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# Energy-adaptive calculation of the most likely path in proton CT

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## Abstract

This note addresses an issue faced by every proton computed tomography (CT) reconstruction software: the modelling and the parametrisation of the multiple Coulomb scattering power for the estimation of the most likely path of each proton. The conventional approach uses a polynomial model parameterised as a function of depth for a given initial beam energy. This makes it cumbersome to implement a software that works for proton CT data acquired with an arbitrary beam energy or with energy modulation during acquisition.

We propose a simple way to parametrise the scattering power based on the measured proton CT list-mode data only and derive a compact expression for the most likely path (MLP) based on a conventional MLP model. Our MLP does not require any parameter. The method assumes the imaged object to be homogeneous, as most conventional MLPs, but requires no information about the material as opposed to most conventional MLP expressions which often assume water to infer energy loss. Instead, our MLP automatically adapts itself to the energy-loss which actually occurred in the object and which is one of the measurements required for proton CT reconstruction. We validate our MLP method numerically and find excellent agreement with conventional MLP methods.

# 1 Introduction

Image reconstruction in list-mode proton computed tomography (CT) is typically performed along the most likely path (MLP) that a proton has taken through the imaged object (Schulte et al., 2008; Rit et al., 2013; Johnson, 2018; Dedes et al., 2020). The reason for this is that protons follow stochastic non-straight trajectories through the object, mainly because of multiple Coulomb scattering (MCS) (Gottschalk, 2010). Most protons which have undergone nuclear scattering are filtered out prior to image reconstruction and MLP algorithms generally assume that only MCS bends the proton trajectory. The MLP attempts to account for MCS by providing curved integration lines to the tomographic reconstruction algorithm. It is estimated based on the position and angle measurement upstream and downstream of the object and considers the likelihood of MCS in the medium. To calculate the latter, a kinematic term essentially equivalent to the protons' scattering power at a given depth needs to be calculated which depends on the proton's kinetic energy. In most MLP formalisms, this term is integrated along depth and therefore has a significant impact on the computational speed of the reconstruction code. A practical approach to speed up the computation is to approximate the kinematic term by a polynomial as a function of depth and to perform the integration analytically (Williams, 2004; Schulte et al., 2008). The result is again a polynomial which is computationally efficient to calculate. The polynomial coefficients need to be determined *a priori* for a given beam energy, e.g. based on a Monte Carlo simulation or suitable tabulated data such as NIST's PSTAR tables (Berger et al., 2005). While this approach is functional and has been successfully used by several authors, it has a few technical downsides: The value of the coefficients depends on the beam energy making it difficult for a reconstruction software to work with list-mode proton CT data acquired with arbitrary beam energy. Either the code would need to include a large database of such polynomial coefficients to cover an adequate range of beam energies, potentially with interpolation between energies, or the user would need to determine the coefficients and provide them as input to the reconstruction, which is arguably impractical. For image acquisition scenarios where the beam energy varies from one proton to another, e.g. when using pencil beams with varying beam energy, the approach is cumbersome because each proton requires a separate set of coefficients.

In this note, we present a method to parametrise and evaluate the kinematic term in the MLP estimation purely based on the measured data. No external parameters other than established physical constants are required. The resulting MLP expression is compact and easy to implement.

## 2 Materials and Methods

### 2.1 Context

This note does not propose a new formalism to estimate the MLP, but a method to parametrise existing MLP formalisms. For this purpose, we chose the MLP formalism in Krah et al. (2019) because it yields a compact MLP expression.

Most MLP formalisms in proton CT use the following model for the multiple Coulomb scattering power  $T(u)$  as a function of depth in the object:

$$T(u) = \frac{1}{X_0} \frac{\Omega_0^2}{\beta^2(u)p^2(u)} = \frac{1}{X_0} \frac{\Omega_0^2(E(u) + E_p)^2 c^2}{(E(u) + 2E_p)^2 E^2(u)} \equiv \frac{1}{X_0} K(u), \quad (1)$$

with  $\Omega_0 = 13.6 \text{ MeV}/c$  a constant,  $\beta = v/c$  the proton's velocity relative to the speed of light,  $p$  the proton's momentum,  $E_p$  the proton's rest mass energy,  $X_0$  the radiation length of the material, and  $E(u)$  the protons' kinetic energy at depth  $u$ . We defined the unit-less function  $K(u)$  to contain the energy-dependent part of the scattering power. The radiation length  $X_0$  is depth-dependent in a heterogeneous medium, but most MLP formalisms treat objects as

homogeneous material and so do we. Schulte et al. (2008) also includes an empirical correction factor which we omit.

Evaluating the MLP from Krah et al. (2019) involves four variants of integrals over  $K(u)$ ,

$$\begin{aligned} A(u) &= \frac{1}{X_0} \int_0^u dv K(v); & C(u) &= \frac{1}{X_0} \int_0^u dv \int_0^v dw K(w); \\ B(u) &= \frac{1}{X_0} \int_0^u dv K(v)v; & D(u) &= \frac{1}{X_0} \int_0^u dv \int_0^v dw K(w)w \end{aligned} \quad (2)$$

where  $u, v, w$  are variables indicating depth in the object.

The MLP, or more precisely the most likely transverse position  $t_{\text{MLP}}$  at depth  $u$ , is calculated as

$$t_{\text{MLP}}(u) = t_{\text{in}} + \theta_{\text{in}}u + c_0C(u) + c_1D(u), \quad (3)$$

where  $t_{\text{in}}$  and  $\theta_{\text{in}}$  are the transverse position and angle of the proton entering the object. The factors  $c_0$  and  $c_1$  are independent of depth and given by

$$\begin{aligned} c_0 &= \frac{1}{A_{\text{out}}D_{\text{out}} - B_{\text{out}}C_{\text{out}}} (-B_{\text{out}}(t_{\text{out}} - t_{\text{in}} - \theta_{\text{in}}u_{\text{out}}) + D_{\text{out}}(\theta_{\text{out}} - \theta_{\text{in}})) \\ c_1 &= \frac{1}{A_{\text{out}}D_{\text{out}} - B_{\text{out}}C_{\text{out}}} (A_{\text{out}}(t_{\text{out}} - t_{\text{in}} - \theta_{\text{in}}u_{\text{out}}) - C_{\text{out}}(\theta_{\text{out}} - \theta_{\text{in}})), \end{aligned} \quad (4)$$

with  $t_{\text{out}}$  and  $\theta_{\text{out}}$  the exit position and angle, respectively, and  $u_{\text{out}}$  the exit depth. We used the short-hand notation  $A_{\text{out}} = A(u_{\text{out}})$  for brevity. Determining  $u_{\text{out}}$  requires knowledge of the external contour of the object to be reconstructed – an assumption common to all MLP formalisms. In a proton CT reconstruction algorithm, equation 3 is evaluated independently for both perpendicular directions transverse to the beam, i.e.  $t_{\text{MLP},x}$  and  $t_{\text{MLP},y}$  (assuming the beam along  $z$ ). Throughout this work, we ignore this technicality and let “transverse direction” refer to either of these two directions.

## 2.2 Conventional parametrisation of the scattering power

The term  $K(u)$  needs to be adequately parametrised in a proton CT reconstruction code to evaluate the integrals in equation 2. The conventional way is to obtain  $E(u)$  from a Monte Carlo simulation for a given proton beam energy and material and fit a polynomial  $\mathcal{P}(u) = \sum_{n=0}^N a_n u^n$  to the so-derived  $K(u)$  (Williams, 2004; Schulte et al., 2008; Krah et al., 2019), with  $N = 5$  suggested in Schulte et al. (2008). The integration can then be performed analytically. As explained in the introduction, one inconvenience of this approach is that  $\mathcal{P}(u)$  depends on the beam energy.

## 2.3 New parametrisation

The new parametrisation proposed in this work starts from an observation depicted in the left panel of figure 1, namely that the reciprocal of the kinematic term in the scattering power as a function of depth in a homogeneous material is approximately linear, i.e.

$$1/K(u) \approx au + b, \quad \text{so that} \quad K(u) \approx \frac{1}{au + b} \quad (5)$$

where we choose  $u$  by convention so that protons enter the object at  $u_{\text{in}} = 0$ . To generate figure 1, we determined the proton energy as a function of depth and calculated the scattering power as in equation 1. More specifically, we integrated  $u(E) = \int_{E_{\text{in}}}^E 1/S_w(E) dE$  numerically, using the stopping power  $S_w(E)$  of water from NIST’s PSTAR table (Berger et al., 2005) and obtained  $E(u)$  by numerical inversion of the relation. The dots in figure 1 are examples of the

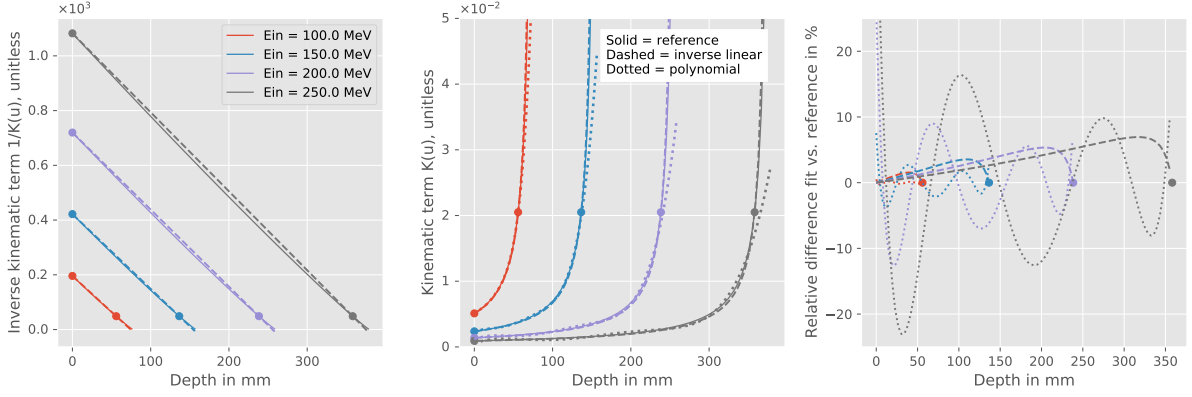


Figure 1: Left: Inverse scattering power calculated according to equation 1 (solid). The linear approximation (dashed line) was determined as the line connecting the two dots which represent the scattering power at the object entry and exit. Centre: Reciprocal of the left plot. The dotted line was obtained as a polynomial fit of order 5 to the solid line between the two dots. Right: Relative difference of the fitted scattering powers to the reference.

proton's entry and exit depths and, for this figure, we chose  $u_{\text{out}}$  to be 2 cm less than the proton range for the given beam energy.

In practice, the coefficients  $a$  and  $b$  can be determined via equation 1 from the proton's incoming and outgoing energy,

$$b = \frac{1}{K(u_{\text{in}})} \quad a = \frac{1}{u_{\text{out}}} \left( \frac{1}{K(u_{\text{out}})} - \frac{1}{K(u_{\text{in}})} \right). \quad (6)$$

The right panel in figure 1 compares the scattering power approximated according to equation 5 (dashed) with the exact scattering power from which  $a$  and  $b$  were derived (solid), as well as a polynomial fit  $\mathcal{P}(u)$  of order  $N = 5$  with the exact scattering power (dotted). Visually, the approximation in equation 5 is at least as good as the polynomial fit. Quantitatively, the right panel in figure 1 shows that equation 5 approximates the scattering power to within a few percent, depending on the initial energy and depth.

Using equation 5, the integrals in equation 2 can be evaluated analytically, as outlined in the Appendix, yielding:

$$A(u) = \frac{1}{a} \log \left( \frac{a}{b} u + 1 \right) \quad (7)$$

$$B(u) = \frac{b}{a^2} \left( \frac{a}{b} u - \log \left( \frac{a}{b} u + 1 \right) \right) \quad (8)$$

$$C(u) = \frac{b}{a^2} \left( \left( \frac{a}{b} u + 1 \right) \log \left( \frac{a}{b} u + 1 \right) - \frac{a}{b} u \right) \quad (9)$$

$$D(u) = \frac{b^2}{a^3} \left( \frac{1}{2} \left( \frac{a}{b} u \right)^2 + \frac{a}{b} u - \left( \frac{a}{b} u + 1 \right) \log \left( \frac{a}{b} u + 1 \right) \right). \quad (10)$$

Inserting  $A(u)$ ,  $B(u)$ ,  $C(u)$ , and  $D(u)$  into equations 3 and 4 and grouping terms yields the new expression for the MLP,

$$t_{\text{MLP}}(u) = t_{\text{in}} + \left( \theta_{\text{in}} - c_0 \frac{1}{a} + c_1 \frac{b}{a^2} \right) u + \frac{1}{2a} c_1 u^2 + \left( c_0 \frac{b}{a^2} - c_1 \frac{b^2}{a^3} \right) \left( \frac{a}{b} u + 1 \right) \log \left( \frac{a}{b} u + 1 \right), \quad (11)$$

i.e. a quadratic function plus an additional linear-logarithmic term. This expression for the MLP does not depend on any external parametrisation of the scattering power  $T(u)$  (or the term  $K(u)$ )

therein) and can be fully determined via equations 1 and 6 based on measurements only, i.e. the proton's entry and exit coordinates as well as the entry and exit energy.

## 2.4 Implementation

The MLP in equation 11 can be implemented according to the following scheme: For each proton, project the entry and exit coordinates (position and angle) onto the external contour of the object to be reconstructed. This yields  $u_{\text{in}}$ ,  $u_{\text{out}}$ ,  $t_{\text{in}}$ ,  $t_{\text{out}}$ ,  $\theta_{\text{in}}$  and  $\theta_{\text{out}}$ . Next, determine the parameters  $a$  and  $b$  via equation 6 based on the proton's entry and exit energy. Calculate and store the parameters  $c_0$  and  $c_1$  (equation 4). Finally, calculate the most likely transverse position  $t_{\text{MLP}}$  at all desired depths  $u$  using  $a$ ,  $b$ ,  $c_0$ ,  $c_1$ . It can be shown that the case  $a = 0$  (no energy loss) does not constitute a true singularity because in that case  $K(u) = 1/b$  and all integrals simplify. This case must be handled separately to avoid numerical instability.

## 2.5 Validation and simulation

We validated the new MLP parametrisation by comparison with conventional MLP expressions. In particular, we chose the methods from Schulte et al. (2008) and Krah et al. (2019). The former is well-established and was one of the first to appear in the literature on proton CT and the latter is the method to which the adaptive parametrisation in this work is applied.

To quantify how well the new MLP agrees with conventional MLP expressions, we performed a GATE Monte Carlo simulation (Sarrut et al., 2014) of protons propagating through water and traced their true trajectory in 1 mm depth intervals. We chose water because this is the underlying assumption of both reference MLPs. We used the *emstandard\_opt4* physics list to ignore nuclear interactions as these are not considered by the MLP formalisms. In practice, most nuclear events are filtered out from proton CT data, but that would have been an unnecessary complication for the purpose of this validation.

For each proton, we calculated the MLP using the three different MLP methods. We compared the MLPs among each other as well as with the true paths from Monte Carlo. Regarding the latter, we generated the distribution of the difference between MLP estimate and true position,  $t_{\text{MLP}} - t_{\text{MC}}$ , at a certain depth.

## 3 Results

The upper left panel in figure 2 shows a few example MLPs in a 20 cm thick box of water for protons of 200 MeV and calculated using the MLP method from this work as well as those from Schulte et al. (2008) and Krah et al. (2019). The lower left panel illustrates how much these MLPs vary among each other. The right panels depict the error of  $t_{\text{MLP}}$  compared to the transverse position from Monte Carlo for 200 MeV (upper) and 150 MeV (lower) protons. The position was evaluated at the central depth and the water boxes were 20 cm and 12 cm thick, respectively.

The differences among MLPs are no greater than a few tens of micrometers and much smaller than the statistical uncertainty of the MLP estimate itself. The MLP uncertainty, which directly influences the spatial resolution in the reconstructed image, is essentially identical for all MLPs. We also verified these results at other beam energies and depths and came to the same conclusions.

## 4 Discussion and Conclusion

In this work, we have presented a new method to parametrise the energy dependence in the scattering power which is part of the most likely path formalism in proton CT. The method relies on the fact that the reciprocal of the scattering power as a function of depth in an object is

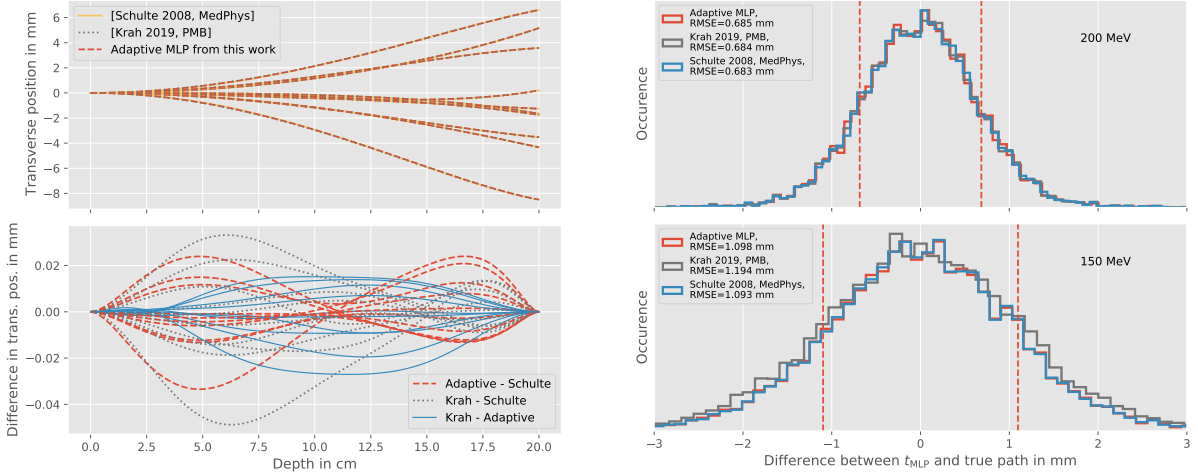


Figure 2: Upper left: Example of most likely paths for 200 MeV protons in water calculated with different MLP methods. Lower left: Difference between the MLPs. Right: Distributions of the difference between  $t_{\text{MLP}}$  and true position (from Monte Carlo) at the centre of a 20 cm (upper) and 12 cm (lower) thick water box. Beam energies are indicated in the graphics. The vertical lines indicate  $\pm$  one root mean square error of the distributions, with specific numbers provided in the legend.

approximately linear, which we have verified for the range of beam energies relevant for proton CT. Our new MLP parametrisation automatically adapts to the energy-loss of a proton in a given object because it uses the actually measured exit energy.

From the practical point of view, the new MLP parametrisation presented in this work greatly simplifies the implementation of a proton CT reconstruction software. Indeed, with a conventional MLP, either the software or the user need to provide the coefficients of the polynomial which approximates the scattering power as a function of depth. The new method can calculate the MLP for protons of any initial energy only relying on the proton CT list-mode data, i.e. proton coordinates and energies. This also makes reconstruction of images acquired with energy-modulated proton beams (Dickmann et al., 2021) technically easier than it would be with the conventional MLP methods.

It is worth remarking that the scattering power term  $K(u)$  (equation 1) in a homogeneous object is also well approximated by a power law of the form  $K(u) = \epsilon(R - u)^\delta$ , where  $R$  is the proton range in the given material and  $\epsilon$  and  $\delta$  are model parameters, similar to the model used in Bortfeld et al. (1996). In a known material,  $\epsilon$  and  $\delta$  could be determined using  $K(u_{\text{in}})$  and  $K(u_{\text{out}})$  (which can be calculated from  $E_{\text{in}}$  and  $E_{\text{out}}$ ). For the example data in water shown in figure 1, we find  $\delta \approx -1.05$ , which is coherent with our inverse linear model. In practice, however, the material of an imaged object and the proton range  $R$  therein is not known. One could use the range in water as an approximation, but that would incorrectly represent the relation  $K(u)$  in materials which are on average denser or less dense than water. In mathematical terms, the power law model in an unknown material has three free parameters ( $\epsilon$ ,  $\delta$ ,  $R$ ), but only two data points ( $E_{\text{in}}$ ,  $E_{\text{out}}$ ) are available, so the model remains underdetermined.

Interestingly, the new MLP expression in equation 11 does not make any assumption about the material of the imaged object, contrary to the conventional MLP parametrisation. For example, in an object which is less dense than water such as the lungs, protons lose less energy and  $K(u)$  does not increase as much as it would in water. Consequently, the slope parameter  $a$  in equation 6 is smaller than it would be in the same object filled with water. The conventional parameterisation, which uses a polynomial  $\mathcal{P}(u)$  fitted to data simulated in water, would overestimate the energy loss in the less dense material. In this context, we also note that the



radiation length  $X_0$  (and other constant factors) which appear in the scattering power actually cancel out in the MLP expression, specifically in the terms  $c_0C(u)$  and  $c_1D(u)$  in equation 3. In other words, in a homogeneous medium, the MLP depends only on  $K(u)$  and not on the radiation length.

We point out that our MLP expression does not account for heterogeneous material composition along the particle path, and neither do the conventional MLP from Schulte et al. (2008) and similar variants. There are MLP methods available in the literature which use a priori knowledge about the object to account for inhomogeneous tissue composition (Collins-Fekete et al., 2017; Brooke et al., 2020). A comparison of such methods, both in terms of image quality and computation speed, was beyond the scope of this work.

The purpose of this work was to find a convenient way of parametrising the scattering power in proton CT reconstruction. We concentrated on a specific MLP formalism, namely the one in Krahl et al. (2019), because it leads to a compact expression for the MLP. We point out, however, that other MLP formalisms could also use equations 5 and 6 when evaluating scattering integrals, e.g. equations 7-9 in Schulte et al. (2008).

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## Appendix

Evaluating the integral terms  $A(u)$ ,  $B(u)$ ,  $C(u)$ , and  $D(u)$  in equation 2 with the new parametrisation of the scattering power involves two similar types of integral expressions which can be found in common mathematical handbooks, namely

$$\int_0^u \frac{1}{av+b} dv = \frac{1}{a} \log(au+b) - \frac{1}{a} \log(b) = \frac{1}{a} \log\left(\frac{a}{b}u+1\right) \quad (12)$$

$$\int_0^u \frac{v}{av+b} dv = \frac{u}{a} - \frac{b}{a^2} \log(au+b) + \frac{b}{a^2} \log(b) = \frac{u}{a} - \frac{b}{a^2} \log\left(\frac{a}{b}u+1\right), \quad (13)$$

where we have assumed  $u_{\text{in}} = 0$  for simplicity and without loss of generality.  $A(u)$  is directly equivalent to equation 12.  $C(u)$  is obtained by integrating equation 12 and using the substitution  $v' \equiv av/b + 1$ , so that

$$\int_0^u \int_0^v \frac{1}{aw+b} dw = \frac{b}{a^2} \int_1^{a/bu+1} \log(v') dv', \quad (14)$$

which is solved recalling that

$$\int \log(x) dx = x \log(x) - x = x (\log(x) - 1). \quad (15)$$

$B(u)$  is directly given by equation 13 and  $D(u)$  follows from it by integration and substitution  $v' \equiv av/b + 1$ , in analogy to  $C(u)$ .



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