Comparison of accuracy of parameterized individual proton range models

Introduction

An accurate calculation of proton ranges in phantoms or detector geometries is crucial for correct decision making in proton therapy and related activites such as proton imaging. The measurement of ranges in phantoms performed during commissioning and quality assessment serves as a ground truth for the calculation between range and energy in water. For benchmarking and calibration of proton range telescopes, it is important to have an accurate calculation scheme between arbitrary ranges and energies (Rinaldi et al. 2014; Pettersen et al., n.d.). To this end, several parameterizations of the range-energy relationship exist, exhibiting different levels of complexity and thus accuracy. In addition, ranges are often expressed in units of *Water Equivalent Thickness* (WET): by using the energy as the connection between range in material and range in water, the WET can be calculated. In order to calculate the pristine depth-dose curve for the depth-dependent energy deposition of individual proton tracks, a differentiation of the energy-range parameterization can be used. In this study we compare the accuracy of some of the different parameterizations of the range-energy relationship when applied in this context.

Materials and Methods

In this study, different models for the relationship between range and energy are evaluated based on their ability to correctly reproduce the proton range in water at different energies as found in the Continuous Stopping Down Approch from the PSTAR database (Berger et al. 2005).

Four models are placed under consideration: These are either semi-empirical or based on interpolation. The semi-empirical models are derived from the Bethe equation and fitted to experimental data in order to find the parameters arising from the particular parameterization scheme. The interpolation-based models use different approaches to interpolate from look-up-tables from tabulated range data.

The models and analysis are created using ROOT 5.34/19 using C++ code, and the range-energy data are downloaded from the PSTAR webpage and loaded in the program. The data fitting library TMinut in ROOT has been used to find the model parameters.

It is not in the scope of this study to validate the accuracy of the experimental data from the different sources, such as PSTAR (Berger et al. 2005), SRIM (Ziegler 2015), Janni (Janni 1982) or ICRU49 (Wyckoff 1993). Previous studies, such as (Paul 2013), has estimated that the ICRU49 values should be accurate to the 0.5% level, depending on the value of the mean ionization potential I. The question is to which degree the different models are able to reproduce the tabulated data after being properly trained.

Semi-empirical models

The Bethe equation (K.A. Olive and Particle Data Group 2014) describes the stopping power of protons in a homogeneous material. Its integral is needed in order to find the proton range. It is not trivially integrable, however by performing series approximations one may obtain a simplified range-energy relationship. Several such approximations have been suggested: The Bragg-Kleeman rule is the 1st order Taylor series, and due to its simple form one may both invert and and differentiate the formula in order to find the dose curve (Thomas Bortfeld and Schlegel 1996). The Bragg-Kleeman rule for a proton's range R_0 with initial energy E and depth dose curve $-\mathrm{d}E/\mathrm{d}z$ is given below:

$$R_0 = \alpha E^p$$
$$E(z) = \alpha^{-1/p}(R_0 - z)^{1/p}$$
$$-\,\mathrm{d}E/\mathrm{d}z = p^{-1}\alpha^{-1/p}(R_0 - z)^{1/p-1}.$$

Here, α and p can be obtained from the Bethe equation or found by model fits to experimental data.

Alternatively, a series of exponential terms (Ulmer 2007) has been suggested as a more accurate model for range calculations. Two separate approximations are offered to calculate R_0 and $E(z)$, respectively, and the differentiation of the latter gives rise to the depth dose curve:

$$R_0 = a_1 E_0 \left[1 + \sum_{k=1}^{N_1} (b_k - b_k \exp(-g_k \cdot E_0)\right]$$

$$E(z) = (R_0 - z) \sum_{k=1}^{N_2} c_k \exp\big(-\lambda_k (R_0 - z)\big)$$

$$-\frac{\mathrm{d}E}{\mathrm{d}z} = \frac{E(z)}{R_0 - z} - \sum_{k=1}^{N_2} \lambda_k c_k (R_0 - z) \exp\big(-\lambda_k (R_0 - z)\big)$$

The different parameters a_1, b_k, b_k, λ_k and c_k are described in (Ulmer 2007), and may be found by fitting the model to range-energy data. A recommendation on the number of terms was also made in the same study, where $N_1 = 2$ and $N_2 = 5$ would yield a good accuracy. In this work the same choice has been made.

Data interpolation models

When considering proton ranges in homogenenous phantoms of known elements or compounds, it is possible to use tabulated data from different experiments: however one needs to interpolate between the data if the required value pairs are not available. The same is also true for more complex geometries such as detector geometries, where the tabulated data is made during Monte Carlo simulations of varying initial proton energies.

A linear interpolation is the simplest way to interpolate between two data points in a look-up-table, as a straight line is used for evaluation between values in the look-up-table. A spline interpolation is performed by calculating a (here) 3rd order polynomial function around each of the data points in the look-up-table, and stiching them together in a piecewise fashion. It is possible to extract the depth-dose curve from range-energy look-up-tables by calculating the difference in range between each energy step, however the end result is a stepwise curve.

A larger number of measurements at different energies are required for a interpolation-based range calculation scheme compared to the simple Bragg-Kleeman rule with two parameters or even the exponential sum from Ulmer (Ulmer 2007) with 15 parameters. On the other hand, interpolation-based calculations enables for more accurate calculations over the therapeutic span of energies.

Comparison of the parameterization models

150 CSDA range values for protons in water, up to therapeutic energies, are split into two groups. One training group ($N_T = 25$) is used for finding the model parameters, the remaining control group ($N_C = 125$) is used to evaluate the model calculations at small range intervals. After each model has been trained, it is then used to calculate the range at all the energy values in the control group. Each model calculated range is then compared to the corresponding value from the control group.

Comparison of the number of data values for model training

In the above analysis, the 75% percentile value of the range deviation between the calculated range and the PSTAR range has been calculated. This value is calculated for a varying number of data points used for training the different models, ranging from $N_T = 3$ to $N_T = 125$.

Comparison of the shape of the Bragg Curve

The depth dose distribution of a single proton incident on water is obtained from a differentiation of the energy-range relationship. If it is convoluted with the statistical range straggling of a proton beam, the result is the depth-dose curve for a proton beam, in contrast to the pristine depth-dose curve of a single proton. The different parameterizatons give rise to depth-dose curves of slightly different shapes. The Bragg Peak position is kept constant by using the same parameter R_0 for all the models.

Results

The results for the training of the models is shown in Table 1 and Table 2. The results are compared to similar results in the literature. The accuracy of the proton range calculation using different models is shown in Figure 1, the training stability of the models is shown in Figure 3.

	α	p
This work	$0.00262\ \mathrm{MeV/cm^{-1}}$	1.736
(T. Bortfeld 1997)	$0.00220\ \mathrm{MeV/cm^{-1}}$	1.77
(Boon 1998)	$0.00256\ \mathrm{MeV/cm^{-1}}$	1.74

Table 1: The parameters for proton range calculation using the Bragg-Kleeman rule, as found in this work and as compared with others.

	a_1	b_1	g_1	b_2	g_2
This work	0.0081	11.782	0.0009	30.003	0.0029
(Ulmer 2007)	0.0069	15.145	0.0012	29.844	0.0033
	c_1	c_2	c_3	c_4	c_5
This work	29.440	11.605	5.775	6.226	2.457
(Ulmer 2007)	96.64	25.05	8.807	4.190	9.273
	λ_1^{-1}	λ_2^{-1}	λ_3^{-1}	λ_4^{-1}	λ_5^{-1}
This work	1.003	5.294	297.04	26.44	1.1223
(Ulmer 2007)	0.098	1.245	5.700	10.65	106.73

Table 2: The parameters for proton range calculation models using a sum of exponentials, as found in this work and as compared with others. Note that since this model is a series approximation, a number of combinations of terms will yield similar results, and as such the comparison with (Ulmer 2007) is somewhat arbitrary.

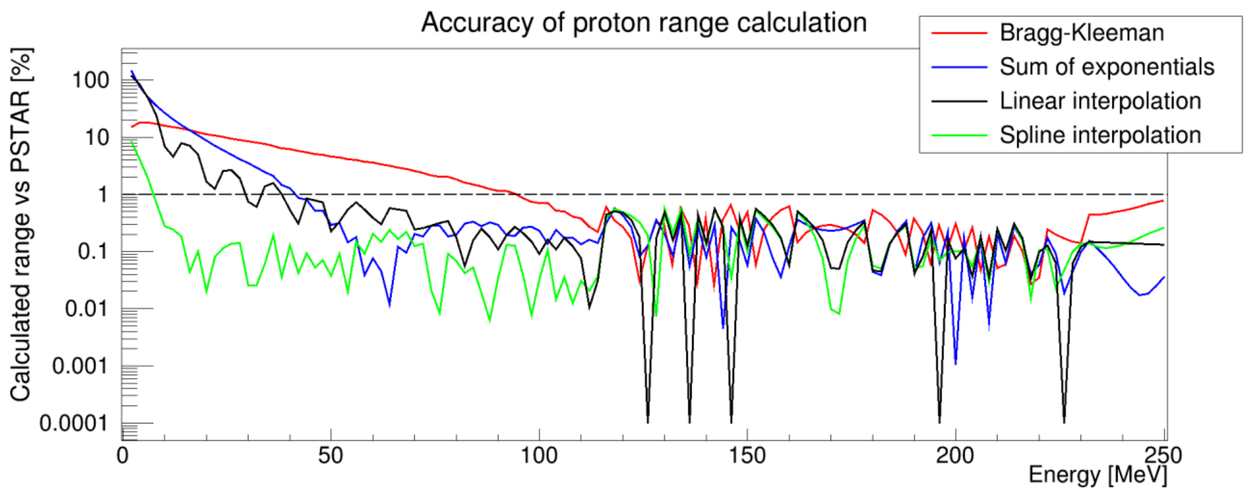

Figure 1: The accuracy of the proton range calculations using different parameterization models. The range error is the relative difference between the calculated or interpolated range using the model, and the PSTAR dataset. The energies used here are from the control group, and not from the training group.

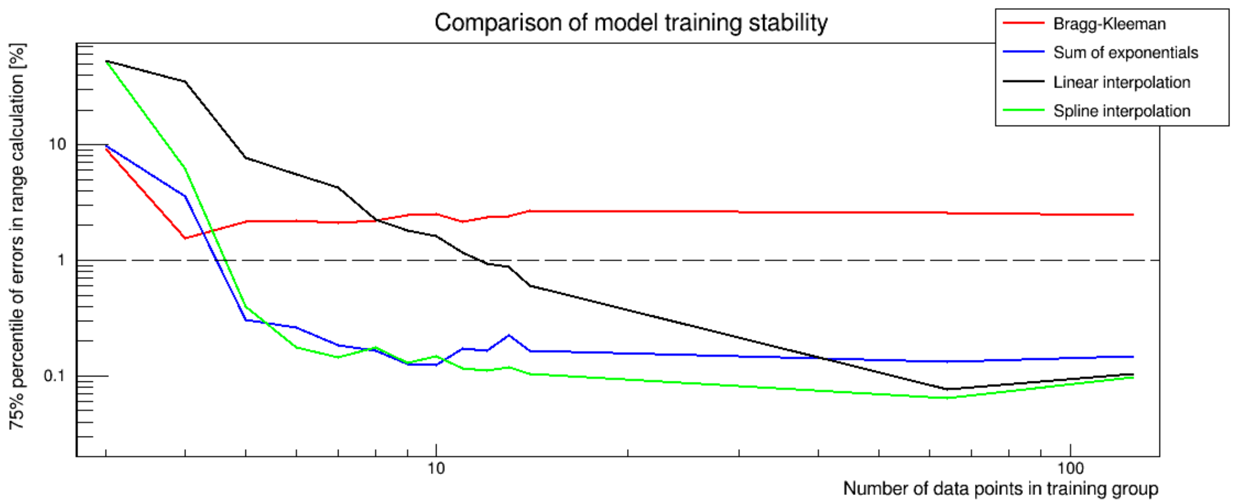

Figure 2: The training stability of the models. The models are trained with different number of data points. The more complex the model, such as the interpolated models or the sum of exponentials, the more data points are needed in order to reduce the calculation errors. The error is calculated as the 75% percentile of all the relative errors as shown in Figure 1 for each of the parameterization models.

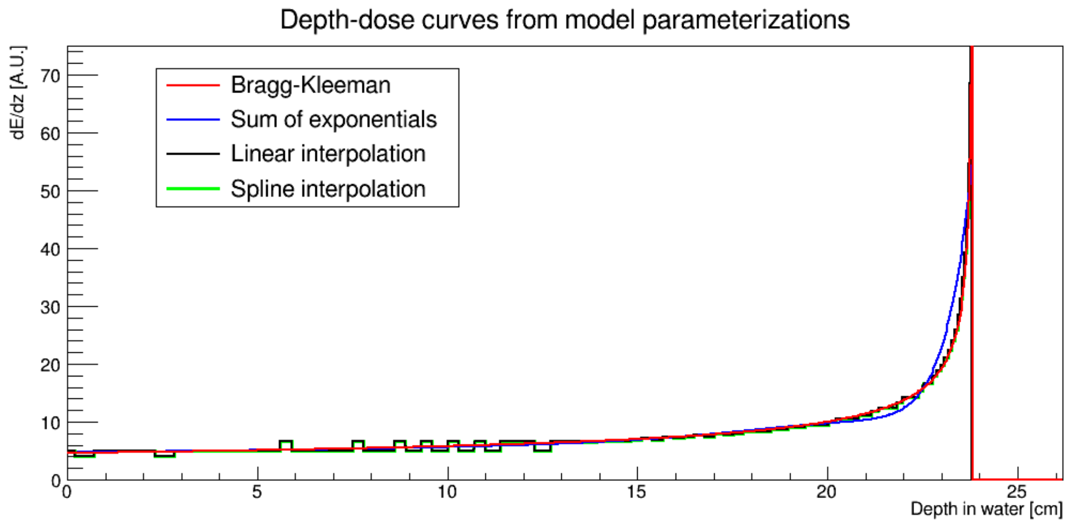

Figure 3: The depth-dose curves calculated obtained by differentiating the parameterization models. The two interpolated models as well as the Bragg-Kleeman model are seemingly identical, while the sum of exponentials model exhibits some differences close to the Bragg Peak.

Discussion

Overall, the spline interpolation model shows the highest accuracy. A sub-percent range calculation accuracy is shown for all models above 100 MeV, and for the spline model above 10 MeV.

By using at least 20 data points for training the model, the accuracy is kept at an acceptable level, and the 75% percentile of the errors in the range calculation is at 0.1% of the range when using the spline interpolation, the linear interpolation or the sum of exponentials. Due to the low number of parameters in the Bragg-Kleeman parameterization, it is stable even when as low as four data points are used for training.

For the shapes of the depth-dose curves, the data-driven methods are assumed to be the ground truth since they represent measurement data, or in the case of PSTAR, accurate calculations of the Bethe equation. Since the number of data points are limited, however, the curves created in this fashion are stepwise functions.

The shapes of the depth-dose curves originating from the interpolations and the Bragg-Kleeman model are visually identical, and as such the shape of the Bragg Peak of individual protons is accurately represented by using the simple differentiated Bragg-Kleeman formula. By using the sum of exponentials the shape exhibits some artefacts due to contributions from the different exponential terms used in the sum.

An application for this work is found in the range calculations for the proton telescope and digital tracking calorimeter (Pettersen et al., n.d.). A look-up-table of range-energy values is created using Monte Carlo simulations, and arbitrary range-energy values are readily calculated during analysis using spline interpolation. The depth-dose curve for individual protons, from both experimental measurements and Monte Carlo simulations, are compared to the depth-dose curve originating from the differentiated Bragg-Kleeman formula which has been shown here to be an accurate representation. The result is a high accuracy of both range calculation of arbitrary energies as well as realistic parametric depth-dose curves for individual protons.

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