CTmod - Mathematical Foundations

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Chapter 1

Introduction

1.1 Foreword

1.2 Intent of this report

CTmod is a set of C++ class libraries primarily designed for the simulation of energy imparted to a CT-scanner detector array using the Monte Carlo method. This report describes mathematical methods and formulas that are used in the code. It is a supplement to the article “CTmod - a toolkit for Monte Carlo simulation of projections including scatter in computed tomography” by A. Malusek, M. Sandborg, and G. Alm Carlsson.

1.3 Notation

In this report, random variables are denoted by a hat. For instance \( \hat{x} \) is a random variable and \( x \) is its sample. Points in space are denoted by bold capital letters, e.g. \( \mathbf{P} \). Directions are denoted by bold small letters, e.g. \( \mathbf{u} \). Inconsistencies in the current notation will be corrected in the next update of this report.

1.4 Revision history

2007-07-06 First version presented on the web.

2007-10-09 Small typographical changes. Corrected a typing error in (3.177). Added timing comparison for photon sources, section 3.3.8.
Chapter 2

General principles

2.1 Sampling of random variables

Computer libraries provide functions which return random numbers from the interval $(0, 1)$. Mathematically speaking, they sample a random variable $\hat{\gamma} \sim R(0, 1)$. The following sections show how to use these samples to obtain random variables with known distributions. Both direct sampling methods and acceptance-rejection methods are discussed.

2.1.1 Direct sampling

Proposition 1 in this section shows how to transform a random variable $\hat{\gamma} \sim R(0, 1)$ into a random variable $\hat{x}$ with a known cumulative distribution function $F(x)$. Proposition 2 then shows, how to transform a pair of independent random variables $\hat{\gamma}_1, \hat{\gamma}_2 \sim R(0, 1)$ into a pair of random variables $\hat{x}, \hat{y}$ with the cumulative distribution function $F(x, y)$.

One variable

Proposition 1: Let $f(x) > 0$ and $F(x)$, where $a < x < b$, be the probability density function and cumulative density function of a random variable with a continuous distribution $D$. Then the random variable $\hat{x}$ defined as

$$\hat{x} \equiv F^{-1}(\hat{\gamma}), \quad (2.1)$$

where $\hat{\gamma} \sim R(0, 1)$, has the $D$ distribution.

Proof: Let $F_x(x)$ be the cumulative distribution function of $\hat{x}$. Since $x = F^{-1}(\gamma)$ and $\hat{\gamma} = F(\hat{x})$, we get

$$F_x(x) = \Pr(\hat{x} < x) = \Pr(\hat{x} < F^{-1}(\gamma)) = \Pr(F(\hat{x}) < \gamma) = \Pr(\hat{\gamma} < \gamma) \quad (2.2)$$

$$= \gamma = F(F^{-1}(\gamma)) = F(x) \quad (2.3)$$

□
Two variables

**Proposition 2:** Let \( f(x, y) > 0 \) and \( F(x, y) \) be the probability density function and cumulative density function of random variables with a continuous distribution \( D \). Let the random variables \( \hat{x} \) and \( \hat{y} \) be defined as

\[
\hat{y} \equiv F_y^{-1}(\infty, \hat{\gamma}_1),
\]

(2.4)

where \( \hat{\gamma}_1 \sim R(0, 1) \), and

\[
\hat{x} \equiv G_y^{-1}(\hat{\gamma}_2),
\]

(2.5)

where \( \hat{\gamma}_2 \sim R(0, 1) \). Here, \( G_y^{-1}(\hat{\gamma}_2) \) is the inverse function of

\[
G_y(x) = \int_{-\infty}^{x} f(u, y) \, du \int_{-\infty}^{\infty} f(u, y) \, du
\]

(2.6)

Then \( \hat{x} \) and \( \hat{y} \) have the distribution \( D \).

**Proof:** The transformation between random variables \( (\hat{x}, \hat{y}) \) and \( (\hat{\gamma}_1, \hat{\gamma}_2) \) is defined via the following formulas

\[
\gamma_1 = F(\infty, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{y} f(u, v) \, dv \, du
\]

(2.7)

\[
\gamma_2 = G_y(x) = \int_{-\infty}^{x} f(u, y) \, du \int_{-\infty}^{\infty} f(u, y) \, du
\]

(2.8)

According to [7], the joint probability density function \( f'(\gamma_1, \gamma_2) \) can be calculated as

\[
f'(\gamma_1, \gamma_2) = f(x, y)|J(x, y)|^{-1},
\]

(2.9)

where the \( 2 \times 2 \) determinant \( J(x, y) \) is

\[
J(x, y) = \begin{vmatrix}
\frac{\partial \gamma_1}{\partial x} & \frac{\partial \gamma_1}{\partial y} \\
\frac{\partial \gamma_2}{\partial x} & \frac{\partial \gamma_2}{\partial y}
\end{vmatrix} = \begin{vmatrix}
0 & \int_{-\infty}^{\infty} f(u, y) \, du \\
\int_{-\infty}^{\infty} f(u, y) \, du & 0
\end{vmatrix} = -f(x, y)
\]

(2.10)

Inserting (2.10) into (2.9) and realizing that \( f(x, y) > 0 \), we get

\[
f'(\gamma_1, \gamma_2) = f(x, y)| - f(x, y)|^{-1} = 1
\]

(2.11)

The joint distribution function \( f'(\gamma_1, \gamma_2) \) corresponds to independent \( \hat{\gamma}_1 \) and \( \hat{\gamma}_2 \) from \( R(0, 1) \). Since we assume the inverse transformation exist, \( \hat{\gamma}_1, \hat{\gamma}_2 \sim R(0, 1) \) will produce \( (\hat{x}, \hat{y}) \) with the joint probability distribution function \( f(x, y) \). \( \square \)
2.1.2 Acceptance-rejection method

The basic acceptance-rejection method is described in proposition 1. In practice, a combination of composition and rejection methods is very useful, this combined method is described in proposition 2.

**Proposition 1:** Let \( f(x) \), where \( a \leq x \leq b \) be a probability density function and let \( f_{\text{max}} = \max\{f(x)\} \). If \( \hat{x} \) is sampled according to the following recipe, then \( f(x) \) is its probability density function.

1. Sample \( \gamma_1, \gamma_2 \)

\[ \gamma_1 \leftarrow R(a,b), \quad \gamma_2 \leftarrow R(0,1) \] (2.12)

2. If \( \gamma_2 f_{\text{max}} < f(x) \) then \( \hat{x} \leftarrow \gamma_2 \). Otherwise go to step 1.

**Proof:** See xx

**Proposition 2:** Suppose \( f \) and \( f_i \) are probability density functions, \( \alpha_i \) are positive real numbers, and \( g_i(x) \in [0,1] \). Sample \( \hat{x} \) as follows:

1. Pick \( \gamma_1 \) and let \( i \) be such that

\[ \sum_{j=1}^{i-1} \alpha_j < \gamma_1 \sum_{j=1}^{n} \alpha_j \leq \sum_{j=1}^{n} \alpha_j. \] (2.13)

2. Pick \( x \) from \( f_i(x) \), possibly by solving

\[ \int_{-\infty}^{x} f_i(x) \, dx = \gamma_2 \] (2.14)

3. Pick \( \gamma_3 \). Terminate the algorithm and accept value of \( x \) if

\[ \gamma_3 < g_i(x). \] (2.15)

4. Otherwise, go back to step 1.

As a result, \( \hat{x} \) has the probability density function

\[ f(x) = \sum_{i=1}^{n} \alpha_i f_i(x) g_i(x) \] (2.16)

2.2 Coordinate system transformations

Let \( S = (O, e_1, e_2, e_3) \) be a coordinate system in a three dimensional affine space [4] with the origin \( O \) and the orthonormal base \( E = (e_1, e_2, e_3) \). Let \((P)_S\) denote the three dimensional column matrix of coordinates of the point \( P \) in the coordinate system \( S \) and let \((u)_E\) denote the three dimensional column matrix of coordinates of the direction \( u \) in the base \( E \). The distinction between points and directions (also called free vectors) is made to emphasize their coordinates are transformed in different ways.
2.2.1 Transformation of directions

Let $\mathcal{E}^i = (e^i_1, e^i_2, e^i_3)$ and $\mathcal{E}^j = (e^j_1, e^j_2, e^j_3)$ be bases of coordinate systems $\mathcal{S}^i$ and $\mathcal{S}^j$, respectively. Coordinates of a vector $\mathbf{u}$ in the base $\mathcal{E}^i$ are

$$ (\mathbf{u})_{\mathcal{E}^i} = (e^i_1\mathbf{u}, e^i_2\mathbf{u}, e^i_3\mathbf{u})^T, $$

(2.17)

where $e^i_k \mathbf{u}$ is the scalar product of vectors $e^i_k$ and $\mathbf{u}$, the symbol $T$ denotes the transposition of the row matrix. The vector $\mathbf{u}$ can be written as a linear combination of vectors from the base $\mathcal{E}^i$ as

$$ \mathbf{u} = \sum_{k=1}^{3} (e^i_k \mathbf{u}) e^i_k. $$

(2.18)

**Proposition 1:** Coordinates of a vector $\mathbf{u}$ in a base $\mathcal{E}^i$ can be calculated from its coordinates in a base $\mathcal{E}^j$ as

$$ (\mathbf{u})_{\mathcal{E}^i} = R^{i\rightarrow j} (\mathbf{u})_{\mathcal{E}^j}, $$

(2.19)

where the transformation (rotation) matrix, $R^{j\rightarrow i}$, is

$$ R^{j\rightarrow i} = \begin{pmatrix} e^i_1 e^j_1 & e^i_1 e^j_2 & e^i_1 e^j_3 \\ e^i_2 e^j_1 & e^i_2 e^j_2 & e^i_2 e^j_3 \\ e^i_3 e^j_1 & e^i_3 e^j_2 & e^i_3 e^j_3 \end{pmatrix}. $$

(2.20)

**Proof:** According to (2.18), vectors $e^i_m$, $m = 1, \ldots, 3$, from the base $\mathcal{E}^i$ can be written as superpositions of vectors from the base $\mathcal{E}^j$ as

$$ e^i_m = \sum_{k=1}^{3} (e^j_k e^i_m) e^j_k. $$

(2.21)

Using (2.17), (2.21), and simple algebraic manipulation, we get

$$ (\mathbf{u})_{\mathcal{E}^i} = \begin{pmatrix} e^i_1 \mathbf{u} \\ e^i_2 \mathbf{u} \\ e^i_3 \mathbf{u} \end{pmatrix} = \begin{pmatrix} \sum_{k=1}^{3} (e^j_k e^i_1) e^j_k \mathbf{u} \\ \sum_{k=1}^{3} (e^j_k e^i_2) e^j_k \mathbf{u} \\ \sum_{k=1}^{3} (e^j_k e^i_3) e^j_k \mathbf{u} \end{pmatrix} = R^{j\rightarrow i} (\mathbf{u})_{\mathcal{E}^j}, $$

(2.22)

(2.23)

Columns of the matrix $R^{j\rightarrow i}$ contain coordinates of base vectors of the base $\mathcal{E}^j$ in the base $\mathcal{E}^i$. Since the scalar product is commutative, $R^{i\rightarrow j} = (R^{j\rightarrow i})^T$. The matrix $R^{i\rightarrow j}$ is unitary and $(R^{i\rightarrow j})^{-1} = (R^{j\rightarrow i})^T$, see [xx].
2.2.2 Transformation of positions

A point \( \mathbf{P} \) can be expressed via its coordinates \( p_k^j \) in a coordinate system \( S^j \) as

\[
\mathbf{P} = \mathbf{O}^j + \sum_{k=1}^{3} p_k^j \mathbf{e}_k^j,
\]

(2.24)

Coordinates of the point \( \mathbf{P} \) in the system \( S^i \) are

\[
(\mathbf{P})_{S^i} = (p_1^i, p_2^i, p_3^i)^T = (e_1^i(\mathbf{P} - \mathbf{O}^i), e_2^i(\mathbf{P} - \mathbf{O}^i), e_3^i(\mathbf{P} - \mathbf{O}^i))^T.
\]

(2.25)

**Proposition 1:** The coordinates of a point \( \mathbf{P} \) in a system \( S^i \) can be calculated from its coordinates in a system \( S^j \) as

\[
(\mathbf{P})_{S^i} = T^{j \rightarrow i} \mathbf{P}_{S^j} + R^{j \rightarrow i} (\mathbf{P})_{S^j},
\]

(2.26)

where \( R^{j \rightarrow i} \) is the rotation matrix

\[
R^{j \rightarrow i} = \begin{pmatrix}
    e_1^j & e_1^j & e_1^j \\
    e_2^j & e_2^j & e_2^j \\
    e_3^j & e_3^j & e_3^j 
\end{pmatrix}
\]

(2.27)

and \( T^{j \rightarrow i} \) is the translation matrix

\[
T^{j \rightarrow i} = (e_1^i(\mathbf{O}^j - \mathbf{O}^i), e_2^i(\mathbf{O}^j - \mathbf{O}^i), e_3^i(\mathbf{O}^j - \mathbf{O}^i))^T.
\]

(2.28)

**Proof:** Using (2.25) and simple algebraic manipulation, we get

\[
(\mathbf{P})_{S^i} = \begin{pmatrix} p_1^i \\ p_2^i \\ p_3^i \end{pmatrix} = \begin{pmatrix} e_1^i(\mathbf{P} - \mathbf{O}^i) \\ e_2^i(\mathbf{P} - \mathbf{O}^i) \\ e_3^i(\mathbf{P} - \mathbf{O}^i) \end{pmatrix} = \begin{pmatrix} e_1^i(\mathbf{O}^j - \mathbf{O}^i) + \sum_{k=1}^{3} (e_1^k e_1^j) e_k^j(\mathbf{P} - \mathbf{O}^j) \\ e_2^i(\mathbf{O}^j - \mathbf{O}^i) + \sum_{k=1}^{3} (e_2^k e_2^j) e_k^j(\mathbf{P} - \mathbf{O}^j) \\ e_3^i(\mathbf{O}^j - \mathbf{O}^i) + \sum_{k=1}^{3} (e_3^k e_3^j) e_k^j(\mathbf{P} - \mathbf{O}^j) \end{pmatrix} = T^{j \rightarrow i} \mathbf{P}_{S^j} + R^{j \rightarrow i} (\mathbf{P})_{S^j}.
\]

(2.29)

(2.30)

(2.31)

\[\square\]

Note that the rotation matrices \( R^{j \rightarrow i} \) defined in (2.20) for directions and in (2.27) for positions are the same.

2.2.3 Rotation matrices

**Proposition 1:** Let \( \mathbf{n} \) be a unit vector and let the matrix \( R(\mathbf{n}, \alpha) \), where \( \alpha \) is an angle, be defined as

\[
R(\mathbf{n}, \alpha) = \begin{pmatrix}
    q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_1 q_2 - q_0 q_3) & 2(q_1 q_3 + q_0 q_2) \\
    2(q_1 q_2 + q_0 q_3) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2(q_2 q_3 - q_0 q_1) \\
    2(q_1 q_3 - q_0 q_2) & 2(q_2 q_3 + q_0 q_1) & q_0^2 - q_1^2 - q_2^2 + q_3^2 
\end{pmatrix},
\]

(2.32)
where \( q_0 = \sin(\alpha/2) \) and \( q_i = n_i \cos(\alpha/2), \ 1 \leq i \leq 3 \). Then \( R(n, \alpha) \) rotates vectors \( u \in \mathbb{R}^3 \) about the vector \( n \) by an angle \( \alpha \).

**Proof 1:** See [2], page 146.

The Proposition 1 can be used to construct the rotation matrix \( R(u, u') \) which rotates the vector \( u \) into \( u' \) about an axis which is perpendicular to both \( u \) and \( u' \): The rotation angle is \( \alpha = \arccos(u \cdot u') \). If \( \alpha \neq 0 \) and \( \alpha \neq \pi \) then the rotation axis is given by the vector

\[
n = \frac{u \times u'}{|u \times u'|}
\]  

(2.33)

**Proposition 2:** Let the rotation matrix \( R(\omega, \theta, \phi) \), where \( \omega, \theta, \text{and} \phi \) are rotation angles be defined as

\[
R(\omega, \theta, \phi) = 
\begin{pmatrix}
\cos \omega \cos \phi \cos \theta - \sin \omega \sin \phi & -\cos \phi \cos \theta \sin \omega - \cos \omega \sin \phi & \cos \phi \sin \theta \\
\cos \phi \sin \omega + \cos \omega \cos \theta \sin \phi & \cos \omega \cos \phi - \cos \theta \sin \omega \sin \phi & \sin \phi \sin \theta \\
-\cos \omega \sin \theta & \sin \omega \sin \theta & \cos \theta
\end{pmatrix}
\]  

(2.34)

Then \( R(\omega, \theta, \phi) \) performs a rotation of the angle \( \omega \) about the z-axis, followed by a rotation of the angle \( \theta \) about the y-axis and, finally, a rotation of the angle \( \phi \) about the z-axis.

**Proof:** See [xx].

### 2.3 Interpolation

Let a function \( y = f(x) \) be sampled at a set of points \((x_i, y_i), 1 \leq i \leq n\). Then the linear-linear (\( \text{lin-lin} \)) interpolated \( y \) corresponding to \( x_i \leq x < x_{i+1} \) is

\[
y = y_i + \frac{y_{i+1} - y_i}{x_{i+1} - x_i} (x - x_i)
\]  

(2.35)

and the \( \text{log-log} \) interpolated \( y \) is

\[
y = \exp \left[ \ln y_i + \frac{\ln y_{i+1} - \ln y_i}{\ln x_{i+1} - \ln x_i} (\ln x - \ln x_i) \right].
\]  

(2.36)
Chapter 3
CTmod objects

3.1 Positioning of objects

Let the global coordinate system be defined as $\mathcal{U} = (O, e_1, e_2, e_3)$, where $O = (0, 0, 0)$ is its origin and $e_1 = (1, 0, 0)$, $e_2 = (0, 1, 0)$, and $e_3 = (0, 0, 1)$ are its base vectors. Each CTmod object has an associated local coordinate system, $\mathcal{L} = (O_\mathcal{L}, e_x, e_y, e_z)$, where $O_\mathcal{L}$ and $(e_x, e_y, e_z)$ are its origin and base, respectively. When a new CTmod object is created, its local coordinate system coincides with the global one, $\mathcal{L} = \mathcal{U}$. To position the object in space, the user provides a rotation matrix $R$ and a translation vector $T$. Coordinates of a point in the local coordinate system, $(P)_\mathcal{L}$, are then transformed to the coordinates of the global coordinate system $(P)_\mathcal{U}$ according to (2.24) as

$$(P)_\mathcal{U} = R(P)_\mathcal{L} + T. \quad (3.1)$$

Directions are transformed according to (2.22) as

$$(u)_\mathcal{U} = R(u)_\mathcal{L}. \quad (3.2)$$

3.1.1 Photon sources

Point sources emit photons from the point $(0, 0, 0)_\mathcal{L}$, the beam axis is $(0, 0, -1)_\mathcal{L}$.

3.1.2 Point detector array

Planar point detector array

The local coordinate system of an individual point detector with indices $(i, j)$, where $1 \leq i \leq N_x$ and $1 \leq j \leq N_y$, is defined as $(O_{ij}, e_1, e_2, e_3)$. Positions of origins $O_{ij}$ are

$$O_{ij} = (i - 1)\Delta xe_1 + (j - 1)\Delta ye_2 - \left(L_x/2, L_y/2, 0\right) \quad (3.3)$$

Here, $L_x$ and $L_y$ are the sizes of the point detector array, see figure 3.2a. If $N_x = 1$ then
Figure 3.1: Local coordinate systems of point detector arrays and individual point detectors. (a) A planar point detector array, (b) A cylindrical point detector array. X-, y-, and z-axes are drawn in red, green, and blue colors, respectively.

Figure 3.2: Parameters and default positions of (a) planar and (b) cylindrical point detector arrays.
$L_x = 0$ and similarly for $N_y$ and $L_y$. The distance between two adjacent point detectors, $\Delta x$, is

$$
\Delta x = \begin{cases} 
  L_x/(N_x - 1) & N_x > 1 \\
  0 & N_x = 1 
\end{cases}
$$

and similarly for $\Delta y$.

**Cylindrical point detector array**

Local coordinate systems of individual point detectors are defined as $(O_{ij}, e_1, e_y, e_z)$, where positions of origins $O_{ij} = (x_{ij}, y_{ij}, z_{ij})$ are given as

$$
x_{ij} = (i - 1)\Delta x - W/2 
$$

$$
y_{ij} = R \cos \alpha_j 
$$

$$
z_{ij} = R \sin \alpha_j. 
$$

Here $1 \leq i \leq N_W$, $1 \leq j \leq N_L$, $R$ is the radius, $W$ is the width, and $L$ is the length of the point detector array, see figure 3.2b. If $N_W = 1$ then $W = 0$ and similarly for $N_L$ and $L$. The initial angle, $\alpha_1$, is

$$
\alpha_1 = 3\pi/2 - L/(2R) 
$$

and the angular step, $\Delta \alpha$, is

$$
\Delta \alpha = \begin{cases} 
  L/[R(N_L - 1)] & N_L > 1 \\
  0 & N_L = 1 
\end{cases}
$$

The base vectors $e_y$ and $e_z$ are calculated using the rotation matrix $R(e_1, \alpha)$ with rotation angle $\alpha$ about the axis $e_1$, as

$$
e_y = R(e_1, \alpha_i - 3\pi/2)e_2 
$$

$$
e_z = R(e_1, \alpha_i - 3\pi/2)e_3 
$$

### 3.1.3 Gantry and table movement

In CTmod, (i) the patient represented by a geometrical model stays stationary, (ii) the source and the detector array perform both rotational and translational movements according to the selected scanning mode. This approach was chosen to avoid the recalculation of transformation matrices of the geometry (section 3.4.2) after each projection.

In the following, sequential and helical scanning modes are described. $R$ and $T$ are rotation and translation matrices, respectively, that define the default position of the photon source or the point detector array. $R(n, \alpha)$ is an active rotation matrix that represents a rotation about the angle $\alpha$ around the unit vector $n$, see section 2.2.3.
Figure 3.3: Local coordinate systems of an object moving on a trajectory in (a) sequential and (b) helical scanning modes. X-, y-, and z-axes are drawn in red, green, and blue colors, respectively.

**Sequential scanning mode**

For a sequential scanning mode, figure 3.3a, positions of photon sources and detector arrays are controlled via rotation angle, \( 0 \leq \alpha \leq \pi \), and slice number, \( s \in \mathbb{Z} \). The matrices \( R' \) and \( T' \) that define object positions during the scan are defined as

\[
R' = R(e_1, \alpha)R \quad (3.12) \\
T' = R(e_1, \alpha)T + s\Delta x e_1, \quad (3.13)
\]

where \( \Delta x \) is the distance between two consecutive slices and \( R(e_1, \alpha) \) is the rotation matrix defining rotation about the axis \( e_1 \).

**Helical scanning mode**

For a helical scanning mode, figure 3.3b, positions are controlled via the rotation angle, \( \alpha \), only and the corresponding matrices are

\[
R' = R(e_1, \alpha)R \quad (3.14) \\
T' = R(e_1, \alpha)T + \alpha (2\pi)^{-1} \Delta x e_1, \quad (3.15)
\]

where \( \Delta x \) is the distance traveled in the x-direction during a full rotation (the pitch).

### 3.2 Photons

#### 3.2.1 Sampling of interactions

Let \( \Sigma_{\text{In}} \), \( \Sigma_{\text{Co}} \), and \( \Sigma_{\text{Ph}} \) be the macroscopic cross sections of the incoherent scattering, coherent scattering, and photoelectric effect, respectively, for a given material and photon energy \( E \). Let \( \Sigma_t = \Sigma_{\text{In}} + \Sigma_{\text{Co}} + \Sigma_{\text{Ph}} \) be the total cross section. If a photon interaction occurs
then the ratios $\Sigma_{\text{in}}/\Sigma_{t}$, $\Sigma_{\text{co}}/\Sigma_{t}$, and $\Sigma_{\text{ph}}/\Sigma_{t}$ give the probability of the corresponding type of interaction. The sampling of the interaction type can thus be performed using the direct method:

1. Sample $\gamma$ from $R(0,1)$.
2. Select interaction according to the condition

\[
\begin{align*}
0 < \gamma &\leq \frac{\Sigma_{\text{in}}}{\Sigma_{t}} \Rightarrow \text{incoherent scattering} \quad (3.16) \\
\frac{\Sigma_{\text{in}}}{\Sigma_{t}} < \gamma &\leq \frac{\Sigma_{\text{in}} + \Sigma_{\text{co}}}{\Sigma_{t}} \Rightarrow \text{coherent scattering} \quad (3.17) \\
\frac{\Sigma_{\text{in}} + \Sigma_{\text{co}}}{\Sigma_{t}} < \gamma &\leq 1 \Rightarrow \text{photoelectric effect} \quad (3.18)
\end{align*}
\]

**New direction**

The azimuthal angle $\phi$ is sampled from the uniform distribution $R(0,2\pi)$ Sampling of the scattering angle $\theta$ is described in sections 3.2.2 and 3.2.3. If $|u_3| = 1$, the new direction is calculated as

\[
\begin{align*}
u_1 &\leftarrow \sin \theta \cos \phi \quad (3.19) \\
u_2 &\leftarrow \sin \theta \sin \phi \quad (3.20) \\
u_3 &\leftarrow \operatorname{sign}(u_3) \cos \theta \quad (3.21)
\end{align*}
\]

Otherwise it is calculated as

\[
\begin{align*}
u_1 &\leftarrow u_1 \cos \theta + (u_2 \sin \phi - u_1 u_3 \cos \phi) \frac{\sin \theta}{\sqrt{1 - u_3^2}} \quad (3.22) \\
u_2 &\leftarrow u_2 \cos \theta - (u_1 \sin \phi + u_2 u_3 \cos \phi) \frac{\sin \theta}{\sqrt{1 - u_3^2}} \quad (3.23) \\
u_3 &\leftarrow u_3 \cos \theta + \cos \phi \sin \theta \sqrt{1 - u_3^2} \quad (3.24)
\end{align*}
\]

**3.2.2 Coherent scattering**

Coherent scattering is simulated according to the method described by Persliden [6]. The differential cross section of coherent scattering is

\[
\frac{d\sigma_{\text{coh}}}{d\theta} = \frac{d\sigma_{\text{Th}}}{d\theta} F_m^2(x),
\]

where $\theta$ is the scattering angle, $F_m^2(x)$ is the form factor of material $m$, and

\[
\frac{d\sigma_{\text{Th}}}{d\theta} = (1 + \cos^2 \theta)2\pi \sin \theta
\]

is the classical Thompson differential cross section. The parameter

\[
x = \frac{E}{hc} \sin(\theta/2),
\]

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where $h$ is Planck’s constant and $c$ is the speed of light in vacuum, is related to the momentum transfer of the interaction.

Let $x_{\text{max}} = \max_{\theta \in (0, \pi)}(x) = E/(hc)$, $y = x^2$, and $y_{\text{max}} = x_{\text{max}}^2$. Since

$$y = \frac{E^2}{(hc)^2} \sin^2 \frac{\theta}{2} = \frac{E^2}{(hc)^2} \frac{1 - \cos \theta}{2}, \quad (3.28)$$

the scattering angle can be calculated as

$$\cos \theta = 1 - 2y/y_{\text{max}} \quad (3.29)$$

The differential cross section can be written as

$$\frac{d\sigma_{\text{coh}}}{dy} = \frac{d\sigma_{\text{coh}}}{d\theta} \left( \frac{dy}{d\theta} \right)^{-1} \quad (3.30)$$

$$= \frac{4\pi r_e^2 (hc)^2}{E^2} \int_0^{y_{\text{max}}} F_m^2(\tau) \, d\tau \left[ \frac{1 + \cos^2 \theta}{2} \right] \frac{F_m^2(\sqrt{y})}{\int_0^{y_{\text{max}}} F_m^2(\sqrt{\tau}) \, d\tau}. \quad (3.31)$$

In (3.30), we used

$$\frac{dy}{d\theta} = \frac{d}{d\theta} \left[ \frac{E^2}{(hc)^2} \sin^2 \left( \frac{\theta}{2} \right) \right] = \frac{E^2}{(hc)^2} \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{\theta}{2} \right) = \frac{E^2 \sin \theta}{2(hc)^2} \quad (3.32)$$

Let the probability density function $f(y)$ be

$$f(y) = \frac{\int_0^y F_m^2(\sqrt{\tau}) \, d\tau}{\int_0^{y_{\text{max}}} F_m^2(\sqrt{\tau}) \, d\tau} \quad (3.33)$$

and let the corresponding rejection function $0 \leq g(y) \leq 1$ be

$$g(y) = \frac{1 + \cos^2 \theta}{2} \quad (3.34)$$

Then the sampling of $y$ can be performed according to Proposition 1 in section 2.1.2.

The material-dependent integral

$$A_m(y) = \int_0^y F_m^2(\sqrt{\tau}) \, d\tau \quad (3.35)$$

is calculated numerically at the beginning of the run for a set of points $y_i$. Linear interpolation is used for both $A_m(y)$ and its inverse function $A_m^{-1}(y)$.

The sampling routine is:

1. Calculate $y_{\text{max}}$ and $A_{\text{max}}$:

$$y_{\text{max}} \leftarrow \left[ E/(hc) \right]^2, \quad A_{\text{max}} \leftarrow A(y_{\text{max}}) \quad (3.36)$$

2. Sample $y$ and calculate $\cos \theta$:

$$y \leftarrow A_{m}^{-1}(\gamma_1 A_{\text{max}}), \quad \cos \theta \leftarrow 1 - 2y/y_{\text{max}} \quad (3.37)$$

3. If $\gamma_2 > (1 + \cos \theta)/2$ go to step 2
Functions $A_m$ and $A_m^{-1}$

The function $A_m(y)$ is evaluated using lin-lin interpolation (2.35) between pre-calculated values $A_i$ and $A_{i+1}$ as

$$A_m(y) = A_i + \frac{A_{i+1} - A_i}{y_{i+1} - y_i} (y - y_i),$$

(3.38)

where the index $i$ is chosen so that $y_i \leq y < y_{i+1}$. The values $A_i$ are calculated from the recursive formula

$$A_i = A_m(y_i) = \int_0^{y_i} F_m^2(\sqrt{t}) \, dt = \int_0^{y_i-1} F_m^2(\sqrt{t}) \, dt + \int_{y_i-1}^{y_i} F_m^2(\sqrt{t}) \, dt$$

(3.39)

$$= A_{i-1} + \int_{y_{i-1}}^{y_i} F_{i-1}^2 + \frac{F_i^2 - F_{i-1}^2}{y_i - y_{i-1}} (t - y_{i-1}) \, dt$$

(3.40)

$$= A_{i-1} + \frac{F_i^2 + F_{i-1}^2}{2} (y_i - y_{i-1})$$

(3.41)

$$= A_{i-1} + \bar{F}_i^2 (y_i - y_{i-1}),$$

(3.42)

where

$$\bar{F}_i^2 = \frac{(F_{i-1}^2 + F_i^2)}{2}$$

(3.43)

are pre-calculated and $A_0 = A_m(0) = 0$. In (3.39), the lin-lin interpolation was used to approximate the values of $F_m^2(\sqrt{y})$ via pre-calculated $F_i^2 = F_m^2(\sqrt{y_i})$, $0 \leq i < i$:

$$F_m^2(\sqrt{y}) = F_{i-1}^2 + \frac{F_i^2 - F_{i-1}^2}{y_i - y_{i-1}} (y - y_{i-1})$$

(3.44)

From (3.42) we get

$$\frac{A_{i+1} - A_i}{y_{i+1} - y_i} = \bar{F}_i^2$$

(3.45)

and thus (3.38) can be simplified to

$$A_m(y) = A_i + \bar{F}_i^2 (y - y_i).$$

(3.46)

The inverse function, $A_m^{-1}$, is obtained from (3.46) as

$$A_m^{-1}(A) = y_i + \frac{A - A_i}{\bar{F}_i^2},$$

(3.47)

where the index $i$ is chosen so that $A_i \leq A < A_{i+1}$.

### 3.2.3 Incoherent scattering

Incoherent scattering of photons is simulated according to methods described in the EGS4 documentation [5] and in Persliden [6]. The Klein-Nishina’s differential cross section modified with the incoherent scattering function, $S_m(x)$, is

$$\frac{d\sigma_{\text{incoh}}(\theta)}{d\theta} = \frac{r^2}{2} \left( \frac{E'}{E} \right)^2 \left( \frac{E}{E'} + \frac{E}{E'} - \sin^2 \theta \right) S_m(x) 2\pi \sin \theta,$$

(3.48)
where $E$ and $E'$ are the energies of the incident and scattered photons, respectively, $\theta$ is the scattering angle, and $x = E/(hc) \sin(\theta/2)$ is a parameter related to the momentum transfer of the interaction. The energy of the scattered photon $E'$ is given by the Compton’s formula

$$E' = \frac{E}{1 + (1 - \cos \theta) E/(m_e c^2)}$$

(3.49)

The incoherent scattering cross section differential in energy of the scattered photon is

$$\frac{d\sigma_{\text{incoh}}(E')}{dE'} = \frac{d\sigma_{\text{incoh}}(\theta)}{d\theta} \left( \frac{dE'}{d\theta} \right)^{-1} = \frac{\pi r^2 m_e c^2}{E^2} \left( \frac{E}{E'} + \frac{E}{E} - \sin^2 \theta \right).$$

(3.50)

The derivative $dE'/d\theta$ was calculated from (3.49) as

$$\frac{dE'}{d\theta} = \frac{E^2 \sin \theta}{m_e c^2}$$

(3.51)

The sampling of $E'$ and $\theta$ is performed in two steps: (i) The energy $E'$ is sampled from the Klein-Nishina’s cross section using a method described in EGS4 and the corresponding scattering angle is calculated, (ii) the scatter-rejection method described in Persliden [6] is applied to account for the incoherent scattering function.

**Sampling from the Klein-Nishina cross section**

The content of this section was taken from [5] with modifications to account for different notations only. Let the energy of the scattered photon be described via the fraction

$$\varepsilon = E'/E$$

(3.52)

The Klein-Nishina cross section differential in $\varepsilon$ is

$$\frac{d\sigma_{\text{KN}}(\varepsilon)}{d\varepsilon} = \frac{d\sigma_{\text{KN}}(E')}{dE} \frac{dE}{d\varepsilon} = \frac{\pi r^2 m_e c^2}{E} \left( \frac{1}{\varepsilon} + \varepsilon - \sin^2 \theta \right).$$

(3.53)

It can be written as

$$\frac{d\sigma_{\text{KN}}(\varepsilon)}{d\varepsilon} = \frac{\pi r^2 m_e c^2}{E} \left[ \frac{1}{\varepsilon} + \varepsilon \right] \left[ 1 - \frac{\varepsilon \sin^2 \theta}{1 + \varepsilon^2} \right] \propto f(\varepsilon) g(\varepsilon),$$

(3.54)

The function

$$f(\varepsilon) = \frac{1}{\varepsilon} + \varepsilon$$

(3.55)

will be sampled over $(\varepsilon_0, 1)$, where $\varepsilon_0 = 1 + 2E/(m_e c^2)$ is the minimum fractional energy given by (xx). The function

$$g(\varepsilon) = \left[ 1 - \frac{\varepsilon \sin^2 \theta}{1 + \varepsilon^2} \right]$$

(3.56)
will be the rejection function. We factorize \( f(\varepsilon) \) over \((\varepsilon_0, 1)\) as follows

\[
f(\varepsilon) = \frac{1}{\varepsilon} + \varepsilon = \sum_{i=1}^{2} \alpha_i f_i(\varepsilon),
\]

(3.57)

where

\[
\begin{align*}
\alpha_1 &= \ln(1/\varepsilon_0), \quad f_1(\varepsilon) = \frac{1}{\ln(1/\varepsilon_0)} \frac{1}{\varepsilon}, \quad \varepsilon \in (\varepsilon_0, 1) \\
\alpha_2 &= (1 - \varepsilon_0^2)/2, \quad f_2(\varepsilon) = \frac{2\varepsilon}{1 - \varepsilon^2}, \quad \varepsilon \in (\varepsilon_0, 1)
\end{align*}
\]

(3.58)

(3.59)

We sample \( f_1 \) by letting

\[
\varepsilon = \varepsilon_0 \exp(\alpha_1 \zeta),
\]

(3.60)

where \( \zeta \) is a random number drawn uniformly on the interval \((0, 1)\). We could sample \( f_2 \) by taking the larger of two random numbers if we were willing to reject sampled values less than \( \varepsilon_0 \); but this would get very inefficient for low energy photons. Instead we make a change of variable. Let

\[
\varepsilon' = \frac{\varepsilon - \varepsilon_0}{1 - \varepsilon_0}
\]

(3.61)

Then, in order to give \( \varepsilon \) the proper distribution, \( \varepsilon' \) must have the distribution

\[
f'_2(\varepsilon') = f_2(\varepsilon) \frac{d\varepsilon}{d\varepsilon'} = \alpha'_1 f'_1(\varepsilon') + \alpha'_2 f''_1(\varepsilon'),
\]

(3.62)

where

\[
\begin{align*}
\alpha'_1 &= \frac{k'_0}{k'_0 + 1}, \quad f'_1(\varepsilon') = 2\varepsilon', \quad \varepsilon' \in (0, 1) \\
\alpha'_2 &= \frac{k'_0}{k'_0 + 1}, \quad f''_1(\varepsilon') = 1, \quad \varepsilon' \in (0, 1)
\end{align*}
\]

(3.63)

(3.64)

Here, \( k'_0 = E/m_e c^2 \). Both of these distributions are easily sampled.

To compute the rejection function it is necessary to get \( \sin^2\theta \). Let

\[
t = \frac{m(1 - \varepsilon)}{E\varepsilon}
\]

(3.65)

Then using (3.49), we have

\[
\cos \theta = \frac{(E + m_e c^2)E - E m_e c^2}{EE'} = 1 + \frac{m_e c^2 \varepsilon - m_e c^2}{E\varepsilon} = 1 - t.
\]

(3.66)

Thus

\[
\sin^2 \theta = 1 - \cos^2 \theta = (1 - \cos \theta)(1 + \cos \theta) = t(2 - t).
\]

(3.67)

When the value of \( \varepsilon \) is accepted, then \( \sin \theta \) and \( \cos \theta \) are obtained via

\[
\begin{align*}
\sin \theta &= \sqrt{\sin^2 \theta} \\
\cos \theta &= 1 - t.
\end{align*}
\]

(3.68)

(3.69)

The sampling procedure is as follows:
1. Calculate $\varepsilon_0$, $\alpha_1$, and $\alpha_2$:

$$
\varepsilon_0 \leftarrow 1 + 2E/(m_e c^2), \quad \alpha_1 \leftarrow \ln(1/\varepsilon_0), \quad \alpha_2 \leftarrow (1 - \varepsilon_0)/2 \quad (3.70)
$$

2. If $\alpha_1 \geq (\alpha_1 + \alpha_2)\gamma_1$ use $\varepsilon = \varepsilon_0 \exp(\alpha_1 \gamma_2)$. Else, use $\varepsilon = \varepsilon_0 + (1 - \varepsilon_0)\varepsilon'$ where

$$
\varepsilon' = \begin{cases} 
\max(\gamma_3, \gamma_4) & \text{if } k'_0 \geq (k'_0 + 1)\gamma_2 \\
\gamma_3 & \text{otherwise}
\end{cases} \quad (3.71)
$$

3. Calculate $t$, $\sin^2 \theta$ and $g(\varepsilon)$:

$$
t \leftarrow m_e c^2 (1 - \varepsilon)/\varepsilon E/m_e c^2, \quad \sin^2 \theta \leftarrow t(2 - t), \quad g(\varepsilon) \leftarrow 1 - \frac{\varepsilon \sin^2 \theta}{1 + \varepsilon^2} \quad (3.72)
$$

4. If $\gamma_5 < g(\varepsilon)$ reject and go to step 1. Otherwise accept.

**Sampling with the incoherent scattering function**

Assume the new energy $E'$ and scattering angle $\theta$ have been sampled from the Klein-Nishina cross section. The differential cross section (3.48) can be sampled using Preposition 1 in section 2.1.2 with $g(x) = S(x)/S_{\text{max}}$

$$
x_{\text{max}} \leftarrow E/(hc), \quad S_{\text{max}} \leftarrow S(x_{\text{max}}) \quad (3.73)
$$

If $\gamma_1 < S(x)/S_{\text{max}}$, accept $E'$ and $\theta$. Otherwise resample them from the Klein-Nishina cross section.

### 3.3 Photon sources

A photon source generates new photons. Each photon is assigned a position $r$, a direction $u$, an energy $E$, and a statistical weight $w$. The position $r$ is the same as the position of the point source, see section 3.1.1. Sampling of the direction $u$ for circular, planar, and cylindrical beams is described in sections 3.3.3 – 3.3.5. Sampling of the energy $E$ is described in section 3.3.6.

The mathematical model assumes that (i) a point isotropic source is used, (ii) the source intensity corresponds to one photon emitted into the solid angle $4\pi$, (ii) ideal collimator absorb all photons heading outside the solid angle $\Omega$ which defines the beam shape, and (iii) the direction $u$ and the energy $E$ are independent random variables.

Let $s_{\Omega,E}(\Omega, E) \, d\Omega \, dE$ be the number of photons with energy from $E$ to $E+dE$ emitted into the solid angle $d\Omega$ in the direction $\Omega$. Assumptions of the mathematical model can be written as

$$
s_{\Omega,E}(\Omega, E) = S s_{\Omega}(\Omega) s_E(E) \quad (3.74)
$$
where $s_\Omega(\Omega) = (4\pi)^{-1}$ sr$^{-1}$ and $s_E(E)$ are the directional and spectral probability density functions, respectively, and $S = 1$ is the total number of photons emitted from the source. The normalization conditions are $\int_{4\pi} s_\Omega(\Omega) \, d\Omega = 1$ and $\int_0^\infty s_E(E) \, dE = 1$.

To increase efficiency, the code produces photons with directions $\mathbf{u} \in \Omega$ only. To account for the biasing, the statistical weight of photons produced by the source is set to

$$w \left\{ \begin{array}{ll} \Delta\Omega/(4\pi) & \Omega \in \Omega \\ 0 & \text{otherwise} \end{array} \right. \quad (3.75)$$

The statistical weight can further be decreased by an optional bowtie filter, see section 3.3.7.

3.3.1 Classification of beam sources

Consider a point source located at $O = (0, 0, 0)^T$ which emits particles into a solid angle $\Omega$. The solid angle is specified as a set of directions $\Omega = (\theta, \phi)$ given by the polar, $\theta$, and azimuthal, $\phi$, angles, see figure xx, or by a region $A$ on a convex solid surface surrounding the vertex $O$, see figure yy. 

- **Circular beam**, figure 3.4a, is defined as a set of rays with directions $\Omega \in \Omega$, where

$$\Omega = \{ (\theta, \phi) : \omega < \theta \leq \pi, \ 0 \leq \phi < 2\pi \} \quad (3.76)$$

and $0 \leq \omega \leq \pi$ is the cone angle. 

- **Planar fan beam**, figure 3.4b, is defined as a set of all rays that originate in the vertex $O = (0, 0, 0)^T$ and intersect the rectangular area $A$

$$A = \{ (x, y, z) : -w < x < w, \ -l < y < l, \ z = -h \} \quad (3.77)$$

positioned at the distance $h$ from the origin. 

- **Cylindrical fan beam**, figure 3.4c, is defined as a set of all rays that originate in the vertex $O = (0, 0, 0)^T$ and intersect the cylindrical area $A$

$$A = \{ (x, y, z) : y^2 + z^2 = R^2, \ -w < x < w, \ z < z_{\text{max}} \} \quad (3.78)$$
with radius $R$. The bound $z_{\text{max}}$ can be specified via the fan angle $0 < \alpha < \pi/2$ using the relation
\[
\tan \alpha = \left| \sqrt{R^2 - z_{\text{max}}^2} / z_{\text{max}} \right|.
\] (3.79)

### 3.3.2 Auxiliary formulas and methods

#### Solid angle size

**Proposition 1:** Let $A$ be the defining region of a solid angle $\Omega$ with vertex $O = (0,0,0)^T$. Then the size $\Delta \Omega$ of the solid angle $\Omega$ is
\[
\Delta \Omega = \int_{\Omega} 1 \, d\Omega = \int_A \hat{r} n / r^2 \, dA
\] (3.80)
where $dA$ is a surface element, $n$ is a normal to the surface, $r$ is the radius, $r = |r|$ and $\hat{r} = r^{-1}r$ is a unit vector in the direction of $r$.

**Proof:** The proposition directly follows from the definition of the solid angle, see for instance [8].

Proposition 1 can be used to calculate the size of the solid angle for all three considered sources. Derivations are in following sections.

#### Acceptance-rejection sampling using a defining surface

To derive formulas for the acceptance-rejection method, consider the following configuration. The photons are emitted from a point source and pass the geometry without any interaction. Let the number of photons passing the area $dA$ be $dN = N_A(x) \, dA$, where $N_A(x)$ is the planar fluence at point $x$. The directional source intensity pdf is then
\[
s_{\Omega}(\Omega) = \frac{1}{N} \frac{dN}{d\Omega} = \frac{N_A(x,y) \, dA}{N} = \frac{N_A(x,y)}{N} \frac{d^2}{|n n'|},
\] (3.81)
where $d$ is the distance between the source and the point $x$, $n$ is a normal to the surface element $dA$ and $n'$ is a direction to the source; both $n$ and $n'$ are taken at the point $x$.

To make $s_{\Omega}(\Omega)$ independent of the position $x$, the ratio $N_A(x)/N$ can be defined as
\[
\frac{N_A(x)}{N} = \frac{|n n'|}{4\pi d^2}.
\] (3.82)

Let $N_{A,\text{max}}$ be the maximum planar fluence at the surface $A$. The acceptance-rejection algorithm is then applied as follows. A position $x$ is sampled on the surface $A$. The position is accepted if
\[
\gamma \frac{N_A(x)_{\text{max}}}{N} < \frac{|n n'|}{4\pi d^2},
\] (3.83)
where $\gamma \sim R(0,1)$, and re-sampled otherwise. Application of 3.83 for planar and cylindrical fan beams is in sections 3.3.4 and 3.3.5, respectively.
Functions J and K

**Proposition 1:** Let the function \( j(x) \) be defined as
\[
j(x) \equiv \frac{R}{4\pi(x^2 + R^2)^{3/2}},
\]
see equation xx for the meaning of \( x \) and \( R \). Then its antiderivative \( J(x) \) is
\[
J(x) \equiv \int j(x) \, dx = \frac{x}{4\pi R\sqrt{x^2 + R^2}}
\]
and the inverse function of the antiderivative, \( J^{-1}(x) \), is
\[
J^{-1}(x) = \text{sign}(x) \frac{R}{\sqrt{(4\pi R)^2 - 1}}
\]

**Proof:** It can be shown (e.g. using the Mathematica software) that
\[
\frac{\partial}{\partial x} J(x) = j(x)
\]
and that
\[
J^{-1}(J(x)) = x.
\]

□

Apparently, \( J(x) \) is an odd function, i.e.
\[
J(-x) = -J(x)
\]

**Proposition 3:** Let the function \( j(x, y) \) be defined as
\[
j(x, y) \equiv \frac{h}{4\pi(x^2 + y^2 + h^2)^{3/2}},
\]
see equation xx for the meaning of \( x \), \( y \), and \( h \). Then its antiderivative in \( x \) is
\[
J_y(x) \equiv \int j(x, y) \, dx = \frac{hx}{4\pi(h^2 + y^2)\sqrt{h^2 + x^2 + y^2}}
\]
and the inverse function of the antiderivative, \( J_y^{-1}(x) \), is
\[
J_y^{-1}(x) = \text{sign}(x) \sqrt{\frac{h^2 + y^2}{h^2/(4\pi x(h^2 + y^2))^2 - 1}}
\]

**Proof:** It can be shown (e.g. using the Mathematica software) that
\[
\frac{\partial}{\partial x} J_y(x) = j(x, y)
\]
and that
\[ J_y^{-1}(J_y(x)) = x. \]  
(3.94)

Proposition 4: Let the function \( k_x(y) \) be defined as
\[ k_x(y) \equiv J_y(x), \]  
(3.95)
where \( J_y(x) \) is defined in Proposition 3. Then its antiderivative in \( y \) is
\[ K_x(y) \equiv \int k_x(y) \, dy = \frac{1}{4\pi} \arctan \frac{xy}{h\sqrt{h^2 + x^2 + y^2}} \]  
(3.96)
and the inverse function of the antiderivative, \( K_x^{-1}(y) \), is
\[ K_x^{-1}(y) = \text{sign}(xy) \sqrt{\frac{x^2 + h^2}{x^2/[h\tan(4\pi y)]^2 - 1}} \]  
(3.97)

Proof: It can be shown (e.g. using the Mathematica software) that
\[ \frac{\partial}{\partial y} K_x(y) = k_x(y) \]  
(3.98)
and that
\[ K_x^{-1}(K_x(y)) = y. \]  
(3.99)

Note that Mathematica sometimes does not simplify complex expressions containing the \( \text{sign}(x) \) function. In this case, it helps to realize that \( K_x(y) \) is an odd function of the product \( xy \) and therefore its inverse function, \( K_x^{-1}(y) \), must also be an odd function of the product \( xy \). □

It can be easily shown that
\[
\begin{align*}
J_y(-x) &= -J_y(x) \\
J_{-y}(x) &= J_y(x) \\
K_x(-y) &= -K_x(y) \\
K_{-x}(y) &= -K_x(y) \\
K_x(y) &= K_y(x)
\end{align*}
\]  
(3.100-3.104)

3.3.3 Circular beam

Solid angle size

Corollary 1: The circular fan beam solid angle size \( \Delta\Omega \) is
\[ \Delta\Omega = 2\pi(1 - \cos \omega), \]  
(3.105)
where the cone angle $\omega$ is defined in section 3.3.1.

Proof: According to Proposition 1 in section 3.3.2

$$\Delta \Omega = \int_0^\omega 1 \, d\Omega = \int_0^{2\pi} \int_0^\omega 1 \sin \theta \, d\phi \, d\theta = 2\pi \int_0^\omega \sin \theta \, d\theta = 2\pi (1 - \cos \omega).$$  \hspace{1cm} (3.106)

\[ \square \]

### Direction-inside condition

The direction $\Omega$ is inside the beam if its deflection, $\alpha$, from $-e_3 = (0, 0, -1)$ is lower or equal to the cone angle, $\omega$. This is equivalent to the condition

$$\cos \omega < \cos \alpha = -e_3 \Omega = -\Omega_3$$ \hspace{1cm} (3.107)

### Direct sampling of directions

Proposition: Consider a point isotropic source emitting photons into the solid angle $\Omega = \{ \Omega : \theta_1 < \theta \leq \pi \}$, where $\theta$ is the polar angle. The cumulative distribution function, $F(\theta)$, is then

$$F(\theta) = \frac{\cos \theta - \cos \theta_1}{1 + \cos \theta_1}$$ \hspace{1cm} (3.108)

Proof: The probability of emitting a photon into a solid angle $d\Omega$ is

$$dP = f_\Omega(\Omega) d\Omega,$$ \hspace{1cm} (3.109)

where $f_\Omega(\Omega) = \Delta \Omega^{-1} = [2\pi (1 + \cos \theta_1)]^{-1}$ is the probability density function. Note that the relation between the cone angle $\omega$ in 3.105 and the polar angle $\theta$ is $\omega = \pi - \theta$. The probability can also be written as

$$dP = f_\theta(\theta) d\theta$$ \hspace{1cm} (3.110)

Combining 3.109 and 3.110 and using the well known relation $d\Omega = 2\pi \sin \theta d\theta$ we get

$$f_\theta(\theta) = \frac{1}{\Delta \Omega} \frac{d\Omega}{d\theta} = \frac{\sin \theta}{1 + \cos \theta_1}.$$ \hspace{1cm} (3.111)

The cumulative distribution function is then

$$F(\theta) = \int_{\theta_1}^{\theta} f_\theta(\theta) d\theta \int_{\theta_1}^{\theta} \frac{\sin \theta}{1 + \cos \theta_1} d\theta = \frac{\cos \theta_1 - \cos \theta}{1 + \cos \theta_1}.$$ \hspace{1cm} (3.112)

\[ \square \]

Let the parameter $\gamma$ be defined as $\gamma = F(\theta)$. The inverse function, $F^{-1}(\gamma)$, is then

$$\theta = F^{-1}(\gamma) = \arccos[\cos \theta_1 - \gamma (1 + \cos \theta_1)]$$ \hspace{1cm} (3.113)
or, when expressed via the cone angle $\omega$,

$$\theta = F^{-1}(\gamma) = \arccos[-\cos \omega - \gamma(1 - \cos \omega)] \quad (3.114)$$

If $\hat{\gamma} \sim R(0,1)$ then, according to Proposition 1, $\theta$ samples directions corresponding to a point isotropic source emitting particles into a cone with the cone angle $\omega$.

In practice, it is better to work with $\cos \theta$ instead of $\theta$. The direct sampling routine is then

$$\cos \theta \leftarrow -\cos \omega - \gamma(1 - \cos \omega) \quad (3.115)$$

$$\sin \theta \leftarrow \sqrt{1 - \cos^2 \theta} \quad (3.116)$$

$$\phi \leftarrow 2\pi\gamma \quad (3.117)$$

$$(u)_L \leftarrow (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)^T \quad (3.118)$$

### 3.3.4 Planar fan beam

#### Solid angle size

**Corollary 1:** The planar fan beam solid angle size $\Delta \Omega$ is

$$\Delta \Omega = 4 \arctan \left( \frac{lw}{h\sqrt{h^2 + l^2 + w^2}} \right), \quad (3.119)$$

where the distance $h$, width $w$, and length $l$ are defined in section 3.3.1.

**Proof:** Let $r = (x, y, -h)^T$ be a point at the defining surface $A$. Its distance from the origin is $r = \sqrt{x^2 + y^2 + h^2}$ and the normal to the surface $A$ at this point is $n = (0, 0, -1)^T$. Then according to the proposition 1 in section 3.3.2

$$\Delta \Omega = \int_{-w}^{w} \int_{-l}^{l} \frac{h}{(x^2 + y^2 + h^2)^{3/2}} \, dx \, dy = K_w(l) - K_w(-l) -$$

$$-K_{-w}(l) + K_{-w}(-l) = 4K_w(l) = 4 \arctan \frac{lw}{h\sqrt{h^2 + l^2 + w^2}} \quad (3.120)$$

The function $K_x(y)$ is defined in section 3.3.2. $\square$

#### Direction-inside condition

The direction $\Omega$ is inside the beam if the ray $x = t\Omega$ intersects the plane $x_3 = -h$ inside the $w \times l$ rectangle

$$-w \leq x_1 \leq w \land -l \leq x_2 \leq l, \quad (3.121)$$

where $x_1 = t\Omega_1$, $x_2 = t\Omega_2$, and $t = -h/\Omega_3$. If $t < 0$ then $\Omega$ is outside the beam.
Direct sampling of directions

The planar fluence \( N_A(x, y) \) at the planar surface for the position \((x, y, -h)\) is

\[
N_A(x, y) = \Phi(x, y) |\mathbf{n'}| = \frac{h}{4\pi(x^2 + y^2 + h^2)^{3/2}}, \tag{3.122}
\]

where \( \Phi(x, y) \) is the corresponding fluence and \( \mathbf{n} \) and \( \mathbf{n'} \) are the normal to the surface and the direction to the source, respectively. The joint probability distribution function \( f(x, y) \) is thus

\[
f(x, y) = \frac{N_A(x, y)}{\int_{-l}^{l} \int_{-w}^{w} N_A(u, v) \, du \, dv} = \frac{N_A(x, y)}{\int_{-l}^{l} k_w(v) - k_{-w}(v) \, dv} = \frac{N_A(x, y)}{K_w(l) - K_{-w}(l) - [K_w(-l) - K_{-w}(-l)]} = \frac{N_A(x, y)}{4K_w(l)} \tag{3.123}
\]

\[
f(x, y) = \frac{N_A(x, y)}{\int_{-l}^{l} \int_{-w}^{w} N_A(u, v) \, du \, dv} = \frac{N_A(x, y)}{\int_{-l}^{l} k_w(v) - k_{-w}(v) \, dv} = \frac{N_A(x, y)}{K_w(l) - K_{-w}(l) - [K_w(-l) - K_{-w}(-l)]} = \frac{N_A(x, y)}{4K_w(l)} \tag{3.124}
\]

Here, the properties of functions \( k_x(y) \) and \( K_x(y) \) defined in section 3.3.2 were used.

Direct sampling of \( \hat{x}, \hat{y} \) can be performed according to Proposition 2 in section 2.1.1.

The function \( F(\infty, y) \) is

\[
F(\infty, y) = \int_{-l}^{l} \int_{-w}^{w} f(u, v) \, du \, dv = \frac{\int_{-l}^{l} \int_{-w}^{w} N_A(x, y) \, du \, dv}{4K_w(l)} \tag{3.125}
\]

\[
F(\infty, y) = \frac{\int_{-l}^{l} k_y(v) - k_{-w}(v) \, dv}{4K_w(l)} \tag{3.126}
\]

\[
F(\infty, y) = \frac{K_y(l) - K_{-w}(l) - [K_w(-l) - K_{-w}(-l)]}{4K_w(l)} \tag{3.127}
\]

\[
F(\infty, y) = \frac{K_l(y) + K_w(l)}{2K_w(l)} \tag{3.128}
\]

Here, the properties of \( K_x(y) \) listed in (3.102) – (3.104) were used. The inverse function \( F^{-1}(\infty, y) \) is thus

\[
y = F^{-1}(\infty, \gamma_1) = K_l^{-1}((2\gamma_1 - 1)K_w(l)), \tag{3.129}
\]

where the inverse function \( K_l^{-1} \) is given by (3.97).

The function \( G_y(x) \) is

\[
G_y(x) = \frac{\int_{-w}^{w} f(u, y) \, du}{\int_{-w}^{w} f(u, y) \, du} = \frac{J_y(x) - J_y(-w)}{J_y(w) - J_y(-w)} = \frac{J_y(x) + J_y(w)}{2J_y(w)} \tag{3.130}
\]

The inverse function \( G_y^{-1}(\gamma_2) \) is

\[
x = G_y^{-1}(\gamma_2) = J_y^{-1}((2\gamma_2 - 1)J_y(w)), \tag{3.131}
\]

where the inverse function \( J_y^{-1} \) is given by (3.92).
Using (3.129) and (3.131), the direction $u$ can be sampled as

$$
y \leftarrow K_{w}^{-1}((2\gamma_1 - 1)K_{w}(l)) \tag{3.132}
$$

$$
x \leftarrow J_{y}^{-1}((2\gamma_2 - 1)J_{y}(w)) \tag{3.133}
$$

$$
d \leftarrow \sqrt{x^2 + y^2 + h^2} \tag{3.134}
$$

$$(u)_L \leftarrow d^{-1}(x, y, -h)^T \tag{3.135}
$$

Functions $J_y(x), J_y^{-1}(x), K_x(y),$ and $K_x^{-1}(y)$ are defined in section 3.3.2.

**The acceptance-rejection sampling of directions**

Let the defining surface $A$ be defined as a rectangle at the distance $h$ from the origin, see figure xx. Since $|\mathbf{nn'}| = h/d$, the right side of relation 3.83 is

$$
\frac{N_A(x)}{N} = \frac{h}{4\pi d^3}. \tag{3.136}
$$

The maximum $N_{A,\text{max}}$ is achieved for the position $(0, 0, -h)$ where $d = h$. The left side of relation 3.83 is thus

$$
\frac{N_{A,\text{max}}(x)}{N} = \frac{h}{4\pi h^3} = \frac{1}{4\pi h^2}. \tag{3.137}
$$

The condition 3.83 becomes

$$
\gamma \frac{1}{4\pi h^2} < \frac{h}{4\pi d^3} \tag{3.138}
$$

which can be simplified to

$$
\gamma < \frac{h^3}{d^3}. \tag{3.139}
$$

The sampling routine is

1. Calculate $(x, y, z)$ and $d$:

   $$(x, y, z) \leftarrow ((2\gamma_1 - 1)w, (2\gamma_2 - 1)l, -h), \quad d \leftarrow \sqrt{x^2 + y^2 + h^2} \tag{3.140}$$

2. If $\gamma_3 > h^3/d^3$ then go to step 1.

3. Calculate the direction

   $$(u)_L \leftarrow d^{-1}(x, y, -h)^T \tag{3.141}$$

**3.3.5 Cylindrical fan beam**

**Solid angle size**

*Corollary 1:* The cylindrical fan beam solid angle size $\Delta\Omega$ is

$$
\Delta\Omega = 4\alpha w(w^2 + R^2)^{-1/2}, \tag{3.142}
$$
where the radius $R$ and width $w$ are defined in section 3.3.1, also see figure 3.5.

**Proof**: Let $r = (x, R \cos \alpha, R \sin \alpha)^T$ be a point at the cylindrical surface $A$ expressed via cylindrical coordinates $(x, \alpha, R)$. Its distance from the origin is $r = \sqrt{x^2 + R^2}$ and the normal to the surface $A$ at this point is $n = (0, \cos \alpha, \sin \alpha)^T$. Since $dA = R \, dx \, d\alpha$, then according to the proposition 1 in section 3.3.2

$$
\Delta \Omega = \int_{-\omega}^{\omega} \int_{-w}^{w} \frac{R^2}{(x^2 + R^2)^{3/2}} \, d\alpha \, dx = 2 \omega \left[ J(w) - J(-w) \right] = 4 \frac{\omega w}{\sqrt{w^2 + R^2}} \quad (3.143)
$$

The function $J(x)$ is defined in section 3.3.2. □

**Direction-inside condition**

The direction $\Omega$ is inside the beam if (i) the deflection $\alpha$ from the plane $y = 0$ is lower or equal to the fan angle $\omega$, and (ii) the ray $x = t \Omega$ intersects the cylindrical surface at the band of width $2w$. The first condition is

$$
\cos \omega < \cos \alpha = \frac{(0, 0, -1)(0, \Omega_2, \Omega_3)}{\sqrt{\Omega_2^2 + \Omega_3^2}} = \frac{-\Omega_3}{\sqrt{\Omega_2^2 + \Omega_3^2}} \quad (3.144)
$$

The second condition is

$$
-w \leq x \leq w, \quad (3.145)
$$

where $x = t \Omega_1$ and $t = R/\sqrt{\Omega_2^2 + \Omega_3^2}$.

**Direct sampling of directions**

The planar fluence $N_A(x, \alpha)$ at the cylindrical surface for the position $(x, \alpha, R)$ is

$$
N_A(x, \alpha) = \Phi(x, \alpha) |\mathbf{n} \cdot \mathbf{n}'| = \frac{R}{4\pi(x^2 + R^2)^{3/2}}, \quad (3.146)
$$

where $\Phi(x, \alpha)$ is the corresponding fluence and $\mathbf{n}$ and $\mathbf{n}'$ are the normal to the surface and the direction to the source, respectively. The planar fluence does not depend on the angle $\alpha$ which can be sampled separately from a uniform distribution $R(-\omega, \omega)$. Let $j(x) \equiv N_A(x, \alpha)$. The probability density function for $x$ is then

$$
f(x) = \frac{j(x)}{\int_{-w}^{w} j(x) \, dx} \quad (3.147)
$$
The corresponding cumulative distribution function is

\[ F(x) = \int_{-w}^{x} f(t) \, dt = \frac{\int_{-w}^{x} j(t) \, dt}{\int_{-w}^{w} j(t) \, dt} \]

\[ = \frac{J(x) - J(-w)}{J(w) - J(-w)} \]

\[ = \frac{J(x) + J(w)}{2J(w)}, \]

where the function \( J(x) \) is defined in section 3.3.2. The inverse function can be obtained from 3.150 as

\[ x = F^{-1}(y) = J^{-1}(2y - 1)J(w) \]

Direct sampling of \( x \) can be performed from 3.151 according to Proposition 1 in section 2.1.1. The sampling of direction \( u \) is summarized in the following algorithm:

\[ \alpha \leftarrow (2\gamma_1 - 1)\omega \]

\[ x \leftarrow J^{-1}((2\gamma_2 - 1)J(w)) \]

\[ d \leftarrow \sqrt{x^2 + R^2} \]

\[ (u)_L \leftarrow d^{-1}(x, R \sin \alpha, -R \cos \alpha)^T \]

The acceptance-rejection sampling of directions

Let the defining surface \( A \) be defined as a cylindrical surface with radius \( R \), see figure xx. Since \( |\mathbf{n}\mathbf{n}'| = R/d \), the right side of relation 3.83 is

\[ \frac{N_A(x)}{N} = \frac{R}{4\pi d^3}. \]

The maximum \( N_{A,max} \) is achieved for positions with \( x = 0 \) where \( d = R \). The left side of relation 3.83 is thus

\[ \frac{N_{A,max}(x)}{N} = \frac{R}{4\pi R^3} = \frac{1}{4\pi R^2}. \]

The condition 3.83 becomes

\[ \gamma \frac{1}{4\pi R^2} \leq \frac{R}{4\pi d^3} \]

which can be simplified to

\[ \gamma \leq \frac{R^3}{d^3} \]

The sampling routine is

1. Calculate \( \alpha \):

\[ \alpha \leftarrow (2\gamma_1 - 1)\omega, \]
2. Calculate $x$, and $d$:

$$x \leftarrow (2\gamma - 1)w, \quad d \leftarrow \sqrt{x^2 + R^2}$$  \hspace{1cm} (3.161)

3. If $\gamma_3 > R^3/d^3$ go to step 2.

4. Calculate the direction

$$(u)_{L} \leftarrow d^{-1}(x, R\sin\alpha, -R\cos\alpha)^T$$  \hspace{1cm} (3.162)

### 3.3.6 Photon spectrum

The probability density function, $s_E(E)$, in (3.74) consists of continuous and discrete parts. Let the probability that the photon is produced from the continuous and discrete parts be $P_c$ and $P_d$, respectively, where $P_c + P_d = 1$. First, the direct sampling is used to determine which part of the spectrum the photon comes from. If $\gamma_1 < P_c$ then the continuous part is selected. Otherwise the discrete part is selected.

#### The continuous part

The continuous part is approximated by a histogram with equidistant bins. Let the bin width be $\Delta E$ and let the bin weights be $w_0, \ldots, w_{n-1}$. In CTmod, $\Delta E = 1$ keV and the weights $w_i$ correspond to bin centers with energies $1\Delta E, \ldots, n\Delta E$, see figure xxa. The normalization condition is $P_c = \sum_{i=0}^{n-1} w_i$. The photon energy, $E$, is sampled using the acceptance-rejection method as follows

$$E' \leftarrow \gamma_1 n\Delta E$$  \hspace{1cm} (3.163)

$$i \leftarrow \lceil E'/\Delta E \rceil,$$  \hspace{1cm} (3.164)

where $[x]$ stands for the largest integral value not greater than $x$. Accept $E'$ if $\gamma_2 w_{\text{max}} < w_i$, where $w_{\text{max}} = \max_{i=0,\ldots,n-1} w_i$. Otherwise resample $E'$. It can be easily seen, that the PDF of $E'$ is shifted by $0.5\Delta$ towards the zero, figure xxb. To correct for the shift, the photon energy $E$ is calculated as

$$E \leftarrow E' + 0.5\Delta E$$  \hspace{1cm} (3.165)
The discrete part

Direct sampling is used to sample the photon energy $E$ from the discrete part. Let $p_i$, $1 \leq i \leq n$, is the probability of producing a photon with energy $E_i$ from the discrete part. Let $F_i = \sum_{j=1}^{i} p_j$ be the corresponding cumulative distribution function. A random number $\gamma$ is sampled. The values $F_i$ are searched from $i = 1$ to $n$; the index $k$ of the first one for which $F_k > \gamma$ is then accepted and the corresponding $E_k$ is used.

3.3.7 Bowtie filters

A bowtie filter in CTmod decrease the statistical weight, $w$, of a photon generated in the source as

$$w \leftarrow w T(\mathbf{u}, E),$$

(3.166)

where $T(\mathbf{u}, E)$ is the transmission function of the bowtie filter which depends on the photon direction, $\mathbf{u}$, and energy, $E$. For homogenous bowtie filters, the transmission function is calculated as

$$T(\mathbf{u}, E) = \exp[-\Delta t(\mathbf{u}) \mu(E)],$$

(3.167)

where $\Delta t(\mathbf{u})$ is the thickness of the filter in the direction $\mathbf{u}$ and $\mu(E)$ is the energy dependent linear attenuation coefficient of the material. In the following, only the 1D-table and the water-cylinder-compensator bowtie filters (which are homogenous) are described. Information about the P45 form filter from Siemens (which is not homogenous) is covered by a non-disclosure agreements and thus the filter is not described here. In general the argument of the exponential function in (3.167) is replaced with the line integral $\int \mu(E) \, dx$ for non-homogenous bowtie filters.

1D table

Proposition 1: Let $\mathbf{P} + t \mathbf{u}$, $t > 0$, be a ray intersecting a bowtie filter (a general cylinder) defined as

$$V = \{(x_1, x_2, x_3) : f(x_2, x_3) < 0, \quad x_3 > 0, \quad a < x_1 < b\},$$

(3.168)

see figure xx. Then (i) the fan angle, $\alpha$ is given as

![Figure 3.7: 1D table bowtie filter](image-url)
\[
\cos \alpha = \frac{-u_3}{\sqrt{u_2^2 + u_3^2}}, \tag{3.169}
\]

and (ii) the line segment of the ray, \(\Delta t\), is

\[
\Delta t = \frac{\Delta t'}{\sqrt{u_2^2 + u_3^2}}, \tag{3.170}
\]

where \(\Delta t'\) is the line segment of the ray projected to the plane \(x = 0\).

**Proof:** The distance, \(t\), to intersection of the ray \(\mathbf{P} + tu\) with the surface \(f(x_2, x_3) = 0\) is a solution of the equation

\[
f(P_2 + tu_2, P_3 + tu_3) = 0 \tag{3.171}
\]

The projection of the ray to the plane \(x = 0\) is the ray \(\mathbf{P} + t'u'\), \(t' > 0\), where

\[
u' = (0, \frac{u_2}{\sqrt{u_2^2 + u_3^2}}, \frac{u_3}{\sqrt{u_2^2 + u_3^2}}) \tag{3.172}
\]

The distance, \(t'\), to intersection of the projected ray \(\mathbf{P} + t'u'\) with the surface \(f(x_2, x_3) = 0\) is a solution of the equation

\[
f(P_2 + t'u'_2, P_3 + t'u'_3) = 0 \tag{3.173}
\]

It is easily seen that \(t'\) is a solution of (3.173) if and only if \(t = t' / \sqrt{u_2^2 + u_3^2}\) is a solution of (3.171). The same is true for the intersections of both rays with the plane \(x_3 = 0\) since it is a special case of \(f(x_2, x_3) = 0\). Thus the same relation must be true for the corresponding differences in (3.170).

The fan angle is the angle between \(-\mathbf{e}_3\) and \(u'\), thus

\[
\cos \alpha = -\mathbf{e}_3 \cdot u' = (0, 0, -1) \cdot \left(0, \frac{u_2}{\sqrt{u_2^2 + u_3^2}}, \frac{u_3}{\sqrt{u_2^2 + u_3^2}}\right) = -\frac{u_3}{\sqrt{u_2^2 + u_3^2}} \tag{3.174}
\]

\(\Box\)

The 1D table defines the thickness, \(t_{1D}(\cos \alpha)\), of the bowtie filter at the plane \(x = 0\) as a function of the cosine of the fan angle \(\alpha\). The line segment \(\Delta t\) corresponding to the direction \(u\) is calculated as

\[
\Delta t(u) = t_{1D}(\cos \alpha) / \cos \beta, \tag{3.175}
\]

where \(\beta\) is the angle between \(u\) and \(u'\) and thus

\[
\cos \beta = u \cdot u' = \sqrt{u_2^2 + u_3^2} \tag{3.176}
\]

**Water cylinder compensator**

This bowtie filter compensates for a water cylinder with radius \(R\) at the distance \(h\) from the point source.
Proposition 1: Let $t \mathbf{u}$, $t > 0$, be a ray that intersects a cylinder with radius $R$ described as

$$x_2^2 + (x_3 + h)^2 = R^2.$$  \hfill (3.177)

Then the length of the intersection is

$$l = 2 \sqrt{R^2(u_2^2 + u_3^2) - h^2 u_2^2 \over u_2^2 + u_3^2}$$  \hfill (3.178)

Proof: Inserting $x_2 = t u_2$ and $x_3 = t u_3$ into (3.177) gives quadratic equation with coefficients $A = (u_2^2 + u_3^2)$, $B = u_3 h$, $C = h^2 - R^2$, see (3.207). Its solutions are given by (3.208), their difference is

$$l(u) = t_2 - t_1 = 2 \sqrt{B^2 - AC \over A} = 2 \sqrt{u_3^2 h^2 - (u_2^2 + u_3^2)(h^2 - R^2) \over u_2^2 + u_3^2} =$$

$$= 2 \sqrt{R^2(u_2^2 + u_3^2) - h^2 u_2^2 \over u_2^2 + u_3^2}$$  \hfill (3.179)

$$= 2 \sqrt{R^2(u_2^2 + u_3^2) - h^2 u_2^2 \over u_2^2 + u_3^2}$$  \hfill (3.180)

The maximum of $l$ is reached for the direction

$$\mathbf{u}_{\text{max}} = (\sin \delta, 0, -\cos \delta),$$

where $\delta$ is the beam angle. The corresponding thickness, $l_{\text{max}}$ can be obtained by inserting (3.181) into (3.178) which gives

$$l_{\text{max}} = 2R / \cos \delta$$  \hfill (3.182)

Also note that this equation directly follows from (3.175) for $\beta = \delta$ and $t_{1D}(\cos \alpha) = 2R$.

The thickness of the bowtie filter is then given as

$$\Delta t(u) = l_{\text{max}} - l(u)$$  \hfill (3.183)

3.3.8 Timing comparison

CPU times of routines for generating photons from an x-ray source based on direct sampling and acceptance-rejection methods are compared in table 3.1. The measurement was performed using GCC version 4.1.2 on a dual CPU machine with AMD Opteron 250 (2.4 GHz) and reg. ECC PC400 memory modules. The source–detector distance was 100 cm, 10 samples of a 20 cm $\times$ 90 cm beam and 10 samples of a 0.2 cm $\times$ 20 cm beam were used. (The difference in CPU time due to beam size was not statistically significant.) Corresponding source routines were called in a loop, the CPU time per one invocation was evaluated. Mean values and standard deviations were calculated from 20 samples.

The difference between CPU time of the direct sampling and acceptance-rejection methods when no optimization was used (the O0 option) was small but, for the commonly used optimization option O2, the acceptance-rejection method was 199.2/167.2 = 1.19 and 202.7/169.2 = 1.20 times faster for the cylindrical and planar fan beams, respectively.
Table 3.1: CPU times in nanoseconds of routines based on direct sampling (D) and acceptance-rejection (R) methods for four optimization levels of the GCC compiler. The coverage factor is $k = 1$, i.e. the statistical uncertainty is ±1 standard deviation.

### 3.4 Geometry

#### 3.4.1 Transformations during ray tracing

The user specifies positions of objects via rotation and translation matrices $R_{L\rightarrow U}$ and $T_{L\rightarrow U}$, respectively. Positions, $(P)_U$, and directions $(u)_U$ in the global coordinate system can be calculated via

\[
(P)_U = R_{L\rightarrow U}(P)_L + T_{L\rightarrow U} \tag{3.184}
\]

\[
(u)_U = R_{L\rightarrow U}(u)_L \tag{3.185}
\]

In CTmod, positions of photons are given in the local coordinate system of the solid where the particle is located. The solid is referred to as the current solid. When a photon enters a new solid, its position and direction are transformed from the current coordinate system $C$ to the new coordinate system $N$ as

\[
(P)_N = R_{C\rightarrow N}(P)_C + T_{C\rightarrow N} \tag{3.186}
\]

\[
(u)_N = R_{C\rightarrow N}(u)_C \tag{3.187}
\]

#### 3.4.2 Initialization of transformation matrices

Transformation matrices $R_{c\rightarrow n}$ and $T_{c\rightarrow n}$ are initialized at the beginning of the simulation for each pair of solids which share a boundary as

\[
R_{c\rightarrow n} = (R_{N\rightarrow U})^T R_{c\rightarrow U} \tag{3.188}
\]

\[
T_{c\rightarrow n} = (R_{N\rightarrow U})^T (T_{c\rightarrow U} - T_{N\rightarrow U}) \tag{3.189}
\]

The derivation of (3.188) and (3.189) can be performed by expressing the coordinates of a point $P$ in the coordinate system $N$ via the coordinates in the coordinate system $C$, see figure 3.8. To do so, we use the fact that transformations $C \rightarrow U$ and $N \rightarrow U$ are known. Using

\[
(P)_U = R_{N\rightarrow U}(P)_N + T_{N\rightarrow U} \tag{3.190}
\]
Figure 3.8: Using known transformation matrices, coordinates of a point in the coordinate system $\mathcal{N}$ can be expressed via its coordinates in the coordinate system $\mathcal{U}$ which can be expressed via coordinates in the coordinate system $\mathcal{C}$. The resulting expression gives transformation matrices $\mathcal{C} \rightarrow \mathcal{N}$.

we get

\[(P)_N = (R^{N \rightarrow U})^T ((P)_U - T^{N \rightarrow U}) \]  

Thus

\[(P)_N = (R^{N \rightarrow U})^T ((P)_U - T^{N \rightarrow U}) = (R^{N \rightarrow U})^T (R^{C \rightarrow U} (P)_C + T^{C \rightarrow U} - T^{N \rightarrow U}) \]  

\[(R^{N \rightarrow U})^T R^{C \rightarrow U} (P)_C + (R^{N \rightarrow U})^T (T^{C \rightarrow U} - T^{N \rightarrow U}) \]

(3.188) and (3.189) follow directly from (3.194).

In early versions of CTmod (TVpSolidNeighbor.h version 1.2 and older), the transformation from the current coordinate system to the new one was defined as

\[(P)_N = R^{C \rightarrow N} ((P)_C - T^{C \rightarrow N}) \]

(3.195)

and the translation $T^{C \rightarrow N}$ was defined as

\[T^{C \rightarrow N} = (R^{C \rightarrow U})^T (T^{N \rightarrow U} - T^{C \rightarrow U}). \]

(3.197)

The equivalence of transformations (3.195) and (3.186) can be shown by inserting (3.197) and (3.188) into (3.195):

\[(P)_N = (R^{N \rightarrow U})^T R^{C \rightarrow U} ((P)_C - (R^{C \rightarrow U})^T (T^{N \rightarrow U} - T^{C \rightarrow U})) = (R^{N \rightarrow U})^T R^{C \rightarrow U} (P)_C + (R^{N \rightarrow U})^T (T^{C \rightarrow U} - T^{N \rightarrow U}) \]

The expression on the right side of (3.199) is the same as in (3.194).

3.4.3 Free and optical paths

In CTmod, the transport of a photon in the geometry and the scoring of a contribution to a point detector are based on the calculation of the free path from the optical path and
vice versa. The relation between the optical path, $o$, and the free path, $\lambda$, is

$$o = \int_0^\lambda \mu(P + tu)\lambda,$$  \hspace{1cm} (3.200)

where $\mu$ is the linear attenuation coefficient. In an infinite medium, it simplifies to

$$o = \mu \lambda.$$  \hspace{1cm} (3.201)

In a geometry consisting of homogenous solids, the evaluation of (3.200) reduces to the task of finding an intersection between the ray $P + tu, t > 0$, and a surface of a solid; corresponding methods are in section 3.5. The evaluation of (3.200) becomes noticeably more difficult if the geometry contains a voxel array, a corresponding method is in section 3.5.6.

### 3.5 Solids

In CTmod, solids are (i) convex, and (ii) bounded by planar or quadratic surfaces. Currently implemented solids are shown in figure 3.9. An intersection between a ray

![Solids implemented in CTmod: (a) a sphere, (b) an ellipsoid, (c) a cylinder, (d) a box, (e) a voxel array. Local coordinate systems and parameters defining the solids are also shown.](image)

Figure 3.9: Solids implemented in CTmod: (a) a sphere, (b) an ellipsoid, (c) a cylinder, (d) a box, (e) a voxel array. Local coordinate systems and parameters defining the solids are also shown.

$$x = P + tu, \quad t \geq 0, \quad |u| = 1,$$  \hspace{1cm} (3.202)

where $P$ and $u$ are the ray’s origin and direction, respectively, and a plane defined as a set of points $x$ satisfying

$$(x - P_0)n = 0,$$  \hspace{1cm} (3.203)
where $P_0$ and $n$ are the plane’s point and normal, respectively, is a point

$$Q = P + tu,$$  

(3.204)

where the parameter $t$ can be obtained by inserting (3.202) into (3.203) and solving the resulting linear equation

$$At + B = 0$$  

(3.205)

with coefficients $A = un$ and $B = (P - P_0)n$. Similarly, intersections between the ray and a quadratic surface described as

$$ax_1^2 + bx_2^2 + cx_3^2 + 2fx_2x_3 + 2gx_3x_1 + 2hx_1x_2 + 2px_1 + 2qx_2 + 2rx_3 + d = 0$$  

(3.206)

are given by solutions of the quadratic equation

$$At^2 + 2Bt + C = 0.$$  

(3.207)

Its solutions, $t_1$ and $t_2$, where

$$t_1 = \frac{-B - \sqrt{B^2 - AC}}{A}, \quad t_2 = \frac{-B + \sqrt{B^2 - AC}}{A}$$  

(3.208)

are real numbers if the discriminant

$$D = 4(B^2 - AC)$$  

(3.209)

is greater than or equal to 0, see figure 3.11. Also note that in this case $t_1 < t_2$.

The intersection point $Q$ is then

$$Q = P + tu$$  

(3.210)
3.5.1 Volume of a solid

The volume, \( V \), of a solid which does not contain any overlapping solids is calculated from table 3.2.

<table>
<thead>
<tr>
<th>solid</th>
<th>volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>sphere</td>
<td>((4/3)\pi R^3)</td>
</tr>
<tr>
<td>ellipsoid</td>
<td>((4/3)\pi abc)</td>
</tr>
<tr>
<td>cylinder</td>
<td>(\pi R^2h)</td>
</tr>
<tr>
<td>box</td>
<td>(abc)</td>
</tr>
</tbody>
</table>

Table 3.2: Volumes of solids.

3.5.2 Spheres

The surface of a sphere is defined as a set of points \( x = (x_1, x_2, x_3) \) satisfying

\[
x_1^2 + x_2^2 + x_3^2 = R^2,
\]

(3.211)

where \( R \) is the radius of the circle, see figure 3.9. Intersections between the ray (3.202) and the surface (3.211) are given by solutions of (3.207) with coefficients

\[
A = 1, \quad B = Pu, \quad C = |P|^2 - R^2
\]

(3.212)

Ray intersection - point inside

Since the point \( P \) is inside the sphere, the intersection \( Q = P + tu \) exists and is given by \( t_2 \) in (3.208).

Ray intersection - point outside

The intersection \( Q = P + tu \) exists if \( B^2 - C > 0 \) and is given by \( t_1 \) in (3.208).

Point inside condition

A point \( P = (P_1, P_2, P_3) \) is inside the sphere if

\[
|P|^2 < R^2
\]

(3.213)

3.5.3 Ellipsoids

The surface of an ellipsoid is a set of points \( x = (x_1, x_2, x_3) \) satisfying

\[
\left(\frac{x_1}{a}\right)^2 + \left(\frac{x_2}{b}\right)^2 + \left(\frac{x_3}{c}\right)^2 = 1,
\]

(3.214)
where \(a\), \(b\), and \(c\) are the lengths of main axes, see figure 3.9. Intersections between the ray (3.202) and the surface (3.214) are solutions of (3.207) with coefficients

\[
A = \left( \frac{u_1}{a} \right)^2 + \left( \frac{u_2}{b} \right)^2 + \left( \frac{u_3}{c} \right)^2 
\]

\[
B = \frac{P_1 u_1}{a} + \frac{P_2 u_2}{b} + \frac{P_3 u_3}{c} 
\]

\[
C = \left( \frac{P_1}{a} \right)^2 + \left( \frac{P_2}{b} \right)^2 + \left( \frac{P_3}{c} \right)^2 - 1 
\]

**Ray intersection - point inside**

Since the point \(P\) is inside the ellipsoid, the intersection \(Q = P + tu\) exists and is given by \(t_2\) in (3.208).

**Ray intersection - point outside**

The intersection \(Q = P + tu\) exists if \(B^2 - AC > 0\) and is given by \(t_1\) in (3.208).

**Point inside condition**

A point \(P = (P_1, P_2, P_3)\) is inside the ellipsoid if

\[
\left( \frac{P_1}{a} \right)^2 + \left( \frac{P_2}{b} \right)^2 + \left( \frac{P_3}{c} \right)^2 < 1, 
\]

\[
(3.218)
\]

**3.5.4 Cylinders**

The cylinder in figure 3.9 is bounded by the cylindrical surface

\[
x_1^2 + x_2^2 = R^2, 
\]

\[
(3.219)
\]

where \(R\) is the radius of the base, and planes \(x_3 = 0\) and \(x_3 = h\), where \(h\) is the height of the cylinder. Intersections between the ray (3.202) and the surface (3.219) are given by solutions of (3.207) with coefficients

\[
A = u_1^2 + u_2^2, \quad B = P_1 u_1 + P_2 u_2, \quad C = P_1^2 + P_2^2 - R^2. 
\]

**Ray intersection - point inside**

Since the point \(P\) is inside the cylinder, the intersection \(Q\) exists. First, calculate the intersection \(Q\) of the ray (3.202) with the base plane from (3.205) and (3.204); if \(u_3 < 0\), use \(t = P_3/u_3\), else use \(t = (h - P_3)/u_3\). If \(Q\) is inside the base, i.e. \(Q_1^2 + Q_2^2 < R^2\), accept it. Otherwise calculate \(t_2\) for the cylindrical surface from (3.207).
Ray intersection - point outside

First, calculate the intersection $Q$ of the ray (3.202) with the base plane from (3.205) and (3.204); if $u_3 > 0$, use $t = -P_3/u_3$, else use $t = (h - P_3)/u_3$. If $Q$ is inside the base, i.e. $Q_1^2 + Q_2^2 < R^2$, accept it. Otherwise calculate the discriminant $D$ from (3.209). If $D < 0$ then there is no intersection. Else obtain $t$ for the cylindrical surface from (3.207) as

$$t \leftarrow -\frac{B - \sqrt{B^2 - C}}{A}$$

(3.221)

and the corresponding $Q$ from 3.210. If $0 < Q_3$ and $Q_3 < h$, accept the point. Otherwise there is no intersection.

Point inside condition

A point $P = (P_1, P_2, P_3)$ is inside the cylinder if

$$0 < P_3 \land P_3 < h \land P_1^2 + P_2^2 < R^2$$

(3.222)

3.5.5 Boxes

The box is bounded by surfaces

$$x_1 = 0, \quad x_1 = a, \quad x_2 = 0, \quad x_2 = b, \quad x_3 = 0, \quad x_3 = c,$$

(3.223)

where $a$, $b$, and $c$ are lengths of edges. Intersections between the ray (3.202) and surfaces (3.223) are solutions of (3.207).

Ray intersection - point inside

Directions $u$ are divided into 8 octants according to signs of coordinates $u_i$. In the following, the algorithm is described for the first octant, $(u_1 > 0 \land u_2 > 0 \land u_3 > 0)$ only. Formulas for other octants can be obtained by permutation of indices.

The intersection $Q$ of the ray (3.202) with the plane $x_1 = a$ is obtained from xx using $t = (a - P_1)/u_1$ from (3.205). If $Q$ is on the surface, i.e. $0 < Q_2 \land Q_2 < b \land 0 < P_3 \land p_3 < c$, it is accepted. If not, the remaining two surfaces $x_2 = 0$ and $x_3 = c$ are tested in the same way.

Ray intersection - point outside

As in the case with $P$ inside, directions $u$ are divided into 8 octants according to signs of coordinates $u_i$. Intersection $P$ with the surface $x_1 = 0$ obtained from xx and xx is accepted if $0 < Q_2 \land Q_2 < b \land 0 < P_3 \land p_3 < c$. Otherwise the surfaces $x_2 = 0$, and $x_3 = 0$ are tested in a similar way.
Point inside condition
A point $\mathbf{P}$ is inside the box if

$$0 < P_1 \land P_1 < a \land 0 < P_2 \land P_2 < b \land 0 < P_3 \land P_3 < c \tag{3.224}$$

3.5.6 Voxel arrays
A voxel array is treated like a box with an internal structure. Intersections between a ray and a voxel array surface are calculated using the corresponding routines for a box.

3.5.7 Calculation of the optical path from a free path
3.5.8 Calculation of the free path from an optical path

3.6 Point detectors

3.6.1 Scored quantities
3.6.2 Antiscatter grids

Grid transmission formula
The transmission function $T = T(u_1, u_2)$ for photons impinging with uniform positional distribution is

$$T = \exp \left[ -\frac{\mu_s (t_1 + t_2)}{u_3} \right] \frac{AB}{C}, \tag{3.225}$$

where

$$A = \exp \left( -\frac{\mu_i h}{u_2} - \frac{nd}{\alpha} \right) \tag{3.226}$$

$$B = D - q + 2\alpha + (d - q - 2\alpha) \exp(-q/\alpha), \quad 0 \leq q < d$$

$$B = D - q + 2\alpha + (q - d - 2\alpha) \exp(-d/\alpha), \quad d \leq q < D$$

$$B = (q - D + 2\alpha) \exp[-(q - D)/\alpha] + (q - d - 2\alpha) \exp(-d/\alpha), \quad D \leq q < C \tag{3.227}$$

$$C = D + d \tag{3.228}$$

Here,

$$\alpha = |u_1|/(\mu_s - \mu_i) \tag{3.229}$$

$$q = P - nC \tag{3.230}$$

$$P = h|u_1|/u_2 \tag{3.231}$$

$$n = \text{int}(P/C) \tag{3.232}$$
3.7 Acknowledgment

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