Reconstruction of multiple Compton scattering events in MeV gamma-ray Compton telescopes using a physics-based probabilistic model

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Abstract

Aimed at progress in MeV gamma-ray astronomy which has not yet been well-explored, Compton telescope missions with a variety of detector concepts have been proposed so far. One of the key techniques for these future missions is an event reconstruction algorithm that is able to determine the scattering orders of multiple Compton scattering events and to identify events in which gamma rays escape from the detectors before they deposit all of their energies. We revisit previous event reconstruction methods, and propose a modified algorithm based on the maximum likelihood method. First, we present a general formalism of likelihood functions describing physical interactions inside the detector and measurement processes. Then, we also introduce several approximations in the calculation of the likelihood functions for efficient computation. For validation, the developed algorithm has been applied to simulation data of a Compton telescope using a liquid argon time projection chamber, which is a new type of Compton telescope proposed for the GRAMS mission. We have confirmed that it works successfully for up to 8-hit events, including correction of incoming gamma-ray energies for escape events. The proposed algorithm can be used for next-generation MeV gamma-ray missions featured by large-volume detectors, e.g., GRAMS.

Keywords: Compton camera, MeV gamma-ray, event reconstruction

1. Introduction

Astrophysical observations of gamma rays from a few 100 keV to a few 10 MeV remain to be ex-
of multi-messenger astronomy including gravitational wave [3] and neutrino observations [4], this curtailed window of electromagnetic waves is drawing increasing attention. Towards high-sensitivity observations in the 2020s or 2030s, several MeV gamma-ray missions have been proposed at this moment (GRAMS [5], AMEGO [6], e-ASTROGAM [7], COSI [8], SMILE [9] e.t.c.).

All of the missions above utilize Compton telescopes which are one of the most promising techniques for imaging gamma-ray sources in the sub-MeV/MeV bands [10][11][12]. A Compton telescope measures the position and deposited energy at each interaction, and calculates the scattering angle by the kinematics of Compton scattering. Then, the incoming gamma-ray direction is constrained on a circle in the sky. If recoiled electron trajectories can be measured additionally, then the gamma-ray direction is constrained on an arc-shaped region [13][14][15]. After an accumulation of many events, the incoming gamma-ray direction can be identified as intersections of the constrained circles or arcs. This is a basic principle of Compton imaging, which is called a back-projection method. Statistical approaches of the image reconstruction methods have been also proposed [16][17].

To calculate the scattering angle of a gamma-ray event, it is required to identify the scattering order of the detected signals and estimate the incident gamma-ray energy accurately. The scattering order determination becomes more complicated in a higher energy band because gamma rays can easily be scattered multiple times in a detector and escape from it before they are absorbed inside the detector. These multiple scattering events are considered to be dominant in large-volume detectors such as proposed in GRAMS [5]. Since in this project it is difficult to measure time-of-flight between signals, the scattering order cannot be determined directly, and thus, one has to determine it based on the detected energies and positions. In this paper, we focus on this order determination problem of the multiple scattering events.

Several approaches have been studied in a variety of fields e.g. astrophysics [18][19][20][21][22][23][24], homeland security [25][26][27][28][29][30][31][32], and nuclear physics [33][34][35]. A popular method is known as the mean squared difference (MSD) method [19][31]. For events with $n \geq 3$ interactions, the scattering angle at $i$-th ($2 \leq i \leq n-1$) interaction site can be calculated in two ways, i.e., from kinematics or geometrical information. Then, by comparing the calculated angles at each site, the most plausible scattering order is estimated based on a figure-of-merit. Another popular method is to calculate the probability of Compton scattering assuming the scattering order and choose one with the highest probability (deterministic method [31]). The Bayesian method [23] and the neural network method [24] are also proposed, and sometimes they outperform the above approaches. However, these approaches require large simulation data sets and a lot of computer resources.

Usually, events such that gamma rays escape from the detector (escape events) are rejected in many algorithms. However, in a high energy band, gamma rays become harder to be photo-absorbed in the detector, and the escape events become non-negligible to achieve high detection efficiency. Then, reconstruction methods should also correct the escape energy and distinguish the events from those that deposit all of their gamma-ray energies in the detector (full-deposit events). If the number of interactions is three or more, the gamma-ray energy of escape events can be estimated by combining the position and energy information (see, e.g., [20][22]). For example, using the MSD method, [33] proposed an algorithm for germanium spectrometers in nuclear physics experiments [35]. They demonstrated that the gamma-ray detection efficiency can be increased by identifying escape events and estimating their escape energies correctly. This consideration is also essential for astronomical observations in a high energy band.

In this work, we revisit the classical approaches and propose an event reconstruction algorithm including the escape gamma-ray events based on the maximum likelihood method. To derive the quantities for the event reconstruction deductively, first we formulate likelihood functions for both full-deposit and escape events considering physical and measurements processes in Compton telescopes. The mathematical formulas of the likelihood functions are shown in Sections 2 and 3. In Section 4, we implement the algorithm, introducing several approximations to calculate the likelihood function efficiently. Here we consider a Compton telescope that measures the interaction positions and deposited energies not including recoiled electron trajectories. A summary of the developed algorithm is given in Section 5. As a numerical test, we apply it to simulation data sets of a liquid argon detector considering the GRAMS experiment in Section 6. Finally, we summarize our results and
discuss further improvements in Section 7.

2. Basic Concept

In a Compton telescope, gamma rays deposit their energies at interaction sites via Compton scattering or photoabsorption. In general, measured values at each site are a tuple of several physical quantities, which is denoted by $D_I$. The index $I$ is the label of each tuple in an event, and here the scattering order is unknown. When a Compton telescope measures deposit energies and interaction positions, $D_I$ is a pair of them:

$$D_I = (r_I, \varepsilon_I),$$

where $r_I$ and $\varepsilon_I$ are the measured position and energy, respectively. Since a gamma ray is scattered multiple times or absorbed by a detector, in experiments we obtain a list of $D_I$:

$$(D_I) = (D_1, D_2, \ldots).$$

We define a hit as a measured interaction with $D_I$. When the number of hits in an event is $n$, we refer to the event as an $n$-hit event.

In the reconstruction of Compton scattering events, the task is divided into the following:

1. to determine the event type, i.e., a full-deposit event or an escape event for a given event.
2. to determine the scattering order of detected hits:

$$(D_I)_{\text{ordered}} = (D_{\tau(1)}, D_{\tau(2)}, \ldots, D_{\tau(n)})_{\text{ordered}},$$

where $(D_I)_{\text{ordered}}$ is a re-ordered list of $(D_I)$ by determining or assuming the scattering order. Here we define the function $\tau(\cdot)$ which maps the scattering order to the data label $(I)$, i.e., $i$-th interaction corresponds to $D_{\tau(i)}$. Figure 1 shows the scattering order candidates and their corresponding map functions $\tau(\cdot)$ for a 3-hit event.

3. to estimate the incident gamma-ray energy.
4. to estimate the incoming gamma-ray direction.

In the MSD method [18, 19, 21, 31, 33], the scattering angles are calculated redundantly from kinematics and from geometrical information, and they
are compared by a figure-of-merit. For example, \[19\] defines the following quantity:

\[
\chi^2_c = \frac{1}{N - 2} \sum_{i=2}^{N-1} \frac{(\cos \vartheta_i^{\text{kin}} - \cos \vartheta_i^{\text{geo}})^2}{\Delta \cos^2 \vartheta_i^{\text{kin}} + \Delta \cos^2 \vartheta_i^{\text{geo}}} \quad (N \geq 3),
\]

where $\vartheta_i^{\text{geo}}$ and $\vartheta_i^{\text{kin}}$ are $i$-th scattering angles calculated by kinematics and geometrically, respectively; $\Delta \cos^2 \vartheta_i$ is the measurement uncertainty, and $N$ is the number of hits. This quantity is interpreted as a generalized chi-squared value. For all $N!$ scattering order candidates, $\chi^2$ are calculated and the best scattering order is determined as one that yields the smallest $\chi^2$.

In order to consider escape gamma-ray events, so-called three-Compton method is usually used \[20, 22\]. If the energy loss at the first and second sites ($\varepsilon_1, \varepsilon_2$) and the scattering angle at the second interaction ($\vartheta_2$) are known, then the incident gamma-ray energy ($\hat{E}_0$) can be calculated as

\[
\hat{E}_0 = \varepsilon_1 + \frac{\varepsilon_2}{2} + \sqrt{\frac{\varepsilon_2^2}{4} + \varepsilon_2 m_e c^2 \varepsilon_1 \cos \vartheta_2}. \quad (5)
\]

For example, \[33\] calculates incident gamma-ray energy for escape events using the three-Compton method, and defines figure-of-merits for both full-deposit and escape events when the gamma-ray generation position is known.

In this work, aiming at MeV gamma-ray telescopes in astrophysics, we formulate a probabilistic model of Compton scattering in the detector instead of the figure-of-merit approaches mentioned above. The most plausible event type and scattering order can be determined as those that yield the maximum likelihood value. The basic concept is similar to the deterministic methods (e.g. \[31\]), but to identify and reconstruct escape events which are usually rejected, we derive likelihood functions for both full-deposit and escape events in the following section. Furthermore, in order to include physical probabilities and detector response functions adequately, the physical and measurement processes are separately considered.

The main advantage of this approach is that the quantity for the event reconstruction can be deductively derived from the likelihood function. Especially, the relative ratio of the quantities for the full-deposit and escape events can be determined based on physics. It is different from heuristic approaches in the MSD methods. Additionally, when more information is obtained, the proposed algorithm can be naturally extensible by determining response functions for the new information (see Section \[7.2\]).

3. Formalism

In this section, we formulate the likelihood function. Here we assume that an incoming gamma ray is scattered in the detector $n-1$ times and photo-absorbed at last, or is scattered $n$ times and escapes from the detector. In both cases, the number of interactions is $n$. Also, we assume that all interactions are measured and a list of the measurement values ($D_i = (D_1, D_2, ..., D_n)$) are obtained. Note that in reality there is a case that some interactions are not detected due to interactions in passive materials, the detector threshold, and multiple scattering in the same spatial resolution element of the detector. The probability of these events strongly depends on the actual detector configuration, and we ignore these possibilities in the likelihood formulation presented in this section.

As shown in Figure 2, the gamma ray changes its energy and its direction of travel every time it interacts with the detector. Then, the gamma ray after $i$-th interaction in the detector can be described with the quantities $\hat{q}_i$, defined as

\[
\hat{q}_i = \left( \hat{r}_i, \hat{E}_i, \hat{\theta}_i, \hat{\phi}_i \right),
\]

\[
\hat{r}_i = \left( x_i \right),
\]

\[
\hat{\theta}_i = \left( \sin \hat{\theta}_i \cos \hat{\phi}_i \right),
\]

\[
\hat{\phi}_i = \left( \sin \hat{\theta}_i \sin \hat{\phi}_i \right), \quad (6)
\]

where $\hat{r}_i$ represents the $i$-th interaction position; $\hat{E}_i$ and $\hat{\theta}_i$ represent the energy and momentum vector, respectively, of the gamma ray after the $i$-th interaction (see Figure 2); $\hat{\theta}_i$ and $\hat{\phi}_i$ describe the direction of travel of the gamma ray. We refer to the quantity $\hat{q}_i$ as gamma-ray state in this work. To distinguish explicitly the parameters in the gamma-ray state and those measured by experiments, we put hats on the former ones. Note that $\hat{q}_0$ represents the initial gamma-ray state. In astrophysical observations, $\hat{q}_0$ is described by just three parameters:

\[
\hat{q}_0 = \left( \hat{E}_0, \hat{\theta}_0, \hat{\phi}_0 \right), \quad (7)
\]
since incoming gamma rays originate from distant sources.

The gamma-ray state \( \hat{q}_i \) \((i \geq 1)\) can be determined when we assume the initial position and energy of the gamma ray \((\hat{r}_0, \hat{E}_0)\) and the position of each interaction \((\hat{r}_{i(\geq 1)})\). Except for \(i = n\), \(\hat{\theta}_i\) and \(\hat{\phi}_i\) are determined from the interaction positions:

\[
\hat{p}_i \parallel \frac{\hat{r}_{i+1} - \hat{r}_i}{|\hat{r}_{i+1} - \hat{r}_i|}.
\]

The gamma-ray energy \(\hat{E}_i\) is determined by the kinematics of Compton scattering:

\[
\hat{E}_i = \frac{\hat{E}_{i-1}}{1 + \frac{\hat{E}_{i-1}}{m_e c^2} \left(1 - \cos \hat{\theta}_{i}^{\text{scat}}\right)},
\]

where \(\hat{\theta}_i^{\text{scat}}\) is the \(i\)-th scattering angle which is calculated as

\[
\cos \hat{\theta}_{i}^{\text{scat}} = \frac{\hat{p}_{i-1} \cdot \hat{p}_i}{|\hat{p}_{i-1}| |\hat{p}_i|}.
\]

In the escape events, \(\hat{\theta}_n\) and \(\hat{\phi}_n\) should be also assumed to determine the direction of escape. Note that Eq. 9 does not take account of the uncertainty of \(\hat{E}_i\) due to the finite momentum fluctuation of the target electrons in the detector material, which is also known as the Doppler broadening effect \cite{50}. We will discuss a possible treatment to include this effect in Section 7.

To construct the likelihood function, it is useful to describe the graphical representation of a Compton scattering event as shown in Figure 3. The change of the state \(\hat{q}_i\) is a probabilistic process determined by the physics of Compton scattering. Then, the parameters of the state are related to the measured values \((\mathbf{D}_i)\) through measurement processes. For example, \(\hat{E}_{i-1} - \hat{E}_i\) is measured as the deposit energy at \(i\)-th interaction.

As a general expression, the likelihood function for full-deposit events is described as

\[
L_{\text{fulldep}}((\hat{q}_i), \tau(\cdot); (\mathbf{D}_i)) = \prod_{i=1}^{n} P_{\text{scat}}(\hat{q}_i, \mathbf{D}_{\tau(i)} | \hat{q}_{i-1}) (n \geq 2).
\]

It is the probability density function (PDF) that a gamma ray with the initial state of \(\hat{q}_0\) is scattered at \(\hat{r}_i \) \((1 \leq i \leq n - 1)\) and is absorbed at \(\hat{r}_n\), and the deposit energy and position at \(i\)-th interaction are measured as the obtained data sample \(\mathbf{D}_{\tau(i)}\). In the likelihood calculation, model parameters are \(\hat{q}_0\), \((\hat{r}_{i(\geq 1)})\) and \(\tau(\cdot)\). The gamma-ray energy \(\hat{E}_i\) and the direction of travel \((\hat{\theta}_i, \hat{\phi}_i)\) after \(i(\geq 1)\)-th interaction are determined from the model parameters (see Eqs. 8 and 9).

Here \(P_{\text{scat}}(\hat{q}_i, \mathbf{D}_{\tau(i)} | \hat{q}_{i-1})\) is the PDF that a gamma ray with \(\hat{q}_{i-1}\) is scattered with changing its state to \(\hat{q}_i\), and the interaction is measured as \(\mathbf{D}_{\tau(i)}\). It is described as the product of three functions:

\[
P_{\text{scat}}(\hat{q}_i, \mathbf{D}_{\tau(i)} | \hat{q}_{i-1}) = P_{\text{path,scat}}(\hat{r}_i | \hat{q}_{i-1}) \times P_{\text{KN}}(\hat{\theta}_i, \hat{\phi}_i | \hat{q}_{i-1}) P_{\text{det}}(\mathbf{D}_{\tau(i)} | \hat{q}_{i-1}, \hat{q}_i),
\]

where \(P_{\text{path,scat}}(\cdot)\) is the PDF that a gamma ray of \(\hat{q}_{i-1}\) is scattered at \(\hat{r}_i\); \(P_{\text{KN}}(\cdot)\) is the PDF that the scattering direction is \((\hat{\theta}_i, \hat{\phi}_i)\) and it is determined by Klein-Nishina formula \cite{37}. \(P_{\text{det}}(\cdot)\) corresponds to the PDF related to the detector response. Also, \(P_{\text{abs}}(\hat{q}_n, \mathbf{D}_{\tau(n)} | \hat{q}_{n-1})\) is the PDF that a gamma ray of \(\hat{q}_{n-1}\) is absorbed at \(\hat{r}_n\), and the interaction is measured as \(\mathbf{D}_{\tau(n)}\):

\[
P_{\text{abs}}(\hat{q}_n, \mathbf{D}_{\tau(n)} | \hat{q}_{n-1}) = P_{\text{path,abs}}(\hat{r}_n | \hat{q}_{n-1}) P_{\text{det}}(\mathbf{D}_{\tau(n)} | \hat{q}_{n-1}, \hat{q}_n),
\]

where \(P_{\text{path,abs}}(\cdot)\) is the PDF that a gamma ray that a gamma ray with \(\hat{q}_{i-1}\) is absorbed at \(\hat{r}_i\). In the following subsections, we explain these PDFs in detail.

Besides, the likelihood function for escape events is described as

\[
L_{\text{escape}}((\hat{q}_1), \tau(\cdot); (\mathbf{D}_i)) = \prod_{i=1}^{n-1} P_{\text{scat}}(\hat{q}_i, \mathbf{D}_{\tau(i)} | \hat{q}_{i-1}) \times P_{\text{esc}}(\hat{q}_n, \mathbf{D}_{\tau(n)} | \hat{q}_{n-1}) (n \geq 2).
\]

The only difference between Eq. 11 and Eq. 14 is the treatment of the last interaction. Here we introduce \(P_{\text{esc}}(\hat{q}_n, \mathbf{D}_{\tau(n)} | \hat{q}_{n-1})\), which is the PDF that a gamma ray of \(\hat{q}_{n-1}\) is scattered with changing its state to \(\hat{q}_n\) and escape from the detector, and the
interaction is measured as $D_{r(n)}$. It is described as

$$
P_{\text{esc}} (q_n, D_{r(n)} | q_{n-1}) = P_{\text{path,scat}} (r_n | q_{n-1}) \times \int d(\theta_n) d\phi_n P_{\text{KN}} (\theta_n, \phi_n | q_{n-1}) \times P_{\text{det}} (D_{r(n)} | q_{n-1}, q_n) P_{\text{path,esc}} (q_n),
$$

(15)

where $P_{\text{path,esc}}(q_n)$ is the probability that the gamma ray with a state of $q_n$ escapes from the detector. Since we cannot know the momentum direction of the escape gamma ray, we integrate the functions over $\phi_n$ and $\cos \theta_n$.

### 3.1. Probability functions related to physical processes

In the above equations, $P_{\text{path,scat}}(r_i | q_{i-1})$ and $P_{\text{path,abs}}(r_i | q_{i-1})$ describe the PDFs that a gamma ray of $q_{i-1}$ is scattered or absorbed at $r_i$. They are defined as

$$
P_{\text{path,scat}} (r_i | q_{i-1}) \, d^3 r_i = \frac{\rho \sigma_{\text{scat}}}{|r_i - r_{i-1}|^2} \exp (-\rho \sigma_{\text{all}} |r_i - r_{i-1}|) \, d^3 r_i ,
$$

(16)

$$
P_{\text{path,abs}} (r_i | q_{i-1}) \, d^3 r_i = \frac{\rho \sigma_{\text{abs}}}{|r_i - r_{i-1}|^2} \exp (-\rho \sigma_{\text{all}} |r_i - r_{i-1}|) \, d^3 r_i,
$$

(17)

where $\sigma_{\text{abs}}, \sigma_{\text{scat}}$ are the cross sections of photoabsorption, Compton scattering at an energy of $E_{i-1}$, respectively; $\rho$ is the number density of the detector material; $\sigma_{\text{all}}$ is the sum of the cross sections of physical processes. When only the pair creation ($\sigma_{\text{pair}}$) is considered additionally, it is equal to $\sigma_{\text{abs}} + \sigma_{\text{scat}} + \sigma_{\text{pair}}$. The term $\frac{1}{|r_i - r_{i-1}|^2}$ corresponds to the solid angle of the volume element at $r_i$ seen from $r_{i-1}$. When incoming gamma rays are considered to be parallel light as in astrophysical observations, this term with $i = 1$ can be removed and Eq. 16 is described as

$$
P_{\text{path,scat}} (r_1 | q_0) \, d^3 r_1 \propto \rho \sigma_{\text{scat}} \exp (-\rho \sigma_{\text{all}} r_{\text{first}}) \, d^3 r_1,
$$

(18)
where \( \ell_{\text{first}} \) is the length of the gamma-ray path inside the detector before it arrives at \( \hat{r}_1 \). Note that here it is assumed that the detector consists of a single material. If a Compton telescope consists of several detectors with different materials, e.g., semiconductor detectors and scintillators, then \( \sigma_{\text{abs/scat/pair}} \) and \( \rho \) also depend on the position. In this case, Eq. [10] is modified as

\[
P_{\text{path,scat}} (\hat{r}_1 \mid \hat{q}_{i-1}) \, d^3 \hat{r}_1 = \frac{\rho(\hat{r}_1) \sigma_{\text{scat}}(\hat{r}_1)}{|\hat{r}_1 - \hat{r}_{i-1}|^2} \exp \left( - \int_C \rho(\hat{r}) \sigma_{\text{all}}(\hat{r}) d|\hat{r}| \right) \, d^3 \hat{r}_1 ,
\]

where \( C \) is the straight line from \( \hat{r}_{i-1} \) to \( \hat{r}_1 \). The same applies to Eqs. [17] and [19].

The function \( P_{\text{KN}} \left( \hat{\theta}_i, \hat{\phi}_i \mid \hat{q}_{i-1} \right) \) is the PDF that the gamma ray of \( \hat{q}_{i-1} \) is scattered to the direction described by \( (\hat{\theta}_i, \hat{\phi}_i) \). Namely it is the normalized differential cross section of Compton scattering. Following Klein-Nishina’s formula [37], it is defined as

\[
P_{\text{KN}} \left( \hat{\theta}_i, \hat{\phi}_i \mid \hat{q}_{i-1} \right) \, d\Omega_i = \frac{1}{\sigma_{\text{scat}}} \frac{d\sigma_{\text{scat}}}{d\Omega_i} \, d\Omega_i = \frac{1}{2} \frac{r_c^2}{E_i} \times \left( \frac{E_i}{E_{i-1}} \right)^2 \left( \frac{E_{i-1}}{E_i} + \frac{E_{i-1}}{E_i} \sin^2 \hat{\theta}_{i,\text{scat}} \right) \, d\Omega_i ,
\]

where \( r_c \) is classical electron radius and \( E_i \) is the energy of the scattered gamma ray calculated by Eq. [9] and \( \hat{\theta}_{i,\text{scat}} \) is the \( i \)-th scattering angle defined in Eq. [10] and \( d\Omega_i \) is equal to \( d(\cos \hat{\theta}_i) d\hat{\phi}_i \). Note that the polarization effect is ignored here to reduce the amount of calculation because the target position is unknown. The treatment of the polarization with known target position is discussed in [38] [33].

Finally we define \( P_{\text{path,esc}} (\cdot) \) as the probability that a gamma ray escapes from the detector without any interaction. It is described as

\[
P_{\text{path,esc}} (\hat{q}_n) = \exp \left( -\rho \sigma_{\text{all}} \hat{t}_n \right) ,
\]

where \( \hat{t}_n \) is the length between \( \hat{r}_n \) and the boundary of the detector from \( \hat{r}_n \) along the direction of escape.

### 3.2. Probability functions related to measurements

The function \( P_{\text{det}} (\cdot) \) corresponds to the measurement process, and then it is determined by the

![Figure 3: A graphical representation of Compton scattering in a detector and measurement in Compton telescopes. The red arrows correspond to probabilistic processes that take place only in escape events.](image-url)
the interaction position of $\hat{\varepsilon}$ is detected as $\varepsilon$, which is equal to $\hat{\varepsilon}$ where $\hat{\varepsilon}$

4.1. Detector response

The interaction positions. However, it is not practical in terms of computational time because the parameter space becomes of high dimensions, i.e., $(3n + 3)$ dimensions when the number of interactions is $n$.

In this section, we implement the order determination algorithm by focusing on a Compton telescope that measures the interaction positions and deposited energies and does not obtain the trajectories of recoiled electrons. First, we introduce specific forms for the detector response terms. Then, we introduce several approximations to eliminate integral calculations and parameter space search in the likelihood calculation.

4.1. Detector response

To describe the detector response terms $P_{\text{ene}}(\varepsilon | \hat{\varepsilon})$ and $P_{\text{pos}}(\mathbf{r} | \hat{\mathbf{r}})$, we adopt the Gaussian function, which is sufficient in most cases. Namely, these functions are formulated as

$$P_{\text{ene}}(\varepsilon | \hat{\varepsilon})\,d\varepsilon = \frac{1}{\sqrt{2\pi}\sigma^2_{\varepsilon}} \exp\left(-\frac{(\varepsilon - \hat{\varepsilon})^2}{2\sigma^2_{\varepsilon}}\right)\,d\varepsilon ,$$

(23)

$$P_{\text{pos}}(\mathbf{r} | \hat{\mathbf{r}})\,d^3\mathbf{r} = \frac{1}{\sqrt{2\pi}\sigma^2_{\mathbf{r}}} \exp\left(-\frac{(\mathbf{r} - \hat{\mathbf{r}})^2}{2\sigma^2_{\mathbf{r}}}\right)\,d^3\mathbf{r} ,$$

(24)

where $\sigma_{\varepsilon}$, $\sigma_{\mathbf{r}}$, and $\sigma_{\mathbf{y}}$ are the energy and positional resolutions of the detector, respectively.

4.2. Approximations in the likelihood calculation

4.2.1. full-deposit events

For the full-deposit events, $\hat{E}_0^{\text{ML}}$ and the interaction positions are estimated by a good approximation as the sum of the measured deposited energies and the measured positions, respectively:

$$\hat{E}_0^{\text{ML}} \simeq \sum_{i=1}^{n} \hat{\varepsilon}_i ,$$

(25)

$$\hat{\mathbf{r}}_i^{\text{ML}} \simeq \mathbf{r}_{\tau(i)} \quad (i \geq 1) .$$

(26)

In this approximation, we ignore the positional errors of the interaction sites. To compensate for this, we modify the energy resolution in Eq. 23. At $i$-th interaction ($2 \leq i \leq n - 1$), the scattering angle can be calculated geometrically, and the positional errors produce the uncertainty on it, to which we refer as $\Delta(\cos \theta^\text{cat}_{i})_{\text{pos}}$. Considering the propagation of the positional errors as discussed in the classical approach [19], $\Delta(\cos \theta^\text{cat}_{i})_{\text{pos}}$ can be calculated. Then, the partial derivative of Eq. 3 with respect to $\cos \theta^\text{cat}_{i}$ yields

$$\Delta \hat{\varepsilon}_i = \frac{\hat{E}_i^2}{m_e c^2} \Delta(\cos \theta^\text{cat}_{i})_{\text{pos}} ,$$

(27)

which means that the positional errors produce uncertainty on the estimation of the gamma-ray energy through the scattering angle calculation. In our algorithm, to include this effectively, for $2 \leq i \leq n - 1$, we modify the energy resolution as

$$\sigma_{\varepsilon}^2 \rightarrow \sigma_{\varepsilon}^2 + \left(\frac{\hat{E}_i^2}{m_e c^2} \Delta(\cos \theta^\text{cat}_{i})_{\text{pos}}\right)^2 .$$

(28)
The incoming direction \((\hat{\theta}_0^\text{ML}, \hat{\phi}_0^\text{ML})\) should be also determined. In Compton telescopes, the incoming gamma-ray direction is constrained on a circle in the sky. We calculate the first scattering angle under assumption of the incident energy \((E_0^\text{ML})\) and the deposit energy \((\varepsilon_{\tau(1)})\) and the first and second interaction positions \((r_{\tau(1)}, r_{\tau(2)})\), and then the circle can be obtained as the solutions of \((\hat{\theta}_0^\text{ML}, \hat{\phi}_0^\text{ML})\) that satisfies the Compton kinematics:

\[
E_0^\text{ML} = \tilde{E}_1(E_0^\text{ML}, \hat{\theta}_0^\text{ML}, \hat{\phi}_0^\text{ML}, r_{\tau(1)}, r_{\tau(2)}) + \varepsilon_{\tau(1)}. \tag{29}
\]

Here \(\tilde{E}_1\) is calculated by Eqs. [9] and [10].

The function \(P_{\text{path,scat}}(\hat{r}_1 | \hat{q}_0)\) also depends on \(\hat{\theta}_0^\text{ML}\) and \(\hat{\phi}_0^\text{ML}\). Here we assume a constant value for the path length in Eq. [18]

\[
\hat{l}_{\text{first}} = L_0. \tag{30}
\]

This should be comparable to the size scale of the detector. Then, the likelihood values are the same for the parameters \((\hat{\theta}_0^\text{ML}, \phi_0^\text{ML})\) that satisfy Eq. [29], i.e., on a Compton circle, and they are considered to be the approximation of the likelihood value for the assumed scattering order.

### 4.2.2. Escape events

For escape events, the incident gamma-ray energy \(E_0^\text{ML}\) is estimated using the scattering angle measured from geometrical information [13]. Here we calculate the incident gamma-ray energy at each \(i\)-th interaction site \((2 \leq i \leq n - 1)\), and use the averaged value as the estimation. Based on the three-Compton method [20, 22], \(E_0^\text{ML}\) is estimated as

\[
E_0^\text{ML,m} = \frac{1}{n - 2} \sum_{m=2}^{n-1} E_0^\text{ML,m} (n \geq 3), \tag{31}
\]

where,

\[
E_0^\text{ML,m} = \sum_{i=1}^{m} \varepsilon_{\tau(i)} + E_m', \tag{32}
\]

\[
E_m' = -\varepsilon_{\tau(m)} + \sqrt{\left(\varepsilon_{\tau(m)} \right)^2 + \frac{\varepsilon_{\tau(m)} m_e c^2}{1 - \cos \hat{\vartheta}^\text{scat,G}_m}}, \tag{33}
\]

\[
\cos \hat{\vartheta}^\text{scat,G}_m = \frac{(r_{\tau(m)} - r_{\tau(m-1)}) \cdot (r_{\tau(m+1)} - r_{\tau(m)})}{|r_{\tau(m)} - r_{\tau(m-1)}||r_{\tau(m+1)} - r_{\tau(m)}|}. \tag{34}
\]

In the calculation of the likelihood function for escape events, the term \(P_{\text{esc}}(\hat{q}_n, D_{\tau(n)} | \hat{q}_{n-1})\) needs the integration over the direction of escape (see Eq. [15]). To calculate it approximately without integral computation, here we assume that

\[
P_{\text{esc}}(\varepsilon_{\tau(n)} | \varepsilon_n) \simeq \delta (\varepsilon_{\tau(n)} - \varepsilon_n). \tag{35}
\]

We also approximate \(\hat{l}_n\) in Eq. [21] as a constant value:

\[
\hat{l}_\text{esc} = L_\text{esc}, \tag{36}
\]

where \(L_\text{esc}\) should be also comparable to the detector size scale like \(L_0\). Then these approximations yield

\[
P_{\text{esc}}(\hat{q}_n, D_{\tau(n)} | \hat{q}_{n-1})
\]

\[
= \int d(\varepsilon_{\tau(n)} \varepsilon_n) |P_{\text{esc}}(\hat{q}_n, D_{\tau(n)} | \hat{q}_{n-1})| \int d(\varepsilon_{\text{esc}}) |P_{\text{esc}}(\varepsilon_{\text{esc}})\|
\]

\[
\times \int d(\varepsilon_{\tau(n)} \varepsilon_n) |P_{\text{esc}}(\hat{q}_n, D_{\tau(n)} | \hat{q}_{n-1})| \int d(\varepsilon_{\text{esc}}) |P_{\text{esc}}(\varepsilon_{\text{esc}})\|
\]

\[
\times \int d(\varepsilon_{\tau(n)} \varepsilon_n) |P_{\text{esc}}(\hat{q}_n, D_{\tau(n)} | \hat{q}_{n-1})| \int d(\varepsilon_{\text{esc}}) |P_{\text{esc}}(\varepsilon_{\text{esc}})\|
\]

\[
\times \int d(\varepsilon_{\tau(n)} \varepsilon_n) |P_{\text{esc}}(\hat{q}_n, D_{\tau(n)} | \hat{q}_{n-1})| \int d(\varepsilon_{\text{esc}}) |P_{\text{esc}}(\varepsilon_{\text{esc}})\|
\]

Note that here the direction of escape is described with the scattering angle \(\hat{\vartheta}^\text{scat}\) at the last interaction and the azimuth angle \(\hat{\vartheta}^\text{scat,G}\) along \(r_{\tau(n)} - r_{\tau(n-1)}\), not \(\hat{\theta}_n\) and \(\hat{\phi}_n\), because it makes the calculation simpler, e.g., \(d \cos \hat{\vartheta}^\text{scat,G} / d \varepsilon_{\text{esc}}\).

### 5. Algorithm Summary

By calculating the likelihood as described in the previous section, the scattering order and the event type (full-deposit or escape) can be determined as follows.
1. One selects a scattering order from all candidates. Here the selected order is labeled with $k$:

$$(D_{I})_{\text{ordered}}^{k} = (D_{r_a(1)}, D_{r_a(2)}, \ldots, D_{r_a(n)})_{\text{ordered}}.$$  

(38)

When the number of the hits is $n$, the number of the candidates is $n!$, i.e., $1 \leq k \leq n!$.

2. One calculates the likelihood value using the approximated formula introduced in Section 4.2. Then, for each scattering candidate, one obtains the two likelihood values $L_{\text{fulldep}}^{k}$ and $L_{\text{escape}}^{k}$, which correspond to the full-deposit and escape events, respectively. The calculation procedure of $L_{\text{fulldep}}^{k}$ and $L_{\text{escape}}^{k}$ is described in the following subsections.

3. One determines the scattering order and the event type as a set of them that yield the maximum value in all of the calculated $L_{\text{fulldep}}^{k}$ and $L_{\text{escape}}^{k}$.

5.1. Calculation of $L_{\text{fulldep}}^{k}$

1. The incoming gamma-ray energy is calculated as the sum of the detected deposit energy (Eq. 25), and the interaction positions are assumed to be the same as the detected ones (Eq. 26).

2. The first scattering angle is calculated by Eq. 29 and the incoming gamma-ray direction is constrained on a Compton circle in the sky.

3. The likelihood value is calculated using Eq. 11 by applying the approximations described in Eq. 28, 30.

5.2. Calculation of $L_{\text{escape}}^{k}$

1. The incoming gamma-ray energy is calculated by Eq. 31, and the interaction positions are assumed to be the same as the detected ones (Eq. 26).

2. The first scattering angle is calculated by Eq. 29 and the incoming gamma-ray direction is constrained on a Compton circle in the sky.

3. The likelihood value is calculated using Eq. 14 by applying the approximations described in Eq. 28, 30, 37.

When the number of hits is two or fewer, the escape gamma-ray energy cannot be estimated in Eq. 31. Thus, this algorithm can work for 3 or more hit events. Note that if the incident gamma-ray energy is known a priori, then this algorithm can also work for 2-hit events with minor modification (see Section 7.1).

The derived algorithm differs from the MSD methods in that it compares the energy deposit rather than the scattering angle. Effectively, this algorithm calculates the energy deposit at each site assuming the incident gamma-ray energy and interaction positions, and compares it with the measured value directly through the energy response function. Moreover, by adopting the maximum likelihood approach, the physical processes are naturally taken into account in the scattering order determination.

6. Numerical Experiments

In order to test the reconstruction algorithm developed in this work, we apply it to a simulation data set generated by ComptonSoft, a software package of Geant4-based simulation and data analysis for Compton telescopes [39, 40, 41]. The algorithm has a great advantage in the event reconstruction of Compton telescopes with a large sensitive volume. The GRAMS experiment utilizes such a large volume detector using a liquid argon time projection chamber [5]. We choose this type of Compton telescope for a numerical demonstration of the reconstruction algorithm, and evaluate the performance of the algorithm, i.e., the event classification (full-deposit or escape events), the incident gamma-ray energy, the scattering order and the angular resolution.

6.1. Simulation Setup

We assume a simple cubic detector with a size of $30 \times 30 \times 30$ cm$^3$ filled with liquid argon as shown in Figure 4. The energy resolution $\sigma_\varepsilon$ of the detector is set to as follows [5]:

$$\sigma_\varepsilon^2 = (5 \text{ keV})^2 + 0.25 \times (\varepsilon/\text{keV}).$$  

(39)

This equation is also adopted in the likelihood calculation in Eq. 23. The X-Y positions of signals are pixelized with a size of 3 mm, and we set $\sigma_x$ and $\sigma_y$ to be $3/\sqrt{12}$ mm in Eq. 24. It is the standard deviation of X or Y positions of events distributed uniformly in a single pixel. The resolution of the Z position is assumed to $\sigma_z = 1$ mm. In this simulation, the signals in adjacent pixels are merged into a single signal, and the position of the merged signal is set to the center of gravity weighting with the detected energies in the pixels. The energy threshold
of each pixel is set to 25 keV. In this demonstration, we set $L_{\text{first}}$ in Eq. 30 and $L_{\text{esc}}$ in Eq. 36 to be 15 cm, one-half of the detector size.

![Geometry of Geant4 simulation](image)

**Figure 4:** The geometry of Geant4 simulation.

### 6.2. Results of Event Classification and Energy Reconstruction

Here we simulated $10^7$ events of 1 MeV gamma-ray beam incoming from the top of the detector, i.e., $\theta_0 = \pi$. The beam has a radius of 10 cm and is co-aligned at the detector center. Figure 5 shows the count of the detected events with the number of hits. The counts of the full-deposit event reach the maximum at 4 hits. Here we focus on the events with the number of hits from 3 to 8. The ratio of the number of the events with more than 8 hits to the total detected events is just 0.07% and they are negligible.

First, we examine the algorithm performance against full-deposit events qualitatively. Figure 6 shows the energy spectra of all detected events (blue, dotted) and those classified as full-deposit events (red, solid). We confirmed that the events peaking around 1 MeV is correctly classified as full-deposit events and the continuum component below 1 MeV is reduced successfully after the reconstruction algorithm was applied. As the number of hits is increased, the events around 1 MeV are classified as full-deposit more accurately. This is because as the number of hits gets larger, the Compton scattering angle can be calculated redundantly at more sites.

Next, the algorithm performance against escape events is checked. Figure 7 shows energy spectra of events classified as escape events. The blue solid lines are spectra of the sum of deposit energies of events classified as escape events. We confirmed that most of the continuum components are successfully reconstructed as escape events. Moreover, the spectra of incident gamma-ray energy corrected by Eq. 31 (red, solid) shows a clear peak at 1 MeV. It confirms that the algorithm estimates the escape energy correctly.

The shape of the reconstructed energy spectrum of escape events strongly depends on the number of hits; when the number of hits is small, the spectrum has relatively long tails. Figure 8 shows the standard deviation of the reconstructed energy spectra in 900–1100 keV, with different number of hits. The energy resolution of full-deposit events does not depend on the number of hits so much. On the other hand, the energy resolution of escape events becomes better as the number of hits gets larger, due to the different method of the energy estimation. Though the absolute value of the energy resolution varies by the assumed detector response, in general the energy resolutions of the full-deposit and escape events are different from each other, and they have different dependence on the number of hits. This feature should be treated accurately when one performs spectral analysis or image reconstruction quantitatively.

### 6.3. Accuracy of the Event Reconstruction

In order to quantify the performance of the developed algorithm, we define the reconstruction ac-

![Energy spectra of detected events](image)

**Figure 5:** The count of the detected events with the number of hits. Here $10^7$ events of 1 MeV gamma rays are simulated. Note that 0 hit represents the event that gamma ray escapes from the detector without any interaction or all the produced signals are lower than the threshold.
Figure 6: The energy spectra of 1 MeV gamma-ray events classified as full-deposit events. The blue dashed and red solid lines represent the spectra of the total energy deposit of all events and those of the events classified as full-deposit events by the algorithm, respectively.

Figure 7: The energy spectra of 1 MeV gamma-ray events classified as escape events. The blue solid lines represent the spectra of the total energy deposit of events classified as escape events by the algorithm, and the red solid ones represent the spectra of the incident energy of those events, estimated by the algorithm (see Eq. 31). The blue dashed lines are the same as in Figure 6.
accuracy $A_{\text{full}}$ and $A_{\text{esc}}$ as

$$A_{\text{full}} = \frac{N_{\text{full,acc}}}{N_{\text{full}}} \quad \text{(40)}$$

$$A_{\text{esc}} = \frac{N_{\text{esc,acc}}}{N_{\text{esc}}} \quad \text{(41)}$$

where $N_{\text{full}}$ is the total number of detected full-deposit events and $N_{\text{full,acc}}$ is the number of full events that are reconstructed as full-deposit events with the accurate scattering order; $N_{\text{esc}}$ is the total number of detected escape events and $N_{\text{esc,acc}}$ is the number of escape events that are reconstructed as escape events with the accurate scattering order.

We show the reconstruction accuracy for 1 MeV gamma-ray events in Figure 9. In the calculation of $A_{\text{esc}}$, we used only events in which the sum of the actual energy deposits is less than 900 keV because the escape energy is too small to detect due to the detector energy resolution when it is close to 1 MeV. At 6–7 hit and 4–5 hit events, $A_{\text{full}}$ and $A_{\text{esc}}$ get their maximum, respectively. This result can be interpreted qualitatively as follows. As the number of hits is increased, we obtain more information about Compton scattering which occurred in the detector, which helps to determine the scattering order accurately. On the other hand, the number of the scattering order candidates is also increased as the factorial of the number of hits, which would make the event reconstruction more complicating. The trade-off between these two factors is considered to determine the number of hits that yields the highest accuracy.

To further investigate the proposed algorithm’s performance for different incoming gamma-ray energies, we also calculated $A_{\text{full}}$ and $A_{\text{esc}}$ for gamma rays from 500 keV to 10 MeV. The results are shown in Figure 10. Below ~ 1 MeV, 40–50% of 3-hit events and 50–70% of 4 or more hit events are reconstructed accurately. As the incoming energy is increased, $A_{\text{full}}$ and $A_{\text{esc}}$ are decreased, especially above ~ 3 MeV. In the argon detector, at ~ 5 MeV the cross section of pair creation becomes comparable to that of Compton scattering. The contamination of these pair creation events makes the accuracy worse. Moreover, electrons with above few MeV produce gamma rays via bremsstrahlung emission, and these gamma rays are not considered in the algorithm. It also reduces the performance of the event reconstruction. We will discuss it in Section 7.

6.4. Angular Resolution and its dependence on the number of hits

We also investigated the angular resolution of the reconstructed events and its dependence on the number of hits. The angular resolution is evaluated by the angular resolution measure (ARM), which is defined as

$$\text{ARM} = \theta_K - \theta_G \quad \text{(42)}$$

where $\theta_K$ is the estimated first scattering angle:

$$\theta_K = \arccos \left( 1 + m_e c^2 \left( \frac{1}{E_0^{\text{ML}}} - \frac{1}{E_0^{\text{ML}} - E_1} \right) \right) \quad \text{(43)}$$

and $\theta_G$ is the first scattering angle calculated from the detected positions of the first and second hits.
Figure 10: The energy dependence of the accuracy for both full-deposit (left) and escape (right) events. For the escape events, we used only events in which the actual escape energy is more than 100 keV.

Figure 11 shows distributions of ARM for both full-deposit and escape events up to 6 hits. Here the incoming gamma-ray energy is 1 MeV, and the incoming direction is the same as that in Sec. 6.2. In both cases, as the number of hits increases, the tail components and a sub-peak at ∼90 degrees are reduced.

The angular resolution depends on the number of hits. Figure 12 shows FWHMs of the obtained ARM distributions for different number of hits. While the FWHMs for the escape events are nearly constant, those of the full-deposit events depend on the number of hits significantly. This is because full-deposit events with a small number of hits have large scattering angles at the first interaction. Then, the angular resolution becomes worse by the Doppler broadening effect. For example, in the full-deposit case, the ratio of the events with the first scattering angle larger than 60 degrees is ∼70% for 3-hit events and ∼10% for 8-hit events. This can be interpreted as that if the scattering angle is small the scattered gamma rays still have large energy and can be easily scattered in the detector many times. On the other hand, in the escape events, the ratio of the forward scattering events does not depend on the number of hits so much, and the angular resolution is almost constant over the number of hits. This dependence of the angular resolution on the event type and the number of hits should be also treated accurately in the quantitative imaging analysis.

We show a simple back-projection image of the 1 MeV gamma-rays events using both full-deposit and escape events in Figure 13. Here the number of hits is from 3 to 8. It demonstrates that the gamma-ray source is reconstructed successfully by using the multiple Compton scattering events.

7. Discussion and Conclusion

In this work, we have formulated probability functions of physical processes and measurements in Compton telescopes and developed the reconstruction algorithm for the multiple Compton scattering events based on the maximum likelihood method. It can treat both full-deposit and escape events simultaneously. The developed algorithm can be used in large volume Compton telescopes aiming at up to ∼10 MeV. A promising application is the GRAMS experiment which uses a large single-material detector with liquid argon.

We also verified its performance using simulation data sets of a $30 \times 30 \times 30$ cm$^3$ liquid argon detector, and confirmed that the algorithm works well for up to 8-hit events for 1 MeV gamma rays. The reconstruction accuracy defined in Eq. 40 gets its maximum of $A_{\text{full}} \sim 0.5$ at the number of hits of 6–7 for the full-deposit events. In the case of escape events, it was maximized at 4-5 hit events with $A_{\text{esc}} \sim 0.7$. The information about the Compton scattering in the detector increases as the number of hits increases, but also the number of the scattering order candidates increases as the factorial of the number of hits. The trade-off between these two factors determines the reconstruction accuracy and its corresponding number of hits.
Figure 11: ARM distributions of 1 MeV gamma rays with different number of hits. The left and right panels correspond to full-deposit and escape events, respectively.

Figure 12: The angular resolutions of 1 MeV gamma rays for full-deposit and escape events. The FWHMs of the ARM distributions in Figure 11 are shown for different number of hits. The filled round and open square markers correspond to the full-deposit and escape events, respectively.

Figure 13: The simple back-projection image of 1 MeV gamma rays for full-deposit and escape events with the number of hits from 3 to 8.

result suggests that optimizing the number of hits in the detector for a target gamma-ray energy band is an essential factor to achieve good performance of Compton telescopes.

7.1. The use of the likelihood for background reduction and measurement of gamma rays with known energy

The maximum likelihood value obtained from the algorithm is considered to use for background reduction, e.g., random coincidence events. The blue line in Figure 14 shows the distribution of the likelihood value of 3-hit full-deposit events using the 1 MeV gamma-ray simulation data set in Section 6.2. To simply make the random coincidence events, we randomized the positions of the hits in this data set, and applied the reconstruction algorithm to them. The red line in the figure corresponds to the distribution of the likelihood value of these randomized events. As clearly seen, the randomized events have much smaller likelihood values than the gamma-ray events. Thus, such background events can be removed by setting a threshold in the obtained likelihood value, though more realistic simulation is needed to conclude this application.

As another possibility, our algorithm could be used in other fields, e.g., imaging in nuclear medicine therapy or monitoring of high-intensity radiation fields. In these cases, incoming gamma-ray energy is often known a priori, and the reconstruction algorithm can be modified by fixing the incoming energy instead of estimating it by Eq. 25 or 31. This additional information can improve the
reconstruction performance, and allow us to analyze 2-hit events. Figure 15 shows the accuracy of 1 MeV gamma-ray event when fixing the incoming energy. The reconstruction accuracy is improved, especially for full-deposit events with a small number of hits and escape events with any number of hits. Moreover, this method could be also useful to estimate the in-orbit instrumental background of a Compton telescope or to search for gamma-ray emission lines from celestial objects because the energy of the target gamma rays is usually known in these cases.

7.2. Possible extension of the algorithm for electron-tracking Compton telescopes

Though this paper focuses on the case that only the deposit energies and positions are measured, our approach could be extensible even when a Compton telescope can also measure the trajectories of recoiled electrons and estimate their initial momentum directions [13, 14, 15]. In this case, \( D_I \) is needed to be redefined as

\[
D_I = (r_I, \varepsilon_I, p_{e,I}) 
\]

where \( p_{e,I} \) is the measured momentum direction of a recoiled electron. Then, we modify the detector response function \( P_{\text{det}}(D_I | \hat{q}_{1-1}, \hat{q}_I) \) by including the electron trajectory information. Here we introduce a function \( P_{\text{track}}(\cdot) \) that compares the expected direction of a recoiled electron \( \langle \vec{p}_I - \vec{p}_{I-1} \rangle \) and measured one \( \langle p_{e,I} \rangle \). The definition of \( P_{\text{track}}(\cdot) \)
would depend on the configuration of Compton telescopes because the obtained electron images vary by the detectors. As an example, if the 3-dimensional trajectories can be obtained and the difference from the expected recoil direction obeys the Gaussian function, then $P_{\text{track}}(\cdot)$ is determined as

$$P_{\text{track}}(p_{\text{e},l} | \hat{p}_i - \hat{p}_{i-1}) \text{d}\Delta \theta_e = \frac{1}{\sqrt{2\pi\sigma^2_{\Delta\theta_e}}} \exp\left(-\frac{\Delta \theta_e^2}{2\sigma^2_{\Delta\theta_e}}\right) \text{d}\Delta \theta_e,$$  

(45)

$$\Delta \theta_e = \arccos\left(\frac{(\hat{p}_i - \hat{p}_{i-1}) \cdot \hat{p}_{\text{e},l}}{|\hat{p}_i - \hat{p}_{i-1}| |\hat{p}_{\text{e},l}|}\right),$$  

(46)

and $P_{\text{det}}(\cdot)$ is reformulated as

$$P_{\text{det}}(D_I | \hat{q}_{i-1}, \hat{q}_i) = P_{\text{ene}}(\xi_I | \hat{\xi}_i) \times P_{\text{pos}}(r_I | \hat{r}_i) \times P_{\text{track}}(p_{\text{e},l} | \hat{p}_i - \hat{p}_{i-1}) \cdot$$  

(47)

After modifying $P_{\text{det}}(\cdot)$, the scattering order can be determined in the same way as in Section 5 but with one exception. In this case, even if the incoming gamma-ray direction is constrained on a Compton circle, the likelihood value becomes to depend on the location in the circle because the direction of electron recoil varies depending on it. Thus, one needs to specify the gamma-ray incoming direction in a Compton circle, where the likelihood is maximized.

7.3. For further improvement

The developed algorithm successfully reconstructs multiple Compton scattering events with high accuracy. However, two essential factors are not considered. One is the momentum distribution of electrons in the detector materials. When the initial electron momentum is not zero, the scattered gamma-ray energy differs from Eq. 9. This effect is known as the Doppler broadening effect and limits the angular resolution. Effectively, this effect could be considered by adding a function $\sigma_{\text{Doppler}}$ in Eq. 25, which is an uncertainty in the energy determination at each interaction site due to the Doppler broadening effect. Since it depends on the gamma-ray energy, the scattering angle, and detector materials, the function $\sigma_{\text{Doppler}}$ should be carefully modeled. When the Doppler broadening effect is comparable to or dominates over the position and energy resolutions, then such a modification would improve the reconstruction accuracy.

The other factor is bremsstrahlung from scattered electrons in the detectors. Bremsstrahlung becomes the dominant energy loss in high energy band, for example, in argon detector it dominates over the ionization losses at a few MeV. Gamma rays emitted by this process make additional signals, which makes the event reconstruction more complex. Decreasing the accuracy above a few MeV is considered to be partially due to bremsstrahlung (see Figure 10). To treat this process is not straightforward because it is a stochastic process without any strong restriction like Eq. 6. A possible way is to calculate the probability that a given signal is produced by a bremsstrahlung photon, considering energies and lengths to other interaction sites, and then merge it to nearby signals if the calculated probability is large. This calculation is expected to be too complicated to be described by analytic expressions.

In a high energy band, it is also needed to distinguish pair creation events. To consider these factors (the Doppler broadening, bremsstrahlung, and pair creation), other statistical methods using large data sets might be effective, e.g., deep neural network technique. We expect that the combination of the analytical method like this work and simulation-based statistical methods can be one of the promising ways to achieve even better reconstruction performance.

Code availability

The code for the reconstruction algorithm is available at https://github.com/odakahirokazu/ComptonSoft.

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References

[1] V. Schönfelder, The Imaging Gamma-Ray Telescope COMPTEL Aboard GRO. Advances in Space Research 11 (8) (1991) 313–322. doi:10.1016/0273-1177(91)90183-K
[2] V. Schönfelder, et al., The first comptel source catalogue Astronomy and Astrophysics Supplement Series 143 (2) (2000) 145–179. doi:10.1051/aas:2000101
URL https://doi.org/10.1051/aas:2000101
[3] B. P. Abbott, et al., GW170817: Observation of Gravitational Waves from a Binary Neutron Star Inspiral, Physical Review Letters 119 (16) (2017) 161101. doi:10.1103/PhysRevLett.119.161101.

[4] IceCube Collaboration, Neutrino emission from the direction of the blazar TXS 0506+056 prior to the IceCube-170922A alert, Science 361 (6398) (2018) 147–151. doi:10.1126/science.aat2890.

[5] T. Aramaki, P. O. H. Adrian, G. Karagiorgi, H. Odaka, Dual MeV gamma-ray and dark matter observatory - GRAMS Project, Astroparticle Physics 114 (2020) 107–114. doi:10.1016/j.astropartphys.2019.07.002.

[6] J. M. Jaworski, Compton Imaging Algorithms for Position-Sensitive Gamma-Ray Detectors, Ph.D. thesis, The University of Michigan (2018).

[7] K. Vetter, D. Chivers, B. Plimley, A. Coffer, T. Aucott, T. Tanimori, et al., MeV\gamma J. A. Lockwood, L. Hsieh, L. Friling, C. Chen, D. Herzo, A large double scatter telescope for gamma rays and neutrons, Nuclear Instruments and Methods 107 (1973) 385–394. doi:10.1016/0029-554X(73)90257-7.

[8] J. A. Tomskick, et al., The compton spectrometer and detector (CSD) for the lunar gamma-ray observatory (LGO), Journal of Geophysical Research 107 (2002) 1–106. doi:10.1016/j.jheap.2018.07.001.

[9] V. Schönfelder, A. Hirner, K. Schneider, A telescope for soft gamma ray astronomy, Nuclear Instruments and Methods 107 (1973) 385–394. doi:10.1016/0029-554X(73)90257-7.

[10] D. Herzo, A large double scatter telescope for gamma rays and neutrons, Nuclear Instruments and Methods 123 (3) (1975) 583–597. doi:10.1016/0029-554X(75)90257-7.

[11] J. A. Lockwood, L. Hsieh, L. Friling, C. Chen, D. Swartz, Atmospheric neutron and gamma ray fluxes and energy spectra, Journal of Geophysical Research 84 (A4) (1979) 1402–1408. doi:10.1029/JA084iA04p01402.

[12] T. Tanimori, et al., Mev γ-ray imaging detector with micro-tpc, New Astronomy Reviews 48 (1-4) (2004) 263–268. doi:10.1016/j.newar.2003.11.038.

[13] K. Vetter, D. Chivers, B. Plimley, A. Coffer, T. Aucott, Q. Looker, First demonstration of electron-tracking based Compton imaging in semiconductor detectors, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 652 (1) (2011) 599–601. doi:10.1016/j.nima.2011.01.131.

[14] H. Yokoda, S. Saito, S. Watanabe, H. Ikeda, T. Takahashi, Development of Si-CMOS hybrid detectors towards electron tracking based Compton imaging in semiconductor detectors, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 912 (2018) 269–273. doi:10.1016/j.nima.2017.11.078.

[15] S. Wilderness, N. Cleinborne, J. Fessler, W. Rogers, List-mode maximum likelihood reconstruction of compton scatter camera images in nuclear medicine, in: 1998 IEEE Nuclear Science Symposium Conference Record. IEEE Nuclear Science Symposium and Medical Imaging Conference (Cat. No.98CH36255), Vol. 3, 1998, pp. 1716–1720 vol.3. doi:10.1109/NSSMIC.1998.773871.

[16] S. Ikeda, H. Odaka, M. Uemura, T. Takahashi, S. Watanabe, S. Takeda, Bin Mode Estimation Methods for Compton Camera Imaging, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 760 (2014) 46–50. doi:10.1016/j.nima.2014.05.081.

[17] T. Kamae, R. Enomoto, N. Hanada, A new method to measure energy, direction, and polarization of gamma rays, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 260 (1) (1987) 254–257. doi:10.1016/0168-9002(87)90414-0.

[18] S. E. Boggs, P. Jean, Event reconstruction in high resolution Compton telescopes, Astronomy and Astrophysics Supplement Series 145 (2) (2000) 311–321. doi:10.1051/asap:2000107.

[19] J. D. Kurfess, W. N. Johnson, R. A. Kroeger, B. F. Philips, Considerations for the next Compton telescope mission, AIP Conference Proceedings 510 (1) (2000) 789–793. doi:10.1063/1.1303306.

[20] U. G. Oberlack, E. Aprile, A. Curioni, V. Egorov, K.-L. Giboni, Compton scattering sequence reconstruction algorithm for the liquid xenon gamma-ray imaging telescope (LxGrIT), in: Hard X-Ray, Gamma-Ray, and Neutron Detector Physics II, Vol. 4141, International Society for Optics and Photonics, 2000, pp. 168–177. doi:10.1117/12.407578.

[21] R. Kroeger, W. Johnson, J. Kurfess, B. Philips, W. Wulf, Three-compton telescope: theory, simulations, and performance, in: 2001 IEEE Nuclear Science Symposium Conference Record (Cat. No.01CH37310), Vol. 1, 2001, pp. 68–71 vol.1. doi:10.1109/NSSMIC.2001.1008411.

[22] A. Zoglauer, S. E. Boggs, Application of neural networks to the identification of the compton interaction sequence in compton imagers, in: 2007 IEEE Nuclear Science Symposium Conference Record, Vol. 6, 2007, pp. 4436–4441. doi:10.1109/NSSMIC.2007.4437096.

[23] D. Shy, Super-MeV Compton Imaging and 3D Gamma-Ray Imaging Using Pixelated CdZnTe, Ph.D. thesis, The University of Michigan (2020).

[24] J. Chu, Advanced Imaging Algorithms with Position-Sensitive Gamma-Ray Detectors, Ph.D. thesis, The University of Michigan (2018).

[25] J. M. Jaworski, Compton Imaging Algorithms for Position-Sensitive Gamma-Ray Detectors in the Presence of Motion, Ph.D. thesis, The University of Michigan (2013).

[26] C. G. Wahl, Imaging, Detection, and Identification Algorithms for Position-Sensitive Gamma-Ray Detectors, Ph.D. thesis, The University of Michigan (2011).

[27] D. Xu, Gamma-ray imaging and polarization measure using 3-d position-sensitive CdZnTe detectors, Ph.D. thesis, The University of Michigan (2006).

[28] C. E. Lehner, 4-pi Compton imaging using a single 3-d position sensitive CdZnTe detector, Ph.D. thesis, The University of Michigan (2004).

[29] D. Xu, Z. He, C. E. Lehner, F. Zhang, 4-pi Compton imaging with single 3D position-sensitive CdZnTe de-
[32] D. Shy, Z. He, Gamma-ray tracking for high energy gamma-ray imaging in pixelated CdZnTe, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 954 (2020) 161443, symposium on Radiation Measurements and Applications XVII. doi:https://doi.org/10.1016/j.nima.2018.10.121

[33] S. Tashenov, J. Gerl, Tango—new tracking algorithm for gamma-rays, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 622 (3) (2010) 592–601. doi:https://doi.org/10.1016/j.nima.2010.07.040

[34] S. Tashenov, Circular polarimetry with gamma-ray tracking detectors, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 640 (1) (2011) 164–169. doi:https://doi.org/10.1016/j.nima.2011.03.011

[35] A. Korichi, T. Lauritsen, Tracking $\gamma$ rays in highly segmented HPGe detectors: A review of AGATA and GRETINA, European Physical Journal A 55 (7) (2019) 121. doi:10.1140/epja/i2019-12787-1

[36] A. Zoglauer, G. Kanbach, Doppler broadening as a lower limit to the angular resolution of next-generation Compton telescopes, in: X-Ray and Gamma-Ray Telescopes and Instruments for Astronomy, Vol. 4851, International Society for Optics and Photonics, SPIE, 2003, pp. 1302 – 1309. doi:10.1117/12.461177

[37] O. Klein, Y. Nishina, Über die streuung von strahlung durch freie elektronen nach der neuen relativistischen quantendynamik von dirac, Zeitschrift für Physik 52 (11) (1929) 853–868. doi:10.1007/BF01366453

[38] J. Fernández, Polarization effects and gamma transport, Applied Radiation and Isotopes 46 (6) (1995) 383–400. doi:https://doi.org/10.1016/0969-8043(95)00030-5

[39] H. Odaka, et al., Development of an integrated response generator for Si/CdTe semiconductor Compton cameras, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 624 (2) (2010) 303–309, new Developments in Radiation Detectors. doi:10.1016/j.nima.2009.11.052

[40] H. Odaka, et al., Modeling of proton-induced radioactivation background in hard X-ray telescopes: Geant4-based simulation and its demonstration by Hitomi’s measurement in a low Earth orbit, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 891 (2018) 92–105. doi:10.1016/j.nima.2018.02.073

[41] S. Agostinelli, et al., Geant4—a simulation toolkit, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 506 (3) (2003) 250 – 303. doi:10.1016/S0168-9002(03)01368-8