IMPLEMENTATION AND EVALUATION OF SCATTER ESTIMATION ALGORITHMS IN POSITRON EMISSION TOMOGRAPHY

CHARALAMPOS TSOUMPAS

ATHENS 2004
INTERDEPARTMENTAL POSTGRADUATE COURSE IN BIOMEDICAL ENGINEERING

SCHOOL OF MEDICINE, UNIVERSITY OF PATRAS
ELECTRICAL & COMPUTER ENGINEERING
AND MECHANICAL ENGINEERING DEPARTMENTS
NATIONAL AND TECHNICAL UNIVERSITY OF ATHENS

IN COLLABORATION WITH HAMMERSMITH IMANET LTD,
HAMMERSMITH HOSPITAL, LONDON, UK

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CHARALAMPOS TSOUMPAS

LONDON 2004
Three-member Examining Committee:

Associate Professor Konstantina Nikita
Professor Dionysios Dimitrios Koutsouris
Professor Nikolaos Ouzounoglou

External Supervisor at Hammersmith Imanet Limited: Dr. Kris Thielemans
Honorary Lecturer at Imperial College of London
Acknowledgments

This master thesis is an attainment of a more than 15 months work. To be fulfilled plenty of people have provided their valuable help and knowledge.

The first part of the thesis has taken place at the Department of Computer and Electrical Engineering in the National and Technical University of Athens, where my supervisor Associate Professor Konstantina Nikita and Dr Giorgos Loudos have introduced me in the growing field of the Emission Tomography, and particularly in the subject of Iterative Reconstruction Algorithms and STIR (Software for Tomographic Image Reconstruction). In the meantime, Dr Giorgos Kontaxakis, who has been guiding my very first steps sharing his expertise in the field, suggested me to implement this scatter algorithm in the STIR library. I am really grateful to all my professors in the Biomedical Engineering Course and especially to Pr Konstantina Nikita and Pr Nikolaos Pallikarakis for encouraging me to proceed in this particular project.

The main part of the master thesis has taken place in the Hammersmith Imanet Limited, in the Hammersmith Hospital of London. I am deeply thankful to all the people in the Hammersmith Imanet Ltd that have accepted me as a dynamic member by my very first day there; and to contribute to my general understanding in PET. Especially, I have to thank Dr Terry Spinks and Mr Leonard Schnorr, for providing experimental data and Dr Timothy Borgeaud for sharing his great knowledge in computer software. Finally, the greatest thank is to my supervisor in Hammersmith Imanet, Dr Kris Thielemans; without our numerous discussions and his fabulous critical comments, suggestions, ideas, knowledge and help, this work would not have been successfully accomplished. I also wish to thank Pablo Aguiar, not only for providing the results of the valuable Monte Carlo simulations that have been used to evaluate our implementation but also for the many valuable discussions and his useful contribution to the Monte Carlo chapter.
Last but by no means least; I have to thank my parents not only for providing me the financial support during my living in London without any second thought, but also for their continuous encouragement.

*Dedicated to the memory of my grand mother and grand father, who left us during this MSc course.*

«Αγνάντευε το σκοτεινό πέλαγο χωρίς να τρεκλίζεις, κοίταξε κατάματα την άβυσσο κάθε στιγμή, χωρίς φαντασία, αναίδεια και φόβο. Μα δε φτάνει· κάμε ένα βήμα ακόμα: πολέμησε να δώσεις νόμιμα στ’ ασυνάρτητα παλέματα του ανθρώπου.»

Νικόλαος Καζαντζάκης. Ασκητική, 1927.

“Survey the dark sea without staggering, look straight in the abyss each moment, without imagination, impudence and fear. But it’s not enough· do one more step· fight to give a meaning to the incoherently wrestling of the humanity.”


Summary

In positron emission tomography the trends are to use the fully 3D capabilities of a scanner to increase sensitivity and hence improve the quality of the data or reduce the scanning time. To make this feasible, some problems have to be addressed. The most significant effect of image degradation in 3D PET is the Compton scatter, since the scatter coincident photons can be more than 70% of the total coincidences in many whole body studies. Many different scatter correction algorithms have been proposed to estimate the scatter distribution.

In the presented work, a model-based scatter simulation (MBSS) algorithm has been implemented in the Open Source software library called STIR (Software for Tomographic Image Reconstruction). The MBSS is based on the single scatter simulation algorithm (SSS). The main advantage of the SSS algorithm is its good accuracy at small computational time. The aim of the current work is to validate the implementation, investigate the influence of several parameters, as for example the detector sampling and the voxel size of the transmission image, and improve on the existing SSS algorithm, if feasible. The results of the implementation are compared both with data from the SimSET Monte Carlo simulation package and with measured data. The flexibility of our code can help us to understand the influence of many parameters of the algorithm, such that optimal values can be found for given time constraints. This implementation will be included in future distributions of STIR.

In the first chapter PET is briefly described in order to introduce basic concepts and physical quantities that will be referred to in the whole thesis, like the Compton scatter cross-section (known by the Klein – Nishina equation). A historical overview is presented. The scanner geometry and characteristics are also described, to give an idea of how the commercial scanners have been developed.

The scatter issue specific to the 3D PET modality is discussed in the second chapter. A brief description of existing algorithms, used in most commercial and research systems, is given. The methods of measuring and evaluating the scatter
accuracy of the scatter correction algorithms are also introduced, either computational or experimental.

A more detailed description of the Monte Carlo techniques and especially of the SimSET package is given in the third chapter, which will be the main tool to evaluate the implemented scatter estimation algorithm.

Our implementation of the SSS algorithm is presented on the fourth chapter. The effect of the scatter points and the detector sampling in the scatter estimation and the needed computational time is investigated. The idea of using a wider energy window for the simulation, instead of the original is proposed ($W$-SSS). The remainder of the chapter discusses various tests that were performed to evaluate the accuracy of the SSS implementation. Comparing profiles of the estimated single scatter component is achieved by using (i) different SSS parameters; (ii) profiles constructed with SimSET and (iii) measured sinograms of a line source. The same is done for the $W$-SSS. The comparison shows that our SSS implementation has an excellent agreement to the single scatter distribution produced with SimSET. The estimation of the total scatter is satisfactory (when using $W$-SSS) but not ideal, as expected.

For that reason, in the fifth chapter, the possibility of extending the SSS algorithm to include the double scatter component and progressively to a multiple scatter simulation MSS is investigated in order to integrate them into a fully Model Based Scatter Simulation (MBSS). We discuss how to implement the double scatter simulation (DSS) and a preliminary evaluation is included. The results are quite satisfactory even if the needed time for DSS is far slower than for SSS. However, some suggestions for speeding up the DSS and consequently the MBSS are given.

In the last chapter, a brief overview of the results of this work is given, together with a discussion on future work. Moreover, the possibility of introducing the SSS or even the MBSS as a method to estimate scatter into the attenuation image is discussed, which is of great interest, as well.

The STIR software is briefly described and some basic PET terminology is explained in the Appendices.
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Chapter 1. Introduction to 3D PET

Tomography (Greek tomos = section + graphien = to write) is defined as a method of producing an image of the internal structures of a solid object by the observation and recording of differences in the effects on the passage of waves of energy impinging on those structures. Different tomographic imaging modalities provide different kinds of information depending on the data recording means. The traditional X-ray based computerized tomography (CT) produces images of photon attenuation in the tissue whereas magnetic resonance imaging (MRI) describes the proton or water density. Both are concerned with anatomical definition and localisation. Emission tomography (ET) is intended to express functional properties of the tissue. Emission refers to the fact that the energy source is not external but it is introduced into the tissue. There are two ET modalities that share some common properties: Positron Emission Tomography (PET) where two gamma rays (with energy 511keV) are emitted from the body and Single Photon Emission Tomography (SPET) with one gamma ray emitted from the body. Emission Tomography (PET) is an imaging modality that uses positron-emitting radioisotopes to provide measurements of regional tissue function in vivo. [Mustafovic 2003]

1.1 Historical Overview

Positron emission tomography (PET) is rapidly becoming the main nuclear imaging modality of the present century. Although PET technology has existed for some decades, the cost of the procedures and lack of reimbursement for clinical studies delayed the wide application of PET in the clinical setting.
1.1.1 Discovery of the Positron

The prediction, and subsequent discovery, of the existence of the positron, $e^+$, constitutes the great success of the theory of relativistic quantum mechanics. When Dirac developed his electron theory [Dirac 1930], he realised that the negative energy solutions are representations of the existence of a new particle with the rest mass of the electron and an equal but opposite charge – the positron. [Charlton and Humberston 2001]

The annihilation of positrons was discovered in 1933 [Joliot 1933; Thibaud 1933], almost two years after the detection of positrons in cosmic radiation [Anderson 1932]. It was subsequently showed that in general two photons are simultaneously emitted from an annihilation process [Klemperer 1934] in almost exactly opposite directions [Beringer and Montgomery 1942] with a deviation from antiparallelism in the order of 0.3º [DeBenetti et al. 1950].

1.1.2 Early Applications of Positrons in Medicine

The first use of positrons in medicine appears to be the study in 1945 [Tobias et al. 1945] of the elimination of $^{11}$CO from the body, using non-coincidence detection of the annihilation photons. However, the detection of positron annihilation photons in coincidence for the localisation of radioactive substances in humans was first suggested in 1951 [Wrenn et al. 1951] and was used at the Massachusetts General Hospital for the localisation of brain tumours [Brownell and Sweet 1953]. The benefits of this new concept of coincidence detection [Brownell et al. 1968], included:

(i) High detection efficiency in the absence of physical collimation,

(ii) Depth-independent response,

(iii) Use of a number of very attractive radioisotopes with close affinity to biological molecules, and

(iv) Potential for improved localisation based on time-of-flight (ToF) measurements.
Other uses of positrons included $^{15}\text{O}_2$ autoradiography studies of murine tumours [Ter-Pogossian and Powers 1957] and $^{18}\text{F}$ bone scanning [Blau et al. 1962], however, in non-coincidence mode. Early experiments with short-lived isotopes had stimulated interest in the area leading to the building of the first hospital – based cyclotron dedicated to medical applications, in 1955 at Hammersmith Hospital, London. In the late 50’s $^{15}\text{O}_2$ and coincidence detection were used at Hammersmith Hospital to perform lung ventilation and oxygen metabolism studies in humans [Dyson et al. 1958; Dyson 1960]. Around the same time the scintillation camera was proposed by Anger [Anger 1958] and subsequently the positron scintillation camera [Anger 1959] based on coincidence detection, which soon found uses in the localisation of brain tumours with $^{68}\text{Ga}$-EDTA [Anger and Gottschalk 1963] This trail of development of tomographs based on large-area detectors was later to be resumed with the design of PET systems using multi-wire proportional chambers. In the 60’s an early design of a positron camera with 32 NaI(Tl) detectors implemented at Brookhaven National Laboratory was reconsidered and the detectors rearranged into a circular array to improve spatial resolution [Rankowitz et al. 1962]. The device was used to measure regional cerebral blood flow with positron emitting radiotracers [Yamamoto and Robertson 1966]. However, the use of such a device was limited at that time by the lack of the appropriate image reconstruction methods, which were soon to be introduced and accelerate the development of transmission and emission tomography. [Livieratos 2002]

1.1.3 Development of Positron Emission Tomography

Early work [Kuhl and Edwards 1963] introduced the concept of emission reconstruction tomography by providing non-focal plane tomographic images from a series of rectilinear scans at a number of discrete angles. This approach was a first, non-filtered, analogue version of filtered – back-projection (FBP) and although the theoretical basis had been existed in the area of radio – astronomy [Bracewell 1956], its application was restricted by lack of computerised techniques available at the time. The concept of positron tomography was introduced in the early 70’s [Chesler 1971; Chesler 1973] to provide emission,
transmission and absorption – corrected emission tomographic images with the first “Positron Camera” at the Massachusetts General Hospital [Brownell and Burnham 1973], a system based on two rotating opposing banks of detectors. The concept of tomographic reconstruction was developed in the field of X-ray CT in 1973 [Hounsfield 1973] and SPECT in 1974 [Budinger et al. 1974].

The availability of algorithms for tomographic image reconstruction gave rise to the development of a number of PET systems. An early design of a positron emission transaxial tomograph (PETT) at the University of Washington, St Louis consisted of a hexagonal array of 24 NaI(Tl) crystals where each detector was in coincidence with the directly opposite detector [Phelps et al. 1975; Ter-Pogossian et al. 1975]. Its later design, PETT-III, was a whole-body, single-slice tomograph consisting of 48 NaI(Tl) crystals arranged in a hexagonal array [Hoffman et al. 1976]. Each detector was in coincidence with all opposite detectors achieving increased sensitivity compared to earlier versions and it soon found clinical application in imaging of the human brain and heart with $^{13}$NH$_3$ and $^{11}$CO-hemoglobin. Initial experience with the PETT series led to the development of the first commercial positron tomograph, the ECAT (Emission Computed Axial Tomograph) developed by the Ortec Company (Oak Ridge, TN) in collaboration with the St Louis group [Phelps et al. 1978a; Soussaline et al. 1979]. An increase in sensitivity compared to PETT was achieved by employing 66 detectors with a thicker crystal than the prototype system. The design was further modified to include delay circuitry for random coincidence subtraction in the ECAT-II model [Williams et al. 1979]. A modified ECAT-II with the additional feature of a built-in retractable ring source of $^{68}$Ge for transmission scanning for attenuation correction was installed at Hammersmith Hospital in 1979 [Jones 1980].

In the meantime, the use of $^{14}$C-deoxyglucose to measure local cerebral glucose utilisation and subsequently images of $^{18}$F-fluorodeoxyglucose (FDG) was described [Sokoloff et al. 1977], which was to become the most commonly used PET tracer, were acquired in SPECT [Kuhl et al. 1977] and PET [Phelps et al. 1978b; Phelps et al. 1979].

The need to scan over a wider axial field simultaneously led to the development of multi-slice tomographs such as the PETT-IV [Ter-Pogossian et
This series of scanners consisted of a circular array of 48 NaI(Tl) detectors. Since fully three-dimensional reconstruction schemes and ways to account for scatter were not yet available, slice separation was achieved by the use of inter-plane lead shields (septa) and event location within the axial width of the detector was based on one-dimensional Anger-type logic. Other features included rotational capability of the detector array and ‘wobble’, a movement of the centre of the detector array about a small circle, in order to improve spatial sampling [Brooks and DiChiro 1975].

Demand for increased scanner sensitivity stimulated interest in seeking a more efficient detector material than NaI(Tl). Bismuth Germanate (Bi$_2$Ge$_3$O$_{12}$, or BGO) was suggested as a potential alternative detector in positron tomographs [Cho and Farukhi 1977] due to its higher density and hence, increased photoelectric efficiency and was first used in Positome-II at the Montreal Neurological Institute [Thompson 1979].

The time-of-flight (ToF) capabilities of annihilation coincidence detection were explored in a number of systems using alternative detector materials with faster resolving times. In ToF systems, the time difference between the detection of the two photons was used to determine the approximate location of the annihilation and improve spatial resolution by incorporating this information into the reconstruction process [Mullani 1980]. A number of ToF PET systems were developed exploring the timing properties of CsF [Ter-Pogossian et al. 1982; Mullani et al. 1983] and BaF$_2$ [Mazoyer et al. 1990]. However, due to the low density and therefore low efficiency of these scintillators, non-TOF PET based on BGO detectors remained the dominant design for the commercially available systems.

Another major step in the evolution of PET technology was the development of the block detector [Casey and Nutt 1986], where a single BGO crystal cut to smaller individual elements was coupled with a light-guide and four photomultiplier tubes (PMT). Anger-type logic was used to determine the position of the interaction within the detector block from the light shared among the PMTs. This was a major development towards reducing the cost of PET and improving spatial resolution by allowing smaller detector size and higher packing ratio. The
block detector was first introduced in the ECAT 931 tomograph [Spinks et al. 1988] and until now has remained the dominant design for commercial scanners. [Livieratos 2002]

### 1.1.4 From 2D to 3D Mode

Despite the obvious benefit in sensitivity by removing the septa and acquiring all available data (an acquisition mode referred to as 3D mode), even at the expense of increased acceptance of scatter and random coincidences, this was not feasible until the late 80’s when reconstruction algorithms capable of handling these data became available. These reconstruction schemes emerged from work originally developed for systems based on large-area detectors. Attempts to explore the use of large-area detectors for positron tomographs, a concept originating from Anger’s positron camera [Anger 1959], were parallel to the development of ring systems based on individual detector elements. In 1976 the concept of the Anger positron camera was re-introduced [Muehllehner 1976], almost simultaneously with the first use of multi-wire proportional chambers (MWPC) [Lim et al. 1975], which were explored by a number of groups [Jeavons et al. 1978; Jeavons et al. 1983; Townsend et al. 1987; Ott et al. 1988; Charpak et al. 1989; Tavernier et al. 1992]. Although large-area systems found limited clinical application due to low intrinsic detection efficiency, they contributed to the development of low-cost 3D PET, such as the rotating BGO tomograph ECAT ART [Townsend et al. 1993], and the introduction of gamma-camera based PET [Nellemann et al. 1995].

As large-area systems inherently acquired data in 3D mode, work in this area stimulated the development of fully 3D reconstruction algorithms [Colsher 1980; Kinahan and Rogers 1989; Townsend et al. 1989]. The concept of 3D acquisition mode was introduced in multi-ring systems in 1988 when 3D data were acquired on the ECAT 931 with the septa physically removed [Colsher 1980; Kinahan and Rogers 1989; Townsend et al. 1989]. The significant improvement in sensitivity in 3D mode led to the development of the first commercial scanner with mechanically retractable septa [Spinks et al. 1992] and the feature was available in subsequent commercial multi-ring systems [Wienhard 1992; Wienhard et al.
1994; Brix et al. 1997]. The dramatic improvement in sensitivity of 3D mode, compared to 2D, was the driving force for advances in methodology with developments in 3D image reconstruction [Defrise et al. 1994; Defrise et al. 1997] and correction schemes [Grootoont et al. 1991; Bailey and Meikle 1994; Ollinger 1996; Watson 1996b] for quantitative measurements [Wienhard 1998], especially for low count-rate neurotransmitter, drug binding and pharmacokinetic studies or repeat studies [Bailey et al. 1993; Cherry 1993]. A number of 3D-only, septa-less scanners have been commercially produced, including the NaI(Tl) based GE (General Electric) Quest [Karp et al. 1990], the ECAT ART [Bailey et al. 1993; Townsend et al. 1993] and gamma-camera PET systems. The desire to follow regional tissue kinetics of radio-labelled ligands, pharmaceuticals and physiological tracer molecules with enhanced sensitivity, spatial resolution and field of view [MRC 1994] led to the development of a large axial field-of-view, 3D-only multi-ring scanner, the ECAT EXACT3D [Jones et al. 1996].

The experience drawn from existing 3D PET systems and the continuous demand for higher sensitivity and resolution have fuelled a quest to explore new detector materials [Melcher and Schweitzer 1992; Melcher 2000] and designs [Moses et al. 1993; Lecomte et al. 1998; Jones 1999; Schmand et al. 1999; Wienhard et al. 2000] as well as new strategies for data processing and analysis [Badawi et al. 1999; Bettinardi et al. 2000]. [Livieratos 2002]

1.2 Applications of PET

The advantages described above make PET research highly advantageous. A large number of applications exist where PET is used and some of them are outlined below:

- Clinical research:
  - Psychiatry: schizophrenia, depression, anxiety and addiction;
  - Neurology: Alzheimer, Parkinson, dementia, stroke recovery and movement disorders; [Livieratos 1995]
  - Oncology: whole body scanning for detection of tumours and metastases and malignancy assessments;
• Cardiology: Heart failure, imaging of blood flow and metabolism using different compounds. [Livieratos 2002]

➢ Drug discovery and development:
  • Determination of action and efficiency of a new therapy especially in early stages thus reducing cost and animal testing;
  • Testing of kinetics of a drug in early stages as almost 50% of new drugs fail because of pharmacokinetics.

➢ Biology:
  • Scanning of animal models in development of therapeutic strategy.

The above is by no means an exhaustive account of PET wide-ranging applications [Bendriem and Townsend 1998]. Further research and improvements of PET instrumentation open many more exciting options and that is the reason for the on-going research in this field.

1.3 PET Principles

As discussed previously, PET provides a kind of metabolic information that other imaging modalities are unable to provide. Positron emitting radio nuclides tend to be low atomic mass elements, many of them naturally found in the human body, like carbon, oxygen and nitrogen. Radioisotopes of these elements and others of low atomic weight can label metabolically active compounds and be used for imaging a large number of physiologic and metabolic processes. In addition, the dual positron annihilation gamma radiation of 511 keV makes easy the localization of the positron emission by external detectors as well as photon attenuation correction and radiotracer uptake quantification.

1.3.1 Radiotracers

Positron emission tomography is an imaging technique in nuclear medicine that allows in vivo measurement of the radioisotopes concentration, bound to molecules with known biological properties. PET acquires images of physiological function, thereby providing important information on biochemical
and biological activity inside a living organism in a non-invasive way. The importance of this technique lies in the existence of neutron–deficient isotopes of $^{11}$C, $^{15}$O, $^{13}$N, $^{18}$F and $^{82}$Rb listed in Table 1:1.

These are the only radioactive forms of the natural elements ($^{18}$F is used as a substitute for hydrogen), which emit radiation that will pass through the body for external detection. Hence, these radioactive markers can be used to label organic molecules without the need to use artificial, inorganic elements that could cause perturbation of the metabolic process of interest. This is an advantage of PET over single-photon emission tomography (SPECT) where heavy isotopes, such as $^{201}$Tl and $^{99}$Tc, must be incorporated. In addition, the synthesis of physiologically useful tracers using these isotopes is a challenging process since they do not occur naturally in biologically active molecules. In contrast to SPECT, the major problem in PET is the cost since the short-lived isotopes require a cyclotron on-site and also the scanners are appreciably more expensive than single-photon cameras. The short half-life of the isotopes, shown in Table 1:1 represents additional technological and complication since a team of radio chemists must process them efficiently [Livieratos 2002].

Table 1:1 Radionuclides Characteristics

<table>
<thead>
<tr>
<th>Radio Nuclide</th>
<th>$t_{1/2}$ (min)</th>
<th>Productive Reaction</th>
<th>Radiotracer</th>
<th>Range in Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{15}$O</td>
<td>2.03</td>
<td>$^{14}$N(d, n)$^{15}$O</td>
<td>O$_2$, CO, CO$_2$, H$_2$O</td>
<td>7.3</td>
</tr>
<tr>
<td>$^{17}$N</td>
<td>9.96</td>
<td>$^{16}$O(p, a)$^{17}$N</td>
<td>NH$_3$, NO$_x$</td>
<td>5.1</td>
</tr>
<tr>
<td>$^{13}$C</td>
<td>20.4</td>
<td>$^{14}$N(p, a)$^{13}$C</td>
<td>CO, CO$_2$, HCN, many organic molecules</td>
<td>4.1</td>
</tr>
<tr>
<td>$^{18}$F</td>
<td>109.8</td>
<td>$^{16}$O(p, n)$^{18}$F</td>
<td>F – DG, F, organic molecules</td>
<td>2.4</td>
</tr>
<tr>
<td>$^{82}$Rb</td>
<td>1.25</td>
<td>Without Cyclotron</td>
<td>RbCl</td>
<td>14.1</td>
</tr>
</tbody>
</table>

1.4 Positron physics

A PET study begins with the injection or inhalation of a radio-pharmaceutical. The radio-isotope is an unstable proton-rich nucleus that decays by emitting a positron and a neutrino like shown in the following nuclear reaction:

$$ N \ (Z, A) \rightarrow N \ (Z-1, A) \ + \ e^+ \ + \ \nu_e $$
where $Z$ and $A$ the atomic number and weight of the nuclei, while $e^+$ and $\nu_e$ are the positron and the neutrino of the electron.

The decay of an unstable nucleus is a statistical phenomenon, which follows the exponential distribution. The probability $p$ of decay of 1 atom in time $T$ follows the exponential law:

$$p = 1 - e^{-\lambda T} \quad \text{Eq. 1:1}$$

For many applications in PET, we need to know the probability distribution for decay of multiple atoms. This is usually assumed to be Poisson, where the Poisson distribution with mean $m$ has as equation

$$\text{Poisson}(n; m) = \frac{m^n}{n!} e^{-m} \quad \text{Eq. 1:2}$$

This is only approximately true.$^1$ As all atoms are independent, the probability of $n$ decays of $M$ atoms is binomial (i.e. $M$ indistinguishable atoms, each of these can decay with probability $P$):

$$\text{Binomial} (n; M, p) = \binom{M}{n} p^n (1 - p)^{M-n} \quad \text{Eq. 1:3}$$

$$P_{\text{decay}}(n \mid M) = \text{Binomial}(n; M, P) \quad \text{Eq. 1:4}$$

The binomial distribution is Poisson approximately if $M \gg n$ and $p \ll 1$ and it has then mean value $Mp$. For the case of decaying atoms the first condition is satisfied, but the second (i.e. $\lambda T \ll 1$) is not really. Luckily, in PET, the probability of detection by two detector pairs of decay is of main importance. If the detector pair has efficiency $\varepsilon$, then the probability $P'$ of a detected decay is $P \varepsilon$. Again; the probability for $n$ detections is binomial,

$$P'_{\text{creation}}(n \mid M) = \text{Binomial}(n; M, P \varepsilon) \quad \text{Eq. 1:5}$$

But now with a $P'$ which is a lot smaller than $P$. So, the Poisson approximation for the detected decays is fine.

$$P(n, t) = \frac{nt}{n!} e^{-nt} \quad \text{Eq. 1:6}$$

---

$^1$ This is a summary of a derivation available at [http://www.HammersmithImanet.com/~kris/PETbasics/PETstatisticsnorandomsHTML/](http://www.HammersmithImanet.com/~kris/PETbasics/PETstatisticsnorandomsHTML/)
The $\beta^+$ radiation is due to the decay of a proton of the unstable nuclei into a neutron with the exchange of a $W^+$ boson and the $\beta^-$ radiation is when a neutron decays into a proton, with the exchange of a $W$ boson, as can be represented by the Feynman diagrams [Feynman 1985; Mandl and G. 1993; Charlton and Humberston 2001] in the Figure 1:1.

Figure 1:1 Feynman diagrams for the $\beta$ decay.

Current theories of particle physics predict that, in vacuum, the positron is a stable particle and laboratory evidence in support of this comes from experiments in which a single positron has been trapped for periods of the order of three months [Van Dyck Jr. et al. 1987]. When a positron encounters normal matter it eventually annihilates with the electron after a lifetime, which is inversely proportional to the local electron density. Annihilation of a positron with an electron may proceed by a number of mechanisms, and the Feynman diagrams for the radiation process, which results in electron emission and for the single-, two- and three- gamma processes, are given in Figure 1:2 [Charlton and Humberston 2001]. The positron can also annihilate with an inner shell electron in a radiationless process, the consequent energy release giving rise to a nuclear excitation [Saigusa 1994].
The most probable of these annihilation processes, when the positron and electron are in singlet spin state, is the two gamma process, the cross section for which was derived by Dirac [Dirac 1930] to be when $v \ll c$:

$$\sigma_{2\gamma} = \frac{4\pi r_o^2 c}{v}$$  \hspace{1cm} \text{Eq. 1:7}

where $r_o = e^2/4\pi \varepsilon_0 m_e c^2$, is the classical radius of the electron, and $v$ is the speed of the positron relative to the stationary electron.

At low incident positron energies the two gamma-rays are emitted almost collinearly, the energy of each is close to $m_e c^2 (=511keV)$. Annihilation can also occur with the emission of three (or more) gamma-rays, and [Ore and Powell 1949] calculated that the ratio of the cross sections for the three- and two-gamma-ray cases is approximately 1/370. The two other processes, shown in Figure 1:2, are the radiation-less and single quantum annihilations and both need to involve the nucleus or the entire atom in order to conserve energy and momentum simultaneously. As such, they are much less probable than the two-gamma-ray process and they can be ignored in the application of PET. [Charlton and Humberston 2001]

Sometimes, it is possible to have the formation of an exotic atom, called Positronium. Positronium is the name given to the quasi-stable neutral bound state of an electron and a positron. It is hydrogen-like, but because the reduced mass is $m_e/2$, where $m_e$ is the rest electron mass. That is the reason the values of the
energy levels are decreased to half of those found in the hydrogen atom. Positronium can exist in the two spin states, $S = 0, 1$. The singlet state ($S = 0$), in which the electron and positron are antiparallel, is termed para-positronium (Para-Ps), whereas the triplet state ($S = 1$) is termed ortho-positronium (Ortho-Ps). The spin state has a significant influence on the energy level structure of the Positronium, and also on its lifetime against self-annihilation. The need to conserve angular momentum and to impose CP invariance, for ground state Positronium, causes the annihilation of the singlet ($1^1S_0$) and triplet ($1^3S_1$) spin states to proceed only by the emission of even and odd numbers of photons, respectively. Thus, in the absence of any perturbation the annihilation of Para-Ps proceeds by the emission of two, four etc gamma rays and the annihilation of Ortho-Ps proceeds by the emission of three, five etc. gamma-rays. It is expected from spin statistics that Positronium will in general be formed with a population ratio of ortho- to para- equal to 3:1, and in the absence of any significant quenching most of the Ortho-Ps, which is formed, will annihilate in this state. Thus, the three-gamma-ray annihilation mode will be much more prolific for Positronium than it is for free positron annihilation. There are ideas that Positron annihilation into three photons, although quite rare, could still be used as a new imaging modality of positron emission tomography. The information gained when the three decay photons are detected is significantly higher than in the case of two-gamma annihilation [Kacperski et al. 2004a; Kacperski and Špyrou 2004b] and it might be feasible in new generation PET systems, which is expected to use semiconductor technology with smaller energy resolution.

The positrons that are coming from the PET radiotracers have small energy, which they lose rapidly by collisions with surrounding atoms [Bendriem and Townsend 1998]. When the energy becomes sufficiently small an encounter with a free electron results in annihilation where, as analytically discussed in the previous paragraph, most of the time two high energy (~511keV) photons are emitted in nearly opposite directions. Detection of these gamma rays makes possible to reconstruct roughly the distribution of the concentration of the radioactive tracer within the body. The finite range positrons travel before annihilation contributes uncertainty to the localisation of the originating radiotracer and is an area of great interest in positron emission tomography as it
imposes a lower limit in the spatial resolution of the technique. Positron range (Table 1:1), and consequently the uncertainty in spatial localisation associated with it, increases with increasing initial energy of the positron. In many cases a non-zero momentum before the annihilation results in the photon pair not to be emitted strictly at 180°. This contributes a further uncertainty to the localisation of the nuclear decay event of 0.5° full width at half maximum (FWHM) from strictly 180°, which can degrade resolution by a further 1.5mm (dependent on the distance between the two coincidence detectors).

1.5 Gamma interaction with matter – Scatter Effect

In general, high-energy photons interact with matter via a number of mechanisms, depending on their energy, which include: the photoelectric effect, the Compton Effect, coherent (Rayleigh) scattering, and pair production. These are the main mechanisms involved both with the detection of the annihilation photons in PET as well as the problems of attenuation and scatter which will be discussed later. For the energy of 511 keV of the photons produced by positron annihilation, Compton scattering is the dominant mechanism of interaction in human tissue. [Zaidi and Koral 2004]

When a photon beam passes through matter, it becomes weaker or attenuated as photons are progressively removed from it. Scattering losses refer to the energy removed from the beam by photons that are redirected by scattering events, mainly Compton. The energy is carried away from the site of the primary interaction. Absorption losses refer to the energy removed from the beam and transferred locally to the lattice in the form of heat. Absorbed energy is derived from the photoelectron in photoelectric interactions and from the recoil electron in Compton events [Barrett and Swindell 1981]. A parallel beam of monochromatic photons in a homogeneous medium is attenuated according to Beer’s law:

\[ \Phi(x) = \Phi_0 e^{-\mu x} \]  

Eq. 1:8

Where \( \Phi_0 \) is the incident photon fluence (photons per square centimetre), \( \Phi(x) \) is the incident photon fluence after travelling distance \( x \) in the medium and \( \mu \) is
the linear attenuation coefficient. The mass attenuation coefficient \((\mu/\rho)\) is defined by:

\[
\text{Mass attenuation coefficient} = \text{linear attenuation coefficient} / \text{density} = (\mu/\rho).
\]

It is useful for calculating the mass of material required to attenuate a primary beam by a prescribed amount, i.e.

\[
\frac{\Phi(x)}{\Phi_0} = e^{-(\mu/\rho)x_n}
\]

Eq. 1:9

where \(x_m\) is the mass of attenuator per unit area of beam. The quantity \(x_m\) is simply \(\rho x\). It has typical dimensions of \(g/cm^2\) while \(\mu/\rho\) has dimensions of \(cm^2/g\). The attenuating material, usually, is described by a volume density, \(n\) per \(cm^3\), of attenuating particles (i.e. electrons/cm\(^3\), with collision cross section \(\sigma_c\) for Compton interaction), each of which presents a cross-sectional area \(\sigma\) to the incident beam. A thin slab of material of thickness \(dx\) will thus remove a fraction \(n\sigma dx\) of the incident photons from the beam:

\[
-d\Phi / \Phi = n \sigma dx
\]

Eq. 1:10

which integrates to Beer’s law, if we make the formal substitution:

\[
\mu = \sigma n
\]

Eq. 1:11

As said, in the area of 511keV the main scatter effect is the Compton one (~99% depending on the attenuation material) [Zaidi 2001]. For that it is not a big approximation to assume that \(\sigma \approx \sigma_c\) for the area of 300keV– 511keV. So, for a single attenuating material volume density \((n)\) does not depend to the energy at that area, as well, the simple formula coming from Eq. 1:11 can be used, to calculate the \(\mu\) in a different energy value:

\[
\mu(E') = \mu(E)\sigma(E')/\sigma(E)
\]

Eq. 1:12

The biological organs are consisted of complicated molecules. Thus, the mass attenuation coefficient of a compound or mixture of elements is of main importance and is given by [Knoll 1989]:

\[
\frac{\mu}{\rho} = \sum \omega_i (\mu/\rho)_i
\]

Eq. 1:13

Where \(\omega_i\) represents the relative weight fraction of the \(i\)-th element in the mixture.
Table 1:2 Linear attenuation coefficient for different kind of absorbers at the energy of 511 keV.

<table>
<thead>
<tr>
<th>Absorber</th>
<th>Linear attenuation coefficient at the energy of 511 keV (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>0.095</td>
</tr>
<tr>
<td>Soft tissue</td>
<td>0.096</td>
</tr>
<tr>
<td>Perspex (1.1 g/cm³)</td>
<td>0.104</td>
</tr>
<tr>
<td>Bone (cortical)</td>
<td>0.173</td>
</tr>
<tr>
<td>Bismuth Germanate (BGO)</td>
<td>0.95</td>
</tr>
<tr>
<td>Sodium Iodide (NaI)</td>
<td>0.34</td>
</tr>
<tr>
<td>Lead (Pb)</td>
<td>1.83</td>
</tr>
</tbody>
</table>

### 1.5.1 Compton Scattering

In a Compton event, the incoming photon with energy $E_0$ is scattered by a free electron through angle $\theta$. Energy $E_e$ is imparted to the electron, which recoils at angle $\phi$; the remaining energy $E_\gamma$ stays with the scattered photon, Figure 1:3 [Young and Freedman 1996]. Actually, this equation is a result of the assuming photon interactions with some electrons [Feynman 1985].

![Figure 1:3 Compton effect. Gamma photon of medium energy strikes outer orbital electron and releases it from its orbit. This results in production of a secondary gamma of reduced energy.](image)

With $\alpha = E_0/m_0c^2$, $(m_0c^2=511 \text{ keV})$, the energy $E_\gamma$ of the scattered photon is given by:

$$E_\gamma = E_0 \left( 1 + \alpha - \alpha \cos \theta \right)^{-1} \quad \text{Eq. 1:14}$$

The collision cross section $\sigma_C$, as mentioned, determines the probability that an incident photon will undergo a Compton scatter. The expression for $\sigma_C$ was first deduced by Klein and Nishina [Knoll 1989]:
\[
\sigma_c = \frac{3}{4} \sigma_0 \left[ \frac{2(1+\alpha)^2}{\alpha^2(1+2\alpha)} + \frac{\ln(1+2\alpha)\left(\frac{1+\alpha}{2} - \frac{1+\alpha}{\alpha^2}\right)}{(1+2\alpha)^2} \right] 
\]

Eq. 1:15

Where \( \sigma_0 = \frac{8\pi r_0^2}{3} \) is the cross section for (classical) Thomson scattering, and the classical electron radius \( r_0 \) = \( \frac{e^2}{(m_0c^2)} \) = 2.818 \( \times 10^{-13} \) cm. In terms of Avogadro’s number \( N_0 \), the electron density \( n_e \) (cm\(^{-3}\)) is

\[
n_e = N_0 \phi Z/A 
\]

Eq 1:16

If we assume that all atomic electrons participate in Compton scattering equally, and then using Eq. 1:11 we can write

\[
(\mu/\rho)_C = \sigma_C(N_0Z/A) 
\]

Eq 1:17

Thus, the mass attenuation coefficient \( (\mu/\rho)_C \) due to the Compton process depends only on \( Z/A \) (in addition to the energy dependence). Notice that for all but the lightest elements, \( Z/A \approx 0.5 \). Therefore, almost all matter has essentially the same Compton mass attenuation coefficient. Consequently, the scaling in the Eq. 1:12 can be used for any mixture of the human tissue without any problem, in the area of Compton Scatter.

The differential cross sections are useful because they permit the calculation of the angular distribution of the various quantities involved [Barrett and Swindell 1981]. The collision differential cross section is defined such that \( d\sigma_C \) is the probability that an incident photon will be deflected into the elemental solid angle \( d\Omega \) when passing through an attenuator containing one scattering centre per unit area. If the radiation is not polarized, the collision differential cross section (known as \( d\sigma_C/d\Omega \)) depends only on \( \theta \), the angle of deflection of the photon. Thus, it follows that \( \sigma_C \) and \( (d\sigma_C/d\Omega)_\theta \) are related by

\[
\sigma_c = \int_0^{\pi} \left( \frac{d\sigma_c}{d\Omega} \right)_\theta 2\pi \sin \theta d\theta 
\]

Eq. 1:18

The collision differential cross section is given by

\[
\left( \frac{d\sigma_c}{d\Omega} \right)_\theta = r_0^2 \left( 1 + \frac{\alpha^2(1-\cos \theta)^2}{1+\cos^2 \theta[1+\alpha(1-\cos \theta)]} \right) \frac{1+\cos^2 \theta}{1+\alpha(1-\cos \theta)} 
\]

Eq. 1:19
In the Figure 1:4 the ratio of the energy of the Compton scattered photon \((E_\gamma)\) to the energy of the incoming photon \((E_0 = 511 \text{ keV})\) is it is shown as a function of scattering angle, in a polar plot [Accorsi et al. 2004].

Figure 1:4 Ratio of the Compton scattered photon energy \((E_\gamma)\) to the energy of the incoming photon \((E_0 = 511 \text{ keV})\) as a function of scattering angle (thin line): \(E_\gamma/E_0 = 1/(2 - \cos \theta)\). Number – versus – angle distribution of the Klein – Nishina cross - section \((d\sigma/d\theta, \text{thick line})\).

1.6 3D PET Scanner Description

1.6.1 Annihilation Coincidence Detection

The fundamental measurement in PET is the detection of the two (almost) antiparallel photons that emerge from a positron annihilation event. This relies on the principle of annihilation coincidence detection \((ACD)\) (Figure 1:5). ACD takes advantage of the fact that the two annihilation photons are emitted in opposite directions and emerge simultaneously from the same event. Therefore if two photons are detected by two opposing detectors simultaneously (i.e. within a narrow time interval), their originating positron annihilation event is placed along the volume defined by the two detectors, ignoring scatter, which is referred to as a line of response \((LoR)\), like this shown in Figure 1:5.
Since ACD defines the annihilation event within a specific LoR without the use of physical collimation, it is often described as an electronic collimation technique. Unlike single-photon detection where physical collimation is used to provide positional information, electronic collimation allows the detection of events for each detector in coincidence with multiple opposing detectors. This results in a significant increase in sensitivity of 10 - 20 times in 2D mode and \(~150\) times in 3D compared to single-photon detection such as in SPECT [Bailey and Meikle 1994]. Since with electronic collimation the position of the annihilation event is confined within the LoR between the two detectors involved, another consequence of ACD is the uniform spatial response in PET. This is demonstrated by the point spread function (PSF), the spatial profile of a point source as a function of position, which remains fairly constant within the field of view of the two detectors, unlike single-photon detection where the PSF is significantly depth-dependent [Phelps et al. 1975].

1.6.2 PET Scanner Geometry: the ECAT EXACT HR⁺

The new generation scanners, as discussed in the historical overview, are consisted of a huge amount of small detectors, arranged in parallel rings. The
neighbour detectors are arranged in a detector block, which has one photomultiplier tube (PMT) like shown in Figure 1:6 [Tsoumpas 2003].

For example, in the case of the ECAT® EXACT® HR+ (CTI / Siemens, Knoxville, TN), a commercial system for brain and whole body PET, the detectors are consisted of BGO crystals; each one of them has dimensions$^2$ (4.39×4.05×30) mm$^3$. In total, the scanner has 18432 crystals. All of them arranged in 64 (8×8) crystals per detector block. Each detector block is connected to 4 PMTs. Then, 6 (3×2) detector blocks are attached vertically to a bucket. Each bucket has a different view of the centre (i.e. 15 total views) of the scanner to preserve the cylindrical arrangement$^3$.

![Figure 1:6 Detector Block, with four PMTs](image)

So, there are 288 detector blocks in 48 buckets, which give 32 rings of about 412mm radius. The system, which is shown in the Figure 1:7 [Tsoumpas 2003], can operate in 2D and 3D mode, the latter measures direct and indirect sinograms, which can be arranged into a Michelogram format (APPENDIX II-II). The a-FoV (axial Field-of-View) is 155 mm, and the t-FoV (Transaxial Field-of-View) is 583 mm, while the radius of the r-FoV (Radial Field-of-View) is 291.5 mm.

---

$^2$ Azimuthal, axial and radial direction, respectively.
$^3$ Not shown in the Figure 1:7.
Figure 1:7 Detector Block Arrangement of the ECAT EXACT HR+ PET, not taking into account the buckets arrangement, for simplification.
Chapter 2. Scatter modelling and correction techniques in fully 3-D PET

2.1 Introduction

As discussed, PET offers the possibility of quantitative measurements of tracer concentration in vivo. However, there are several issues that must be considered in order to take advantage of its full potential. Two of the most significant effects are the photon attenuation in the patient and the contribution in the images of events arising from photons scattered in the patient and the gantry. The non-homogeneous distribution of attenuation within the thoracic cavity complicates the interpretation of PET images and precludes the application of simple scatter correction methods developed for homogeneous media. The development of more sophisticated techniques for quantification of PET images is still required. Progress in 3D PET instrumentation and image reconstructions, by removing the septa, has created a need for a review of the scatter correction techniques. Of course, to obtain a satisfactory scatter and attenuation correction many parameters should be minimised, such us the patient motion.

While it is well accepted by the nuclear medicine community that the detection of Compton-scattered events degrade image quality, a common question asked by most nuclear medicine physicians is to what extent does scatter affect image interpretation and clinical decision making. The physicists are convinced that scatter correction is a vital component in the production of artefact-free, quantitative data.
2.2 Investigation of the Scatter Component in 3D PET

Extensive investigation of the scatter in PET by Monte Carlo (M-C) simulations can show interesting results for the scatter component in 3D PET [Adam L. E. et al. 1999]. Adam has simulated the scatter for the ECAT EXACT HR+ tomograph based on EGS4 [Nelson et al. 1985]. In the simple case of a point source in the centre of a water-filled cylinder that nearly fills out the patient port, with inter-plane septa (2D mode) one of the three events are scattered, and without septa (3D mode) about two out of the three detected events. This is significantly higher than for a classical 2D scanner with a smaller axial FoV and demonstrates the increased importance of the scatter correction.

Adam shows also that the scatter fraction, and also the scatter distribution, varies significantly with the axial position in the FoV and that there is no simple function to describe the scatter kernels. This mainly affects convolution-subtraction algorithms and suggests the use of a simulation to estimate the scatter kernel or, alternatively, an energy window based algorithm which intrinsically accounts for positron-dependent effects of scatter as well as SoFoV, such as Ferreira’s [Ferreira et al. 2002], see § 2.5.3. For an accurate scatter correction it is necessary to take the activity and scattering media outside the field of view into account. It is also shown that for extended attenuation media the HR+ detects a considerable amount of multiple scatter which has a different spatial distribution from single scattered events [Adam L. E. et al. 1999]. This means that the multiple scatter can only partially be corrected by rescaling the single scatter component. If this approximation a little or not is, depends strongly on the type of crystals (i.e. the energy resolution) and the energy window of the scanner.

2.3 Finding An Optimal Scatter Model

Scattered photons arise from the whole attenuating medium, including the imaging table and the PET tomograph itself. In addition to a decrease in the image contrast, events may also appear in regions of the image where there is no activity (e.g. outside the patient). Several studies have reported that the scatter fraction
(SF) defined as the ratio of the scattered photons to the total photons (scattered and unscattered) detected, represents from 30% (brain scanning) to even more than 50% (whole-body scanning) of the data acquired in the 3-D mode, depending mostly on the scanner geometry, the energy window setting, the region to be explored and patient size [Zaidi 2000b]. The issue of scatter detection, modelling and correction in PET is addressed in many publications.

The ideal research tool for scatter modelling and evaluation of scatter correction techniques is the M-C method [Adam L. E. et al. 1999; Zaidi 1999; Zaidi 2000a]. Nevertheless, the complexity and computing requirements of M-C simulation led to the development of analytical simulation tools based on simplifying approximations to improve the speed of operation. For instance, a fast analytical simulator of tomographic projection data developed for SPECT taking into account attenuation, distance-dependent detector response, and scatter based on an analytical point spread function (PSF) model [Beekman et al. 1997].

Much research and development has been concentrated on the scatter compensation required for quantitative 3-D PET. Historically, once one had obtained the best projection data feasible, one typically applied compensations for these degradations either prior to or after reconstruction with filtered back-projection. However, the most reliable method for determining the actual amount of scatter in the image is physical modelling of the scatter process in order to resolve the observed energy spectrum into its primary (unscattered) and scatter components. Nowadays, scatter correction models based on attenuation maps and the physics of interaction and detection of annihilation photons. Increasingly, sophisticated scatter correction procedures are under investigation, particularly those based on accurate scatter models [Ollinger 1996; Watson et al. 1997], and iterative reconstruction-based scatter compensation approaches [Beekman et al. 1997; Hutton and Baccarne 1998; Kadmmas DJ 1998; Zaidi 2001b].

2.4 Scatter correction techniques

Multiple energy window methods were originally developed for SPECT and have been in use for more than 15 years. The development of the 3-D acquisition
mode in PET and the improvement in the energy resolution of the detector has allowed the implementation of scatter correction based on the analysis of energy spectra [Grootoont et al. 1996]. Several groups investigated the potential of acquiring data in two, three and multiple energy windows to develop corrections for scattering in 3-D PET. The quantitative accuracy is generally improved at the expense of a degradation of signal-to-noise ratio, which can be explained by the scatter subtraction process and the resulting reduction in the statistics of the acquired data sets. The major problem with the window approaches, which usually use a normal and a low energy window, is that the majority of scattered events in the photo-peak window undergo only a single Compton interaction, while the majority of scattered events in the lower energy window undergo multiple interactions [Thompson 1993]. The effect of multiple scatter is to broaden the scatter distribution, so it is much flatter than the singly scattered events. Harrisson has shown that this leads to impaired accuracy [Harrison et al. 1991].

There is continuing interest in the development of non-stationary convolution ± subtraction scatter correction techniques [Bentourkia and Lecomte 1999], which overcome the inherent limitations of the stationary approach [Bailey and Meikle 1994] by taking into consideration the dependence of scatter upon source locations, object size, detector angle, etc. Different methods of non-stationary deconvolution have been proposed for SPECT [Ljungberg and Strand 1990], 2-D PET imaging [Bentourkia and Lecomte 1999] and PET animal imaging [Lubberink et al. 2004]. The extension of such models for 3-D PET, though, does not seem to work better than the model-based simulation algorithms.

Model-based scatter correction methods use both emission and transmission scans together with the physics of Compton scattering to estimate the scatter distribution [Ollinger 1996; Watson et al. 1997]. They essentially perform a simulation of the single scatter distribution, based on a known attenuation and emission map. The emission map is usually reconstructed from scatter corrected emission data in an iterative process. In general, these methods have two problems: multiple scatters and scatter from out of field-of-view (SoFoV). This last effect can be directly taken into account by acquiring short, auxiliary scans.
adjacent to the axial volume being investigated. These algorithms can thus be slightly modified to partially reduce this effect.

Direct $M$-$C$-based scatter compensation approaches intrinsically handle the effect of multiple scatters, but they have identical problems with SoFoV as the model-based methods. An interesting attempt of using $M$-$C$ simulation for scatter correction has been performed by Holdsworth [Holdsworth et al. 2002]. This technique accounts for all the scattered photons, incorporating innovative sampling techniques to increase time efficiency. However, the method is still slower than model-based methods, which is particularly troublesome of multiple iterations are necessary. To partially overcome this, its current implementation uses as input the scatter corrected emission image based on the scatter correction supplied by the scanner software.

In the rest of this thesis, we will further concentrate on model-based methods as they are more accurate than most other methods, while still being not too computer-intensive for practical use.

### 2.5 Scatter models based on Single Scatter

#### 2.5.1 Ollinger’s Approach

As mentioned, the first approach was done by Ollinger [Ollinger 1996], who combines an analytically computed estimate of the distribution of single scatters with a convolutional estimate of multiple scatters. Then based on the estimation of the intensity and attenuation coefficient in the volume being imaged, he estimates the distribution of scattered events. Most of the scatter component is due to single scatter (i.e. most of the cases more than $\sim 70\%$). Multiple-scatter is modelled as an integral transformation of the single - scatter distribution, by convolving the latter with a one-dimensional Gaussian kernel [Goggin and Ollinger 1994], where the kernel of the filter is determined by fitting to representative experimental data. The emission images are corrected for scatter iteratively. This is done, by estimating the scatter component based on the uncorrected emission and attenuation images at the first iteration. Then, based on the first-step-corrected
images, the scatter component is recalculated. This is done just a few iterations in order not to slow down the whole process. The detector efficiency for a scatter coincidence is the same as that for a true coincidence. The energy resolution is modelled as a Gaussian function with a variance determined by the measured energy resolution.

The results of this approach have been evaluated using the SimSET M-C package and have been accurate, even for air-filled and water-filled lung phantoms. It has been noticed, as well, that increasing the sampling rate of the oblique angle does not affect the accuracy, but increasing the spatial sampling significantly improves it.

Concluding, this scatter correction method takes into account many physical and geometrical parameters resulting in very good accuracy, but the computational time was not too fast to run directly into the reconstruction algorithm, in 1996. A potential drawback is the multiple scatter model. The particular empirical model is not robust; since a lot of parameters need to be fit to different scanning situations [Zaidi 2000a] and it is probably the source of a significant component of the overall error of the method. Ollinger did not attempt to compute the multiple-scatter distribution directly because of the computational complexity, but see Chapter 5. Detection efficiency normalization is another difficult problem since scattered photons are detected with different efficiencies from unscattered photons because of their lower energies [Ollinger 1995]. Furthermore, the largest – and the most difficult to solve – problem in patient studies is likely to be the scatter due to the activity outside of the field of view as discussed previously.

Wollenweber managed to develop a fast implementation of Ollinger’s method [Wollenweber 2002], in order to use it commercially into GE PET scanners. This approach utilizes many of the processing steps of Ollinger’s algorithm with the simplification of removing explicit calculation of scatter contribution from oblique azimuthally directions. This approximation allows faster execution time for 3-D scatter correction and it might have small impact on quantitative accuracy. Scatter for the oblique sinogram is not calculated at all. Moreover, he uses only a few numbers of thick slices to sample the axial direction, translating the problem
from 3D to a kind of 2D. Essentially, this implementation samples the images by taking a small number of pixels, in order to make the method faster. These simplifications make the scatter correction algorithm as fast as it is needed to be included in the reconstruction algorithms of a commercial scanner.

2.5.2 Watson’s Approach

The single scatter simulation algorithm (SSS) has been introduced in 1996 [Watson et al. 1996a] and is integrated in the CPS/CTI PET scanners (Siemens). This approach also starts with a numerical computation of the single scatter distribution. In contrast to Ollinger, Watson assumes that the total scatter distribution can be well approximated by scaling the single distribution. However, it does not model the finite positron range and the non-collinearity. All these methods ignore the previous effects, so you should move that to the start presumably. The scatter from out of the FoV (SoFoV) is not simulated.

The basic concept of the SSS algorithm is to select randomly a scatter point in the attenuation image by using a threshold in order to exclude areas that are not inside the area of the patient. Then, for each selected scatter point the probability to be scattered and detected by a detector pair is estimated using the Klein-Nishina formula. The sum of the single scatter probabilities over all scatter points forms the estimate for the single scatter distribution for each detector pair. In order to achieve fast computational times, the attenuation image is sampled and the attenuation and emission line integrals are stored in the cache memory. An analytical description of the SSS is given in §4.1.

After defining the single scatter distribution the result is scaled in order to have the same scatter with the experimental sinogram in the region where only scatter must have occurred, such as the region out of the patient border that can be defined by the attenuation image. There are three versions of the SSS algorithm, introduced by Watson. The most important difference among these algorithms is this scaling factor and the use of iterations. In the 1st SSS version [Watson et al. 1996a], a single scaling factor is used. Aside from taking multiple scatter into account, the scale factor helps to compensate some of the numerical
approximations made in the simulation, such as the use of low-resolution, uncorrected images to present the emitter and attenuation distribution. It also permits the scatter correction to be computed from non-calibrated estimated emission images. Further, the normalization to the data may compensate in part for some physical approximations made in the model, such as the neglect of activity SoFoV, the simple treatment of detector response and coincidence electronics, and the neglect of multiple scattering, finite positron range and the non-collinearity of the annihilation radiation. In the 2nd SSS version [Watson 2000] no scaling factor is used at all. As it is argued, the scaling step of the 1st version is very problematic when the data are very noisy, when the patient occupied most of the FoV, or when little activity was in the FoV. There is some effort to estimate the single scatter sinogram in the correct scale, comparing to the measured sinogram. The multiple scatter is presumed, to be taken into account using the ad-hoc method of not using any iterations at all, i.e. the single scatter estimate is computed during the image reconstruction from the original emission data, which include all scatter. This image estimate is obviously contaminated with scatter, but it is hypothesised in [Watson 2000] that this compensates for not simulating multiple scatters. However, it seems that this simpler method did not show the expected results and this is the reason of the recently 3rd SSS version [Watson et al. 2004a], which again introduces iterations and now uses multiple scaling factor, one per sinogram, to take into account multiple scatter and the SoFoV.

A point worthy to mention is that in all versions of Watson’s SSS, an extended energy window has been employed in the scatter simulation by lowering the LLD (lower limit of discrimination) compared to the one set at acquisition. This was explained in [Watson et al. 1997] by referring to the need of a more accurate representation of the physical threshold. Later on this has been clarified by arguing that there was a different response of the electronics of the particular scanner (i.e. ECAT EXACT HR+), than was expected at the LLD. Particularly, Watson argues [Watson 2004b] that the reason for introducing the LLD deficit in the SSS calculation was not to account for multiple scatter. Moreover, he argues that the multiple scatter does not change the shape of the scatter distribution significantly for LLDs of 350 keV and higher except at large angular distances.
from the source – i.e. for LORs that lie radially well outside of the emitter
distribution, where it doesn’t matter for clinical scatter correction. The LLD deficit
was introduced because the physical threshold of the older generation scanners
(i.e. before Pico-3D digital electronics were introduced) is actually lower than the
nominal value that is set in the user interface. In the 3rd SSS version, though, the
energy window used for the scatter algorithm and the acquisition is the same, at
least for the new HiReZ scanner, since the electronics of the new scanner are well
– calibrated and their response is as expected.

2.5.3 Alternative SSS implementations

Various SSS algorithms have been implemented and applied into the
reconstruction algorithms. We discuss here Werling’s, Poenisch’s, Ferreira’s and
Accorsi’s [Werling 2001; Ferreira et al. 2002; Poenisch 2003; Accorsi et al.
2004].

The Werling’s approach is the first SSS implementation that caches the line
integrals, causing about three times faster calculation\(^4\) [Werling 2001]. It uses the
scaling technique of the original SSS version by defining the scale factor using a
robust estimator. It uses a mask function to ensure that only the scatter region
contributes to the scaling factor. The scaling factor is estimated by an iterated, re-
weighted least squares formula, in order to minimize the difference between the
observation and its fitted value. This implementation uses only direct sinograms,
as well, since it was observed that scatter distributions from oblique projections
are very similar to the direct projections. The acquired 3D emission sinograms
have been rebinned into 2D sinograms using the FORE algorithm [Defrise 1995].
However, theoretically, the application of rebinning algorithms to scatter
contaminated data is expected to produce erroneous results since the scatter
component of the oblique sinograms cannot be estimated from the direct ones
using the same rebinning formula appropriate for unscattered events. Moreover,
the scattering process is considered as an integral part of the image forming
process and, consequently, is modelled in the forward projector of an iterative

\(^4\) However, Ollinger probably cached the line integrals as well, and so did Watson in his 2\(^{\text{nd}}\)
version.
reconstruction algorithm, which is however applied on Fourier Rebinning (FORE) rebinned data. Their obtained results have not been as good as expected. So it was presumed that there might be a problem with the scaling factor. Moreover, it is believed that these systematic errors are caused due to higher order scatter and that the limitation to single scattered events is of limited validity for whole-body measurements. So, they suggest that a more accurate model taking into account multiple scatter could yield significant improvements in these situations. Finally, they argue that the SSS cannot work satisfactory in whole-body cases.

The Poenisch’s approach is the first SSS implementation for the case of an in-beam dual head positron camera, which is used to monitor dose application in situ during the tumour irradiation with ion beams. In this interesting approach, the small number of detectors, comparing to the original PET scanners, gives the opportunity of using more scatter points, which have to be chosen carefully because of the anisotropic spatial resolution of the double head camera. The scaling factor, in contrast to the original SSS procedure, is calculated by means of an additional M-C simulation. The ML-EM (Maximum Likelihood – Expectation Maximisation) algorithm is used to reconstruct the image [Poenisch 2003], but it should be noticed that the system matrix in the back projection do not contain the scatter contribution as it should be for an exact solution.

The Ferreira’s approach uses a hybrid scatter correction method for 3D PET based on an estimation of the distribution of non-scattered coincidences [Ferreira et al. 2002]. The implemented scheme combines two scatter-correction methods in a complementary way. The first is based on the discrimination of the energy of events to estimate the true coincidences. The second is the SSS (the paper also discusses using the convolution – subtraction method as possible 2nd method). The first method gives the opportunity to take into account the SoFoV. The second accounts for events that have scattered with small angles, which have an energy that cannot be discriminated from that of the non-scattered events. This technique, in contrast with the most dual window techniques, uses the data acquired in an upper energy window (550 – 650 keV), to obtain a noisy estimate of the non-scattered events. The second method (i.e. SSS) is used to remove scatter for the upper window. It is argued that in such a high window most of the photons are
true coincidences. The SSS or the convolution – subtraction method gives an approximation of the scatter component, which can be detected, even in this upper energy window due to the detector efficiency. Note that the Single Scatter approximation should be valid for this high-energy window. Then, the estimated distribution of the unscattered events is scaled somehow, to the non – scattered detected events in the normal window (350-650 keV). Then, by a simple subtraction of the true events the total scatter can be estimated. This estimate is noisy however, but this is remedied by using a smoothing step of the total scatter estimate. This technique introduces a sophisticated idea of combining the double energy window method and SSS, in order to include SoFoV and multiple scatter. It seems to be potentially the only way to estimate the SoFoV, aside from using a few different bed positions with the associated difficulties of changing radioactivity distribution. The drawback of this hybrid way is the many steps of using scaling factors and, maybe more importantly, the instability of the higher energy window in current PET scanners. For the scaling, Ferreira does not use a global factor to scale the single scatter and the measured coincidences, in the upper energy window, due to the different shape of the scatter distribution, which depends on the different detector efficiency in the energy window. However, there is a question if the shape is also depended on the different possibility of occurring single scatter events in a different energy window, even if in the subtraction formula it does not contribute directly. If this is true, a different variant scale factor should be used to scale specifically the scatter distribution of the upper window, to represent the small angles scatter of all the true events.

The scaling factor of both the measured and the scatter distribution of the upper window and the corresponds to the product of two components: a space-variant one, only due to the different normalization factors, to the two energy windows and the global scaling to compensate shifts in the energy spectrum. In addition, the global factor that scales the unscattered counts in the two energy windows changes with time. In order to overcome somehow this problem, an ad-hoc method has been used, determining this factor from the observation that errors in the global scaling factor lead to a contamination of the final scatter estimate with unscattered events and to an increase of the correlation between the final scatter
estimate and the distribution of non-scattered events, in the region of the emission object.

In addition, a point to be discussed is the use of a different LLD (i.e. 430 keV) in the scatter estimation, than what is specified during the acquisition (i.e. 550 keV), like in the 1st SSS version for the HR$^+$ scanner [Watson et al. 1997]. As explained [Ferreira et al. 2002], this value corresponded to the best correction for a 20 cm uniform cylinder in the upper window and it is influenced by the scanner design.

Concluding, in cases of much more SoFoV this technique seems to have quite good agreement in comparison to the classical SSS, due to the dual window method. Comparison should be realised in cases with minimum SoFoV, as well. Why Watson’s 3rd version does not include this technique is a spontaneous question. Perhaps all these scaling factors do not give a stable result in some cases. However, this technique seems to be quite exceptional, and might have the potential to be improved in order of adapting it as the most complete scatter correction method, till the computational time for a M-C scatter estimation technique can be reduced to a practical level$^5$.

A well optimised and evaluated single scatter simulation algorithm has been implemented by Accorsi [Accorsi et al. 2002]. In this implementation, scatter and activity that comes out of the are explicitly modelled by loading data and distributing more scatter points to model these effects as well. The effect of the side shields was included, as well by assuming that the shields perfectly absorb all incident photons. SSS predictions are compared to M-C simulations and experimental data from uniform, line and cold-bar phantoms showing that the code is for uniform as well as asymmetric objects. It is also possible to model different energy resolution crystals and LLD settings. However, the current implementation has been evaluated in the case of a GSO-based scanner, which enjoys relatively good energy resolution. For detector crystals with lower energy resolution (e.g. BGO) it is expected to result in different agreement, especially because of a higher fraction of multiple scatter events.

---

$^5$ M-C methods, though, also have SoFoV problems.
An interesting point is the implementation of the detection efficiency, which does not seem to be quite correct. Firstly, the energy resolution is independent of the scattered photon energy. Moreover, the LLD is not the minimum accepted energy value of the incident photon, as it will be shown in the next chapter; there is at least some small but not negligible possibility to detect an event with lower energy than LLD, due to the resolution of the scanner at the particular energy.

Some absolute quantitative studies have been performed [Accorsi et al. 2004] and show that for most applications, the code provides a better scatter estimation than the tail-fitting scatter correction method, which has been used before on the Philips scanner. This is somehow expected, since the SoFoV is modelled and the multiple scatter is negligible.

Finally, really interesting is the extension of the code to the case of transmission scanning which have been validated against M-C data [Accorsi et al. 2002]. SSS has been applied to transmission scanning to obtain a better estimate of the distribution of the scattering medium, which can be used for a more accurate estimate of the emission scatter. More importantly, scattering causes an apparent reduction in the attenuation coefficient, which is more severe for high scatter fractions. For example, a scatter fraction of 25% is enough to cause a variation of 10% or more in the apparent attenuation coefficient. An accurate estimation of the scatter fraction can be used to obtain a better estimate of the attenuation coefficient. The code was modified to estimate the scatter distribution of a transmission scan using a $^{137}$Cs source. Results from SSS were compared to M-C data, as the only method available to estimate the scatter distribution in transmission scans.

### 2.6 Accuracy of scatter correction

#### 2.6.1 Evaluations based on simulated phantoms

Evaluation of scatter correction algorithms is inherently difficult and sometimes unconvincing. Most of the algorithms developed so far have been evaluated using either simulated or experimentally measured phantom studies, in addition to
 qualitative evaluation of clinical data [Zaidi 2000a]. Modelling and simulation of PET imaging is best done with phantom models that match the gross parameters of an individual patient. Recent three- and four-dimensional computer phantoms seek a compromise between ease of use, flexibility and accurate modelling of populations of patient anatomies, and attenuation and scatter properties and biodistributions of radiopharmaceuticals in the patients. Modelling of the PET imaging process has been improved by more accurate simulation of the physics and instrumentation involved in the process. M-C software packages, especially those developed specifically for nuclear medicine and with different performance characteristics, have been found useful in the modelling work. The combination of realistic computer phantoms and accurate models of the imaging process allows simulation of PET data that are ever closer to actual patient data. Simulation techniques have found an increasingly important role in nuclear medicine research, especially scatter modelling and correction. In the present work, the SimSET M-C package, which will be discussed in §3.1, is used extensively in the evaluation of the scatter simulation accuracy. [Zaidi 2001a]

2.6.2 Evaluations based on real phantoms

In a clinical environment, the evaluation is further hampered by the multiplicity of the medical purposes for which the corrections may be studied. For that reason, certain standards have been introduced. The usually followed standards are those that have been proposed by the National Electrical Manufacturers Association (NEMA) [NEMA 1994; NEMA 2001] in order to check the scanner performance. For example, CTI uses the NEMA tests as part of the scanner acceptance test.

For scatter accuracy, the NEMA standard prescribes the following test. The test phantom is a solid right circular cylinder composed of polyethylene with a specific gravity\(^6\) of 0.96 ± 0.01, with an outside diameter of 203 ± 3 mm, and with an overall length of 700 ± 5 mm. A 6.4 ± 0.2 mm hole is drilled parallel to the central axis of the cylinder, at a radial distance of 45 ± 1 mm [NEMA 2001].

\(^6\) The specific gravity (or better the relative density) of a material is defined as the ratio of the density of that material to the density of the water.
The NEMA ‘94 uses a much shorter phantom, and it is filled with water. There are just two more holes at 0 ± 1 mm and 90 ± 1 mm. [NEMA 1994]
Chapter 3. Monte - Carlo Simulations in PET

3.1 Introduction

Monte Carlo (M-C) methods are alternative techniques to solve complex or non-linear problems when analytical formulas are unwieldy. These methods use random numbers as a base to perform a simulation of any specified situation, usually corresponding to naturally random processes, such as radioactive decay. The first reference to the M-C method is Comte de Buffon in 1777. Simulation using computers was first used during the World War II Manhattan project to designate a class of numerical methods based on the use of random numbers. Von Neumann and Ulam named it M-C because one of the most well known centres for gambling is the M-C Casino.

The problems in which M-C techniques can be used must be described by a probability density function (PDF). Then, M-C code performs a random sampling of these functions by using a pseudo random number generator. In Nuclear Medicine, these numbers imitate the stochastic behaviour of photon interactions in matter. Unless variance reduction techniques such as forced detection (see §3.2.3) are used, the process will follow Poisson distributions because the detection of an emitted photon is independent of the others, the number of emitted photons is statistically large and the probability of detection is lower than 0.05.

Several M-C simulators have been developed in order to simulate experiments in scientific fields such as high-energy physics and particle physics. Some of them have been integrated into nuclear medicine, for instance GATE, which is based on GEANT-4, while others have been, developed independently to simulate the physical processes which take place in PET and SPECT (Table 3:1). An extensive
comparison among \( M-C \) packages dedicated in \( SPECT \) and \( PET \) has been presented by Buvat et al. [Buvat and Castiglioni 2002].

<table>
<thead>
<tr>
<th>General Purpose</th>
<th>( PET )</th>
</tr>
</thead>
<tbody>
<tr>
<td>GEANT</td>
<td>GATE</td>
</tr>
<tr>
<td>EGS4</td>
<td>SIMSET</td>
</tr>
<tr>
<td>MCNP</td>
<td>PETSIM</td>
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<tr>
<td>ITS</td>
<td>EIDOLON</td>
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</table>

In the present work, the \( SimSET \) \( M-C \) package has been extensively used for the evaluation of the scatter simulation algorithms.

### 3.2 SimSET

#### 3.2.1 SimSET Code

Simulation System for Emission Tomograph (\( SimSET \)) is open source software, written in the C programming language and developed at the IRL, at the University of Washington, Seattle [Lewellen et al. 1998; SimSET-Collaboration 2004]\(^7\). The purpose of \( SimSET \) package is to simulate the transport of photons generated from a distribution of an isotope in a medium.

It is a useful tool to evaluate interesting situations, which are not possible to study using, measured projections. As input for calculations, \( SimSET \) requires a digital representation of the activity distribution and mass density distribution of the patient. \( SimSET \) controls the mean value and the variance\(^8\) (the statistical noise). The \( SimSET \) outputs are projections file and statistical information file.

The sampling of each history is defined in \( SimSET \) as in the standard \( M-C \) method, but with a significant difference. Whereas in the latter all the results are given per particle emitted, in the former the results are absolute counts. This will change the statistical results of \( SimSET \) in comparison with a standard \( M-C \) code.

\(^7\) For further details see the SimSET’s website: http://depts.washington.edu/SimSET/html/SimSET_home.html

\(^8\) The mean value corresponds to the estimated value for the expectation of a distribution and the variance corresponds to the statistical noise.
Then, in SimSET a variable proportional to the activity is defined as the number of emitted photons at each voxel \( P_k \) and the total emitted photons in the object, \( P \):

\[
P = \sum A_k \Delta V_k \Delta t = \Sigma P_k
\]

Eq. 3:1

Where,

- \( \Delta t \): scan time for the PET acquisition (different in SimSET original code where this parameter was constant).
- \( A_k \): Voxel activity.

- All the voxels in the input of SimSET have a curtain volume represented by \( \Delta V_k \).

Emitted photons are sorted voxel by voxel. The initial weight differs from that of the standard M-C simulation because each history transfers the information of a set of emitted photons.

As an input a digital representation of the activity and density and several parameters of the simulation about scanner characteristics are needed.

The “Photon generator” (PHG) generates photons and transports them from the object to the detector [Aguiar and Cot 2004].

<table>
<thead>
<tr>
<th>Table 3:2 Photon History Generator (PHG) input/output</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PHG input</strong></td>
</tr>
<tr>
<td>Activity Distribution (isotope)</td>
</tr>
<tr>
<td>Density Distribution (attenuating material)</td>
</tr>
<tr>
<td>Data Tables (special operations)</td>
</tr>
<tr>
<td>Simulation options</td>
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<tr>
<td></td>
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</tbody>
</table>

### 3.2.2 Projections file

The SimSET output is normally in the form of a projections file, which contains several sets of sinograms depending on the selected options [Aguiar and Cot 2004]. The first block always contains unscattered trues and the others can have scatter photons in different configurations according to what is wanted to study (i.e. singles, doubles, multiples, scatter photons). How the sinograms are ordered within each block is shown schematically in Figure 3:1. In the first row, the first
sinogram has only LoRs contained in the first ring (direct sinogram), the second sinogram has LoRs between the first and second rings, the third sinogram has LoRs on the plane between the first and third rings, etc. Similarly, the first sinogram in the second row is not a direct sinogram; it has LoRs on the plane described between second ring and first ring. If there are 8 rings, for example, this is the ninth sinogram. We will find the direct sinogram of this row in position tenth (second sinogram in the second row) which corresponds to LoRs on the plane formed by the second ring.

\[
\begin{array}{cccc}
11 & 12 & 13 & 14 \\
21 & 22 & 23 & 24 \\
31 & 32 & 33 & 34 \\
41 & 42 & 43 & 44 \\
\end{array}
\]

Figure 3:1 Example of order of sonogram pairs in SimSET output format (4 rings scanner):

Where each “ij” element represents one sinogram which is formed by LoRs on the plane between \(i^{th}\) and \(j^{th}\) rings. When \(i=j\) direct sinograms and \(i\neq j\) indirect sinograms.

![Figure 3:2. The first row of sinograms in the scanner of eight rings.](image)

3.2.3 SimSET modules and parameters

The SimSET package includes three modules:

I) Collimator module:

It is very important in SPECT, but it is not used in PET.
II) Detector module:

It receives the photons either directly from the \textit{PHG} and it tracks photons through the specified detector.

In the current simulations, a simple case has been used. In this case, it doesn’t track photons when their energy \( E \) comes from the \textit{PHG} and the photons impact in detector, having the same energy \( E \). This means that the output value of detector module for the energy will depend on the energy resolution in that energy \( E \).

III) Binning module:

It is used to process the photons and the detection records. It can be used on-the-fly, but also after the simulation by processing a standard history file. The number of scatter bins can be chosen in order to have “trues” (non-scattered), singles, doubles… multiples, totals scattered events. It can show the results by energy bins in order to have photons separated for different energy values and it writes the characteristics of the sinogram, azimuthal angle bins, transaxial bins, axial bins, as well.

It is possible to simulate \textit{PET} patient studies and obtain the equivalent sinograms to compare them, in two different ways:

a) The user gives a value for \( \Delta t \) to obtain the desired number of detected events, as in the experimental acquisition, and simulate a study with a huge number of emitted photons such that the expectation would be estimated with null uncertainty. In order to reproduce the same noise as the experimental acquisition, the Poisson distribution should be sorted in each bin upon the known estimate of the expectation. In this way the CPU time will be quite long.

b) There is a stopping criterion in \textit{SimSET}, based on the variance of the simulated sinogram. When the expectation estimator of the variance is equal to the experimental sinogram the simulation stops.

Apart from the modules, a number of parameters describe the simulation of some physical effects\(^9\):

\(^9\) More information lies in the statistical files and “nohup” files.
I) Simulate stratification:
When it is used, the outcomes, which are more likely to result in a detected photon, are sampled more frequently. In order to use this feature, a previous simple simulation is needed first to be run, to generate a “productivity table”. This is a very important sampling technique.

II) Simulate forced detection:
When it is used, the scatter angle is forced to be in the direction of the detectors, and the photon weight is appropriately modified to avoid bias. This, as well, is a significant sampling technique.

III) Forced non absorption:
When it is used, modelling of photon interactions prevents absorption as an outcome the photon weight is appropriately modified to avoid bias.

IV) Adjust for positron range:
As already mentioned, before the annihilation, the positron travels some uneven distance. In order to make the simulation faster and simpler, it is possible not to simulate it.

V) Adjust for non-collinearity:
When the positron annihilates, as discussed in the chapter of positron physics, there is a slight possibility of generating two no-collinear photons. This effect, for the same reason as the previous, is possible not to be simulated.

VI) Minimum energy:
A useful parameter to decrease simulation time is the cut-off value. Photons whose energy drops below this value as a result of Compton interactions are discarded from the simulation.

VII) Random seed:
SimSET can use several seeds to create the random numbers. If this parameter is set to zero, SimSET will use a seed taken from the system clock.

VIII) Model coherent scatter:
In photon interaction with matter there is a possibility of coherent scatter, known as the Rayleigh effect. This can be modelled, as well.
In the present work, these parameters have been taken as shown in the Table 3:3. [Aguiar and Cot 2004]

Table 3:3 Parameters of the current Simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulate stratification</td>
<td>YES</td>
</tr>
<tr>
<td>Simulate forced detection</td>
<td>YES</td>
</tr>
<tr>
<td>Forced non absorption</td>
<td>YES</td>
</tr>
<tr>
<td>Adjust for positron range</td>
<td>NO</td>
</tr>
<tr>
<td>Adjust for no-co linearity</td>
<td>NO</td>
</tr>
<tr>
<td>Minimum energy</td>
<td>250keV</td>
</tr>
<tr>
<td>Random seed</td>
<td>0</td>
</tr>
<tr>
<td>Model coherent scatter</td>
<td>NO</td>
</tr>
</tbody>
</table>

3.3 SimSET detection energy efficiency

In the SimSET package the photons are computed one by one, that means:

(1) When a photon hits the target with energy $E$, this photon deposits energy $E_f$ (i.e. $E-E'$), where $E$ is the incident energy and $E'$ is the output energy. To estimate this, an energy photon tracking is needed inside of the detector, but in the current case, where a simple PET detector module has been used, it is not feasible.

(2) Having this $E_f = E-E'$ as energy value, SimSET computes if this photon will be inside of the window. This means if $E'$ is very high it will be difficult to detect that photon.
In the simulations used in this work, since we use a simple detector module, we need an efficiency probability distribution, which will give the possibility to detect a prompt photon of given energy \(E\). In SimSET, photons are tracked one by one, so what is needed is a probability function for the deposited energy \(E_f\). The simple detector module uses a Gaussian function with the photon energy \(E\) input as mean value and standard deviation, which depends on the Scintillation Detectors response [Aguiar and Cot 2004].

The detection efficiency corresponding to the above detection probability is obtained by integrating the detected energy \(E_f\) over all possible values and is thus given by the following combination of the error functions:

\[
\left( \operatorname{erf} \left( \frac{(HLD - E)}{\sqrt{2} \sigma} \right) - \operatorname{erf} \left( \frac{(LLD - E)}{\sqrt{2} \sigma} \right) \right) / 2 \quad \text{Eq. 3:2}
\]

Where,

\[
\sigma = \sqrt{E \cdot 511 \text{keV} \cdot FWHM (511 \text{keV}) / (2 \sqrt{2 \ln 2})} \quad \text{Eq. 3:3}
\]
For a given photon, SimSET then runs a random number from this Gaussian distribution to determine $E_f$. Then they check if the final energy value is inside of the energy window. In the Figure 3:4, for example, the blue (i.e. non-scattered) photon (Gaussian on the right) will almost always be detected because the tails are in the centre of the window, however, for the red photon (Gaussian on the middle), some random numbers will provide energy values out of the window.

![Figure 3:4 Detector Efficiency Windows](image)

Notice that when a scattered photon falls into the detector with energy less than the detector lower energy threshold ($LLD$), there is still a possibility to be detected (pink photon – Gaussian on the left) [Aguiar and Cot 2004].
Chapter 4. The Implementation of the Single Scatter Simulation Algorithm in STIR

4.1 Analytical Description of the SSS algorithm

The single scatter simulation algorithm, as briefly discussed in §2.5, attempts to estimate the single scatter distribution. The parameters on which the single scatter distribution depends are the emission and the attenuation images and the scanner.

Figure 4:1 Single Scatter Effect

The algorithm estimates the possibility $S_{AB}^{S}$ for the scatter occurring around scatter point $S$ to be detected by the detector pair $AB$ [Watson et al. 1996a]. This is then integrated over the whole volume $V_S$. 

46
\[
S_{AB} = \int_{\text{Scatter Volume}} dS \left\{ \frac{\sigma_{AS} \sigma_{BS}}{4\pi R_{AS}^2 R_{BS}^2} \right\} \left[ e_{AS}(E) e^{-\frac{s}{\int \mu(E,s)ds}} \int_{\Omega} \lambda(s) ds \frac{d\mu(E,S,\theta)}{d\Omega} e^{-\frac{s}{\int \mu(E',s)ds}} e_{BS}(E') \right] + e_{AS}(E') e^{-\frac{s}{\int \mu(E',s)ds}} \frac{d\mu(E,S,\theta)}{d\Omega} \int_{\Omega} \lambda(s) ds e^{-\frac{s}{\int \mu(E,s)ds}} e_{BS}(E) \]

Eq. 4:1

where,

\( \sigma_{XS} \) is the vertical area of the detector \( A \) \( X \) or \( B \) to the corresponding line \( XAS \) or \( BS \).

\( R_{XS} \) is the corresponding distance between the detector \( X \) and the scatter point.

\( E \) is the energy of the annihilation photon (i.e. 511keV).

\( E' \) is the energy after scatter at the \( S \).

\( \theta \) is the angle between the scatter point and the corresponding detectors.

\( \mu(E,s) \) is the attenuation value at the scatter point \( s \) of the attenuation image.

\( \lambda(s) \) is the emission distribution.

\( e_{XS}(E) \) is the detection efficiency at detector \( A \) of a photon of energy value \( E \), “coming” from the direction of the scatter point \( S \).

\( \frac{d\mu(E,S,\theta)}{d\Omega} \) is the probability for Compton scatter for the particular angle.

A single event is consisting of one Compton scatter effect \( (P_c = \frac{d\mu}{d\Omega}) \) in the patient and the detection point \( (P_{\text{det}}) \), in each of the two detectors \( (P_{\text{det}} = \frac{\sigma_{AS} \sigma_{BS} e_{AS}(E) e_{BS}(E')}{4\pi R_{AS}^2 R_{BS}^2}) \) The exponential integrals represent the probability of the gamma photon not having any other Compton interaction at all between the scatter point and the detector. The line integral \( \int_{S}^{X} \lambda ds \) represents the possibility of having positron annihilation along the \( SX \) line that joins the scatter point \( S \) and the detector \( X \).
The probability for Compton scatter can be computed as
\[
\frac{d\mu(E,s,\theta)}{d\Omega} = \frac{\mu(E,s)}{\sigma_c(E)} \frac{d\sigma_c(E,s,\theta)}{d\Omega}.
\] The energy after scatter, the \(\sigma_c\) and \(d\sigma_c/d\Omega\) are estimated given by the formulas, which are discussed in §1.5.1.

The integral goes over the location of each scatter point \(S\). Then it is calculated by the summation over all the selected scatter points:

\[
V_s \sum \Box = \int \Box dS
\]  
\text{Eq. 4:2}

\(V_s\) is the volume of the attenuation voxel size.

Doing the same for all the detector pairs, the single scatter sinogram is constructed.

To estimate all these parameters various calculations and approximations are taking place. To have reasonable computation time estimation, the emission and attenuation images are interpolated to larger voxel sizes in order to have less number of voxels. For the same reason, instead of taking all the detectors, just a few of them are selected. Then, the integral over all scatter locations is discretised by taking a single scatter point per voxel of the attenuation image, which is chosen either in the centre of the voxel or in a random position (see §4.3.1). The scatter point is selected only if the attenuation value of the particular voxel is above a given threshold. This is a way to speed up the process skipping many points, which have very slight possibility to create scatter.

Based on the attenuation and emission images, the Attenuation and Emission Integrals (\(\int_s \mu_{\text{det}}\), (\(\int_s \lambda_{\text{det}}\)) are estimated by the length of the line of intersection with the voxels. In order to speed up the process the integrals are estimated once, for each scatter point and detector, and are kept in memory.

Having computed the energy of the photon after its scatter according to Eq. 4:1 the attenuation value at the scattered energy is accurately calculated by the formula, which is based on the Eq. 1:12:

\[
\mu(E) = \mu(511\text{keV}) \frac{\sigma_c(E)}{\sigma_c(511\text{keV})}
\]  
\text{Eq. 4:3}
The detection efficiencies are estimated as in SimSET, shown analytically in the previous chapter, including an energy limit \( E_{\text{lim}} = LLD - 2\sigma \), accounting for more than the 95% of the prompting photons at the minimum accepted energy (LLD). This is just an approximation to the integral, to speed up the process. Moreover, the incident angle is taken into account, as it affects the efficiency, somehow. This is simply modelled at the moment by the: \( \varepsilon_{\text{ls}}(E) = \varepsilon_{\text{s}}(E) \cdot \cos \theta \).

The detection efficiencies in general depend not only on the detector efficiency but also on the direction from where the photon impinges on the detector. The notation in the \( Eq. \) 4:1 does not include that phenomenon. In the case of unscattered photons, this is a geometrical factor that depends on the relative location of the two detectors. These geometrical factors are generally determined in the normalisation process [Casey et al. 1995] and are usually given by the manufacturer. For the scatter, though, the geometric factor which would be used for the detector pair \( AB \) is not appropriate, as the photons come from different directions [Ollinger 1995]. Ollinger argues that it is best to exclude these geometric factors in the scatter simulation and apply them as normalisation factors after scatter subtraction. This is motivated by the fact that the scattered photons come from a ‘cone of response’, and the geometric factors could thus average out. However, in the current simulations it is not taken into account. This is left for further study.

**4.2 STIR-SSS characteristics**

Its logical diagram in APPENDIX I-III, describes the algorithm schematically. As shown, scatter points can be selected either in the centre of each voxel or randomly, depending on an input parameter. The lower and higher levels of discrimination (LLD and HLD) can be given as inputs. This is important not only because the window can be change at acquisition time by the user, but also to find the LLD energy deficit [Watson 1996b], which has been mentioned in section §2.5.2.

Finally, in order to have the correct scale between the scatter and the emission sinograms, the single scatter distribution is scaled (see §2.5.2 and §2.5.3). At this
moment an ad-hoc way is used to do this, but in the near future a mask function onto the emitted sinogram will be used. The scaling factor is supposed to be global or at least partially – global, i.e. global for each 2D sinogram [Watson et al. 2004a]

The current implementation is very flexible since it allows choosing different scanners and different sampling characteristics of those scanners, but also different attenuation and emission voxel sizes. After Due to the interpolation of the images and the scatter sinogram, the whole calculation can be speeded up, depending on the processing power\textsuperscript{10}, such that the simulation time is reasonably small (~min).

In comparison to the commercial approaches [Watson 2000; Wollenweber 2002] which are used for the CTI and GE scanners software, the current implementation gives the significant opportunity to choose among different schemes, depending on the processing power and some given time constraints. Not only the simplest sampling is finer than those used in the commercial implementations as shown in the table below, but it still allows fast scatter estimation.

<table>
<thead>
<tr>
<th>Sampling</th>
<th>Sinogram size</th>
<th>Attenuation Voxel size, mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTI</td>
<td>$17 \times 34 \times 8$</td>
<td>$22.5 \times 22.5 \times 22.5$</td>
</tr>
<tr>
<td>GE</td>
<td>Not Mentioned</td>
<td>$38 \times 22.2 \times 22.2$</td>
</tr>
<tr>
<td>STIR</td>
<td>$36 \times 36 \times 8$</td>
<td>$20 \times 20 \times 20$</td>
</tr>
</tbody>
</table>

### 4.3 Evaluation of the SSS implementation

Several approaches have been used to evaluate this implementation of the scatter estimation. All simulations have used the geometric characteristics of the ECAT EXACT HR\textsuperscript{+} (CPS Innovations, formerly CTI at Knoxville, Tennessee, USA). The energy resolution of the BGO crystals has been set to 25% at 511keV\textsuperscript{11}. Acquisitions and SimSET simulations were performed with a 350-650

---

\textsuperscript{10} The current implementation has taken place on an AMD Athlon MP 1900+ processor.

\textsuperscript{11} The resolution of BGO crystals is set to 22.5% in most of the rest SSS implementations. However, both this SSS and SimSET use 25%.
keV energy window. As mentioned (see 2.5.2 and 2.5.3), the use of a slightly larger energy window in the SSS simulation in order to investigate if this energy deficit should be taken into account. The notation SSS is used for a 350-650 keV energy window and W-SSS for a 320-650 keV energy window.

4.3.1 Comparing different SSS Schemes profiles

Firstly, three simulations were performed for several voxel sizes and detector samplings. A point (simulation A), a line (130 mm length, simulation B) and a cylinder (130 mm length, 100mm radius, simulation C) sources have been put separately in the centre of a cylinder phantom (130 mm length, 100mm radius) filled with water in the centre of the FoV have been simulated.

![Simulation Schemes](image)

In the current implementation the detector sampling characteristics are based on the ECAT EXACT HR$^+$ scanner and are given as an input viewgram template in the executable file (APPENDIX I). Four different schemes have been used to investigate how the scatter estimate depends on the detector sampling and what the capabilities are of the algorithm (Table 4:2). The voxel sizes for both the emission and the attenuation image have been chosen roughly of the same size as the distance between the detectors. For the case where the voxel size is very small compared to the spacing between the detectors, problems occurred that the simulation could miss the isolated sources, and hence return zero scatter. This effect can be explained by the fact that our implementation uses ray tracing between the centre of the detectors and the scatter points. The detector sampling characteristics, the attenuation and the activity image voxel sampling are described at tables below, respectively.
Moreover, using two different ways to find the scatter points has performed simulation A. The first method positions the scatter points in the centre of the selected attenuation voxels. The second method introduces a random displacement as in [Watson et al. 1996a], where it was introduced in order to reduce artefacts occurring at particular detector pairs. Simulations B and C were only performed with the random displacement. For the Simulation B, due to symmetry, it is expected to have the same profile in each angle. So, we have used a Figure of Merit (FoM) given by the relative standard deviation error over all views through the centre of a 2D sinogram. Indeed, as shown in the table below all the schemes have reasonably small relative standard deviation errors.

### Table 4:4 Relative std. error over all views through the centre of a 2D sinogram for Simulation B

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Scatter points</th>
<th>Rel. Std. Dev. (%) for B</th>
</tr>
</thead>
<tbody>
<tr>
<td>I - direct</td>
<td>712</td>
<td>3.20</td>
</tr>
<tr>
<td>II - direct</td>
<td>2331</td>
<td>2.77</td>
</tr>
<tr>
<td>III-direct</td>
<td>1157</td>
<td>3.32</td>
</tr>
<tr>
<td>IV-direct</td>
<td>4329</td>
<td>2.83</td>
</tr>
<tr>
<td>IV–indirect</td>
<td>4329</td>
<td>2.76</td>
</tr>
</tbody>
</table>
Figure 4:3. Profiles for Schemes I – IV along radial direction, through a single view of a direct sinogram, for simulation A, without having randomly positioned the scatter points.

Figure 4:4. Profiles for Schemes I – IV along axial direction, through a single view of a direct viewgram, for simulation A, without having randomly positioned the scatter points.
Figure 4.5. Profiles for Schemes I – IV along radial direction, through a single view of a direct sinogram, for simulation A, using randomly positioned scatter points.

Figure 4.6. Profiles for Schemes I – IV along axial direction, through a single view of a direct sinogram, for simulation A, using randomly positioned scatter points.
Figure 4:7. Direct Sinograms for Scheme IV, (a) with each scatter points positioned in the center of the voxel and (b) with each scatter point randomly positioned in the voxel.

Figure 4:8. Profiles for Schemes I – IV along radial direction, through a single view of a direct sinogram, for simulation C, using randomly positioned scatter points.
As shown in these results, the change of the voxel size and the detector sampling does not affect, mostly, the shape of the scatter distribution, but has a strong influence on the computational time. This is fortunate as the simulation using the Schemes I and III is quite fast (Table 4:2). However, for more complicated attenuation distribution we expect to have better results when using finer sampling. In Figure 4:4 and in 4:5 we notice that the finer the sampling is (Schemes III and IV), the smoother the distribution seems to be. In Figure 4:6 – 4:7, it is clear that there is a discretisation artefact, which is spread-out when placing the scatter points in a random way in the attenuation voxel. In the simulation C, (i.e. Figure 4:8 and 4:9) all the schemes give almost the same distribution, which seems also to be quite smooth, both in radial and axial directions. This shows that for larger objects, the randomly positioned scatter points practically remove the discretisation error.

The simulation of an oblique scatter profile is not plotted since, in these simple cases, it is almost the same as the direct profile [Wollenweber 2002; Tsoumpas et al. 2004a; Watson et al. 2004a], but in non symmetric cases (e.g. whole body imaging) this should be tested more extensively, in order to notice if the indirect
sinogram information gives any further significant information for the scatter distribution.

4.3.2 Comparing SSS to SimSET profiles using experimental data

For the second evaluation, which is based on data acquired during the acceptance tests of the scanner, the results of the simulation B are compared, to single scatter data generated by the SimSET M-C simulation package. The same detection model in the SSS implementation and in SimSET has been used in order to validate our implementation, even though it might not be very accurate. For the comparison, only the simplest sampling (Scheme I) has been used, as all sampling schemes resulted in very similar results in the previous simulations. The SimSET package parameters have been discussed in a previous chapter.

The reason we performed this test is that M-C eliminates any unknown physical parameter from the comparison, such as the exact distribution of the radioactivity and attenuation, and the dependency of the detection efficiencies on photon energy or direction. So, the results of SSS and SimSET should be very close, aside from discretisation artefacts and noise in the M-C simulation.

To reduce the significant statistical noise of the SimSET data, we have performed simulations using the same sinogram characteristics as the SSS simulation. We compare our simulations to the single and the total scattered photons distribution, for the line source lying at radial positions 0 and 8 cm. Comparing profiles, after the appropriate global scaling, we have the following figures.
The two figures above show excellent agreement between our estimation of the single scatter probabilities and SimSET simulation for single scatter. The total scatter distribution is, as expected, wider than the single scatter, but lowering the energy threshold somewhat overcomes this problem. Watson et al., though, argue...
that single and total scatter should have roughly the same shape, which seems not to be correct, looking at these results. Particularly in the figure below, where the SSS profile is scaled in order to show the difference in shapes. Note that although Watson also uses a lower limit for the energy window, this is done to model deficiencies in the electronics [Watson 1996b], see also § 2.5.2.

![Graph showing profiles of SSS and SimSET Total Scatter Simulation (Scheme I) scaled to the same maximum value, along radial direction, through the first single view of the central direct sinogram, for simulation B, based on the acquired experimental data for the line source at ~0mm.](image)

4.3.3 Comparing SSS to Measured Sinogram profiles

The third evaluation test of our code is based on experimental data. The data have been acquired on an ECAT EXACT HR\(^+\) scanner as part of the scanner acceptance tests [NEMA 1994]. A 20cm diameter cylinder filled with water aside from 3 holes (parallel to the cylinder axis) at radial positions at about 0, 4 and 8 cm from the centre was positioned in the scanner. A Ge line source (diameter ~2mm) was inserted into one of the holes and a 3D PET scan was performed with an energy window of 350-650 keV. A calculated attenuation was used for the simulation, and we determined the position of the line source by a fit of a cylinder of 2mm diameter to the reconstructed image. The simulation has been performed with Scheme I, since it is the closer approximation to what ECAT 7.1 uses [Watson et al. 1997; Watson 2000]. The original energy window has been used
(SSS), but also the wider energy window of 320-650 keV ($W$-SSS), as ECAT 7.1 uses. Then, we compare profiles along radial direction for the vertical view of the simulation and the completely normalised measured sinogram, averaged over 40 (out of 63) central sinograms. We have scaled the simulations to the data such that the mean values of the profiles, ignoring the peak of unscattered photons, are the same.

Figure 4:13. Profiles along radial direction for vertical view of the simulation (Scheme I), for SSS, $W$-SSS and completely normalised measured sinogram, for line source at ~0 mm. The y-axis is scaled such that the maximum in the measured data corresponds to 1.

Figure 4:14. Profiles along radial direction for vertical view of the simulation (Scheme I), for SSS, $W$-SSS and completely normalized measured sinogram, for line source at ~80 mm. The y-axis is scaled such that the maximum in the measured data corresponds to 1.
The SSS simulation shows reasonable agreement with the measured data, as shown in the two figures above. The estimated single scatter distribution is too narrow, which is to be expected as only single scatter photons are taken into account. This causes the scaling to compensate and increase the estimated scatter too much. This problem is less severe for objects with more distributed activity. As expected, $W$-SSS has better agreement than SSS. Unfortunately, these results cannot be used to decide if $W$-SSS performs well because it corresponds more to the ‘real’ energy window [Watson 1996b] or because it provides an ad-hoc way to take multiple scatters into account. As can be noticed, in the Figure 4:14, there is an overestimation of the scatter at around -15cm of the plot. This is under of investigation and one possible reason might be the rough approximation of the detector efficiencies [Ollinger 1995] as discussed in section 4.1.

4.4 Conclusion

The SSS algorithm has been implemented in the STIR library [Tsoumpas et al. 2004a; Tsoumpas et al. 2004b]. The discretisation artefact has been investigated and it seems that it does not affect in the scatter distribution, when the source has not too small size. The current implementation has the advantage of the flexible choice of the voxel sizes for the emission, attenuation image and the detector sampling characteristics, as well. This is important, since computational power is increasing, giving the opportunity of using even finer schemes. $W$-SSS has been introduced as an ad-hoc way to allow “artificially” detection of events of lower energy and hence larger scatter angle, such as the multiple photons. The evaluation tests, so far, have shown fine agreement both with Monte Carlo simulations and with experimental data, especially in the case of $W$-SSS, but not so well if the scaled SSS is directly compared to the total scatter profile as shown in the Figure 4:12. Moreover, the SimSET total scatter distribution has been compared to the $W$-SSS, as shown in the Figure 4:10-11, showing that it can represent the total scatter component, somehow, but not quite satisfactory.
All these are generating the challenging issue of finding an even better approximation than the SSS in order to have a better estimate of the scatter component. So, this is the topic of the next chapter.
Chapter 5. Investigating the Multiple Scatter Simulation

5.1 Need for a better total scatter approximation

It is clear that the single scatter simulation is just an attempt to approximate the total Compton scatter effect. It is physically possible that both photons scatter, and potentially more than once. These events are called multiple scatters. As shown by the SimSET simulations in the previous chapter, but also in other M-C simulations [Adam L. E. et al. 1999], the shape of the single scatter distribution can be different to the total scatter distribution. How close this approximation could be depends on how much multiple scattered photons would have been detected, which depends on the energy resolution of the detectors and the used energy window of detection. The multiple scatter is more likely to happen if the attenuation medium has a large volume, and hence more in PET studies of the torso than of the head. Multiple scatters broaden the scatter distribution. Several ad-hoc methods have been proposed to take the multiple scatters into account, which have been extensively discussed in §2.3. All of these methods indeed broaden the SSS estimate, but the computation has no physical grounds. Consequently, these methods are likely to break down for complicated activity and / or attenuation distributions.

In this chapter, we extend the methodology used in the single scatter simulation algorithm to handle double scattered events. This approach is, to our knowledge, completely new. A preliminary evaluation of this algorithm is presented, as well.
5.2 Implementation of the Double Scatter Simulation

Double scatter is defined by the case of two scatter events per coincidence. That means that either one-gamma photon scatters twice, or there is one single scatter event for each photon of the pair, as shown in the figure below.

![Diagram of double scatter](image)

Figure 5.1 Cases of Double Scatter

The double scatter distribution for the detector pair AB can be computed in a similar way to the single scatter result (equation below):

\[
S_{2}^{AB} = \int_{Volume} ds_{1}ds_{2} \left\{ \frac{\sigma_{AS_1}\sigma_{BS_2}}{4\pi R_{AS_1}R_{BS_2}} \right\} \\
\quad \cdot \left\{ e_{AS_1}(E) e^{-\int_{s_1} \mu(E,s_1) ds_1} \int_{\Omega} \frac{d\mu(E,S_1,\theta_{AB})}{d\Omega} e^{-\int_{s_2} \mu(E,s_2) ds_2} \int_{\Omega} \frac{d\mu(E,S_2,\theta_{AB})}{d\Omega} \right\}
\]

\[
e^{\int_{s_1} \mu(E,s_1) ds_1} \int_{\Omega} \frac{d\mu(E,S_1,\theta_{AB})}{d\Omega} e^{\int_{s_2} \mu(E,s_2) ds_2} \int_{\Omega} \frac{d\mu(E,S_2,\theta_{AB})}{d\Omega} \}
\]

Where,

\( \sigma \) is the vertical area of the detector A or B to the corresponding line \( AS_1 \) or \( BS_2 \);

\( R \) is the corresponding distance between the detector (A or B) and the scatter point \( S_1 \) or \( S_2 \);

\( R_{AS} \) is the corresponding distance between the detector \( X \) and the scatter point \( S \).
$E$ is the energy of the annihilation photon (i.e. 511keV)

$E_1, \ E_2$ are the energies after scatter at $S_1$ and $S_2$, correspondingly.

$E_{12}, \ E_{21}$ are the energies after scatter at $S_1$ and then $S_2$ and after scatter at the $S_2$ and then $S_1$, correspondingly.

$\theta_{21A}, \ \theta_{12B}$ are the angles when scatter first happens at $S_2$ and then at $S_1$ and opposite.

$\mu(E,S,\theta)$ is the attenuation value at a scatter point $S$.

$\frac{d\mu(E,S,\theta)}{d\Omega}$ is the probability for Compton scatter for the particular angle $\theta$.

$\lambda(s)$ is the emission distribution.

$\varepsilon_{sA}(E)$ is the detection efficiency at detector $A$ of a photon of energy value $E$, coming from the direction scatter point $S$.

The integral goes over the location of each scatter point $S^{12}$

The scattered energy, the attenuation at that energy and the $\sigma_c$ and $d\sigma_c/d\Omega$ are estimated by the same formulas, as in the SSS, on the fly. The same discretisation approach for the integrals over the scatter locations can be used as in the SSS case.

The whole estimation is much more expensive in computation time, but is nevertheless feasible by saving all the integrals (note that only the integrals between 2 scatter points are new). In addition, a lower energy limit is used, which corresponds to a maximum angle of scatter, below which the detection probability is very small (less than 5% in the simulations below). This maximum scatter angle allows us to skip much useless estimation.

---

$^{12}$ The integrals go over the location of each scatter points $S_1, \ S_2$. Then, they are calculated by a summation over the summation of all the selected scatter points:

$$V_S^2 \sum \sum = \int \int dS_1 dS_2 \quad \text{Eq. 5.1a}$$

$V_S$ is the volume of the attenuation voxel size.
5.3 Evaluation of the Double Scatter Simulation

In order to investigate if the double scatter algorithm can give the expected result, this implementation has been tested using the simplest scheme of detector and attenuation / emission image sampling (Scheme I, Table 5:1).

The same simulations have been used as for the evaluation of the Single Scatter Simulation. In the Figure 5:4 – 5:5 the simulation A is examined without using random scatter points. The estimated single and double scatter distribution and their sum are plotted, either for the axial or for the radial profiles. Then, the double scatter is scaled and compared to the single one, to have the same average, in order to show the difference between the two shapes. In the Figure 5:6 and 5:7, the simulation A is examined by using random scatter points. Finally, radial and axial profiles from the simulation C are plotted in the Figure 5:10 – 11.

Figure 5:2 Single and Double Scatter profiles for scheme I along radial direction, through a single view of a direct sinogram, for simulation A, with scatter points at the centre of the voxels.
Figure 5.3. Single and Double Scatter radial scaled profiles for scheme I, through a single view of a direct sinogram, for simulation A, without having randomly positioned the scatter points.

Figure 5.4. Single and Double Scatter profiles for scheme I along axial direction, through a single view of a direct sinogram, for simulation A, without having randomly positioned the scatter points.
Figure 5:5. Single and Double Scatter scaled axial profiles for scheme I, through a single view of a direct sinogram, for simulation A, without having randomly positioned the scatter points.

Figure 5:6. Single and Double Scatter profiles for scheme I along radial direction, through a single view of a direct sinogram, for simulation A, having randomly positioned the scatter points.
Figure 5.7. Single and Double Scatter scaled profiles for scheme I along radial direction, through a single view of a direct sinogram, for simulation A, having randomly positioned the scatter points.

Figure 5.8. Single and Double Scatter radial profiles for scheme I, through a single view of a direct sinogram, for simulation C, having randomly positioned the scatter points.
Figure 5.9: Single and Double Scatter scaled radial profiles for scheme I, through a single view of a direct sinogram, for simulation C, without having randomly positioned the scatter points.

Figure 5.10: Single and Double Scatter profiles for scheme I along axial direction, through a single view of a direct sinogram, for simulation C, without having randomly positioned the scatter points.
Figure 5: Single and Double Scatter scaled axial profiles for scheme I, through a single view of a direct sinogram, for simulation C, without having randomly positioned the scatter points.

As can be easily noticed in all these profiles, the double scatter distribution has, as expected, a wider shape. Moreover, the ratio between the single and double scatter estimates seems to be quite reasonable, but this and the double scatter distribution have not been investigated, yet, using SimSET. However, in the case of the cylinder, the single scatter and double scatter have almost the same shape, as Watson et al. supports. The simulation is too slow for the simulation C but not so slow for the simulations A and B (table below). As it is estimated the Total Single to Total Double Scatter ratio is small for the simulations A and B but high for the case of the simulation C.

<table>
<thead>
<tr>
<th>Scheme 1 / Simulation</th>
<th>Sinogram size</th>
<th>Attenuation / Activity Voxel, mm³</th>
<th>Single / Double Scatter</th>
<th>DSS Time, min</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>36×36×8</td>
<td>20×20×20</td>
<td>14.16%</td>
<td>59.4</td>
</tr>
<tr>
<td>B</td>
<td></td>
<td></td>
<td>14.57%</td>
<td>67.8</td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
<td>27.47%</td>
<td>111.3</td>
</tr>
</tbody>
</table>

Table 5:1. Attenuation/Emission Scanner Sampling Characteristics (Scheme I)
5.4 Incorporating the Multiple Scatter Simulation (MSS)

Since single and double scatter work reasonably well, it is logical to argue that multiple scatter could work as well. How could it be feasible? It is not too difficult to see that it can be implemented as a kind of iterating steps using the already calculated integrals and recalculating the energy and the other parameters depending on it. The \( n^{th} \) level of scatter can be estimated by the equation 5:2:

\[
S_n^{4B} = \int \ldots \int d^n S \left( \frac{\sigma_{AS} \sigma_{BS_n} \left( I_n^{4S} + I_n^{4S_2} + \ldots + I_n^{4S_n} + I_n^{4S_{B_n}} \right)}{4\pi R_{AS}^2 R_{BS_n}^2} \right)
\]

Eq. 5:2\(^{14}\)

Where:

\[
I_n^{4S} = e_{AS_n}(E) e^{-\int \frac{\mu(E,\theta,\phi) dS}{\lambda}} \left\{ \frac{d\mu(E,\theta,\phi)}{d\Omega} e^{-\int \frac{\mu(E,\theta,\phi) d\theta}{d\Omega}} \right\} \]

\[
\ldots \left\{ \frac{d\mu(E_{i-1,\theta_{i-1},\phi_{i-1}})}{d\Omega} e^{-\int \frac{\mu(E_{i-1,\theta_{i-1},\phi_{i-1}}) d\theta_{i-1}}{d\Omega}} \right\} \left\{ \frac{d\mu(E,\theta,\phi)}{d\Omega} e^{-\int \frac{\mu(E,\theta,\phi) d\theta}{d\Omega}} \right\} e^{-\int \frac{\mu(E,\theta,\phi) d\theta}{d\Omega}} e_{BS_n}(E)
\]

Equation 5:4

\(^{13}\) The term “Total” corresponds to the total single (or double) scatter probability and is estimated by adding all the values of the single (or double) scatter distribution.

\(^{14}\) The integrals go over the location of each scatter points \( S_1, S_2 \). Then, they are calculated by a summation over the summation of all the selected scatter points:

\[
V_3 \sum \sum \sum \ldots = \int \ldots \int dS_1 dS_2 \ldots dS_n \quad \text{Eq. 5:2a}
\]

\( V_3 \) is the volume of the attenuation voxel size.
\[ I_{n}^{S_{,\theta}} = e_{\lambda S_{1}}(E_{n,1})e^{-\frac{\mu(E_{n,1},\theta)}{d\Omega}} \left( \frac{d\mu(E_{n,1},S_{1},\theta_{1,1,1})}{d\Omega} \right) \]

\[ \cdots \left( \frac{d\mu(E_{n,n,1},S_{n,1},\theta_{n,1,1,1})}{d\Omega} \right) e^{-\frac{\mu(E_{n,1},\theta)}{d\Omega}} \int_{S_{n}}^{S_{1}} \lambda(s) ds e^{-\frac{\mu(E_{n,1},\theta)}{d\Omega}} e_{\lambda S_{1}}(E_{n,1}) \]

\[ I_{n}^{S_{,\theta}} = e_{\lambda S_{1}}(E_{n,1})e^{-\frac{\mu(E_{n,1},\theta)}{d\Omega}} \frac{d\mu(E_{n,1},S_{1},\theta_{1,1,1})}{d\Omega} \]

\[ \cdots \frac{d\mu(E_{n,n,1},S_{n,1},\theta_{n,1,1,1})}{d\Omega} e^{-\frac{\mu(E_{n,1},\theta)}{d\Omega}} \int_{S_{n}}^{S_{1}} \lambda(s) ds e^{-\frac{\mu(E_{n,1},\theta)}{d\Omega}} e_{\lambda S_{1}}(E_{n,1}) \]

where the integer \( k \) travels over the scatter points.

### 5.5 Integration to a full Model Based Scatter Simulation (MBSS)

A recursive scheme is not too difficult to be implemented by using an \( n^{th} \)-level class template in STIR software, which will correspond to the \( n^{th} \) level scatter and then the calculation will be based on a recursive method of the scatter class.

The \( (n-1)^{th} \) level of scatter is given by just substituting the \( n \) by \( n-1 \), at the equation 5:2:

\[ S_{n-1}^{\lambda S_{1}} = \left( \frac{\sigma_{\lambda S_{1}} \sigma_{\lambda S_{1}} \left( I_{n-1}^{S_{1}} + I_{n-1}^{S_{1}} + \cdots + I_{n-1}^{S_{1}} + I_{n-1}^{S_{1}} \right)}{4\pi R_{1}^{2} R_{2}^{2}} \right) \]

\[ I_{n-1}^{S_{,\theta}} = e_{\lambda S_{1}}(E_{n-1,1})e^{-\frac{\mu(E_{n-1,1},\theta)}{d\Omega}} \frac{d\mu(E_{n-1,1},S_{1},\theta_{1,1,1})}{d\Omega} \]

\[ \cdots \frac{d\mu(E_{n,n-1,1},S_{n-1,1},\theta_{n-1,1,1,1})}{d\Omega} e^{-\frac{\mu(E_{n-1,1},\theta)}{d\Omega}} \int_{S_{n-1}}^{S_{1}} \lambda(s) ds e^{-\frac{\mu(E_{n-1,1},\theta)}{d\Omega}} e_{\lambda S_{1}}(E_{n-1,1}) \]

\[ \cdots \frac{d\mu(E_{n,n-1,1},S_{n-1,1},\theta_{n-1,1,1,1})}{d\Omega} e^{-\frac{\mu(E_{n-1,1},\theta)}{d\Omega}} \int_{S_{n-1}}^{S_{1}} \lambda(s) ds e^{-\frac{\mu(E_{n-1,1},\theta)}{d\Omega}} e_{\lambda S_{1}}(E_{n-1,1}) \]
\[
\int_{s_n} I_{n+1}^a = \left( -\frac{\partial^2}{\partial s_{n+1}} \right) \int_{s_{n-1}}^b \lambda(s) ds \cdot e^{\int_{s_{n-1}}^b \frac{-\nu_1}{\nu_{E_{22}}(s)} ds} - \frac{\partial^2}{\partial s_{n+1}} \int_{s_{n-1}}^b \lambda(s) ds \cdot e^{\int_{s_{n-1}}^b \frac{-\nu_1}{\nu_{E_{22}}(s)} ds} \right) \int_{s_n} \frac{d\mu(E_{n-1}, S_{n-2}, \theta_{n-1}, \theta_{n-2})}{d\Omega} d\Omega \quad \text{Eq. 5:9}
\]

where \( E' \) is the scattered energy, from the \( S_n \) to \( S_{n-1} \) scatter point.

\[
I_{n}^a(E) = I_{n+1}^a(E') \quad \text{Eq. 5:9}
\]

\[
S_{n}^{AB} = \int_{S} d^n S \left\{ \frac{\sigma_{4S} \sigma_{SR} \sigma_{RS_{n-1}} \left( I_{n}^{4S} + I_{n}^{S_{n-1}} + \cdots + I_{n}^{S_{n}} \right) }{4\pi R_{AB}^2 R_{BS_{n}}^2} \right\} \quad \Leftrightarrow
\]

\[
S_{n}^{AB}(E) = \int_{S} d^n S \sigma_{AB} \sigma_{BS_{n}} \sigma_{RS_{n-1}} \left( I_{n}^{4S}(E') + I_{n}^{S_{n-1}}(E') + \cdots + I_{n}^{S_{n}}(E') \right) \quad \Leftrightarrow
\]

\[
S_{n}^{AB}(E) = S_{n-1}^{AB}(E') \cdot \int_{S} d^n S \sigma_{BS_{n-1}}^2 \sigma_{RS_{n}}^2 + \int_{S} d^n S \sigma_{AB} \sigma_{BS_{n}} \sigma_{SR} \sigma_{RS_{n-1}} \left( I_{n}^{S_{n}}(E') + I_{n}^{S_{n}}(E') - I_{n}^{S_{n}}(E') \right) \quad \text{Eq 5:10}
\]
Actually, all of them have been calculated (i.e. equations 5.1 – 5.9) and potentially, cached. The only difference is the energy\textsuperscript{15}, which actually introduces only some multiplication factors.

The MBSS is consisting of the following infinite summation:

$$S_{\text{total}}^{4B} = \sum_{n=1}^{\infty} S_n^{4B}$$  \hspace{1cm} Eq. 5.11

The whole algorithm can be built in a recursive function and the simulation can be speed up perceptibly.

### 5.6 Difficulties and Limitations of the MBSS

#### 5.6.1 Multiple scatter in a single voxel

The proposed method has some limitations and some difficulties that have to be resolved. It has to be mentioned, that the discretisation approximation, that is to say the scatter caused by a voxel is proportional to the scatter caused by a single point in the voxel, breaks down for double scatters when the voxels are close to each other. In these cases the algorithm seems to be strongly depended on the selection of the scatter points, especially if they are very few. Moreover, there is a possibility of more than one scatter in one particular voxel, since so far the approximation takes into account only a single scatter in each voxel. This causes an underestimation of the multiple scatter events, since it is quite possible to happen twice or more in a voxel, especially with size of 8cm\textsuperscript{3}. This should be sorted out by multiplying with a factor $f_i$ each voxel, which will depend on the attenuation coefficient, $f(\mu)$. However, it is expected that the contribution of these terms is almost negligible.

---

\textsuperscript{15} In the case $n > 2$. For the case of double scatter, the new integrals between the scatter points have to be computed just once and then are stored.
5.6.2 Time Constraints

All the integrals over the emission and attenuation distributions are already cached by using the single and double scatter approach. Nevertheless, the whole procedure is expected to be very slow. On the other hand it is expected one can use a smaller number of scatter point combinations when an \( n^{th} \) - level of scatter is computed. This is feasible by using a maximum scatter angle (i.e. a lower energy limit for detection) reducing the number of scatter combinations significantly. So, it is a matter of investigation how many scatter point combinations are needed.

At present, even the DSS, as shown, has very slow computational time which can be easily improved by using an even smaller detector and scatter point sampling, reducing time in a way to be used directly in the reconstruction algorithms.

Actually, the only new parameter that needs to be estimated each time is the scattered energy after every Compton interaction. Look-up tables for the efficiencies and attenuation values at the particular energies perhaps can speed up the whole procedure and make it faster.

The whole algorithm could be organized such that a grid of computers or even a cluster can be used to do many calculations in order to run some simulations and evaluate the proposed MBSS algorithm.

5.6.3 Scaling Factor

So far, all the profiles have been scaled in order to compare to simulated or measured data. In effect, we have compared the shape and not the values. It is needed to have a robust scale factor, which should give the correct value of single, double, and multiple scatter, comparing to a Monte Carlo technique. It would be also very interesting to change the algorithm, in order to obtain a sinogram of non-scatter \( S_0 \) (i.e. simulation of the true events). Then, using the ratios of total scatter \( S_{0, tot}/S_{1,tot}/S_{2,tot}/\cdots \) it should be feasible to scale to the true events directly each scatter sinogram, and therefore no one particular scale factor would be expected.
anymore. On the other hand, it might be needed to use a scale factor for the $n+1$ multiple scatter level and as it is discussed on the following chapter, to take the $SoFoV$, somehow, into account.
Chapter 6. Future Work – Conclusive Comments

6.1 Improving the Scatter Correction

As can be noticed in the polar plot at Figure 1:4, the most probable angle of a scattered photon between its original direction is 0°. However, scatter of very small angles (~0°) will not introduce wrong spatial information after detection, and hence could be excluded from the scatter sinogram. In that case, we would retain more counts without actually reducing the resolution. This might be quite useful in the case of sparser detector sampling. This effect is expected to be even more visible in the cases of the double and multiple scatter simulations and could be used to speed up the calculation, as well.

6.2 Scatter out of the Field of View (SoFoV)

The proposed MBSS (Model Based Scatter Simulation) should be able to give a very good estimation of the scattered events if the complete activity and the attenuation distribution are known. However, except in whole body imaging, this is never the case. SoFoV cannot adequately be addressed by any model based scatter estimation approach.

This can be overcome with various approaches such as:

- Short acquisition of neighbouring regions (using bed movement). This can be done in a short period of time, as the quality of the data need not be very high to obtain reasonable scatter estimates.

- Modelling of the neighbouring regions based on population data. For instance, for tracers with high uptake in the liver, the liver might be
modelled as a uniform region so it could be taken into account even if only a part of the liver is imaged.

- Hybrid scatter methods such as Ferreira’s [Ferreira et al. 2002] but then combined with a more accurate method than SSS (Single Scatter Simulation).
- Scatter tail fitting such as used in [Watson et al. 1996a] where it is suggested that this can work to account for out of SoFoV scatter. See also [Spinks et al. 1998].

6.3 Integration with the reconstruction algorithms

Since the scatter sinogram is estimated, the scatter correction may still be applied either pre- or post-reconstruction [Watson 2000]. Usually, the scatter correction is applied pre-reconstruction by subtracting the estimated scatter sinogram, from the measured data, prior to attenuation correction and reconstruction. However, as long as the reconstruction operator \( R \) is linear, FBP (filtered back-projection) for example, then it is strictly mathematically equivalent to separately reconstruct the measured total uncorrected image \( A \), and the estimated scatter image \( A_s \), using the same multiplicative attenuation correction factors, \( a \), and normalization factors, \( n \), and then subtract these two images:

\[
R[an(S - S_o)] = R(anS) - R(anS_o) = A - A_s \tag{6.1}
\]

One advantage to the image-space subtraction alternative is that it does not require access to the measured data, making it more modular and applicable in cases where the measured data no longer exist\(^\text{16}\).

On the other hand, most of the currently popular iterative reconstruction algorithms are non-linear, and they generally apply pre-reconstruction scatter correction. In these cases, is suggested that a typical OSEM algorithm suggests that pre- and post-reconstruction scatter correction do produce very similar results in this case [Watson 2000]. However, a third and theoretically more correct alternative is to include the scatter estimate as part of the forward model in maximum likelihood [Shepp and

\(^{16}\) However, Watson maybe has suggested this because he thought he did not need tail fitting anymore.
Vardi 1982; Hudson and Larkin 1994] or Bayesian [Green 1990] type reconstruction algorithms, and a variation of the SSS algorithm has to be adapted to this purpose [Werling et al. 2002; Wollenweber 2002; Poenisch 2003].

Prior to the integration into the reconstruction algorithm, or to subtract the scatter estimate from the measured data, the scatter sinogram needs to be interpolated to the same size as the emission data. To do this one of the already known interpolation techniques needs to be implemented. The linear interpolation seems to cause some artifacts, when used with a sampling with a small number of detectors [Accorsi et al. 2002], which disappear when the cubic interpolation is used [Werling et al. 2002; Accorsi et al. 2004]. However, b-splines might be an interesting alternative [Kybic et al. 2000], which has not been used so far.

### 6.4 Development of a scatter correction technique for transmission images

Since the scatter estimation algorithm is evaluated and seems to work quite satisfactory, the next step is to investigate if it can work as well in the transmission image. The main difference will be that instead of the positron annihilation into two photons, there is only one photon beam. It is, then, of main importance to consider the acquisition type. This is usually a rotating source, a positron annihilator or single photon emitter such as $^{137}$Cs, and the source can be collimated or not collimated. Taking this into account, instead of the activity concentration a scatter component can be constructed, based on a rough estimation of the attenuation sinogram in the first simulation. Then, the same process should be repeated iteratively, using the corrected attenuation sinogram, in each of the iteration steps. This will give a final attenuation sinogram or transmission image, which will be used into the emission Model-Based Scatter Simulation.

In the case of a transmission image based on a Computerized Tomography (CT) acquisition, though, this might be more difficult, since the produced X-rays have lower energy, which means that the photoelectric and Rayleigh effects are more severe, especially for the scattered photons.
6.5 Evaluations Based on Phantoms using fully 3D acquisitions

So far, only simple simulations based on point, line and cylinder sources have been evaluated. The intention is to evaluate the whole algorithm in order to ensure it works for more complicated phantoms as well, before including it into patient studies. The Hoffman, Zubal and Utah phantoms will be used to test the scatter correction accuracy, not only using SimSET Monte Carlo simulations, but also GATE [Jan et al. 2004] and of course real acquisition tests. These tests will take place, not only in the ECAT EXACT HR⁺ scanner, but also in the ECAT EXACT HR++. The latter is a PET prototype, which has no septa, meaning that the acquisition is only in 3D mode. The main difference to the HR⁺ is that it has 48 rings instead of 32, which is promising for better quality of the reconstruction images. Apparently, accurate scatter correction has not been yet feasible in all cases, not only due to the insufficient scatter correction, but primary due to the low quality of the transmission images, on which the algorithm is strongly depended. Here, though, the MBSS or even the SSS for the attenuation could become a valuable tool.

6.6 Concluding Comments

This work discussed a new implementation of the SSS algorithm and explored extending the algorithm to take multiple scatters into account. The current implementation of the scatter estimation algorithm has been designed to be as flexible as possible (e.g. in the choice of the voxel sizes for the emission, attenuation image and the detector sampling characteristics, but also in the scanner characteristics). This is important in a research context to be able to use it in a variety of context, and to optimise the algorithm for particular situations. Also, since computational power is increasing, it gives the opportunity of using finer sampling schemes to improve the accuracy of the simulation.

Applying the single scatter simulation algorithm in the ECAT EXACT HR⁺, the scatter estimation produces reasonable results comparing to Monte Carlo simulations and some experimental data. To be able to take multiple scatter into account, we studied an ad-hoc way of lowering the energy threshold during the simulation (W-SSS
for “Wide energy window SSS”), but it should be tested further for more complicated cases to define the most accurate Lower Level Discriminator (LLD).

An alternative method for handling multiple scatters has been proposed in this work. The Double Scatter Simulation (DSS) was proposed and has been implemented. Preliminary evaluations have shown quite reasonable behavior compared to experiments, although there are some computation time difficulties, but potential solutions have been proposed. Then, the idea of MBSS has been introduced which can in principle compute scatters of any order, giving the spark to do more evaluations based on simulated and experimental data as well.

So far, experience shows that the scatter correction problem is really complicated and difficult. There are numerous topics where further improvement is possible. As discussed, the performance of a particular scatter correction scheme is strongly depended on the specific scanner and its hardware, meaning that for each scanner one among several scatter approaches might be the best. Considering the many problems and complications that arise with the scatter in 3D PET, the most promising approach seems to be a Monte-Carlo (M-C) based correction algorithm which could be used within an iterative reconstruction algorithm, replacing the forward projection. However, clinical application requires fast and practical data processing, which motivates continued investigation of simpler correction algorithms. It remains to be seen if MBSS will be able to provide a bridge between SSS and full M-C methods. It is the intention of the General Electric Healthcare who owns Hammersmith Imanet Limited, where the most part of this thesis has taken place, to patent this invention as soon as possible, in order to be able to use it in the commercial scanners.

The SSS implementation will be integrated into analytic and iterative reconstruction algorithms available in STIR\textsuperscript{17} and will then be included in STIR under the Lesser GNU Public License. So, the main part of this work will be freely available to the PET community.

\textsuperscript{17} Further details can be found at STIR website: http://www.stir.irls.org (12/2004).
APPENDIX I

I-I STIR SOFTWARE [Thielemans 2004c]

STIR (Software for Tomographic Image Reconstruction) is Open Source software (written in C++) consisting of classes, functions and utilities for 3D PET image reconstruction, although it is general enough to accommodate other imaging modalities\textsuperscript{18} [Labbé et al. 1999; Labbé et al. 1999]

STIR consists of two parts:

(i) Library providing building blocks for image and projection data manipulation; and

(ii) Image reconstruction algorithms.

Applications using this library including basic image manipulations file format conversions and of course image reconstructions. The library has been designed so that it can be used for many different algorithms and scanner geometries. The library contains classes and functions to run parts of the reconstruction in parallel on distributed memory architectures, although these are not distributed yet. This will enable the software to be run not only on single processors, but also on massively parallel computers, or on clusters of workstations.

STIR is portable on all systems supporting the GNU C++ compiler or MS Visual C++ (or hopefully any ANSI C++ compliant compiler). The library is fully documented. The object-oriented features make this library very modular and flexible. This means that it is relatively easy to add new algorithms, filters, projectors or even a different type of image discretisation. It is even possible to select at run-time which version of these components you want to use.

The software is freely available for downloading under the GNU LGPL (the library) or GNU GPL (the applications) license. It is the hope of the collaborators of the STIR project that other researchers in the PET community will use this library for their own work, extending it and

\textsuperscript{18} Further details can be found at STIR website: http://www.stir.irsl.org (12/2004).
making their work available as well. In its current status, the software is mainly a research tool. It is probably not yet friendly enough to use in a clinical setting.

I-II A bit more detail on the library [Thielemans 2004b]

The STIR software library uses the object-oriented features of C++:

- Self-contained objects hide implementation details from the user (encapsulation);
- Specialisation of concepts is implemented with hierarchies of classes (inheritance);
- Conceptually identical operations are implemented using functions with identical names (polymorphism).

The building block classes included in this library are as follows:

- Information about the data (scanner characteristics, study type, algorithm type, etc.);
- Multi-dimensional arrays (any dimension) with various operations, including numeric manipulations;
- Reading and writing (I/O) data in Interfile format (for which a 3D PET extension is proposed), reading of GE Advance sinogram data, limited reading and writing of ECAT6 and ECAT7 and conversion between ECAT6 and Interfile;
- Classes of projection data (complete data set, segments, sinograms, viewgrams) and images (2D and 3D);
- various filter transfer functions (1D, 2D and 3D);
- Forward projection and back-projection operators;
- Classes for sparse projection matrices, both for on-the-fly computation and pre-stored trimming and zooming utilities on projection and image data;
- Classes for iterative reconstruction algorithms;
- Stream-based classes for message passing between different processes, built on top of PVM (Parallel Virtual Machine) or EPX (the native library provided with Parsytec CC systems)
I-III Scatter Simulation – Logical Diagram [Tsoumpas 2004c]

- Scatter Buildblock
- Scatter Inline

**INPUT:**
- Reconstructed Image
- Attenuation Map
- Sinogram Template
- Scatter Sinogram Name
- Attenuation Threshold
- Lower & Upper Energy
- Use Random Points (?)
- Use of cache (?)
- Single (1) or Double (2) ?

**Scatter** (EXECUTABLE)

- Estimate Scatter from all Scatter Points
  - 1 or 2
- Estimate Scatter from one/two Scatter Points
- Create Scatter Viewgram
- Write statistics
- Sample Scatter Point
- Random Points

**Differential and Total Cross Section**
**Detection Efficiency**

**Cache Factors (1 and 2)**

**No Cache**
**Cache**

- 1 or 2
- Scatter Point to Detector Integrals
- Emission and Attenuation
I-IV Header File

/*!
\file Scatter.h
\ingroup scatter
\brief A collection of functions to measure the scatter component
\author Charalampos Tsoumpas
\author Kris Thielemans
\author Pablo Aguiar
$Date: 2004/11/03 17:41:57 $
$Revision: 1.14 $
*/

#include "stir/VoxelsOnCartesianGrid.h"
#include "stir/DiscretisedDensityOnCartesianGrid.h"
#include "stir/round.h"
#include "stir/ProjData.h"
#include <vector>
#include <cmath>

START_NAMESPACE_STIR

const double Qe = 1.602E-19;
const double Me = 9.109E-31;
const double C = 2.997E8;
const double Re = 2.818E-13;
enum image_type{act_image_type, att_image_type};
template <class coordT> class CartesianCoordinate3D;
class ProjDataInfoCylindricalNoArcCorr;
struct ScatterPoint
{
   CartesianCoordinate3D<float> coord;
   float mu_value;
};
extern std::vector< ScatterPoint> scatt_points_vector;
extern std::vector<CartesianCoordinate3D<float> > detection_points_vector;
extern int total_detectors;

void sample_scatter_points(
   const DiscretisedDensityOnCartesianGrid<3,float>& attenuation_map,
   int & scatt_points, const float att_threshold, const bool random);

//@{
86
float detection_efficiency(const float low, const float high, const float energy, const float reference_energy, const float resolution);

float detection_efficiency_BGO(const float low, const float high, const float energy);

float integral_scattpoint_det(const DiscretisedDensityOnCartesianGrid<3,float>& discretised_image, const CartesianCoordinate3D<float>& scatter_point, const CartesianCoordinate3D<float>& detector_coord);

float cached_factors(const DiscretisedDensityOnCartesianGrid<3,float>& discretised_image, const unsigned scatter_point_num, const unsigned det_num, const image_type input_image_type);

float cached_factors_2(const DiscretisedDensityOnCartesianGrid<3,float>& discretised_image, const unsigned scatter_point_1_num, const unsigned scatter_point_2_num, const image_type input_image_type);

float scatter_estimate_for_one_scatter_point(const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, const std::size_t scatter_point_num, const unsigned det_num_A, const unsigned det_num_B, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache);

double scatter_estimate_for_two_scatter_points(const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, const std::size_t scatter_point_1_num, const std::size_t scatter_point_2_num, const unsigned det_num_A, const unsigned det_num_B, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache);

float scatter_estimate_for_all_scatter_points(const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, const unsigned det_num_A, const unsigned det_num_B, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache, const int scatter_level);

float dif_cross_section_511keV(const float cos_theta);

float dif_cross_section(const float cos_theta, float energy);

float dif_cross_section(const CartesianCoordinate3D<float>& scatter_point, const CartesianCoordinate3D<float>& detector_coordA, const CartesianCoordinate3D<float>& detector_coordB, const float energy);

float dif_cross_section(const float cos_theta, const float energy, const CartesianCoordinate3D<float>& scatter_point, const CartesianCoordinate3D<float>& detector_coordA, const CartesianCoordinate3D<float>& detector_coordB, const float energy, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache, const int scatter_level);

float scattering_estimate_for_one_scattering_point(const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, const std::size_t scatter_point_num, const unsigned det_num_A, const unsigned det_num_B, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache);

double scattering_estimate_for_two_scattering_points(const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, const std::size_t scatter_point_1_num, const std::size_t scatter_point_2_num, const unsigned det_num_A, const unsigned det_num_B, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache);

float scattering_estimate_for_all_scattering_points(const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, const unsigned det_num_A, const unsigned det_num_B, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache, const int scatter_level);

float scatting_estimate_for_all_scattering_points(const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, const unsigned det_num_A, const unsigned det_num_B, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache, const int scatter_level);
float diff_cross_section_511keV(const CartesianCoordinate3D<float>& scatter_point, const CartesianCoordinate3D<float>& detector_coordA, const CartesianCoordinate3D<float>& detector_coordB);
/**
\ingroup scatter
\brief computes the total cross section
This function computes the total cross section for Compton scatter, based on the
inline float total_cross_section(float energy);
inline float energy_after_scatter_511keV(const float cos_theta);
inline float total_cross_section_relative_to_511keV(const float energy);
*/
//@
/*! \ingroup scatter
\brief lower accepting limit of the energy and corresponding scattering angle to speed up the process.
These functions return the limit of the Detected Energy or its scattering angle in order to speed up the simulation. It is set at approx*sigma lower than the lower energy threshold (low). This means that we keep the 95.45% of the distribution integral.
*/
//@
inline float max_cos_angle(const float low, const float approx, const float resolution);
inline float max_cos_angle_BGO(const float low, const float approx);
inline float energy_lower_limit(const float low, const float approx, const float resolution);
inline float energy_lower_limit_BGO(const float low, const float approx);
//@
/*! \ingroup scatter
\brief uses the given proj_data writes the scatter viewgram */
void scatter_viewgram(ProjData& proj_data, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_activity, const DiscretisedDensityOnCartesianGrid<3,float>& image_as_density, int& scatt_points, const float att_threshold, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache, const int scatter_level, const bool random);
#endif
/* !\ingroup scatter
\brief Temporary implementation of the error function for Visual C++
*/
extern "C" double erf(const double x);
#endif /* !\ingroup scatter
\brief Temporary implementation of writing log information
The log information is written in the statistics.txt file */
//@
void writing_log(const DiscretisedDensityOnCartesianGrid<3,float>& activity_image, const DiscretisedDensityOnCartesianGrid<3,float>& density_image, const ProjDataInfoCylindricalNoArcCorr * proj_data_info_ptr, const float given_attenuation_threshold, const int total_scatt_points, const int total_scatt_points, const float lower_energy_threshold, const float upper_energy_threshold, const bool use_cosphi, const bool use_cache, const bool random, const int simulation_time, const int scatt_points_vector_size, const int scatter_level, const float total_scatter);
//@
// Temporary Function that could be in the BasicCoordinate Class
template<int num_dimensions>
inline BasicCoordinate<num_dimensions,float> convert_int_to_float(const BasicCoordinate<num_dimensions,int>& cint);
END_NAMESPACE_STIR
#include "local/stir/Scatter.inl"
**APPENDIX II**

**II-I Abbreviations**

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACD</td>
<td>Annihilation Coincident Detection</td>
</tr>
<tr>
<td>BGO</td>
<td>Bismuth germinate (Bi$_2$Ge$<em>3$O$</em>{12}$)</td>
</tr>
<tr>
<td>CT</td>
<td>Computerised tomography</td>
</tr>
<tr>
<td>ECAT</td>
<td>Emission Computed Axial Tomograph</td>
</tr>
<tr>
<td>ET</td>
<td>Emission Tomography</td>
</tr>
<tr>
<td>DSS</td>
<td>Double Scatter Simulation Algorithm</td>
</tr>
<tr>
<td>FBP</td>
<td>Filter back projection</td>
</tr>
<tr>
<td>FDG</td>
<td>$^{18}$F – fluorodeoxyglucose</td>
</tr>
<tr>
<td>FoM</td>
<td>Figure of Merit</td>
</tr>
<tr>
<td>FORE</td>
<td>Fourier Rebinning</td>
</tr>
<tr>
<td>FoV</td>
<td>Field of View</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full Width at Half Maximum</td>
</tr>
<tr>
<td>GE</td>
<td>General Electric</td>
</tr>
<tr>
<td>(L)GPL</td>
<td>(Lesser) General Public License</td>
</tr>
<tr>
<td>GNU</td>
<td>GNU not Unix</td>
</tr>
<tr>
<td>LLD (HLD)</td>
<td>Lower (Higher) Limit of Discrimination</td>
</tr>
<tr>
<td>LoR</td>
<td>Line of response</td>
</tr>
<tr>
<td>MBSS</td>
<td>Model Based Scatter Simulation</td>
</tr>
<tr>
<td>M-C</td>
<td>Monte Carlo Technique</td>
</tr>
<tr>
<td>ML-EM</td>
<td>Maximum Likelihood – Expectation Maximisation</td>
</tr>
<tr>
<td>MRI</td>
<td>Magnetic Resonance Imaging</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td><strong>MSS</strong></td>
<td>Multiple Scatter Simulation</td>
</tr>
<tr>
<td><strong>MWPC</strong></td>
<td>multi-wire proportional chambers</td>
</tr>
<tr>
<td><strong>NEMA</strong></td>
<td>National Electrical Manufacturers Association</td>
</tr>
<tr>
<td><strong>Ortho-Ps</strong></td>
<td>Ortho-Positronium</td>
</tr>
<tr>
<td><strong>OSEM</strong></td>
<td>Ordered Subset Expectation Maximisation</td>
</tr>
<tr>
<td><strong>Para-Ps</strong></td>
<td>Para-Positronium</td>
</tr>
<tr>
<td><strong>PET</strong></td>
<td>Positron Emission Tomography</td>
</tr>
<tr>
<td><strong>PETT</strong></td>
<td>Positron Emission Transaxial Tomography</td>
</tr>
<tr>
<td><strong>PDF</strong></td>
<td>Probability Density Function</td>
</tr>
<tr>
<td><strong>PHG</strong></td>
<td>Photon History Generator</td>
</tr>
<tr>
<td><strong>PMT</strong></td>
<td>Photo Multiplier Tube</td>
</tr>
<tr>
<td><strong>PSF</strong></td>
<td>Point Spread Function</td>
</tr>
<tr>
<td><strong>SimSET</strong></td>
<td>Simulation System for Emission Tomograph</td>
</tr>
<tr>
<td><strong>SoFoV</strong></td>
<td>Scatter from activity out of the Field of View</td>
</tr>
<tr>
<td><strong>SPE(C)/T</strong></td>
<td>Single Photon Emission (Computed) Tomography</td>
</tr>
<tr>
<td><strong>SSS</strong></td>
<td>Single Scatter Simulation Algorithm</td>
</tr>
<tr>
<td><strong>STIR</strong></td>
<td>Software for Tomographic Image Reconstruction</td>
</tr>
<tr>
<td><strong>ToF</strong></td>
<td>Time of Flight scanners</td>
</tr>
<tr>
<td><strong>W-SSS</strong></td>
<td>Wider (energy widow) Single Scatter Simulation Algorithm</td>
</tr>
</tbody>
</table>
BASICS

Geometry
A cylindrical geometry has been chosen to describe positron tomographs made of a number of adjacent detector rings and reconstructed image volumes. The geometry supports consequently two principal directions axially along the scanner cylinder and transaxially perpendicular to the cylinder axis.

Scanner
Geometrically associated to the cylindrical volume defined by the inner dimensions of the positron tomograph.

Detector ring
Geometrically associated to the cylindrical volume defined by the dimensions of a detector ring. Note that because currently the Depth of Interaction is not taken into account, the ring radius in the building blocks is ~1 cm larger than the actual ring radius (corresponding to the average depth of interaction for BGO).

Detector
Sometimes called detector crystal. Geometrically associated to the inner face of a detector element. The scanner is then considered as a tessellation of detectors constructing adjacent rings.

LoR (Line of Response)
Line joining the centres of two detectors. Ignoring scatter, attenuation and other physical effects, the average number of coincidences observed between two detectors can be estimated as the line integral of the tracer distribution along the LoR. This does not take the finite width of the Tube of Response (ToR) into account, nor scatter within the detectors. It can be shown that this line integral approximation works best for LoRs that do not run parallel to edges within the object. We say that the projector that uses this model is a ray-tracing projector.

ToR
Tube joining two detectors.
**Sinogram**
Set of bins corresponding to 1 segment and 1 axial position. Before axial compression, this corresponds to LoRs in a detector ring (direct sinogram) or between two different detector rings (oblique sinogram). For a scanner of n detector rings, there are n direct sinograms and \( n^2 - 1 \) oblique sinograms for a total of \( n^2 \) sinograms. With axial compression, the number of direct sinograms is \( 2n-1 \). Conventionally, the view angle in an oblique sinograms runs only over 180°, meaning that only half of the detectors in each ring are covered. The other half corresponds to the sinogram in the opposite segment (with minus the average ring difference).

**View**
The azimuthal angle of an LoR (ignoring interleaving)

**Bin**
A single element in a sinogram, completely specified by its segment, axial position, view and tangential position.

**Ring difference**
Number of rings between two rings associated to a sinogram. If ring \( A \) and ring \( B \) are the ring numbers, the ring difference is given by ring \( B - ring A \). Thus there can be positive and negative ring differences.

The (average) ring difference of a direct sinogram is zero.

**Michelogram**
Representations of sinograms on a square grid in order to take into account the indirect sinograms, as well.

**Segment**
Set of merged sinograms with a common average ring difference.

**Viewgram**
Set of equal azimuth merged LoRs of a segment.

**FoV**
Geometrically associated to the volume for which there is at least 1 bin with non-zero detection probability. In many cases, the term is also used for the smaller volume for which there is at least 1 bin with non-zero detection probability for every view. The latter FoV is usually cylindrical.
Septa

Inter–plane lead shields used for slice separation.

Image slice

Geometrically associated to a cylindrical volume defined by a slice of the FoV. By convention, a slice is half the width of a ring. For a scanner of $n$ detector rings, there are $2n-1$ image slices.

Direct plane

Image slice centred on a ring. For a scanner of $n$ detector rings, there are $n$ direct planes. Two direct planes centered on the first and last rings are the ends the FoV.

Cross plane

Image slice in between two consecutive direct planes. Direct planes are adjacent to cross planes. For a scanner of $n$ detector rings, there are $2n-1$ cross planes.

Wobble

A movement of the centre of the detector array about a small circle in order to improve the spatial sampling.

DIFFERENT DATA COMPRESSIONS USED IN PET

Trimming

Reduction of the number of bins in tangential direction without changing the size of bins.Trimming is a type of bin truncation.

Angular compression

Reduction of the number of views by a multiple of two. As an example, doing a mashing of 2 means that pairs of views have been added 2 by 2 to form only one view.

Axial compression

Reduction of the number of sinograms at different ring. Span is a number used by CPS to say how much axial compression has been used. It is always an odd number. Higher span, more axial compression. Span 1 means no axial compression. Note that the GE Advance uses mixed data, where segment 0 has span 3, while other segments have span 1.
APPENDIX III

III-1 Gaussian Function

In one dimension, the Gaussian function\(^{19}\) is the probability function of the normal distribution, sometimes also called the frequency curve.

\[
f(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}
\]

The full width at half maximum (FWHM) for a Gaussian is found by the half-maximum points \(x_o\). The constant scaling factor can be ignored, so we must solve:

\[
e^{-\frac{(x_0-\mu)^2}{2\sigma^2}} = \frac{1}{2} f(x_{\text{max}})
\]

But, \(f(x_{\text{max}})\) occurs at \(x_{\text{max}} = \mu\), so:

\[
e^{-\frac{(x_0-\mu)^2}{2\sigma^2}} = \frac{1}{2} f(x_{\text{max}}) = \frac{1}{2}
\]

Solving,

\[
e^{-\frac{(x_0-\mu)^2}{2\sigma^2}} = 0.5 \Leftrightarrow (x_0 - \mu)^2 / 2\sigma^2 = -\ln 2 \Leftrightarrow (x_0 - \mu)^2 = 2\sigma^2 \ln 2 \Leftrightarrow x_0 = \pm \sigma \sqrt{2\ln 2} + \mu
\]

The FWHM therefore given by: \(FWHM \equiv x_+ - x_- = 2\sqrt{2\ln 2}\sigma \approx 2.3548\sigma\)

\(^{19}\) For more details see in the website: \(http://mathworld.wolfram.com/\)
**III-II Error Function**

$erf(z)$ is the “error function”\(^{20}\) encountered in integrating the normal distribution (which is a normalized form of the Gaussian function). It is an entire function defined by:

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_{0}^{z} e^{-t^2} dt$$

Note that some authors define $erf(z)$ without the leading factor of $2/\sqrt{\pi}$

\(^{20}\) For more details see in the website: [http://mathworld.wolfram.com/](http://mathworld.wolfram.com/)
BIBLIOGRAPHY