Assessment and Correction of Image Degradation in MeV Cone Beam Computed Tomography

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Every scientific statement is provisional. Politicians hate this. How can anyone trust scientists? If new evidence comes along, they change their minds.

The Science of Discworld IV: Judgement Day
Terry Pratchett, Ian Stewart and Jack Cohen
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Abstract

This work represents a detail assessment of all image degrading effects present in a mega-electronvolt (MeV) X-ray Cone Beam Computed Tomography (CBCT) system. A combination of Monte-Carlo (MC) simulations and validating measurements were able to determine the object, with its scattered radiation and its non-linear effects on the X-ray spectrum as well as the detector and its non-linear X-ray conversion and signal spread as the main sources of signal degradation. The studies served as an input for correction methods improving the quality of the reconstructed images. The developed correction algorithms contained a fast MC evaluation of object scattered radiation paired with a hardware based detector filter optimization and a statistical reconstruction. Examples of steel objects showed the success of the optimization and correction approach.

Keywords: X-ray imaging; Monte-Carlo simulation; Industrial Computed Tomography; Reconstruction.
Kurzfassung

Diese Arbeit beinhaltet eine detaillierte Untersuchung aller bildschwächen-
den Effekte in der MeV Röntgencomputertomographie mit Kegelstrahlgeometrie. Eine Kombination von MC Simulationen und validierenden Messungen konnten das Objekt mit seiner Streustrahlung und dem nicht-
linearen Effekt auf das Röntgenspektrum und den Detektor mit seiner nichtlinearen Signal Umwandlung und seiner Unschärfe, als Hauptkomponenten der Bildschwächung bestimmen. Die Untersuchungen dienten als Vorraussetzung und Input für die Entwicklung von Korrekturalgorith-
men zur Verbesserung der Bildqualität. Die entwickelten Algorithmen bestehen aus einem beschleunigten MC Verfahren zur Auswertung der Streustrahlung und der Spektren des Objekts in Kombination mit einer Systemoptimierung basierend auf detektorseitiger Filterung des Rönt-

Stichworte: Röntgentechnik; Monte-Carlo simulationen; Industrielle Röntgencomputertomographie; Rekonstruktion.
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Acronyms

CT Computed Tomography
CBCT Cone Beam Computed Tomography
eV electronvolt
keV kilo-electronvolt
MeV mega-electronvolt
EMPA Eidgenössische Materialprüfungs- und Forschungsanstalt
POD probability of detection
SNR signal-to-noise ratio
RF radio frequency
SPR Scatter to Primary Ratio
FDK Feldkamp-David-Kress
PSF Point Spread Function
MTF Modulation Transfer Function
LSF Line Spread Function
ESF Edge Spread Function
QAE Quantum Absorption Efficiency
MC Monte-Carlo
EM Expectation Maximization
**FDK**  Feldkamp-Davis-Kress

**FT**  Fourier Transform
Part I

Introduction and Basics
Chapter 1

Introduction

1.1 High Energy Industrial X-ray Computed Tomography

Industrial X-ray Computed Tomography (CT) is a non-destructive measurement technique that uses irradiation for the inspection and metrology of the interior and exterior features of an object. The basics of the technique of industrial X-ray CT do not differ greatly from its medical counterpart, however, as opposed to medical applications of X-rays, the radiation doses do not play such an important role in the industrial field of X-ray measurements. As a result, a wide range of X-ray energies can be used for industrial CT applications. Conventional systems use X-ray spectra of tens of kilo-electronvolt (keV) up to several hundred keV dependent on the use case. Deciding factors for the X-ray energy are mainly the size of the object, the density of the material as well as the desired resolution of the resulting reconstructed 3D volume. Generally speaking, the energy of the X-rays limits their penetration length in a given object. As a consequence, for the investigation of larger objects such as truck engines or very dense objects such as turbine blades high X-ray energies exceeding 1 MeV are needed in order to achieve measurable transmission values.

In the following the term high energy will refer to these types of X-ray CT systems with source spectra exceeding 1 MeV. These high energy systems do not only differ in energy from lower energy CT setups.
The high energetic radiation can not be produced in a traditional X-ray tube any more, but has to be created with a linear accelerator with a transmission target. Moreover, as opposed to most lower energetic X-ray CT setups, most current high energy CT employ a line detector and scan in fan beam geometry. While cone beam geometry has the advantage of faster acquisitions due to the 2D capabilities, the increased impact of scattered radiation on the radiographic images discouraged users of its use in high energy applications. The physical interactions present at several mega-electronvolt (MeV) are mainly photoelectric absorption, Compton scattering, Rayleigh scattering and Pair Production. For a reliable investigation with a high energy Cone Beam Computed Tomography (CBCT) setup the influence of these processes on radiographic signal quality have to be understood and reduced. So far, these type of investigations of physical interactions have been performed for low and medium energy X-ray radiation up to 450 keV. This project should address the field of high energy X-ray inspection by performing a detailed analysis of all parameters influencing the quality of radiographic images. The aim is to gain a deep understanding of the sources of artefacts in high energy CT systems. The examination will specifically incorporate the effects of environmental scattering and deteriorating effects coming from the detection system itself.

To carry out the research in this project a combination of simulations and measurements will be performed. The work will start with a series of Monte-Carlo simulations of the CT system. The results will help to understand and quantify the influence of the system components as well as the contribution of the physical processes on the radiographic images. The knowledge of the deteriorating effects in the CT system shall be used to find new algorithms correcting artefacts in the radiographic images. The final goal of this work is the improvement of both scanning speed and image quality of a high energy CBCT system.

1.2 State-of-the-Art

The task of modeling the radiographic imaging process has been approximated by first order effects using a deterministic simulation [36]. This method is fast, but does not simulate higher-order effects such as multiple scattering. A Monte-Carlo simulation is able to incorporate higher-order effects but the accuracy of Monte-Carlo simulations comes
with much higher computation time. In most cases, where the amount of single scattered photons dominate over the amount of multi-scattered photons, a deterministic approach can be used, while neglecting the effects of multi-scattering. This fact constrains the applicability to configurations where the multi-scattered photons are negligible [80]. For a fast simulation that still incorporates higher-order effects, hybrid methods that use both the deterministic and the Monte-Carlo method have been proposed [3], [78]. The existing X-ray simulation frameworks employed at the Center for X-ray analytics of Eidgenössische Materialprüfungs- und Forschungsanstalt (EMPA) covered an energy range up to 450 keV. For energies exceeding 1.022 MeV the list of physical effects has to be extended to incorporate the effect of pair production, which is not present at lower energies.

Inspections of large objects with energies above 1 MeV have been performed for more than a decade [37]. These CT systems consist of a linear accelerator to produce X-rays at several MeVs combined with a line detector which uses individually collimated detector channels. Simulations of the source spectrum and attenuation behaviour have been examined [42] and several artefact correction schemes have been suggested [64]. Moreover, the importance of scattered radiation in radiographic imaging has been analytically examined [80].

The variety of measurement tasks in industrial CT imposes another important task in the analysis of high energy CT systems. Aspects, such as probability of detection (POD) and measurement uncertainty, rely on properly chosen measurement parameters, such as voxel size, contrast and signal-to-noise ratio (SNR) [23], [40]. Algorithms and simulations for the calculation of these parameters have been developed for systems with energies ranging up to 450 keV [63]. For systems with higher energies, these algorithms do not exist yet and trial-and-error runs are needed for the inspection of each new sample type.

1.3 Motivation

In order to assess the capabilities and challenges posed by the CBCT system with MeV source, the setup seen in Figure 1.1 was employed at the Center for X-ray analytics at EMPA and a CT scan of a steel casting part (seen in Figure 1.2) was performed. The data was reconstructed
with a Feldkamp-Davis-Kress (FDK) algorithm and a Hamming filter. The measurement settings of source and detector can be found in table 1.1.

**Table 1.1:** Acquisition parameters corresponding to the measurement of the steel cast part shown in Figure 1.2.

<table>
<thead>
<tr>
<th>X-ray Source - Pulstar Linac PSL-6D</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
<td>6.0</td>
<td>MeV</td>
</tr>
<tr>
<td>Frequency</td>
<td>125</td>
<td>pps</td>
</tr>
<tr>
<td>Dose rate at 1m distance</td>
<td>94</td>
<td>mGy/s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Detector - XRD 1621 AN14 ES</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Gain</td>
<td>0.5</td>
<td>pF</td>
</tr>
<tr>
<td>Binning mode</td>
<td>no binning</td>
<td></td>
</tr>
<tr>
<td>Integration time</td>
<td>1500</td>
<td>ms</td>
</tr>
</tbody>
</table>

**Figure 1.1:** Experimental setup.

The slices of the reconstructed volumes that can be seen in Figure 1.4 show the typical artefacts originating from scattered radiation and the effect of beam hardening. The first artefact that can be noticed are streaks artificially connecting parts of the object. It is known that these
1.3 Motivation

Figure 1.2: Object for the naive scan.

Figure 1.3: Selected projections from a scan of a steel casting part. The scan was performed with a 6 MeV spectrum created by a linear accelerator. The flat panel detector is from Perkin Elmer with a pixel pitch of 0.2 mm, the scan was taken with a binning factor of 2 and an angular increment of 0.25°.

streaks can be caused by photon starvation, however, beam hardening and scattered photons add to the degradation effect leading to the streak artefacts. In addition to that, a non-uniform grey value distribution can be observed in large areas of single materials, specifically in Figure 1.4a. This artefact is known as cupping. A cupping artefact typically results
from beam hardening, but can be caused by scattered radiation as well. Generally, a loss of contrast stemming from these effects can be noticed in the reconstructed slices. Particularly, dimensional measurements suffer from the blurred edges, which hinder an accurate surface detection, and thus, prevent the exact measurements of sizes and wall thicknesses. On top of that, the blurring as well as the artefacts can lead to a decreased flaw detection capabilities masking imperfections such as cracks or voids.

### 1.4 Structure of the thesis

This dissertation is divided into four main parts. The first part addresses the basics of X-ray imaging, reconstruction and simulation. In part II the MeV CBCT setup will be studied in detail. Simulations paired with validating measurements investigate the possible sources of signal degradation in the X-ray system. The results from part II will serve as an input for the corrections developed in the third part of this work. These correction methods will consist of a combined simulation, hardware and software based approach. A fast evaluation of object scattered radiation by simulation will help optimize a hardware based filter correction of signal degradation. Additionally, a reconstruction based on a statistical pixel neighbourhood prior model will be introduced. In the last part of this work, the results of this dissertation will be summarized and discussed.
Chapter 2

Basics of X-ray Computed Tomography

Just as visible light, X-rays are photons and as such a form of electromagnetic radiation. In the electromagnetic spectrum, X-rays cover an energy range corresponding to ionizing radiation with photon energies ranging from a few keV up to several MeV. Depending on their energy X-rays can be further classified in three categories. Soft X-rays at the lower end of the electromagnetic spectrum, hard X-rays around hundred keV and Gamma rays exceeding one MeV. Due to their higher energy and lower wavelength compared to visible light, X-rays have the ability to penetrate materials, which makes them useful for imaging and investigating the inside of objects as well as humans or animals. The biggest advantage of X-ray imaging is the non-destructive nature of the technique. This chapter will go into details about the fundamentals of X-ray physics as well as the basics of X-ray imaging and X-ray CT.

2.1 X-Ray Production

The first and arguably most essential part of an X-ray CT scanner is its source. Here, the radiation is created by shooting electrons on a target. To be able to describe the physics behind this form of beam production, the interaction of charged particles with matter have to be described first. Afterwards the X-Ray production and the energy spectrum that results from it can be investigated.
2.1.1 Interactions of charged particles in matter

A charged particle passing through matter will interact either with an electron of an atom in the material or with its nucleus. The interactions are dominated by the Coulomb force and can be categorized using the so-called impact parameter [4]. This parameter describes how close an incoming charged particle gets to the nucleus of an atom of the material it is passing through. A sketch of the different impact parameters can be found in Figure 2.1. In this section we will focus on interaction between electrons and matter as they occur in the source of an X-ray system.

![Figure 2.1: Impact parameter b characterizes the charged particle interaction with an atom.](image)

If the impact parameter is big compared to the size of the atom, the incident particle will interact with the atom as a whole. The result of this interaction can be either the excitation or the ionization of the atom. This kind of interaction is classified as a soft collision of the particle with the atom, which leads to a rather small amount of energy transfer. Soft collisions are the most probable kind of interaction for charged particles in matter. In the case of a smaller impact parameter in the range of the size of the atom the most probable type of interaction will be with one of the electrons of the atom rather than with the whole atom itself. The incident charged particle can cause the ejection of an electron from the atom. The subsequent recombination at the atom will result in
radiation which can be detected as characteristic spectral lines. This characteristic radiation from electron matter interactions is known as fluorescence. For an impact parameter that is much smaller than the size of the atom, the interaction will most probably take place between the incident charged particle and the nucleus of the atom. The interaction between the nucleus and the electron can either be an elastic or inelastic scattering event. In the case of elastic scattering, the electron will change direction, but not loose a significant amount of energy. This is not the case for inelastic scattering. Here, the electron looses a part of its energy, which in turn is radiated away in form of a photon. This is the famous effect of Bremsstrahlung, which is the basis of X-ray imaging.

2.1.2 The Source of a CT Scanner

Generally, in a common X-ray tube, electrons are accelerated and shot onto a so-called X-ray target. In the target material two of the previously described processes will result in the production of X-rays, the fluorescence and the Bremsstrahlung. The kinetic energy of the electrons sets an upper limit to the energy of the created X-ray radiation. However, most of the time the deceleration of the electron via the effect of Bremsstrahlung will not be a single event where the electron looses all of its kinetic energy. It is rather a chain of events, each of which results in an X-ray photon with a given energy corresponding to the electrons energy loss. Due to this multitude of possible deceleration cascades in the material, the resulting X-ray Bremsstrahlung spectrum will be continuous. The effect of fluorescence transitions will add characteristic spectral lines to this spectrum given by the energy of the electrons as well as the target material.

Most X-ray systems employ a so-called X-ray cathode or X-ray tube as source. Here, electrons are emitted from an electron gun and then accelerated in a vacuum tube by applying an electric field (see Fig 2.2). In this case the electron emission is a thermionic one, which means the cathode of the system is heated. This leads to electrons being liberated on the surface of a wire, because their thermal energy is higher than the work function of the material the wire is made of. The anode is situated at the end of the tube and acts as a reflection and transmission target for the production of X-rays. A special geometrical form of the target makes sure, that the resulting X-Ray beam is directed on the right trajectory. This can be seen in Fig 2.2.
For the production of X-rays with energies exceeding one MeV another type of source known as linear accelerator is necessary. Just like in the case of the X-ray tube, an electron gun is used in a linear accelerator for the production of electrons. In contrast to lower energetic X-ray sources, the electrons cannot be accelerated by simply applying a voltage to a cathode and anode configuration. For higher energy X-ray production, the accelerating structure of the source is an evacuated tube with cylindrical electrodes of varying lengths. This linear accelerator is fed through a waveguide by a magnetron or a klystron, which acts as a radio frequency (RF) generator. The RF generator creates either a travelling or standing wave which is able to accelerate the electrons towards the target. An additional set of magnets in the tube help focus the beam, which tends to defocus due to space charges. In contrast to traditional X-ray tubes, the electrons and the produced X-rays are at opposite sides of the target. A sketch of a linear accelerator can be seen in Figure 2.3.

2.2 X-ray Physics

After their creation, the X-Rays propagate through the air, hit the object and propagate through it. When the X-ray beam propagates through
the object, naturally, its intensity will be attenuated. This is described by the Lambert-Beer Law. The physics behind this attenuation contains several different processes. In this section, the Lambert-Beer Law will be described shortly and afterwards, the different interactions of X-Ray with matter will be investigated.

### 2.2.1 Lambert-Beer Law

A beam of X-Rays which travels through a piece of material, will experience a decrease in intensity. This attenuation can be described by a parameter that is called attenuation coefficient \([12]\). Let \(I(x)\) be the intensity of the X-Ray beam at position \(x\) along a line. After passing through a slice of material of thickness \(dx\), the intensity will have decreased.

\[
I(x + dx) < I(x)
\]

For infinitesimal steps \(dx\), this can be used to define the attenuation coefficient \(\mu(x)\) at each position along the line.
\[ I(x + dx) = I(x) - \mu(x)I(x)dx \]
\[ \frac{I(x + dx) - I(x)}{dx} = -\mu(x)I(x) \]

This last differential equation can easily be solved assuming a linear attenuation, that means the attenuation coefficient is constant with respect to \( x \), \( \mu(x) = \mu \). The result is the Lambert-Beer Law.

\[ I(x) = I_0e^{-\mu x} \]

The linear attenuation coefficient \( \mu \) contains all physical processes that lead to the attenuation. It is a combination of the attenuation coefficient concerning scattering \( \mu_{scatter} \) and the attenuation coefficient for absorption \( \mu_{absorption} \).

\[ \mu = \mu_{scatter} + \mu_{absorption} \]

The linear attenuation coefficients are proportional to the cross sections of the interaction processes that are involved in the attenuation. That means, finding the physical processes that are involved and their cross sections can lead to a prediction of the attenuation of an X-Ray beam. This will be done in the next section.

### 2.2.2 Interactions of X-Rays with matter

While travelling through matter, X-Rays undergo several interactions, which either result in scattering or absorption of the photon. The proba-
bility of these events depends on the energy of the photon and on the atomic number of the material [4]. In X-ray CT, the four most important interactions are the Photoelectric Effect, the Rayleigh Scattering, the Compton Effect and Pair Production. The probability of occurrence of the different interactions is given by their physical interaction cross section. This quantity depends on the atomic number of the material as well as the energy of the incident photon. The following sections describe the physics behind these main interactions in X-ray CT. Moreover, the rate of occurrence with respect to the atomic number and the energy of the X-ray photon will be assessed.

**Photoelectric Effect**

![Figure 2.5: Photoelectric Effect](image)

In the Photoelectric Effect, or Photoelectric Absorption, the X-Ray will be absorbed by the atom. The energy transfer will cause one of the inner shell electrons to be kicked off the atom. As a result, the outer shell electrons will fill the vacancy left by the emitted electron. The excess on energy will be radiated away in form of a photon. A sketch of the process of Photoelectric Absorption can be seen in Fig. 2.5. The maximum of the kinetic energy of the emitted electron can be calculated using energy momentum conservation.

\[
E_e = E_{\text{photon}} - E_b
\]  

(2.1)

The term \(E_b\) describes the binding energy of the electron. The energy of the X-Rays that originate in the recombination process depends on the transition levels between the shells. Because of the shell like arrangement, as described by the Bohr model of the electrons of an atom, there are a limited number of transitions that can occur and thus, the result
are X-Ray photons with specific energies, that form a characteristic line spectrum for the material. The cross section for the Photoelectric Absorption depends on the atomic number $Z$ of the material and the photon energy $E$.

$$\sigma \propto \frac{Z^n}{E^{3.5}}, \ n \in [4, 5]$$

Equation 2.2 shows that the cross section of the photoelectric effect is inversely proportional to the energy of the X-ray photons. This means that the occurrence of the photoelectric effect will decrease drastically at higher X-ray energies. However, the actual cross section is more complex. In reality the cross section will be decreasing up until the energy of the photon is high enough to excite the next available electron shell of the atom, at this point the cross section will have a jump. This effect can be seen as characteristic absorption edges. A sketch of the cross section of the photoelectric effect can be seen in Figure 2.6.

![Figure 2.6](image)

**Figure 2.6:** Sketch of the cross section of photoelectric absorption with respect to the energy of the photon for lead. Data was taken from the NIST database of cross sections [58].

The binding energies in equation 2.1 depend on the atom that is investigated, but in general they can reach from a few electronvolt (eV) up to about 100 eV. This means, that the cross section will have the spectrum shown in Figure 2.6 up to the highest binding energy and
for higher photon energies, it will decrease with $\frac{1}{E^{3.5}}$. As a result, the photoelectric absorption will be the dominant effect for low energy photons of a few eV, but other effects will be dominating for photon energies above 100eV.

**Compton Effect**

The Compton Effect is also known by the name Compton Scattering. It describes an inelastic scattering interaction of a photon by an electron. This electron is typically assumed to be free, but in most cases the electron is actually lightly bound to one of the atoms. The photon will be deflected and it will transmit a part of its energy to the electron, which can be kicked of the atom. A sketch of the Compton interaction can be seen in Figure 2.7.

![Figure 2.7: Sketch of Compton Scattering.](image)

The energy transferred between the photon and the recoil electron and the scattering angle $\theta$ are linked by energy and momentum conservation. The resulting Klein-Nishina formula describes the energy $E$ of the scattered photon dependent on its scattering angle $\theta$, and its initial energy $E_0$.

$$E(\theta) = \frac{E_0}{1 + \frac{E_0}{m_e c^2} (1 - \cos \theta)}$$  \hspace{1cm} (2.3)

From equation 2.3 the so-called Klein-Nishina differential cross section can be derived (see equation 2.4). Compared to the cross section, a differential cross section describes the interaction probability with respect
to a solid angle \( d\Omega = \sin \theta d\theta d\phi \). This means, the Klein-Nishina differential cross section illustrates the interaction probability per scattering angle with respect to the energy of the incident photon.

\[
\frac{d\sigma}{d\Omega} = \frac{1}{2} \left( \frac{e^2}{4\pi \epsilon_0 m_e c^2} \right)^2 \left( \frac{E}{E_0} \right)^2 \left( \frac{E_0}{E} + \frac{E}{E_0} - \sin^2 \theta \right)
\]

\( r^2_e \), classical electron radius

Figure 2.8 shows the cross section with respect to the scattered angle for various photon energies. It can clearly be seen here, that for higher energies the dynamic of the interaction becomes more forward directed.

\[ \text{Figure 2.8: Klein-Nishima Cross section with respect to the scattered angle for different energies} \]

At the limit of low photon energies in the range of the rest energy of the electron, the Klein-Nishina differential cross section becomes the Thomson cross section. Equation 2.5 shows that in contrast to the Klein-Nishina cross section, the Thomson cross section does not depend on the energy of the photon.
\[ \frac{d\sigma}{d\Omega} = \frac{r_e^2}{2} \left( 1 + \cos^2 \theta \right) \] (2.5)

**Rayleigh scattering**

Just as Compton scattering, Rayleigh scattering describes the interaction of a photon with an electron that results in the scattering of the photon. However, in contrast to Compton scattering, the Rayleigh interaction results in almost no energy transfer between the photon and the electron. This means, Rayleigh scattering falls into the category of so-called elastic scattering events. Rayleigh scattering angles are typically much smaller than Compton scattering angles. As a result, the effect of Rayleigh scattering becomes important on narrow beam applications. Similar to the photoelectric effect, the cross section for Rayleigh scattering is inversely proportional to the energy $E$ of the incident photon as can be seen in Equation 2.6. Thus, equivalently to the photoelectric effect, Rayleigh interactions have to be considered mainly in low energy applications. Rayleigh scattering dominates at energies of several tens of keV over all other physical interactions.

\[ \sigma \propto \frac{Z^n}{E^n}, \quad 2 \leq n \leq 2.5 \] (2.6)

**Pair Production**

![Figure 2.9: Pair production due to interaction with the nucleus of an atom.](image)

In the presence of a nucleus or an electron a photon can create a pair of a particle and its antiparticle, namely an electron and a positron
(see Figure 2.9). The photon energy itself will be completely converted, which means, the photon is destroyed in the process. This interaction is called Pair Production. For a photon to be able to create the two particles, it needs an energy that is at least twice times the rest energy of the electron. That means, the interaction of Pair Production does not occur for photon energies below 1.022 MeV. Typically, the positron that is created in a Pair Production event annihilates with one of the electrons in the material. In this annihilation event two photons will be created. If we consider a frame of reference without linear momentum, the direction of the resulting annihilation photons will be opposite to each other, due to momentum conservation. Commonly, the energy of the two photons created in an annihilation event is equal to the rest mass of the electron and the positron (0.511 MeV).

The kinetic energy of the electron and the positron created in a Pair Production event depends on the type of Pair Production that took place. If the Pair Production is a result of the interaction of a photon with the nucleus of an atom the two resulting particles will split the remainder of the photon energy after the rest mass of the created particles has been subtracted (see equation 2.7).

\[
E_{\text{photon}} = 2m_ec^2 + T_{e^+} + T_{e^-}
\]  

(2.7)

Where \(T_{e^+}\) and \(T_{e^-}\) describe the kinetic energy of the created electron and positron. If the Pair Production is a result of the interaction between a photon and an electron of the atom this electron will gain part of the energy as well. The resulting energy and momentum conservation equation can be seen in equation 2.8.

\[
E_{\text{photon}} = 2m_ec^2 + T_{e^-,interaction} + T_{e^+} + T_{e^-,produced}
\]  

(2.8)

Here \(T_{e^-,interaction}\) describes the kinetic energy of the electron that initially interacted with the photon after the interaction. \(T_{e^-,produced}\) is the kinetic energy of the electron that was produced in the pair production interaction. Francis Perrin [60] showed, that due to momentum conservation, the threshold for this second process is 2.044MeV = 4\(m_ec^2\), which is higher than the threshold for general Pair Production interactions. This means the cross section \(\sigma_{\text{pair}}\) of the pair production for photon energies between 1.022MeV and 2.044MeV is given by the cross section for the Photo-nuclear interaction \(\sigma_{\text{photon-nucleus}}\) that creates the particle pair.
1.022\,MeV \leq E_{\text{photon}} < 2.044\,MeV :
\sigma_{\text{pair}} = \sigma_{\text{photon} - \text{nucleus}}

For photon energies above 2.044\,MeV, the total cross section of Pair Production is the sum of the two cross sections for Pair Production due to interaction with the electric field of an electron and Pair Production due to interaction with a nucleus.

2.044\,MeV \leq E_{\text{photon}} :
\sigma_{\text{pair}} = \sigma_{\text{photon} - \text{nucleus}} + \sigma_{\text{photon} - \text{electron}}

Here $\sigma_{\text{photon} - \text{electron}}$ describes the component of the cross section belonging to the interactions with the electric field of an electron. It is worth noting at this point that Pair Production dominates all other physical interaction process for energies above 10\,MeV. Furthermore, from 100\,MeV on the cross section of Pair Production is saturated, that means it can be characterized by a constant.

Interestingly, it has been pointed out by [43], that on the level of Feynman diagrams, Pair Production is similar to Bremsstrahlung. In a Feynman diagram the direction of travelling helps to distinguish between particles and antiparticles. For example, an electron travelling backwards in time is actually an antiparticle, the positron. In Figure 2.10 the two processes of Bremsstrahlung and Pair Production in the form of Feynman diagrams can be seen. It is clear, that by turning the diagram clockwise such that the incident particle is the photon and the formerly incident electron becomes an emitted positron, the Feynman diagram for Bremsstrahlung becomes the Feynman diagram for Pair Production. Feynman developed a set of rules for these diagrams, which make it possible to easily derive transition amplitudes $\mathcal{M}$, which are proportional to the differential cross section, $\frac{d\sigma}{d\Omega} \propto |\mathcal{M}|^2$.

Bethe and Heitler [7] were the first to derive the differential cross section for the process of pair production. They distinguished three different cases, depending on the energy of the incident photon.

- $E_{\text{photon}} \sim m_e c^2$ :
- $m_e c^2 \ll E_{\text{photon}} \ll \frac{137 m_e c^2}{Z^{1/3}}$ :
• \( \frac{137m_ec^2}{Z^{4/3}} \lesssim \frac{E_e^- E_e^+}{E_{\text{photon}} m_ec^2} : \)

Later work of several other authors resulted in corrections the Bethe-Heitler cross section formulas including a Coulomb Correction, a correction for Screening and radiative corrections. The formulas and corrections are summed up in [35].

### 2.2.3 Relative Importance of the different Interactions

Especially for a simulation, it is important to know the relative importance of the different effects of photon interactions to find the most important, dominating effects and to be able to neglect highly improbable effects or even effects that cannot take place in a given situation. Here it is useful to look at the relative occurrence rates of the effects with respect to the incident photon energy. Figure 2.11 shows the cross sections of the different physical interactions for photon energies up to 20 MeV. It is clear that the effect of Photoelectric Absorption dominates at low photon energies, while Compton Scattering starts to dominate at energies of 100 keV and higher. The two different types of pair production come into play above 1 MeV and 2 MeV respectively. However, not only the energy of the incident, but also the atomic number of the material is of importance when discussing the relative importance of physical interactions in X-ray CT. Figure 2.12 shows three regions of importance for the various physical effects. It can be seen, that for low atomic numbers the Compton effect is the main dominant interaction for almost all photon energies. At higher values of the atomic number \( Z \) and low
2.3 X-Ray Detection

Now that the production and the propagation of X-rays have been discussed, the detection of the radiation is the last missing piece for a working X-ray CT system. Detection systems for X-rays can be classified into three general categories: Gas Detectors, Scintillation Detectors and Solid State Detectors. The choice of detector in a given X-ray setup depends on the energy range of the photons as well as resolution and speed requirements of the application. This section will give a short overview over the detection principle of the various detectors. The corresponding advantages and weaknesses of the detectors will be discussed.

### 2.3.1 Gas-filled Ionization Detector

In a gas detector the incident X-Ray interacts with an atom of the gas thereby creating an electron through a process called photo-ionization. These electrons are measured by collecting them on a positive electrode.

Figure 2.13 shows a sketch of a gas-filled ionization chamber. Since the photo-ionization has a rather low probability, these detectors operate

**Figure 2.11:** Relative importance of the main photon interaction cross sections on the example of aluminum. Data was taken from the NIST database [58].

Photon energies photoelectric absorption dominates over the other effects. Pair Production is dominating only for photons at higher energies.
Figure 2.12: Plot of the relative importance of the main photon interaction cross sections with respect to energy and atomic number of the material. Data was taken from the NIST database [58].

Figure 2.13: Sketch of a gas-filled ionization detector.

with high gas pressure. Combined with a tall ionization chamber gas detectors can double as a collimator. This is due to the fact that the signal of photons exceeding a specific entrance angle will generally have a smaller travelled path in the detector resulting in a suppression of their signals [12]. In order to get a good spatial resolution in these types of detectors, several cathodes and anodes have to be set up in an array parallel to each other. Nevertheless, gas-filled ionization detector arrays
typically don’t reach the same spatial resolutions compared to the other possible detectors. However, gas detectors possess the general benefit of having almost no dead time. This means, the time the detector needs after an event before it is able to detect the next event is close to zero.

### 2.3.2 Scintillation Detector

A Scintillation Detector consists of a slab of luminescent material, that has the ability to absorb the total energy or part of the energy of incident photons. The absorbed energy is re-emitted in the form of photons with another wavelength (typically visible light) than the incident photon. This light can be detected with a photomultiplier tube, which converts the light signal into a measurable electric signal while simultaneously amplifying the signal. A photomultiplier consists of a photocathode as well as a range of dynodes and a final anode for charge collection. At the photocathode the incident visible light photons will create electrons due to the photoelectric effect. These electrons will be accelerated and multiplied in a vacuum tube by the Dynodes in order to create a measurable electrical signal at the anode. Another way of detecting the light from the scintillator would be a CCD camera. A sketch of a detector using a luminescent material combined with a photomultiplier tube can be seen in Figure 2.14.

![Sketch of a scintillation detector and its photomultiplier tube.](image)

**Figure 2.14:** Sketch of a scintillation detector and its photomultiplier tube.

The efficiency of a scintillating detector highly depends on the chosen scintillating material. The choice of material defines the after-glow and therefore the dead time of the detector. Scintillation detectors can be arranged in a line or also as flat panel detector. The resolution of a scintillator depends on the readout matrix behind the scintillator, but
also on the size of the scintillating medium. Thick scintillators will have a higher spread of the photons in the luminescent material and thus diminish the resolution of the detector itself. Typical commercial scintillators in flat-panel configuration will reach pixel sizes of 100 µm nowadays. In contrast to the other detectors, scintillation detectors are generally operated as integrating detectors. This means that incident radiation will be measured over a given period of time and the total deposited energy will be recorded. As a result, scintillation detectors can not resolve the energy of the incident radiation.

2.3.3 Solid State Detector

Solid state detectors are build on the basis of semiconductors. This means, incident radiation creates charge carriers in the semiconductor material, which can be measured. The resulting signal will subsequently be amplified and measured. Typically solid state detectors are more sensitive then the other detectors. They should be operated at low temperatures to suppress the formation of charge carriers due to thermal vibrations. However, compared to gas ionization detectors, the energy resolution of solid state detectors is higher. Their time resolution is also high or in other words, their dead time is small.

Figure 2.15: Sketch of a solid state detector.
2.4 X-ray Computed Tomography

Now that the three main parts of a typical X-ray CT scanner have been analyzed, this section will give an overview over typical industrial X-ray CT system configurations. In most industrial CT scanners, the source and the detector stay fixed, while the object is moved in the beam. There are two main architectures that can be distinguished here: A fan beam scanner and a cone beam scanner [12].

**Figure 2.16:** Sketch of a fan beam scanner. As can be seen in the side view in 2.16a, the object can be moved to be able to scan it line by line. The top view 2.16b shows

The main difference between the fan beam geometry (Fig 2.16) and the cone beam geometry (Fig 2.17) is that the former uses a detector that works in 1 dimension, while the latter detects a 2 dimensional image at once. A detector for a fan beam scanner consists of a line of pixels. Here, either the object is moved up and rotated or the source and detectors move up in a synchronized manner in order to scan the
object slice by slice. This up and down movement of the object or the source and detector is typically not necessary for cone-beam systems. The main advantage of a cone beam over a fan beam system is the shorter acquisition time. However, flat panel detectors have a given size limit which means fan beam scanners are usually the only choice for the X-ray analysis of very large objects. Another advantage of fan beam systems over cone-beam CT is the possibility of collimation. In a fan beam geometry the initial X-ray beam as well as the incident beam at the detector can be highly collimated thus reducing the amount of scattered radiation in the image. The detrimental effect of scattered radiation on cone beam measurements will be discussed later in this work. Another consideration on flat-panel over line detector system is the thickness of the scintillating medium. State-of-the-art commercial flat-panel detectors tend to employ very thin scintillating material for the detection of the radiation. While this decreases the spread of the signal and thus increases the resolution capabilities of the detector, it also decreases the efficiency of the detector. Thinner scintillating mediums also result in fewer detected photons generally. Line detectors on the other hand can be chosen with much larger scintillators typically. They usually have a worse resolution than flat-panel detectors, however, their dynamic range is commonly much better. As a result, the choice between a fan-beam and a cone-beam geometry depends on a large set of parameters. The energy of the X-ray beam as well as the object size, desired resolution and acquisition speed play a big role here.

![Figure 2.17: Sketch of a cone beam scanner.](image)
2.5 Image Reconstruction

During a CT scan, the object is measured from different angles. This results in several projections of the object. In order to get the actual CT image from the measurement, the data has to be combined and transformed. This section will introduce the mathematical description of the measurement and give a short introduction into the topic of reconstruction. The following material is a summary of the work in [12, 28, 32]. It is meant to outline the general concepts and ideas behind the various reconstruction concepts.

2.5.1 The Radon Transform

The measured data per angle is the intensity of the X-Ray beam with respect to the position on the detector. This is called the projection of the object. To be able to describe the transformations necessary to reconstruct the object from all of the projections, the coordinate systems have to be defined first. There are two main coordinate systems, one corresponding to the object, and the other one corresponding to the source-detector system.

Let \((ξ, η)\) be the source-detector system and \((x, y)\) the system of the object. A sketch of this configuration can be seen in Fig 2.18. Since the object is rotated, these coordinate systems do not coincide at all.
times. The change in coordinates between the two coordinate systems is a simple polar coordinate transformation.

\[
\begin{align*}
\xi &= x \cos \phi + y \sin \phi \\
\eta &= -x \sin \phi + y \cos \phi
\end{align*}
\]

(2.9)

The projection of the object for angle \( \phi \) at position \( \xi \) on the detector is called \( p_\phi(\xi) \). The attenuation values in the object system are called \( f(x,y) \). The convolution between this function of the attenuation values and the travelled path of the X-Rays \( L \) results in the projection \( p_\phi(\xi) \). This is called the two dimensional Radon transform of the object.

\[
f * \delta(L) = \int f(r)\delta(r - L)dr
\]

\[
= \int_{r \in L} f(r)dr
\]

\[
= p_\phi(\xi)
\]

That means, the object function \( f \) can be determined by measuring \( p_\phi(\xi) \).

The function \( f(x,y) \) describes the attenuation of the object, that is why it is equivalent to the attenuation coefficient \( \mu(x,y) \) introduced in section 3.1. If we define the Lambert-Beer equation in this context, it has to be considered, that the attenuation coefficient is dependent on the travelled path by the X-Rays.

\[
\ln \left( \frac{I}{I_0} \right) = \int_{r \in L} \mu(x,y)dr
\]

\[
= p_\phi(\xi)
\]

2.5.2 Reconstruction and the Fourier Slice Theorem

In the previous section a relation between the measured projection \( p_\phi(\xi) \) and the attenuation function \( \mu(x,y) \) was found. That means, in order to reconstruct the distribution of the attenuation values \( \mu(x,y) \) from the
measured projection values $p_\phi(\xi)$, the Radon transform has to be inverted. There are numerous methods that solve the inverse problem. Generally, the Analytic Reconstruction Methods and the Iterative Reconstruction Methods can be distinguished. A possible approach to invert the Radon Transform relies on the Fourier Transform (FT). The Fourier Slice Theorem uses the FT and the inverse FT to get $\mu(x, y)$ from $p_\phi(\xi)$. Let $\mathcal{F}$ denote the FT and $\mathcal{R}$ the Radon Transform of a function.

$$p_\phi(\xi) = \mathcal{R}(f(x, y)) = \int_{r \in L} \mu(x, y) dr$$

$$\mathcal{F}(p_\phi(\xi)) = \mathcal{F}(\mathcal{R}(\mu(x, y)))$$

This equation can also be written out

$$\mathcal{F}(p_\phi(\xi)) = P_\phi(q) = \int p_\phi(\xi)e^{-2\pi iq\xi} d\xi = \int \mathcal{R}(\mu(x, y))e^{-2\pi iq\xi} d\xi = \int \int \mu(x, y)e^{-2\pi iq\xi} d\xi dr = \int \int \mu(x, y)e^{-2\pi iq(x\cos \phi + y\sin \phi)} dx dy$$

In the last step, the coordinate transformation (2.9) was used. This can now be written as two Fourier Transformations in $x$ and $y$ for $\mu(x, y)$.

$$\mathcal{F}(p_\phi(\xi)) = \int \int \mu(\xi, \eta)e^{-2\pi iq x \cos \phi}e^{-2\pi iq y \sin \phi} dxdy = \mathcal{F}(\mu(q \cos \phi, q \sin \phi)) = M(q \cos \phi, q \sin \phi)$$

The desired distribution of attenuation values $\mu(x, y)$ results by calculating the inverse $\mathcal{F}^{-1}$ of the function $M(q \cos \phi, q \sin \phi)$.

$$\mu(x, y) = \mathcal{F}^{-1}(M(q \cos \phi, q \sin \phi)) = \int \int M(q \cos \phi, q \sin \phi)e^{2\pi ij(x \cos \phi + y \sin \phi)} dq d\phi$$
Because of the relation between the measured projected data and the object data given by the Fourier Slice Theorem, a reconstruction algorithm can be inferred (see Fig 2.19).

**Figure 2.19:** Flow Chart of the Fourier Slice Algorithm for the reconstruction of projected data.

**Figure 2.20:** Spectral representation $P_\phi(q)$ in the spatial domain. The values of $P_\phi(q)$ are only known on radial lines (crossed data points), which means the data gets sparser the farther away from the origin it is. The coordinates used in this picture are $u = x \cos(\phi)$ and $v = y \sin(\phi)$. For the inverse FT the data needs to be interpolated onto a 2D Cartesian grid (gray points).
Although this reconstruction algorithm based on the Fourier Slice Theorem seems to be exact, it has to be noticed here, that the discretization introduced in the measurement process leads to a loss in accuracy specifically outside of the central domain of the reconstructed volume. Figure 2.20 shows, how the discretization in the angular domain effects the accuracy in the reconstruction. This means additional calculations have to be performed in the form of cartesian regridding as well as a filling of the Fourier space in order to be able to use the Fourier Transformation Algorithm as reconstruction.

2.5.3 Reconstruction by Simple Back Projection

The naive way of approaching back-projection is to take the measured values per projection angle \( \theta \) and sum them up over the image space. As equation an operation like this can be put as follows:

\[
g(x, y) = \int_0^\pi p_\theta(\rho) d\theta
\]

\[
= \int_0^\pi p_\theta(x \cos(\theta) + y \sin(\theta)) d\theta
\]

The last line of the above equations contains the inner product between the two vectors \((x, y)\) and \((\cos(\theta), \sin(\theta))\). This computation actually relates to lines on the image for each fixed projection angle \( \theta \) (cf. Figure 2.21). Performing the integration now consists of adding up the values for each integration angle \( \theta \) over all displacements along the detector \( \rho \) along each of the lines over the image. That leads to the projection...
being smeared out over the image space from all angles. The operation performed here, is the adjoint or transpose operation of the projection itself. It can be seen as reversing the projection process but shouldn’t be confused with the inverse of the projection. In fact, this adjoint operation only equals to the inverse projection if the following equation holds

$$ A^T = A^{-1} \quad (2.12) $$

which means that the operator describing the projection has to be orthonormal, a property that cannot be assumed in most cases. The downside of the simple backprojection can be seen by taking a closer look at the calculations that go into forming the reconstructed image:

$$ g(x, y) = \int_0^\pi p_\theta(x \cos(\theta) + y \sin(\theta)) d\theta \quad (2.13) $$

The sampling along lines \( L = x \cos(\theta) + y \sin(\theta) \) through the object described in the last step can be substituted using the following equation

$$ f(x, y) \ast \delta(L) = \int_{\mathbb{R}^2} f(r) \delta(r - L) dr $$

$$ = \int_{\mathbb{R}^2} f(x', y') \delta \left( \begin{pmatrix} x' \\
 y' \end{pmatrix} - \begin{pmatrix} x \\
 y \end{pmatrix} \right) dx' dy' $$

Which results in

$$ g(x, y) = \int_0^\pi \int_{\mathbb{R}^2} f(x', y') \delta(r - L) dx' dy' d\theta \quad (2.15) $$

$$ = \int_{\mathbb{R}^2} f(r') \left( \int_0^\pi \delta \left( \begin{pmatrix} x' \\
 y' \end{pmatrix} - \begin{pmatrix} x \\
 y \end{pmatrix} \right) \cdot \begin{pmatrix} \cos(\theta) \\
 \sin(\theta) \end{pmatrix} \right) d\theta \right) dr' $$

$$ = \int_{\mathbb{R}^2} f(r') \left( \int_0^\pi \delta(\theta - \theta_0) \right) \frac{1}{|r - r'| \sin(\pm \pi/2)} d\theta \right) dr' $$

$$ = \int_{\mathbb{R}^2} f(r') \frac{1}{|r - r'|} dr' $$

$$ = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x', y') \frac{1}{|(x - x', y - y')|} dr'$$
2.5 Image Reconstruction

This last line corresponds to the convolution of the original image with the function \( h(x, y) = \frac{1}{|x, y|} \):

\[
g(x, y) = f(x, y) * h(x, y).
\]  

(2.16)

The convolution function \( h(x, y) \) is called the point-spread function (PSF) or impulse response of the imaging system. These equations show explicitly how the simple back-projection process leads to a blurred image. By substituting the delta function for \( f(x, y) \) the above equations yield \( g(x, y) = h(x, y) = \frac{1}{|x, y|} \). Although \( f(x, y) \) will be measured correctly as a point distribution in the projection the simple backprojection the density of the function \( g(x, y) \) is geometrically decreasing with the radius. For images that don’t consist of delta distributions, but extended objects, the blurring by the point spread function \( h(x, y) \) will occur at any point of the reconstructed object.

Figure 2.22 shows a simple example of the back projection discussed here. The differences between the original and the back projected image point out the effect of the back projection operation on the reconstructed image. In summary this means, that in most cases the simple form of the back-projection can not be recommended, since it leads to non-negative contributions from all other points of the original image. Especially points outside of an object, which should be equal to zero in the reconstruction, end up having positive values. Other backprojection methods compensate for this blurring effect with deconvolution filters.

### 2.5.4 Filtered Back Projection

The basis of the back-projection method can be found by taking a closer look at the inverse FT of the object function:

\[
f(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(u, v)e^{2\pi ij(xu+vy)}dudv.
\]  

(2.17)

Performing a coordinate transform to the variables

\[
u = \rho \cos(\theta)
\]

\[
v = \rho \sin(\theta)
\]

\[
\Rightarrow \quad J = det \left( \frac{\partial (u, v)}{\partial (\rho, \theta)} \right) = \rho (\cos^2(\theta) + \sin^2(\theta)) = \rho
\]

(2.20)
Figure 2.22: Example of a Naive Back Projection. In the last line on the right the back projected image has been normalized to stress the similarities and differences with respect to the original image on the left.

where $J$ describes the Jacobian matrix. This coordinate transform leads to the following equation:

\[
 f(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(u, v) e^{2\pi ij(xu+yv)} du dv
\]

\[
 = \int_{0}^{\pi} \int_{-\infty}^{\infty} P_{\theta}(\rho) e^{2\pi ij(x\rho \cos(\theta)+y\rho \sin(\theta))} |\rho| d\rho d\theta
\]

\[
 = \int_{0}^{\pi} \int_{-\infty}^{\infty} |\rho| P_{\theta}(\rho) e^{2\pi ij(x\rho \cos(\theta)+y\rho \sin(\theta))} d\rho d\theta
\]

\[
 = \int_{0}^{\pi} g_{\theta}(x \cos(\theta) + y \sin(\theta)) d\theta
\]
Which means that we can write

\[ g_{\theta}(t) = \int_{-\infty}^{\infty} |\rho| P_{\theta}(\rho) e^{2\pi i \rho t} d\rho \]  
(2.25)

which has the form of an inverse FT

\[ = \text{CTFT}^{-1} \{ |\rho| P_{\theta}(\rho) \} \]
(2.26)

this last equation can be written as the convolution

with a high pass filter \( h(t) = \text{CTFT}^{-1} \{ |\rho| \} \)

\[ = h(t) * p_{\theta}(r) \]  
(2.27)

Geometrically this high-pass filter corresponds to the incremental slices in the plane corresponding to all projections, which can be seen in Figure 2.23. The area of the incremental slice increases linear with \( \rho \), which leads directly to the form of the high-pass filter \( h \). In the sinogram the filter will be applied to each row and accentuate the edges before the backprojection is performed.

![Figure 2.23: Increment in High Pass Filter.](image)

In general the formulas for the backprojection and filtering all go to infinity, but if the measured object signal is bandlimited this is not necessary and it is useful to impose bandlimiting on the filter. This means, the filter needs to be cut off at a certain frequency in order to avoid creating additional noise (cf. Figure 2.24).
\[ H(\rho) = |\rho| - f_c \]

Figure 2.24: Bandlimited High Pass Filter with cut-off frequency \( f_c \). 
\[ H(\rho) = f_c [\text{rect}(f/(2f_c)) - \Lambda(f/f_c)] \]
\[ h(t) = f_c^2 [2 \text{sinc}(2tf_c) - \text{sinc}^2(tf_c)] \]

The result of the reconstruction using a filtered backprojection will get better the more projections are used. Roughly the number of projections needed to reconstruct an \( N \times N \) image is \( N \), because the sinogram needs to contain about the same amount of information as the image we try to reconstruct. The theory suggests that an infinite number of backprojections will lead to a perfect reconstruction result. This theoretical consideration is conditioned on the assumption that the original signal was bandlimited, though. Due to the fact that this is not the case there will still be some smearing at the edges in the reconstruction due to sampling, even if we assume the hypothetical case of an infinite number of projections and therefore there will be no perfect reconstruction.

2.5.5 Algebraic and Statistical Reconstruction

In contrast to the backprojection method, the problem statement in algebraic reconstruction already contains the discretized nature of the CT measurement process. On the one hand the discretization of the detector array is given by the equipment itself and on the other hand the number of voxels in the picture to be reconstructed has to be predefined in algebraic reconstruction as well.

Model of the forward projection

Typically, the object or image to be reconstructed will be represented by a discrete set of values corresponding to the pixels and their respective attenuation value \( \mu_i \). The X-rays pass through several of those pixels on their way to the detector and get attenuated accordingly. This leads to the detected value \( p_j \) on the detector.
As can be seen in Fig 2.25 the projections can be expressed as a system of linear equations, which can be solved for the attenuation values in order to reconstruct the image.

\[
\begin{align*}
\mu_1 + \mu_4 + \mu_7 &= p_1 \\
\mu_2 + \mu_5 + \mu_8 &= p_2 \\
\mu_3 + \mu_6 + \mu_9 &= p_3 \\
\mu_7 &= p_4 \\
\mu_1 + \mu_5 + \mu_9 &= p_5 \\
\mu_3 &= p_6 \\
\mu_7 + \mu_8 + \mu_9 &= p_7 \\
\mu_4 + \mu_5 + \mu_6 &= p_8 \\
\mu_1 + \mu_2 + \mu_3 &= p_9
\end{align*}
\]

The example in Fig 2.25 is simplified, in general it can not be assumed that if a X-ray crosses a voxel it will experience its full attenuation. This effect is shown in Fig 2.26. The X-ray beam gets not only attenuated by the main two cells \(\mu_2\) and \(\mu_6\), but is also affected by adjacent cells \(\mu_1\), \(\mu_5\) and \(\mu_9\). This effect can be expressed in the system of equations by introducing weights corresponding to the illuminated area of the cell:
weight \( a_{i,j} = \frac{\text{illuminated area of pixel } j \text{ by ray } i}{\text{total area of pixel } j} \). \hspace{1cm} (2.28)

With this definition for the weight, the generalized set of equations becomes:

\[
\sum_{j=1}^{N} a_{i,j} \mu_j = p_i. \hspace{1cm} (2.29)
\]

This can also be presented in matrix notation

\[
p = A \cdot \mu \hspace{1cm} (2.30)
\]

Measured transmission values: \( p = (p_1, \ldots, p_M) \)

Object attenuation values: \( \mu = (\mu_1, \ldots, \mu_N) \)

Design or System matrix: \( A = \begin{pmatrix}
a_{11} & a_{12} & \cdots & a_{1N} \\
a_{21} & a_{22} & \cdots & a_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
a_{M1} & a_{M2} & \cdots & a_{MN}
\end{pmatrix} \)

![Figure 2.26: ART Principle - weights](image)

This matrix approach has some advantages, compared to the backprojection method. Different geometries of the CT system can be incorporated without much effort by applying an adequate operator corresponding...
to the system change. Furthermore, the discrete formalization makes it easy to account for detector sensitivities and widths. Nevertheless, there are also several challenges to using this system for the reconstruction of the image. First of all, in order to theoretically get a unique solution to the problem number of measurements $M$ has to be equal to the number of pixels $N$. If $M < N$ or $M > N$, the system is under- or over-determined and a solution can only be estimated. But even for the perfect case $M = N$ the formalism in this ART approach only covers ideal physical conditions, that means the X-Rays get attenuated by the image cells perfectly following Lambert-Beers law. In a real measurement the data in $\mathbf{p}$ will contain noise from different sources, either noise from physical interactions such as scattering or electronic noise from the detector. That means that by solving the above equations, only an approximate solution for the image can be found. The solution of the system of equations bares another problem. Inverting the matrix $\mathbf{A}$ is not possible most of the time, because it becomes singular. Moreover, it is typically very large, making inversions computationally really costly. Nevertheless, $\mathbf{A}$ can be sparse, since it correlates to all pixels that contribute to each entry in the Radon space, which is normally a small number in the order of $\sqrt{N}$. This condition holds as long as the noise is not a function of the angle for all projections.

**Solution of the ART equations**

The general equation (2.30) has to be solved for $\mu$, which corresponds to the image. As it was already mentioned before, most of the time there is no exact solution and the problem to be solved takes the form of an optimization problem. By taking a closer look at the problem at hand it becomes clear, that it results in minimizing

$$\chi^2 = |\mathbf{A}\mu - \mathbf{p}|^2$$

(2.31)

which is clearly a least squares problem. This means the solution vector can be estimated using the Moore-Penrose pseudo inverse $\mathbf{A}^+$:

$$\hat{\mathbf{f}} = \mathbf{A}^+\mu$$

(2.32)

Another way of solving the above equation uses the singular value decomposition of $\mathbf{A}$, which also leads to a pseudo inverse of $\mathbf{A}$.
\[ \mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^T \]  
\[ \mathbf{A}^+ = \mathbf{V} \cdot \text{diag} \left( \frac{1}{\sigma_j} \right) \cdot \mathbf{U}^T \]

which can be used in the same way as in equation 2.32. Here, \( \Sigma \) is a diagonal matrix with entries \( \sigma_j \) corresponding to the nonzero singular values of \( \mathbf{A} \).

The issue with this approach of the pseudo inverse lies in the fact that the problem is typically ill-posed and very sensitive to even small measurement errors, which will be accentuated by the term \( \frac{1}{\sigma_j} \). A diagonalized version of the set of equations would directly solve the problem as it was the case in the Fourier based reconstruction at the beginning of this chapter. The diagonal form is unfortunately not given and moreover, the matrix gets extremely large in reality, which poses problems especially for the inversion of it. A typical matrix has the size

\[
\text{size}(\mathbf{A}) = \frac{M_i}{\text{size of image}} \times \left( \frac{M_d}{\# \text{ detector pixels}} \cdot \frac{M_a}{\# \text{ projection angles}} \right)
\]

\[
= 10^5 \times (10^3 \cdot 10^3)
\]

\[
= 10^5 \times 10^6
\]

Therefore most ART algorithms nowadays use iterative ART techniques to circumvent the problem of inverting this matrix.

### 2.5.6 General Iterative Reconstruction Methods

In contrast to the analytic reconstruction method of Filtered Back Projection, there are also reconstruction techniques which are based on an iterative procedure. Iterative reconstruction consists of successively estimating and comparing results with the hope of fast converging to the same result.

Naturally, this method is computationally much more expensive than any form of analytic reconstruction. Nevertheless, there are limitations in analytic reconstruction methods like filtered back projection for example,
because they don’t allow an accurate handling of attenuation corrections. Iterative reconstruction can help here, because features like the geometry of detector and source and the spectrum of the beam can be incorporated in the procedure. There are two main classes of iterative reconstruction methods, the conventional ones and the statistical methods. The basic algorithm of iterative reconstruction is given in Fig 2.27.

2.5.7 Reconstruction for Cone Beam Geometry

The examples shown previously used a two dimensional image space for the reconstruction. The projection data consisted of one dimensional array like projection data for each angle. However, a lot of the common measurements is performed with two dimensional detectors allowing the measurement and reconstruction of three dimensional volumes. The 3D reconstruction of the central slice of the 2D projection data follows the same rules as previously discussed. For the introduction of the third dimension in ART, the remaining X-rays beam paths have to be mapped out and added to the system matrix. For backprojection reconstructions a third angle and spatial coordinate has to be incorporated into the backprojection equations in order to account for the additional data.

\textbf{Figure 2.27:} Sketch of the Iterative Reconstruction Method.
as well as the third dimension in the resulting reconstructed volume. Moreover, filters have to be adapted to account for the additional spatial dimension. The required formalism has been developed by Feldkamp-Davis-Kress [22].

2.6 Sources of Artefacts

As mentioned before, X-Rays undergo several interactions while propagating through the CT machine. These effects lead to artefacts in the final image, which can be divided in two categories. Either they arise from Scattered Radiation or from Beam Hardening.

2.6.1 Scattered Radiation

As mentioned before, there are several interactions of the photon with the matter of the object, or even with the CT machine or generally the environment. These interaction lead in many cases to elastic or inelastic scattering of the photon. The ratio of scattered radiation with respect to the photons of the original beam is called the Scatter-to-Primary Ratio (SPR).

Mainly, scattering radiation results in a reduction of the contrast in the final image. However, it can also lead to specific artefacts, especially when different materials or different thicknesses are present in the object. Then the scattering can differ between certain regions of the objects and the attenuation can be under- or overestimated in different parts of the final image. When the object that is scanned is not rotationally symmetric, the effect of scattering also depends on the projection direction of the scan. This leads to streaks and cupping artefacts, which can also be observed as a result of the beam hardening effect.

2.6.2 Beam Hardening

The phenomenon of Beam Hardening is a result of the polychromaticity of the X-Ray source. The various X-ray photon energies in a beam have to be taken into account, due to the fact that beam attenuation depends on the energy of the photons. Beam hardening describes the shifting of the mean energy of the X-Ray Beam to higher energies. This happens due to the fact that low energetic photons are more likely to be absorbed than higher energetic ones. The artefacts on the final image resulting
from Beam hardening are Cupping Artefacts or Streaks.

Cupping Artefacts occur, when there are big differences in the regions the photons travelled through. If on one part of the object they travel through little material, while on another part of the object they travel through a lot material, the beam hardening will turn out to differ much over the image. Because a harder beam has a lower attenuation, the attenuation effect will be overestimated.

Streaks occur, when there are several dense regions in an object for example. Depending on the angle from which the object is scanned, the beam will go through only a few or many of these objects and will thus experience different levels of beam hardening. This can lead to dark and bright streaks on the resulting image.

2.6.3 State of the art scatter correction methods

As we discussed in [73] common scatter correction methods can be classified in three categories. Scatter can either be reduced by hardware optimization in the form of a redesign and optimization of the X-ray setup, it can be estimated and corrected after the measurement or it can be guessed using X-ray simulations.

Optimizing the system setup with respect to scattered radiation is recommendable in any case. Specifically reducing scatter from peripheral sources such as collimators and mounting can be a simple way of increasing radiographic image quality. Moreover, as shown in [11, 14] additional anti-scatter grids can help reduce the amount of scattered radiation detected in the X-ray images. A simpler scatter reduction method, mostly used in the field of medical X-ray CT is the air gap method [55]. It involves increasing the distance between the object and the detector. The angles of scattered radiation with respect to the surface normal of the detector are typically larger than the equivalent angles of primary radiation, which can result in scattered radiation missing the detector for larger photon travel distances. It has to be noted, however, that the object size limits the maximal object to detector distance.

Estimation of scattered radiation can be either hardware or software based. For methods using hardware based scatter estimation, a part of the detector is typically blocked from the primary X-ray beam and the
scatter signal is quantified from the measured signal in the blocked part of the detector. Examples of these hardware estimation techniques are the beam shadow method [72], the beam stop method [61,69] as well as the method of primary modulation of the X-ray beam [70]. All of these estimation methods introduce material into the beam that either reduce the total information in the measurement by blocking various parts of the detectors surface from radiation. This means that a reduction in the total measured information has to be ultimately accepted in favour of a correction of scattered radiation in the other parts of the radiography, or a second scan without the estimation device has to be performed.

Software based scatter estimation generally refers to an analytical determination of the scatter in the radiographies. These analytical calculations rely on the dominance of the Compton interactions over all other physical effects. In this case, radiographies are typically corrected using a deconvolution of the images with the calculated scatter kernels [9]. Other analytical approaches to scattered radiation assume a gray value dependency of the amount of scattered radiation leading to a similar concept as in beam hardening corrections [71].

The last category of scatter correction methods involves the simulation of the X-ray images. Simulations allow the differentiation of the various physical effects and the assessment of their impact on radiographic image quality. There are several X-ray simulation options, they can either be deterministic, based on ray-tracing or based on a Monte-Carlo approach. Despite their accuracy, X-ray simulations are typically rejected for other scatter estimation methods due to their computational complexity. Efforts have been made to increase computational efficiency in the form of hybrid simulations [79] or the so called forced detection approach [54]. However, simulations still require a large amount of previous knowledge about the X-ray beam, the system and the object in order to be correct.
Chapter 3

X-ray Simulation

The previous chapter gave an overview of the different physical processes involved in X-ray imaging including their corresponding mathematical formulation. A common method of modelling a system like an X-ray CT scanner involves the simulation of the X-ray imaging process. But before analysing the different simulation techniques and frameworks we have to answer the question why we should do simulation work, when we already know a lot about the underlying mechanisms of an X-ray setup. Simulations are mainly used when the model of a system is complex and involves a large set of parameters and components. Particularly, if the relationship between the model parameters is nonlinear or if some parameters are random in nature, analytical solutions might not be feasible or sufficient. In the case of X-ray simulations the underlying mechanism of beam generation, propagation and detection is governed by particle physics. More precisely, the interactions of particles with matter and the resulting processes such as absorption and scattering form the basis of X-ray imaging. Due to the large number of processes involved and their inherent random nature, the X-ray imaging model becomes unsolvable analytically. An X-ray simulation code can help navigate the parameter space of physical interactions and system components and thus help deepen the understanding of the X-ray imaging process. Moreover, the simulations can help improve the X-ray system as well as support the development of correction algorithms for all deteriorating effects in the image formation process. The field of X-ray simulations is large and the various simulation codes are based on a range of different simulation techniques. This work will focus on particle simulations on
the basis of the Monte Carlo technique in order to assess and correct image deteriorating effects. Other X-ray imaging techniques are based on analytical estimations, transfer matrix approaches or ray tracing algorithms. This chapter will provide a detailed description of the Monte Carlo method as well as the Monte Carlo simulation framework used for the results in this work. A second section will describe other simulation techniques and discuss their respective advantages and weaknesses.

## 3.1 Monte Carlo Simulations

### 3.1.1 Basics

The Monte Carlo method is used to numerically find a solution to a given problem. In order to achieve this, the method makes use of random sampling from a probability distribution of possible input values. This way, the dynamics of a system can be simulated. This means, that a large part of the reliability of a Monte Carlo simulation depends on its random number generator. The numbers from this kind of number generator are not really random, but rather derived mathematically, that is why they are sometimes referred to as pseudo random number generators. Although, the random numbers generated this way are not random in a natural way, a lot of research led to algorithms that produce sufficiently random sets of numbers. Moreover, with a pseudo random number generator the user has the advantage, that the Monte Carlo simulation can be repeated in the exact same way by feeding the generator the same initial value, the so-called seed.

Most random number generators deliver a random number between 0 and 1. The random numbers are uniformly distributed over the intervall \((0, 1]\). However, the aim of a Monte Carlo simulation is not to sample the random variable \(x\) according to this uniform distribution, but to do the random sampling according to a probability distribution function \(f(x)\). This distribution function has to be integrable, non-negative and in the best case normalized.

\[
\begin{align*}
  f(x) &\geq 0 \\
  \int f(x) \, dx &= 1
\end{align*}
\]

Let \(y\) be the uniformly distributed random number, \(y \in (0, 1]\). Then
it can be related to the uniform distribution by determining the inverse of the integrated function. This is enough to simulate the random variable $x$ according to the probability distribution function $f(x)$ using the uniformly distributed random variable $y$.

\[ f(x)dx = 1dy \]
\[ F(x) = \int_{-\infty}^{x} f(x)dx = y \]
\[ \Rightarrow F^{-1}(y) = x \]

This direct method of random sampling is not always possible. It highly depends on the probability distribution function and the possibility of inverting its integral. The Acceptance-Rejection Method is an alternative way of performing the random sampling if the direct method fails. The basis is again a random variable of the interval $y \in (0, 1]$, but another distribution function $g(x)$ is needed to do the sampling. This function should be a suitable bound on the probability distribution function $f(x)$. That means there exists a constant $M$, such that for all possible values of $x$, the probability distribution function $f(x)$ is always smaller than the product between $M$ and $g(x)$.

\[ f(x) < M \cdot g(x), M > 1 \]

Then in the Acceptance-Rejection Method $x$ is sampled from $g(x)$ like in the direct method above. The variable $x$ will then be accepted or rejected in the following way:

\[ \begin{align*}
    &y < \frac{f(x)}{Mg(x)} \quad \text{accept } x \\
    &y > \frac{f(x)}{Mg(x)} \quad \text{reject } x
\end{align*} \]

There are numerous other methods, some of them are a mix of this two methods. A famous extension to the Acceptance-Rejection Method is for example the Metropolis Algorithm. The differences between the methods are mainly in computational efficiency, which highly depends on the problem.

\section*{3.1.2 Error estimation}

Let $x$ be the quantity to be simulated by a Monte Carlo simulation using $N$ particle histories. If the simulation of all $N$ particle histories happens
in one run, a direct error estimation can be carried out [8]. The quantity that can be directly computed is the mean value \( \bar{x} \). Using the mean value, the variance of \( x \) and the variance of the mean value \( \bar{x} \) can be found.

\[
\text{Mean value} \quad \bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i
\]

Variance associated to \( x \)
\[
\sigma_x^2 = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2
\]

Variance associated to \( \bar{x} \)
\[
\sigma_{\bar{x}}^2 = \frac{\sigma_x^2}{N}
\]

Result
\[
x = \bar{x} \pm \sigma_{\bar{x}}
\]

It is possible that the simulation is not only carried out in one run, but in several independent runs. Nevertheless, the simulation results can be combined into one result with an estimate on the variance as before. Let the simulation consist of \( m \) independent runs such that the total number of simulations is \( N = \sum_{k=1}^{m} N_k \).

\[
\text{Mean value for each run} \quad \bar{x}_k = \frac{1}{N_k} \sum_{i=1}^{N_k} x_i
\]

Variance associated to set \( x_k \)
\[
\sigma_{x_k}^2 = \frac{1}{N_k-1} \sum_{i=1}^{N_k} (x_i - \bar{x}_k)^2
\]

Variance associated to \( \bar{x}_k \)
\[
\sigma_{\bar{x}_k}^2 = \frac{\sigma_{x_k}^2}{N_k}
\]

Mean value for all runs
\[
\bar{x} = \sum_{k=1}^{m} \left( \frac{N_k}{N} \right) \bar{x}_k
\]

Variance associated to all runs
\[
\sigma_{\bar{x}}^2 = \sum_{k=1}^{m} \left( \frac{N_k}{N} \right)^2 \sigma_{\bar{x}_k}^2
\]

Result
\[
x = \bar{x} \pm \sigma_{\bar{x}}
\]

In the calculation of the variance associated to all runs combined a first order propagation of the errors was assumed [8].

### 3.1.3 Monte Carlo simulation frameworks for X-ray imaging

Monte Carlo methods have been developed extensively in the field of particle physics and the underlying models and databases of interaction processes are typically updated with each new finding. This is why Monte Carlo simulations are generally seen as the golden standard of
particle transport simulations in X-ray imaging. Not only the accurate modelling of interactions, but also the possibility of investigating complex geometries constitute a big advantage with respect to other simulation methods. Moreover, the detailed information about all aspects of the simulation and the underlying physical mechanisms that can be retrieved even exceed the information that can be gathered experimentally. All of these aspects make the Monte Carlo method arguably the most versatile and accurate simulation technique in the field of X-ray simulations.

Even when choice of Monte Carlo simulation as the X-ray simulation technique has been made, there are still several different options for the simulation framework. Some Monte Carlo simulation frameworks are specialised for X-ray imaging or radiation physics applications, others are general particle simulations.

The EGS (Electron Gamma Shower) Monte Carlo simulation code can be considered one of the earliest simulation codes. It was developed at SLAC (Stanford Linear Accelerator Center) and is build for the simulation of electrons and photons. The EGS code is known to be especially useful for the purpose medical dose radiation calculation. The original EGS code is no longer actively supported, however different forks of the software such as EGS4 [56], EGS5 [33] and the EGSnrc [41] code are still being maintained and developed. MCNP (Monte Carlo N-Particle Transport Code) [10] is a Monte Carlo simulation for neutron, photon and electron simulations. MCNP was developed at the Los Alamos National Laboratory. Later version of the MCNP code specialised in the simulation of nuclear systems. The current version of the MCNP code is MCNP6. Just as the EGS code, PENELOPE (Penetration and ENergy LOss of Positrons and Electrons) [66] is a Monte Carlo simulation code for electron and photon transport. GEANT (GEometry ANd Tracking) [15] is a Monte Carlo code developed at CERN. The fourth version of the GEANT series will be used for the simulation work here. The next section will go into details about the mechanics and specifics of the GEANT4 simulation code. These are only a small selection of the wide variety of Monte Carlo particle simulation codes. Most of them are based on another older simulation code and add to it.

3.1.4 GEANT4

The GEANT (GEometry ANd Tracking) series is a simulation toolkit developed at CERN [15]. It uses the Monte Carlo Method discussed in the previous section to simulate particle dynamics and interactions. The
predecessors of GEANT4 were written in FORTRAN, but GEANT4, the version that will be used here, is based on object oriented C++ programming. GEANT4 has broad application due to the provided energy ranges and effects. It is used in medical physics as well as in astrophysics or high energy physics.

The GEANT4 simulation toolkit is able to simulate so-called single particle transport. This means each of the particles is transported through the system individually. Therefore, no interactions between two particles can be simulated. Geometries in GEANT4 can either be given as voxelized data or build out of a set of primitives. For the simulation of the interactions the database for the physical interactions can be choses from a set of libraries. The choice of this library depends on the specific problem on hand is is crucial for the quality of the outcome of a simulation. Besides the database of physical interactions, the random number generator is also a crucial part of the simulation. The next sections will go into details about the choice of library as well as the choice of random number generator will be discussed. Furthermore, the tracking of particles and their physical interactions will be described.

**Random number generator**

The module for random number generation in GEANT4 is based on the corresponding module of the Computing Library for High Energy Physics (CLHEP). There are several random engines and distributions implemented in this library to get the random generator. The only one used within the GEANT4 framework is the static random number generator of the HEPRandom class. Several different random engines can be executed in this class. The default engine is the HEPJamesRandom engine, which relies on a pseudo-number generation algorithm described in [39]. Other engines that can be set are DRand48Engine and RandEngine, which use the standard C library, the RanluxEngine and the RanecuEngine, which come from the original implementation of the MATHLIB HEP library. The latter two are also described in [39]. Besides the random engine, random distributions can be specified as well. Distributions that can be implemented are for example the RandFlat distribution, shooting flat random numbers from a given interval or the RandGauss distribution, shooting random numbers that are gaussian distributed.
3.1 Monte Carlo Simulations

Libraries

The subject of this thesis addresses all processes that describe interactions between photons, electrons, positrons and matter, which means covering the electromagnetic implementation of GEANT4 will be sufficient. For these electromagnetic processes GEANT4 provides two different packages, the Standard and the Low Energy package. The Standard Package is able to describe physics which covers the energy range from 1keV to 100TeV, while the Low Energy Package is able to cover an energy range from 10eV up to 100GeV, depending on the used sub-package. These sub-packages describe the library that has been used, there are the Livermore library, the Penelope model, the Ion model or the Geant4-DNA project.

The Livermore model is based on the libraries EADL (Evaluated Atomic Data Library), EEDL (Evaluated Electrons Data Library) and EPDL97 (Evaluated Photons Data Library) to describe electron and photon interactions. It provides cross sections and energy spectra and is able to describe processes of an energy up to 100GeV and including atoms with an atomic number between 1 and 100. For the described electromagnetic processes it is even possible to include effects from polarized photon interactions.

The Penelope model in GEANT4 includes models from the Penelope (Monte Carlo) code (PENetration and Energy LOss of Positrons and Electrons). Its energy range is restricted to energies from 250eV to 1GeV, which is less than described by the Livermore model. Nevertheless, Penelope has the advantage that it is able to describe positrons. This feature is not present in the Livermore model.

The Ion model is especially designed to describe the energy loss of heavier ions. It is able to provide stopping powers and it can describe the production of $\delta$-rays. This model includes the ICRU73 model with revised tables. The energy range covered here goes from 250eV up to 10MeV. The Geant4-DNA project was initiated by ESTEC (European Space Research and Technology Centre). It is used for microdosimetry in radiobiology. That means this sub-package models the interaction of radiation with a biological system like cells for example.

Since the processes of interest here will take place at an energy of a few MeV and Pair Production should be included, the Low Energy
sub-package Penelope will be the best choice. A list of the implemented particles and physical processes with their respective physical interaction model can be found in table 3.1.

<table>
<thead>
<tr>
<th>Physical interaction</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compton interaction</td>
<td>Analytic parameterization (with atomic binding and Doppler broadening)</td>
</tr>
<tr>
<td>Rayleigh scattering</td>
<td>Analytic parameterization</td>
</tr>
<tr>
<td>Photoelectric effect</td>
<td>Sauter distribution</td>
</tr>
<tr>
<td>Pair Conversion</td>
<td>Bethe-Heitler cross section with Coulomb correction (semi-empirical model)</td>
</tr>
<tr>
<td>Bremsstrahlung</td>
<td>Total cross section calculated from data</td>
</tr>
<tr>
<td>Ionisation</td>
<td>Calculated analytically</td>
</tr>
</tbody>
</table>

**Table 3.1:** Implemented physical models of the low energy electromagnetic interaction library Penelope (empenelope).

**Particle tracking**

In the following simulations, the physical interactions that occur during the GEANT4 simulations are assigned to the propagating particles via interaction trees. Children of particles that are created through the interactions inherit all of their parents physical interactions. The assignment of physical interactions to the particles is done in binary form, which means that the number of times a physical interaction occurred will not be measured. However, another parameter measures the order of scattering. At the detector the kinetic energy as well as the number of all incident photons is recorded including the information about physical interactions as well as order of scattering.

**3.2 Other X-ray simulation methods**

**3.2.1 Ray tracing**

In ray-tracing simulations a set of virtual rays is emitted from the source towards each of the detector elements. The intersection lengths with the different object materials combined with the X-ray attenuation law give rise to the measured intensity at the detector. This algorithm will result
in a realistic X-ray image, however, all other effects besides the simple X-ray attenuation are not taken into account. Processes like scattering that add to the measured signal are not considered in simple ray tracing approaches. An example of a ray tracing implementation is virtual X-ray imaging (VXI) code [21].

### 3.2.2 Analytical and deterministic simulations

The modelling of scattering processes is not restricted to Monte Carlo simulations. Analytical approximations of the physical interactions can be done. Typical deterministic simulations combine a ray-tracing approach and superimpose a simulated scatter projection onto the simulated X-ray image. Current deterministic simulations approximate both the Rayleigh and the Compton scattering in the X-ray image [25,46]. However Compton scattering is generally only modelled to a first order of scattering. Multiple scattering is often only estimated as a constant or from the single scattering distribution.

### 3.2.3 Hybrid simulations

Another class of X-ray simulations combines the concepts of Monte Carlo simulations with the deterministic simulation approaches. The aim of these so-called hybrid simulations is typically to speed up Monte Carlo simulations without loosing the accuracy of the Monte Carlo approach. Hybrid simulations will therefore often use deterministic algorithms for the calculation of the X-ray image containing the single-scatter contribution [44]. For multiple scatter estimations, crude Monte Carlo simulations will be performed.
Part II

Signal degradation in the MeV CBCT setup
Introduction to Part II

The goal of the following work is to identify and quantify all image degrading processes in a high energy X-ray Cone Beam Computed Tomography (CBCT) system. The X-ray source in this high energy setup is a linear accelerator capable of producing a mega-electronvolt (MeV) X-ray beam. A first chapter will describe the geometry of the high energy CBCT system for both the measurements as well as the geometry implemented in the Monte-Carlo simulation framework. The aim of the Monte-Carlo simulation work is to gain insight into the influence of all physical interactions on the measured radiographies. Additionally, the impact of the various system components on image quality can be assessed. Each part of the X-ray setup will be studied individually in order to assess its impact on radiographic image quality.

When studying the simulation results particular attention will be paid to the investigation of scattered radiation. The physical interaction of scattering of X-ray photons is one of the two types of processes that forms the basis of X-ray attenuation and subsequently X-ray imaging. Alongside X-ray absorption, X-ray scattering leads to a loss of intensity of a X-ray beam when travelling through material. However, scattered photons do not vanish in the process, they are merely redirected. This means scattered photons can reach the detector, where they produce an additional signal in the radiography which does not correspond to the classical theory of X-ray attenuation described by the Beer-Lambert law. This increase in signal caused by scattered radiation is one of the main contributions to image degradation in industrial X-ray Computed Tomography (CT). It leads to a high non-linearity in the scan, which causes blur and general loss of contrast in the reconstructed images.

Three main sources of scattered radiation in an X-ray CT setup can be
distinguished: The object, the detector and the remaining components of
the X-ray CT setup. These three elements of the X-ray measurement will
be investigated in detail in the following chapters. The studies will focus
on the contribution of physical interactions on the scattered radiation as
well as the order of scattering. It is important to notice that these three
sources of scattering are not decoupled from each other. On the contrary,
scattered photons from system components outside of the field of view of
the beam are more likely to be the results of a scattering from several
of these sources as opposed to the result of a single scattering event.
Accordingly, it can be assumed that scattering from these kind of sources
is of high order. The last chapter in this part will address the issue of
the combined scattering sources. Simulations of the complete X-ray CT
system will be performed in order to analyse the influence of the system
components on image quality as well as the relative importance of the
various scattering sources. Spectral investigations will complement the
scatter simulations, starting with the spectrum simulations of the X-ray
source. Other studies of the spectrum will involve the effect of beam
hardening as well as the energy dependency of the detector image transfer
characteristics. Finally, measurements will complement and validate the
simulation work. Measurements of system characteristics such as the
Modulation Transfer Function (MTF) of the detector as well as different
materials and various attenuation lengths intend to validate simulation
results.
Chapter 1

Experimental and simulation setup

The X-ray CT setup studied in this work is a MeV X-ray CBCT setup. This means, the setup consists of a high energetic X-ray source of MeV energy and a two dimensional detector. The MeV X-ray source is a linear accelerator with a focal spot size of 2 mm. The linear accelerator can be operated at X-ray energies of 4 MeV and 6 MeV. X-rays are generated in a transmission target at the end of the linear accelerator in a 0.85 mm thick tungsten target. Details about the MeV X-ray source can be found in Table 1.1. Additionally, two source sided collimators shape the beam to a 5° opening angle. The technical drawings of the source collimators can be seen in Figure 1.1.

Figure 1.1: Sketch of the primary collimator (left) and secondary source collimator (right).
Table 1.1: Specifications of the linear accelerator PSL-6D from U.S. Photon Service employed in the system.

<table>
<thead>
<tr>
<th>Pulstar Linac - PSL-6D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer</td>
</tr>
<tr>
<td>Linac Design</td>
</tr>
<tr>
<td>Electron Beam Energy</td>
</tr>
<tr>
<td>Maximum Dose Rates</td>
</tr>
<tr>
<td>at 1m distance</td>
</tr>
<tr>
<td>Target material</td>
</tr>
<tr>
<td>Focal spot size</td>
</tr>
</tbody>
</table>

The detector in this high energy X-ray setup is an active matrix flat-panel imager from Perkin Elmer with pixels of size 200 µm. It is an indirect detection detector, which means that incident X-ray photons are converted into visible light in a scintillating medium. Here, the scintillator is a 208 µm thick terbium doped gadolinium oxysulfide ($Gd_2O_2S : Tb$), which is added in the form of a powder, on top of the amorphous silicon array and thin film transistors. Further specifications of the detector can be found in Table 1.2. The active area of the detector was reduced by 25 mm at each side to a size of 1798 × 1798 pixels by a lead shielding. A shielding thickness of 60 mm was chosen in order to protect the electronics of the detector from the high energy X-ray radiation. A sketch of the detector with the shielding in its mobile mounting can be seen in Figure 1.2.

Figure 1.3 shows a drawing of the MeV X-ray CBCT setup employed at the Center for X-ray analytics at Empa. The source to detector distance was chosen to be at a maximum 4.5 m. A large distance between source and detector will allow us large variations in the object to detector distance. Moreover, the large travel distance of the beam will lead to a more parallel beam at the detector. Compared to a more diverging beam, this will minimize distortions and thus increase the accuracy at the border of the reconstructions.
Table 1.2: Specifications of the detector XRD 1621 from Perkin Elmer employed in the system [59].

<table>
<thead>
<tr>
<th></th>
<th>XRD 1621 AN14 ES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer</td>
<td>Perkin Elmer</td>
</tr>
<tr>
<td>Pixel number</td>
<td>2048 × 2048</td>
</tr>
<tr>
<td>Pixel pitch</td>
<td>200 µm</td>
</tr>
<tr>
<td>Area</td>
<td>409.6 × 409.6 mm²</td>
</tr>
<tr>
<td>Scintillator</td>
<td>DRZ-Plus, 208 µm Gd₂O₂S:Tb</td>
</tr>
<tr>
<td>Radiation energy</td>
<td>40 keV - 15 MeV</td>
</tr>
</tbody>
</table>

Figure 1.2: Sketch of the flat panel detector in its housing with the lead shielding.
**Figure 1.3:** Side view of the experimental setup. To the right, the linear accelerator can be seen, the detector is placed to the left. Behind the flat panel detector to the left, another detector for a fan beam setting of the system is located.
Chapter 2

The Source

The goal of this set of first simulations is the creation of correct X-ray source spectra for use in the later simulation work. A correct source spectrum is the basis of a working simulation of an X-ray CT setup. The spectra simulated in the following will serve as a database for all other simulations performed in this work. As a result, a speed-up of the further simulation work can be achieved by eliminating the part of the X-ray production.

However, the aim of the following simulations is not only to create a set of X-ray spectra for later simulations, but also serve the purpose of studying the angular distribution of the X-ray beam. The results should emphasize, if intensity drops for larger cone beam angles are an issue in the given X-ray setup. Additionally, it is interesting to check if changes in the spectrum of the X-ray beam with the angle can be expected. Additionally, a study on secondary particle generation is of interest. Specifically secondary electrons created at the source and their relative importance with respect to the X-ray photons created at the target has to be investigated.

The first part of this chapter will discuss the detailed source setup employed in the Monte-Carlo simulations. Further sections will go into detailed analysis on the angular distribution of X-ray radiation as well as influences of system components on spectral composition. A study of secondary particle influence shall reveal their impact. Finally, a set of source simulations employing different filters will complete the database.
of spectra for further simulations.

2.1 Simulation setup

As described in the previous chapter, the X-ray source of the MeV X-ray CBCT setup is a linear accelerator that can be operated at the two electron beam energies 4 MeV and 6 MeV. The geometrical setup of the X-ray source implemented in the Monte Carlo source simulations is shown in Figure 2.1. It includes all accelerator components that are essential for the spectrum simulations such as the housing as well as the water cooling. The X-ray photons are created in a 0.85 mm thick tungsten target at the end of the electron acceleration tube. The simulations performed here do not incorporate the electromagnetic field used to accelerate the electrons onto the X-ray target. The electrons in the simulations are either shot onto the target with a given mono-energy or with a randomly sampled energy from a given distribution around one energy.

![Figure 2.1: The target geometry employed in the source spectrum simulations matches the linear accelerator employed in the experimental high energy CBCT setup. The electrons are accelerated in a vacuum tube surrounded by copper housing and water cooling.](image)

The simulation setup includes a source collimation equal to the collimation of the experimental setup. Figure 2.2 shows a sketch of the
source simulation setup with the two collimators (see Figure 1.1) and their placement with respect to the linear accelerator.

![Diagram](image)

**Figure 2.2:** Sketch of the two source collimators and their placement with respect to the target at the end of the linear accelerator.

The resulting spectrum is recorded on a virtual sphere around the detector. This enables us to investigate the angular dependence of the spectrum and the amplitude of the generated X-ray beam. The detector itself is an ideal detector, recording the total energy of any particle incident onto a detector element. The detector geometry can be seen in Figure 2.3.

### 2.2 Spectra for different electron energies

These first simulations analyse the X-ray spectrum in forward direction for different initial electron energies. This means only photons in an angle range of $[-0.5, +0.5]^\circ$ will be analysed. Different mono-energetic electron beams incident on the X-ray target will be evaluated.

The resulting spectra are shown in Figure 2.4. The curves were normalized such that the integral over all counts is one. It is interesting to notice, that the spectra do not reflect the large differences in the initial electron energies. Comparing the peaks of the X-ray spectra (see Table 2.1) the differences between the 1 MeV and the 6 MeV only results in a peak distance of 30 keV. However, the normalized peak intensities differ significantly, which is a result of the larger spread of the higher energetic...
Figure 2.3: A spherical detector around the X-ray target records the produced X-ray beam allowing an investigation of the angular dependence of spectrum and intensity.

Figure 2.4: Spectra for different initial electron energies.

spectra. Obviously the tails of the higher energetic spectra reach farther, given that only the electron energy is the limiting factor for the photon energy at the higher end. It is worth noting that in all cases of MeV X-ray spectra, the high energy tails of the spectrum seem to play a much
smaller role given their relative importance with respect to the total spectral distribution. However, for the inspection of very large and dense objects X-ray spectra containing photons of several MeV will still be crucial for acceptable transmission values.

Table 2.1: Energies corresponding to the peak of the spectra

<table>
<thead>
<tr>
<th>Electron energy</th>
<th>Peak spectral energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 MeV</td>
<td>240 keV</td>
</tr>
<tr>
<td>4 MeV</td>
<td>260 keV</td>
</tr>
<tr>
<td>6 MeV</td>
<td>270 keV</td>
</tr>
<tr>
<td>9 MeV</td>
<td>260 keV</td>
</tr>
</tbody>
</table>

2.3 Spectrum angular distribution

The following simulations were performed with a monoenergetic 6 MeV electron beam. As opposed to the first set of simulations, the resulting photons are recorded on the spherical detector shown in Figure 2.3. This allows us to look at the angular distribution of the spectrum as well as the intensity for the different cone beam angles. In order to study the angular dependence of the intensity of the spectrum for the different cone beam angles, the spectra were normalized by the integral of the curve of the spectrum in $0^\circ$ direction.

Figure 2.5 shows the spectrum for different angles with respect to the initial electron momentum vector. It can be seen, that the spectrum starts to change only for large angles exceeding $20^\circ$. This means we can safely assume an isotropic spectral distribution for the small cone beam angles that are considered in this X-ray setup. Figure 2.6 shows a close up on the small angles up to $5^\circ$. This is the angular range that is significant for the high energy X-ray CBCT setup employed in the experiments. No change in the spectrum can be observed for angles smaller than $5^\circ$, which leads us to the conclusion that an angular dependence of the spectrum does not have to be included into the further simulation work.
Figure 2.5: Spectrum for different outgoing angles. The spectra were normalized to the sum of the spectrum in $0^\circ$ direction.

2.4 Source components and secondary radiation

So far only photons resulting from the simulations have been studied. However, in a typical X-ray source a certain amount of electrons could reach the detector as well. Moreover, in the case of high energy X-rays the creation of positrons has to be considered. Here, we checked the relative amount of electrons and positrons that reach the detector with respect to the X-ray photons. Additionally, the distribution of the secondary radiation will be examined. Knock-off simulations, where different parts of the X-ray source are left out, will reveal their impact on the secondary radiation.
2.5 Different source filtrations

In order to complete the database for the further X-ray simulations a set of different source filtration configurations were simulated. The filter material was introduced behind the first collimator as it would be placed in the experiments. Table 2.2 shows the different source filtration configurations that have been simulated.

The resulting filtered spectra can be seen in Figure 2.8. The impact of filtration on the form of the spectrum is in accordance with the density

**Figure 2.6:** Spectrum for outgoing angles in forward direction. The spectra were normalized to the sum of the spectrum in 0° direction.

Figure 2.7 shows the distribution of secondary radiation for different angles with respect to the initial electron momentum in the linear accelerator. It can be seen that the number of secondary particles in the form of electrons is 3 orders of magnitude lower. Furthermore, the number of positrons is 5 orders of magnitude below the number of photons. This means that it will be sufficient to use a pure photon beam in the Monte-Carlo (MC) simulations of the following chapters.
Figure 2.7: Total Count of photons, electrons and positrons for various angles with respect to the initial electron direction in the linear accelerator. Plots are normalized to the total number of recorded particles.

Table 2.2: Configurations of the source filtration simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron energy</td>
<td>6 MeV</td>
</tr>
<tr>
<td>Filter materials</td>
<td>[aluminium, brass, lead]</td>
</tr>
<tr>
<td>Filter lengths</td>
<td>[10 mm, 25 mm, 50 mm]</td>
</tr>
</tbody>
</table>

and thickness of the filter material. As opposed to the low density aluminium filter, the lead filter is able to cut off low energy photons and shift the peak of the spectrum to a higher X-ray energy. However, it has to be kept in mind, that a large and dense filter lead to a significant reduction in the overall X-ray flux. This typically leads to increased detector integration time and subsequently to an increase in measurement time.
2.5 Different source filtrations

(a) Aluminium filtered spectra in comparison to the unfiltered spectrum.

(b) Brass filtered spectra in comparison to the unfiltered spectrum.

(c) Lead filtered spectra in comparison to the unfiltered spectrum.

Figure 2.8: Spectra for the different configurations of filters detailed in Table 2.2.
Chapter 3

The object

3.1 Scattering

This section will investigate object scattered radiation and its impact on image quality. The object is the most evident source of scattering in the system. It is subject to the direct X-ray beam and as such the cause of most of the scattered photons created during the imaging processes. Amount and distribution of object scattered radiation highly depends on transmission lengths and as such on the geometry of the object. Additionally, the material of the object plays an important role as well as the spectrum of the incident radiation. In order to investigate the scattering of photons at the object in detail, a simplified version of the X-ray CT setup was simulated.

Figure 3.1 shows the simulation setup used in the following object scatter simulations. The object is placed close to the detector with a distance of 20 cm. The detector used in these simulations is implemented as an ideal detector made of vacuum. In contrast to a real detector made out of a scintillating material, this ideal detector will integrate the total energy of any incident radiation. The simulations will be performed with the pre-simulated non-filtrated 6 MeV input spectrum from the previous chapter as well as mono-energetic X-ray beams ranging from 0.1 MeV up to 6 MeV. The source is placed at a large distance of 50 m with respect to the detector in order to obtain an approximately parallel beam. This means that differences arising from the angle of the incident radiation will be minimal and can be neglected. The objects employed in the following
The object 20 cm

Detector

Source at 50 m

Rotation

Object

20 cm

Figure 3.1: Sketch of simulation setup

simulations are boxes and cylinders. The corresponding dimensions and materials can be seen in figure 3.2.

X = 10 cm
Y = 10 cm
Z = 10 cm

Height = 8 cm
Diameter = 10 cm

Materials

<table>
<thead>
<tr>
<th>Name</th>
<th>Composition</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>PVC</td>
<td>[ H: 50 %, C: 33.33 %, Cl:16.67 % ]</td>
<td>1.35 $g/cm^3$</td>
</tr>
<tr>
<td>Aluminium</td>
<td>[ Al: 100 % ]</td>
<td>2.70 $g/cm^3$</td>
</tr>
<tr>
<td>Steel</td>
<td>[ Fe: 99.82 %, C: 0.18 % ]</td>
<td>7.87 $g/cm^3$</td>
</tr>
</tbody>
</table>

Figure 3.2: Sketch of the objectes used in the object scatter simulations dimensions are denoted to the right of the sketches. The simulated materials with the corresponding composition is shown below the sketches.
The total amount of scattered radiation as well as the detailed distribution of the scattered photons in the radiography will be studied. This will include the composition of the scattered radiation with respect to the physical interaction processes responsible for the scattering processes and the order of scattering. Furthermore, the Scatter to Primary Ratio (SPR) will be calculated and compared for the different materials and different transmission lengths.

\[
SPR(i,j) = \frac{\text{Amount of scattering at pixel } (i,j)}{\text{Amount of primary radiation at pixel } (i,j)}
\] (3.1)

Finally, a reconstruction of the simulated projections will show the influence of the scattering on the reconstructed volume.

### 3.1.1 Physics and order of scattering

The first simulations relate to the box objects in Figure 3.2. The following simulations corresponding to figures 3.3, 3.4 and 3.5 were performed with the 6 MeV input spectrum. Figures 3.3 and 3.4 show the distribution of the different physical interactions for the box at a $0^\circ$ and $45^\circ$ rotation angle respectively. This means that the results in figure 3.3 correspond to equal transmission path lengths throughout the image of the object due to the near parallel beam geometry. It can be seen that Compton scattering clearly dominates over all other physical effects. Moreover, Compton scattering events seem to be centered in the middle of the detector and spread over the whole radiography. In contrast to this, Rayleigh scattering is rather short ranged, hence its common name small angled scattering. It is interesting to notice that the distribution of Rayleigh scattering resembles the form of the object. The remaining two effects shown in figure 3.3 are Bremsstrahlung and Pair Production. The intensity of both of these effects show that they constitute a negligible contribution to the radiographies compared to the effects of Compton and Rayleigh scattering. Furthermore, both effects are evenly speckled over the radiographic image. This means not only the overall intensity of the effects is minor, but also their distribution will not have a significant effect on the reconstruction result. Comparing the results of the different materials it is clearly noticeable that the intensity of scattered radiation is highly decreased for steel. This result seems illogical at first, since the physical interaction cross sections described in section 2.2 all seem to generally increase with the atomic number of the material. However,
Figure 3.3: Boxes of different materials with respective distributions of physical processes for a simulation with a 6 MeV X-ray beam. The projection angle of the box is 0°.
Figure 3.4: Boxes of different materials with respective distributions of physical processes for a simulation with a 6 MeV X-ray beam. The projection angle of the box is 45°.
for the steel box not only the general interaction cross section of the material, but also the absorption behaviour of the scattered photons is of importance. This means low transmission values of the X-rays also correspond to the transmission of scattered photons. This difference in absorption of photons due to the transmission lengths becomes clear in the configuration shown in Figure 3.4. The shortened path lengths through the material to the sides of the detector lead to a significant increase in transmitted Rayleigh scattered radiation in the case of the steel box. Comparing the distribution of Compton Scattering for $0^\circ$ and $45^\circ$ shows that the distribution of the scattering does not change significantly despite the different transmission lengths throughout the image.

Figure 3.5 shows the profiles corresponding to a line through the scatter projections given in Figures 3.3 and 3.4. It can be seen that in the case of the less dense objects of material PVC and aluminium, the Compton scattered radiation changes little with the projection angle. In contrast to this, the case of the steel box shows a significant increase of Compton scattered radiation with angle. This can be attributed to the overall increase in transmission specifically at the sides of the box with increasing angle. Due to the high angular distribution of the Compton scattering angle, the distribution of Compton scattering still evens out throughout the image as opposed to the distribution of Rayleigh scattered radiation. The third column in Figure 3.5 shows the amount of Rayleigh scattered radiation. Particularly in the case of the steel box, this form of scattering becomes enhanced with the projection angle. This clearly corresponds to the smaller transmission lengths to the side of the object. This effect is smaller but still visible in the case of the aluminium box, but vanishes in the case of the PVC box. This can be attributed to the low density of the object. Here reabsorption of scattered photons is low compared to the other two cases.

The results for the PVC and the aluminium box shown in Figure 3.5 might lead us to believe that a simple estimation of the Compton profile dependent on the material might be possible. The almost non-existent change of the distribution of Compton scattered radiation as well as the relative dominance of Compton scattering over Rayleigh scattering seem to support this hypothesis. However, the case of the steel box shows a completely different picture. Not only does the intensity of Compton scattered radiation double with the rotation by $45^\circ$, but also the significance of Rayleigh scattered radiation increases with respect
3.1 Scattering

Figure 3.5: Plot of the simulated scatter profile as well as the profiles for Compton and Rayleigh scattering for a 6 MeV X-ray beam and boxes of size $10 \times 10 \times 10$ cm$^3$ composed of different materials. The profiles were taken through the middle line of the radiographies. The distance between the object and the detector was 20 cm. The distance between the source and the detector was 50 m in order to have a near parallel beam geometry.

to Compton scattering. The cause of this are of course the overall low transmission values, which enhance the problem as the ratio of scattered to primary signal will be more likely to increase.
3.1.2 Energy dependence of scattered radiation

In the following, the scattered radiation will be investigated for a set of mono-energetic X-ray beams. Figure 3.6 shows the exemplary case of the steel box with the SPR measured at the transmission region as well as in the air for photon energies ranging from 0.1 MeV up to 6 MeV. Moreover, the respective percentage of physical interactions on the scattered radiation are plotted for each energy. It is interesting to notice that for an X-ray beam with an energy of 0.1 MeV the amount of scattered photons exceeds the amount of primary transmission leading to a SPR of over 100%. Generally, the SPR is higher for lower energetic X-ray beams, which is directly correlated to the energy dependent transmission capabilities of the X-ray photons. In contrast to this, the amount of scattering in the air region, shown in Figure 3.6b, shows a slight increase with energy. This can be explained by the contribution of physical interactions detailed in Figure 3.6d. With an increasing contribution of Compton scattering, the small angled Rayleigh scattering becomes less important and the wider angled Compton interactions lead to increased amounts of radiation scattered farther away from the object. This is of course the same effect seen in the spectral simulations corresponding to Figure 3.3, where the wide ranged effect of Compton scattering can be directly compared to the short ranged influence of Rayleigh scattered photons. It is worth noting however, that the amount of scattering at the air region is significantly lower than the scatter at the transmission region.

3.1.3 The scatter to primary ratio vs the gray value

The second set of simulations were performed on the cylinder object shown in Figure 3.2. All of the following simulations were performed with the 6 MeV input spectrum. The geometry of the simulation setup such as the object to detector distance as well as source detector distance was chosen according to the setup in Figure 3.1. Figure 3.7 shows the three different radiographies for the cylinders corresponding to the three materials detailed in Figure 3.2. Mean values of the SPR have been computed at various locations on the detector. For the computation of the mean values a circular region of interest spanning a diameter of 10 pixel at each of the chosen detector positions was averaged. This procedure was performed on the results of a set of 10 simulations each executed with $10^7$ initial photons. The mean values as well as the standard deviation of the hereby retrieved results can subsequently be calculated.
### 3.1 Scattering

(a) Simulated radiography of the steel box.

(b) SPR corresponding to the air region shown as blue box in Figure 3.6a.

(c) SPR corresponding to the transmission region shown as red box in Figure 3.6a.

(d) Percentage of the different physical interactions on the composition of the scattered radiation.

**Figure 3.6:** SPR and physical interactions for the steel box and monoenergetic X-ray beams ranging from 0.1 MeV up to 6 MeV. Figures 3.6b and 3.6c show the SPR at the air (blue box) and transmission region (red box) shown in Figure 3.6a.
Figure 3.7: SPR of cylinders with a diameter of 10 cm for a 6 MeV X-ray beam, at different locations throughout the detector. Object to detector distance as well as source detector distance was chosen according to the setup in Figure 3.1.
3.1 Scattering

from the dataset. Figure 3.7d outlines the resulting mean SPR values and their respective standard deviation at the various positions across the detector for the respective materials. In all three cases the measured SPR decreases with decreasing transmission lengths. Furthermore, an increase of scattered radiation with the density of the material can be observed. It is interesting to notice that despite the large differences in SPR at the transmission region, all three material cases seem to result in a similar amount of scattered radiation at the air region in a distance of 6 cm from the center of the detector. This is in accordance with the findings of the previous investigations shown in Figure 3.6. The SPR in air is relatively small compared to the SPR at the transmission region and only small differences between the material cases can be observed.

**Figure 3.8:** The SPR plotted against the measured intensity for different materials and a 6 MeV X-ray beam, corresponding to the scatter projection shown in Figure 3.4.

The results might suggest that a relation between the SPR and the intensity can be deduced. In order to test this hypothesis the measured intensity is plotted against the corresponding SPR for all three materials (see Figure 3.8). The values in this plot were deduced from the box measurement at a 45 degree angle shown in Figure 3.4. As expected, the SPR decreases with intensity for all three materials. However, the relationships between the SPR and the measured intensity do not coincide. This means, a simple deduction of the SPR from a transmission measurement is not possible. The reason for the discrepancy is the distinct interplay between both scatter probability and re-absorption of scattered radiation for a given object.
3.1.4 Impact of scattered radiation on reconstructions

In order to assess the impact of the scattered photons on the reconstructed images, 360 projections of the cylinder objects were simulated. Each projection resulted from a simulation performed with $10^7$ photons and a different random seed. The pixel size of the detector was chosen to be 1 mm, the distances between object, detector and source were chosen according to Figure 3.1. The pre-simulated 6 MeV spectrum was used as an input spectrum. The resulting simulated data allows the reconstruction of both the total measured signal as well as the pure primary signal without scattered radiation. A simple Feldkamp-Davis-Kress (FDK) algorithm in combination with a Ramp filter and a Hamming window [30] was chosen for the reconstruction. In addition to the Hamming filter, the projections were filtered with a median filter of neighbourhood 3 in order to reduce the noise in the reconstructions. Figure 3.10 shows the middle slices of the reconstructed volumes. The underestimation of gray values in the center of the slice of the reconstruction of the total signal can be observed for all three cylinder materials. Moreover, the scatter corrected reconstruction clearly reduces this effect.

![Profiles of the cylinder reconstructions with and without scatter.](image)

**Figure 3.9:** Profiles of the cylinder reconstructions with and without scatter.

The profiles shown in Figure 3.9 highlight this result. The different magnitudes of cupping that can be observed in the reconstructed volumes
Figure 3.10: FDK cylinder reconstructions of the total signal and the primary signal without scatter for the cylinders of various materials.
is of course directly correlated to the amount of scatter and in particular the SPR in the measurement. As already shown in Figure 3.7, the steel cylinder exhibits much larger amounts of scattered radiation compared to the lighter materials. It is noteworthy however, that the removal of scattered radiation still can not completely get rid off the cupping artefact. Particularly in the case of the denser steel cylinder a remaining underestimation of gray values can be observed. This can be attributed to the fact that the simulations were performed with a spectrum rather than a mono-energetic X-ray beam. This means the non-linear attenuation of the different energetic X-ray photons has an influence on the resulting reconstruction. This artefact resulting from the poly-energetic nature of a X-ray beam will be investigated in the next section.

### 3.2 Spectral investigations and Beam hardening

Another source of image degradation is the poly-energetic nature of the X-ray beam. While passing through an object the lower-energetic photons of the beam will be attenuated more or sometimes even completely absorbed whereas higher energetic photons are able to pass with ease. The different attenuation and absorption behaviour of the photons is a consequence of the energy dependent attenuation coefficients, which are larger at lower energies. This increases the mean value of the spectrum of the X-ray beam. This effect is called the hardening of the spectrum or the beam hardening effect. Beam hardening is highly dependent on material and transmission lengths. Figure 3.11 shows the exemplary case of a steel cylinder head simulated with the previously determined 6 MeV input spectrum. The resulting spectra after X-ray transmission at various transmission lengths are shown. The shift in mean energy for long transmission regions that is typical for beam hardening cases can clearly be seen in the plot.

The influence of material on the spectrum of the X-ray beam has already been shown in the source simulation chapter. Through different materials and material thicknesses the spectrum can be changed. In this chapter a series of measurements and the corresponding simulations on the effect of beam hardening are performed. The Monte Carlo simulations allow us to additionally investigate the difference between the spectra for the primary and the scattered radiation.
3.2 Spectral investigations and Beam hardening

Figure 3.11: Exemplary case of beam hardening from the simulation of a small steel cast part. The spectra are normalized with respect to their total intensity.

The effect of beam hardening on the reconstructed volume is similar to scatter artefacts. Beam hardening will appear in a reconstructed volume as a cupping artefact. This effect of the different absorption of the poly-energetic X-ray beam could be seen already in the reconstruction in Figures 3.9 and 3.10. Here, it is apparent that the reconstructed volume exhibits a residual amount of cupping even after the removal of all scattered photons. As a matter of fact, the object material does behave in the same way as the source filters that have been discussed in the source simulation chapter. This means we can accordingly expect large spectral changes in the form of low energy cut off and peak energy shifts for large and dense transmission volumes.

In addition to the effect of beam hardening, the spectrum of the primary and the scattered radiation incident on the detector will differ greatly. Scattered radiation will be skewed to lower energies compared to the spectrum of the primary radiation. This is a direct result of the physics involved in the scatter interactions, which are largely inelastic in the high energy X-ray case and thus lead to a redistribution of energy between the particles and subsequently to an overall loss of energy for the incident photons.
The goal of this chapter is the study of the beam hardening for different materials and transmission lengths. Moreover, the spectrum of the scattered radiation will be compared to the spectrum of the primaries. Figure 3.12 shows a sketch of the simulation setup used in the beam hardening simulations. The simulations were performed with the unfiltered 6 MeV spectrum presented in the source simulation chapter. A total of $10^9$ events were simulated. For the analysis of the spectral changes the total energy of the outgoing photons will be recorded behind the wedges on an ideal detector with a pixel pitch of 0.2 mm. The energy will be recorded in energy bins of 100 keV. Moreover, the spectrum will be evaluated at positions along the vertical axis of the detector for each material. In addition to the recorded energy, the photons will be classified in scattered and primary radiation. This will help us to quantify the difference in scattered and primary spectra.
Table 3.1: Table with the material properties for the wedge objects in the beam hardening simulations shown in Figure 3.12.

<table>
<thead>
<tr>
<th>Materials</th>
<th>Composition</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminium</td>
<td>[ Al: 100 % ]</td>
<td>2.70 g/cm³</td>
</tr>
<tr>
<td>Copper</td>
<td>[ Cu: 100 % ]</td>
<td>8.96 g/cm³</td>
</tr>
<tr>
<td>Brass (MT - MS 60)</td>
<td>[ Cu: 59 %, Zn: 40 %, Si:0.5 %, Sn:0.5 % ]</td>
<td>8.44 g/cm³</td>
</tr>
<tr>
<td>Steel (St37)</td>
<td>[ Fe: 99.82 %, C: 0.18 % ]</td>
<td>7.7 g/cm³</td>
</tr>
<tr>
<td>Stainless steel (X5 Cr Ni 18 - 9)</td>
<td>[ C: 0.03 %, Si: 1 %, Mn: 2 %, P: 0.045 %, S: 0.03 %, Cr: 19.5 %, Ni: 10.5 %, N: 0.1 %, Fe: 66.795 % ]</td>
<td>7.9 g/cm³</td>
</tr>
</tbody>
</table>

3.2.1 Material and transmission dependent spectral changes

The leftmost plots in Figure 3.13 show the spectra of the X-ray beam exiting the metal wedges for the two exemplary cases of the aluminium and the steel wedge. The thin end of the wedge corresponds to a pixel value of 80 with increasing transmission lengths up to the largest end of the wedge corresponding to a pixel value of 930. The overall decrease in intensity with increasing pixel numbers can be attributed to the increasing transmission lengths and thus increasing absorption of X-ray photons. The decrease in intensity is more noticeable for low energy photons. The beam hardening effect can be quantified by comparing the resulting mean energy of the different spectra. Figure 3.14 shows an exemplary spectrum and the calculation of its mean energy. The relation between material, transmission length and mean energy can be seen in Figure 3.15. The shift in mean energy to higher energies for larger transmission length, which is typical for the effect of beam hardening, can be observed. The weighted mean energies (calculated according to Figure 3.14 show however, that the effect is much less severe in the case of the aluminium wedge compared to the other four wedges. This can be attributed to the large difference in density between the aluminium wedge with a density below 3 g/cm³ and the other four wedges, which
have densities exceeding $7 \, \text{g/cm}^3$ (cf Table 3.1).

Besides the investigation of the spectral changes and shifts in mean energy of the primary radiation, a study distinguishing scattered and primary radiation might be worthwhile. As discussed before, due to inelastic scattering event, we expect the spectrum of scattered radiation to be generally focused at lower energies compared to the primary beam. However, the previous studies of object scattered radiation showed the complex dependencies between both the amount of scattering and the re-absorption of scattered radiation for different materials and transmission lengths. As a result, we can not directly anticipate the spectrum of scattered radiation behind the object to be shifted to lower mean energies with respect to the primary radiation.

The second plot in Figures 3.13a and 3.13b shows the spectra of the scattered radiation exiting the aluminium and steel wedge. It can be clearly seen, that most of the scattered radiation has an energy below 2 MeV. Interestingly, scattered radiation shows a clear increase with growing transmission lengths in the case of the aluminium wedge, while the scatter component of the spectrum resulting from the steel wedge simulation stays constant with respect to distribution and intensity for the complete pixel range. A plot of the SPR (cf. rightmost plot of Figure 3.13) shows the increasing severity of the scatter contribution with increasing material size. For particularly large transmission lengths, the transmitted primary intensity drops to undetectable values leading to a SPR of over 100%. However, due to the fact that these large scatter contributions only occur at very low energies, the overall integrated SPR will not turn out to be as extreme, as shown in Figure 3.16.

### 3.2.2 Verification with measurements

In order to verify the simulation results, measurements of the beam hardening wedges have been performed (cf. Figure 3.17). Table 3.1 shows the detailed materials of the beam hardening wedges and Table 3.2 shows the acquisition parameters of the measurements.

Figure 3.18 shows the comparison between the simulated and the measured wedge profiles. The profiles are extracted along the colored lines depicted in the simulated and measured radiography. Especially in the case of the steel wedge, both the simulated and measured results show the
Table 3.2: Acquisition parameters of the Beam Hardening measurements.

<table>
<thead>
<tr>
<th>X-ray Source - Pulstar Linac PSL-6D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
</tr>
<tr>
<td>Frequency</td>
</tr>
<tr>
<td>Dose rate at 1m distance</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Detector - XRD 1621 AN14 ES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gain</td>
</tr>
<tr>
<td>Integration time</td>
</tr>
<tr>
<td>Binning mode</td>
</tr>
</tbody>
</table>

A non-linear profile common to beam hardening. The differences between the measured and simulated profiles likely stem from the fact, that an ideal detector, integrating the total energy of all incident radiation, was used. In reality, the detector will likely have a non-linear conversion of photons of different energies, particularly when the spectral range is as large as in this example. Additionally, scattering in detector and environment could lead to an added signal. These effects will be subject of the subsequent chapters.
(a) Aluminium Wedge. (b) Steel Wedge.

**Figure 3.13:** Spectra of the X-ray beam exiting the metal wedges. The spectra are plotted against the pixel along the wedge from the thinnest to the longest part of the wedge. This means a pixel value of 80 corresponds to the thin upper part of the wedge shown in Figure 3.12 and a pixel value of 930 corresponds to the largest material transmission, which means the large lower part of the wedge shown in Figure 3.12.
3.2 Spectral investigations and Beam hardening

Figure 3.14: Sketch of the mean energy calculations for an exemplary spectrum. The mean energy corresponds to the energy, where the upper and lower sum of the spectrum bins are equal. On the left the calculation of the mean energy for a normalized spectrum is shown. On the right, the corresponding calculation of the weighted mean energy is depicted. The each histogram bin is weighted with respect to its corresponding energy.

Figure 3.15: Mean energy and weighted mean energy corresponding to the positions along the various wedges in the radiography calculated according to Figure 3.14. A pixel value of 80 corresponds to the thin upper part of the wedge (cf. Figure 3.12) and a pixel value of 930 corresponds to the large lower part of the wedge (cf. Figure 3.12).
Figure 3.16: Simulated radiographies for a 6 MeV X-ray spectrum and the simulation setup shown in Figure 3.12. The simulated primary signal as well as the scatter signal and the resulting scatter to primary ratio are depicted.
Figure 3.17: Pictures of the setup used in the beam hardening measurements.
Figure 3.18: Comparison of the measurement of the beam hardening wedges with the corresponding simulations. The radiography on the left shows the simulation of the metal wedges and the radiography on the right depicts the corresponding measurement. The colored lines indicate the positions where the profiles were extracted. The resulting profiles shown below the radiographies correspond to the aluminium and the steel wedge.
Chapter 4

The detector

The detector is a crucial part of the X-ray imaging system turning the attenuated radiation into a digital signal. Current X-ray Computed Tomography scanners mostly use indirect detection detectors in the form of active matrix flat-panel scintillation detectors for the measurement of the radiographies. The detector employed in this high energy MeV X-ray CBCT system is described in Table 1.2. Figures 1.2 shows the detector in its mobile mounting with the required 60 mm lead shielding around the edges. The shielding allows the use of the flat-panel detector with the MeV X-ray source, however, the performance of these digital detectors in high energy X-ray settings is not known so far. The performance characterisation of a detector in an imaging system is not independent of the rest of the system. Focal spot, spectrum and scattering influence the signal transfer of the imager. This chapter aims to quantify the detector performance characteristics by measuring and simulating the employed imager in the X-ray setup. The performance quantification will be done by measuring the detectors MTF using the standard edge method [16]. Furthermore, detailed Monte-Carlo simulations will help understand the response of the detector. An investigation of the detectors response to different energies in the form of the Quantum Absorption Efficiency (QAE) will be performed and the impact of the different detector components on the imagers Point Spread Function (PSF) will be studied. The final goal of these studies is to be able to describe the signal transfer of a incoming high energy spectrum of radiation into the digital signal.
4.1 PSF simulations

An X-ray systems PSF describes its response to a pencil beam. Assuming a linear behaviour of the detector and an artefact free measurement, we can define the detected X-ray image to be the true image of the object convoluted with the PSF of the system. As such, the measured image is a blurred version of a virtual ideal measurement. There are several different reasons for a blur of the image in the detection chain. Scattering inside the detector caused by the various detector components as well as a spread of the optical photons in the scintillator can be the origin of this type of image degradation. This section aims to understand the impact of these effects on the detectors PSF. In order to do this a realistic model of the detector in the MeV CBCT setup will be implemented and its response to the high energy beam will be simulated. Detailed simulations of the detector response with respect to different X-ray energies as well as various incident angles of incoming radiation allow the accurate assessment of the detector response to the high energy X-ray signals. Figure 4.1 shows the model of the detector implemented in the Monte Carlo simulation framework. Dimensions and materials were kept as close as possible to the values of the flat panel imager employed in the high energy CBCT setup (see Table 1.2). Figure 4.2 shows the simulation setup in GEANT4 visualized with HepRA[13]. Besides the detector geometry, 100 simulated events consisting of 1 MeV photons are shown.

Figure 4.1: Sketch of the detector employed in the simulations analysing the internal detector scatter and cross talk. The black box shows a close up on the layered structure of the detector with the corresponding materials and layer-thicknesses.

4.1.1 Simulated PSF for different energies

A first set of simulations investigates the spread of the signal in the scintillator for various X-ray energies ranging from 0.1 MeV up to 6 MeV.
Figure 4.2: Sketch showing the detector employed in the GEANT4 simulations and 100 simulated events with 1 MeV (visualized with HepRApp [13]). In dark blue, the aluminium entrance window and the aluminium housing are shown. The scintillator is depicted in red and the amorphous silicon in yellow. The teal block shows the glass base. The green tracks show the photons and the red tracks show charged particles, namely electrons and positrons.

To do this, the mono-energetic X-ray beam was directed perpendicular to the detector onto the middle pixel of the active matrix. $10^7$ photon histories are evaluated per energy and the deposited energy in the scintillator is recorded. Figure 4.3 shows the exemplary case of the simulated...
detector response for the low and the high end of the energy range. The two dimensional intensity profiles were smoothed with a median filter of neighbourhood 2. The color axis was scaled logarithmically and normalized to one at the center pixel in order to illustrate the difference between the signal spread in both cases. Figure 4.4 shows the top view of the same plot for various energies. The plots clearly show an increase in signal blur for higher energetic radiation. This impact of the energy on the signal blur can have various possible causes. First of all, the low energetic photons are more likely to be completely absorbed in the scintillator right away. High energetic X-rays on the other hand are more likely to deposit in a cascade of physical interactions. In addition to that, high energetic photons are more likely to pass through the active matrix and TFT layer without depositing energy. The subsequent interactions with the glass base and the housing of the detector can possibly lead to backscattered photons that superimpose the initial signal in the scintillator. Lastly, the entrance window of the detector can be a source of scattered radiation. The interaction probability of this scattering interactions increases with energy as well. Moreover, very low energetic photons can be filtered out by the entrance window material.

Figure 4.3: Images of two PSFs for 0.1 MeV and 6 MeV monoenergetic X-ray beams. The 3d profiles were smoothed with a median filter. Both PSF profiles were normalized to one at the center pixel and plotted logarithmically in intensity.

For a more detailed analysis of the difference between the PSFs shown in Figure 4.4, the images are now radially integrated in order to extract their profiles. All profiles are normalized to one at the center pixel. Figure 4.5 shows the extracted radial PSF profiles. The center pixel was excluded from the plot in order to enhance the differences in the slope for
4.1 PSF simulations

Figure 4.4: Images of the PSFs for various mono-energetic X-ray beams. The color axis is scaled logarithmically and the images are normalized to one at the center pixel.

the different energetic X-ray beams. A correlation between the energy of the X-rays and the spread of the signal can be observed. In the low energy case of the X-ray beam of 0.1 MeV energy almost no signal spread can be observed, whereas in the case of the 3 MeV and 6 MeV beam, 2% of the signal are still present at 1mm distance to the center pixel, where the incident beam hit the pixel. Interestingly, while the 3 MeV and 6 MeV beam sit seem to be largely similar, it can be observed that the 6 MeV beam drops to 0 faster than the 3 MeV case. This means a direct relation between energy and signal spread might not be deducible in this case.

4.1.2 Impact of detector internal scattering

The PSF of the detector is not only determined by the signal spread in the scintillator, it is also dependend on the thickness of the scintillator
Figure 4.5: Plot of the radial integrated PSF profiles for mono-energetic X-ray beams of different energies. All profiles were normalized to one at the center pixel. The center pixel is left out in the plot in order to highlight the differences between the different cases.

and it is influenced by scattered radiation in the detector. The latter can be caused by components of the detector such as the entrance window and the housing. Furthermore, the scintillator itself can be considered as a source of scattered radiation involving mainly the produced visible light photons. This section aims to understand the impact of the detector components on the blur of an incoming signal. The simulations allow the virtual removal of detector parts shown in Figure 4.1 in order to investigate the change in image blur, which can be quantified by the detectors PSF. In order to investigate the impact of the different detector components on the form of the PSF, different configurations of the imaging system were simulated. The various configurations of the detector can be seen in Table 4.1. The simulations were performed with an X-ray beam sampled from a 6 MeV input spectrum.

Figure 4.6 shows, that the different configurations detailed in Table 4.1 basically lead to two different forms of the PSF. The signal in the detector exhibits a wider spread for configurations 0, 1, 2 and 4, whereas the signal
Table 4.1: Detector configurations for the PSF simulations to assess the impact of the different detector components on the signal spread in the detector.

<table>
<thead>
<tr>
<th>Configurations</th>
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<th>3</th>
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<td>✘</td>
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<td>✘</td>
<td>✔</td>
</tr>
</tbody>
</table>

EW: Entrance Window, GB: Glass Base, HS: Housing

is narrower in the case of the remaining configurations 3, 5, 6 and 7. To understand this signal blurring behaviour we have to investigate what is common to the corresponding configurations. A comparison between the two sets of the configurations and the table shows that the signal spread seems to directly correspond to the first column in table 4.1. This means that the entrance window has the largest impact on the PSF compared to the other detector components.

4.1.3 PSF for different angles of incidence

For a complete modelling of the detector response the signal spread corresponding to different angles of the radiation has to be studied. A deviation from the normal direction with respect to the detector surface can have various causes. Primary radiation that arrives at a pixel which is not the center of the detector will have a slight angle of incidence due to the cone beam geometry. In addition to that, scattered radiation will tend to arrive at the detector in an angle that deviates from the direction of the primary beam. It is important to examine if these events change the PSF significantly. Especially for a possible deconvolution, it has to be determined beforehand if the PSF can be assumed isotropic throughout the detector or if a spatial dependency has to be taken into consideration.

Figure 4.7 shows the profile in x of the simulated PSF for varying
Figure 4.6: Plot of the radial integrated PSF profiles for X-ray beams with the 6 MeV input spectrum corresponding to the different configurations detailed in table 4.1. All profiles were normalized to one at the center pixel. The center pixel is left out in the plot in order to highlight the differences between the different cases.

angles of incident from $0^\circ$ to $20^\circ$, where the angular deviation from $0^\circ$ happens in x direction. Since the opening angle of the cone beam in the studied MeV X-ray CBCT setup is $2.5^\circ$, this range of simulated angles largely exceeds the maximal incident angle a primary photon might experience. For the angle range shown in Figure 4.7 only a slight change in PSF can be observed. As expected, the PSF skews in direction of the incident photons. The small extent of the change can be explained by the geometry of the detector. The thin scintillation layer does respond with a large signal spread for tilted incident radiation. From this it can be concluded, that the assumption of an isotropic PSF is justified.

4.1.4 Optical photons

It is important to notice that the previous simulations did not include optical photons. The recorded signal was deduced from the deposited energy of the photons. In reality each energy deposit will cause a shower
of visible light photons in the scintillating medium that subsequently are converted into the digital signal by the active matrix array. This means, this shower of visible light photons could add to the blur of the signal in the imaging chain. In order to assess the impact of optical photons on the PSF, simulations including optical photon creation will be performed here.

Figure 4.8 shows the comparison of the simulation results with and without optical photons. It is obvious that the additional optical photons lead to a significant increase in signal spread compared to the simulated signal without optical photons. However, the simulations with optical photons are computationally far more expensive, because the additional processing of the large stacks of visible light photons. Moreover, the result highly depends on the optical properties of the material given to the simulation program. Not only the slow and fast component of the scintillation yield but also the density of the material significantly impact the overall signal spread caused by visible light radiation in the scintillator. Even though the density of the scintillating material is known, due to the fact that it is employed in powder form, the correct density of the bulk scintillator in the simulations might be less than the density of Gadox. In order to obtain a quantification of the signal transfer properties of
the detector in the MeV CBCT setup, a measurement of the PSF is necessary. This measurement will be performed in a subsequent section of this chapter.

### 4.2 Quantum absorption efficiency

Signal degradation at the detector does not only involve detector internal scattering and signal spread. A non-linear conversion of photons of different energies in the scintillator leads to a skewed spectral sensitivity of the detector [38]. In order to investigate this energy dependent conversion efficiency of the detector simulations of the so called QAE will be performed here. The QAE measures the ratio of detected photons with respect to the total amount of incident photons.

\[
\text{QAE}(E) = \frac{\text{Number of detected photons}(E)}{\text{Number of simulated photons}(E)}
\]  

The QAE will be simulated for each energy \( E \) of incident photons on the detector. It is noteworthy, that this quantity does not measure the quality of the signal in anyway. It does not distinguish or favour detected primary over scattered radiation as it is a binary measure of detection.
4.2 Quantum absorption efficiency

Table 4.2: Optical properties of the gadolinium oxysulfide (Gd$_2$O$_2$S, Gadox) scintillator employed in the GEANT4 simulations (* room temperature values, taken from [82]).

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
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<tr>
<td>Density</td>
<td>7.32 g cm$^{-3}$</td>
</tr>
<tr>
<td>Peak E$_\gamma$</td>
<td>2.275 eV, 545 nm</td>
</tr>
<tr>
<td>Z</td>
<td>[64, 8, 16]</td>
</tr>
<tr>
<td>Refractive index</td>
<td>2.3</td>
</tr>
<tr>
<td>Scintillation yield*</td>
<td>70000 MeV$^{-1}$</td>
</tr>
<tr>
<td>Efficiency*</td>
<td>16%</td>
</tr>
</tbody>
</table>

Figure 4.9: Plot of the simulated QAE of the flat panel detector shown in Figure 4.1.

Figure 4.9 shows the resulting detection efficiency for various energies up to 6 MeV. It is obvious, that low energy photons are detected much more efficiently than high energy photons. Detection efficiency of photons above 1 MeV even drops below 1%. A reason for this is most likely the size of the scintillation layer of the detector. The thin scintillating powder layer is ideal for decreasing signal spread in the detector. However, high energy photons would generally need a longer path in order to increase
4.3 Measured MTF

The Modulation Transfer Function (MTF) quantifies the image sharpness of a CT system, by measuring the transfer of contrast in the system. The real contrast of the measured object is compared to the output contrast of the detection system. The MTF is commonly plotted as a function of spatial frequency, which refers to the ability of the system to image a black and white line pattern of a given periodicity. For the measurement of this system performance characteristic, several different test objects can be used. Most commonly used methods use a bar pattern object, a thin slit or a simple edge from a rectangular plate.

Measuring the MTF using a bar pattern is probably the most straightforward of those three methods. The input spatial frequency is already given by the bar pattern object and the output contrast per frequency can be directly computed from the image. However, this method returns only discrete values and the continuous MTF can only be approximated by a fit to the measured values.

The measurement of a slit requires an object made of two long and dense plates that are able to block out almost all of the X-ray beam. The slit in between the plates should be aligned with the X-ray beam and the detector. The resulting image leads to the determination of a Line Spread Function (LSF) perpendicular to the slit in the image, which can then be transformed into the MTF by performing a Fourier transformation. In contrast to the bar pattern method, the slit method directly results in a continuous MTF without the need for approximations. Nevertheless, this method is not generally superior, since it often yields noisy tails in the LSF. Moreover, this method can be complicated to measure because of the precise alignment that is needed between the source and the slit.

The edge method, as described in the international standard for the characterisation of digital X-ray imaging devices [16], is arguably the easiest of the methods in terms of the data acquisition process. It requires a thin object with a sharp edge being placed in front of the detector, which blocks almost all of the incident X-ray radiation in the best case. The edge is placed at a slight angle with respect to the image axis to
4.3 Measured MTF

rule out an influence of the detector matrix on the measurement. Ideally, the edge is also measured at different positions of the detector and along different directions since the MTF is not necessarily shift-invariant for a flat-panel detector. To extract the MTF from an edge measurement, the Edge Spread Function (ESF) has to be determined in a first step. The ESF is measured perpendicularly to the edge in the image and normally averaged over several pixels. From the ESF, the LSF can be calculated by differentiation. The resulting LSF is smoothed using a gaussian fit and additionally normalized. Finally, the MTF can be determined by performing a Fourier transform on the LSF.

The edge measurement is the defined standard measurement for digital imaging devices in the field of X-ray imaging. However, the standard is defined only for lower energetic X-ray spectra. The applicability of the method in the context of MeV industrial X-ray measurements is questionable. The edge object is favourably constructed as a sharp edge made of a dense and thick enough material to block out all of the incident X-ray radiation. In this case of a high energy X-ray CBCT system this condition can not be met. An opaque edge would require a thick layer of material and thus negate the sharp edge requirement. This means that the only option for the edge method in a high energy X-ray system is the semi-transparent edge method. This means we have to consider a trade-off between the sharpness of the edge of the object and the contrast in the image.

Even though a perfect MTF measurement with the edge method is not possible in the high energy application, the edge method chosen here is still advantageous compared to the other mentioned methods. Measurements of the MTF using the bar-pattern test object only return discrete values and the final continuous MTF has to be approximated by interpolation [67]. A measurement using a slit object, will be able to yield a continuous MTF, however, the method requires a good alignment of the slit with the source and has been known to yield noisy tails in the deduced LSF [67].

In [74] we investigated the influence of different plate thicknesses and their impact on the derived MTF. No significant differences between the derived, which means that all thicknesses of the edge objects are equivalent for the measurements. However, it could be seen that the semi-transparent edge method introduces scattered radiation into the
Table 4.3: MTF Measurement parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
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<td>X-ray source settings: Pulstar Linac PSL-6D</td>
<td></td>
</tr>
<tr>
<td>Energy</td>
<td>[4.0, 6.0] MeV</td>
</tr>
<tr>
<td>Frequency</td>
<td>122 pps</td>
</tr>
<tr>
<td>Dose rate at 1 m distance</td>
<td>[57.9, 91.7] mGy/s</td>
</tr>
<tr>
<td>Detector settings: XRD 1621 AN14 ES</td>
<td></td>
</tr>
<tr>
<td>Gain</td>
<td>0.5 pF</td>
</tr>
<tr>
<td>Integration time</td>
<td>1568 ms</td>
</tr>
<tr>
<td>Binning mode</td>
<td>no binning</td>
</tr>
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</table>

ESF. Selected results from the measurements performed for the work in [74] will be shown in the next sections. For the measurements, each plate was placed directly in front of the entrance window of the flat-panel detector. The acquisition parameters of the source and the detector used in the MTF measurements can be found in table 4.3. The edge plate was arranged at a slight angle of about $1.5^\circ$ with respect to the image axis to rule out an influence of the detector matrix on the measurement (see Figure 4.10).

4.3.1 Measured ESF

In Figure 4.11a the extracted ESF from the plate measurements of the 2mm edge is shown. The computation of the LSF from the ESF is a simple differentiation paired with a gaussian fit (cf. Figure 4.11b). It is interesting to notice, that opposed to an ideal edge, the ESF shows a negative and positive jump right before and after the edge. As discussed in detail in [74], we trace this phenomenon back to the object scattered radiation, which is highly forward directed and enhanced through the proximity between the edge object and the scintillator. Figure 4.12 shows a sketch of this effect. It is shown, that scattered radiation leads to a contribution to both the air and the transmitted signal. The measured superposition of object scattered radiation and signal leads to a reduced signal close to the edge of the object as well as an excess signal due to the additional scattered radiation at the air region close to the object. For larger object to detector distances effects like this even out because the scattered radiation spreads out farther. This effect will be discussed
4.3 Measured MTF

Figure 4.10: Edge measurement of the 2 mm edge device. Indicated in red is the $1.5^\circ$ angle in which the edge device is placed with respect to the image axis.

(a) ESFs extracted perpendicular to the edge of the 2 mm edge object.

(b) ESF and the corresponding LSF.

Figure 4.11: On the left, Figure 4.11a shows the ESF of the 2 mm edge device corresponding to Figure 4.10. Figure 4.11b on the right shows the ESF and the calculated LSF of the same edge object corresponding to the 6 MeV measurement in horizontal direction.
in detail in the next chapter. The hypothesis shown in Figure 4.12 was verified by a Monte-Carlo simulation (see [74]). Equivalently to the measurements, the simulated signal exhibits the same jumps around the edge. The simulation results can be seen in Figure 4.13. In order to investigate the source of the jumps, scatter volumes were recorded and tracked in the simulations. Figure 4.13 clearly shows the characteristic form of the object scatter that leads to the observed effect.

4.3.2 Deduced MTF

As described earlier, with the help of a gaussian fit and a Fourier transform the LSF yields the MTF. Figure 4.14 shows the resulting MTFs corresponding to the various configurations in table 4.3. A comparison of the MTF corresponding to the same edge object for different directions (see Figure 4.14a) shows that the resolution of the detector is isotropic. Furthermore, the MTFs of all edge objects compared in Figure 4.14b seem to exhibit only small differences, that can be explained by a misalignment of the edge object with the beam (see [74]). An average of all measured MTF at 6 MeV allows a statement about the resolution capabilities of the high energy X-ray setup. At 2 line pairs per mm the MTF was found to be at 14.6% and the visibility limit, commonly retrieved at a MTF value of 10% was deduced to be at 2.3 line pairs per mm.
Figure 4.12: Sketch of the effect of object scattering on the measured ESF.
4.4 Measured vs simulated PSF

The measured MTF can be converted into the detectors PSF with the Matlab function otf2psf. A comparison between the two PSFs from mea-

Figure 4.13: Resulting simulated ESF and the corresponding contributions of the system components from the simulations described in [74].

Figure 4.14: The MTF in the two major directions for different energies and edge thicknesses.
measurement and simulation showed a good agreement. Here, the simulation with optical photons for a 6 MeV X-ray spectrum were used. Accordingly, the comparison is made with the MTF from the measurement with the 6 MeV spectrum. The data from the vertical measurement performed with the 1 mm edge was used.

**Figure 4.15:** Comparison of the simulated PSF and the measured PSF for a 6 MeV X-ray spectrum.
Chapter 5

The complete X-ray CT setup

The previous chapters showed, that the object as well as the detector contribute to the image degradation of the measured signal in the MeV CBCT setup. However, the impact of the remaining system components of the X-ray CT setup on image quality can not be ignored. Peripheral system components, collimation, shielding and laboratory walls all are able to contribute to scattered radiation in the measured signal. Due to the fact that the scattering components in this case are not in the direct imaging path, we can expect environmental scattered radiation to consist mostly of multiple scattered radiation. It is either object scattered radiation that missed the detector at first but scattered back from a system component to the detector or radiation that exited the detector at the back that backscattered at the wall back into the detector. The latter is presumably a considerable amount for high energy photons due to the fact that a large amount of photons do not interact with the scintillator as shown by the small high energy QAE of the detector in the previous chapter.

This last set of simulation studies investigates image degrading radiation in the complete MeV CBCT setup as described in chapter 1. The different physical interactions and their respective impact on the scatter signal from the object have been discussed in chapter 3. Here, we will focus on discussing the contribution of the various system components. Additional parameter studies on source to detector and object to detector
distance were studied as previously described in [76].

5.1 Simulation setup

Figure 5.1 shows a sketch of the MeV CBCT simulation setup highlighting the various system components studied in the following simulations. The source to wall distance is fixed at 6600 mm, while other distances in the setup can be varied. Specifically the source to detector as well as the object to detector distance will be studied. These two acquisition parameters are variable in the experimental setup as well. The pre-simulated 6 MeV X-ray spectrum with a circular focal spot of radius 1 mm is used for the simulations. Moreover, all simulations are performed using a 5° cone beam angle. For each configuration $10^8$ photons were simulated and for each photon track and its secondary particles scattering events are registered. All system components where a particle has scattered are recorded and handed on to all following secondary particles. The exception to this method of scatter event inheritance are scattering interaction in the scintillator. The energy deposited in the scintillator leads to the simulated detector signal.

Figure 5.1: Sketch of the top view of the simulation setup used for the complete MeV X-ray CBCT system simulations.

For the simulations, a steel step cylinder was chosen as sample. It
offers a range of different transmission lengths allowing us to simulate the different amounts of object scatter and their respective effect on the other scatter contributions. A sketch of the step cylinder with its geometrical dimensions can be found in Figure 5.2.

**Figure 5.2:** Sketch of the steel step cylinder used in the MeV X-ray CBCT system simulations.

### 5.2 Contribution of system components on the scatter signal

The simulations point out the detector entrance window as main contributor to scattered radiation measured in the MeV CBCT setup (cf. Figure 5.3). However, due to the fact that the detector entrance window is placed in close proximity to the scintillator, this effect has a very predictable impact. The highly forward directed scatter radiation at high photon energies (as described in the first part, see compton process) as well as the short distance between the scatter medium and the detector can be
modelled as a blurring of the radiographies. We noticed this blurring of the detector PSF by the entrance window already in the knock-off simulations of the detector PSF in chapter 4. The following investigations will focus on the other system components besides the entrance window.

![Graph showing percentage of total scattered radiation](image)

**Figure 5.3:** Total amount of scattered radiation from the various system components.

Figure 5.4 shows qualitatively the simulated radiographies corresponding to object scatter as well as scatter from peripheral system components and the detector shielding. As described in [76], the peripheral equipment describes system components such as walls and mountings of other machines. It is interesting to notice the significant difference in the distribution of the scattering for the different system components. While the shape of the object scattered radiation is clearly influenced by the geometry of the object, peripheral equipment contributes more evenly to the scatter projection showing only a shadow of the form of the object. The shielding of the detector adds a scatter signal mostly to the outer borders of the radiographies and becomes insignificant several tens of pixel away from the shielding. A profile of these scattering components can be seen in Figure 5.5. The shape of the scattered radiation originating from the shielding hints at a possible CT system optimization. An improvement of the distance between the source and the detector might reduce the amount of primary radiation that hits the shielding.
As a result, this will reduce the shielding scatter component and thus the overall scatter in the radiography.

**Figure 5.4:** Simulated distributions of scattered radiation from the MeV X-ray CBCT system components (adapted from the results shown in [76]).

**Figure 5.5:** Scatter profiles of the scattered radiation from the MeV X-ray CBCT system components (adapted from the results shown in [76]). The profiles correspond to the detector pixel line shown in red in the image at the right.
5.3 Impact of acquisition parameters on the scatter contribution

Besides the study of the amount and distribution of scattered radiation from CT system components, the simulations allow the investigation of the impact of various acquisition parameters on image quality. Two system parameters in the experimental setup detailed in chapter 1 are modifiable, the source to detector distance and the object to detector distance. A parameter sweep over both of these distances was performed and the amount of scattering from the various system components was studied. The result is shown in Figure 5.6. Distances are changed with respect to the reference distance corresponding to a configuration with a source to detector distance of 4.5 m and a object to detector distance of 1 m. Positive distance changes describe a change of distance away from the source, while negative distances describe a movement into the direction of the source.

(a) Change of the object to detector distance.
(b) Change of the source to detector distance.

Figure 5.6: Relative changes of the scattered radiation for changes in object to detector and source to detector distances.

The variation of the object to detector distance shows that the closer the object gets to the detector, the larger is its contribution to the overall scattered radiation (cf. Figure 5.6a). This effect can be attributed to the cone like nature of scatter events. Scattering is typically forward directed, in direction of the photon that was the origin of the interaction. However, for inelastic scattering events, not only a change in energy, but
also a change in direction occurs. The deflection angle depends on the interaction and the energy of the photon as described in part I chapter 2. For small distances between object and detector it can be expected, that almost all forward directed object scattered radiation is measured. With increasing object to detector distance, more object scattered radiation can miss the detector. This effect is known as the air gap principle [27]. Using the distance in order to reduce object scattered radiation is a simple solution. However, the size of the object or the field of interest does not allow large deviations in object to detector distance.

A change in the source to detector distance mainly has an effect on the scatter component originating in the shielding (cf. Figure 5.6b). At closer detector distances the lead shielding in front of the detector is not hit by the X-ray beam directly any more, leading to the reduction in scattered radiation. The remaining scattering from the shielding stems from multiple scatter events.
Part III

Development of correction algorithms
In the previous part of this work it was determined that there are three different sources of image degradation in the X-ray Computed Tomography (CT) setup. The object under investigation leads to scattered radiation and a change of the X-ray spectrum resulting in non-linear signals. As a consequence, reconstructed volumes will suffer from cupping artefacts as well as a loss of contrast. Besides the object, the commercial flat panel detector is another image degrading factor in the megaelectronvolt (MeV) X-ray Cone Beam Computed Tomography (CBCT) system. An assessment of the detector determined the resolution capabilities of the high energy X-ray system. Moreover, the simulations revealed a highly non-linear conversion effect concerning the various photon energies of the 6 MeV X-ray beam. In particular for photons at very high energies, a significant drop in detection rate measured by the detectors Quantum Absorption Efficiency (QAE) could be observed. The rest of the setup can be classified as the environment, contributing mostly to the multiple scattered radiation in the measured signal. As such it is lower in signal and can be described as uniformly distributed over the X-ray image.

In the following, algorithms and methods for the reduction and correction of the image degrading effects are developed. A procedure for the fast assessment of the Scatter to Primary Ratio (SPR) of an object is presented based on irregular sampling in both the spatial as well as the angular dimension of a CT scan. Based on the amount of scattered radiation and the spectral changes for a given measurement task a hardware optimization based on detector sided filtration is developed. The size and material of the filter is chosen such that the measured SPR is minimized while the additional blurring introduced by the detector filter is kept at a minimum as well. Finally, pre-simulated Point Spread Function (PSF)s of the detector filter combination will be used in a statistical reconstruction
procedure based on scalar Gaussian Message Passing.
Chapter 1

Fast MC evaluation of object SPR

Monte-Carlo (MC) simulations of the signals in a X-ray CT system provide a reliable and accurate approach of determining image degrading contributions in the measured radiographies. Part II of this thesis showed in detail how the X-ray MC simulations allowed us to investigate the amount of scattering, the change in spectrum as well as the contribution of system components to the signal at the detector. However, the simulation speed limits the ability to perform a full MC simulation of all projections per scan.

This section presents a speed-up procedure for the determination of object SPR as well as spectral behaviour based on irregular down-sampling of the dataset of a given scan. Besides spatial and angular down-sampling procedures, different interpolation methods for the re-upscaling of the dataset will be discussed. The results will be used as input for a measurement task specific hardware optimization introduced in the next chapter.

The following calculations presume that either a CBCT scan of the object has already been performed, or that simulated scan data of the object exists. The latter can be generated with a fast analytical simulation program such as Scorpius XLab® [24]. The measured radiographies serve as an input for the irregular down-sampling procedures in both angular and spatial dimensions. As a result, a set of projection angles
will be selected for the simulation. Moreover, the spatial grid of each projection that was selected for simulation will be down-sampled as well. The angular and corresponding spatial sampling point will serve as an input for the MC simulations. The reduced number of simulations will lead to an overall speed-up of the simulations of object SPR. This concept is visualized in Figure 1.1.

\[ \text{CBCT measurement} \quad \xrightarrow{\text{angular downsampling}} \quad \text{selected projection angles: } \phi_i, i \in \{0, \ldots, N_p\}, \ldots \quad \xrightarrow{\text{spatial downsampling per selected projection } \phi_i} \quad \text{Quadtree nodes } q_{\phi_i}^{j} \]

\( \Rightarrow \) Object SPR

**Figure 1.1:** Concept of the fast MC evaluation approach by irregular angular and spatial downsampling of a X-ray CBCT measurement.

Hereinafter, the various procedures shown in Figure 1.1 will be explained. Chapter 1.1 will explain the simplification of the X-ray CBCT setup geometry for the fast MC simulations. Chapter 1.2 gives an overview on the concept of sampling and a motivation for the irregular sampling approach chosen here. Chapters 1.3 and 1.4 will go into detail about the downsampling algorithms for the angular and the spatial dimension.

### 1.1 Simplification of the detector geometry

In the previous part of this work all parts of the X-ray CBCT system were discussed in detail. The studies involved the source geometry, source and detector collimation, peripheral system equipment, stages and mountings and even the wall at the back of the laboratory. However, it was determined, that image degradation is governed by the scattered radiation and the beam hardening caused by the object as well as the signal transfer in the detector. The signal transfer in the detector can be modelled by transfer functions, however, scattered radiation from the object highly depends on the object under investigation. In order to speed up the simulation of this scatter component, the simulation setup can be stripped down to the bare minimum. This means the source will be
1.2 Measurement specific automated resolution reduction

A typical dataset from a X-ray CBCT scan consists of a set of two-dimensional projections. This means the sampling space corresponding to the CBCT scan includes three dimensions, the two spatial dimensions of the radiographies and a third dimension that belongs to the projection angle, as detailed in Figure 1.2.

\[
\mathcal{O} (N_{\text{scan}}) = \mathcal{O} (N_{\text{pixel},x}) \cdot \mathcal{O} (N_{\text{pixel},y}) \cdot \mathcal{O} (N_{\text{projections}})
\]

**Figure 1.2:** Sketch of the sampling space of a MeV CBCT scan.

In this case, the size of a complete dataset of a scan can easily be estimated by determining the upper limit of all three dimensions.
\[ N_{\text{pixel}, x} = \text{number of pixels in x direction} \]
\[ N_{\text{pixel}, y} = \text{number of pixels in y direction} \]
\[ N_{\text{projections}} = \text{number of projections} \]

This rough estimation of the order of magnitude of the dataset of a CBCT scan demonstrates the computational complexity of a full simulation of the problem. However, for the correction of image degrading effects and the development of optimized scan setups a full simulation of the complete system is not necessary. As discussed previously, a simplification of the detector geometry can be easily achieved by replacing most of the system components with pre-simulated inputs and functions. This means, the remaining need for a MC simulation is the determination of the object scattered radiation and the SPR. Considering the previously acquired results concerning the distribution and magnitude of object scattered radiation with regard to a simulation speed up, a set of important take-away points can be listed.

- The distribution of scattered radiation in a projection is varying with the gray values of the projection, however, a gray value to SPR relation could not be found.
- Compared to the primary signal, the signal of scattered radiation is less varying and generally smoother.
- The material of the object as well as the spectrum of the beam play an important role for the SPR.
- For small angular changes, the distribution of scattered radiation in the projection will not change significantly.

In the following, we assume that a CBCT scan has already been performed and we want to use the resulting radiographies in combination with their angular information for the estimation of the object SPR via MC simulation. As a result of the slow varying nature of the object SPR in both the spatial and angular dimension, a downsampling of the spatial and angular dimension of the X-ray CBCT scan seems to be a good option for a simulation speed-up. The complete set of scatter projections can then be retrieved by interpolation in all three dimensions. Hereafter, various approaches for the downsampling of the measured CBCT data will be discussed. The resulting sampling grid can subsequently be used
for a reduction of the MC simulation time of the object and its scattered radiation.

A straightforward approach for achieving this downsampling for subsequent MC simulation speed-up would be a systematic sampling of the previously acquired X-ray CT data. This means, after a starting point is chosen for all three dimensions each subsequent point in a given interval is selected. In the spatial dimension, downsampling of the projections is typically accomplished by a binning of the images. A regular downsampling in the angular dimension of the scan would lead to a set of projection angles in a regular angular interval. These systematic downsampling procedure linearly decreases simulation time. However, these crude regular resolution reduction methods don’t take into account any prior knowledge from the scan. Moreover, they can leave out important projections necessary for the correct interpolation of spatial and angular scatter projections. This can be illustrated by the case of the coin scan shown in Figure 1.3. Here, the fixed interval for the downsampling of the angular dimension leaves out an important projection angle corresponding to the 90° rotation angle which will leave us with a smoother interpolation of the scatter projection where in reality a jump in scatter intensity is possible.

![Diagram showing regular sampling points and interpolation](image)

**Figure 1.3:** Example of a regular projection selection for the case of a turning coin-like object. It is shown that a naive selection of projections in a given fixed interval can lead to errors in the interpolation in the angular up-scaling of the dataset.
Moreover, not only angular sampling can suffer from the regular downsampling approach. Figure 1.4 shows the problems that can occur in regular spatial downsampling of a measured radiography achieved by a binning procedure. In this case, the spatial sampling leaves us with undersampled object edges which appear to be far from the original round projection. At the same time, the central part of the projection, which contains the same gray values (marked in red) seems to be oversampled. Due to the same material and transmission lengths in this area, we can expect the SPR values to be equal. This means, if we would want to achieve an optimized sampling for the use in a MC simulation a less regular sampling grid could help accomplish a more accurate simulation result while retaining the same number of sampling positions. Here, a more efficient distribution of sampling points would emphasize the edges of the object, while larger areas of similar signal could be presented by a smaller number of sampling points.

![Figure 1.4: Example of a regular spatial downsampling of a projection of the coin-like object discussed in Figure 1.3.](image)

All of these sampling problems shown in Figures 1.3 and 1.4 can be alleviated by decreasing the sampling distances subsequently increasing the spatial and angular sampling points. However, this will linearly increase simulation time, curbing the initial effort of simulation speed-up.

The following procedures are based on the fact that the measured projections of a CT scan already provide us with a large amount of information. The air in a radiography can easily be distinguished from the object and a similarity between projections can be measured. While all three dimensions of the sampling space of a scan (as detailed in Figure 1.2) are obviously connected, the following resolution reduction techniques will cover the spatial and the angular components of the
data separately. A first method will determine angular sampling points singling out significant projections to be simulated. A second procedure will irregularly downsample the selected projections based on the gray values present in the images. Finally interpolation methods for the upscaling in all three dimensions are discussed.

1.3 Image guided irregular down-sampling in angular dimension

As shown in the previous section of this chapter, a fixed sampling distance in the angular space of a dataset from a measured CBCT scan might not be the best solution for an angular resolution reduction. In particular for objects whose projected area varies largely for the different rotation angles it is important to single out significant projections such that a subsequent upscaling via interpolation has the best chance of success. As discussed previously, hereinafter, we presume that a CBCT scan of the object has already been performed, which means that a dataset containing the projections at various angles $\varphi$ is available. If this is not the case the corresponding projection data could be pre-simulated using a similar primitive object or a CAD version of the object in combination with a fast analytical simulation program.

In order to understand the aspects necessary for a successful sampling of the angular dimension of a CT scan it is useful to first take a look at the simpler case of the sampling of a one dimensional signal. For simplicity we will additionally assume that the signal is bandlimited with bandwidth $M$ and that the signal has a finite length $N$. In the case of regular sampling with fixed interval, the sampling rate should satisfy the so-called Nyquist criterion $f \leq N/M$ in order to be able to fully recover the original signal. Given the Nyquist frequency $f$ the sampling interval easily calculates as $N/f$. Considering that our final goal is to reduce the number of sampling points in order to speed up the simulation time, we now want to find a reduced set of sampling points of the signal that represent the total signal well enough that an adequate reconstruction of the signal from these points is possible. Consider the simple one dimensional signal detailed in Figure 1.5a. Here, it is easy to find sampling points from which we can fully recover the original signal. They are given by the points where the trend of the signal changes (marked in red). For more complex signals as shown in Figure 1.5b, choosing a set of sampling
points becomes less obvious. Particularly when we want to restrict the total number of sampling points used, a full reconstruction of the signal will not be possible.

(a) A simple one dimensional signal with ideal sampling points (marked in red).

(b) An intricate one dimensional signal. A choice of sampling points is less obvious.

Figure 1.5: Examples of one dimensional signals for sampling considerations.

In the case we are interested in here, of the sampling of a CBCT scan in angular space, however, recovering the full original signal is not of interest. The aim of the simulations is to get an accurate estimate of the scatter projections as well as the overall scatter to primary ratio in all projections. These values are not as detailed and varied as the radiographies of the scan. As shown in the simulations in the previous part of this work, object scatter projections will typically be matched with the projection of the object, while at the same time showing less variation. This means, for a precise simulation of the scatter projections, a lower amount of sampling points in angular space is acceptable. Moreover, the scan itself already carries a large amount of information about the variation in the SPR even though it is not measured. The radiographies can serve as a guide showing variations in transmission lengths throughout the scan. Additionally, it is important to notice that the data is sorted. Assuming that the CT scan was performed at an adequate sampling rate in angular space, we can expect neighbouring projections to be similar.

Ideally, a scatter projection should be simulated as soon as it has
changed significantly with respect to the previous projection. As the scatter projections follow the measured signals, we can use the radiographic images for the determination of these sampling points. This means, in order to find the angular sampling points for the simulations we have to find measures to judge the image similarity between the projections. A straightforward way to measure the similarity between two images is the absolute value of the difference of both images.

\[ \text{Diff}_{\text{imgs}} = \sum_{i,j} |\text{Im}_2(i,j) - \text{Im}_1(i,j)| \] (1.2)

However, differences between neighbouring projections are not of interest here. Due to the fact, that the angular spacing is typically chosen small for a CT scan, measuring this difference for each pair of subsequent projections results in small values that are influenced more from a variation in the illumination from the X-ray beam than the actual image difference. A more suitable measure for the selection of angular sampling points would be the absolute image difference between a projection \( i \) chosen as sampling point and all later projections \( i + n \). This way, a threshold can be applied enabling the next sampling point choice. The pseudocode shown in Algorithm 1 details this sampling algorithm. It is important to note that this algorithm is highly sensitive to changes in the X-ray beam, reacting highly to changes in the pulse frequency of the LinAc. This means that a first pre-processing step is needed in order to normalize all projections.

The result of a angular sampling based on the algorithm detailed in Algorithm 1 on the example of a cylinder head scan can be seen in Figure 1.6. The threshold incrementally increased by \( 5 \cdot 10^6 \) (a value that roughly corresponds to about 5 times the neighbour image difference) until less than ten projections were selected for sampling. This random threshold selection shows the weakness of the approach. A good threshold is not innately given by the problem. However, the selection can be chosen such that a suitable number of sampling points is returned, which can be chosen on time and computation power considerations. Moreover, the dataset provides more information than simply the gray values of the radiographies. In contrast to using the overall pixel values to measure image similarities other image features can be used for the task of projection selection. Specifically the extend and orientation of the object in a given projection can be computed for both the gray scale and binarized
**Algorithm 1** Angular sampling by absolute image difference thresholding. Returns a list of angles containing the sampling points.

```python
1: function ComputeImageDifference(img0, img1)
2:     imgdiff ← 0
3:     for i < NX do
4:         for j < NY do
5:             imgdiff ← imgdiff + abs(img0[i][j] - img1[i][j])
6:     return imgdiff

7: procedure ChooseAngularSamplingPoints
8:     img0 ← projections(0)
9:     SamplingPoints ← add(0)
10:    diff ← 0
11:    for angle in ListOfAngles do
12:        img1 ← projections(angle)
13:        diff ← diff + ComputeImageDifference(img0, img1)
14:        if diff > threshold then
15:            SamplingPoints ← add(angle) ▷ Add new sampling point
16:            img0 ← img1
17:            diff ← 0
```

(a) Total image difference  (b) Accumulated image difference

**Figure 1.6:** The total image difference between neighbouring projections and the image measure based on the algorithm described in Algorithm 1 with the selected projections.
images. Due to the fact that these features represent an abstraction of the image, they give a more robust image descriptor since they are less sensitive to variations in the X-ray flux as well as imperfections of the measurements such as saturating or defect pixels.

Feature detection in images constitutes a large field of computer vision and image processing. The specific features that are extracted highly depend on the application and the images itself. Many algorithms, especially when image classification or object detection is concerned, need a so called feature vector in order to produce the desired output. This feature vector is a n-dimensional vector, where n represents the number of numerical features that are extracted from an object. In this case the objects are the radiographies. The most popular feature detection methods include the Harris–Stephens algorithm (based on corner and edge detection [31]), the SIFT(local Scale-Invariant Features [49]) and SURF(Speeded-Up Robust Features [5]) image features, the FAST(Features from Accelerated Segment Test [65]) feature detector as well as the BRISK(Binary Robust Invariant Scalable Keypoints [45]) method. However, these feature detection algorithms are often build to deal with a set of highly different images such as the tracking of cars in videos or the detection of a specific object in a large set of images.

In this case, due to the nature of a CBCT scan, we can simplify the feature problem significantly. The data range will be limited and all projections are gray value, which means that the different color channels do not have to be examined. Moreover, we can already expect neighbouring images to be similar, which means there is a pre-defined order to the dataset. For the following feature vectors we will additionally assume that the object can be distinguished from the background. This condition is a necessity due to the fact that the following features are based on the abstraction of the form of the object in the projection. In the case of a CBCT scan with limited field of view, where in some of the projections the object fully covers the radiographies a binarization of the object is no longer possible. In this case the previous image measure using the total image difference might be the better option for angular sampling. Algorithm 2 shows the image features and the feature vector extracted for the irregular angular sampling method.
Algorithm 2 Function for image feature extraction on a binarized and gray scale projection.

1: function GetImageFeatureVector(image)
2:     binaryImage ← Binarize(image) \ Binarize operation: automatic imaging threshold (Otsu’s method) with subsequent morphological closing using a circular structuring element of radius 3

3:     Area ← sum(binaryImage)
4:     FeatureVector ← add(Area)

5:     [x, y] ← index(binaryImage)
6:     Centroid ← [mean(x), mean(y)]
7:     FeatureVector ← add(Centroid)

8:     ConvexHull ← Hull(binaryImage) \ Determine the smallest convex polygon that contains the binary region
9:     FeatureVector ← add(ConvexHull)

10:    Extrema ← OutmostRegionPoints(binaryImage) \ Set of eight outmost points of the binary region
11:    FeatureVector ← add(Extrema)

12:    MinorAxis ← length(min(axes(ConvexHull)))
13:    MajorAxis ← length(max(axes(ConvexHull)))
14:    Orientation ← angle(MajorAxis, x-axis)
15:    Axes ← [MinorAxis, MajorAxis, Orientation]
16:    FeatureVector ← add(Axes) \ Length and orientation of the largest and smallest axis contained in the convex hull

17:    MaxIntensity ← max(image)
18:    MeanIntensity ← mean(image)
19:    MinIntensity ← min(image)
20:    IntensityMeasures ← [MaxIntensity, MeanIntensity, MinIntensity]
21:    FeatureVector ← add(IntensityMeasures)

22:    [x, y] ← indx(image)
23:    WeightedCentroid ← [mean(x), mean(y)]
24:    FeatureVector ← add(WeightedCentroid)

25: return FeatureVector
1.3 Image guided irregular down-sampling in angular dimension

Figure 1.7: Example projections with the features extracted by the algorithm detailed in Algorithm 2. The green and yellow circle display the centroid and the weighted centroid respectively. The blue lines show the major and minor axis of the smallest ellipse containing the object.
(a) Area of the binarized projection given in number of pixels.

(b) Position of the centroid of the binarized projection in x.

(c) Position of the centroid of the binarized projection in y.

(d) Length of the major axis of the smallest convex hull enveloping the binarized area.

(e) Length of the minor axis of the smallest convex hull enveloping the binarized area.

(f) Orientation of the major axis with respect to the x axis of the image.

(g) Mean intensity of the object gray values.

(h) Position of the weighted centroid of the projection in x.

(i) Position of the weighted centroid of the projection in y.

**Figure 1.8:** The various projection features extracted by the algorithm detailed in Algorithm 2 plotted against the projection angles.
Figure 1.7 shows these features for the exemplary case of two radiographies extracted from a CT scan of a small steel cylinder head. All image features of this example case extracted with the help of Algorithm 2 are shown in Figure 1.8. For some of the plotted outlines of the one dimensional features in angular space it seems natural to extract sampling points. Both the centroid (cf Figure 1.8b) and the intensity weighted centroid (cf Figure 1.8h) exhibit a clear maximum and minimum that could lead us to believe that both points might be good angular sampling positions. The area (cf Figure 1.8a) and the length of the minor axis (cf Figure 1.8e) likewise show four distinct turning points that seem suitable for sampling positions. However, we don’t want to rely on extrema computation for the angular sampling in this case. Figures 1.8c, 1.8g and 1.8i show that a peak-finding algorithm might not be the most suitable approach to measure the image similarity. Here, we rely on the fact that we already extracted a set of $N_{proj}$ observations (where $N_{proj}$ is the number of projections of a CBCT scan), each containing the feature vector obtained with Algorithm 2. We want to group these projections into a set of subgroups that are similar. This image classification based on the available feature vector data can be solved by a simple clustering approach. First, the ELBOW method [57] described in Algorithm 3 is used in order to find the number of clusters in the set of data in the list above. As shown in the final algorithm for projection clustering based on the image feature vector detailed in Algorithm 4 an additional step sorts the cluster indices based on their projection number creating a new set of cluster indices that favours neighbouring projections. Figure 1.9 shows the preliminary clustering result and the re-sorted cluster indices. As we can expect the projections per cluster index to be similar an angular sampling point per projection should be chosen. Here, we’ll choose the central projection of each cluster.

Figure 1.10 shows a comparison of the first four sampling positions extracted for the two suggested angular sampling approaches. Additionally, the mean projection of the first four clusters for the clustering approach is shown. This mean projection is calculated as the average image of all images corresponding to the cluster.

$$\text{Mean projection}_{\text{cluster } i} = \frac{1}{\# \text{ elements in cluster } i} \sum_{j \in \text{ cluster } i} \text{Projection}_j$$

(1.3)
Algorithm 3 Function that uses the ELBOW method [57] in order to determine the ideal number of clusters. The cluster number as well as a vector with the cluster indices is returned.

1: function $K\text{MEANSELBOW}(\text{FeatureMatrix})$
2:  \hspace{1em} \text{distortion\_list} \leftarrow \{}$
3:  \hspace{1em} \text{for } ktmp \text{ do}$
4:  \hspace{2em} [\text{KIndex}, \text{Centroid}] \leftarrow \text{kmeans}(\text{FeatureMatrix}, ktmp) \triangleright$
5:  \hspace{2em} \text{Performs kmeans algorithm on the feature vectors}$
6:  \hspace{1em} \text{dist} \leftarrow \text{sum of point to centroid distances per cluster}$
7:  \hspace{1em} \text{for } n < 10 \text{ do } \triangleright \text{Perform 10 kmeans clusterings per number of cluster } ktmp$
8:  \hspace{2em} [\text{KIndex}, \text{Centroid}] \leftarrow \text{kmeans}(\text{FeatureMatrix}, ktmp)$
9:  \hspace{2em} \text{dist\_new} \leftarrow \text{sum of point to centroid distances per cluster}$
10:  \hspace{2em} \text{dist} \leftarrow \text{min}(\text{dist}, \text{dist\_new})$
11:  \hspace{1em} \text{distortion\_list} \leftarrow \text{add}([ktmp, \text{dist}])$
12:  \hspace{1em} \text{distortion\_result} = \text{var}(\text{distortion\_list}) \triangleright \text{Calculate the percentage of variance explained for the cluster configurations}$
13:  \hspace{1em} \text{KResult} \leftarrow k, \text{such that } \text{distortion\_result} > \text{threshold}$
14:  \text{return } [\text{KResult}, \text{kmeans}(\text{FeatureMatrix}, \text{KResult})]$

Algorithm 4 Angular sampling by feature clustering of the projections. The following algorithm uses the previously defined functions for feature extraction and kmeans cluster number determination.

1: procedure $\text{ClusterProjections}$
2:  $\text{ListOfFeatures} \leftarrow \{} \triangleright \text{Stores the feature vectors of all projections.}$
3:  \hspace{1em} \text{for } angle \text{ in } \text{ListOfAngles} \text{ do}$
4:  \hspace{2em} \text{image} \leftarrow \text{projections}(\text{angle})
5:  \hspace{2em} $\text{FeatureVector} \leftarrow \text{GetImageFeatureVector}(\text{image})$
6:  \hspace{2em} \text{ListOfFeatures} \leftarrow \text{add}(\text{FeatureVector})$
7:  \hspace{1em} [K, \text{ClusterIndx}] = \text{KMEANSELBOW}(\text{ListOfFeatures}) \triangleright \text{Determine the number of clusters}$
8:  \hspace{1em} \text{NewClusters} \leftarrow \text{Sort}(\text{ClusterIndx} \text{ by } \text{angle}) \triangleright \text{Sort the clusters in new sets of neighbouring projections with the same cluster index}$
9:  \hspace{2em} \text{SamplingPoints} \leftarrow \text{Centers}(\text{NewClusters}) \triangleright \text{Extract one sampling point per cluster}
1.3 Image guided irregular down-sampling in angular dimension

(a) Result of the angular clustering according to Algorithm 3.

(b) Resorting of the cluster indices in Figure 1.9a and sampling point selection.

Figure 1.9: Clustering of projections based on image features and the ELBOW method. Three clusters were found, with the sorting procedure based on projection numbers this results in 8 final clusters (and thus 8 sampling points).

Comparing the images outlined in blue and the green we can see that the clustering approach detailed in Algorithm 4 successfully groups similar projections. A comparison between the projections in the red frames and the projections in the green frames shows, that even though both approaches select the same number of angular sampling points, different sampling positions were reached with the two methods. As opposed to the total image difference method (cf. Algorithm 1), the clustering approach using the ELBOW method (cf. Algorithm 4) results in a fixed number of sampling points given by the geometry of the object and the scan. In the first case, the threshold parameter can be chosen optimally with respect to the computational prerequisites. However, this degree of freedom involves guessing the minimum number of angular sampling points that sufficiently describe the scan. While the second sampling approach (cf. Algorithm 4) does not allow us to choose the size of the sampling set, it naturally groups the projections such that a sufficient sampling distance is ensured.

In order to compare the various results, a pixel wise linear and a spline interpolation is performed for the sampling points of the image difference method, the clustering method with sampling points chosen at the beginning of each cluster (method 1) and the clustering method with
Mean projection for cluster index $k$ (cf Figure 1.8)

Sampling points of clustering method (cf Figure 1.8)

Sampling points of image difference method (cf Figure 1.5)

**Figure 1.10:** Comparison of the two angular sampling methods detailed in Algorithm 1 and 4. The first four sampling points were selected for comparison.

sampling points chosen at the center of each cluster (method 2). The interpolated projections are compared to the original dataset and the total absolute image difference is summed. Figure 1.11 shows the resulting
differences normalized to the first configuration, the image difference method. Compared to the image difference method, both interpolations of the projection clustering method with sampling points chosen in the center lead to a decrease in the deviation from the original dataset. The resulting interpolations from the projection clustering method with the sampling points chosen at the beginning of each cluster is close to the result from the total image difference, while the projection clustering method 2 leads to a slightly better result. This can be attributed to the fact, that the central projections of each cluster are the farthest away from the borders between the clusters. Thus, they present the extrema of image feature differences and subsequently the best sampling option. However, the robustness introduced through the use of abstraction in the form of feature detection only leads to an improvement of around 25% in this case. Additionally, the projection clustering method results in a fixed number of sampling points, while the total image difference method gives the option of choosing the sampling point number by variation of difference threshold. This means, if the smallest number of sampling points has to be chosen, the projection clustering method with sampling points in the center of each cluster is the better option. However, if the evaluation time allows for considerably more sampling points, the total image difference method is the better choice.

![Figure 1.11: Comparison of the interpolated data using the sampling points of the various sampling methods with respect to the original data. The data was normalized with respect to the total image difference method.](image-url)
1.4 Irregular downsampling of radiographies

As shown in section 1.2, specifically in Figure 1.4, a regular downsampling of projections leads to two possible problems. First of all, a large amount of angular sampling points are distributed over an area of similar gray values. For the simulation of a correct scatter projection we can assume that these areas exhibit similar SPR values as well. Additionally sampling points at the edges or in regions where gray values change seem to be too sparse to correctly sample the form of the object in the projection. This means, a sampling based on the variation of gray values in the projection is likely to be optimal for the simulation of a scatter projection. Just as in the previous section detailing angular sampling approaches we presume in the following, that either a dataset containing the projections at various angles $\varphi$ is available. Here, particularly the projections corresponding to the angular sampling points selected previously are of interest, since all other projections will be determined by interpolation.

![Figure 1.12: Quadtree concept.](image)

1.4.1 Irregular downsampling by quadtree decomposition

A simple way to irregularly sample an image based on the gray values and the gray value variation is its Quadtree decomposition. A quadtree describes the representation of two-dimensional data by splitting the data recursively into four subregions [2]. This means, at each iteration the region nodes of the spatial dimension can get divided into four children
nodes. This concept is shown in Figure 1.12. The criterion that defines whether a node is split into four children or not can be chosen based on the particular problem. Here, the data range in the region is evaluated and a mean value as well as the corresponding error is computed. If the gray values of the region are contained in a pre-defined value range, the node will not be split any more. Additionally, a limit on the iteration depth of the algorithm specifies the minimal size of a node. Algorithm 5 shows this quadtree concept.

Figure 1.13: Spatial downsampling of the projection of a coin. On the left the original projection is presented. The middle projection shows the quadtree decomposition of the projection. On the right a binned version of the projection is displayed. Both the middle and the right downsampled projections are designed to have the same amount of spatial sampling points (729).

In order to point out the difference between the irregular sampling achieved by a quadtree decomposition of a projection and the regular binned projection we can revisit the example coin projection discussed at the beginning (cf Figure 1.4). Figure 1.13 shows the projection as well as the quadtree decomposition and a binned projection. The two latter were chosen such that 729 spatial sampling points were created. It is clearly visible that the circular structure is represented in a finer way for the quadtree decomposition due to the increased amount of sampling points clustered around the edges of the circle. The regular downsampled projection however, has many sampling points representing the same gray values. For the purpose of simulating the SPR of the projection we can expect them to be similar for these regions of equal gray value due to the fact that the material and the transmission lengths are likely to be equal.
Algorithm 5  Quadtrees decomposition of a projection.

1: function WeightedAverage(ImageRegion)  
2:     Histogram ← hist(ImageRegion); NormValue ← sum(Histogram)  
3:     MeanValue ← 0; Deviation ← 0  
4:     for i < length(Histogram) do  \> Calculate mean value of histogram  
5:         MeanValue ← MeanValue + i · Histogram(i)  
6:     MeanValue ← MeanValue/NormValue  
7:     for i < length(Histogram) do  \> Calculate deviation in histogram  
8:         Deviation ← Deviation + Histogram(i) · (MeanValue - i)^2  
9:     Deviation ← sqrt(Deviation/NormValue)  
10:    return Deviation

11: function Split(Quad)  \> Split a quad region into four child nodes  
12:     Children ← {}; [m,n] ← size(Quad)  
13:     Children.insert(Quad[1:floor(m/2)][1:floor(n/2)])  
14:     Children.insert(Quad[1:floor(m/2)][floor(n/2)+1:n])  
15:     Children.insert(Quad[floor(m/2)+1:m][1:floor(n/2)])  
16:     Children.insert(Quad[floor(m/2)+1:m][floor(n/2)+1:n])  
17:    return Children

18: procedure QuadtreeDecomp(projection, IterationDepth)  
19:     ListOfNodes ← {projection}; FinishedTree ← {}  
20:     while NOT(ListOfNodes.isempty()) AND i<IterationDepth do  
21:         CurrentLength ← length(ListOfNodes)  
22:         for j < CurrentLength do  \> Go through all nodes of the current quad tree  
23:             CurrentQuad ← ListOfNodes.pop()  
24:             Deviation ← WeightedAverage(CurrentQuad)  
25:         if Deviation < threshold then  
26:             FinishedTree.insert(CurrentQuad)  
27:         else  
28:             Children ← Split(CurrentQuad)  
29:             ListOfNodes.insert(Children)  
30:         i ← i + 1  
31:     return FinishedTree
This means for the binned projection, large regions are oversampled leading to an unnecessary extension of the SPR computation time.

![Original projection](image1.png) ![Iteration depth 3](image2.png) ![Iteration depth 4](image3.png)

![Iteration depth 5](image4.png) ![Iteration depth 6](image5.png) ![Iteration depth 7](image6.png)

**Figure 1.14:** Quadtree decomposition for the exemplary case of a projection of the small steel cylinder head part.

The coarseness of the sampling as seen in the middle image of Figure 1.13 can be tuned by the threshold and the iteration depth in the Algorithm 5. Figure 1.14 shows the quadtree decomposition of one of the projections of the small steel cylinder head part at different iteration depths. With the increasing quadtree layers, the edges of the object in the image become more defined and gray value differences within the projection are represented more accurately. At an iteration depth of seven (cf Figure 1.14f) the smallest children in the tree are of size $2 \times 2$ pixels of the original projection. The resulting quadtree decomposition resembles the original projection reasonably well with a number of 3073 spatial sampling points. It is interesting to compare this result with the original spatial sampling given by the size of the projection in Figure 1.14a, which consists of $866 \times 866$ pixels.
\[
\frac{\text{\# quadree sampling points}}{\text{\# pixels in the original projection}} = \frac{3073}{866 \cdot 866} \approx 0.41\% \quad (1.4)
\]

Equation 1.4 shows, that the quadtree decomposition of a typical X-ray projection constitutes a significant reduction in spatial sampling. At the same time it can be seen in Figure 1.14 that the distribution of gray values as well as the outline of the edges of the object are kept close to the original image. It has to be pointed out, that there are a number of more sophisticated two-dimensional downsampling methods that are similar to the quadtree structure. Most of these methods differ in the form of the nodes, the Delaunay triangulation [20] for example uses a triangular node form as opposed to the square quadtree nodes. However, due to the fact, that the basis of our decomposition is already comprised of square pixels the square super-sampling seems to arise naturally. Moreover, the resulting rectangular structure of the quadtree algorithm fits in perfectly with the resulting simulation procedure for the projection. This will be discussed in detail in the following.

### 1.4.2 Weighted Quadtree SPR Simulation Procedure

The quadtree decomposition discussed previously results in an irregularly sampled projection consisting of differently sized square nodes that are linked to a mean gray value. This means the datastructure of a quadtree projection has the following form:

<table>
<thead>
<tr>
<th>Position(_x)</th>
<th>Position(_y)</th>
<th>Size</th>
<th>Mean gray value</th>
</tr>
</thead>
</table>

Where Position\(_x\) and Position\(_y\) describe the position of the left upper corner of the quadtree node square.

In the example shown in Figure 1.14 it is also interesting to notice, that the resulting children of the quadtree carry more information than just the position and size of the sampling square. Additionally, the gray value of the quadtree node is stored. This value basically measures the mean intensity of the X-ray beam at a given spatial sampling position. As such it is directly related to the number of photons reaching the detector. For the simulations that means at darker gray values, less simulated events will contribute to the SPR computation. As a result, this additional information can be used in order to weight the number of
events simulated per quadtree node in order to obtain sufficient statistics for each simulated SPR value.

Let us for now assume that the conversion of photons into gray values is linear. This would mean that the measured intensity or equivalently the gray value of the projection at a given pixel is directly related to the measured number of photons. This is of course a simplification of the process leaving out the different energies of the photons as well as the energy dependent conversion probability of the detector. In this naive view we can deduce for a given measured gray value $v_{\text{pixel}}$ and a measured air value $v_{\text{air}}$ the number of transmitted photons will be given by:

$$N_{\text{transmitted}} = N_{\text{original}} \cdot \frac{v_{\text{pixel}}}{v_{\text{air}}}$$  \hspace{1cm} (1.5)

As discussed in the first part of this thesis, the uncertainty of a measured result obtained by a MC simulation will decrease with $\sqrt{N}$, where $N$ is the number of simulated events. As we want to measure the ratio of scattered to primary photons here, however, it is important to consider only the amount of transmitted photons per sampling position, which is the amount of measured photons. This means the error of the SPR value scales with $\sqrt{N_{\text{transmitted}}}$, where $N_{\text{transmitted}}$ is given by

$$N_{\text{transmitted}} = N_{\text{primary}} + N_{\text{scattered}}$$  \hspace{1cm} (1.6)

From the rules of error propagation it is known that for quantities formed by addition, the uncertainties add in quadrature and for quantities formed by division, the fractional uncertainties add in quadrature:

\[
\begin{align*}
\text{Addition} & \quad M = A + B \\
\delta M & = \sqrt{(\delta A)^2 + (\delta B)^2} \\
\text{Division} & \quad M = \frac{A}{B} \\
\frac{\delta M}{|M|} & = \sqrt{(\frac{\delta A}{A})^2 + (\frac{\delta B}{B})^2}
\end{align*}
\]

This means the error on the SPR value can be computed as

$$\frac{\delta \text{SPR}}{\text{SPR}} = \sqrt{\left(\frac{\delta N_{\text{scattered}}}{N_{\text{scattered}}}\right)^2 + \left(\frac{\delta N_{\text{primary}}}{N_{\text{primary}}}\right)^2}$$  \hspace{1cm} (1.7)

Remaining with the initial assumption of equation 1.5. If the same statistics should be maintained for all quadtree nodes the same number
of samples should be used for the SPR calculation. As a result, if the transmitted and thus measured number of photons should be roughly the same per spatial sampling point the simulated number of photons have to be scaled inversely according to the gray value. Accordingly for a quad of the normalized gray value $v_{n} = \frac{v_{\text{pixel}}}{v_{\text{air}}}$ the number of simulated events should be increased by $\frac{1}{v_{n}}$. This procedure is sketched in Algorithm 6. Additionally to the SPR value per node of the quadtree the simulations allow the retrieval of the spectrum of both the scatter and the primary photons.

As mentioned before, for this simulation procedure to work, the object has to be represented in the detector geometry of GEANT4. There are two different scenarios here. The form of the object can already be known, for example as a CAD file. On the other hand, a first scan of the object could have already been performed. The angular as well as the spatial sampling algorithms both depend on this knowledge as well. Appendix A describes the procedures needed for the import of the object into the GEANT4 simulation. If a triangulated mesh of the object exists already, Appendix A.2 describes this import procedure using a GEANT4 CADMesh library developed by Poole et al [62]. Otherwise, the a first reconstruction of the object has to be performed. The reconstructed volume than has to be segmented and triangulated. This procedure is described in detail in Appendix A.1.
Algorithm 6 Pseudocode describing the weighted irregularly sampled SPR simulation procedure.

1: procedure WeightedQuadSPRSimulation
2:   ImportObject(TriangulationFile, MaterialReference, MeasurementProperties) ▷ Import the object as triangulated volume surface and the corresponding material names for the object representation in the simulation. MeasurementProperties describes positioning of object with respect to source and detector.
3:   for i < length(Quadtree) do ▷ Perform one simulation run per quadtree node of the projection
4:     quad ← Quadtree.getElement(i)
5:     weight ← 1/quad.MeanGrayValue()
6:     posx ← quad.PositionX()
7:     posy ← quad.PositionY()
8:     size ← quad.Size()
9:     ConfigureXRayBeam(posx, posy, size) ▷ Align the X-ray beam with the current quadtree position on the detector
10:    NumberOfPhotons ← weight · NumberOfEvents ▷ Calculate the number of photons for the simulation of the current quadtree node
11:    [currentSPR, SpectrumPrimaries, SpectrumScatter] ← RunSimulation(NumberOfPhotons) ▷ Simulate the detector signal corresponding to the current quadtree node and extract SPR and spectra
12:   ListOfSPR ← add(currentSPR)
13:    ListOfPrimarySpectra ← add(SpectrumPrimaries)
14:    ListOfScatterSpectra ← add(SpectrumScatter)
15: return [ListOfSPR, ListOfPrimarySpectra, ListOfScatterSpectra]
Chapter 2

Efficiency optimization by detector sided filtration

The results obtained in the simulations and measurements performed in the previous part of this work yielded starting points for tomographic image quality improvement. A reduction of the object SPR, a decrease of the impact of beam hardening as well as an increase in the high energy detector QAE would significantly improve the signal and contrast in the radiographies. This improvement of the measured X-ray images will result in an enhancement of the reconstructed three dimensional volumes.

Other image degrading effects, especially other scatter components were shown to be either negligible with respect to the object SPR. Examples of these other effects are the scattered radiation from walls or peripheral equipment, which consists of mainly multiple scattered radiation. However, this significance of object SPR over the other scatter contributions is not owed to the total amount of object scattered radiation, but to the distribution of the various scatter components. Other parts of the scattered radiation such as the environmental scatter contribution of the peripheral equipment and walls were shown to contribute isotropically to the total scatter signal. This is of course a result of the high order of scattering present for these types of events. In contrast to this isotropically distributed contribution, the signal originating from
object scattered radiation is highly influenced by the form of the object as well as material and transmission lengths. Additionally, object scatter simulations not only showed that a simple gray value to SPR relation can not be deduced. They also emphasized the effects of this type of image degradation for the reconstructed volumes. Combined with beam hardening, cupping and streaking artefacts are the result of a non-optimized MeV CBCT investigation.

The low detector QAE becomes an issue particularly for larger and denser objects with low transmission values. Not only is the probability for scattering interactions higher at lower energies, but due to the non-linear conversion efficiency of the detector, the lower energy part of the spectrum is more likely to be detected. Furthermore, considering that beam hardening shifts the mean energy of the primary radiation to higher energies, this non-linear spectral detection effect worsens the detected SPR.

This chapter aims on improving radiographic imaging quality using a hardware optimization based on detector sided filtration. The filter material will amend both the effects of SPR and beam hardening while at the same time increasing the detector QAE for the high energy photons. A first section explains the overall concept of the detector sided efficiency optimization. Afterwards, a model of the filter system will be developed in order to find the best filter combination for a given CT scan.

2.1 Concept of detector sided filtration

The proposed hardware optimization aims on reducing the amount of scattered radiation in the radiography, diminishing the effects of beam hardening and increasing the detector QAE for the high energy photons. The concept is based on a filter placed in front of the detector. The filter is a metal plate that can either be a single material or a set of different materials.

The concept of detector sided filtration is not new to the field of X-ray investigations and measurements. The decrease in signal and contrast for high energy X-ray photons and flat panel detectors, described by the QAE of the detector, has been studied extensively in MC simulations [38]. Additional investigations of the X-ray signal conversion
inefficiency focused on medical applications, specifically radio-therapeutic measurements [77]. In the medical field of intensity modulated radiotherapy (IMRT) flat-panel detectors have been used in combination with metal-foils placed in front of the detector in order to diminish the non-linear QAE effect by increasing the sensitivity of the detector for the high energy photons [29]. This increase in sensitivity is especially important for dosimetric measurements. Here, the metal filter materials are called build-up materials [53]. Detector-sided beam filtration has been known not only in the medical field of X-ray investigations, but also in the field of radiographic non-destructive testing, particularly for inspections using X-ray films [68]. However, here the reason for the application of filter materials is the reduction of scattered radiation in the X-ray images. The filter materials absorb a large part of the low energy spectrum of the beam and thus filter out the main part of the scattered radiation.

Here, the filter at the detector should serve several purposes explained in the sketch in Figure 2.1. The material should filter out unwanted scattered radiation. The scattered photons are typically at the lower end of the spectrum making them more likely to be absorbed by an additional layer of material. Furthermore, cutting the lower energy photons from the detection will decrease artefacts caused by beam hardening. In this case, the filter at the detector acts in a similar way as a source sided filter. While a filter at the source pre-hardens the beam reducing the low energy radiation incident on the object as well as the detector, a filter at the detector will do the same for the X-ray beam exiting the object. With respect to the hardening of the spectrum in general both concepts work equally good, however, the detector sided filter can filter out low energy radiation created in the object, which will be detected for a configuration with only source filtration. Besides decreasing the detection of low energetic image degrading radiation, the filter will serve as an enhancer for the high energy photons. For configurations without filter, detection probability of high energy photons in the thin scintillation layer is extremely low. However, when measuring large and dense objects, these high energy photons carry a lot of the information. By forcing a part of the high energy radiation to scatter at the filter material, the energies will be broken down into a scatter cone of photons and electrons with lower energies. This way, the detection of this component of the X-ray beam will be increased.

When talking about the advantages of the detector sided filter such
**Figure 2.1:** Sketch of the concept of detector sided filtration. In the configuration without filter high energy photons have a lower probability of being detected due to the thin detector scintillation layer. On the other hand, the detector is very sensitive to low energy radiation, which contains most of the scattered radiation. The configuration with a filter added in front of the detector increases the likelihood of scattering for high energy photons. The photons scattered in the filter (see the green scatter cone) have lower energy and thus are more likely to be detected at the scintillator. Low energy photons shown in red are more likely to be absorbed in the filter reducing the amount of detected scattered radiation.
as artefact reduction and signal enhancement, the drawbacks of the filter concept have to be kept in mind as well. While close range scattering events increase high energy photon detection, they also increase the signal blur in the radiographies. The detector filter can be viewed as an additional stage in the imaging stage that introduces an additional increase in the overall PSF.

This chapter aims to investigate the effects of the filter material including the impact on the low energy part of the spectrum, the increase in detection efficiency as well as the introduced blurring by the filter stages. A set of simulations in combination with CT measurements performed on the steel step cylinder sample introduced in Part II Chapter 6, will give insights into the impact of the additional filter stages.

A model for the filters will be developed that can be used as an optimization algorithm. Finally, for a given sample, with the help of the fast MC evaluation of object SPR introduced in the previous chapter, an optimal filter configuration should be chosen from an initial naive X-ray scan as well as a set of available filters.

2.2 Effect of the filter on the detector QAE

In this first study, the impact of the filter material on the spectral detection sensitivity will be examined. For this purpose, the model of the detector introduced in Part II section 4 is used in combination with various materials of different thicknesses placed flush with the entrance window of the detector as shown in Figure 2.1. Subsequently, the change in the detectors QAE for various incident energies, as defined in Part II section 4.2, is measured.

Figure 2.2 shows the change in the detectors QAE for various materials and thicknesses. The choice of filter configurations is based on the available filter material in the laboratory. The filter material has opposite effects on the low and high energy QAE of the detector. While the detection of low energy photons is decreased, detection of high energy photons is enhanced by roughly 15%. The denser filters are more efficient in cutting off the low energy end of the incident X-ray spectrum. In the case of the 2 mm lead filter the detection of photons with energies below 0.2 MeV can be presumed to be completely cut off. Alternatively, the
5 mm copper filter has the biggest effect of the high energy detection efficiency.

It is interesting to take an additional look at the relative importance of physical interactions involved in the scattering at the detector filter. A simulation of a 6 MeV X-ray pencil beam with a total of $10^8$ photons incident on a 2 mm lead filter is performed and the total energy of photons entering the scintillator including their inherited physical interactions is recorded. Figure 2.3 shows the resulting distributions for the four main effects: Compton scattering, Rayleigh scattering, Pair Production (with annihilation events) and Bremsstrahlung. The interactions and their relative importance is quantified in the radial profiles shown in Figure 2.4. Compared to the pair production events in object scattered radiation shown in part II section 3, the pair production signal is still less significant than Compton scattered radiation by two orders of magnitude. However, in contrast to the pair production distribution present in object scattered radiation of the X-ray CT setup [75, 76], which was evenly distributed over the radiography, the pair production radiation here...
shows a cone like distribution resembling the form of Compton scattered radiation. This can be explained by the interaction chain linked to a pair production event. The positron created in a pair production event typically annihilates resulting in two photons (see Part I section 2.2 for details). In the case of object scattered radiation, pair production and the subsequent annihilation lead to large deflection of the photons
making them less probable to reach the scintillator. Moreover, the annihilation radiation that reaches the detector will be spread out over the whole radiography. Here, however, due to the close proximity of the filter material to the scintillating medium, annihilation radiation has a distribution resembling a PSF. In addition to that, it has to be noted, that the detector is highly sensitive to the energy of these annihilation photons (0.511 MeV). Aside from the annihilation radiation, Compton scattering, and specifically multiple scattering, will lead to a decrease in energy of high energy photons.

2.3 Effect of the filter on image degradation

The previous investigation of the impact of the filter material on the detectors QAE showed that the forced scattering events in combination with the annihilation photons lead to a non-linear change in the detectors sensitivity for incident low and high energy radiation. Cutting the low energy end of the spectrum will not only have an effect on beam hardening, but also exclude a large part of the scattered radiation from detection. As shown in Part II section 3.2, the spectra of primary and scattered radiation differ largely. While the spectra of scattered radiation peak at low energies and diminish at high energies, spectra and specifically the mean energy corresponding to primary radiation shift to higher energies as explained by the beam hardening effect.
2.3 Effect of the filter on image degradation

In order to investigate the effect of the filter material on both the scattered radiation as well as beam hardening, simulations of the steel step cylinder shown in part II section 5 will be performed. At first the exiting spectra corresponding to the center of each of the step cylinder steps is evaluated. Additionally, the mean energy and the SPR is computed. Afterwards, the previously computed QAE is convolved with the spectra in order to investigate the impact of the various filter configurations on the SPR and the mean energy of the X-ray beam.

Figure 2.5 shows the spectra corresponding to the various steps of the step cylinder. The spectra were normalized with respect to the total intensity of the combined primary and scattered spectrum for each step. A shift of the primary spectra to high energies for larger transmission lengths can be observed. On the contrary, the largest part of scattered radiation is concentrated at lower energies. Moreover, the offset between the curves shows an overall increase of scattered radiation with increasing transmission length. Figure 2.6 shows the SPR calculated from the curves shown in Figure 2.5. The dominance of scattered radiation over primary radiation at low energies is clearly visible. Moreover, the increasing severity of scattered radiation with increasing transmission lengths is visible.

**Figure 2.5:** Spectra of the primary and scattered radiation for each of the steps of the steel step cylinder. The spectra are normalized by the total intensity of the combined primary and scattered spectrum per step.
Figure 2.6: Scatter to primary ratios for the step cylinder steps computed from the spectra in Figure 2.5.

Figure 2.7: On the left: Mean energy and weighted mean energy of the step cylinder spectra. On the right: Plot of the mean SPR for each of the steps of the steel step cylinder.

Figure 2.7a shows the mean energy as well as the weighted mean energy of the spectra corresponding to the various steps of the cylinder. The calculation of these two mean energies has been performed according to the method introduced in the beam hardening chapter in part II.
2.3 Effect of the filter on image degradation

The increase in beam hardening is clearly visible in the rising mean energy of the X-ray beam. Both the mean energy as well as the weighted mean energy show the same behaviour. Figure 2.7b shows the mean SPR for each of the cylinders steps. A significant increase of the overall scattered radiation for cylinder step numbers 7 and 8 is observable.

![Graphs showing mean energy and SPR for various filter configurations.](image)

(a) Weighted mean energy  
(b) Mean SPR

**Figure 2.8:** Mean energy and SPR of the step cylinder steps for various filter configurations.

<table>
<thead>
<tr>
<th>Difference calculated for</th>
<th>Mean Energy</th>
<th>Mean Energy, weighted</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Filter</td>
<td>0.4546</td>
<td>0.2414</td>
</tr>
<tr>
<td>Copper Filter, 2 mm</td>
<td>0.4286</td>
<td>0.1282</td>
</tr>
<tr>
<td>Copper Filter, 5 mm</td>
<td>0.3913</td>
<td>0.1282</td>
</tr>
<tr>
<td>Lead Filter, 2 mm</td>
<td>0.2593</td>
<td>0.1000</td>
</tr>
<tr>
<td>Tungsten Filter, 1 mm</td>
<td>0.2593</td>
<td>0.1000</td>
</tr>
</tbody>
</table>

**Table 2.1:** Difference between the largest and smallest mean energy in Figure 2.8a (calculated as \( \frac{\text{max}(E) - \text{min}(E)}{\text{max}(E) + \text{min}(E)} \)).

A convolution of the spectra in Figure 2.5 allows the investigation of the impact of the filters on the mean energy as well as the SPR. Figure 2.8b shows, that for high transmission lengths corresponding to step 6 and higher, the filter configurations decrease the mean detected SPR. The tungsten and the lead filter are the most effective in decreasing the SPR in the signal. Moreover, Figure 2.8a and Table 2.1 show, that
the increase in mean energy from step 1 to step 8 is less severe for the filter configurations. This means the rise in mean energy of the detected spectrum is less with detector filters, which in turn indicates an overall decrease in beam hardening. This of course is a consequence of the overall cut-off of detected low energy photons. It is an equivalent situation as with a pre-hardened beam by source filters, with the difference that in this case the artificial hardening of the beam is applied after the object and not directly at the source. The effect of both the source and the detector filter on the beam hardening artefacts is still the same, as both equalize the overall detected mean energy. However, the detector filter has the added effect on the detected object SPR, leading to a further improvement of radiographic image quality.

2.4 Filter Point Spread Functions

The positive effects of the detector sided filter concept discussed in the previous section is countered by their negative impact on image blur. The forced scattering events that lead to the enhancement of the signal will also cause a broadening of the detectors PSF introduced by the cone-like scatter behaviour as shown in Figure 2.1. This change in the detectors PSF is worsened by the air gap between the entrance window and the scintillator of the detector. This section aims to study the impact of the filter material on the detectors PSF. Herefore, simulations of X-ray pencil beams incident onto various filter materials will be performed. The aluminium entrance window as well as the glas base and the housing of the detector are included in the simulation setup.

Figure 2.9 shows the distribution of the X-ray beam exiting the 5 mm copper filter simulated with a 6 MeV X-ray spectrum. The signal spread is quantified in Figure 2.10. The material dependent differences in the normalized PSFs are apparent. In order to quantify the signal spread a model has to be fitted to the radial distribution of the PSF. There are several different analytical shapes that are commonly used in PSF modelling:

- **Gaussian fit**: \( A \cdot \exp \left( -\frac{x^2}{\sigma^2/2} \right) \)
- **Lorentz fit**: \( A \cdot \left( \frac{x^2}{\sigma^2} + 1 \right)^{-1} \)
- **Moffat fit**: \( A \cdot \left( \frac{x^2}{\sigma^2} + 1 \right)^{-\beta} \)
2.4 Filter Point Spread Functions

Figure 2.9: PSF of the X-ray beam exiting the 5 mm copper filter simulated with a 6 MeV X-ray spectrum.

Figure 2.10: Radial profiles of the PSFs for different detector filters simulated with a 6 MeV X-ray spectrum. All profiles were normalized to one at the center pixel. The center pixel is excluded from the plot in order to enhance the tail of the PSFs.

Empirically, it was determined that the last model performed best in fitting the filter PSFs. The best model fit has been found using the smallest sum of square distance (Least Squares). The central pixel was not fitted. Figure 2.11 depicts the possible radial profile created by a Moffat model. From the behaviour of the curves to a change of the
various parameters it can be deduced that for a small signal spread $A$ and $\sigma$ should be as small as possible and $\beta$ should be maximized.

![Graphs showing distributions](image)

**Figure 2.11:** Example of the distributions originating from an analytical shape following the Moffat model. An increase in the parameter $A$ while keeping $\sigma$ and $\beta$ fixed leads to an offset of the curves. Changing the parameters $\sigma$ and $\beta$, changes the form of the tail.

Figure 2.12 shows two exemplary simulated PSFs for two different filter configurations and their corresponding PSF fits. The fit models the simulated data well for pixel values close to the central pixel. At far pixels the Moffat fit and the simulated data start to disagree. The real filter PSF is likely a superposition of various different models. However, due to the fact that the differences are small, we can expect the model to work well here. In addition to the filter optimization here, the learned fit parameters can be used for a PSF deconvolution.
2.5 Validation through Measurements

In order to verify the studied impact of the filter material on the scattered radiation, the beam hardening, the QAE as well as the PSF in a MeV X-ray CBCT measurement, a set of scans of the steel step cylinder as well as Modulation Transfer Function (MTF) measurements have been performed.

2.5.1 X-ray CT measurements of the steel step cylinder

For the investigation of the image enhancement by detector sided filters a set of measurements of the steel step cylinder object shown in Part II section 5 have been carried out. For comparison reasons, two scans with the lead and the tungsten filter positioned at the source behind the primary collimator (cf. Part II section 2.1) were performed. Each scan was performed and reconstructed using the same parameters and an in-house FDK reconstruction tool. Specifically software based corrections, such as polynomial beam hardening corrections or a ring artefact correction, were disabled in order to be able to study the impact of the detector filter on the measurement in an unimpeded manner. The only correction that was applied to the radiographies, besides the standard
dark and flat field correction, was a normalization based on the air values in the radiographies. This normalization aims to correct fluctuations in the pulse rate of the linear accelerator leading to fluctuations in intensity. The measurement settings of the source and the flat panel detector can be found in Table 2.3. The integration time of the flat panel detector was adjusted for each filter configuration in order to exploit the maximal dynamical range of the detector in each measurement. Table 2.2 shows the filter configurations with the corresponding integration times.

**Table 2.2:** Filter configurations and corresponding integration times for the filters positioned at the detector as well as the source sided filter configurations

<table>
<thead>
<tr>
<th>Filter positioned at the detector</th>
<th>Material</th>
<th>Thickness</th>
<th>Integration Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>-</td>
<td></td>
<td>1500 ms</td>
</tr>
<tr>
<td>Copper</td>
<td>2 mm</td>
<td></td>
<td>1500 ms</td>
</tr>
<tr>
<td>Copper</td>
<td>5 mm</td>
<td></td>
<td>1450 ms</td>
</tr>
<tr>
<td>Lead</td>
<td>2 mm</td>
<td></td>
<td>2000 ms</td>
</tr>
<tr>
<td>Tungsten</td>
<td>1 mm</td>
<td></td>
<td>1900 ms</td>
</tr>
<tr>
<td>Copper &amp; Tungsten</td>
<td>2 mm &amp; 1 mm</td>
<td></td>
<td>1600 ms</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Filter positioned at the source</th>
<th>Material</th>
<th>Thickness</th>
<th>Integration Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lead</td>
<td>2 mm</td>
<td></td>
<td>1650 ms</td>
</tr>
<tr>
<td>Tungsten</td>
<td>1 mm</td>
<td></td>
<td>1600 ms</td>
</tr>
</tbody>
</table>

For each step of the step cylinder 100 slices of the reconstructed volume were averaged and the radial profiles were extracted. In order to evaluate the impact of the filter configurations on the scan, cupping and contrast per step and configuration were computed. In the following we define cupping to be the difference between the highest and lowest material gray value ($G$) of a slice (cf. Figure 2.13).

$$Cupping = \frac{G_{max} - G_{min}}{G_{max}}$$  \hspace{1cm} (2.1)
Table 2.3: Acquisition parameters corresponding to the detector filter measurements of the steel step cylinder.

<table>
<thead>
<tr>
<th>X-ray Source - Pulstar Linac PSL-6D</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy 6.0 MeV</td>
<td></td>
</tr>
<tr>
<td>Frequency 125 pps</td>
<td></td>
</tr>
<tr>
<td>Dose rate at 1m distance 94 mGy/s</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Detector - XRD 1621 AN14 ES</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Gain 0.5 pF</td>
<td></td>
</tr>
<tr>
<td>Binning mode no binning</td>
<td></td>
</tr>
<tr>
<td>Integration time 1450 - 2000 ms</td>
<td></td>
</tr>
</tbody>
</table>

Contrast will be computed at the inner hole of the various steps of the step cylinder. This means the contrast compares the average gray value of the air in the middle of the step with the adjacent material gray value (cf. Figure 2.13).

\[
\text{Contrast} = \frac{G_{material} - G_{air}}{G_{material} + G_{air}} \tag{2.2}
\]

Figure 2.14 shows the reconstruction of the step cylinder measured without detector filter. The central slice on the left shows that the contrast between the material and air values in the middle of the cylinder steps decreases significantly with an increase in cylinder diameter. Additionally, the reconstructed slices shown on the right display a large amount of cupping.

Figure 2.15 shows the exemplary cases of the reconstructed slices corresponding to step 5 and 6 for various detector filter configurations. Both the 5 mm copper filter as well as the 2 mm lead filter lead to a significant decrease in cupping compared to the reconstructed slices of the configuration without filter. It has to be noted, that cupping is commonly corrected by a filter employed at the source. In order to compare the source sided with the detector sided filtration two scans with equivalent source sided filters have been performed. Figures 2.15a
Figure 2.13: Exemplary case of the calculation of cupping and contrast on the radial profile of the step cylinder.

Figure 2.14: Reconstruction of the step cylinder measured without detector filter.
(a) Extracts of the reconstructed slices corresponding to step 5 for 4 exemplary cases.

(b) Extracts of the reconstructed slices corresponding to step 6 for 4 exemplary cases.

(c) Radial profiles corresponding to step 5 and step 6 for all detector filter configurations.

**Figure 2.15:** Reconstructed slices of step 5 and 6 of the step cylinder measured with various filter configurations. Figure 2.15c shows the extracted radial profiles.

and 2.15b show show that the 2 mm lead filter employed at the source does not remove as much cupping as the equivalent filter material at the detector. This difference in effectiveness can be explained by the impact
of the filters on object scattering. While both the detector and the source sided filter reduce beam hardening, only the detector sided filter can filter out scattered radiation created at the object. The radial profiles shown in Figure 2.15c quantify this filter impact on cupping. For the two steps shown here, step 5 and 6, the 5 mm copper detector filter seems to perform better than all the other filter configurations detailed in table 2.2. Both configurations where the filter was positioned at the source, are clearly less effective than their equivalent detector filter configurations.

![Graph showing cupping and contrast for different filter configurations.](image)

**Figure 2.16:** Cupping and contrast for all step cylinder steps and detector filter configurations computed according to Figure 2.13.

In order to assess the impact of the detector filter configurations on the various transmission lengths present in the step cylinder all reconstructed slices and specifically all radial profiles are now evaluated with respect to cupping (cf. equation 2.1) and contrast (cf. equation 2.2) as shown in Figure 2.13. The results are shown in Figure 2.16. It is interesting to see, that while the 5 mm copper filter performs better than all other filters for step cylinder steps 1 to 6, the same filter has the worst performance with respect to contrast correction for small step cylinder steps. For the largest transmission lengths, the 2 mm lead filter leads to the best contrast correction and the combined copper and tungsten filter show the best improvement of cupping. This shows that the optimal detector filter configuration highly depends on the material, the transmission length...
2.5 Validation through Measurements

and the purpose of the measurement task.

2.5.2 MTF measurements of the various filters

As already done for the non filtered configuration, the signal transfer characteristics and specifically the resolution capabilities of the MeV CBCT setup with detector filters can be assessed by measuring the systems MTF. The method will be the same as in part II section 4.3. Here, the 1 mm tungsten plate will be chosen as edge object for all measurements. Furthermore, only the horizontal MTF will be calculated, as the isotropy of the detector was already established in the previous measurements and there is no reason to believe that the filters will introduce an anisotropy into the signal. In accordance with all other filter measurements, MTF measurements were performed with an unfiltered 6 MeV spectrum corresponding to the settings shown in Table 2.3.

![Figure 2.17](image)

**Figure 2.17:** For the measurement of the MTF a 1 mm edge device is placed flush with the detector filter. Shown are the measurement setup for the 2 mm copper filter on the left and the 2 mm lead filter on the right.

Figure 2.17 shows the exemplary cases of the MTF measurements for
the 2 mm copper filter and the 2 mm lead filter configuration. The edge object is placed on top of the filter material. For each edge radiography, 10 frames were averaged and the Edge Spread Function (ESF) was extracted perpendicular to the measured horizontal edge of the tungsten plate. Figure 2.18 shows the Line Spread Function (LSF)s extracted from the measured edges. The difference in impact of the various filters on the resolution capabilities of the system can already be inferred here. The 1 mm tungsten filter leads to the widest LSF, while the 2 mm copper filter as well as the 2 mm lead filter and the combined copper and tungsten filter seem to have equal wide spread LSFs.

![Figure 2.18: LSFs deduced from the edge measurements for all detector sided filter configurations.](image)

The calculated MTFs of the MeV CBCT system for each of the measured filters is shown in Figure 2.19. Additionally, the MTF of the configuration without filter deduced in part II section 4.3 is shown. In comparison to the non filtered setup, all detector filters show an either equally good MTF of the detector or they worsen the resolution capabilities. The 1 mm tungsten filter leads to the largest deviation from the MTF measurement without filter. These MTF curves show, that a simple relation between density, transmission length or material and the resulting PSF can not be deduced. This stems from a combination of effects. While the forced scattering in the detector leads to a blur in the image, a longer transmission length can lead to reabsorption of the scattered radiation thus reversing the image degrading effect. The
additional blur seen in the 5 mm copper filter compared to the 5 mm copper filter can be attributed to a larger amount of scattering. It is also interesting to notice the improvement shown in the MTF of the combined copper tungsten filter with respect to the single tungsten filter. For the single tungsten filter configuration, we can assume that a large amount scatter events originating in the thin material could reach the detector. Scattering introduced in the copper material of the combined filter however, already has a lower energy and thus is likely to get absorbed in the adjacent second filter, the 1 mm tungsten filter. Of course these measurements are all performed with the unfiltered 6 MeV spectrum from the linear accelerator X-ray source. It can be assumed that a different incident spectrum leads to a different PSF, shown previously by the spectral simulations of the PSF in part II section 4.1. This means, if an object is introduced into the transmission path between the source and the detector, depending on the change in spectrum, a specific filter might work optimally. The optimization of the filter setup will be discussed in the next section.

**Figure 2.19:** MTFs deduced from the edge measurements for all detector sided filter configurations.
2.6 Measurement task specific filter optimization

The previous sections showed that the optimal filter for a measurement depends on the object and the inspection task. Cupping and contrast in the reconstructed slices (cf. Figure 2.16) show that specifically for various transmission lengths different filters are more efficient in reducing cupping and correcting contrast. Moreover, the best filter configuration for the reduction of cupping might not be the best filter for a cupping correction and vice versa. Here, an optimization model will be developed that allows the determination of the most fitting filter configuration based on a first scan of the object or a CAD file of the object. A set of available filters will be presumed.

In the following the optimization technique will be discussed and tested for a set of four filters: a 2 mm copper filter, a 5 mm copper filter, a 2 mm lead filter and a 1 mm tungsten filter. Even with this finite, small set of filters, the total number of all possible measurements becomes very large when considering all possible combinations and different sequences of filters:

\[
C(n) = \sum_{k=1}^{n} \frac{n!}{(n-k)!} \quad (2.3)
\]

\[
C(4) = \sum_{k=1}^{4} \frac{4!}{(4-k)!} = 64
\]

Here, \(C(n)\) describes the number of possible filter combinations for \(n\) different filters. In the measurements shown in the previous section three single material filters as well as two filter combinations were tested, the 5 mm filter consisting of 2 mm and 3 mm copper filter and the copper tungsten filter configuration. Of course, due to the fact that two of the four filters have the same material some of the configurations are redundant.

The number of possible filter combinations would be even smaller if the filter system can be considered linear. If the system of filter combinations would be linear, then the order of the filters would not matter in a measurement. This means it wouldn’t matter if a filter of
Figure 2.20: Two examples of filter configurations with two filters. On the left a lead copper filter combination is shown, on the right a double copper filter is shown.

Figure 2.21: An example of a triple filter configuration with a copper, a lead and a tungsten filter is shown.

material 1 is placed in front of or after a filter of material 2. Figures 2.20 and 2.21 show examples of various filter configurations and their respective impact on the QAE. With the exception of the trivial case, where the configuration consists of two equal materials, it can be noted that
QAE(Filter\(_1\), Filter\(_2\)) \neq QAE(Filter\(_2\), Filter\(_1\)) \quad (2.4)

for most filter combinations.

**Simulation**

*Fast MC evaluation of object SPR*

- Primary radiation
  - Set of spectra \( S_p(E) \)
- Scattered radiation
  - Set of spectra \( S_s(E) \)

\[
S(E) = S_p(E) + S_s(E)
\]

\[
SPR(E) = \frac{S_s(E)}{S_p(E)}
\]

**Library**

(pre-simulated)

- \( QAE(E, \text{Filter-Configuration}) \)
- \( PSF(E, \text{Filter-Configuration}) \)

**Optimal filter for the measurement**

**Figure 2.22:** Task Specific Filter Optimization Model.

In order to find the filter combination that is best suited for a measurement we have to consider the impact of the filter on both the detected object SPR as well as the detectors PSF. The goal is to reduce the SPR while keeping the signal blur caused by the detector and filter PSF as
small as possible. To assess the impact of the filter combinations on both of these quantities for a given measurement task, the significant spectra corresponding to the primary and scattered radiation have to be known as well. We will assume either that a scan has already been performed or that a CAD file or a former scan of a similar object exists. With this data, the methods developed in the previous chapter can be used to extract and simulate significant projections. The simulations will give an overview over the range of spectra present in the scan. Additionally, scattered and primary radiation can be distinguished and the SPR can be deduced. An exemplary case of this kind of simulation was shown in one of the previous sections, where the spectra corresponding to a step cylinder measurement were deduced. Figures 2.5 and 2.6 show the resulting spectra that can be used as an input for an optimization algorithm. With this information about spectra and the SPR, each filter combination could be simulated and all results could be compared. However, this approach would be very computationally demanding and slow. Alternatively, spectral signal transfer through the filters can be simulated beforehand. This means the spectral response of a filter configuration on the SPR as well as the PSF can be pre-calculated and the input spectra of a given measurement task can be evaluated by simple convolution with the pre-determined transfer functions. Figure 2.22 shows a sketch of this object specific filter optimization. The optimal filter will be chosen based on the calculated SPR and PSF.

The PSF for the pre-simulated library in Figure 2.22 will be evaluated per configuration for a set of mono-energetic X-ray beams of energy \( E_i \in \{0.1, ..., 6.0\} \) MeV. For a given discrete incident spectrum \( S_0(E) \) we can then determine the object and filter specific PSF by calculating the weighted superposition

\[
\text{PSF} = \sum_{i=1}^{N_E} S_0(E_i) \cdot \text{PSF}(E_i, \text{configuration}). \tag{2.5}
\]

For the filter optimization, the parameters \( A, \sigma \) and \( \beta \) determined by the Moffat fit of the PSF are determined and compared to the total measured SPR (cf. section 2.4). Figures 2.23 and 2.24 show the resulting fit parameters versus the calculated total SPR for steps 1 and 5 of the steel step cylinder. The filter combinations corresponding to the configuration numbers in the plot can be found in appendix B. It can be seen that larger filter combinations of two to four filters decrease the overall measured
spr more than the single filter configurations. However, a simultaneous optimization of both the $\sigma$ and $\beta$ parameter proves to be difficult, as different configurations maximize $\beta$ and minimize $\sigma$. Table 2.4 shows the configuration numbers of the various filter combinations that optimize the PSF fit and the SPR. It is noteworthy that these filter combinations all include three or more filters. The amount of material likely kills all low energy radiation decreasing the overall percentage of scattered radiation in the signal. However, the general signal intensity will be decreased as well, which means that the integration time per radiography has to be increased significantly in order to reach the same dynamic range in the measured images. This increase in integration time directly impacts the total measurement time. Restricting the filter optimization to a maximum of two filter combinations will keep measurement time at an acceptable level. The result of this optimization can be found in Table 2.5. Configuration 11, the Lead 2 mm & Copper 2 mm filter combination, seems to be the best option for a measurement of this steel step cylinder object. It both minimizes $A$ and maximizes $\beta$. While it doesn’t lead to the smallest measured SPR, the difference between
2.7 Image sharpness restoration by deconvolution

Figure 2.24: Moffat Model fit parameters versus the total SPR for all filter configurations and the input spectrum of step 5 of the steel step cylinder.

The results of the filter optimization model in the previous section do not only provide a map for choosing the optimal filter combination for a specific measurement task, they also provide an estimate on the detectors PSF for the given filter combinations. This information about signal spread can be used in order to restore a part of the original image sharpness of the radiographies. Of course, due to the down-sampling of the radiographies introduced in the previous chapter, the information about spectra and as a result the knowledge about PSF kernels can not be provided for each projection and each pixel. However, an interpolation of the Moffat model parameters in both spatial and angular dimension
Table 2.4: Filter configuration numbers that optimize the given parameter of the Moffat Fit or the SPR for all filter combinations.

<table>
<thead>
<tr>
<th>Step</th>
<th>A</th>
<th>σ</th>
<th>β</th>
<th>SPR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>25</td>
<td>42</td>
<td>37</td>
<td>44f</td>
</tr>
<tr>
<td>2</td>
<td>25</td>
<td>28</td>
<td>37</td>
<td>44f</td>
</tr>
<tr>
<td>3</td>
<td>25</td>
<td>28</td>
<td>37</td>
<td>44f</td>
</tr>
<tr>
<td>4</td>
<td>25</td>
<td>28</td>
<td>37</td>
<td>44f</td>
</tr>
<tr>
<td>5</td>
<td>25</td>
<td>28</td>
<td>37</td>
<td>44f</td>
</tr>
<tr>
<td>6</td>
<td>25</td>
<td>28</td>
<td>37</td>
<td>44f</td>
</tr>
<tr>
<td>7</td>
<td>25</td>
<td>28</td>
<td>37</td>
<td>44f</td>
</tr>
<tr>
<td>8</td>
<td>48</td>
<td>28</td>
<td>37</td>
<td>43e</td>
</tr>
</tbody>
</table>

- Copper 3 mm & Lead 2 mm & Copper 2 mm
- Copper 3 mm & Tungsten 1 mm & Lead 2 mm
- Tungsten 1 mm & Copper 3 mm & Copper 2 mm
- Copper 2 mm & Copper 3 mm & Tungsten 1 mm & Lead 2 mm
- Copper 2 mm & Lead 2 mm & Copper 3 mm & Tungsten 1 mm
- Copper 2 mm & Lead 2 mm & Tungsten 1 mm & Copper 3 mm
- Copper 3 mm & Copper 2 mm & Tungsten 1 mm & Lead 2 mm

provides an estimate on the PSF kernels of the measurement:

- Simulate projections $p_{\phi}$ where $\phi \in \{1, ..., N_p\}$, and $N_p$ describes the number of projections (projection indexes $\phi$ were chosen according to the algorithm introduced in chapter 1)

  $\Rightarrow$ Spectrum at detector per pixel $(i, j)$

- Determine the PSF using the library (cf. Figure 2.22) and perform the Moffat fit

  $\Rightarrow$ Fit parameters $A_{(i,j)}^{(\phi)}$, $\sigma_{(i,j)}^{(\phi)}$ and $\beta_{(i,j)}^{(\phi)}$ for simulated projections $\phi$ per pixel $(i, j)$

- Determine the parameters in the missing projections per interpolation

Finally, the PSF fit parameters will be known for each projection and each pixel. The size of the convolution kernel will be fixed to a value
2.7 Image sharpness restoration by deconvolution

Table 2.5: Filter configuration numbers that optimize the given parameter of the Moffat Fit or the SPR for one to two filter combinations.

<table>
<thead>
<tr>
<th>Step</th>
<th>A</th>
<th>σ</th>
<th>β</th>
<th>SPR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11b</td>
<td>4a</td>
<td>11b</td>
<td>15c</td>
</tr>
<tr>
<td>2</td>
<td>11b</td>
<td>16d</td>
<td>11b</td>
<td>15c</td>
</tr>
<tr>
<td>3</td>
<td>11b</td>
<td>16d</td>
<td>11b</td>
<td>15c</td>
</tr>
<tr>
<td>4</td>
<td>11b</td>
<td>16d</td>
<td>11b</td>
<td>15c</td>
</tr>
<tr>
<td>5</td>
<td>11b</td>
<td>16d</td>
<td>11b</td>
<td>15c</td>
</tr>
<tr>
<td>6</td>
<td>11b</td>
<td>4a</td>
<td>11b</td>
<td>15c</td>
</tr>
<tr>
<td>7</td>
<td>11b</td>
<td>4a</td>
<td>11b</td>
<td>15c</td>
</tr>
<tr>
<td>8</td>
<td>11b</td>
<td>4a</td>
<td>11b</td>
<td>15c</td>
</tr>
</tbody>
</table>

a Tungsten 1 mm
b Lead 2 mm & Copper 2 mm
c Tungsten 1 mm & Copper 3 mm
d Tungsten 1 mm & Lead 2 mm

$M_x \times M_y$ with $M_x \ll N_x$ and $M_y \ll N_y$, where $N_x$ and $N_y$ denote the number of pixels in both dimensions of the projection. Additionally, for symmetry reasons, the values of $M_x$ and $M_y$ will be chosen such that they are even. For simplicity we will discuss the detailed form of this convolution in one dimension. For each $p_{\phi}(i)$ we can determine its filter convolution kernel using the corresponding Moffat fit parameters $A_{i}^{(\phi)}$, $\sigma_{i}^{(\phi)}$ and $\beta_{i}^{(\phi)}$

$$k_{i}^{(\phi)} = \left[ k_{i}^{(\phi)}(i - M/2) \cdots k_{i}^{(\phi)}(i) \cdots k_{i}^{(\phi)}(i + M/2) \right]$$  \hspace{1cm} (2.6)

where the entries $k_{i}^{(\phi)}(j)$ are calculated using the Moffat model

$$k_{i}^{(\phi)}(i + j) = A_{i}^{(\phi)} \cdot \left( \frac{j^2}{(\sigma_{i}^{(\phi)})^2 + 1} \right)^{-\beta_{i}^{(\phi)}}, \forall j \neq 0$$  \hspace{1cm} (2.7)

The value of the central pixel is not modelled by the Moffat model. It will be determined by the normalization of the convolution kernel.
\[ k_i^{(\phi)}(i) = 1 - \sum_{j=-\frac{M}{2}}^{\frac{M}{2}} k_i^{(\phi)}(i+j) \quad (2.8) \]

which will help conserve the total signal intensity from the original to the convolved image. The full convolution can then be described by the following equation

\[ \bar{p}^{(\phi)} = K \ast p^{(\phi)} \quad (2.9) \]

where

\[
K = \begin{pmatrix}
  k_1^{(\phi)}(0) & k_1^{(\phi)}(1) & \cdots & k_1^{(\phi)}(\frac{M}{2}) & 0 & 0 & \cdots & 0 & 0 \\
  k_2^{(\phi)}(-1) & k_2^{(\phi)}(0) & \cdots & k_2^{(\phi)}(\frac{M}{2} - 1) & k_2^{(\phi)}(\frac{M}{2}) & 0 & \cdots & 0 & 0 \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
  0 & 0 & \cdots & k_m^{(\phi)}(-1) & k_m^{(\phi)}(0) & k_m^{(\phi)}(1) & \cdots & 0 & 0 \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
  0 & 0 & \cdots & 0 & 0 & k_N^{(\phi)}(-\frac{M}{2}) & \cdots & k_N^{(\phi)}(-1) & k_N^{(\phi)}(0)
\end{pmatrix}
\]

and

\[ p^{(\phi)} = \begin{pmatrix}
p_1^{(\phi)} \\
p_2^{(\phi)} \\
\vdots \\
p_N^{(\phi)}
\end{pmatrix}, \]

Restoration of image sharpness ultimately means, that equation 2.9 has to be inverted

\[ p^{(\phi)} = K^{-1} \ast \bar{p}^{(\phi)} \quad (2.10) \]

In order to prove invertibility of \( K \) it is useful to look at its intrinsic matrix properties. Due to the fact that the filter kernels always effect the pixel and its direct neighbours, matrix \( K \) has elements on the diagonal and \( M - 1 \) minor diagonals and as such takes the form of a band matrix. Additionally, from equation 2.8 and using the fact that the Moffat fit kernels are positive, we can deduce that
\[ \sum_{j=-\frac{M}{2}}^{\frac{M}{2}} |k_i^{(\phi)}(i+j)| = 1 - k_i^{(\phi)}(i) \quad (2.11) \]

\[ < k_i^{(\phi)}(i) \quad (2.12) \]

\[ \text{if } k_i^{(\phi)}(i) > \frac{1}{2} \quad (2.13) \]

This means, as long as the diagonal elements of the matrix \( K \) are larger than \( \frac{1}{2} \), the matrix can be considered to be strictly diagonally dominant. Under this premise, the Levy-Desplaques theorem [34] states that \( K \) is non-singular.

In practice, the radiography in question will first be reduced to its Quadtree representation. As described in chapter 1 of this part, a weighted simulation per Quadtree node will be performed. Additionally, nodes with air values will not be simulated. This will result in the spectral information at the detector per object Quadtree node. For a given filter combination, the spectral information in combination with the pre-simulated library (cf. Figure 2.22) can be used to deduce the PSF by superposition as shown in the previous section. With the help of the Moffat fit, this information allows the definition of the fit parameters \( A, \sigma \) and \( \beta \) per Quadtree node. A sketch of this procedure can be found in Figure 2.25. Upsampling in the spatial domain, in order to define the (de)convolution kernel per pixel, will be simply done by assigning all values of a Quadtree node to its corresponding daughter pixels.

For the example of the steel step cylinder, all projections are similar enough, that we can use only one projection as angular sampling point. Figure 2.26 shows the Quadtree decomposition of the first step cylinder radiography. The image was reduced to 188 Quadtree nodes from the original size of 1648 × 1648 pixels. Figure 2.27 shows the result of the simulations. Air values have an assigned value of \( NaN \) due to the fact that they are not included in the simulations. Figure 2.28 shows the tails of the PSF corresponding to the quadtree nodes of the central slice of the step cylinder for a signal blur caused by a 2 mm copper filter.
Efficiency optimization by detector sided filtration

Measured Radiography

Quadtree Decomposition

Simulation

For each Quadtree node $q$:
Spectra $S_q(E)$, $S_q,\text{primaries}(E)$
and $S_q,\text{scatter}(E)$

Weighted superposition:
$\text{PSF} = \sum_E S_q(E) \cdot \text{PSF}(E,\text{Filter Configuration})$

Pre-simulated Library
cf. Figure 2.22

Moffat fit of PSF: $A$, $\sigma$, $\beta$

Figure 2.25: Sketch of the procedure for the determination of the PSF for the deconvolution of images measured with a specific filter configuration.
2.7 Image sharpness restoration by deconvolution

Figure 2.26: Quadtree decomposition of a radiography of the steel step cylinder.

Figure 2.27: Results of the simulation of the steel step cylinder split with respect to the various energies.
Figure 2.28: PSF tails corresponding to the quadtree nodes of the central slice of the step cylinder for a signal blur caused by a 2 mm copper filter.
Chapter 3

Reconstruction

In [51, 85] we developed a reconstruction based on a statistical model using on a voxel domain prior and a distance driven algebraic reconstruction [18, 19]. Voxel values in the reconstruction are updated using an expectation maximization approach in combination with iterative scalar gaussian message passing. The basic reconstruction algorithm was tested on simulated data and compared to state of the art statistical reconstructions, see [85]. In the following chapter the fundamental aspects of the model will be explained and the reconstruction will be applied to the step cylinder measurements introduced in chapter 2. Additionally, the algorithm will be extended incorporating the blurring and simulated scatter into the measurement model.

In the following, we will establish a two dimensional statistical model for the reconstructions corresponding to fan-beam measurement data. The third dimension can be deduced by adding the additional voxel dimension and pixel neighbour connections (see [51]). Generally, we will use the term voxel domain in order to refer to the image that we wish to reconstruct and the term measurement domain, corresponding to the measured projections. Both the voxel domain and the measurement domain are connected by the system matrix containing the measurement model (as introduced in the common algebraic reconstruction introduced in part I section 2.5.5).
3.1 Pixel-Domain Prior Model

Statistically, the value of each pixel in the reconstruction can be associated with a real random variable $X_{s_{l}}$, $l \in \{1, ..., L\}$, where $s_{l} = (i, j)$ describes the spatial index of the pixel in the image and $L$ is the total number of pixels. We will restrict ourselves to images with square pixels. As a result, the reconstructed image is represented by the random vector

$$X = (X_{s_{1}}, ..., X_{s_{L}}) \in \mathbb{R}^{L}$$  \hspace{1cm} (3.1)

For the calculations it is interesting to impose an order on this pixel dataset $X$. In the following we will define the following order on two pixels $s_{l} = (i, j)$ and $s_{l'} = (i', j')$

$$s_{l} \prec s_{l'} \iff (i < i') \text{ or } ((i = i') \& (j < j')) \hspace{1cm} (3.2)$$

Based on this order two pixels $s_{l}$ and $s_{l'}$ are defined as neighbouring pixels if and only if

$$\|s_{l} - s_{l'}\| \triangleq |i - i'| + |j - j'| = 1.$$  \hspace{1cm} (3.3)

Hereinafter, a set of two neighbouring pixels like this will be denoted by $\Delta$

$$\Delta = \{(\ell, \ell') : \|s_{\ell} - s_{\ell'}\|_{1} = 1 \text{ and } (s_{\ell} \prec s_{\ell'}) \}.$$ \hspace{1cm} (3.4)

Figure 3.1 shows that this pixel neighbourhood model connects bordering pixels while leaving out diagonally connected pixels. In this two-dimensional case, each pixel neighbours two to 4 pixels, depending on whether the pixel is a corner pixel, a border pixel or any of the other pixels in the image.

For the prior model, the statistical relation between two neighbouring pixel values should be described. The straightforward approach would be to define a pixel value to either belong to one of the materials or the air. In this scenario, two neighbouring pixels either have the same pixel value, or completely different pixel values. Considering this pixel domain model, we can try to implement a simple thresholding algorithm. The value $X_{s_{\ell}}$ of pixel $s_{\ell}$ will be updated to the value $\tilde{X}_{s_{\ell}}$ based on its neighbour pixel $X_{s_{\ell'}} ((s_{\ell}, s_{\ell'}) \in \Delta)$.
Figure 3.1: Sketch of the image pixel domain. In green, pixel $s_\ell = (i, j)$ with its corresponding neighbours.

$$\tilde{X}_{s_\ell} \begin{cases} = X_{s_{\ell'}} & \text{if } \|X_{s_\ell} - X_{s_{\ell'}}\| \leq \text{threshold} \\ \neq X_{s_{\ell'}} & \text{if } \|X_{s_\ell} - X_{s_{\ell'}}\| > \text{threshold} \end{cases} \quad (3.5)$$

It has to be noted, that this method requires, and depends on, a definite sequence of pixels ($1 \leq \ell \leq L$). Figure 3.2 depicts this simple pixel neighbourhood model applied to a line profile through step 5 of the step cylinder described earlier. Despite the fact, that the step cylinder consists of one single material, the cupping artefact leads to a step like profile that could be mistaken for several different materials of various densities.

In order to avoid artefacts like these, the prior model of the pixel domain employed here, will be based on the following principle: neighbouring pixels are either approximately equal or completely different. This leads to a resulting signal which consists of smooth material regions while at the same time abrupt changes are allowed. When thinking about the possible structures in the reconstructed images, it can be noted that in most cases there will be significantly fewer border pixels than pixels
belonging to a region of a material or air.

For the description of the pixel-domain prior model we will characterize the variation between two neighbouring pixels \((\ell, \ell') \in \Delta\) as

\[
X_{s_{\ell'}} = X_{s_{\ell}} + U_{\ell, \ell'} \tag{3.6}
\]
\[
U_{\ell, \ell'} = \tilde{U}_{\ell, \ell'} + \bar{U}_{\ell, \ell'} \tag{3.7}
\]

with mutually independent \(\tilde{U}_{\ell, \ell'} \sim \mathcal{N}(0, \sigma_\epsilon^2)\) and \(\bar{U}_{\ell, \ell'} \sim \mathcal{N}(0, \sigma_{\ell, \ell'}^2)\). Both \(\tilde{U}_{\ell, \ell'}\) and \(\bar{U}_{\ell, \ell'}\) describe the pixel neighbourhood model described earlier, favouring similar pixel values while allowing abrupt jumps in the image. \(\tilde{U}_{\ell}\) describes a random-walk model favoring similar pixel neighbour values. The parameter \(\sigma_\epsilon^2\) in the model is fixed and can be assumed to be known. \(\bar{U}_{\ell, \ell'}\) on the other hand describes a normal random variable with unknown variance. It will allow the occasional jumps in the image corresponding to two bordering materials [48, 86]. The parameters \(\sigma_{\ell, \ell'}^2\) will be estimated by the algorithm. Due to the fact that material borders are assumed to be rare in the image, the vector \(\tilde{U}\) containing all \(\tilde{U}_{\ell, \ell'}\) will likely be sparse. Figure 3.3 depicts the factor graph corresponding to equations 3.6 and 3.7.
3.1 Pixel-Domain Prior Model

Figure 3.3: Factor graph describing the pixel domain prior model between neighbouring pixels in the one dimensional and in the two dimensional case.
The pixel domain prior model in equations 3.6 and 3.7 can be rewritten

\[ X_{s_\ell} = X_{s_{\ell'}} + U_{\ell,\ell'} \]
\[ U_{\ell,\ell'} = X_{s_{\ell'}} - X_{s_\ell} \]

which allows the representation of the model in matrix form

\[ U = DX. \]  

We can now use these properties to compute the probability density function of the signal \( X \), \( p_X(x|\sigma^2) = p(x|\sigma^2) \). From equation 3.7, we can deduce that \( U \) follows a normal distribution.

\[ p(u|\sigma^2) = \prod_{(\ell,\ell') \in \Delta} \frac{1}{\sqrt{2\pi(\sigma^2_\epsilon + \sigma^2_{\ell,\ell'})}} \exp \left( -\frac{u^2_{\ell,\ell'}}{2(\sigma^2_\epsilon + \sigma^2_{\ell,\ell'})} \right) \]  

Using the relation between \( U \) and \( X \) introduced in equation 3.9 we can rewrite this as

\[ \hat{p}(x|\sigma^2) = p_U(Dx|\sigma^2) \]
\[ = \prod_{(\ell,\ell') \in \Delta} \frac{1}{\sqrt{2\pi(\sigma^2_\epsilon + \sigma^2_{\ell,\ell'})}} \exp \left( -\frac{(x_{s_{\ell'}} - x_{s_\ell})^2}{2(\sigma^2_\epsilon + \sigma^2_{\ell,\ell'})} \right) \]

This final prior model on \( X \) is similar to the model used in [17], which is based on the composite likelihood in [47]. These calculations were of course performed under the assumption that all the \( U_{\ell,\ell'} \) are independent of each other. This is correct in the one dimensional case shown in Figure 3.3a. Figure 3.3b shows, that in the two dimensional case, some of the random variables \( U_{\ell,\ell'} \) are in fact dependent on each other. This introduces cycles in the factor graphs. In fact, the dependencies were introduced by the relation between \( U \) and \( X \) described in equation 3.9. This becomes obvious when rewriting equation 3.12 as

\[ \hat{p}(x|\sigma^2) = \int \delta(u - Dx)p(u|\sigma^2)du \]

The term \( \delta(u - Dx) \) signifies the dependencies between \( u \) and \( x \). Additionally, \( \hat{p}(x|\sigma^2) \) can not be called a probability function any more.
when it comes to the two dimensional case (as well as in the extension to the three dimensional case). This is due to the fact that its integral over \( \mathbb{R}^L \) is not equal to one. However, \( \tilde{p}(x|\sigma^2) \geq 0 \) for all \( x \in \mathbb{R}^L \), which means it can be described as the density of a finite measure on \( \mathbb{R}^L \).

Normalisation of \( \tilde{p}(x|\sigma^2) \) is generally possible, as described in [51], we can define a matrix \( \Sigma \triangleq \sigma^2 \epsilon I + \text{Diag}(\sigma^2) \), with \( \sigma^2 \in \{\sigma^2_{\ell,\ell'}\}_{(\ell,\ell') \in \Delta} \) and \( I = \text{identity matrix} \), that allows us to replace the exponent in the exponential of equation 3.12

\[
-\frac{(x_{s_{\ell'}} - x_{s_{\ell}})^2}{2(\sigma^2_{\ell} + \sigma^2_{\ell,\ell'})} = -\frac{x^T D^T \Sigma^{-1} D x}{2}
\]

(3.14)

where \( D^T \Sigma^{-1} D \) is symmetric positive definite (see [51]). This makes the normalization of the finite measure \( \tilde{p}(x|\sigma^2) \) possible, leading to the probability density function

\[
p(x|\sigma^2)_{\text{norm}} = (2\pi)^{-L/2} \sqrt{\det(D^T \Sigma^{-1} D)} \exp \left( -\frac{x^T D^T \Sigma^{-1} D x}{2} \right)
\]

(3.15)

Due to the computation complexity of calculating the normalization factor \( \sqrt{\det(D^T \Sigma^{-1} D)} \) in this probability density function, and specifically due to the fact that this factor contains \( \sigma^2 \) impeding their algorithmic optimization, the original finite measure \( \tilde{p}(x|\sigma^2) \) will be used in the following as the prior model.

### 3.2 Joint measurement and pixel prior model

In the previous section we have only concerned ourselves with the statistical pixel neighbourhood relations in a reconstructed image. However, each pixel value is connected to a set of measurements. In order to express the relation between the pixel values \( X \in \mathbb{R}^L \) and the measured projections (from now on observations) \( Y \in \mathbb{R}^N \) the model described in part I section 2.5.5 will be used. This means pixel values and observations are connected by the system matrix \( A \in \mathbb{R}^{N \times L} \):

\[
Y = AX + Z
\]

(3.16)

The term \( Z \) describes an isotropic Gaussian noise on the measurements \( (Z \sim \mathcal{N}(0, \sigma^2_Z)) \). Matrix \( A \) depends on the volume of the reconstructed
picture as well as the size of the measurements and the distances between the source, the object and the detector. This means it can be pre-computed once for a given measurement. The likelihood of the observations can therefore be expressed as

\[
p(y|x) \triangleq p_y(y|x) = \frac{1}{(2\pi\sigma_Z^2)^{N/2}} \exp\left(\frac{\|y - Ax\|^2}{2\sigma_Z^2}\right). \tag{3.17}
\]

However, as we know from our previous investigations, the imaging chain involves an additional blurring of the data y. This blurring can be described as a convolution with the detectors PSF given by the convolution kernel K.

\[
Y = K \ast (AX) + Z \tag{3.18}
\]

Which means that the likelihood of the observations will carry the blur as well

\[
p(y|x) \triangleq p_y(x|y|x) = \frac{1}{(2\pi\sigma_Z^2)^{N/2}} \exp\left(\frac{\|y - K \ast (Ax)\|^2}{2\sigma_Z^2}\right). \tag{3.19}
\]

The convolution kernel can be assumed to be finite, however, as we saw in the previous chapters, it can depend on the spectrum of the X-ray beam. From the fast MC simulations described in chapter 1 used in the filter optimization, the convolution kernel of each observation can be estimated. As a result, the factor graph representation of the joint voxel domain model with the measurement developed in [51] can be extended to include the blurring by introducing an additional stage. Figure 3.4 shows both the factor graph of the original joint model as well as the extended factor graph that includes the convolution matrix K. This joint model connects the observations y with the \(\sigma^2\) of the pixel domain prior that we aim to optimize.

\[
\bar{p}(y|\sigma^2) = \int \int p(y|x)p(x|\sigma^2)dx
\]

\[
= \int \int p(y|x)\delta(u - Dx)p(u|\sigma^2)du\,dx \tag{3.20}
\]

The mapping corresponding to the line integrals of the measurement described by system matrix A is described in detail in [51]. In the
Figure 3.4: Factor graph describing the joint density \( p(y|x)\delta(u - Dx)p(u|\sigma^2) \). The pixel domain prior as well as the measurement in form of the mapping described by system matrix \( A \) is included. Figure 3.4a depicts the model developed in [51] and Figure 3.4b extends this model by including the signal blurring using the matrix \( K \).

Following, we will take a closer look at the additional blurring described by convolution matrix \( K \). From the calculations performed in the previous chapter, we can assume that we know the convolving element \( w_n \) for
each observation $\tilde{y}_n$, where $n \in \{1, ..., N\}$. We will assume the size of $w_n$ to be finite and fix it to a maximum length of $M$ ($M$ even) such that

$$w_n = \left( w_{n,-M/2}, \ldots, w_{n,0}, \ldots, w_{n,M/2} \right). \quad (3.21)$$

This means each value $\bar{y}_n$ (corresponding to the measured value $y_n$ without added white noise $\mathcal{N}(0, \sigma_Z^2)$) is influenced by its $M$ neighbouring pixels to each side. The impact of the values is defined by the weights corresponding to the blur of the pixels $\bar{y}_k$ with $k \in \{n-M/2, \ldots, n+M/2\}$. Figure 3.5 shows the exemplary case of the normalized PSFs of five neighbouring pixels. The computation of the resulting value $\bar{y}_4$ from its neighbouring pixels under consideration of their own PSFs is depicted.

**Figure 3.5:** The normalized PSFs of five neighbouring pixels is shown. The resulting value at pixel 4 can be computed using the PSFs and anterior pixel values of the neighbouring pixels.

$$\bar{y}_n = \sum_{k=n-M/2}^{n+M/2} w_k(n) \bar{y}_k \quad (3.22)$$

Figure 3.6 shows the factor graph of the signal blur matrix $K$ in the context of the joint prior and measurement model. It is a detailed version of the factor graph shown in Figure 3.4 for blur kernels of size 3 split component wise. For the complete set of observations, we can write
Figure 3.6: Factor Graph system matrix and detector PSF for exemplary case of a kernel that has a length of 3.
Due to the fact, that we restrict each kernel to a size $M \ll N$ most of the $w_i(j)\ i, j \in \{1,\ldots,N\}$ will be zero, making $K$ a sparse matrix. It can be noted that the kernel only applies to the $M$ neighbouring observations (cf. equation 3.22), which means that $K$ forms a so called band matrix with bandwidth $M$

$$w_i(j) = 0 \text{ if } j < (i - M/2) \text{ or } j > (i + M/2).$$

Furthermore, as shown in the previous chapter 2.7, as long as the signal spread introduced by the filter material is not too severe, it can be assumed that $K$ is strictly diagonally dominant and as such nonsingular [34].

### 3.3 Maximum "Likelihood" Estimation

The final goal of the reconstruction technique introduced here is to optimize the likelihood of the joint model introduced in equation 3.20. This means we want to find the $\sigma$ that maximize equation 3.20. A maximization of this type of likelihood is not possible in closed form. However, the joint model in equation 3.20 has the form of a type-II likelihood [6] with the exception that, as explained earlier in this section, the non-normalized version of the density $\tilde{p}(x|\sigma^2)$ was used. For the maximization of this type of likelihood, an approximated version of the Expectation Maximization (EM) algorithm was used. An EM algorithm generally uses an iterative method of applying a so called expectation and maximization step in order to find the parameters that maximize the given likelihood. Here, $U$ is considered as the hidden variable and the $\sigma^2$ are updated iteratively. This means, the following expectation and maximization steps will be performed in step $k$ of the iterative algorithm:

**Expectation**

$$P(\sigma^2 | (\sigma^2)^{[k]}) = \mathbb{E} \left[ \ln p(\mathbf{y}, U | (\sigma^2)^{[k]}) \right]$$

**Maximization**

$$(\sigma^2)^{[k+1]} = \arg \max_{\sigma^2} \left( P(\sigma^2 | (\sigma^2)^{[k]}) \right)$$
The algorithm will start with an initial guess of the $\sigma^{[0]}$. In [51] it was shown that the maximization step can in fact be reduced to the maximization of the neighbour model $U_{\ell,\ell'}$ and split for each individual $\sigma^2_{\ell,\ell'}$ with $(\ell, \ell') \in \Delta$:

$$(\sigma^2_{\ell,\ell'})^{[k+1]} = \max \left( 0, \mathbb{E} \left[ (U^2_{\ell,\ell'})^{[k]} \right] - \sigma^2_{\epsilon} \right)$$

(3.25)

It is interesting to notice that the fixed parameter $\sigma^2_{\epsilon}$ of the model plays a role in the maximization of the $\sigma^2_{\ell,\ell'}$. In fact, the parameter controls the sparsity of the final estimate of $\sigma^2_{\ell,\ell'}$. As a result, setting a suitable value for the parameter of $\sigma^2_{\epsilon}$ is crucial for the success of the algorithm. An overestimation of $\sigma^2_{\epsilon}$ in equation 3.25 can in the worst case set all $\sigma^2_{\ell,\ell'}$ to zero. The realization of this expectation maximization algorithm requires us to compute $\mathbb{E} \left[ U^2_{\ell,\ell'} \right]$ for each iteration step. The computation of this expectation can be done by determining the posterior mean and variance of $U_{\ell,\ell'}$:

$$\mathbb{E} \left[ U^2_{\ell,\ell'} \right] = m^2_{U_{\ell,\ell'}} + \sigma^2_{U_{\ell,\ell'}}$$

(3.26)

The calculation of $m^2_{U_{\ell,\ell'}}$ and $\sigma^2_{U_{\ell,\ell'}}$ will be done by Gaussian message passing using the factor graphs developed in the previous section. The implementation of the corresponding Gaussian message passing algorithm will be addressed in the upcoming section.

### 3.4 Iterative scalar Gaussian message passing algorithm

The scalar factor graph shown in Figure 3.6 allow us to perform scalar Gaussian message passing in order to calculate the quantities $m_{U_{\ell,\ell'}}$ and $\sigma^2_{U_{\ell,\ell'}}$ necessary for the expectation maximization. Due to the fact, that the factor graph corresponding to the two dimensional (as well as the three dimensional) case is not cycle free (cf. Figure 3.3b) convergence of the following algorithm can not be guaranteed. However, applications showed that non-convergence can be prevented in most cases by choosing a suitable set of parameters ($\sigma^2_Z$ and $\sigma^2_{\epsilon}$). Additionally, in case of convergence the calculated means will be correct even though the factor graph contains cycles [52, 83, 84] and the resulting variances will typically converge to approximates of the real variances [83, 84]. Due to the fact that the factor graph contains cycles, the message passing algorithm in
this case has to be implemented in an iterative manner, initializing edges with random or neutral messages and updating them iteratively.

As described in [51] the following algorithm is inspired by the iterative message passing algorithms of the LDPC decoder [26]. After a random initialization, the iterations in the algorithm will send messages along each edge upwards and downwards in sequentially. The updates of the algorithm will focus on comparing upward and downward messages along the edge $X$ shown in the factor graph in Figure 3.3b.

**Figure 3.7:** Detailed version of the factor graph corresponding to the signal blur described by kernel $K$ with weights $w(y_i, j)$ shown here for observation $y_n$.

Let us consider messages from the observations going upwards through the kernel $K$ to node $A$. Figure 3.7 shows the detailed computation for observation $y_n$. As a result, using standard Gaussian message passing rules, we can compute the upward messages corresponding to this observation in the following way:
\[ \hat{m}_{\bar{y}_n} = \frac{1}{w(y_n, 0)} \cdot \left( y_n - \sum_{k=-M/2}^{M/2} w(y_n, k) \cdot \hat{m}_{\bar{y}_{n+k}} \right) + \hat{m}_{\bar{y}_n} \] (3.27)

\[ \hat{\sigma}^2_{\bar{y}_n} = \frac{1}{w(y_n, 0)^2} \cdot \left( \sigma^2 Z + \sum_{k=-M/2}^{M/2} w(y_n, k)^2 \cdot \hat{\sigma}^2_{\bar{y}_{n+k}} \right) - \hat{\sigma}^2_{\bar{y}_n} \] (3.28)

It is obvious that for this computation, not only do we need to know observations \( y_n \) and weights \( w(y_n, k) \) but also downward messages \( \hat{m}_{\bar{y}_k} \) and \( \hat{\sigma}^2_{\bar{y}_k} \). In the iterative algorithm this issue will be dealt with by starting with the computation of downward messages from node \( D \) to node \( A \) (see [51]). Afterward, these messages can be used to compute the downward messages from \( A \) to \( K \):

\[ \bar{m}_{\bar{y}_n} = \sum_{\ell':a_n,s_{\ell'} \neq 0} a_{n,s_{\ell'}} \bar{m}_{\bar{X}_{s_{\ell'}}^{(n)}} \]

\[ \bar{\sigma}^2_{\bar{y}_n} = \sum_{\ell':a_n,s_{\ell'} \neq 0} a_{n,s_{\ell'}}^2 \bar{\sigma}^2_{\bar{X}_{s_{\ell'}}^{(n)}} \]

In the final iterative algorithm the messages at iteration step \( t \) will be calculated in the following order:

- Update messages \( (\hat{m}^{[t]}_{\bar{X}_{s_{\ell}}^{(n)}}, \hat{\sigma}^{2[t]}_{\bar{X}_{s_{\ell}}^{(n)}}) \) from node \( D \) to node \( A \) using the messages of the previous iteration step \( t - 1 \)
- Compute messages \( (\hat{m}^{[t]}_{\bar{y}_n}, \hat{\sigma}^{2[t]}_{\bar{y}_n}) \) from node \( A \) to node \( K \)
- Compute messages \( (\bar{m}^{[t]}_{\bar{y}_n}, \bar{\sigma}^{2[t]}_{\bar{y}_n}) \) from node \( K \) back to node \( A \)
- Compute messages \( (\hat{m}^{[t]}_{\bar{X}_{s_{\ell}}^{(n)}}, \hat{\sigma}^{2[t]}_{\bar{X}_{s_{\ell}}^{(n)}}) \) from node \( A \) to node \( D \)
- For all pixel neighbours \( (\ell, \ell') \in \Delta \) compute messages \( (\hat{m}^{[t]}_{\bar{X}_{s_{\ell}}^{(\ell,\ell')}}, \hat{\sigma}^{2[t]}_{\bar{X}_{s_{\ell}}^{(\ell,\ell')}}) \)
- For all pixels \( \ell \in \{1, ..., L\} \) compute the messages \( (\hat{m}_{\bar{X}_{s_{\ell}}^{(\ell',\ell)}}, \hat{\sigma}^{2[t]}_{\bar{X}_{s_{\ell}}^{(\ell',\ell')}}) \) from node \( D \) back to node \( A \)
The detailed computations corresponding to each of these steps can be found in appendix C. The messages \( \overrightarrow{m}^{[t]}_{X} \), \( \overrightarrow{\sigma}^{2[t]}_{X} \) can be used for the expectation maximization step shown in the previous section.

### 3.5 Results

The reconstruction algorithm introduced in the previous section is tested on several measurements. As the algorithm is only two-dimensional so far, the central slices of the three dimensional MeV CBCT measurement data will be used.

#### 3.5.1 Steel Step Cylinder

A first test of the message passing reconstruction algorithm is performed on the steel step cylinder measurements introduced earlier in this work. The central slice of each of the projections was extracted and rebinned to a size of 512 pixels per projection in favour of computational efficiency. For the same reasons, the angular space of the projection data was rebinned to an angular spacing of \( 0.5^\circ \) from the original data, which was recorded at an angular spacing of \( 0.225^\circ \). This central slice corresponds to step 5 of the steel step cylinder. The reconstruction was performed on an equal sized pixel grid of 512 \( \times \) 512 pixels. For the reconstruction, the following parameter configuration was determined:

\[
\begin{align*}
\sigma_{\epsilon} & = 10^{-2} \quad (3.29) \\
\sigma_{Z} & = 15 \quad (3.30) \\
\text{Number of message passing iterations} & = 15 \quad (3.31) \\
\text{Number of EM updates} & = 5 \quad (3.32)
\end{align*}
\]

At first the original reconstruction algorithm from [51] was used for the reconstruction. Figure 3.8 shows the reconstructed images of the measurements with various filter combinations. The cupping artefacts that arise in the measurements without detector filter do not lead to the step like behaviour that was predicted for the straight forward pixel neighbourhood model discussed in section 3.1. It is interesting to notice that the ring artefacts visible in the original FDK reconstructions of the lead detector filter configuration shown in Figure 2.15 vanish here.
3.5 Results

(a) No Filter  
(b) Lead Filter at Source  
(c) Lead Filter at Detector

Figure 3.8: Reconstruction of the steel step cylinder measurement data with the iterative message passing algorithm without kernel $K$.

For the configuration with the lead filter at the detector, the spectrum and as a result the spatial blurring kernel can be determined (cf. section 2.7). Due to the radial symmetry of the measurement this kernel remains the same for all projections with a slight left to right shift for the various rotation angles accounting for a center of rotation displacement. This lets us construct matrix $K$ of the factor graph model in Figure 3.4b easily. The introduction of this kernel has the same effect as an image sharpening filter on each of the projections. The sharper input data to node $A$ and subsequently node $D$ also leads to a sharper reconstruction. Figure 3.9 shows the resulting reconstruction of the step cylinder step 5.

In order to quantify the sharpness difference, the image sharpness is evaluated using the gradient magnitude metric. This means the sums of all gradient norms of images $I$ are calculated and compared:

$$\text{Sharpness } S = \frac{1}{N_x \cdot N_y} \cdot \sqrt{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \left[ \left( \frac{\partial I}{\partial x} \right)_{(i,j)}^2 + \left( \frac{\partial I}{\partial y} \right)_{(i,j)}^2 \right]} \quad (3.33)$$

Here, $N_x$ and $N_y$ denote the number of pixels in both image dimensions. For the results shown in Figure 3.9 these sharppnesses evaluate to $S_1 = 1.51$ for Figure 3.9a and $S_2 = 1.76$ for Figure 3.9b corresponding to an increase in the sharpness metric of about 16%.
In Figure 3.13 the reconstructed slices are compared with a filtered backprojection. The radial profiles showing the edge of the inner hole of the cylinder show the success of the deconvolution leading to a significantly steeper edge.

### 3.5.2 Small Steel Cast Part

Finally, the the message passing reconstruction algorithm is tested on the steel cast part that was already shown in the introductory chapter of this work. As in the previous reconstruction, the central slice of each of the projections was extracted and rebinned to a size of 512 pixels per projection in favour of computational efficiency. For the same reasons, the angular space of the projection data was rebinned to an angular spacing of 0.5° from the original data, which was recorded at an angular spacing of 0.225°. The same parameter configuration as in the previous example was used for the reconstruction.

Figure 3.11 shows the reconstructions of a non filtered and a filtered measurement. A higher amount of blurring for the measurement with detector filter can be observed. The reconstruction with the additional PSF data is able to recover a large amount of the image sharpness.
3.5 Results

(a) Filtered Backprojection  (b) GaMP without deconvolution  (c) GaMP with deconvolution

(d) Radial Profiles

Figure 3.10: Comparison of the radial profiles for a filtered backprojection with a Ram-Lak Filter, the Gaussian message passing reconstruction and the Gaussian message passing reconstruction with PSF deconvolution for the reconstruction of the steel step cylinder measured with a lead filter.

Line profiles show, that the simulations overestimated the filter PSF slightly, leading to sharp edges but also an overshoot effect. This can be attributed to the fact that the fast MC simulations and subsequently the PSF computation evaluate the worst case scenario, meaning the projections with the largest transmission lengths that have the greatest effect on the spectrum and thus the change in PSF. The central slice here has however, comparatively small material transmission lengths. A finer simulation with more spatial and angular sampling points will improve uncertainties in the PSF simulations.
Figure 3.11: Reconstruction of the steel cast part measurement data with the iterative message passing algorithm without kernel $K$ with and without a detector filter.

Figure 3.12: Reconstruction of the steel cast part measurement data for the configuration with a copper tungsten filter with the iterative message passing algorithm without and with kernel $K$. 
3.5 Results

(a) Filtered Backprojection  (b) GaMP without deconvolution  (c) GaMP with deconvolution

Figure 3.13: Comparison of line profiles for a filtered backprojection with a Ram-Lak Filter, the Gaussian message passing reconstruction and the Gaussian message passing reconstruction with PSF deconvolution for the reconstruction of the small steel cast part measured with a copper tungsten filter.
Part IV

Discussion and Conclusion
Chapter 1

Conclusion

This work represents a detailed assessment of the capabilities and challenges posed by a Cone Beam Computed Tomography (CBCT) system with mega-electronvolt (MeV) X-ray source. Monte-Carlo (MC) simulations combined with measurements identified and quantified all image degrading processes in the X-ray setup. Three different sources of image degradation in the high energy X-ray Computed Tomography (CT) setup were determined: the object, the environment and the detector.

Worsening of the X-ray signal caused by the object is governed by both scattered radiation as well as a non-linear change in the X-ray spectrum, called beam hardening. The MC simulations allowed the investigation of the various physical interactions and their respective impact on the object scatter signal. Bremsstrahlung as well as Pair Production and its subsequent Annihilation radiation showed a very low intensity with respect to the other physical interactions Compton and Rayleigh scattering. Compton scattering proved to be the dominant interaction process in the detected scatter signal. In contrast to Compton scattered radiation, the distribution of Rayleigh scattering is less distributed over the projection. This is a result of the respective angular dominance of the cross sections of both interactions. While Compton scattering governs for most scattering angles, Rayleigh scattering is the dominant interaction process at very small angles. Investigations of scattered radiation for various materials and transmission lengths showed that a simple Scatter to Primary Ratio (SPR) to gray value relation can not be deduced. Beam hardening simulations allowed the investigation of
spectral changes caused by the object in the X-ray setup. Specifically, primary and scattered spectra could be distinguished and compared. It was determined, that scattered radiation is more dominant at the lower end of the spectrum. Additionally, the comparison between simulated and measured beam hardening curves showed that there is an additional image degradation not directly connected to the object in the X-ray setup: the signal conversion in the flat-panel detector.

The detectors Point Spread Function (PSF) was studied by simulations as well as edge measurements. Knock-off simulations allowed the investigation of the various detector component and their respective impact on signal spread. The entrance window showed to be the main contributor to signal spread. Studies of the PSF for various angles of incidence showed that the angular component can be disregarded as only for angles much greater than the system intrinsic $2.5^\circ$ opening angle a skew in the PSF can be noticed. Modulation Transfer Function (MTF) measurements in horizontal and vertical direction demonstrated, that the system is isotropic. The visibility limit extracted from the MTF was determined to be at 2.3 line pairs per mm. Additional investigations showed that the thin scintillating layer is non optimal when it comes to high energy X-ray detection. The ratio of incident versus detected photons described by the detectors Quantum Absorption Efficiency (QAE) decreases significantly for MeV X-rays.

Additional simulations studied the complete X-ray setup in order to determine the contribution of the various peripheral system components on scattered radiation in the radiographies. Scattered radiation from peripheral equipment that is detected in the X-ray image mostly consists of highly multiple scattered radiation. As a result, the contribution of these scatter components is much lower than all other scatter components. Additionally, the distribution of this scattered radiation is typically spread out over the whole radiography. As a result, this spread out scatter contribution will not be a significant contributor to the degradation of the reconstructed CT volume.

The results from the simulations and measurements of the second part of this work allowed the development of fast evaluation and efficient correction methods for the image degradation in the MeV X-ray CBCT setup. A speed up of the MC simulation of X-ray scatter using irregular spatial and angular sampling allow a fast assessment of object SPR as
well as primary and scatter spectra. These results serve as an input for a hardware based and object specific system optimization based on a detector sided filter. The filter optimization aims to reduce the detected object SPR while simultaneously keeping the systems PSF as small as possible. The filter material both filters out a large part of the low energy spectrum, removing the main contributor to scattered radiation. At the same time, high energy photons are forced to additional proximal scatter interactions decreasing their energy and increasing their detection probability. The resulting knowledge about the object and filter specific PSF is used for image sharpness restoration of the filter measurements. The PSF kernel is input into a reconstruction algorithm based on a model using a voxel domain prior combined with an algebraic reconstruction. Examples showed the success of the filter and sharpness restoration method.
Chapter 2

Outlook

This work demonstrated the effect of the developed filter optimization method on steel objects. While the material and size of the objects are representative of typical inspection tasks for MeV CBCT systems, they only consist of a single material. Studies of multi-material samples and specifically an investigation of the impact of the detector filter method on their reconstruction might yield interesting results. On the one hand, it would be worthwhile to see if a contrast improvement between similar materials can be achieved with the filters. On the other hand, an investigation of the image contrast on low density components might be helpful. MeV X-ray systems employing a line detector showed already the capacity of resolving low density materials such as plastics or wood. However, they do have the advantage of longer scintillation crystals. A study of the detector filter method in combination with these different object material configurations will be beneficial for everyday inspection tasks.

The studies performed in this work also provided information about the filter specific signal spread. Especially for the tasks of failure and flaw detection it is useful to pursue this direction and study the impact of the additional signal spread on the probability of detection (POD). In practice it is crucial to know whether a detector filter might mask a certain flaw size. These investigations on the POD can then serve as an additional limiting criterium for the filter specific measurement automation.
Finally, the reconstruction algorithm incorporating the filter specific PSF can be extended to three dimensions. This is specifically useful as the advantage of the presented MeV X-ray CBCT system is the two dimensional detection allowing the three dimensional reconstruction.
Part V

Appendix
Appendix A

Object volume import for the simulations

A.1 Segmentation and triangulation

For the initial segmentation of the 3D volume data we use the algorithm provided by Quan Wang [81]. The procedure uses Gaussian hidden Markov random fields for the segmentation. It requires the definition of the number of clusters as well as the number of connected components. Here, the number of clusters corresponds to the number of materials in the volume. The result will be an indexed 3D dataset, where the index corresponds to the specified materials.

As a next step the dataset will be split into several 3D volumes, each corresponding to one of the materials, i.e. cluster indices. For each material the hull will be extracted using a slice-wise edge detection on the binary data from the clustering approach. For the edge detection, a morphological closing using a square 3 pixel neighbourhood was applied at first in order to amend any errors of the previous clustering approach. A Sobel algorithm was used in order to extract the edge points per slice. The result will be saved as a triangular mesh including the corresponding material index. The 3D mesh is extracted by Delaunay triangulation using a pre-defined search radius. The matlab implementation by Lundgren (Alpha shapes, [50]) was used for the computation.
An example of the clustering result as well as the edge extraction can be seen in Figure A.1. The slices correspond to the small steel cast part discussed previously in part III of this work. Here, the object consists of one single material, which means that the data will be clustered into two clusters corresponding to the material and the air.

The resulting point cloud of the edges (cf Figure A.1c) are shown in
A.1 Segmentation and triangulation

Figure A.2: Resulting point cloud extracted from the edge data as seen in Figure A.1.

Figure A.2. This data can be used as input for the Delauny triangulation in order to create a closed hull. The result of the delauny triangulation computed with the alphavol function [50] can be seen in Figure A.3.

The triangulated mesh is saved in the Polygon File Format (Standford Triangle Format). The polygon file format (ply) consists two subsequent lists of vectors. The first list contains the \((x,y,z)\) vector of all points of the mesh. The second list connects the indices of the previous point cloud to triangular meshes called faces. Each face is linked to a face color as well, meaning it could theoretically be connected to different face properties such as the material for example. Here, however, the faces will all have the same color, since the different materials are saved in several mesh files resulting in each ply file containing only meshes of the one material. The header of the ply files describe the properties of the point cloud. Information on the number of points (number of vertices \(NV\)) as well as the number of mesh triangles (number of faces \(NF\)) are given. An outline of this ply file format is given in Table A.1.
**Figure A.3:** Triangulation of the point mesh shown in Figure A.2.

**Table A.1:** Outline of the Polygon File Format.

```
ply
format ascii 1.0
element vertex
  Number of vertices \( NV \)
  property float x
  property float y
  property float z
element face
  Number of faces \( NF \)
  property list uchar int vertex_indices
end_header

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<th>vertex(_z,1)</th>
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```
A.2 Import into GEANT4

In order to be able to use the triangulated object data as created in the previous section, it has to be read into the GEANT4 simulation. There are two points to this procedure. First of all, the triangulated meshes need to be imported, correctly interpreted and the volumes need to be assigned to the correct materials. Secondly, the proportional size needs to be correct considering that the goal is a correct simulation of the object SPR. In order to import the previously created polygon files into GEANT4 the CADMesh module is used here [62]. It uses the triangular facets to create a G4TessellatedSolid that can be used in the simulation. The size of the volume can be scaled by converting the units of the data from the ply file to the real volume scale of the original dataset in mm (SetScale(CADVolumeScale*mm)). Figure A.4 shows exemplary case of the imported triangulated mesh of the small steel cast part.

Figure A.4: Visualisation of the imported object via the CADMesh library [62] in GEANT4. The triangulated mesh of the small steel cast part described in the previous section is used. Visualization is performed with the HepRAApp Data Browser [1].
Figure A.5: Examples of simulated projections of the small steel cast part with the help of the triangulated mesh and the CADMesh library [62] in GEANT4.
Appendix B

List of filter configurations

The following tables describe the filter combinations and their corresponding configuration numbers used in part III section 2.5.

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Appendix C

Iterative scalar Gaussian message passing algorithm in detail

1) Update messages from node $D$ downward to node $A$:

\[
\frac{1}{\sigma^2[t]} X_{s\ell}^{(n)} = \frac{1}{\sigma^2[t-1]} X_{s\ell}^{(n)} + \sum_{n': n' \neq n \& a_{n',s\ell} \neq 0} \frac{1}{\sigma^2[t-1]} X_{s\ell}^{(n')}
\]

\[
\overrightarrow{m}[t] X_{s\ell}^{(n)} = \overrightarrow{m}[t-1] X_{s\ell}^{(n)} + \sum_{n': n' \neq n \& a_{n',s\ell} \neq 0} \overrightarrow{m}[t-1] X_{s\ell}^{(n')}
\]

\[
\frac{\sigma^2[t]}{\sigma^2[t]} X_{s\ell}^{(n)} = \frac{\sigma^2[t-1]}{\sigma^2[t-1]} X_{s\ell}^{(n')} + \sum_{n': n' \neq n \& a_{n',s\ell} \neq 0} \frac{\sigma^2[t-1]}{\sigma^2[t-1]} X_{s\ell}^{(n')}
\]

\[
\overleftarrow{m}[t] X_{s\ell}^{(n)} = \sum_{\ell': a_{n,s\ell} \neq 0} a_{n,s\ell'} \overleftarrow{m}[t] X_{s\ell'}^{(n)}
\]

\[
\overleftarrow{\sigma^2[t]} X_{s\ell}^{(n)} = \sum_{\ell': a_{n,s\ell} \neq 0} a_{n,s\ell'}^2 \overleftarrow{\sigma^2[t]} X_{s\ell'}^{(n)}
\]

2) Use the downward messages $\overrightarrow{m}[t] X_{s\ell}^{(n)}$ and $\overleftarrow{\sigma^2[t]} X_{s\ell}^{(n)}$ to update messages from node $A$ downward to node $K$:

\[
\overrightarrow{m}[t] X_{s\ell}^{(n)} = \sum_{\ell': a_{n,s\ell} \neq 0} a_{n,s\ell'} \overrightarrow{m}[t] X_{s\ell'}^{(n)}
\]

\[
\overleftarrow{\sigma^2[t]} X_{s\ell}^{(n)} = \sum_{\ell': a_{n,s\ell} \neq 0} a_{n,s\ell'}^2 \overleftarrow{\sigma^2[t]} X_{s\ell'}^{(n)}
\]
3) Use the downward messages $\overleftarrow{m}_{\tilde{y}_n}^{[t]}$ and $\overleftarrow{\sigma}_{\tilde{y}_n}^{2[t]}$ to update the messages from node $K$ to node $A$:

$$
\overleftarrow{m}_{\tilde{y}_n}^{[t]} = \frac{1}{w(y_n, 0)} \cdot \left( y_n - \sum_{k=-M/2}^{M/2} w(y_n, k) \cdot \overleftarrow{m}_{\tilde{y}_n+k}^{[t]} \right) + \overleftarrow{m}_{\tilde{y}_n}
$$

$$
\overleftarrow{\sigma}_{\tilde{y}_n}^{2[t]} = \frac{1}{w(y_n, 0)^2} \cdot \left( \sigma_Z^2 + \sum_{k=-M/2}^{M/2} w(y_n, k)^2 \cdot \overleftarrow{\sigma}_{\tilde{y}_n+k}^{2[t]} \right) - \overleftarrow{\sigma}_{\tilde{y}_n}^{2[t]}
$$

4) Use the upward messages $\overrightarrow{m}_{\tilde{y}_n}^{[t]}$ and $\overrightarrow{\sigma}_{\tilde{y}_n}^{2[t]}$ to update the messages resulting from node $A$:

$$
\overrightarrow{m}_{X_{s}^{(n)}}^{[t]}_{X_{s}^{(n)}} = \frac{1}{a_{n,s}} \cdot \left( \overrightarrow{m}_{\tilde{y}_n}^{[t]} - \sum_{\ell':a_{n,s,\ell'} \neq 0} a_{n,\ell'} \cdot \overrightarrow{m}_{X_{s}^{(n)}}^{[t]}_{X_{s}^{(n)}} \right) + \overrightarrow{m}_{X_{s}^{(n)}}^{[t]}_{X_{s}^{(n)}}
$$

$$
\overrightarrow{\sigma}_{X_{s}^{(n)}}^{2[t]} = \frac{1}{a_{n,s}^2} \cdot \left( \overrightarrow{\sigma}_{\tilde{y}_n}^{2[t]} + \sum_{\ell':a_{n,\ell'} \neq 0} a_{n,\ell'}^2 \cdot \overrightarrow{\sigma}_{X_{s}^{(n)}}^{2[t]}_{X_{s}^{(n)}} \right) - \overrightarrow{\sigma}_{X_{s}^{(n)}}^{2[t]}
$$

5) Use the messages $\overrightarrow{m}_{X_{s}^{(n)}}^{[t]}_{X_{s}^{(n)}}$ and $\overrightarrow{\sigma}_{X_{s}^{(n)}}^{2[t]}_{X_{s}^{(n)}}$ to compute the messages from node $A$ to node $D$:

$$
\overrightarrow{\sigma}^{2[t]}_{X_{s}^{(n)}} = \sum_{n:a_{n,s} \neq 0} \overrightarrow{\sigma}^{2[t]}_{X_{s}^{(n)}}
$$

$$
\overrightarrow{m}^{[t]}_{X_{s}^{(n)}} = \overrightarrow{\sigma}^{2[t]}_{X_{s}^{(n)}} \sum_{n:a_{n,s} \neq 0} \overrightarrow{m}^{[t]}_{X_{s}^{(n)}}
$$

6) Then on the pixel neighbours $(\ell, \ell') \in \Delta$ compute

$$
\overrightarrow{\sigma}^{2[t]}_{X_{s}^{(\ell,\ell')}} = \overrightarrow{\sigma}^{2[t]}_{X_{s}^{(\ell,\ell')}} + \overrightarrow{\sigma}^{2[t-1]}_{X_{s}^{(\ell,\ell')}} - \overrightarrow{\sigma}^{2[t-1]}_{X_{s}^{(\ell,\ell')}}
$$

$$
\overrightarrow{m}^{[t]}_{X_{s}^{(\ell,\ell')}} = \overrightarrow{\sigma}^{2[t]}_{X_{s}^{(\ell,\ell')}} \left( \overrightarrow{m}^{[t]}_{X_{s}^{(\ell,\ell')}} + \overrightarrow{m}^{[t-1]}_{X_{s}^{(\ell,\ell')}} - \overrightarrow{m}^{[t-1]}_{X_{s}^{(\ell,\ell')}} \right) $$
7) For all pixel neighbours \((\ell, \ell') \in \Delta\) compute

\[
\begin{align*}
\nabla^{-2[t]}_{\sigma_{X_{s_{\ell}}}} &= \nabla^{-2[t-1]}_{\sigma_{X_{s_{\ell}}}} + \sigma_c^2 + \sigma_{\ell, \ell'}^2 \\
\nabla^{m[t]}_{X_{(\ell, \ell')}} &= \nabla^{m[t-1]}_{X_{(\ell, \ell')}}
\end{align*}
\]

The equivalent computation has to be done for the pairs \((\ell', \ell) \in \Delta\).

8) Finally, for all pixels \(\ell \in \{1, ..., L\}\) compute the messages from node \(D\) back to node \(A\):

\[
\begin{align*}
\frac{1}{\sigma^2_{X_{s_{\ell}}}} &= \sum_{\ell' : (\ell, \ell') \in \Delta} \frac{1}{\sigma^2_{X_{s_{\ell'}}}} + \sum_{\ell' : (\ell', \ell) \in \Delta} \frac{1}{\sigma^2_{X_{s_{\ell'}}}} \\
\nabla^{-m[t]}_{X_{s_{\ell}}} &= \sum_{\ell' : (\ell, \ell') \in \Delta} \nabla^{-m[t]}_{X_{s_{\ell'}}} + \sum_{\ell' : (\ell', \ell) \in \Delta} \nabla^{-m[t]}_{X_{s_{\ell'}}}
\end{align*}
\]
Bibliography


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