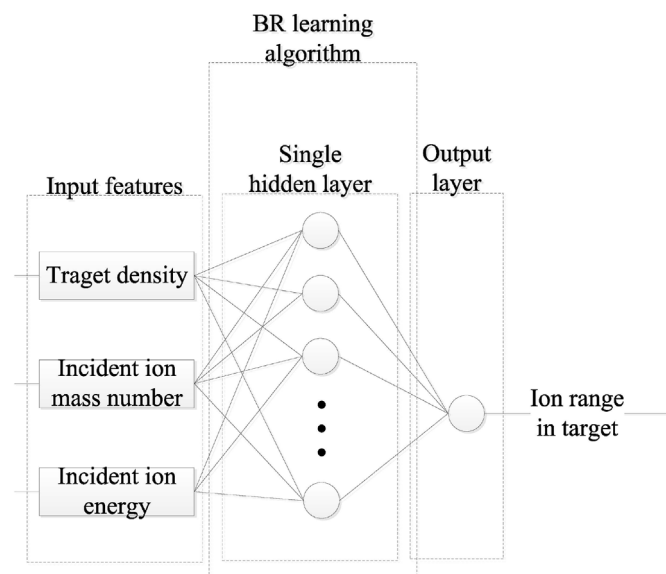


Fig. 1. The schematic view of the applied FFNN-BR.

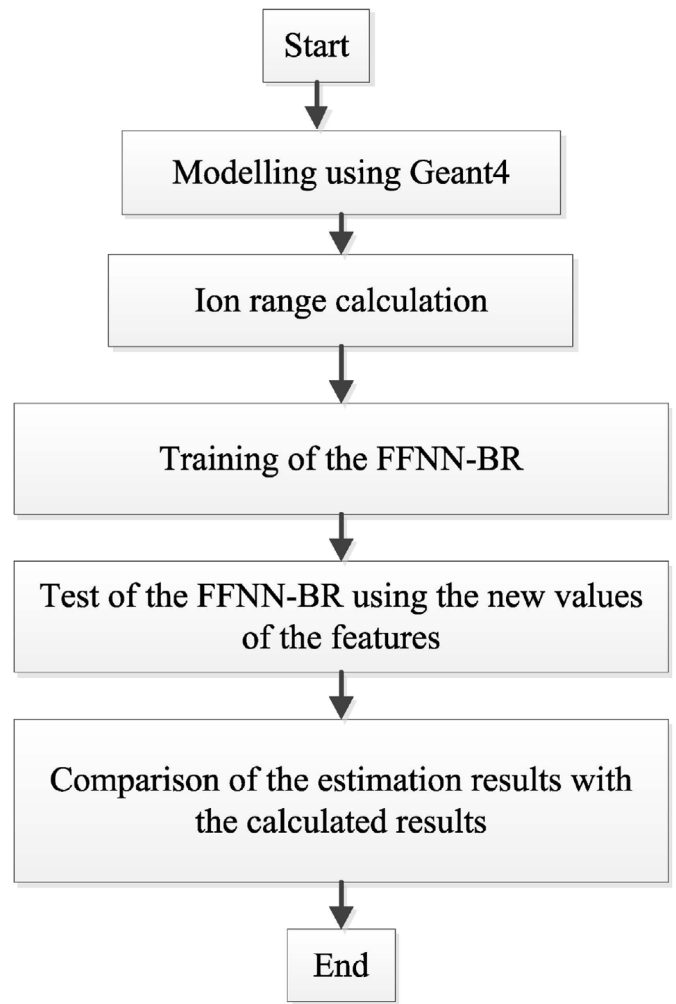


Fig. 2. The illustration of the proposed approach for estimation of ion range in material.

the range of each energy is estimated K times (i.e. using K number of the trained neural networks) and the average of these estimations is presented as the output. The reason for estimating more than once is because the neural network may create a different mapping function between input and target data in each training, and therefore the different created mapping function gives different estimation in the test process. In this manuscript, in order to increase the reliability of the reported estimations, the average estimation of K networks is presented. Therefore, in this paper, CDF and AMRE are intended to make the reported results more reliable.

$$CDF(Error) = \sum_{e=0}^{Error} P(e) \tag{10}$$

where, $P(e)$ is probability of estimation with error equal to e . The $CDF(Error) = 1/100$ means that mean relative error (MRE) defined by Eq. (11) in 1 out of 100 estimations is either less than or equal to $Error$.

$$MRE = \frac{\sum_{E_i=E_1}^{E_n} \frac{|\text{Estimated by FFNN-BR}(E_i) - \text{Calculated by Reference}(E_i)|}{|\text{Calculated by Reference}(E_i)|}}{n} \tag{11}$$

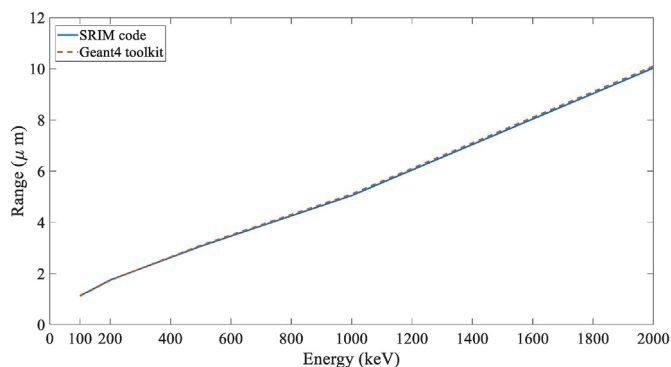


Fig. 3. The calculated values of alpha ion range in water using the Geant4 and the SRIM.

5. The results and discussion

The results of range calculation using the Geant4 show good agreement with the SRIM code [24]. As an example, the range of alpha in water is presented in Fig. 3. The modelling is done for ion energies from 100 to 2000 keV. It should be noted that although ICRU73 is intended for protons and ions heavier than helium, the use of this model to calculate the deuteron range also showed

Table 1

The input features value.

Atomic mass number	Incident energy	Density (g/cm3)
Proton	100–2000 keV	Water
Deuteron	–	Polyethylene
Alpha	–	CD ₂
		CT ₂
		TiD ₂
		TiT ₂

Table 2

The training/test cases for the FFNN-BR.

Ion	Proton	Deuteron	Alpha
The target material	Water	Water	Water
The target material	Polyethylene	Polyethylene	Polyethylene
The target material	–	CD ₂	–
The target material	–	CT ₂	–
The target material	–	TiD ₂	–
The target material	–	TiT ₂	–

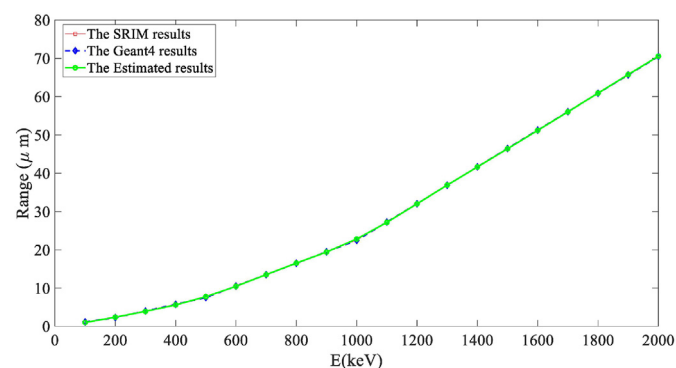


Fig. 4. The estimation range of trained proton ion in Polyethylene in comparison with the Geant4 toolkit and the SRIM code.

Table 3

The deuteron ranges for the different targets by the proposed approach in comparison with the Geant4 toolkit and the SRIM code.

Target	Energy (keV)	SRIM results (μm)	Geant4 results (μm)	Estimation results (μm)
Water	1000	15.58	15.84	15.61
	500	6.15	6.21	6.12
	200	2.48	2.47	2.45
	100	1.48	1.45	1.39
CD ₂	1000	15.73	15.32	15.67
	500	6.02	5.9	6.13
	200	2.30	2.34	2.47
	100	1.34	1.39	1.42
TiD ₂	1000	7.58	7.44	7.57
	500	3.04	2.95	3.01
	200	1.20	1.16	1.19
	100	0.69	0.66	0.67
CT ₂	1000	15.68	15.24	15.58
	500	6.00	5.89	6.00
	200	2.29	2.34	2.37
	100	1.33	1.40	1.35
TiT ₂	1000	7.63	7.44	7.51
	500	3.06	2.95	3.02
	200	1.21	1.16	1.17
	100	0.69	0.66	0.67
Polyethylene	1000	15.33	15.22	15.56
	500	5.85	5.88	6.09
	200	2.23	2.33	2.43
	100	1.29	1.38	1.37

acceptable results. The calculated values of ranges by the Geant4 are utilized to train/test the FFNN-BR.

The input features are the energy and atomic mass number of incident ion as well as the density of the target matter which are presented in Table 1. It is important to mention that the material densities (i.e. CD₂, CT₂, TiD₂, TiT₂) are calculated by the method described in reference [25]. The metal targets TiD₂ and TiT₂ and the organic targets CD₂ and CT₂ are widely used in variety of neutron generators.

The utilized network is a single hidden layer network with 20 neurons. The incident ions/target materials which are used to train/test the FFNN-BR are given in Table 2. Seventy/thirty percent of data by random selection are utilized for training/test of the FFNN-BR. Therefore, there is no predefined regularity in selection of the training patterns. The values of proton range in.

Polyethylene are given comparatively in Fig. 4. Moreover, the range values of deuteron using the proposed approach in comparison with the Geant4 toolkit and the SRIM code for different targets are given in Table 3. The results show good performance of the proposed approach. In order to determine the generalization

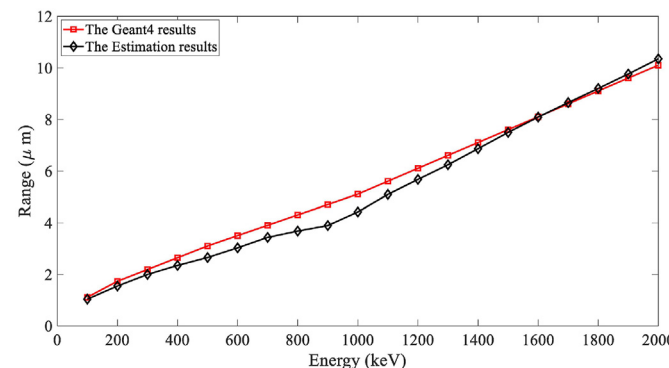


Fig. 5. The estimation range of untrained alpha ion in water in comparison with the Geant4 toolkit.

Table 4
The AMRE of estimating range values for energies 100–2000 keV ($K = 100$).

Estimation results in comparison with Geant4				Estimation results in comparison with SRIM			
	Proton	Deuteron	Alpha		Proton	Deuteron	Alpha
Polyethylene	0.0193	0.0134	0.0199	Polyethylene	0.0195	0.0208	0.0367
CT ₂	–	0.0246	–	CT ₂	–	0.0331	–
TiD ₂	–	0.0644	–	TiD ₂	–	0.0756	–
Water	0.0185	0.0175	0.0193	Water	0.0363	0.0210	0.0218
CD ₂	–	0.0241	–	CD ₂	–	0.0270	–
TiT ₂	–	0.0725	–	TiT ₂	–	0.0725	–

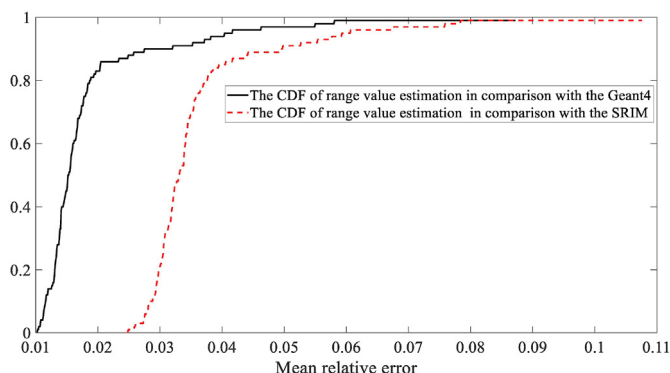


Fig. 6. The CDF of range value estimation for interaction of proton with water.

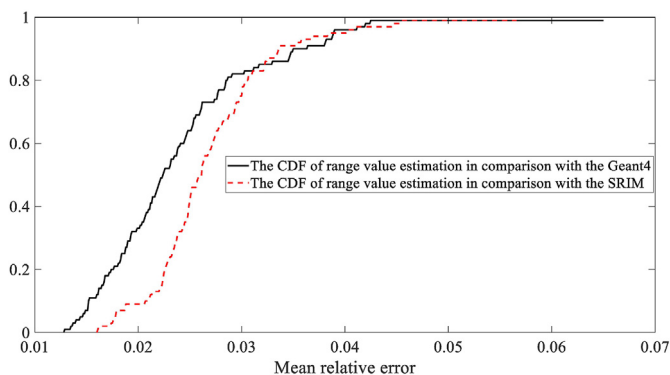


Fig. 7. The CDF of range value estimation for interaction of deuteron with CD₂.

ability of the proposed neural network, the training/test of the neural network is done by the different materials. The presented result in Fig. 5, as an example, show the acceptable performance of the proposed approach for estimation of range of untrained alpha ion.

The AMRE of estimating range values are presented in Table 4. The CDF of the estimating range values of proton interaction with

Table 5
The estimating range values for energies 100–2000 keV ($K = 100$ and $CDF = 0.50$).

Estimation results in comparison with the Geant4				Estimation results in comparison with the SRIM			
	Proton	Deuteron	Alpha		Proton	Deuteron	Alpha
Polyethylene	0.0160	0.0127	0.0153	Polyethylene	0.0162	0.0197	0.0338
CT ₂	–	0.0198	–	CT ₂	–	0.0294	–
TiD ₂	–	0.0308	–	TiD ₂	–	0.0438	–
Water	0.0152	0.0173	0.0143	Water	0.0331	0.0204	0.0171
CD ₂	–	0.0224	–	CD ₂	–	0.0261	–
TiT ₂	–	0.0447	–	TiT ₂	–	0.0447	–

water and deuteron interaction with CD₂ are presented in Fig. 6 and Fig. 7, respectively. The CDF of the estimating range values are presented in Table 5 and Table 6. The CDF accompanied with AMRE are reliable tools to reflect the performance of the proposed approach. The notable advantages of the proposed approach are: 1- The range of ions in different materials is given as quickly as possible and the time needed to estimate the ranges can be neglected (i.e. less than 0.01 s by a typical personal computer). 2- The proposed approach can generalize its ability for estimating the new untrained cases. 3- There is no need for a pre-made lookup table for the estimation of the range values.

6. Conclusion

In this study, a new approach for estimation of ion range values in interaction with materials is developed using a combination of the Geant4 toolkit and the FFNN-BR neural network. The incident ions interactions with materials are modelled by the Geant4. Seventy/thirty percent of the calculated range values are utilized for training/test of the FFNN-BR.

The results are compared with the SRIM code and show good agreement. The notable achievements of the proposed approach are: 1- The range of ions in different materials is given as quickly as possible and the time needed to estimate the ranges can be neglected (i.e. less than 0.01 s by a typical personal computer). 2- The proposed approach can generalize its ability for estimating the new untrained cases. 3- There is no need for a pre-made lookup table for the estimation of the range values.

In this study, the neural network is trained only for ions with energies less than 2 MeV. This makes possible to examine the efficiency of the proposed approach without need for the deep learning. The further development of the proposed approach to cover the full range of energies/ions/targets that require DNNs will be presented in the next work.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Table 6
The estimating range values for energies 100 to 2000 keV ($K = 100$ and $CDF = 0.90$).

Estimation results in comparison with the Geant4				Estimation results in comparison with the SRIM			
	Proton	Deuteron	Alpha		Proton	Deuteron	Alpha
Polyethylene	0.0303	0.0198	0.0371	Polyethylene	0.0336	0.0283	0.0472
CT ₂	–	0.0342	–	CT ₂	–	0.0429	–
TiD ₂	–	0.0910	–	TiD ₂	–	0.1057	–
Water	0.0275	0.0210	0.0356	Water	0.0492	0.0249	0.0361
CD ₂	–	0.0350	–	CD ₂	–	0.0336	–
TiT ₂	–	0.0971	–	TiT ₂	–	0.0971	–

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