Interaction Models for Proton Transport Monte Carlo Simulations based on the PENELOPE code

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Abstract

In this thesis work I have examined the physics models of the PENELOPE based proton transport Monte Carlo simulation code PENH with main focus on the eikonal expansion scattering model.

The eikonal expansion model, used for elastic proton scattering off atoms in PENH, has been compared with several alternative models, and concluded to be a reasonable choice of model for this application. The implementation of the model in PENH was adjusted, so that the masses used in computations account for the two-body nature of scattering. The correction had a small effect on the simulation results. The scattering power in water was seen to decrease slightly while the range was unaffected.

A simulation for benchmarking with experimental depth-dose data from the The Svedberg Laboratory (TSL) in Uppsala displayed errors in range as well as in initial dose. The errors in range are most probably the result of limited knowledge of the energy spectrum of the proton beam used. The error in initial dose originate from the fact that inelastic nuclear scattering is modeled by local absorption in the simulation. The model for inelastic nuclear scattering is the most important part of the code to develop in future work.

This thesis has been carried out at Elekta as a part of an effort to further develop their existing simulation software.
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Symbols used in this thesis

The following symbols are used throughout this thesis.

$M_p$ Proton mass

$m_e$ Electron mass

$Z$ Charge of the target in a scattering process, units of electron charges

$Z_0$ Charge of the projectile in a scattering process, units of electron charges

$e$ Electron charge

$M_1$ Projectile mass

$M_2$ Target mass

$\beta$ Projectile velocity in, units of $c$

$c$ Speed of light in vacuum

$\mathcal{M}$ Mass of the projectile as used in computations

$a_0$ Bohr radius
Chapter 1

Introduction

1.1 Radiation Oncology and Proton Beam Therapy

The practice of radiation oncology - using radiation for treating cancer - ranges back far, with early experiments beginning in the late 1800’s. The mechanism is simple: deliver energy into cells and it will cause damage and possibly kill the cells. Normal tissue is more resistant to damage than cancer cells and has a higher chance of surviving the treatment, implying that even an inaccurate delivery of radiation can lead to a successful treatment.

To improve the treatment, one tries to focus the radiation. As dose to normal tissue decreases, so does the risk of damage to organs. As the dose to tumorous tissue increases, so does the chance that no cancer cells survive. There are several ways to focus radiation. One method is using several different radiation sources with a common focus, thus delivering low doses to a large region of the body and a high dose in a very concentrated volume. This method is used in the Elekta Leksell Gamma Knife, as well as in intensity modulated radiation therapy.

An alternative method was proposed by Robert Wilson as early as 1946: to use beams of protons or other charged ions \cite{wilson1946}. He noted that the dose deposit as a function of depth is very favorable for such particle beams compared to gamma radiation, since the main energy delivery is focused in a so-called Bragg peak, see figure 1.2. The Bragg peak is typically in the order of mm wide, and can in principle be focused to only damage the tumor and sparing all other tissue. The predictions of Wilson were confirmed when the first patient was treated with a proton beam in 1954, and the results were reproduced in Uppsala 1957 \cite{wilson1954}.

A lot of further development has occurred within the field and PBT (Particle Beam Therapy) is currently on the rise as more and more PBT centers are built around the world. There are currently 46 facilities in operation, by which 20 has started operations the last 5 years \cite{pbt}. Despite this trend, the
Figure 1.1: Basic principle of the Leksell Gamma Knife - using several radiation sources with a common focus implies tissue out of focus receives a small dose while the organ in focus high dose. Image used with permission from Elekta.

Evidence for PBT is not clear.

The American Society of Radiation Oncology (ASTRO) reported 2012 that there is medical evidence for using proton beam therapy in a number of cancers, but that there is not enough support to say if it is preferential to photon beam therapy as further clinical trials are needed to collect data on the matter. They were optimistic about the technology as there are a lot of current developments in proton beam therapy [1].

One of the main drawbacks for proton beam therapy (PBT) is the high cost of treatment, with proton cyclo- or synchrotrons being far more costly than linear accelerators used in gamma oncology. So in the 2013 Nature Review on evidence for charged particle therapy [26] (such as proton beams and coal ion beams), while the picture on medical evidence essentially stands, they call for further research to understand the cost to benefit ratio.

1.2 Elekta

Elekta is an international company based in Sweden with main business areas covering neuroscience, oncology, brachytherapy and software engineering. The Leksell Gamma Knife and a variety of linear accelerators are found among the main products.
The Leksell Gamma Knife is a tool for stereotactic radiosurgery. The device has a large number of gamma emitting Co-60 samples with rays focused with a high precision to allow for surgery in the brain or spine. The most typical surgery for the Gamma Knife is tumor eradication. The linear accelerators are developed for oncological use producing high energy x-rays for treatment of cancer.

There is a constant need for predicting, verifying and validating performance in the product development cycle, both in hardware and software development. As experiments are costly and time consuming, the use of simulations have become more and more utilized to heed these needs. Typical applications include computing the dose delivery or radiation safety of linear accelerators, or benchmarking performance of simplified dose calculation engines. The Elekta office in Stockholm administers a computation cluster with a simulation platform based on the simulation software PENELLOPE. Local extensions are programmed as a layer on top of PENELLOPE and includes capabilities of handling voxelized geometry, CAD (computer aided design) model based geometry, simulations with computed tomography (CT) data as geometry and material definition files, advanced variance reduction methods.
and parallel computation. This simulation platform, called Pegasos, is used regularly in daily operations at Elekta [10].

1.3 Monte Carlo Simulations for Proton Transport at Elekta

A contemporary trend in the radiation oncology field is the increasing use of PBT. It offers an alternative to stereotactic radiosurgery and radiotherapy using external photon beams, mainly based on physical considerations as described above. Elekta does not currently offer any hardware products in the PBT field, but does provide dose planning software for PBT. In order to properly benchmark Elekta products against PBT, and to provide validation computations for dose planning software the resources needed to perform simulations of PBT is of interest.

An inherent limitation of PENELOPE is that the simulation only models gamma radiation, electron and positron radiation. This offers no major limitations for current usage, as these are the dominant particles when using the Leksell Gamma Knife and linear accelerators, but a natural step would be to complement Pegasos with proton simulation capabilities. Two naturally arising criteria for such an extension are 1) to base the extension on the PENELOPE model to minimize the business costs associated with software migration and 2) to have a detailed simulation model allowing complex geometries, arbitrary materials and so on.

One such extension to PENELOPE has been presented by the original PENELOPE authors under the name of PENH [35]. The PENH code is not complete, in the sense that it treats several physical processes in a basic manner - strong interactions with nuclei and bremsstrahlung included. Before using such a code system, Elekta needs to revise the code system including the physics models, since these have not been studied extensively in the literature.

1.4 Aim and Structure of This Thesis

The aim for this thesis is to answer the question

What models are used in PENH, what approximations have been made in developing them, and what models must be developed for the simulation code to produce acceptable results?

To approach this question we will go into the physics models of PENH, examine the elastic scattering model in detail and discuss the other scattering models more briefly. An overall benchmark of the PENH code system with experimental data will be presented.

The structure of the thesis is as follows: Chapter 2 provides a background on proton transport physics at the relevant energy scale. All models used later in the thesis are described, including the models currently implemented in
PENH. Monte Carlo simulations for charged particles are described in chapter 3 together with a description of selected Monte Carlo codes to give an overall idea about how the same problem may be solved in different ways. The PENH and PENELPOE codes are also described in chapter 2. The computations and simulations performed to understand the PENH models are described in chapter 4. Results from these simulations and computations are presented in chapter 5. Chapter 6 discusses and interprets the results of chapter 5. Main features of the results are pointed out. The concluding chapter 7 summarizes and puts into context the findings of chapter 6. Topics for future investigations are suggested.
Chapter 2

Proton Transport Physics

2.1 Introduction

To simulate proton transport we have to understand the mechanisms that govern protons propagating space in the presence of ambient matter. Since protons and atoms are composite objects, there are difficulties in applying fundamental theories of particle collisions directly. We need to find models that are sufficiently simple to solve our problem and that produce accurate results in the desired regime (energy, matter phases, particle types etc). Proton beams used in radiotherapy ranges up to 1 GeV [27], so the aim in this chapter is to discuss the energy range of 0.01 – 1,000 MeV. This is an in-between energy range where accurate models for hadron collisions are rare. This is illustrated in figure 2.1 and we will come back to this issue later on.

Figure 2.1: The energy ranges of relevance. PBT is concerned with slightly higher energies than medical linac’s used in high energy x-ray oncology. The code system PENELLOPE covers a wide energy range down to ver low energy, below which chemical processes take over. TALYS and Bertini INC model hadronic collisions in different energy ranges (see section 2.5.4).
Effects of coherent behavior such as effects of molecular structures will in general be disregarded - an approximation called the additivity approximation in which the cross sections for different components of compounds are incoherently added. This is a plausible approximation in general purpose Monte Carlo codes. \[35\]. This implies that the study can be restricted to scattering in media constituted by a single kind of atoms.

There are two different approaches to the study of proton transport connected to the computational capabilities available. One may either study the fundamental collision process for individual protons, or one may study the collective behavior of a beam at a macroscopic level. This is what I will call a detailed vs. compound model. Both of these perspectives are useful in simulation of charged particles.

In the following chapter I will first present some basic fundamnetals, then go into the detailed description of elastic and inelastic scattering processes and their importance for proton transport simulations, and finally outline some compound description theory. This constitutes the models needed for Monte Carlo simulations.

2.1.1 Basic Concepts

2.1.1.1 Cross Section

Proton transport is governed by the interaction of protons with ambient matter. The physical properly that describes the collisions is called a cross section, which may be defined by

\[\sigma = \frac{N}{N \Phi}\]

where \(N\) is the number of scatter events per unit time, \(N\) is the number density of scatterers per area and \(\Phi\) is the flux density (number of incident particles per unit area and unit time). One may interpret the cross section as a probability for interactions - the larger the cross section, the more scattering events will occur.

2.1.1.2 Differential Cross Section

The cross section \(\sigma\) is often restricted to scatter events for which the projectile is emitted in some specific solid angle \(\Omega\) or in which the particle loses some energy \(E\). These quantities are called differential cross sections and are denoted:

\[\frac{d\sigma}{d\Omega}\]  and  \[\frac{d\sigma}{dE}\]

respectively.
Note that these are differential in the sense that we might recover the full cross section using for example

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega.$$  

The final direction of the particle may either be described of the exit solid angle $$\Omega$$, but alternative parameterization may be useful. Sometimes the deflection angles ($$\theta, \phi$$) are more useful. The angles $$\theta$$ and $$\phi$$ are the polar and azimuthal angles in a spherical coordinate system with the $$z$$-axis along the projectile velocity and $$\phi = 0$$ implying along the lab system $$z$$-axis.

Since the differential cross section encodes the probability of certain scatter events to happen, our goal to describe proton transport may be fulfilled by calculating all relevant the differential cross sections. Elastic scattering are processes where the particle does not lose kinetic energy. The relevant differential cross section is differential in solid angle only: $$\frac{d^2\sigma}{d\Omega dQ}$$. Inelastic scattering are processes where the particle may lose kinetic energy. The cross section is normally parameterized in energy loss $$W$$ and in recoil energy $$Q$$: $$\frac{d^2\sigma}{dW dQ}$$. The $$Q$$ is the kinetic energy for an electron with momentum equal to the momentum lost by the projectile, i.e. $$Q(Q + 2m_e c^2) = q^2 c^2$$ where $$q$$ is the 4-momentum transfer in the collision.

### 2.1.1.3 Relativistic Effects

The protons under consideration will have kinetic energies $$E$$ in the range up to 1 GeV, which corresponds to $$\beta \lesssim 0.9$$ in the lab system. This indicates the need for relativistic kinematics. The relation between velocity, energy and momentum is shown in figure 2.2. These relations, which is the most important relations for this work, are contained in the well known formulas

$$E = \sqrt{m^2 c^4 + \vec{p}^2 c^2} - mc^2$$

$$\vec{p} = m\vec{v} \gamma = mc \vec{\beta} \gamma$$

where $$\vec{v} = \vec{\beta} c$$ is the velocity, and $$\gamma = (1 - |\vec{\beta}|^2)^{-1/2} = (E + mc^2)/mc^2$$.

The relativistic velocities has two main effects on the computations.: First, it has effect on the scattering calculations as such, making nonrelativistic quantum mechanics inappropriate. Second, it means that any change of coordinates must be made with the Lorentz transformation. It is often convenient to calculate cross sections in the center-of-momentum frame. The transformation of cross sections rests on the idea of a scaling factor

$$\frac{d\sigma}{d\Omega_{lab}} = \frac{d\sigma}{d\Omega_{CM}} \left| \frac{d\Omega_{CM}}{d\Omega_{lab}} \right|.$$
In the equation \(d\Omega_{CM}\) denotes a solid angle element in the center of mass frame, whereas \(d\Omega_{lab}\) is the corresponding solid angle element in the lab frame when the angles are transformed via the Lorentz transform. The details can for example be found in [35].

### 2.1.1.4 Interaction Channels

When there are several possible qualitatively different ways for the particle to scatter, these are all associated with their respective cross section. I will call these different ways of interaction different channels. There are 4 distinct channels that I will discuss in this thesis, as presented in table 2.1. The first level categorization is whether the interaction is elastic or inelastic. The second level categorization is based on the choice of models, trying to separate the effect from electromagnetic scattering and electrons from the effect of the nucleus.

Bremsstrahlung has a small effect on the stopping of protons since the radiated power is quite small. If the simulation aims to use the spectrum of secondary gammas, such as in spectrum sensitive detector modeling, one has to include this effect [21]. In dosimetry, the bremsstrahlung can most probably be neglected [35].

The activation of stable nuclei into elements with considerable half-life is an issue in proton beam therapy. A treatment session has a beam-on time for about a minute but activated components should not be handled until after initial cool down, taking about 15 minutes for copper gantry parts [35]. The dosimetry contribution from these isotopes is assumed to be of relatively low importance for dosimetry simulations which is the prime interest of this thesis, and will be neglected.

One interaction channel often neglected in the discussion of proton beam therapy physics is the Coulomb excitation of the nucleus. I will not discuss its
2.1. INTRODUCTION

### Channel Characteristics

<table>
<thead>
<tr>
<th>Channel</th>
<th>Characteristics</th>
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<tbody>
<tr>
<td>Elastic</td>
<td>Assumes nucleus and proton are pointlike. Only electromagnetic forces are modeled.</td>
</tr>
<tr>
<td>Residual</td>
<td>Includes strong interaction and the effect of nucleus size.</td>
</tr>
<tr>
<td>Inelastic</td>
<td>Ionization. Production of secondaries: * Auger electrons * Delta rays * Fluorescence</td>
</tr>
<tr>
<td>Nuclear</td>
<td>Absorption Secondary production of: * Gamma * Conversion electrons * Protons * Alphas * Neutrons * Other heavy fragments</td>
</tr>
</tbody>
</table>

Table 2.1: Reaction channels and phenomenon discussed in this thesis.

importance for dosimetry, but note that a full treatment of inelastic scattering should include this effect.

#### 2.1.2 Detailed and Compound Models

Low energy radiation transport physics normally rely on calculation of cross sections to describe the transport phenomenon. This is the approach of PENELOPE, why I use this perspective in this thesis. One should keep in mind that there is one cross section for each possible interaction and for high projectile energy, there is a large number of available interactions channels. If the energy is high enough, the approach of using tabulated cross section is unwieldy since the memory needed is very large. Alternative methods include calculating collision cross sections in run-time or relying on Monte Carlo engines to model each collision process. One has to consider what kind of model is applicable given the resources one has at disposal.

When lacking computational power, the method of modeling each and every scattering event is impossible to utilize. I will call physical models in which several scattering events are bundled together “Compound models”. Developing these compound models using analytical methods, the need for computational power is greatly reduced. Modern Monte Carlo transport codes often use these compound models as a benchmark or as a way to simplify and speed up simulations.

I will return to this subject in section 2.6 where I discuss the Bethe-Bloch equation and multiple scattering theory, and in section 3.1 where I discuss
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2.2 Elastic Scattering: Pure EM

2.2.1 General Considerations

The interaction I call “Pure EM” will be defined by the model we put forward for it, as opposed to being defined by the physical behavior we want to describe.

The starting point is elastic scattering mediated by electromagnetic forces. Next is to approximate nucleus to be pointlike. Further, we may consider several different models and simplifications which we will explore in the coming subsections.

One important approximation is the static-field approximation. In this regime, the charge density of the atom is assumed to be constant in time (no polarization of the atom). This is true for all small angle scatter events and slow projectiles. This aspect of the approximation should only have minute effect on transport studies [35]. Another aspect of the static-field approximation is that the recoil of the target should result in a photon exchange. This transverse excitation of the field is radiative and not included in the normal electrostatic interaction. In the worst case, when the target is a hydrogen atom and the projectile has an incident energy of 1 GeV, the two protons have a relativistic $\beta \approx 0.5$ in the center-of-mass frame. Under this consideration, the recoils should be large and the static field approximation less appropriate. The static field approximation will nevertheless be made for all our models under consideration but for the one-photon-exchange model.

Another simplification is to consider the projectile and target to be spin zero particles. By comparing Dirac and spin zero particles scattered by a coulomb potential in the Born approximation, a factor of $[1 - \beta^2 \sin \theta/2]$ is present in the differential cross section for particles with spin [35]. A useful approximation is thus to treat all particle as scalar, and at the end introduce said multiplicative factor. All models but the one-photon-exchange models will make this approximation.

After these two simplifications, we have a scalar two-body relativistic scattering process. Assuming the target to be stationary, we would have a single particle Klein-Gordon problem, but since we also consider light targets, we must consider a two-body problem. We will now, with some heuristics reduce this to a 1-particle Schrödinger scattering problem. We start off with the system Hamiltonian:

$$E = \sqrt{p_1^2 c^2 + M^2 c^4} + \sqrt{p_2^2 c^2 + M^2 c^4} + V(x_1 - x_2)$$

To reduce the problem to a tractable form, we go to the center-of-mass coordinates ($\sum_i p_i = 0$ so that $p_1 = -p_2 \equiv p$) and assume equal masses.
(M_1 = M_2 \equiv M). Use shorthand notation V(x_1 - x_2) = V. After resolving the square root, we arrive at

\[ E^2 - 2EV + V^2 = 4p^2c^2 + 4M^2c^4. \]

For infinite particle separation, the total energy of the system is \( E = 2\gamma Mc^2 \), i.e. the energy of two free particles with identical mass and velocity. The total energy is also conserved in this problem. Inserting and rearranging yields

\[ \frac{p^2c^2}{\gamma Mc^2} + V(1 - \frac{V}{4\gamma Mc^2}) + \frac{M^2c^4}{\gamma Mc^2} - \frac{\gamma^2 M^2c^4}{\gamma Mc^2} = 0. \]

Identifying \( M^2c^4 - (\gamma Mc^2)^2 \equiv -k^2c^2 \) as the negative squared momentum of the particles at infinite separation. Also, introduce a computational mass \( \mathcal{M} \).

\[ \mathcal{M} = \gamma M/2 \] (2.1)

and rearrange. This might be compared with the corresponding reduced mass used in classical mechanics, which for this problem would be \( \mu = M_1M_2/(M_1 + M_2) = M/2 \). The expression found,

\[ \frac{k^2}{2\mathcal{M}} = \frac{p^2}{2\mathcal{M}} + V(1 - V/4\mathcal{M}c^2) \]

needs just one more approximation to be useful. Since \( 4\mathcal{M}c^2 \) is typically in the order of GeV for proton collisions, and the potential \( V \) may never exceed the Coulomb barrier which is of the order of \( MeV \), we may assume \( 4\mathcal{M}c^2 \gg V \) and we arrive at a one-particle Schrödinger equation

\[ \frac{k^2}{2\mathcal{M}} = \frac{p^2}{2\mathcal{M}} + V. \]

The mass present in the equation is the computational mass \( \mathcal{M} \) which corrects for both the relativistic mass correction (\( \gamma \) factor) and for the classical phenomenon of reduced mass. Possible generalizations particles with different masses are possible, as presented in table 2.2.

In the following, based on the approximations above, we may use models for non-relativistic single-particle quantum mechanics despite the nature of the real problem - as long as we use a computational mass \( \mathcal{M} \) instead of the invariant mass of the projectile.

Finally, the potential \( V \) must be realistic. One effort in this regard is performing self-consistent Dirac-Hartree-Fock-Slater computations and parameterizing the result with a sum of Yukawa-terms. Coefficients from such computations are tabulated in [34]. The potential takes the form
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### Table 2.2: Possible formulations of computational mass $M$ in scattering problems.

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<th>Non-relativistic</th>
<th>Relativistic</th>
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<td>Single particle</td>
<td>$M_1$</td>
<td>$\gamma M \equiv \gamma_1 M_1$</td>
</tr>
<tr>
<td>Reduced mass</td>
<td>$\mu \equiv \frac{M_1 M_2}{M_1 + M_2}$</td>
<td>Symmetric formula: $\mu^* \equiv \frac{\gamma_1 M_1 \gamma_2 M_2}{\gamma_1 M_1 + \gamma_2 M_2}$</td>
</tr>
<tr>
<td></td>
<td>$\gamma \mu \equiv \frac{\gamma_1 M_1 M_2}{M_1 + M_2}$</td>
<td>Asymmetric formula: $\gamma \mu \equiv \frac{\gamma_1 M_1 M_2}{M_1 + M_2}$</td>
</tr>
</tbody>
</table>

The two relativistic reduced masses are not provable to be correct, but both reproduce the exact formulation in equation (2.1) in both the non-relativistic limit as well as the same-mass-limit, which is imperative. The $\gamma_i$ are the respective gammas in the center-of-momentum frame.

$$V(r) = \frac{Z_0 Z e^2}{r} \sum_{i=1}^{3} A_i \exp \left[-\alpha_i r \right] \quad (2.2)$$

and the tables cover values of $A_i$ and $\alpha_i$. The screening phenomenon is the fact that the electron cloud surrounding the nucleus modifies the electrostatic potential. At large distances, the electron cloud should mask the nucleus completely, since the atom as a whole is a neutral object. Only when penetrating into the electron cloud will the charge of the nucleus be noticeable.

### 2.2.2 Classical two-body Cross Sections

The classical two body problem in mechanics may be solved exactly. This is done fully in many books, example in Landau & Lifshitz Mechanics [25]. The solution is:

$$\frac{d\sigma}{d\Omega} = \rho(\theta) \frac{\sin \theta}{\sin \phi_0} \left| \frac{d\rho}{d\Omega} \right|$$

The scattering angle $\theta = |\pi - 2\phi_0|$ corresponds to the quantity $\phi_0$. The half deflection angle is in turn possible to relate to the impact parameter $\rho$ via the integral

$$\phi_0 = \int_{r_{min}}^{\infty} \frac{(J/r^2)dr}{\sqrt{2M[E - U(r)] - J^2/r^2}}$$

The energy $E$ of the incident particle is the kinetic energy at infinite separation. The angular momentum of the system $J$ is related to the mass, velocity at infinite separation and impact parameter $J = M \rho v_\infty$.

The integration limit $r_{min}$ is the minimal radius throughout the scattering event - also called the collision diameter. It is found by the relation where all
2.2. ELASTIC SCATTERING: PURE EM

kinetic energy at infinite separation minus the potential energy is exactly the centrifugal energy from pure angular motion.

\[ E - U(r_{\text{min}}) = \frac{J^2}{2Mr_{\text{min}}^2} \]

Normally this method is used for classical problems, so that \( M = \mu \equiv M_1M_2/(M_1 + M_2) \) - i.e. the classical reduced mass.

2.2.3 Rutherford Cross Section

The result of Rutherford for scattering, which is the solution to the classical scattering problem for a Coulombic potential \( V(r) = ZZ_0e^2/r \) is one of the more famous results. The differential cross section is well known, and in [35] formulated as:

\[ \frac{d\sigma^{\text{Ruth}}}{d\Omega} = (2Mc^2Z_0Ze^2)^2 \frac{1}{(cq)^2}. \]

The same result may be found by quantum mechanical means, as the first order Born approximation of the cross section for the Coulomb potential scattering.

2.2.4 Born Cross Section

The problem may be treated with Schrödinger quantum mechanics and the Born approximation. Then

\[ \frac{d\sigma^{\text{Born}}}{d\Omega} = \left( \frac{M}{2\pi\hbar} \right)^2 |\langle \vec{R}'|V|\vec{k}\rangle|^2 \]

where \( \vec{R}' \) points into the solid angle \( \Omega \). If the potential has the form (2.2), the matrix elements may be computed analytically to find (see [35])

\[ \frac{d\sigma^{\text{Born}}}{d\Omega} = (2Mc^2Z_0Ze^2)^2 \left( \sum_{i=1}^{n} \frac{A_i}{(ch_i)^2 + (cq)^2} \right)^2. \]

Some of the similarities between the Rutherford and Born cross sections are apparent: They coincide if \( a_i = 0 \) for all \( i \), i.e. when the potential is the Coulomb potential. When \( (cq)^2 \geq (ch_i)^2 \), for large scattering angles, the screening effect is negligible.

There must therefore be some scattering angles for which \( cq = cha_i \) where the effect of a screened potential takes effect. We find this angle by noting that the screening radius is in the order of the Bohr radius \( 1/a_i \approx a_0 \) and that \( q = 2p\sin\theta/2 \) in the center-of-mass frame.
Table 2.3: Order of magnitudes for the screening angles. The Born approximation suggests screening is important when the momentum transfer is equal to or larger than the inverse screening radius - i.e. $cq \geq cha_i$. Inverse screening radii is typically in the order of the inverse Bohr radius, $a_i \approx 1/a_0$. In the center-of-mass frame, we have that $q = 2p \sin \theta/2$. Thus, the screening angle is $\theta_{CM} = 2 \arcsin \frac{1}{2a_0^p}$.

### 2.2.5 Partial Wave Expansion

The single-particle scattering problem is solvable using partial wave expansion and numerics. This should be the preferred method of solution in elastic scattering problems generally, but it is a series expansion method and produce very slow convergence for heavy particles such as protons in the energy range of interest. Therefore, this will not be the method of choice. [35].

### 2.2.6 Eikonal Expansion Cross Sections

One other expansion model that might produce good results efficiently for this problem is the eikonal expansion proposed by Wallace [44]. To the zeroth order, this is the well known eikonal approximation of straight ray propagation through the potential combined with the ansatz that the potential contributes to the phase only, as in the WKB approximation. This approximation is treated in detail in modern books on quantum mechanics such as [33].

The contribution of Wallace is to have developed a series method for calculating correction terms to this first approximation. Thus, the solution method can be regarded as a semi-classical optical model with corrective terms. The expansion scheme is analytically solvable to first order in the case of Yukawa-sum potential models such as the one used in (2.2).

A first order correction to the standard eikonal approximation is used in the PENH code system [35]. I will here simply state the result:

$$\frac{d\sigma}{d\Omega} = \left| \frac{p}{\hbar} \int_0^\infty J_1(qb/\hbar) \exp[i\chi(b)] \frac{d\chi(b)}{db} bdb \right|^2$$
2.2. ELASTIC SCATTERING: PURE EM

\[ \chi(b) = -\frac{2MZ_0e^2}{hp} \sum_i A_i \times \left\{ K_0(\alpha_ib) - \frac{MZ_0Ze^2}{p^2} \sum_j A_j \alpha_j K_0(|\alpha_i + \alpha_j|b) \right\} \]

(2.3)

\[ \frac{d\chi(b)}{db} = -\frac{2MZ_0e^2}{hp} \sum_i A_i \times \left\{ \alpha_i K_1(\alpha_ib) - \frac{MZ_0Ze^2}{p^2} \sum_j A_j \alpha_j [\alpha_i + \alpha_j] K_1(|\alpha_i + \alpha_j|b) \right\} \]

where \( J_i \) and \( K_i \) are Bessel functions of the first kind and modified Bessel functions of the second kind. Please be aware of the small typo in [35].

2.2.7 One-photon-exchange Cross Section

A different approach to the scattering problem is to model the collision as a fermionic electromagnetic collision to first order in perturbation. This is similar to the Möller scattering, but we assume different masses and charges for the two particles. The calculation automatically includes the effect of relativity, reduced masses, spin coupling, longitudinal photon exchange et cetera. On the downside, this method only describes the scattering of a purely Coulombic potential. The more complicated case using atomic relativistic factors will not be considered here.

The scattering of electrons against protons at rest is a model case derived in [15] as electron-electron scattering without the exchange symmetry and with different masses. I will state their result simply:

\[ \frac{d\sigma}{d\Omega} = \frac{M_1^2M_2}{4\pi^2} \frac{|M_{fi}|^2}{|p|} \frac{M_2 + E - E'\frac{p_f}{|p|}}{\cos \theta} \]

and the matrix element is

\[ |M_{fi}|^2 = \frac{Z_i^2Z_0^2e^4(4\pi)^2}{2M_1^2(q^2)^2} \frac{1}{M_2^2} \left\{ 2M_2^2EE' - p_f \cdot p_i \left[ M_1^2 + M_2(E' - E) \right] + M_1^2M_2^2 \right\} \]

where \( p_i = (E, \vec{p}) \), \( p_f = (E', \vec{p}') \) are Minkowski 4-vectors in the lab system, and the momentum transfer \( q = p_i - p_f \). Calculating the \( E' \) as a function of scattering angle is most easily done by first Lorentz transforming to the center-of-mass system, finding the momentum transfer in that frame, and then boosting back to the lab system.
CHAPTER 2. PROTON TRANSPORT PHYSICS

<table>
<thead>
<tr>
<th>Atom</th>
<th>Nucleus charge</th>
<th>Barrier energy [MeV]</th>
<th>Range in water [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1</td>
<td>1.20</td>
<td>0.03</td>
</tr>
<tr>
<td>O</td>
<td>8</td>
<td>3.81</td>
<td>0.24</td>
</tr>
<tr>
<td>Al</td>
<td>13</td>
<td>5.20</td>
<td>0.36</td>
</tr>
<tr>
<td>Ag</td>
<td>79</td>
<td>16.3</td>
<td>2.94</td>
</tr>
</tbody>
</table>

Table 2.4: Barrier and range threshold for nuclear reactions to occur.

2.3 Elastic Scattering: Residual Cross Section

The Pure EM models above all neglect the extension of the nucleus of the target. This means that the EM potential model should have a smearing effect at very small separation, which it does not have currently. Further, the models neglect scattering mediated by strong forces.

The first question to raise is if we can neglect other forces - but the answer is unfortunately “No”. Using nuclei radius \( r_{\text{nuc}} \approx 1.2 \sqrt[3]{A} \text{ fm} \), and \( V(r) = \frac{Ze^2}{r} \), one can find the energy needed to penetrate the Coulombic barrier and make the projectile suffer nuclear interaction. The residual range for protons with such a kinetic energy can be found in the PSTAR database\(^{[4]}\) and give an estimate on whether they will have any effect on simulation results. Table 2.4 shows a compilation of such ranges.

We can clearly see that for a proton to not be able to penetrate any nucleus, and to allow a model without any nuclear modelling, we should have energies below 1 MeV and any geometrical feature of interest must be sub-millimeter.

The way to approach a model for this residual cross section is not clear. The suggested approach in \(^{[35]}\) is to used tabulated experimental data. Several databases are thinkable.

The ENDF (Evaluated Nuclear Data File)\(^{[7]}\) is one option. The residual differential cross section has been measured and tabulated for a selection of elements. For these elements, interpolation to energies of interest may be carried out. Elements covered to lesser or greater extent with energy-angle-distributions and tabulated cross sections include, H, He, C, N, O, F, Na, S, K, Ca and Fe. For the latest version, please see [https://www-nds.iaea.org/exfor/endf.htm](https://www-nds.iaea.org/exfor/endf.htm).

Another database that may be used is the ICRU 63 report \(^{[20]}\) on ”nuclear data for neutron and proton...”. It contains the total inelastic cross section, from which one may subtract the cross section derived analytically. The database only covers scattering angles above 5 degrees and the elements C, N, O, P, Ca. In some cases the subtraction leads to nonphysical results, which must be handled in one way or another.

For proton-proton-collision, which is the case for collisions with hydrogen, the partial-wave-approach expansion may be possible. The SAID partial wave analysis database \(^{[2]}\) includes computation of cross sections for proton-proton
2.4 Inelastic scattering: Electronic scattering

The inelastic scattering is in general a more complicated problem than the elastic scattering process due to the increased number of degrees of freedom.

Based on a relativistic first order Born approximation, one can derive an expression for the cross section as a product of terms dependent on the kinematics of the projectile, and one factor including the internal dynamics of the target called the generalized oscillator strength, or GOS, denoted \( \frac{df}{dW} \) \[1\]. The cross section is differential in energy loss \( E \) and in recoil energy \( Q \). Approximations leading to this formula includes only taking the electrons into account, and assuming the momentum transfer is small \( (q \ll p) \) which should hold for projectile energies below 1 TeV (kinematic constraints for proton-electron scattering).

\[
\frac{d^2\sigma}{dWdE} = \frac{2\pi Z^2 e^4}{m_e^2 \beta^2 c^2} \times \left\{ \frac{2m_e c^2}{WQ(Q+2m_e c^2)} + \frac{2m_e c^2 W}{(Q(Q+2m_e c^2)-W^2)^2 \left( \beta^2 - \frac{W^2}{Q(Q+2m_e c^2)} \right)} \right\} \times \frac{df(Q,W)}{W}
\]

Thus, the inelastic scattering model may be accurately developed if in turn the GOS is modelled correctly. In previous work with PENELOPE, a GOS-model called the Sternheimer-Liljequist model has been implemented\[36\]. It models excitations of individual orbitals in the electron cloud and uses the mean excitation energy of the material in question as the single free parameter of the model.

In the PENH code the same model used, but with minor alterations to account for the heavier mass of proton projectile in contrast with electron/positron projectiles used in PENELOPE. In \[35\], the claim is that this is needed because the assumption on small momentum transfer no longer holds. I would claim that this is not the case - but it does not matter too much since the alteration should not decrease the precision of the code.

If the energy lost from the projectile to an electron in a specific subshell is large enough the electron is excited to a higher energy state or emitted as a delta ray. Relaxation of excited atoms produces x-rays and Auger electrons. This relaxation cascade is described in the PENELOPE manual\[36\].

The Sternheimer-Liljequist model contains errors related to x-ray and Auger electron production that is adjusted in two steps. First - a more detailed relativistic plane wave Born approximation calculation (PWBA) was performed to find the cross section for ionization of inner shells. The Sternheimer-Liljequist model is then adjusted to fit the PWBA-calculations closely. Finally, the PWBA-calculation will not perfectly reproduce the actual stopping power,
so a global adjustment of the GOS model is made so that the full GOS model will yield a stopping power as prescribed by the ICRU 49 [19].

2.5 Inelastic Scattering: Nuclear Scattering

The inelastic scattering of protons off atomic nuclei is a problem with no conclusive solution in the literature. Experimental data is abundant, but limited in energy ranges. No theory does yet provide conclusive answers on how to calculate cross sections for reactions. Several different models have been proposed, and this section will describe a few simpler models briefly.

2.5.1 Pure Absorption

The most primitive modelling of inelastic scattering off nucleus is to have a model for the total cross section and in the event of scattering deposit all energy locally. This approximation should be acceptable for all scattering events that produce very heavy secondaries such as alpha particles. It should be lacking regarding neutron and proton production which may have long range.

One such ”total cross section” model is presented by Preal and Chadwick [29, 30] which was implemented in the simulation code LAHET for inelastic proton cross section to extend the more complicated collision model to lower energies - aiming at a few 100 MeV. Analytical expressions for total cross section in units of mb (millibarn) as a function of atom mass number $A$, atomic number $Z$ and incident proton energy $E$ (in units of GeV) is available in the reference. It is applicable for $Z \geq 4$, and for the combinations $(Z, A)$ being any of $(3, 7), (3, 6), (2, 4), (2, 3)$.

2.5.2 Long- and Short-range Secondaries

Categorizing secondaries in ”long ranged” and ”short ranged” provides a simple and useful model. ”Short range” secondary energy deposit energy locally and ”long range” secondaries are neglected in the simulation altogether. This is very close to the approach in VMCpro [13]. In this code, the inelastic cross section is found by curve fitting a functional form to tabulated ICRU63 stopping powers. When an inelastic nuclear scattering event is sampled, first the secondary particle energy is sampled uniformly, then there is a 50% chance that the secondary is a proton, and otherwise it is ”short range energy” or ”long range energy”. Long range energy are representation of neutrons etc. which deposit the energy outside of the simulated system. ”Short range energy” is heavy particles and fragments with short range such as alphas, deuterium and tritium, which energy is deposited locally. The model is verified to give acceptable results when benchmarked on oxygen collisions with Geant4 and data tables in the ICRU 63 report.
2.5. INELASTIC SCATTERING: NUCLEAR SCATTERING

2.5.3 Proton-like Treatment of Charged Secondaries

The PENH-code has been partially extended to handle nuclear collisions for light elements \[39\]. The cross sectional data is taken from the ICRU 63 report: "Nuclear data for neutron and proton radiotherapy and radiation protection". Charged secondary fragments are tracked as secondary protons, but with a reduced energy and increased statistical weight to account for their mass difference to protons. The statistical weights and energy factors are based on the similarity in the CSDA range of the different particles with protons. Neutrons produced are neglected in the code since they contribute only slightly to the total dose.

The method has been benchmarked to Geant4 with satisfactory results, but is limited to the data availability in the ICRU 63 report. It covers the energy range \(7 \text{ MeV} < E < 250 \text{ MeV} \) and elements C, N, O, P and Ca.

2.5.4 More Complete Handling of Secondaries

In more advanced code systems, the collision of hadrons is based on an intranuclear cascade (INC). In such a simulation method, the projectile and target are decomposed into their nucleons, and a Monte Carlo simulation of nucleon-collisions is performed. No cross sections for the composed targets are needed, but only cross sectional data for nn-, np- and pp-scattering is needed.

Geant uses the Bertini INC as standard for hadron collisions. The model is used for projectile energies in the interval between 100 MeV and 10 GeV, and is valid for a selection of projectiles including neutrons and protons. The INC is supplemented by auxiliary models such as evaporation or fragmentation models to detail different regimes in the collision process. The model is described in detail in the Geant4 physics reference manual \[14\]. A family of similar methods are available in the same category of Monte Carlo codes, including FLUKA and LAHET.

There are several other monte-carlo based software packages that do not track geometry and such, allowing for a simpler interfacing to other codes and often using standard file formats for output. A common task for using these codes is a so to say intelligent interpolation of data otherwise found experimentally. A few that I have stumbled upon in this thesis work are EMPIRE \[16\], McGNASH\[11\], MEND\[8\] and TALYS\[24\]. Usually, they utilize some Hauser-Feshbach theory and or other computational method such as the ones mentioned above. The respective references provides good descriptions both of the respective code systems and their nuclear reaction models. Typical energy ranges for these models are \(0.01 \text{ MeV} < E < 200 \text{ MeV} \).
2.6 Compound Models

2.6.1 Stopping Power and Range

2.6.1.1 Bethe-Bloch Formula

In the energy range below 1 GeV, the dominant interaction mechanism for protons is the electromagnetic inelastic scattering off atomic electrons with a small energy loss and negligible angular deflection. This is called Multiple Coulomb scattering (MCS). The phenomenon applies to all transport of charged particles. The projectile undergoes an immense amount of these interactions with very short free flight in between, why we call the regime Continuously Slowing Down Approximation (CSDA). Computations based on continuously slowing down was used with success to predict penetration depth before more complicated computer programs came to use.

The CSDA can be formulated in the famous Bethe-Bloch formula. It was first derived in the quantum mechanical setting by Bethe 1930, and can neatly be derived from individual scattering events as presented in e.g. [11]. It is a formula for stopping power, which is the energy loss per unit length

\[-\frac{dE}{dx} = \frac{4\pi Z^2 e^2}{M_1 \beta^2 c^2} N Z_0 \left\{ \ln \frac{2M_1 \beta^2 c^2}{I} + \ln \frac{1}{1 - \beta^2} - \beta^2 + \text{corrections} \right\}\]

where \(N\) is the scatterer density in the surrounding material and \(I\) is a parameter called the mean excitation energy. It is often taken as a free parameter in the model even though it in principle may be calculated from microscopic theory. The corrective terms are a power series in \(Z^n\) for \(n = -1, 0, 1, 2, 3,...\). The first two terms has been described by Fano [11]. While the initial terms stem from scattering of the particles off the atomic electrons, several approximations has been made. The first corrective term (called shell correction) account for the fact that atomic electrons are not at rest. The second term (called density effect correction) corrects the assumption that the projectile never polarize the target. A full treatment on the calculations may be found in [46].

By integrating the stopping power, one may calculate the range of a particle given some initial energy.

2.6.1.2 PSTAR and ICRU 49

The database PSTAR is available on the internet http://physics.nist.gov/PhysRefData/Star/Text/programs.html and contains stopping power and range tables for protons. The development of the data set is described in the ICRU report 49 [19]. The PSTAR database is produced by a computer program using a Bethe-Bloch equation with correction terms to compute stopping powers at high energies (\(E \geq 0.5\) MeV), and using experimental data for stopping powers at lower energies. The errors in the high energy region is
about 1 – 2% while the error in the lower energy region increases as energy decrease.

2.6.2 Angular Deflection and Multiple Scattering

The Bethe-Bloch equation does not account for the angular scattering of proton transport and further assumes that the beam has a constant width. This is not true, since the beam broadens as it propagates into matter. Short of computational power in the early 20th century, scientists put forward methods to derive the mean behavior of particles. The starting point for such an approach is a transport equation in the phase space of incoming particles,

\[
\frac{df}{ds} = -\mathbf{\hat{d}} \cdot \nabla f + N \int \left[ f(s; r, \mathbf{\hat{d}}) - f(s; r, \mathbf{\hat{d}}') \right] \frac{d\sigma(\theta)}{d\Omega} d\Omega
\]

for which the solution gives the final distribution of particles at some point after some specified time. The distribution \( f \) is over velocity direction \( \mathbf{d} \) at some space point \( r \) and some distance traversed \( s \). \( N \) is the scatterer (e.g. atomic) density of the medium. The solid angle \( \Omega \) is in the direction \( \mathbf{\hat{d}} \). The quantity \( \frac{d\sigma(\theta)}{d\Omega} \) is called the differential cross section for scattering by a polar angle \( \theta \) and can be interpreted as the (non-normalized) probability to change direction of propagation by an angle \( \theta \). The PDE should be solved with some initial condition: the typical case being

\[
f(0; r, \mathbf{\hat{d}}) = \delta(r)\delta(\mathbf{\hat{d}} - \mathbf{\hat{z}})
\]

which means that particles that have not yet propagated \( s = 0 \) is in the entry point to the medium \( r = 0 \) and travels straight along the beam axis \( \mathbf{\hat{d}} = \mathbf{\hat{z}} \).

Different ways to solve this equation leads to different multiple scattering theories. Some notable examples are the theories of Molière, Goudsmit-Sanderson and Lewis [12]. Based on the theories of Lewis and Goudsmit-Sanderson, analytical expressions for the spreading in the lateral plane can be derived, and they display a simple relation to the cross section and quantities called transport coefficients that are derived from the cross section. To evaluate those expressions, on the other hand, one has to assume some specific scattering potential. Moliere used a specific potential and solved the original problem directly, yielding one special case of the general solution. There are several other multiple scattering theories in use today, but these are the most commonly referred.

The relatively simple form of these multiple scattering laws makes them feasible for fast computations and a few examples of how these are implemented in clinical software for dose calculations can be found in the following articles: [5, 9, 17, 28, 37, 40].
Chapter 3

Charged Particle Monte Carlo

In this chapter I will present some general points on charged particle Monte Carlo and further present some specific simulation code systems as examples on how to deal with the bias/noise trade off problem present in these simulations.

3.1 Transport Simulations for Charged Particles

A Monte Carlo simulation method is a technique using randomness to calculate quantities otherwise difficult to determine. The process can be thought of in the following way:

1. Stochastically generate a state ensemble that represents your system.
2. Compute aggregated properties for this ensemble. These are estimates for the quantities you are computing.
3. Assess the statistical uncertainties in the estimate coming from the fact that you have a finite sample representing the complete ensemble.

Step 2 and 3, collectively called scoring, may in some algorithms be performed in parallel to step 1. The Monte Carlo method we use in particle transport follows the schema:

1. Generate a random particle track. It consists of the different points in space at where the projectile collides with surrounding matter, and the energy lost in each collision. The distance between collisions, the angular deflection and the energy loss in each collision is determined by sampling from probability distributions generated by the differential cross sections.
2. Calculate the mean energy deposition, radiative flux or other properties for some region of interest such as the patient body.
3. Calculate $3\sigma$ error bounds for said quantities.

Because of the stochastic nature of the method, one has to introduce a careful error analysis. The first error of Monte Carlo methods - the noise - is due to the random sampling of the state ensemble. The main way to eliminate this error is to extend the ensemble size, but this may be an impossible approach if the state space is so large that important regions are not sampled from enough. An alternative way is to sample in a strategic way so that important regions of the state space is sampled from more frequently, and then weighted properly so that no new error is introduced - in general called variance reduction. The second error is the model error - or the bias - in the simulation. To reduce the bias a more sophisticated model of the system has to be employed. More sophisticated models often implies more complex ways to sample random states. This further leads to inability to generate large ensembles quickly, which may increase the stochastic error.

While Monte Carlo method may be used to calculate any macroscopic property from fundamental principles, the trade off between the two error types mentioned above can make the calculation unfeasible to do in acceptable precision and time. This trade off is core to the design of Monte Carlo simulation codes. There are specific troubles occurring in the simulation of charged particles though matter. Charged particles exhibit Multiple Coulomb Scattering (MCS) as described in section 2.6.1.1. In the macroscopic behavior this is what motivates the CSDA and allows an analytic approach, but when Monte Carlo simulating this behavior the MCS can become quite prohibiting. Since there is a very large number of collisions, a single particle track may include millions of collisions. Combining the MCS into a compound description will reduce the precision of the simulation since it assumes extra conditions about the scattering (e.g. no material boundary crossings). On the other hand - not combining the multiple scattering into compound schemes makes the number of collisions and the computational power needed immense.

In the 60’s a method was devised to split the physics into what is called soft and hard events. The method is attributed to Martin J. Berger and is today a standard approach in particle transport simulations [32]. Soft events are events with small enough scattering angle and energy deposition, while hard events are all other events. Soft events constitute the majority among the events, but has only small impact on the particle track. The soft events are treated with some multiple scattering formulas such as those from the Lewis or Moliere theory. Every now and then, a hard event will occur. Those are the events in which large momentum transfers occur and they imply large energy deposition and or large angle scattering. These events are treated with the detailed description of the system. Different variants of simulation techniques have been devised ranging from treating all events as soft, to treating no events at all as soft. An overview is provided in table 3.1.
3.2. CHARGED PARTICLE CODE SYSTEMS

<table>
<thead>
<tr>
<th>Simulation type</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pencil beam techniques</td>
<td>A deterministic method assuming the incident radiation is a thin parallel, simple beam that is may be treated with some compound description of the physics. Not a Monte Carlo technique, but often used in dose planning where simulation speed is imperative and precision is even more limited by other factors.</td>
</tr>
<tr>
<td>Detailed Monte Carlo</td>
<td>Each collision is modeled. Sample length of free flight in between. Sample scattering angles and energy loss in each interaction. The method is often computationally unwieldy.</td>
</tr>
<tr>
<td>Condensed Monte Carlo</td>
<td>All energy loss and angular scattering is sampled from a probability distribution based on compound descriptions such as Lewis Theory. Production of secondaries is accounted for after the primary track is finished. High computational speed but has inherent problems with geometry handling.</td>
</tr>
<tr>
<td>Mixed Monte Carlo</td>
<td>Hard and soft events are defined as above or below some angular or energy loss threshold. Hard events are simulated as in detailed simulation. Flight in between hard events follow a compound description of the soft events only.</td>
</tr>
</tbody>
</table>

Table 3.1: Comparison of different computational techniques in charged particle transport.

3.2 Charged particle code systems

3.2.1 PENELOPE

PENELOPE is a Mixed Monte Carlo code system developed by Francesc Salvat at Universitat de Barcelona for simulating coupled electron-photon transport. Energy ranges from 1 keV to 1 GeV can be handled with precision. The original version was released in 1996[3] and has continuously been updated. The latest official release is the 2011 version of the code [36]. The code is managed by OECD Nuclear Energy Agency (NEA). Organizations from countries participating in NEA may request the source code.

The code package is intended to be accompanied by a user written master program handling particle generation, scoring and possibly also geometry. The code is written in FORTRAN 77 standard. The physics model of PENELOPE is a Mixed Monte Carlo for electrons and positrons, but a fully detailed simu-
CHAPTER 3. CHARGED PARTICLE MONTE CARLO

...ation for photons. All collisions are modeled down to microscopic processes. For photons, the following processes are considered:

- Compton scattering (secondary electrons produced),
- Rayleigh scattering,
- Photoelectric absorption (secondary photo-electron and possibly fluorescence and Auger electrons produced),
- Pair production (secondary electrons and positrons produced).

Electrons and positrons, on the other hand, may both undergo

- Elastic scattering via partial wave expansion,
- Inelastic scattering using the Sternheimer-Liljequist GOS model,
- Bremsstrahlung (infrared cutoff set as parameter).

Positrons may also annihilate with electrons. Low energy particles below some cut-off energy (photons, electrons and positrons) are taken out of the simulation and scored as local dose deposit. A specific cascade model is used for relaxation of atoms after inelastic scattering has excited the atomic electrons.

Since the code of PENELOPE is always accompanied by a user written master program, the main mechanics of the simulation loop is presented as it is implemented with the Pegasos code, in section 4.1.

3.2.2 PENH

PENELOPE has been extended to include proton transport. The mechanism mimicks the PENELOPE mechanism for electron transport, but with changes as summarized below. The model has been described in one paper focusing on the general structure and EM interactions by Salvat [35], and a second paper focusing on the implementation of a selection of nuclear reactions, written by Sterpin et al [39].

The elastic EM scattering is the Eikonal scattering model of section 2.2.6. For scattering angles above a threshold, a heuristic extrapolation formula is used. The inclusion of residual cross sections is made in the paper by Sterpin et al using the ICRU 63 data. The model is thus only applicable for a selection of light elements - see section 2.3. Upon finding negative residual cross sections, these are set to zero. Elastic scattering may result in a substantial recoil of the target for light elements. If the recoiling particle is a $H$, it is tracked just as a ordinary proton. If the recoiling particle is some other atom, the energy is absorbed locally.

The inelastic electronic scattering model is the Sternheimer-Liljequist of PENELOPE (see section 2.4 with corrections described earlier. In the paper
by Sterpin et al. [39], the extension to handling inelastic nuclear scattering is made. The strategy in section 2.3.3 is employed. Once again, the method is limited to the scattering off light elements. Also - the energy range of the data is limited.

### 3.2.3 Voxel Monte Carlo (VMC)

The VMC code system was originally developed 1995 for coupled electron-photon transport. [22]. It is based on the codes EGS4 and ETRAN, but includes a set of simplifications. The most notable are using only rectangular voxel geometry (such as the data received from computer tomography), only allowing light elements at low density and restricting the energy range limited to $1 - 30 \text{ MeV}$.

In comparison with EGS4 (at the time a gold standard method for electron beam therapy) the computation time was reduced by a factor of 35 with consistent simulation results.

To use a compound description with the CSDA, the stopping power for soft events has to be determined. The VMC algorithm uses experimental ICRU-data, but corrects it by subtracting contributions for Möller scattering and bremsstrahlung based on elementary theory. The multiple scattering model is not physically motivated, but rather a simplification of the Möller theory that is verified to give acceptable results.

Collision resulting in secondary electrons are assumed to be described by the Möller DCS. It is simplified so much that when sampling secondary electron kinetic energy $E'$, the differential cross section is simplified to be $\propto (E')^{-2}$. Bremsstrahlung is treated similarly. The differential cross section is simplified to behave $\propto 1/k$ where $k$ is the energy of the produced photon. It is a very strong simplification, but has been verified with experiments to give acceptable precision.

### 3.2.4 VMCpro

VMC has been extended to include proton transport and the new code goes under the name of VMCpro [13]. The code runs proton transport in the energy range $0.5 - 500 \text{ MeV}$. The errors in the model is small as long as only transport in human tissue is simulated. I will comment briefly on a number of details in the physics model and what simplifications are made.

Electromagnetic processes are corrected in the following ways in relation to electrons in VMC:

- Ionization is regarded as a separate interaction channel.
- The nuclear contribution to soft stopping power is neglected. ICRU 49 data has been used to derive an analytical formula for material stopping power based on the density of the material.
• No delta rays with energies below the electron absorption energy are produced. Instead, an energy straggling model is imposed on the projectiles in soft stepping to simulate the variance in energy otherwise created by the delta ray emission.

• The multiple scattering for electronic and nuclear interactions are separated through computer experiments based on Geant4 models and fitting curves to the output.

Nuclear processes are handled by first assuming that all matter is water, and then correcting the numbers with relative density corrections obtained from CT pictures. This means that only proton-hydrogen and proton-oxygen has to be modeled with respect to nuclear collisions. Proton-hydrogen cross sections are taken from SAID, and the proton-oxygen collision model is the one described in section 2.5.2.

3.2.5 Geant4

GEANT (GEometry ANd Tracking) was originally a FORTRAN program developed in 1974 at CERN to describe detectors and also perform simulations of particle physics experiments. The underwent substantial development up to version 3.21 extended the functionality further [6].

Version 4 is a new software written from scratch in C++ and maintained by a large international collaboration. First release was in 1998. It covers all components needed for simulation of particle transport and reactions such as geometry handling, material data, physics processes, graphical user interface (GUI) and more. All components are separate C++ libraries and the object oriented programming style allows different research groups to update and maintain the different libraries.

The code is open source and managed by a Collaboration Board and a Technical Steering Board. This development model has led to widespread use in particle physics, medical physics, space research and other areas.

To use the code packages the user has to develop user programs that call upon the different libraries. In some occasions there are competing libraries (different GUI or different physics models) in which case deeper knowledge is required from the user to properly use Geant4.

The physics models are supplied through a set of libraries. The user program supplies a physics list which stipulates what physical laws will govern the simulation. Different physics libraries shows different traits, such as the standard EM module being a Mixed Monte Carlo, while hadronic collisions is a Detailed Monte Carlo.

Geant4, as a full scale and open source Monte Carlo engine has widespread use and is also being used for proton therapy simulations. Other similar advanced, full scale simulation engines that has been used in proton therapy are MCNPx and FLUKA [31].
Chapter 4

Method

This chapter describes the computer experiments and simulations that constitutes the main part of this thesis. The main focus is on the elastic model of the PENH code. The code was supplied by Francesc Salvat in the state as described in [40]. The nuclear models of Sterpin et al [39] was not available. This code was the starting point for investigations as described below. The implementation of the code in the Elekta Monte Carlo environment is described in section 4.1. The investigations started off with comparing the elastic scattering model with others since the eikonal expansion model of PENH was not very well documented and explored in the literature. I present this comparison in section 4.2. After this first comparison, we deduced that the effect of reduced mass in two-body problems must be accounted for. The next investigation was to compare different ways to approximate relativistic and two-body effect on the computational mass. This is the content in section 4.3. After noting this effect, we implemented a reduced mass in the PENH code and conducted a comparative simulation, as described in section 4.4. Finally a benchmark with experimental data was conducted to assess the overall quality of simulation with several present materials and to learn about the challenges in such a benchmark. This is the scope of section 4.5.

4.1 Implementation of PENH code

The PENH code consists primarily of the penh.f FORTRAN program, material database files called PDHEL containing elastic scattering data and a program genelast.f for generating the PDHEL database. It was bundled with PENEOLOPE as it relies on that code for tracking, sampling and more.

The PENH and PENEOLOPE bundle was implemented first on a local Fedora 20 workstation, and later in the Elekta computational cluster environment. The environment constitutes of a GUI called Hermes developed in Java used for defining the geometry and material data in a 3D graphical environment, as well as setting simulation parameters such as scoring, and beam
source definitions. It connects to the second layer called Pegasos through simulation, material and geometry files (*.sim, *.mat, *.pmst, *.pgeo0) either in a local installation, or at the central cluster.

![Figure 4.1: The typical workflow using the Hermes and Pegasos software. Simulations are managed through the Hermes GUI, and then submitted to a remote computer for parallel computing. The results from the separate Pegasos simulations are combined into a total result file and returned for visualizing in Hermes or post processing in MATLAB.](image)

Pegasos is a C++ application designed to work with MPI (Message passing Interface) for running parallel simulations and later combining the result files (*.out) into a total simulation answer (*.tot). When running Pegasos, it handles the particle track, the geometry (supporting many different geometry formats), the scoring and the pseudo-random number generation. PENELOE FORTRAN subroutines are used for sampling step lengths and scattering events. The tot-file format is suitable for post processing in external software such as MATLAB, but may also be put back into Hermes for visualizing the results.

Implementing PENH into this simulation environment means that adapting the Pegasos program to support new particle kinds, adding appropriate options to the Hermes GUI and adapting PENH when needed to properly integrate with Pegasos. The following adaptions were made: Pegasos scoring demands that “energy deposit” should be returned from scattering subroutines instead of “energy loss of primary particle” which is the PENELOE standard. Calls to the PENELOE random number generator was changed to the external Pegasos random number generator.
4.1. IMPLEMENTATION OF PENH CODE

After integration with PENH, the Pegasos software works as in normal PENELOPE mode. The only difference is that PENELOPE subroutine calls are replaced by PENH subroutine calls. Typically, they are similar, but has an $H$ appended. The JUMP subroutine is replaced by the JUMPH subroutine of PENH. The standard simulation process, for a slave process not managing the MPI, is presented in the text below, and illustrated by figure [4.2].

1. Read options from the simulation and geometry files and initialize the random number generator.

2. Initialize PENELOPE and PENH e.g. load material database libraries and prepare interpolation tables.

3. Run the simulation loop for as many primary particles as desired. This is the main body of the simulation.

   • Generation of primary particle is made according to the chosen particle source.
   
   • The “locate” function makes sure that the initial position is known by the geometry handling libraries.
   
   • The PENELOPE subroutine CLEANS simply sets the number of particles in the secondary stack to 0. The START validates that the generates particle has an energy accepted by PENELOPE and initializes helping variables, such as ensuring that the next simulation step is a soft one.
   
   • JUMP is the subroutine for sampling segment length until next collision. It samples the total cross sections at the current energy.
   
   • Moving the particle is handled by the geometry libraries. If the particle crosses fluency scoring planes this is registered. The subroutine also return flags for if the particle leaves the simulation or moves into a new material.
   
   • The subroutine for sampling energy loss, deflection and production of secondaries is the KNOCK subroutine. For charged particles, every second call to KNOCK is a “hinge” which represent a collection of soft scatter events. Every second call simulates a hard event. In connection with this subroutine, the dose deposit is scored.
   
   • When a primary particle track has ended, secondary particles produced earlier in the process are popped from the stack and simulation of these is carried out.

4. Print simulations result to the process result file.
4.2 Elastic Scattering Model

To compare the eikonal expansion scattering model and its implementation in PENH, a set of elastic scattering models were implemented in MATLAB. The implementation followed the formulas in the PENH paper [35], thus using the computational mass $M = \gamma M_1$ in many cases. The classical cross section was implemented as a purely classical calculation in the center-of-mass-frame, and thus, the classically reduced mass was used. The one-photon-exchange model only use rest masses in the expressions. The models were:

- Rutherford cross section, using $M = \gamma M_1$
4.3. REDUCED MASS EFFECT ON EIKONAL CROSS SECTION

- Born cross section, using $\mathcal{M} = \gamma M_1$
- Eikonal expansion to first order cross section, using $\mathcal{M} = \gamma M_1$
- Classical two-body scattering cross section, using $\mathcal{M} = \mu$
- One-photon-exchange cross section, using rest masses $M_1$ and $M_2$
- Interpolating data from the PDHEL database, using $\mathcal{M} = \gamma M$

All these models but the PDHEL database are described in chapter 2 of this thesis.

The PDHEL database contains a table of differential cross sections, cross sections and transport cross sections calculated with the genelast program using the eikonal expansion model. The differential cross sections are supplied in the center-of-mass frame and reduced, in the sense that both spin-correction-factor and the pre-factor $(2MZZ_0e^2)^2$ are excluded. These effects are accounted for at simulation run-time, so when interpolating data for this comparison, this had to be accounted for. The spin-factor is omitted in all plots in my comparison, but the other pre-factor has been post-multiplied to the PDHEL tabulated values.

These models were plotted for a selection of elements and scattering angles at a set of different kinetic energies determined in the lab frame.

Since the PDHEL data are tabulated for the center-of-momentum frame, they have to be transformed to the lab system where I make the comparison. The projectile energy in the lab- and center-of-mass frame differ, and this has lead to minor errors when PDHEL data was not present for the energy under consideration. The closest available energy has been used, and the error in selection of energy is in general less than one percent in the center-of-mass frame.

By including the classical model in the comparison, we may test the assumption that the eikonal model is a semiclassical one. Inclusion of the one-photon-exchange model lets us test the approximation of static potential. The Rutherford and Born cross sections are included simply for checking the validity and consistency of calculations. By testing the PDHEL database together with a separate implementation of the eikonal model we may validate the computations further.

4.3 Reduced Mass Effect on Eikonal Cross Section

The mass models under comparison are:

$\gamma M$ - the relativistic mass of the projectile in the center of mass frame. This is the mass used by Salvat in the PENH code as standard.
\[ \gamma \mu = \gamma M_1 M_2 / (M_1 + M_2) \] - the reduced mass of the projectile, but corrected relativistically. This is the “natural form” if combining a two-body problem and relativity.

\[ \mu^* = \gamma_1 M_1 \gamma_2 M_2 / (\gamma_1 M_1 + \gamma_2 M_2) \] - the classically found “reduced mass” assuming both the projectile and the target are to be treated as relativistic particles.

Since these masses are functions of incident proton kinetic energy, they were all computed with a MATLAB script and compared, including Lorentz transforming to the center-of-momentum frame and finding relativistic \( \gamma \) in this frame. The eikonal differential cross section was thereafter calculated for the two mass options \( \mu^* \) and \( \gamma M \) above, with the MATLAB script from section 4.2.

### 4.4 Reduced Mass Effect on Simulation

In this step, I compared the effect of changing the computational mass used for elastic scattering, in the simulation.

Since the symmetrical form \( \mu^* \) is slightly more complicated (involves adjusting the factor by the current velocity and target mass and so on) I used a more pragmatic way, which is more simple to implement in the code.

First, I changed the program `genelast.f` which generate the PDHEL database, to use the computational mass \( M = \gamma \mu \) in all cross section calculations. Then I changed the subroutine `HELaR` in `penh.f` which loads the PDHEL database at run-time to use the same computational mass. With these two changes, the mass should be replaced in all elastic collisions.

To compare the performance change with this alteration, I simulated protons penetrating into water. A parallel beam with radius 0 and kinetic energy of 180 MeV is incident on a cylindrical water phantom of length 30 cm and radius 20 cm. Two scoring meshes are in use: one scoring integrated depth dose (cylinder of radius 20 cm, length 24 cm, 480 scoring bins in length-direction). The second scoring cylinder has radius 1.6 cm, length 24 cm, 480 scoring bins in length direction and 480 scoring bins in the radial direction. The scorers kept track of mean deposited energy in the scoring volumes.

Since the initial beam is narrow (radius 0 cm), the central axis dose curve will have a prompt fall off as the beam thickens and spreads radially. Because of this, the central-axis depth-dose curve will depend strongly on the scoring volume radius used. Central-axis depth-dose distribution and beam range will be calculated based on several different scoring volume radii.
4.5 **Benchmark with Experimental Data**

The simulation benchmark is based on the depth-dose data measured by Kimstrand et al. [23], which was measured at the The Svedberg Laboratory (TSL) in Uppsala. The full setup and measurement procedure is described in the mentioned reference, but will be described briefly below.

The TSL proton beam setup is scanned beam, meaning that a full field used in therapy is made up of a large number of small elementary beams. Each elementary beam is generated by a proton beam pulse from the accelerator, then deflected by a scanning magnet - first on in the x-plane, and later one in the y-plane. This aims the beam in the lateral plane. After this, a range-shifter made out of Plexiglas slabs reduce the energy of the beam so that the Bragg peak may be localized as desired in the direction of propagation. Gantry parts after the x-scanning magnet is movable to reduce the size of the setup.

A full field of $14 \times 14$ cm was incident on a water phantom of size $15 \times 15 \times 40$ cm. A Hi-pSi diode was used to measure the dose along the central axis as a function of penetration depth. The normalization of the measurement is relative to a reference dose, and not absolute. The data include beams range shifted by 0, 25, 50, 75 and 100 mm PMMA ("Plexiglas").

The energy spectrum of the beam, was characterized to have a normal distribution of mean 180.4 MeV and standard deviation of 0.23 MeV by comparing with results from pre-calculated Geant3 simulations in combination with a TSL-developed Monte Carlo engine producing the beam phase space.

Instead of modeling the scanned spot system in detail, I used a divergent beam model which is a standard component in Pegasos. It allows for a normally distributed energy spectrum just like the one determined from the accelerator. To model the spreading of the beam, an initial thickness equal to the initial width ($1\sigma$ in the beam characterization) of the beam was used. The divergence of the beam was set so that it had a $14 \times 14$ cm cross section when hitting the water phantom. In other words - no magnets have been modeled.

Since the diode size is missing in the specifications, a set of different scoring volumes are used. A typical diode size should correspond to a scoring volume of about $(1 \text{ mm})^3$.

Since data is not absolutely normalized, we may only draw conclusions about the shape of the depth-dose curve. To make the simulations comparable to the measurement data, a range for normalization was chosen, and the reference data was scaled so that the integral over this range was the same for reference data as for simulations. The range was chosen after performing simulations and inspecting results, with the aim at choosing some robust region where the result should be accurate.
Figure 4.3: The TSL measurement setup (top part of figure) is composed of an accelerator (far left), two scanning magnets for the x- and y-plane directing of the beam, and a set of Plexiglas slabs for shifting the range of the beam. The rightmost part is movable to follow the direction of the first scanning magnet. The beam is then scanning to build up a rectangular homogeneous total field. In the simulation setup (lower part of figure), this was modeled by a rectangular divergent field incident on slabs that are stationary. The numbers in the bottom is in units of cm.
Chapter 5

Results

This chapter presents the results obtained in the computer simulations and computations described in chapter 4.

5.1 The Eikonal Scattering Model

Comparison of the different elastic scatter models under consideration yielded plots for a selection of elements and energies. These are presented in this section. The diagrams present elastic differential cross sections for scattering off hydrogen, aluminium and gold at the energies 0.1, 10 and 1000 MeV, since these numbers correspond to the plots as presented in [35]. Please note the typo in the plots in [35] - the energy labeled 1 MeV corresponds to calculation of 10 MeV.

For collisions with hydrogen (figure 5.1), there is a big fall off in cross section for scattering angles greater than 90°. This originates from the fact that back scattering is almost prohibited when the projectile and target mass are similar. The cross section for one-photon-exchange scattering and classical computations differ from the other cross sections substantially. The difference is a multiplicative factor for large angle scattering. For small angle scattering the Rutherford, classical and one-photon-exchange scattering diverge in contrast to the Born, eikonal and PDHEL cross sections. For high energy collisions, there is a discrepancy between the classical and the one-photon-exchange scattering for intermediate angles. At low energy, there is a substantial difference between the eikonal and the Born model for scattering around the screening angle; the eikonal model is more heavily screened than the Born model for screening angle scattering.

For aluminium targets (figure 5.2), the big difference between one-photon-exchange, classical and the other models is gone. The difference between the eikonal and Born models are larger. It is also clear that for low energy scattering, the classical and the eikonal models coincide in the region where the born model is as most differing from the eikonal model. At 1000 MeV and
large angle scattering, the one-photon-exchange cross section shows a small rise in comparison to the Born cross section.

When looking at scattering off the heavier and more charged gold atoms (figure 5.3), the trend from scattering off aluminium has been more pronounced. The region for which the Born and eikonal models diverge is the region for which the eikonal model reproduce the classical scattering model. The phenomenon is more pronounced for low energy scattering. At higher energies, the eikonal and Born models still show the same coincide as for the lighter elements. The small angle relative rise of the one-photon-exchange cross section is present for gold as well as for aluminium.

5.2 Reduced Mass Effect on Eikonal Cross Section

The results from comparing the different models for computational mass is most easily illustrated in the plots for computational mass in relation to the incident proton kinetic energy. These are found in figure 5.4. The difference between the symmetric relativistic reduction ($\mu^* = \gamma_1 M_1 \gamma_2 M_2 / (\gamma_1 M_1 + \gamma_2 M_2)$) and the relativistic corrected classically reduced mass ($\gamma_1 \mu = \gamma_1 M_1 M_2 / (M_1 + M_2)$) is comparably small, and vanishes both for light and heavy elements. It has a maximum for elements that have different masses, but for which the kinetic energy in the center of mass frame is comparable to the rest mass. For $Z=1$ i.e. proton-hydrogen collisions, the mass increases slowly with kinetic energy. In collisions with heavier particles the mass increase faster. For heavy elements, all three expressions are very similar.

The effect of replacing the computational mass used in PENH ($M = \gamma M$) with the asymmetric expression ($M = \gamma \mu$), the cross sections does not change very much, as seen in figures 5.5–5.7. For high energy ($E \geq 10$ MeV), the effect is simply a multiplicative factor, but for lower energies, the behavior is more complicated. Scattering below the screening angle is less affected by the change in computational mass, than scattering above the screening mass. Around the scattering angle, there is a relative increase in the quotient between the two cross sections. This pattern holds for scattering off the lighter elements such as hydrogen and lithium. There is a strange behavior for scattering off gold at large angles. Since there are oscillations in the differential cross section, it is sensitive to perturbation.

5.3 Reduced Mass Effect on Simulation

The effect on simulation of changing the computational mass is presented in two ways: the range along the central axis and the distribution in lateral planes at different depths.
When looking at lateral plane distributions, we see that the reduced mass simulation gives a higher dose deposition close to the central axis. The penetration depths are chosen to be at distances as follows:

- In the Mid-depth region (12.5 cm)
- At the Bragg peak (21.5 cm)
- In the distal fall off (22.0 cm)

The central axis dose distribution differs slightly depending on the scoring volume used to define “central axis”. To illustrate this, a set of different “central axis scoring volumes” were used. Their respective depth dose curves are displayed in figure 5.9. Invariably with the scoring volume radius, the dose is the same for shallow penetration, but it decrease for most scoring volumes after some distance. Simulation using the reduced mass shows a slower falloff.

The ranges for the two simulation does not change much - neither as a function of mass model used, nor as a function of scoring volume. The ranges found varies between 21.623 and 21.633 cm. A comparison, a beam of energy 180 MeV should by PSTAR have a range of 21.628 cm. The maximum difference is thus 0.02% from the reference value of PSTAR.

5.4 Benchmark with Experimental Data

The benchmark simulations yielded depth-dose curves for the different range-modulated beams. These are presented below in figures 5.10 and 5.11. The effect of scoring volume size clearly had an effect on the noise in the scoring; a large scoring volume yields more reliable curves than a smaller volume. The range of the beam is not very dependent on the scoring volume used, as seen in table 5.1. The entrance dose is higher for the simulations than for the reference data - especially in the 0 range-shifted beam, where the dose in simulation shows an initial fall off and data indicates an initial build up. These phenomenon are easier to see in figure 5.11.

The range of the beams are slightly longer than the reference data ranges. Since the dependency on scoring volume is so weak and the statistical noise is large for very small voxel size, see figure 5.10 I calculate the errors in range based on the 4 mm squared scoring voxel. The error in range is 2 – 3 mm and seems to increase with range shifter thickness. The relative error ranges 1 – 3% and shows suggests the same.

Normalization was performed for the 0 mm thickness range-shifted beam for the penetration depth between 6 and 17.5 cm penetration. In this region, the errors in nuclear effect should be reduced (lower energy of the protons after initial penetration) and the Bragg peak should be avoided. Judging from the levels of the Bragg peaks, the normalization of the reference data to gives a slightly too low level of dose deposition.
### Table 5.1: Ranges of beams in simulations for different scoring voxel sizes, in comparison with the measurement data, in units of cm.

<table>
<thead>
<tr>
<th>Reference data</th>
<th>Scoring voxel cross section area</th>
<th>Simulated range</th>
<th>Error</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<td>(2 mm)&lt;sup&gt;2&lt;/sup&gt;</td>
<td>(4 mm)&lt;sup&gt;2&lt;/sup&gt;</td>
<td>(8 mm)&lt;sup&gt;2&lt;/sup&gt;</td>
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<td>18.55</td>
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<td>10.08</td>
<td>10.08</td>
<td>10.08</td>
</tr>
</tbody>
</table>

### Table 5.2: Ranges of beams in simulations for different scoring voxel sizes, in comparison with the measurement data, in units of cm.

<table>
<thead>
<tr>
<th>Reference range [cm]</th>
<th>Simulated range [cm]</th>
<th>Error [cm]</th>
<th>Relative error</th>
</tr>
</thead>
<tbody>
<tr>
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<td>21.70</td>
<td>0.306</td>
<td>1.4%</td>
</tr>
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<td>18.55</td>
<td>18.75</td>
<td>0.201</td>
<td>1.1%</td>
</tr>
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<td>15.86</td>
<td>0.272</td>
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</tr>
<tr>
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<td>12.98</td>
<td>0.335</td>
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</tr>
<tr>
<td>9.75</td>
<td>10.08</td>
<td>0.328</td>
<td>3.4%</td>
</tr>
</tbody>
</table>
5.4. BENCHMARK WITH EXPERIMENTAL DATA

Figure 5.1: The elastic scattering differential cross sections for hydrogen collision: Rutherford (■), Born ( ), classical ( ), eikonal ( ), one-photon-exchange ( ) and PDHEL ( ). Note that the PDHEL data is missing for 1,000 MeV. Plots to the left are absolute values. The figures to the right corresponds to data divided by the eikonal cross section.
Figure 5.2: The elastic scattering differential cross sections for hydrogen collision: Rutherford (--), Born (-----), classical ( ), eikonal ( ), one-photon-exchange ( ) and PDHEL ( ). Plots to the left are absolute values. The figures to the right corresponds to data divided by the eikonal cross section.
Figure 5.3: The elastic scattering differential cross sections for scattering off gold: Rutherford (- - -), Born (-----), classical ( ), eikonal ( ), one-photon-exchange ( ) and PDHEL ( ). Plots to the left are absolute values. The figures to the right corresponds to data divided by the eikonal cross section.
Figure 5.4: Computational mass dependency on the kinetic energy. The different computational masses used are $\mu^* = \gamma_1 M_1 \gamma_2 M_2 / (\gamma_1 M_1 + \gamma_2 M_2)$, the relativistic corrected classically reduced mass $(\gamma_1 \mu = \gamma_1 M_1 M_2 / (M_1 + M_2)$ and the relativistically corrected projectile invariant mass $\gamma_1 M_1$. 
Figure 5.5: Relation between reduced-mass $\frac{d\sigma}{d\Omega}$ and full-mass $\frac{d\sigma}{d\Omega}$ differential cross section for collisions with hydrogen in the center-of-mass frame shown on left hand y-scale. Quotient $\left(\frac{d\sigma_{\text{red}}}{d\Omega}\right) / \left(\frac{d\sigma_{\text{full}}}{d\Omega}\right)$ on right hand scale.
Figure 5.6: Relation between reduced-mass and full-mass differential cross section for collisions with lithium in the center-of-mass frame shown on left hand y-scale. Quotient on right hand scale.
Figure 5.7: Relation between reduced-mass and full-mass differential cross section for collisions with gold in the center-of-mass frame shown on left hand y-scale. Quotient on right hand scale.
Figure 5.8: Dose distribution in the lateral plane. The plots represent cross sections at 12.5 (top left), 21.5 (top right) and 22.0 (bottom) cm penetration depth. The solid line represent the simulation with full mass, the dots denote the reduced mass simulation.
5.4. **BENCHMARK WITH EXPERIMENTAL DATA**

Figure 5.9: Central axis dose-depth curves for full-mass and reduced-mass simulations. The solid lines represent full mass simulations. The dots represent data points for the reduced mass simulation. The curves correspond to a central axis scoring volume that has a radius of (top to bottom) 200, 16, 8, 4, 2, 1 mm.

Figure 5.10: Simulation (curves) and experimental data (markers) for different range shifter thickness (0, 25, 50, 75 and 100 mm Plexiglas). Scoring voxel size is $1 \times 1 \times \frac{1}{2}$ mm.
Figure 5.11: Simulation (curves) and experimental data (markers) for different range shifter thickness (0, 25, 50, 75 and 100 mm Plexiglas). Scoring voxel size is $140 \times 140 \times \frac{1}{2}$ mm.
Chapter 6

Discussion

This chapter discusses the results presented in chapter 5. The first topic is the behavior of eikonal scattering model as implemented in the PENH code in comparison with other elastic scattering models. Secondly, it deals with the effect of using a reduced projectile mass in the calculation of the eikonal cross section its effect on simulation results. Third and lastly, the benchmark with experimental data is discussed.

6.1 The Eikonal Scattering Model

The PENH database covering elastic cross sections is based on the eikonal scattering model. By implementing the eikonal model in a MATLAB together with a set of other models we hope to understand this model. Analysis of the assumptions underlying the eikonal model and inspection the differential cross sections for the different models provides insight on whether the static potential assumption holds, what the screened regime looks like, and uncovers the eikonal expansion models relation to classical assumptions.

The most striking insight from comparing the models is that the classical model and the one-photon-exchange model produce cross section that differ from all other models by a multiplicative factor in the large angle scattering regime. This is seen clearly in figure 5.1 showing the cross sections for scattering off hydrogen, where the projectile and the target have similar masses. The factor can be explained by the fact that different computational masses have
been used for the different models. The computational mass enters most of the expressions for cross section as a power of 2, so changing the computational mass changes the cross section. In the classical model, the classically reduced mass ($\mathcal{M} = \mu$) has been used. For the one-photon-exchange model, only rest masses ($M_1$ and $M_2$) are used, but the formalism takes the two body nature of the problem into account. The other models (Born, Rutherford, eikonal and PDHEL) use the relativistic mass ($\mathcal{M} = \gamma M$). By changing the computational mass, this discrepancy between the two groups of models should disappear.

When comparing the plots further, there are three clear regimes in scattering angels: Forward scattering (angle less than the screening radius), scattering around the screening angle, and large angle scattering (angle greater than the screening radius). The eikonal model is compared to the other models in the list below.

**Compared to the Rutherford cross section** The Rutherford cross section is not screened, which means it diverge for small angles, opposed to the behavior of the eikonal model. For larger angles the two cross sections coincide.

**Compared to the Born cross section** The Born cross section differ by a multiplicative factor at forward scattering. The eikonal cross section is more strongly screened. This effect is larger for low energies. When scattering around the screening angle, the difference has a maximum. This discrepancy increases with the charge of the atom. For large angle scattering, the two cross sections coincide.

**Compared to the Classical cross section** For forward scattering, the classical model diverge, which differ from the eikonal model. As long as any of the screenings are penetrated (scattering around the screening angle and strong scattering), the classical and the eikonal cross section coincide, apart from a multiplicative factor arising from using different computational mass.

**Compared to the one-photon-exchange cross section** The one-photon-exchange model diverges for forward scattering, as expected from a model in which the interaction potential is not screened. This is the same behavior as Rutherford scattering. For scattering around the screening angle, the behavior differs - only for scattering above all three screening angles do the models coincide. The one-photon-exchange model deviates from the other models for high energies. This is an indication that the static potential approximation may fail for high energy scattering.

**Compared to the PDHEL cross section** In these plots, no difference can be seen between the pretabulated PDHEL database and the MATLAB-computed eikonal cross section. This is a validation of the code.
6.2. SIGNIFICANCE OF USING THE REDUCED MASS IN COMPUTATION

Based on these observations we may say that the eikonal model in PENH shows no clear reasons to be rejected as long as the mass used in computations is adjusted properly. It is an in-between model for the classical and the Born cross sections. When the scattering process penetrates all screening, it behaves classically and quantum mechanical alike - just like the Rutherford cross section. For smaller angles, it behaves classically in the sense that it captures the scattering effects arising from the Yukawa sum potential. For the small angle scattering, it is more strongly screened than any of the other models.

Model errors are rather coming from other approximations such as the spin decoupling or from treating the Klein-Gordon as a mass modified Schrödinger equation than coming from the treatment of that very problem with the eikonal scattering model.

6.2 Significance of Using the Reduced Mass in Computation

As discovered in the comparison of different elastic cross sections, the mass used in computations must be adjusted to reproduce the classical limit. The mass model of choice must take into account both the relativistic effects as well as the classical two-body reduction of mass. Possible options for computational masses to use are found in \( \mu^* \). From theoretical considerations, the \( \mu^* \) mass is the most reasonable - it takes both effects into consideration and treats the target and projectile on equal grounds. The other two models \( \gamma M \) and \( \gamma \mu \) may be seen as approximations.

The plot showing computational mass dependency on kinetic energy shows that the choice stands between \( \mu^* \) and \( \gamma \mu \), since \( \gamma M \) differ considerably. The two options should produce similar results as long as the kinetic energy of the projectile is small compared to the target rest mass.

6.2.1 Eikonal Model Dependency on the Computational Mass

For high projectile kinetic energy, (10 MeV - 1 GeV), the eikonal cross section dependency on mass is simply through a multiplicative factor. This is seen in figures 5.5, 5.6 and 5.7. This factor is very close to \( M^2 \) for 10 MeV, and quite close to this value for 1 GeV. This reduction in cross section thus corresponds to the reduction as described by table 6.1. The \( M^2 \) factor enters the cross section through the eikonal phase derivative \( d\chi/db \) in equation 2.3, that derivative also introduce higher powers of \( M \) into the cross section. If the only dependency on \( M \) was through the square, then the quotient in said figures be equal to the classically reduced mass.
Table 6.1: Classically reduced masses $\mu$. The reduced mass $\mu = M_1M_2/(M_1 + M_2)$ where $M_1 = M_p$ is the proton mass and $M_2$ is the mass of the target atom. This factor $(\mu/M_p)^2$ describes the change eikonal cross section when changing from $M = \gamma M_1$ to $M = \gamma \mu$.

<table>
<thead>
<tr>
<th>$Z$</th>
<th>$M_2/M_p$</th>
<th>$(\mu/M_p)^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.001</td>
<td>25%</td>
</tr>
<tr>
<td>3</td>
<td>6.890</td>
<td>76%</td>
</tr>
<tr>
<td>79</td>
<td>195.544</td>
<td>99%</td>
</tr>
</tbody>
</table>

For 0.1 MeV, the differential cross section dependency on mass is slightly more complicated. For forward scattering, the cross section is higher than the $M^2$ factor explains for hydrogen and lithium. In hydrogen and lithium collisions, the cross section is still high even in the screening angle scattering. This behaviors may be explained by the screening angle increase as the computational mass is reduced.

At the even lower 1 keV energy level, the model seems to break down. A discontinuity is seen in the cross section for collisions with gold and similar tendencies are seen in collisions with hydrogen and lithium. It is not advised to use this model for such low energy levels without further validation of the model. This will not impose limitation of the usability of the PENH code however - typically, spatial resolution of 0.1mm will be enough, and removing protons with 0.1mm residual range in water corresponds to a cutoff energy of about 2 MeV.

### 6.2.2 Simulation Dependency on Computational Mass

The comparative simulation shows that a reduced mass in the elastic model leads to a higher dose density along the central axis. This seems reasonable as the reduction in cross section decrease the scattering power.

The range of the beam is affected just slightly, so this change should be neglected for all practical reasons. The change is of the order 0.02%, where the error in reference values constituted by the PSTAR database may be a factor 100 larger. One should note, however, that the simulations show good agreement to PSTAR, which is a sign that the implementation of the code is correct.

An extra insight produced in this simulation is offered by figure 5.9. The range, defined by a 80% falloff after the Bragg peak, shows no strong dependency on the scoring volume used. As when the beam is collinear enough, the scoring volume used does not affect the range appreciably. One can suspect that the discrimination between central axis- and integrated depth dose is more important when the incoming beam has a greater distribution of different initial directions as well as an initial diameter greater than 0.
6.3 Challenges with Benchmarking Monte Carlo Simulations

The simulation of the TSL measurement setup shows discrepancies to the actual measured data. There are two dominating errors present - the range of the beam is longer than the range of the measured data, and the dose at the beginning of the depth dose curve (shallow penetration) is relatively high which ruins the normalization of the curves.

6.3.1 The Error in Range

The simulation overshoots the measurement data in range by approximately 1-3%. Since the inelastic scattering model is adjusted to PSTAR data, and the error present in PSTAR data is of this order of magnitude, it is difficult to assess the source of error. A few sources are possible:

One probable error source is that the kinetic energy spectrum for the incident protons is off from the actual energy spectrum. By PSTAR, the 180.4 MeV main energy component should have a range of 21.71 cm. This is a slight bit off from both the simulation result (just slightly, and we expect this since the beam is not monochromatic), but quite far off from the measurement range. The energy used is the energy determined to fit with the simulations by Kimstrand [23]. If the stopping power and range in any of the software used in that simulation does not correspond to the PSTAR values, discrepancy is to be expected. We can at this stage not determine if this difference between measurement and data is an error in the model or in the energy used in the simulation. An independent energy measurement is needed to draw final conclusions.

More errors are possibly introduced at other points. The modeling of the beam source is very crude (path length through the range shifter differ for central and lateral parts of the beam, for example) to name one. The density of the Plexiglas is also a source of possible error, since this is a component with large effect to the beam. The energy shift needed at the source to correct the 3 mm range difference is about 0.06 MeV so the range shifter is a sensitive part to model correctly.

As a final remark, the range error accepted at Massachusetts General Hospital, where a similar (but more complete) TOPAS benchmark was conducted [42], is +1/-2 mm, so the +3 mm error present here is unacceptable for those criteria. By adjusting the energy in the simulation, we should be able to drastically reduce the range error though.

6.3.2 The Entrance Dose and Normalization Error

When looking at the low-noise depth-dose curves in figure 5.11 one can note that the entrance dose in simulation is higher than the reference data. This
is especially true for the long-range beam where the protons have a higher energies at entry.

This is expected considering that the inelastic nuclear model deposit all dose locally instead of producing secondaries. Secondaries would propagate and smear the dose deposit into deeper penetration. This behavior also contaminate the normalization of the reference data. Since one is advice to use the plateau region for normalization (the Bragg peak shows too large gradients to be well suited for this), the integral is slightly too large in this region. Relatively speaking, the Bragg becomes low, and this is what we see in the plots.

In the TOPAS benchmark mentioned above, the entry dose in simulation was found to overestimate the entrance dose by $1 - 2\%$. While the overestimation in this study is far greater, one can still note that the much more complicated model of Geant4 still overestimate the entrance dose considerably.
Chapter 7

Conclusion and Outlook

The work with finding efficient tools for simulation of proton transport is essential to support the increased research and investment into proton beam therapy.

Available software frameworks such as Geant4 are made more easy-to-use by the TOPAS initiative and this is an important step forward, but that software still operates through text files for input/output. This is a step backwards in the simulation workflow for those who use 3D modeling and graphical user interfaces. At Elekta, the PENH extension to PENELOPE is a good opportunity to extend simulation capabilities to the PBT area while still maintaining existing workflows.

This thesis has explored some aspects of the models underlying the PENH code and thus scraped at the surface in terms of building knowledge of proton simulations at Elekta. The conclusions to this are presented below. Further work has to be conducted to fully draw conclusions about to what extent the PENELOPE approach to proton transport Monte Carlo is a successful one.

7.1 Elastic Scattering Models: Pure EM and Residual Scattering

The eikonal expansion model with a Yukawa-sum potential is an in-between model behaving like a classical model for large and intermediate angle scattering and displaying Born-like screened behavior for small angle scattering. This is expected from theoretical considerations and also found when comparing the calculated cross section with other models. Errors arising from using this model for elastic proton scattering is more likely to arise from the spin-decoupling assumption when simplifying the scattering problem than from using the eikonal expansion to a nonrelativistic Schrödinger scattering problem.

When comparing the eikonal expansion model with other models, the implementation of the eikonal model in the PENH code seems to treat the mass
erroneously. Using a reduced mass as done in this thesis has shown to have a
limited effect to the propagation of protons through water by increasing the
scattering power.

Further exploration of the elastic model in PENH should either look at
implementing residual cross sections as described in the original PENH paper
[35], but an alternative way forward could be to look at the effect of having an
non-pointlike nucleus, leading to the need for other potential parameterization
than the Yukawa-sum model. To further develop an elastic scattering model
does on the other hand not constitute the prime interest for future research,
as the model errors in the inelastic model is of greater concern.

7.2 Inelastic Scattering Models: Electronic and
Nuclear Scattering

The inelastic scattering model of PENH is today separated into two parts -
the scattering off atomic electrons and the scattering off the nucleus. This
separation of interaction modes is in line with how other simulation codes
design the structure of the program. The model for scattering off atomic
electrons have been examined in detail in the electron scattering case, and
been even more improved through the work of Salvat with PENH [35]. One
should not expect to find major errors originating from this model. In contrast,
the absorption model used for nuclear interactions is very crude and must be
improved for the code to be useful in applications. This was indicated in [35]
and verified through this thesis.

The following two approaches are suggested for future work:

1. Implement a model along the lines of inelastic nuclear scattering off
   oxygen in VMCpro. The differential cross sections for production of
   secondary protons, short-range and long-range secondaries should be
deducible to some approximation from available data.

2. Construct a more complete model utilizing proton transport mechanism
   for all charged fragments like in the PENH extension of Sterpin et al,
   but take cross sections from some evaluated data like TALYS.

7.3 Benchmark to Data

The comparison of simulation to experimental data made in this thesis illus-
trates how difficult it is to properly make a benchmark. Detailed knowledge
of the experimental setup is needed to fully understand what kind of errors
are present.

The errors between simulation and experiment are quite large. They at
least partially originate from the crude nuclear inelastic scattering model,
but they also come from the limited knowledge of the energy spectrum of
the proton beam. Finally, the uncertainty in the range calculations of the
reference data will introduce errors in simulation results. Independent emergy
measurements and a more thorough treatment of the model adjustment to
reference data might overcome these errors. A more complete modeling of
the experimental setup, such as properly constructing the total field from
elementary beams of using a proper phase space as input to the simulation
might also reduce error.

Further benchmark using inhomogeneous phantoms or describing the lat-
eral plane is also of use to determine the simulation quality, since even a quite
rudimentary model should be able to reproduce the range of protons. It is
by showing agreement in the more complicated cases that any Monte Carlo
proton transport model might excel.
Bibliography


[31] S D Randeniya, P. J. Taddei, W. D. Newhauser, and P. Yepes. Intercomparison of Monte Carlo Radiation Transport Codes MCNPX, GEANT4,


