Monte Carlo Simulation of Proton and Neutron Transport Based on the PENELOPE Code

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Abstract

This master thesis is a continuation of previous work done at Elekta Instrument AB for the joint objective of developing the Monte Carlo simulation program, Pegasos, for proton therapy. For this purpose, neutron transport with nuclear interactions has been implemented into the Pegasos framework. Nuclear data is provided from the TALYS nuclear code and for neutron-hydrogen nuclear interactions, the ENDF database, through the Los Alamos LA150 library, is used. Furthermore, angular distribution of neutron elastic scattering is implemented as well as neutron radiative capture to deuterium.

Benchmarks of the Pegasos software, with implemented neutron as well as the initial Pegasos code, were executed against the Monte Carlo program Geant4 and against experimental data provided from Proton Therapy Center (PTC), Prague, and The Svedberg Laboratory (TSL), Uppsala.

The results show a relatively good agreement for all benchmarks, except against PTC resulting from uncertainties in the proton beam’s energy spectrum. A small deviation of the Bragg peak’s position against Geant4 may result from the different databases used, which is called for further investigation. In addition, further implementation of angular distribution for proton nuclear reaction, including hydrogen and helium, and transport of heavier charged particles is recommended in future endeavours with the objective of simulating clinical cases.
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Chapter 1

Introduction

In this section an introduction to proton therapy is first presented, followed by a presentation of Elekta Instrument AB, where this thesis has been conducted. Ultimately, earlier works and the aim of this thesis is described.

1.1 Proton Therapy

The interest in proton therapy has drastically increased in the last couple of years. In the *Physics in Medicine and Biology* journal there are, at the moment of writing, 476 hit results when searching for “proton therapy” where 60% are written in the last five years [1]. In addition, of the total 1584 hits on proton therapy in the *Medical Physics* journal, 34% are written in the last 5 years [1]. This increase in interest is mainly due to advances in clinical studies and technological development which has been achieved in the last decade, making the field more commercial.

The proton therapy concept was initialized after the method proposed by Robert R. Wilson in 1946 [2]. Wilson, also known for his participation in the Manhattan Project building the atomic bomb, proposed that charged particles could be favourable for the treatment of deep-seated cancer cells due to their characteristic dose distribution when interacting with matter. In comparison to the gamma, whose dose delivery in matter decreases as a function of the penetration depth, charged particles manifests a peak dose just before the particle comes to rest, known as the Bragg peak. An illustration of the dose delivery differences between a proton of energy 170 MeV and a gamma of energy 1.25 MeV is presented in figure 1.1. Thus by adding proton beams of different energies the dose can be maximized at the cancer cell, the target volume, while the dose on surrounding healthy tissues is minimized. This is a key advantage of proton, or other heavier ion, therapy in comparison to traditional radiotherapy.

The first patient treated with proton beams were at the Lawrence Berkeley Laboratory in California, 1954 [3]. Since 1954 to the end of 2014, more than
CHAPTER 1. INTRODUCTION

Figure 1.1: Comparison of the dose deliver between a proton and a gamma in water. The dose is normalized to the maximum dose delivery point for the proton and the gamma respectively.

118,000 patient had been treated with proton therapy worldwide [4]. In the Scandinavian countries, the first proton therapy clinic, Skandionkliniken, was installed in Uppsala, Sweden, with its first patient treatment in August, 2015 [5]. In four years, the facility expects to be treating around 15,000 patients per year. However, earlier treatment of proton therapy in Sweden had been conducted in The Svedberg Laboratory (TSL), with a total amount of around 1,500 patients from year the 1957 until its last patient in June, 2015 [4] [6].

1.2 Elekta Instrument AB

Elekta Instrument AB, later in this thesis referred to as Elekta, is a world leading provider of radiotherapy equipment for cancer treatment and is probably most famous for the Leksell Gamma Knife used for treating cancer tumours in the brain. The Swedish company was founded in 1972 by Lars Leksell, a Professor of Neurosurgery at the Karolinska Institute, and has since its establishment expanded to more than 3000 employees worldwide. This thesis has been carried out at Elekta’s headquarters in Stockholm, Sweden.

1.3 Objectives and Earlier Works

This thesis has been carried out with the composed objective, together with earlier efforts done by first Ludvig Hult and secondly Martin Björnmalm, to make Elekta’s Monte Carlo engine, Pegasos, compatible to proton therapy sim-
1.4. AIM OF THIS THESIS

Ludvig Hult investigated the proton extension provided by Francesc Salvat, that was integrated into the Pegasos framework [7]. Subsequently, Martin Björnmalm implemented nuclear reactions with the generation of secondary particles [8].

1.4 Aim of this Thesis

At beginning of this thesis, Pegasos benchmark had only been carried out against the experimental data provided by Proton Therapy Center (PTC), Prague, with the newly implemented nuclear reactions [8]. Furthermore, nuclear reaction data against air, present in the PTC benchmark, had not been implemented. Thus additional benchmark was needed for further validation of the initial Pegasos, in this thesis called "old Pegasos", code before proceeding with implementing neutron transport. For this purpose, implementation and benchmark against the Geant4 Monte Carlo software and subsequent benchmark against experimental data from The Svedberg Laboratory (TSL), Uppsala, and PTC (with nuclear reaction data for air) was called for.

The aim of this work can thus be divided into two parts. Firstly, as stated above, benchmark of the initial Pegasos, with the main objective of implementing and setting up a functional Geant4 environment. Secondly, the aim was to implement neutron transport into the Pegasos framework. Though not contributing considerably to the therapeutic dose due to their relative high mean free path (MFP), it is crucial in commercial and clinical cases to know where these secondary neutrons interact, for radiation protection of clinical personnel and of course for the patient her-/himself. As one can study in figure 1.2, above about 50 MeV, neutrons are the second most probable secondary particle for the proton-oxygen interaction.

The structure of the thesis is as follows. First, in chapter 2 basic concept are presented as well as a description of the components that incorporates the Pegasos framework. Later, in chapter 3 the Geant4 environment and implementations are described. Subsequently the neutron implementation is described in chapter 4 and chapter 5 contains the simulation procedure at Elekta and simulation setups. These results are then presented in chapter 6 to later be discussed in chapter 7. In chapter 8 conclusions are presented together with this thesis’ progress summary and an eventual outlook for future works.
Figure 1.2: Cross sections for a proton-$^{16}\text{O}$ interaction at 1 MeV to 260 MeV. The interaction channels are proton, neutron, deuteron, triton, $^3\text{He}$, alpha and gamma. Picture generated from TALYS data [9].
Chapter 2

Background

2.1 Basic Concepts

In this section, first the cross section, $\sigma$, and the mean free path (MFP) concept is briefly over-viewed, both essential components in the physics model of interaction probability. Secondly an introduction to the different particle interactions prominent for dosimetry in proton therapy will be presented.

2.1.1 Interaction Cross Section and Mean Free Path

The total cross section is a fundamental quantity in nuclear collisions and directly linked to the likelihood of an event to occur. It can be expressed as

$$\sigma = \frac{N}{\Phi}, \quad (2.1)$$

where $N$ equals the number of interactions per unit time per target and the flux, $\Phi$, is the number of incident particles per area and unit time. Consequently, a larger cross section is equivalent with a higher probability of an interaction to take place. To determine the probability of different reaction channels corresponding cross section are used, e.g. elastic cross section and non-elastic cross section.

In addition to the total cross section, the differential cross section (DCS) is a helpful quantity to present the particle’s change in direction, through a solid angle $\Omega$, or/and kinetic energy loss, $W$. Thus the DCS are defined through the total cross section, $\sigma$, by

$$\sigma \equiv \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^E \left( \int \frac{d^2\sigma}{d\Omega dW} d\Omega \right) dW, \quad (2.2)$$

where $E$ is the particle’s kinetic energy. Through the DCS and the total cross section essential data about the nuclear interaction is obtained and used for probabilistic calculation in the Monte Carlo program.
An important quantity in the Monte Carlo framework of particle transport, derived from the cross section, is the MFP which represents the average path length travelled by the particle between successive collisions. Mathematically, the MFP, $\lambda$, is defined as an expected value of the path length $s$,

$$\lambda \equiv \langle s \rangle = \int_0^\infty sp(s)ds,$$  \hspace{1cm} (2.3)

where $p(s)$ is the probability distribution function for a particle travelling a path length, $s$, until its next interaction [10]. Thus the product $p(s)ds$ represents the probability of the next interaction occurring in the path length interval $(s, s + ds)$. Consequently, the probability that a particle travels path length $s$ without an interaction is

$$F(s) = \int_s^\infty p(s')ds'.$$  \hspace{1cm} (2.4)

In addition, the probability of an interaction within $ds$ can be expressed as $n\sigma ds$, where $n$ represents number of molecules in the (homogeneous) medium per unit volume and $\sigma$ is the total cross section [10]. It is now clear that the product $F(s) \cdot n\sigma ds$ is the probability of the particle travelling the path length $s$, without interaction, and subsequently interacting in $ds$, i.e.

$$p(s)ds = F(s)n\sigma ds$$

$$p(s) = n\sigma \int_s^\infty p(s')ds'.$$  \hspace{1cm} (2.5)

By solving Eq. 2.5 with the boundary condition $p(\infty) = 0$, one gets

$$p(s) = n\sigma e^{-n\sigma s}.$$  \hspace{1cm} (2.6)

Eventually, the MFP in Eq. 2.3 is obtained,

$$\lambda \equiv \langle s \rangle = \int_0^\infty sp(s)ds = \frac{1}{n\sigma}.$$  \hspace{1cm} (2.7)

The interaction probability per unit path length is then easily obtained through the inverse mean free path (IMFP),

$$\lambda^{-1} = n\sigma.$$  \hspace{1cm} (2.8)

Worth stressing is that the IMFP is linear in the reaction cross section, hence cross section is directly proportional to the interaction probability.

### 2.1.2 Particle Interactions

To give an introduction of the different interactions presented in proton therapy, some basic interactions are presented below in table [2.1] followed with a short overview presented of each and everyone of them.
2.1. BASIC CONCEPTS

<table>
<thead>
<tr>
<th>Interaction</th>
<th>Target</th>
<th>Main product(s)</th>
<th>Influence on projectile</th>
<th>Influence on dosimetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inelastic Coulomb scattering</td>
<td>Atomic</td>
<td>Primary proton, ionization electrons</td>
<td>Energy loss</td>
<td>Determines the range in the material.</td>
</tr>
<tr>
<td></td>
<td>electrons</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Elastic Coulomb Scattering</td>
<td>Nucleus</td>
<td>Primary proton, recoil nucleus</td>
<td>Change in direction</td>
<td>Lateral distribution</td>
</tr>
<tr>
<td>Non-elastic nuclear reactions</td>
<td>Nucleus</td>
<td>Secondary protons, heavier ions, neutrons, gamma rays</td>
<td>Primary proton is eliminated</td>
<td>Generation of stray neutrons, prompt gamma</td>
</tr>
<tr>
<td>Bremsstrahlung</td>
<td>Nucleus</td>
<td>Primary proton, Bremsstrahlung photon</td>
<td>Change in direction, Bremsstrahlung energy loss</td>
<td>Negligible</td>
</tr>
</tbody>
</table>

Table 2.1: Short description of the different proton interaction and their dominant effects in proton therapy.

2.1.2.1 Inelastic Coulomb Interaction

In a first-order approximation the, proton primarily loses energy through inelastic Coloumb interaction with the outer electrons of passing nuclei [11] [12]. The proton’s energy loss per electron interaction is small and a continuous slowing down approximation (CSDA) is often used for calculations. However, since the proton has an mass about 1836 times greater than the electron, the proton will travel in a, more or less, straight line. As presented in table 2.1 these small interactions add up to the most significant source of the retardation of the proton, determining the proton range in the transported medium [11]. The ranges of plausible secondary electrons, caused by the passing proton, are small, less than 1 mm, and most of the dose is absorbed locally [12] [13].

The Bethe-Bloch formula implements the CSDA and gives the mean rate of energy loss for a charged particle with mass $m_0 \gg m_e$ [14] [15]. It assumes that the projectile moves much faster than the target electrons. The formula was introduced by Bethe in 1930 and corrections were provided by Bloch in 1933 , in the order of $Z^4$ [16] [14] [15]. The Bethe-Bloch formula is presented below in Eq. 2.9 and a thorough review and derivation of Bethe-Bloch formula,
with different correction terms, can be found in \[17\] \[16\].

\[
- \langle \frac{dE}{dx} \rangle = \frac{4\pi r_e^2 m_e c^2 Z_0^2}{\beta^2} Z_1 n \left[ \ln \left( \frac{2m_e c^2 \beta^2}{I(1-\beta^2)} \right) - \beta^2 + \text{corrections} \right], \quad (2.9)
\]

where \(Z_0\) and \(Z_1\) is the atomic number of the projectile and the medium respectively, \(r_e\) is the classical electron radius, \(n\) is the atomic density in the medium, \(\beta = v/c\) and \(I\) is the average excitation energy of the medium \[17\]. The correction terms of Eq. 2.9 are in order of \(Z^n\), where \(n = -1, 0, 1, 2\ldots\). An important feature of Eq. 2.9 is the first order approximation, \(- \langle \frac{dE}{dx} \rangle \propto v^{-2}\), which, as \(v \to 0\), leads to the characteristic Bragg peak of charged particles illustrated in figure 1.1. From Eq. 2.9 the range, \(R(E)\) in the medium is calculated by

\[
R(E) = \int_0^E \left( -\frac{dE'}{dx} \right)^{-1} dE' \quad (2.10)
\]

and is known as the CSDA range. Eq. 2.9 is accurate at energies higher than 1 MeV \[11\]. However, at lower energies, the projectile cannot longer be assumed to have a much higher velocity than the electrons of the nuclei and the assumption in the Bethe-Bloch formula consequently collapses. However, this restriction causes only a small uncertainty in \(R(E)\) since large \(\frac{dE}{dx}\) only has a small contribution to \(R(E)\) in accordance with Eq. 2.10.

### 2.1.2.2 Elastic Coulomb Interaction

The proton scattering is mainly caused by elastic coulomb interactions with passing nuclei \[11\] \[13\]. These repulsive forces from the positively charged nuclei each give rise to small angular deflections of the proton which combined has a crucial role in the lateral profiles of the beam. Further description of the multiple scattering (MSC) methods used for modelling these small angular deflection, through different Monte Carlo algorithms, will be presented in section 2.1.3.

### 2.1.2.3 Non-elastic Nuclear Reactions

In addition, there are three different types of non-elastic nuclear scattering reactions which are referred to as: direct, compound and pre-compound (or pre-equilibrium). Direct processes have short reaction times, \(10^{-22}\) seconds, in the time order it takes to pass the target nucleus \[18\]. The direct process is characterized with a single step interaction between that the projectile and target nucleus \[19\]. Thus the projectile, target nucleon or a cluster of nucleons in the nucleus, has sufficient energy to escape the composite nucleus directly after impact, taking up the majority of the initial projectile momentum. Compound processes have longer reaction times, \(10^{-18}\) seconds, in time order of the relaxation time. The process is characterized with the nucleus
capturing the target projectile, subsequently producing many collisions within the nucleus [18, 19, 20]. The incident energy is subsequently shared within the nucleons in the nucleus. However, one or more nucleons can accumulate enough energy to escape the nucleus.

Initially, only the compound and the direct processes were used as models for the non-elastic nuclear scattering. However, after comparing the theoretical cross sections with measured data, an effort was undertaken in the late 50’s and early 60’s to introduce a third reaction process, referred to as pre-equilibrium or pre-compound, which demonstrates both direct and compound features [18, 19]. Precompound processes differs from direct processes by emitting particles after the first step of interaction, but, in contrast to compound processes, emission takes place long before thermodynamic equilibrium is achieved. The precompound process takes up a sizeable portion of the nuclear reaction cross section in energies in the 10 MeV to 200 MeV range, and is thus an important concept in medical applications [18]. The concept pre-equilibrium and pre-compound are generally used interchangeable.

The exciton model, which was proposed by Griffin in 1966, was the first quantitative model for precompound nuclear reactions and is still used, as a basis, in many nuclear reaction codes, such as Geant4 and TALYS [21, 19, 22, 23, 9]. The exciton term refers to number of excited particles and holes, i.e. the excited degrees of freedom [19, 22, 21]. The precompound model in Pegasos uses an extension of the exciton model, through the use of TALYS. Further information about the exciton model can be found in [21].

2.1.2.4 Bremsstrahlung

When a charged particle is subject to a deceleration or acceleration, primarily caused by EM interaction with the atomic nucleus, a photon may be emitted by the charged particle, known as bremsstrahlung. The intensity of the radiation, $I_{BS}$ is proportional to the inverse square of its mass,

$$I_{BS} \propto \frac{1}{m^2}$$  \hspace{1cm} (2.11)

[24]. The primarily source of bremsstrahlung radiation thus is from electrons while for heavier charged particles this effect is much weaker. At the clinical energies of proton beams bremsstrahlung effects is negligible [11]. However, the bremsstrahlung caused by the electrons excited in proton-nucleus collisions may have a small contribution to the dosimetry. Bremsstrahlung is not modelled by Pegasos, but should be implemented for a complete program in the future. A thorough overview of bremsstrahlung is presented in the book *The elementary process of bremsstrahlung* [24].
2.1.3 MSC Models and Different Monte Carlo Methods

When each single scattering event is explicitly simulated, the number of steps needed in the simulation, and consequently simulation time, is drastically increase. Thus, for optimization, a multiple scattering (MSC) model is often invoked which simulates the mean effects of these single interactions [22]. Thus the change in direction and energy loss are given by the MSC model over a specific step length. The models used are mainly based of the MSC theories of Molière, Gaudsmit and Sanderson or Lewis [22]. Both in Pegasos and Geant4 the MSC algorithm used is based on the Lewis theory [22, 10] (for more information and derivation of the Lewis theory the reader is referred to [29]). The main challenge when using MSC modelling is implementing an algorithm used for the determining the spatial displacement. None of the above presented MSC theories provide this data, hence own algorithms must be provided which also are subject to most of the uncertainties in the MSC models [22].

There are three different types of Monte Carlo methods used for particle transport: detailed, condensed and mixed [22]. In detailed Monte Carlo each single scattering event is simulated while the condensed Monte Carlo uses a MS model. Mixed Monte Carlo is a combination of detailed and condensed, where all ”soft” events are calculated through the MS algorithm but each ”hard” events are simulated explicitly. Soft events are defined as events which produces angular deflection and energy deposition lower than a chosen angular and energy cut-off, while consequently hard events are all other events. Pegasos uses a mixed Monte Carlo for charged particles (photons and neutrons are detailed) while Geant4 uses a condensed Monte Carlo model [22, 10, 26].

2.2 PENELOPE and PENH

PENELOPE (PENetration and Energy LOss of Positrons and Electrons) is a Monte Carlo simulation code, developed at Universitat de Barcelona by Francesc Salvat in 1996 and is today managed at the Nuclear Energy Agency (NEA) at OECD, with current version PENELOPE-2014 [10]. The code is written in FORTRAN77, and used for simulating the propagation of electrons, positrons and photons in matter. Photons are treated using a detailed simulation scheme while for electrons and positrons a mixed simulation scheme is used, combining a detailed and a condensed simulation procedure. Please see section 2.1.3 for more information of different simulation schemes.

In 2013, PENH was presented as an extension to PENELOPE by Francesc Salvat to also include proton transport [26]. However, PENH does not include nuclear reactions and is thus restricted to EM interactions (inelastic and elastic) which are implemented in a similar manner as for the PENELOPE code [26]. An extensive review of the PENH extension can be found in [26].
2.3 Pegasos

Elekta’s Monte Carlo program, Pegasos, is used for conducting radiotherapeutic simulation of e.g. the Gamma knife and the MRI-guided linear accelerator (MR linac) etc. Through Elekta’s Java application program Hermes, it is possible to import complex CAD geometries, making it a powerful tool for the research and development of radiotherapy at Elekta. The Pegasos’ simulation work flow and algorithms will be described later in chapter 5.

The Pegasos framework encapsulates a modified version of the PENEOPE code, introduced in section 2.2, and thus does not include heavier charged particle transport. An extension to PENH was later added for the transportation of protons with the objective that Pegasos eventually also be used for Monte Carlo simulations of proton therapy. The implementation of the PENH code, with analysis of its models, into Pegasos can be found in [7] and furthermore the implementation of nuclear reactions with secondary protons can be found in [8].

2.4 Geant4

Geant4 (GEometry ANd Tracking) is Monte Carlo simulation software program used to simulate the propagation of particles in matter. Though originally a FORTRAN77 program when introduced at CERN in 1974, version 4 has been rewritten from scratch in C++ using object-oriented programming. It is continuously maintained and developed by scientists and software engineers in a world-wide collaboration. The software is freely available and used in areas such as high energy physics, space studies and medical science. The Geant4 implementation is described in the following chapter.

2.5 Nuclear Databases

2.5.1 TALYS

TALYS is a nuclear reaction code used for generating nuclear data for many different nuclear channels at a given energy and angle-grid [9]. TALYS is a freely available software and was developed in NRG in Petten, Netherlands, and CEA in Bruyères-le-châtel, France, and is continuously maintained. The last version, TALYS-1.6, was released in December 2013 [20]. The nuclear reaction data involves protons, neutrons, deuterons, tritons $^3$He, alpha particles and photons hitting a target nuclei of atomic number greater than 2 with the initial energy range that needs to be above the resonance level (around 1 keV) and is, for accuracy, recommended to be below 200 MeV.

TALYS include the uses the direct, pre-compound and compound nuclear reactions models earlier described in section 2.1.2.3.
2.5.2 ENDF

The ENDF (Evaluated Nuclear Data File) formats and libraries are governed by the Cross Section Evaluation Group (CSEWG), a corporation between industry, national laboratories and universities in Unites States and Canada [27]. In addition, the National Nuclear Data Center (NNDC) is responsible for maintaining these data. Many different Monte Carlo codes for nuclear calculations uses the ENDF data, e.g. Geant4, FLUKA and MCNP [27].

Other important national and international organization has adopted the same nuclear data format, called ENDF-6. These are e.g. the Joint European File (JEF) and the European Fusion File (EFF). JEF and EFF were later merged into JEFF, being a part of the OECD corporation through The Nuclear Energy Agency (NEA) [28].
Chapter 3

Geant4 Implementation

Using Geant4 implies programming in the Geant4 source code, implementing new classes in the Geant4 libraries, which of course requires the user to be familiar with the Geant4 environment. In fact, user implementation of derived classes of the purely virtual classes are mandatory. Fortunately, some basic examples are given in the default Geant4 download which helps the user to become familiar with the different libraries and can be used as a foundation for setting up the experimental setup of choice. An alternative to hard-programming in Geant4, in medical applications, is the encapsulating program GATE and TOPAS which will be presented later in section 3.3. Below, an introduction to the basic concept of Geant4 will be presented, needed for setting up the Geant4 environment.

3.1 Geant4 Environment

In this section, a short introduction is given to the Geant4 environment. As mentioned earlier in this chapter, using Geant4 implies implementing C++ source code. To run a Geant4 application there are three mandatory classes which must be implemented by the user, derived from the purely virtual classes presented below.

**G4VUserDetectorConstructor** Construction of the experimental setup, scoring volumes and materials.

**G4VUserPhysicsList** Construction of particles and physical models which are to govern the simulation.

**G4VUserPrimaryGeneratorAction** Construction of the particle generator where the user describes the initial state of the primary event.

Moreover, there are five optional user action classes which correspond to different actions, user hooks, which the user may want to address to modify default functionality within the simulation.
G4UserRunAction is called in the beginning and end of the run. E.g. used for saving files and generating a run, called a G4Run. In multi-threading, each thread will have a G4Run object.

G4UserEventAction is called in the beginning and end of an event, where an "event" starts with the primary particle and ends when no more particles are traced in the geometry. This class can be used in single threading for saving data after each event, but for multi-threading the data needs to be recorded by member functions, implemented through a user derivation of G4Run.

G4UserStackingAction is called in the beginning of each event and the class, initializing the stack, subsequently sets the framework for stacking G4Track objects (representation of the particle during tracking, i.e. current position/time, pointer to the current physical volume and particle information), through G4StackManager.

G4UserTrackingAction is called in the start- and endpoint of processing a G4Track.

G4UserSteppingAction is called at the end of a particle step. Can be used for collecting desirable data after each step.

In addition to the classes introduced above, further implementation of classes may be needed depending on the application at hand. The application used in this thesis is based on example B4c, provided in the Geant4.10.01.p02 download. However, further implementations was needed in order get energy deposition at each voxel in the scoring volume, multi-threading, different physics models and proton beam structure. For further information about the Geant4 environment the reader is referred to Geant4 User’s guide for Application Developer [29].

3.2 Physics List

A physics list is a composition of different physics models, implemented as C++ classes, used in the Geant4 application. There are many different physics models available in the Geant4 libraries, specialized at different energies, and by combining them the user implements the physics list most appropriate for the application a hand. In table 3.1 a overview of the different name conventions is presented.

In proton therapy application the focus is on low energy physics, thus high energy models (QGS and FTF) do not need to be investigated further. Instead, up to a few GeV, a hadron-nucleus interactions may be modelled as a hadron-nucleon interactions within the nucleus. In Geant4 there are mainly two different hadron-nucleus models being used for low energy physics, these
3.2. PHYSICS LIST

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Model</th>
<th>Energy range</th>
</tr>
</thead>
<tbody>
<tr>
<td>QGS</td>
<td>Quark gluon string</td>
<td>&gt;= 20 GeV</td>
</tr>
<tr>
<td>FTF</td>
<td>FRITIOF</td>
<td>&gt;= 10 GeV</td>
</tr>
<tr>
<td>BERT</td>
<td>Bertoni inspired cascade</td>
<td>&lt;= 10 GeV</td>
</tr>
<tr>
<td>BIC</td>
<td>Binary based cascade</td>
<td>&lt;= 10 GeV</td>
</tr>
<tr>
<td>HP</td>
<td>High precision neutron model</td>
<td>&lt; 20 MeV</td>
</tr>
</tbody>
</table>

Table 3.1: Abbreviation used for choosing physics model in Geant4

are the cascade models BERT and BIC. In addition, there is a possible extension to these two physics list, giving a neutron model, HP, with higher precision for energies below 20 MeV. For simulation involving neutrons, with energies below 20 MeV, the HP model extension is highly recommended since the simulation otherwise may lead to unreliable results \[29\]. Further information about the more precise neutron model can be found in \[30\].

3.2.0.1 Geant4 Cascade models

In an intranucleus cascade model the secondaries, produced from the primary hadron-nucleon collision, in turn interacts with nearby nucleons, like a “cascade”, until the initial kinetic energy has partitioned within the nucleus. Thus the inelastic scattering for hadrons can be generated by simulation of this interaction cascade within the nuclear potential. In the context of Monte Carlo, intranucleus cascade models have been deemed valid after the Goldberger’s calculations presented in \[31\]. Subsequently, Metropolis et. al., did the first Monte Carlo simulations of an intranucleus cascade in 1958 \[32\]. A brief overview of the two Geant4 cascade models, BERT and BIC, are presented below. For a more thorough description of the different cascades the reader is recommended Geant4’s Physics Reference Manual \[22\].

The BERT cascade model is a composition of the Bertini intranuclear cascade model with exitons, an evaporation model, a simple nuclear explosion model, a precompound model and a fission model \[22\]. The BERT cascade is a non-quantum cascade, solving the Boltzmann equation on average. The cascade starts when the projectile hits a nucleon in the target nucleus and produces secondaries which consequently may either be absorbed or generate a chain of secondaries within the nucleus. The cascade ends when all particles, which have enough kinematic energy to do so, have escaped the target nucleus. \[22\]. By using this model there is the condition that

\[
\frac{\lambda_B}{v} \ll \Delta t \quad (3.1)
\]

is satisfied, where \(\lambda_B\) is de Broglie wavelength of the nucleons an \(v\) is the average velocity between two nucleon and \(\Delta t\) is the time interval between
collisions. This is not strictly valid at energies below 200 MeV, thus the precompound model takes over [22]. The precompound model will be described further in section 3.2.0.2.

In contrast to BERT, BIC is a time dependent quantum cascade model, meaning that quantum mechanical effects (e.g. Fermi motion) are taken into account and that the collisions are ordered. Hence the propagation of the particles within the nucleus is done by numerically solving the equation of motion in the nuclear field by a Runge-Kutta integration method [22]. The cascade ends when the maximum energy of produced secondaries is below the threshold, that is when the maximum individual particle kinetic energy is below 75 MeV or when the mean kinetic energy is below 15 MeV [22]. As for the BERT model, the precompound model is subsequently invoked to process the remaining participants, with the initial state defined by the final state of the BIC simulation.

3.2.0.2 Precompound Model

The Geant4’s precompound model is based on the exciton model proposed by Griffin in 1966 [21]. Only emission of protons, neutrons, deuterons, tritons and alphas are possible. The precompound model is invoked on low energy nucleon-nucleus inelastic collision. Hence it is in general used as an extension to Geant4 cascade models, described above, as a transition from the cascade model to the equilibrium stage of reactions described by the equilibrium de-excitations models. However, the precompound model is not derived from the cascade models and can thus explicitly be used without the BERT or BIC frameworks. The system is said to be in statistical equilibrium when the number of exciton, \( n \), which equals the number of holes and excited particles, reaches an equilibrium number of excitons,

\[
 n_{eq} = \sqrt{2gU},
\]

where \( U \) is the excitation energy and \( g \) the density of single particle levels [22].

3.2.0.3 Physics List Setup

After recommendations from the Geant4 web-page, the QGSP_BIC_HP physics list was chosen [33]. Moreover, there are a variety of electromagnetic physics list available for the developer, which can be found at [34]. In the QGSP_BIC_HP a default EM standard model is chosen. However, to increase accuracy at low energy physics another enhanced EM standard model (option 4) was used, recommended for low energy physics (medical applications). This model has a more accurate electron, hadron and ion tracking than the default EM standard model used in QGSP_BIC_HP. Except changing the default EM model, the original QGSP_BIC_HP physics list was used, constituted by the physics models stated below.
3.3. GEANT4 ENCAPSULATING SOFTWARE

G4EMStandardPhysics_option4 - EM physics.

G4EMExtraPhysics - Synchrotron radiation. EM radiation emitted when charged particles are radially accelerated.

G4DecayPhysics - Particle decays.

G4HadronElasticsPhysicsHP - Hadron Elastic Scattering.

G4HadronPhysicsQGSP_BIC_HP - Hadron Physics. QGSP high energy model with the BIC cascade and HP neutron extension.

G4StoppingPhysics - Stopping physics. Provides the nuclear capture at rest of negatively charged particles ($\pi^-$, $\mu^-$ etc.)


3.3 Geant4 encapsulating software

GATE (Geant4 Application for Emission Tomography) is a more user friendly application than the original Geant4, used for simulation in the range of nuclear medicine [35]. GATE encapsulates the Geant4 libraries but does not require any C++ programming by the user, making it a welcomed alternative for the novice Geant4 user. This application has not been used in this thesis, but could be a good option for benchmarking in further research.

TOPAS is another software used in medical physics for radiotherapy [36]. As for GATE, TOPAS encapsulates the Geant4 libraries and is an easier-to-use application than Geant4 since it does not require any programming by the user or knowledge about the Geant4 environment. The software is free for a single user in a non-profit organization in US or in one of the ”least developed countries”, otherwise a fee is required.
Chapter 4

Neutron Implementation

The neutron is often divided into three subgroups depending on its kinetic energy: thermal, intermediate and fast neutrons. The most probable kinetic energy for a neutron at thermal equilibrium at room temperature is 0.025 eV which is categorized as a thermal neutron, being below 0.5 eV. Neutrons in the 0.5 eV < E < 10 keV range are called intermediate and above 10 keV are called fast. In the Pegasos Simulation framework only energies above 10 keV cut-off are simulated corresponding to, so called, fast neutrons. Below 10 keV, the neutron’s dose contribution is dominated by the hydrogen capturing the neutron resulting in an emitted gamma rays of 2.2 MeV. In this thesis it is supposed that most neutrons resulting from proton non-elastic nuclear reactions will leave the patient/phantom a long time before becoming thermal neutrons. Since only fast neutrons are simulated, dose transfers resulting from emitted gammas from these low energetic neutrons will not be taken into account which is a restriction of this implementation. This restriction will be discussed later in section 7.1.4. For fast neutrons, the dominant dose contribution in human tissue is from recoiled protons resulting from elastic scattering to the hydrogen nuclei. The neutron elastic scattering will be described in section 4.4.

In this section, the implementation of the neutron transport is described. First, the handling of the Pegasos’ material file is presented. In section 4.3, the sampling technique is described and subsequently the neutron elastic scattering implementation. Eventually, the special care that has been taken towards the neutron-hydrogen interaction is presented in section 4.5.

4.1 Extending the Material File

This section describes how the nuclear reaction data for neutron transport was implemented. It first gives a short introduction to the TALYS nuclear code, subsequently explaining why another nuclear data library, ENDF, needed to be used. In addition, section 4.1.2 explains how the ENDF database was
incorporated into the Pegasos’ nuclear library and eventually, in section 4.1.3, the implementation of the neutron nuclear reaction data into the material files is presented.

4.1.1 TALYS nuclear code

For the neutron nuclear reaction data of cross sections, angular distribution of elastic scattering and particle emission spectra from non-elastic nuclear interactions, the TALYS nuclear reaction code was used [9]. The choice of TALYS was made to maintain consistency in the physics model, since the nuclear reactions data for protons incorporate data provided by TALYS [8]. In addition, TALYS is a freely available nuclear reaction code and one can thus architect the output data for one’s own purposes (e.g., energy range, elements etc.). TALYS uses the optical model for obtaining its nuclear reaction data. Due to the fact that the the TALYS nuclear physics model already has been investigated in [8], no further investigation is conducted in this thesis about the TALYS physics model. For more information about the models that constitute TALYS, the reader is referred to [8] or the TALYS manual [20].

However, there are two restrictions that need to be stressed when using the TALYS nuclear code. The first restriction is the projectile’s energy range, where TALYS only allows incident energies from around 1 keV [9]. However, Pegasos uses a minimum kinetic energy of about 10 keV throughout the simulation, hence, in this case, the lower bound of TALYS is sufficient. Consequently, as mentioned above, this implies that incident neutrons with energies below 10 keV, e.g. the thermal neutrons, will not be included in this neutron implementation.

The second restriction of TALYS is that the target nucleus must have \( Z \geq 3 \). In other words, nuclear data from hydrogen nor helium, with respective isotopes, cannot be obtained from TALYS. With the objective of implementing neutron transport, this imposes a major restriction, since the main neutron dosimetry contribution in human tissue is excluded when using TALYS, due to the exclusion of hydrogen. Instead, the ENDF (Evaluated Nuclear Data File) was used for obtaining the neutron-hydrogen data. This nuclear data library will now be presented.

4.1.2 ENDF database

As mentioned above in section 4.1.1, the ENDF database was needed in order to obtain nuclear data of hydrogen and helium. The Los Alamos LA150 library was found to have neutron-hydrogen nuclear interaction data up to 150 MeV. However, no neutron-helium interaction data was found above 20 MeV and since helium is not common in humans, it was excluded from this implementation.
4.2 READING THE MATERIAL FILE

The LA150 library is manifested in then compact ENDF-6 format, cryptic to read for the human eye. The data in the ENDF-6 format is structured into a hierarchy, from highest level 'tapes', with subsequent material ('MAT'), file ('MF') and eventually the lowest level, reaction ('MT') (for the novice ENDF-6 user, [39] is recommended). From the ENDF file the elastic cross section, radiative capture cross section and the angular distribution, in terms of Legendre coefficients, were obtained.

To keep user consistency in the Pegasos’ nuclear library format, the ENDF Legendre coefficients and cross section data was interpolated to the energy grid and format used by TALYS. Two external FORTRAN77 programs were created, endfleg.f and endfxs.f, outside of the Pegasos framework, to generate these nuclear data to the nuclear library later used by Pegasos. The cross sections were interpolated by a linear log-log interpolation. Due to the fact that the Legendre coefficients can be negative, linear-logarithmic interpolation was implemented for the Legendre coefficients. Spline interpolation was also tested, resulting in about 20 percent increment at higher energies, but was considered not suitable due to larger uncertainties concerning extrapolation of energies higher than 150 MeV (the TALYS data is set up to 260 MeV).

4.1.3 Integration to Pegasos’ Material File

To handle nuclear reaction data in the material file two subroutines are used in PENH, PHMATW and PHMATR, which writes and reads the material file respectively. PHMATR will be treated in section 4.2 and in this section implementations in PHMATW is presented.

The raw nuclear data, in the TALYS format, is read by the subroutine PHMATW, through invoking the Pegasos program hmaterial, in order to produce the material file of choice. In other words, material files for e.g. water and air are generated by hmaterial, containing all interaction data. In PHMATW, different subroutines are called for handling different types of interaction data for protons and neutrons. For writing elastic and non-elastic neutron cross section to the material file the subroutine NNRAW is invoked. Furthermore, the particle emission spectra, for incident neutrons, is written to the material file by the subroutine NNXSPECW and the Legendre coefficients are written by the subroutine NLLEGW. These implementations are relatively straight forward, mainly transferring the nuclear data from the TALYS format to an extension of the PENELOPE material file. The material file is subsequently processed when starting the Pegasos application in runtime.

4.2 Reading the Material File

In runtime, the material file is read by the subroutine PHMATR. For consistency in the Pegasos code, the neutron implementation follows that of the proton implementation.
CHAPTER 4. NEUTRON IMPLEMENTATION

The subroutine NNRaR handles the neutron elastic and non-elastic cross sections. These cross sections are cubic spline interpolated into a logarithmic energy grid, used in general throughout PENELope and PENH, which is later used for sampling IMFP (the inverse mean free path presented in section 2.1.1). In turn, the IMFP is used for determining type of nuclear interaction in subroutine KNOCK and for sampling discrete translation in JUMP. Of course, these cross sections are also used for sampling to which element the reaction occur, when the reaction channel already has been determined.

The neutron emission spectra of protons, neutrons and gamma, are treated in the subroutines NPREAD, NNREAD and NGREAD respectively, corresponding to the PREAD, NREAD and GREAD for the proton emission spectra. These subroutines perform a cubic interpolation of the yield of each reaction, analogous to the probability of a particle being emitted. In addition, the RITA values (see section 4.3) are stored, used later for sampling the energy of the emitted product.

Eventually, the angular distribution of neutron elastic scattering is handled by the subroutine NLegR. The angular distribution is expressed in terms of Legendre series. The Legendre coefficients and Legendre polynomials, calculated through recursion, are stored locally for subsequent calculation of the probability density function (PDF) at each energy. The PDF is at each energy processed by RITA and stored in RITA values. These RITA values are later used in the NNRANGLE subroutine for sampling the angular distribution and thus energy loss due to target recoil. The RITA sampling technique will now be presented in the following section.

4.3 Sampling Technique

For sampling techniques involving the angular distribution and the particle emission spectra the RITA (Rational Inverse Transform with Aliasing) algorithm is invoked [10]. During the read of the material file, in the subroutine PHMATR, different "RTA values" (such as $a$ and $b$ in Eq. (4.1) and the cumulative probability) are stored to be used during sampling in runtime. In simulation runtime, the sampling starts by generating a random value, $\xi$, and subsequently the cumulative probability interval $i$ is found, $\xi_i \leq \xi < \xi_{i+1}$. Thirdly, $\nu \equiv \xi - \xi_i$ and $\Delta_i \equiv \xi_{i+1} - \xi_i$ are defined and eventually the output value $y$ is generated,

$$y = y_i + \frac{(1 + a_i + b_i)\Delta_i\nu}{\Delta_i^2 + a_i\Delta_i\nu + b_i^2}(y_{i+1} - y_i),$$

(4.1)

where $y_i$ and $y_{i+1}$ are the output values at grid points $i$ and $(i + 1)$ respectively [10].

For sampling in emission spectra and angular distribution, an statistical approach was implemented in order to avoid tedious interpolations of whole
distribution functions, generated by the RITA algorithm, between grid points. This statistical approach is presented in the next section.

4.3.1 Sampling Incident Energy Grid Point

Consider an incident neutron with energy \( E \), in the energy grid interval \( i \), i.e. \( E_i < E < E_{i+1} \). As mentioned above, sampling in angular distribution, \( \cos \theta \), and particle emission spectra, \( E_s(E) \) would require computationally inefficient interpolations, since both the Legendre coefficients, \( a_l(E) \) and the emission spectra are dependent on the neutron’s incident kinetic energy. Instead a statistical approach was invoked to avoid interpolation over the incident neutron’s energy grid interval \( i \). The incident energy grid point, \( i \) or \( i+1 \), is simply chosen by generating a random value \( \xi \) and subsequently compared to a weighted ratio to choose grid point from which \( a_l \) or \( E_s \) will be sampled

\[
\begin{align*}
\xi &\leq \frac{E_{i+1} - E}{E_{i+1} - E_i} \rightarrow E_i, \\
\xi &> \frac{E_{i+1} - E}{E_{i+1} - E_i} \rightarrow E_{i+1}.
\end{align*}
\]

The advantage of this approach is clear, saving a lot of computational time while being statistically valid.

4.4 Neutron Elastic Scattering

4.4.1 Angular Distribution and Legendre Series

For neutron elastic scattering, the angular distribution has been expanded in terms of Legendre series. The representation of the Legendre polynomials for the angular distribution arises from the relationship between the differential cross section, \( \frac{d\sigma}{d\Omega} \) and scattering amplitude, \( s(E_k, \theta) \), with incident energy \( E = E_k \) assuming no polarization and azimuthal dependency,

\[
\frac{d\sigma}{d\Omega} = |s(E_k, \theta)|^2.
\]

A derivation of Eq. (4.3) can be found in most any textbook on quantum mechanics and scattering theory, e.g. [40]. The scattering amplitude can in turn be expanded into a sum of partial waves, in basis of Legendre polynomials, in the domain \(-1 \leq \cos(\theta) \leq 1\)

\[
s(E_k, \mu) = \sum_{l=0}^{\infty} (2l + 1)R_l(k)P_l(\mu),
\]

where \( \mu = \cos \theta \) and the partial wave amplitude, \( R_l(k) = \frac{e^{i\delta_l(k)}}{k} \sin \delta_l(k) \) is determined by the partial wave phase shift \( \delta_l(k) \).
Since the Legendre polynomials represent a complete basis in this domain, the angular distribution can be obtained by a Legendre expansion of the probability distribution function, with normalization $a_0 = 1$,

$$f(E, \mu) = \frac{2\pi}{\sigma(E) d\Omega} \int_0^\infty \frac{(2l + 1)}{2} a_l(E) P_l(\mu),$$

$$\int_{-1}^1 f(E, \mu) d\mu = 1.$$

At low energies, when the particle’s de Broglie wavelength is much larger than the target nucleus, higher order Legendre polynomial can be neglected and the distribution can be approximated with the spheric symmetrical ‘s-wave’ corresponding to the first Legendre polynomial ($l = 0$) \[39\]. It is through this isotropic approximation all nuclear angular distribution earlier has been implemented Pegasos.

In this thesis, an effort has been taken to implement angular distribution for elastic scattering in the neutron implementation of Pegasos. Eq. 4.5 corresponds to the form in which nuclear data of angular distribution has been provided by the TALYS and ENDF libraries.

### 4.4.2 Sampled Angle and Energy Loss to LAB Frame

In this section the neutron elastic scattering implementation will be presented with angle transformation between different frames and energy loss. The relation between the angles in the LAB frame, $\theta$, and CM frame, $\theta'$, is expressed as follows,

$$\tan \theta = \frac{\sin \theta'}{(\tau + \cos \theta') \gamma_{CM}},$$

$$\tau = \sqrt{\left(\frac{M}{M_{\text{target}}}\right)^2 (1 - \beta_{CM}^2) + \beta_{CM}^2},$$

(4.6)

where $\gamma_{CM} = (1 - \beta_{CM}^2)^{-1/2}$ is the Lorentz factor in the CM frame and $\beta_{CM} = \frac{v_{CM}}{c}$ \[26\]. The angular distribution is sampled in the CM frame, $\cos \theta' = \mu'$ and subsequently, by using trigonometric identities, Eq. 4.6 is reformulated in terms of $\mu$ and $\mu'$, used in the Monte Carlo simulations,

$$\mu = \frac{\tau + \mu'}{\sqrt{(\tau + \mu')^2 + (1 - \mu')^{-2}}}.$$  

(4.7)

The energy loss, $W$, is obtained from the kinematics in the CM frame and depends on the sampled scattering angle, $\mu'$,

$$W = \frac{p^2}{M} (1 - \mu').$$

(4.8)
where \( p' \) is the momentum in the CM frame and \( M \) the target’s mass \[26\]. The above formulas are defined in the subroutines NNRANGLE (for neutrons) and NRANGLE (for protons) in the modified PENH subroutine.

## 4.5 Neutron-Hydrogen Interaction

Due to the important dose features characterizing the neutron interaction against hydrogen, special mechanisms were implemented for this interaction. The interaction can occur by either elastic scattering or by the neutron being captured by the hydrogen atom to deuterium. The elastic scattering results in a recoil proton that subsequently is tracked in the Pegasos code if its energy is higher than the absorption (cut-off) energy. The radiative capture of the neutron results in a gamma ray emission of 2.2 MeV.

However, due to the lower energy bound set in Pegasos, thermal neutrons, which are most probable of being captured, are not simulated. In other words, the chance of a neutron being captured in the simulation is smaller than in reality and the larger nuclear channel for neutron interaction is the elastic scattering. The implications of the low energetic neutrons not being simulated will be further addressed in chapter \[7\].

For the neutron-hydrogen elastic collision, the recoiled proton is followed in the simulation if its kinetic energy is higher than the proton absorption energy. The recoil proton is known for being the main dose contributor for fast neutrons and is thus an important aspect that was taken into specific attention in this neutron implementation \[37\] \[38\]. Other energy transfers to recoils, resulting from the neutron elastic scattering, are approximated to be locally deposited.
Chapter 5

Method

This chapter will first present the simulation procedure at Elekta and subsequently the experimental setup of the different benchmarks conducted.

5.1 Simulation and Processing at Elekta

The simulation algorithm of Pegasos has been explained in [7, 8]. However, since the simulation algorithm also is a central concept in this work, a brief overview will also be presented here.

In runtime, after the material file has been read and interaction data saved, an initial primary particle is created and subsequently follows procedure presented in figure 5.1. The simulation shower starts by invoking the subroutine "START" in PENELOPE. The particle is subsequently transported through the subroutine "JUMP" with subsequent position checks where the subroutine START is invoked again if the particle has crossed a boundary between materials. Next the subroutine "KNOCK" is invoked which alternates between simulating either a "hard" or a "soft" event (see section 2.1.3 for more information about the different types of events). However, for uncharged particles, there are no soft events due to the fact that they are not affected by the Coulomb force. Hence, every time KNOCK is called, a hard event is simulated for neutrons (as for photons). The algorithm explained above, from the subroutine JUMP to KNOCK is subsequently repeated until the particle is absorbed in the medium, determined by a cut-off energy unique to each particle, or leaves the simulation region.

Eventually, when the particles have been either absorbed or left the simulation region, the secondary particle stack is checked. If no secondaries are left, the simulation shower is ended. Otherwise, a secondary is popped from the stack and simulated by invoking START.

Pegasos simulations at Elekta has been carried out at their computer cluster for improvements in computational time and thus statistics, using 112 CPUs instead of the local computer’s 8. A schematic sketch of the data pro-
Figure 5.1: Pegasos’ simulation algorithm for particle transport showers. Bold boxes represent routines strongly related to the PENELOE/PENH code while dotted boxes are exclusively implemented in the Pegasos encapsulation program. The picture has been provided by Ludvig Hult [7].

cessing in this thesis is presented in figure 5.2. First simulations parameters and geometries with respective materials are set in the local Java application Hermes. Hermes thus generates different simulation data files which are subsequently transferred to Elekta’s cluster for more computational power.

The application is then simulated through the multiprocessing program PegasosMPI, using the Message Passing Interface (MPI). Results from each node are saved respectively in an output file which is subsequently merged by the program mfcombiner, resulting in a *.tot, which contains the conclusive result of the simulation. Eventually, the result file is transferred to the local computer for post-processing in e.g. MATLAB computational program.
5.2 Benchmarks

All benchmarks are done before (called "old Pegasos") and after the neutron implementation in Pegasos. However, it is crucial to stress that all presented differences cannot solely be contributed to the neutron implementation. Simultaneously, during the neutron extension, other changes of the Pegasos code was also applied. Some bugs and typos of earlier implementations were corrected and furthermore an implementation of proton-nucleus reaction Q-values was done. Nonetheless, all the result presented in this section represents implementations done during the period of this thesis.

5.2.1 Geant4

Three different benchmark were generated against Geant4. These are presented in each subsection below. For each benchmark against Geant4 a uniform parallel beam of radius 3 mm was used.

5.2.1.1 Lateral Dose Distribution

The penumbral sharpness is crucial in clinical application of radiotherapy. For this objective the lateral profiles are investigated through the centre of axis dose in comparison to Geant4. A dose cylinder, of radius 1.6 cm, 200 radial bins and length 1 cm, was placed at four different depths in water to compare
the lateral dose distribution between Pegasos and Geant4. Incident proton kinetic energy was set to 170 MeV and the results are shown in figure.

5.2.1.2 Depth-dose Curve

A depth-dose curve comparison was compared against Geant4 at three different energies, 100 MeV, 135 MeV and 170 MeV in a water phantom of size 50x50x23 cm$^3$ with an radius of 100 mm and 460 z-bins which are. In addition, benchmarks were also executed at incident kinetic proton energy 170 MeV, with cylindrical radius 4 mm, 8 mm and 16 mm.

5.2.1.3 Lateral Halo Dose

Eventually, a halo benchmark was provided against Geant4, to investigate the fringe dose. In this manner, the effects of the neutron implementation could be measured. For this benchmark a cubical water box of length 50 cm positioned and incident protons of energies 170 MeV were bombarded perpendicular to the plane. A dose cylinder, with radius 25 cm, 250 radial bins and length 50 cm, as well as a cubical dose box, with 1 cm$^3$ bins, filling the water phantom.

5.2.2 Experimental Data

Experimental data were provided from The Proton Therapy Center (PTC) and the The Svedberg Laboratory (TSL) [41, 6]. The experimental set-up is described in the two following sections.

5.2.2.1 Proton Therapy Center

The PTC, in Prague, provided experimental data of depth-dose distribution used for comparison against Pegasos and Geant4. The measurements were done in a water phantom, using a Bragg Peak Chamber, type 34070, with radius 40.8 mm and thickness 2 mm [42]. This chamber was subsequently translated, in segments of 0.5 mm, from the Bragg peak towards then incident beam. The source was place 2 meter from the water phantom. Thus the beam first propagated through 2 meter of air before interacting in the water phantom. In addition, the energy deposit was normalised to the Bragg Peak. For comparison against Pegasos and Geant4, the beam radius was assumed to be 3 mm and the water phantom a box of size 50x50x23 cm$^3$.

5.2.2.2 The Svedberg Laboratory

The experimental set-up of the data obtained from TSL will now be presented according to [43]. With the proton beam propagating in the z direction, two scanning magnets first direct the beam in the x and y direction respectively. Thirdly, the beam transverse through an ionization chamber and a multi-wire
ionization chamber to monitor the vertical position of the particles. Subsequently a range shifter was introduced, consisting of PMMA (plexiglas) sheets of different thickness, before propagating through the water phantom. By using the two initial magnets the proton beam was scanned to hit an area of 140x140 mm$^2$ of the water phantom of size 150x150x400 mm$^3$. Hence lateral equilibrium could be ensured when performing the central depth dose measurements with a Scanditronix Hi-pSi diode at the central axis. The experimental data obtained had PMMA thickness of 0, 25, 50, 75 and 100 mm. The experimental set-up is presented in figure 5.3.

Figure 5.3: At the top part of the figure the experimental set-up is illustrated from left to right, magnet in the $x$-plane, magnet in the $y$ plane, range shifter sheets and finally the water phantom. In the lower part of the figure the simulation setup is presented, using a rectangular divergent proton beam and the unit cm is used for the numbers in the bottom. The picture has been provided by Ludvig Hult [7].

To determine the energy spectrum of the beam in the experiment, simulations done by Geant3.21 played a crucial role. Pre-calculated mono-energetic depth doses, $D(z, E_i)$, was generated by Geant3 and subsequently weighted...
and summed to a calculated depth dose:

\[ D_{\text{fit}}(z) = \sum_{i=1}^{n} D(z, E_i) \frac{dN}{dE}(E_i) \Delta E_i, \tag{5.1} \]

where the weighting term, \( \frac{dN}{dE} \), is a Gaussian distribution of the form

\[ \frac{dN}{dE}(E_i) = N_0 \frac{1}{\sqrt{2\pi\sigma_E}} \exp\left(-\frac{(E_i - \langle E \rangle)^2}{2\sigma_E^2}\right). \tag{5.2} \]

The mean energy, \( \langle E \rangle = 180.4 \text{ MeV} \), and standard deviation, \( \sigma_E = 0.23 \text{ MeV} \), where determined by fitting the Eq. 5.1 to the experimental data. However, after a private conversation with the author [43], it was advised that the energy should be reconfigured to fit the penetration depth of the simulation result obtained by Pegasos. This advice was given due to uncertainties in the determination of the mean energy when using the earlier Geant3, presented in Eq. 5.1. By using the NIST database, [44], the difference of the corresponding energy between Pegasos and TSL, when no PMMA range shifter was used, resulted in \( \langle E \rangle = 179.65 \text{ MeV} \). Thus this mean energy was used for the simulations for the subsequent range thicknesses.

At Elekta, the simulation was carried out according to [7], who had done the TSL benchmark at an earlier stage of the Pegasos code and is illustrated in figure 5.3. A scoring cylindrical volume of radius 10 mm was placed inside the water phantom, with voxel thickness 0.5 mm. The larger radius was chosen for statistical improvements in respects to computational time.

The obtained data was provided normalized to an unknown reference dose, \( D_{\text{ref}} \), obtained at a reference plane situated at a 4.5 cm penetration depth within the water phantom, with a 30 mm PMMA energy degrader [43]. However, experimental data with 30 mm PMMA was not available. Instead, data from the 25 mm PMMA energy degrader was used, where the dose deposit at \( z = 5.6578 \text{ cm} \) was closest to the actual reference value, \( D(z = 5.6578 \text{ cm})/D_{\text{ref}} = 1.0043 \). The Pegasos’ simulation results were thus normalized to the dose deposit at \( z = 5.6578 \text{ cm} \), \( D_{\text{Pegas}}(z = 5.6578 \text{ cm}) \) and multiplied by the \( D(z = 5.6578 \text{ cm})/D_{\text{ref}} = 1.0043 \) factor, i.e. the normalized dose deposit with PMMA thickness \( i \), \( D_i(z) \), was obtained by

\[ D_i(z) = \frac{D_{\text{Pegas}}}{D_{\text{Pegas}} \cdot 1.0043}. \tag{5.3} \]

### 5.3 Photon Spectrum

To verify the neutron radiative capture a photon spectrum was obtained. An incident proton beam with kinetic energy 100 MeV was transported in a water phantom of size 50x50x23 cm³. Behind the water phantom, with origo at the central axis, a 70x70 cm² plane was placed to count the number of hitting
photon at each energy. Thus by normalizing to the total number of hits, a photon spectrum could be provided with the probability that a given energy would be encountered. It should be stressed that this does not demonstrate the probability of a photon being emitted at an energy within the water phantom, since the spectrum plane solely was positioned behind the water phantom.

5.4 Angular Distribution

Eventually, to study the impact of a non-trivial angular distribution for elastic neutron scattering these probability density functions were studied. Incidental neutron energies were set to 1 MeV, 10 MeV and 100 MeV against hydrogen and oxygen respectively. For each one of these initial energies and targets, the probability density function (angular distribution), derived from the Legendre coefficients, was saved and subsequently plotted for comparison against a s-wave approximation.
Chapter 6

Results

In this section the different results and data obtained from the simulations and computations introduced in chapter 5 will be presented. All benchmarks are conducted with the initial Pegasos code, called "old Pegasos", and with the current Pegasos code with the neutron implementation. Moreover, the "average difference" is defined as the sum of all absolute differences, at each data point, divided by the sum of the reference data. It can be illustrated as a comparison between different areas, the area corresponding to the difference between the two curves, divided by the area of the reference curve.

6.1 Benchmark against Geant4

Benchmark was performed against Geant4 for the depth-dose curve and for the lateral dose distribution in a water phantom of size 50x50x23 cm$^3$. The lateral dose distribution, with initial proton kinetic energy 170 MeV, is presented at penetration depths 5 cm, 10 cm, 15 cm and 19.2 cm in figures 6.1a to 6.1a respectively.

For the depth-dose curve four different scoring radii were used, 4, 8, 16 and 100 mm with initial proton energy 170 MeV. The results are presented in figures 6.2 to 6.5. In addition, simulations with initial proton energy 100 MeV and 135 MeV, with 100 mm scoring radius, are presented in figure 6.6a and 6.6b.

6.2 Benchmark against Experimental Data

Pegasos and Geant4 was compared against the PTC data at three different energies, 170 MeV, 135 MeV and 100 MeV and are plotted in figures 6.7 to 6.9. In addition, the TSL benchmark was conducted for Pegasos and "old Pegasos" in figures 6.10 and 6.11 respectively. Each figure contains simulation results with PMMA slabs of thickness 0 mm, 25 mm, 50 mm, 75 mm and 100 mm.
6.3 Lateral Halo Benchmark and Photon Spectrum

The lateral halo dose distribution is illustrated in figure 6.12 from central axis radii 75 mm to 250. In addition a photon spectrum is presented in figure 6.13.

6.4 Angular Distribution

The angular distribution for neutron elastic scattering against hydrogen and oxygen in the CM frame can be studied in figures 6.14 and 6.15 respectively. For each element, the angular distribution is plotted against three different energies, 1 MeV, 10 MeV and 100 MeV. Furthermore, to clearer compare the difference against a s-wave approximation, this uniform probability density function is also plotted in each figure.
6.4. **ANGULAR DISTRIBUTION**

(a) Depth 5 cm  
(b) Depth 10 cm  
(c) Depth 15 cm  
(d) Depth 19.2 cm

Figure 6.1: Lateral dose curve comparison between Pegasos and Geant4 at four different depth, 5, 10, 15 and 19.2 cm. Average differences from (a) to (c) are for Pegasos: 7.66%, 5.60%, 2.70% and 4.05% respectively, and for old Pegasos: 10.49%, 8.08%, 4.67% and 4.59% respectively.
CHAPTER 6. RESULTS

Figure 6.2: Depth-dose curve comparison between Pegasos and Geant4 with scoring radius 4 mm. Average differences are 6.15% and 8.36% for Pegasos and old Pegasos respectively.

Figure 6.3: Depth-dose curve comparison between Pegasos and Geant4 with scoring radius 8 mm. Average differences are 8.65% and 10.76% for Pegasos and old Pegasos respectively.
Figure 6.4: Depth-dose curve comparison between Pegasos and Geant4 with scoring radius 16 mm. Average differences are 8.01% and 10.00% for Pegasos and old Pegasos respectively.

Figure 6.5: Depth-dose curve comparison between Pegasos and Geant4 with scoring radius 100 mm. Average differences are 4.71% and 5.84% for Pegasos and old Pegasos respectively.
CHAPTER 6. RESULTS

Figure 6.6: Depth-dose curve comparison between Pegasos and Geant4 with scoring radius 100 mm with energies 100 MeV and 135 MeV. Average differences for (a) and (b) are, for Pegasos 4.93% and 4.47% respectively and for old Pegasos 6.20% and 5.99% respectively.

Figure 6.7: Depth-dose curve comparison between experimental PTC data, Geant4 and Pegasos at energy 170 MeV.
Figure 6.8: Depth-dose curve comparison between experimental PTC data, Geant4 and Pegasos at energy 135 MeV.

Figure 6.9: Depth-dose curve comparison between experimental PTC data, Geant4 and Pegasos at energy 100 MeV.
Figure 6.10: Depth-dose curve comparison between Pegasos (lines) and TSL (dots) with 100, 75, 50, 25 and 0 mm PMMA, following the colour scheme. Average differences are, from 100 mm to 0 mm PMMA, 8.79%, 8.58%, 7.34%, 2.11% and 0.31%.
Figure 6.11: Depth-dose curve comparison between old Pegasos (lines) and TSL (dots) with 100, 75, 50, 25 and 0 mm PMMA, following the colour scheme. Average differences are, from 100 mm to 0 mm PMMA, 4.01%, 5.07%, 5.03%, 0.60% and 0.08%.
CHAPTER 6. RESULTS

Figure 6.12: Lateral halo dose curve comparison between Pegasos and Geant4. Showing radial dose density at radii 75 mm to 250 mm. Average differences are 5.40\% and 7.72\% for Pegasos and old Pegasos respectively.

Figure 6.13: Photon spectrum behind the water phantom.
6.4. ANGULAR DISTRIBUTION

Figure 6.14: The angular distribution, in the CM frame, of elastic neutron scattering against hydrogen at three different energies. The isotropic angular distribution is also plotted for reference.
Figure 6.15: The angular distribution, in the CM frame, of elastic neutron scattering against oxygen at three different energies. The isotropic angular distribution is also plotted for reference.
Chapter 7

Discussion

In this chapter the results presented in chapter 6 are discussed. It is again important to emphasize that all differences between the old Pegasos and Pegasos with neutron implementation cannot solely be contributed to the neutron extension. As mentioned in section 5.2 other corrections were also fixed during the process of this work. Especially, the implementation of proton Q-values, which was conducted simultaneously, has an important contribution to the characteristics of the dose curves.

7.1 Geant4 Benchmark

7.1.1 Bragg Peak

The reason for the discrepancy of the Bragg peak position between Geant4 and Pegasos is unknown. Different Geant4 EM physics models were tested, but the stopping power stayed indifferent. Earlier benchmark, conducted by Sterpin et. al. [45], between then PENH code and Geant4 (through the encapsulating program GATE) in water, with initial proton energies 100 MeV and 250 MeV, also manifests, although smaller, difference in in the Bragg peak position. However, in Sterpin et. al. the thickness of the $z$ bins were 1 mm in comparison to 0.5 mm in this work, which could explain the somewhat smaller discrepancy. Indeed, when reproducing the benchmark conducted by Sterpin et. al., a similar result is obtained by Pegasos.

PENELOPE and PENH both have their own database, which consequently Pegasos inherit [10, 26]. The stopping power is determined from a re-normalization to the ICRU data. In other words, Pegasos should reproduce the range calculated from the ICRU’s stopping power. For more information about the databases used in PENELOPE and PENH, the reader is referred to [10] and [26] respectively.

An important observation is that, in the depth-dose curves presented in figures 6.2 to 6.5, the dose deposit at the Bragg peak is higher for Geant4 at scoring radius $r = 4$ while for larger scoring radii the Pegasos has a higher
dose deposition at the Bragg peak. These observations can also be studied in lateral dose distribution, presented in figures 6.1a to 6.1d. This implies a difference in lateral sharpness between the two codes and thus a probable difference in the MSC model used. Indeed, there has been suggested that the Geant4 multiple scattering model should be revised, which could be a source for this discrepancy [46]. As stated in section 2.1.3, the MSC models of both Pegasos and Geant4 incorporate the Lewis theory. However, the spatial displacement algorithms are not part of the Lewis theory and is the main source of uncertainties, as mentioned in section 2.1.3. Further discussion of the lateral profile between Pegasos and Geant4 will now be presented in the following section.

7.1.2 Lateral Dose Distribution

From the lateral dose of at the Bragg peak, figure 6.1d it is hard to make any clear conclusions since the Bragg peaks lateral dose density is very sensitive at which depth the dose is taken. Consequently a small location difference between two Bragg peaks will have a substantial impact on the lateral dose density at a given depth. As stated above, the Geant4’s total Bragg peak dose is greater for dose radii up to 4 mm, while smaller for 8 mm and greater, in comparison to Pegasos. This behaviour is not displayed in figure 6.1d due to the sensitiveness of measurement position.

For lateral dose distributions shown in figures 6.1a and 6.1b, there is a clear difference between at the initial phase of the simulation, where Pegasos has deposit a large dose than Geant4, equivalent to what characteristics shown in this domain for the depth-dose curve in figure 6.5. In addition, there is also notable differences to the “old Pegasos” which cannot be explained by the neutron implementation. Most probably, the difference arises from the Q-value implementation resulting in lower deposit dose, since most proton non-elastic nuclear reactions towards oxygen are endothermic [9].

7.1.3 Build-up

As one can note from figures 6.2 to 6.6 there is a difference in the initial build-up between Geant4 and Pegasos, as well as the dose at the beginning of the curve. It has been shown in earlier studies that there is a clear difference between the Geant4’s binary cascade and pre-compound model at the initial phase of the dose-curve [45]. The energy dose was shown to be significantly higher for the Geant4 pre-compound model since the model on average transferred a larger fraction of the initial energy to heavier elements whereas the binary cascade, on the other hand, transferred more initial energy to secondary protons and neutron [46]. Since Pegasos used a pre-compound model, this may be a factor of the initial difference in dose at the first phase of the dose between Pegasos and Geant4.
A second explanation of the lack of build-up in the initial phase of Pegasos could be the s-wave approximation applied for all nuclear interactions, except for neutron elastic scattering. At higher energies, the de Broglie wavelength cannot be approximated to be much greater than the target nucleus and the isotropic s-wave approximation of angular distribution is no longer valid. This phenomenon is illustrated in figures 6.14 and 6.15. Since the protons are energetic at the initial stages of the build-up, this could be a contributing factor of the smaller build-up in the Pegasos dose curves, supposing the proton angular distribution will be similar to the neutron’s.

A third explanation could come from heavier secondary charged particles not being transported in the Pegasos framework, but absorbed locally. By studying figure 1.2 at higher proton energies, it is clear that especially creation of alphas and deuterons should not be neglected. Taking into account a non-trivial angular distribution, these heavier particles would transport some dose to a greater penetration depth. It is, however, unclear if this contribution would be significant enough for explaining the lack of build-up or the higher initial dose demonstrated. Probably, the answer is, at least partially, the joint contribution of all three aspects presented above.

### 7.1.4 Lateral Halo Benchmark

To clearly observe the contributions of the neutron extension to the Pegasos code, the lateral halo benchmark was conducted, presented in figure 6.12. One can in figure 6.12 indeed observe a prominent difference to the old Pegasos code, having no neutron implementation. However, Geant4 manifests a still larger dose deposit in this domain. This difference could be explained by two factors. First, this larger dose could be explained by nuclear decay, resulting in emitted gammas. Nuclear decay and a temporal dimension are not implemented into the Pegasos framework and could thus be an possible explanation to the larger dose deposit at the lateral halo benchmark demonstrated by Geant4. Secondly, the less dose manifested in Pegasos could also be due to the fact that neutrons below 10 keV is not simulated, which dominant contribution is through neutron capture to deuterium resulting in an emitted gamma of 2.2 MeV.

### 7.2 Benchmark to experimental data

In this section the benchmarks against experimental data from PTC and TSL will be discussed.

#### 7.2.1 PTC

As shown in figures 6.7 to 6.9, neither Pegasos nor Geant4 reproduces the PTC benchmark. In fact, the agreement between the two Monte Carlo engines is
CHAPTER 7. DISCUSSION

better than to the experimental data obtained from PTC. The difference in the Bragg peak’s position becomes even clearer when the incident proton energy is decreased to 135 MeV and subsequently 100 MeV. Though the dislocation of the Bragg peak between Geant4 and Pegasos stays indifferent, the dislocation towards the PTC’s Bragg peak increases. The essential factor of these illustrated differences arises from the uncertainties of the incident proton beam’ energy spectrum in the PTC data. Hence only conclusions from the shape of the depth-dose curves can be drawn.

Another source of controversy arises regarding the normalization of the PTC data. Since the energy deposit at the Bragg peak is very sensitive to a small translation, normalizing to that energy will consequently contribute to additional uncertainties about the shape of the curve. A better alternative would have been to normalize to the dose in the intermediate region of the depth-dose curve, where it demonstrates a more stable behaviour.

In figures 6.7 to 6.9 the absence of an initial build-up in the Pegasos’ curve, once again becomes observable. Possible reasons for this has already been discussed in section 7.1.3. However, worth noting is that the shape correspondence between Geant4 and Pegasos is good in the PTC benchmark.

7.2.2 TSL

As demonstrated in figures 6.10 and 6.11, the fit against old Pegasos is remarkably good while for the current Pegasos version poorer. In comparison, it appears that Pegasos has too few nuclear reaction in the PMMA, thus depositing an overdose in the water phantom in contrast to old Pegasos. In fact, in the dose cylinder, 1.69% less energy is deposited in the 0 mm PMMA in Pegasos in comparison to old Pegasos. On the other hand, 2.59% more energy is deposited in the 100 mm PMMA benchmark for Pegasos in respect to old Pegasos. The reason for the lesser dose in 0 mm PMMA is most probably due to the Q-value implementation. However, the source of the higher dose in 100 mm PMMA could arise from a "bug" within the Pegasos code handling nuclear reaction cross sections for protons. Changes has been done in these sections of the code during the process of this work, which can have lead to the creation of these bugs.

A danger in the PENH and PENELOPE codes is that they use implicit declarations, leaving room for typos. These bugs can often be hard to notice and a debug editor and/or print-statements is often needed. An alternative would be to remove all these implicit statements by invoking "implicit none" in the FORTRAN77 subroutines. To increase the robustness of the code this would be advised, but, however, this would be a drastic change in the architecture of the source code and thus time consuming.
7.3 Photon Spectrum

The objective of obtaining the photon spectrum was to verify the implementation of neutron radiative capture to deuterium. In figure 6.13 one can clearly observe a peak in at 2.2 MeV corresponding in the gamma emitted from the neutron capture. However, in this thesis, no comparison was done against any experimental data. Nonetheless, figure 6.13 clearly demonstrate the presence of the neutron radiative capture to deuterium.

7.4 Angular Distribution

From figures 6.14 and 6.15 it is clear that the s-wave approximation is poor for heavier target elements or high energetic neutrons. In this thesis the angular distribution implementation has solely been done for neutron elastic scattering. However, it is most likely that the tendencies are similar for all nuclear reactions for neutrons as well as protons. Especially, in dosimetry aspects, angular distribution for proton nuclear interactions needs to be implemented for a more accurate model. It is plausible that the angular distribution contributes to the steeper build-up manifested in the Geant4, as well as the experimental benchmarks.
Chapter 8

Conclusion and Summary

8.1 Conclusion

Some different aspect of the lack of build-up and higher dose, at the earlier stage of the depth-dose curves, has been discussed. These could be partially be explained by a trivial angular distribution, precompound model and local absorption of heavier charged particles. Especially non-trivial angular distribution for protons and transport of heavier charged particles into the Pegasos framework is advised.

The observed range difference between Pegasos and Geant4 could be caused by the fact that different data libraries are used. The discrepancy in range between Pegasos and Geant4 is a subject that would need further investigations before any other conclusions could be drawn. In addition there was a deviation of the lateral distribution manifested between Geant4 and Pegasos, where Pegasos demonstrated a broader lateral profile. However, Geant4’s MSC model had in earlier articles been criticized, which put doubts on the accuracy of that model.

Helium is excluded from this neutron implementation. Though not being prominent a element in human tissues, helium could be present in a commercial setup as cooling device. Thus for a complete Monte Carlo program, ready for simulating clinical cases, these nuclear reaction data at therapeutic energies needs to be obtained. In addition, hydrogen and helium, with respective isotopes, are excluded from the proton nuclear reaction simulation, which is far more pressing. However, external programs have in this work been taken into place with the purpose to translate the ENDF-6 format to the Pegasos nuclear library. Thus the main objective in future editions would be to obtain these nuclear data, preferably in the ENDF-6 format.

Few conclusions could be drawn from the PTC benchmark, due to lack of information of the proton beam’s energy spectrum. Nonetheless, the lack of build-up was again manifested. For the TSL benchmark, a clear difference was observable, probably arising from fewer occurrences of nuclear reactions
in the PMMA, for Pegasos in comparison to old Pegasos. Most probably, this difference resulted from a "bug" within the proton non-elastic nuclear reaction handling the cross sections. Thus future investigation concerning the proton reaction cross section code is necessary to correct this error.

The halo benchmark was performed with the objective of measuring the neutron contribution and subsequently comparing it to the Geant4 engine. In earlier benchmarks presented, there could be many factors responsible for the differences between the two Pegasos codes. Hence the halo benchmark was an important tool for observing the neutron’s dose contribution.

In addition, there has been concluded that the source for the demonstrated dose difference against Geant4 in the lateral halo benchmark could be contributed to extra gammas emitted by radiative nuclei and/or by radiative capture by thermal and intermediate neutrons. There is, however, a clear difference of the halo dose in comparison with Pegasos to old Pegasos. This fact demonstrates the dose contribution from the neutron implementation. Radioactive decay of unstable nuclei is not implemented in Pegasos and is thus an omitted dose contribution. This is an aspect that could be interesting in future developments of the Pegasos framework.

Eventually, the photon spectrum clearly illustrate the presence of neutron capture from hydrogen to deuterium. However, these results has not been compared to any other sources for validation.

### 8.2 Summary

#### 8.2.1 Progress

As stated in section 1.4, the aims of this thesis were divided into two parts. First an benchmark of the initial Pegasos code, in this thesis called "old Pegasos", to primarily Geant4 and subsequently TSL and PTC. The second aim was to incorporate the neutron transport into the Pegasos code. However, to clarify how the actual work process was manifested, i.e. in what time-frame each progress was taken place, this section will present an overall summary of the thesis, in chronological order.

#### 8.2.1.1 Geant4

At the time of this benchmark, only benchmark against the PTC data had been conducted for the proton nuclear reaction implementation, without nuclear data of air [8]. Since the energy spectra of the PTC beam was unknown, only small conclusions could be drawn from this benchmark. From these initial premises the Geant4 benchmarks were conducted, to benchmark against another Monte Carlo engine, well known in the nuclear community. From the Geant4 benchmark we could witness a relatively good agreement, better than to the PTC data. With this in mind, the Geant4 benchmark was essential
8.2. SUMMARY

for the progress of this thesis’ later implementation of the neutron transport. However, before beginning the neutron implementation, another experimental benchmark was first executed, the TSL and PTC benchmark.

8.2.1.2 Experimental Benchmark

The TSL benchmark was conducted in order to have an experimental benchmark where more information of the experimental setup and energy spectrum were available, in order to draw more conclusions than the PTC benchmark. This benchmark, presented in figure 6.11, showed remarkably good agreement between the Pegasos and TSL and, together with data results from the earlier benchmarks, it was subsequently concluded that the initial foundation for Pegasos was sufficiently validated for continuing the progress to the neutron implementation.

8.2.1.3 Neutron implementation

For consistency in the physics model, the neutron implementation has followed that of proton transport, using TALYS as the nuclear data library. However, TALYS does not include nuclear data of hydrogen nor helium, where, especially hydrogen, constitutes an crucial part of the neutron interaction. Hence, the ENDF library was used for obtaining nuclear reaction data of the neutron-hydrogen interaction up to 150 MeV. Unfortunately the ENDF nuclear data of helium- and other hydrogen isotopes were only available up to 20 MeV and their incorporation into Pegasos was thence not carried out in this thesis. External FORTRAN77 programs where used for interpolation and extrapolation of the ENDF data to the TALYS output format.

Special care was taken into account for the neutron-hydrogen interaction. First, through radiative capture a deuterium and an emitted gamma ray of 2.2 MeV is obtained. Secondly, elastic scattering against hydrogen results in a recoil proton subsequently tracked, if higher than the kinetic threshold, in the Pegasos framework.

Instead of an isotropic sampling in the CM frame, angular distribution of elastic neutron scattering was implemented, through the use of the Legendre series. These Legendre coefficients were available both in TALYS and ENDF libraries, and are handled in Pegasos in a general fashion making the implementation easy to extend to protons and heavier charged particles. Figures 6.14 and 6.15 undoubtedly states the importance of non-trivial angular distribution for elastic neutron scattering and the importance of a non-trivial angular distribution is, most probable, equivalent for protons.

The main objective of this thesis has been the implementation of neutron transport into the Pegasos framework. Consequently, for consistency, the focus has been on expanding the neutron code in contrast to expansion of the proton code. It is worth pointing out though, that for dosimetry aspects,
incorporating proton-hydrogen nuclear data and angular distribution for protons would clearly have had a larger effect, in comparison to the neutron’s, and should be a next step in the enhancement of Pegasos. However, the hydrogen interactions plays a crucial role in neutron interactions and excluding them, in favour for hydrogen interaction to proton, would clearly have put doubts on the validity of the neutron implementation. Thus focus in this work has fully been on the neutron extension. To summarize, through this neutron implementation better information is applicable for radiation shielding for personnel and patient in clinical settings.

8.2.2 Outlook

Transport of heavier particles, such as alphas, deuterons and tritons, needs to be implemented in the Pegasos code. By looking at the secondary production cross section in oxygen, showed in figure 1.2, it is clear that at below ≈ 50 MeV the most probable secondary product, except protons, are alpha particles. In addition, at higher incident proton energies, these heavier charged particles would be able to transfer energy farther in the medium. In the current implementation of Pegasos these particles are absorbed locally. The role of heavier charged particle transport has already been discussed in relation to lack of build-up.

For a complete code, the effect of bremsstrahlung should also be modelled. Though the effects in clinical energies are minimal, the excited electrons will produce bremsstrahlung which ought should be taken into account. For this purpose [47] could be helpful.

As a next step, angular distribution for proton nuclear reaction as well as proton nuclear reactions against hydrogen and helium are recommended. These could also play an important role in the build-up demonstrated the initial phase of the dose deposition. For a complete model, ready for clinical and commercial cases, these implementations are essential.
Bibliography


[41] Proton Therapy Center. URL http://www.ptc.cz/


