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Integrated optical and nuclear simulation of a monolithic LYSO:Ce based PET detector module

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\textbf{Abstract}: In the recent years new digital photon counter devices (also known as silicon photomultipliers, SiPMs) were designed and manufactured to be used specifically in positron emission tomography (PET) scanners. Finely pixelated SiPM arrays have opened new opportunities in PET detector development, such as the utilization of monolithic scintillator crystals. We worked out a simulation tool (SCOPE2) to assist the optimization and characterization of such PET detector modules. In the present paper we report the first application of SCOPE2 on the performance evaluation of a prototype PET detector module. The PET detector is based on monolithic LYSO:Ce scintillator crystal and a fully digital, silicon photon-counter, SPADnet-I. A new interface has been developed for SCOPE2 to access GATE simulation results. A combination of GATE and SCOPE2 was used to simulate excitation of the prototype PET detector with an electronically collimated $\gamma$-beam. Measurement results from the collimated $\gamma$-beam experiment were compared with the combined simulation. A good agreement was observed in the tendencies of total count spectrum and point of interaction distribution. We used the performance evaluation to understand and explain the measurement results in detail.

\textbf{Keywords}: Gamma camera, SPECT, PET PET/CT, coronary CT angiography (CTA); Gamma detectors (scintillators, CZT, HPG, Hgl etc); Scintillators, scintillation and light emission processes (solid, gas and liquid scintillators); Simulation methods and programs

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1 Introduction

Positron emission tomography (PET) is one of the widely used 3D imaging techniques in today’s medical diagnosis besides computer tomography (CT) and magnetic resonance imaging (MRI). Its principle of operation is based on the detection of pairs of annihilation $\gamma$-photons that are emitted due to the interaction of the patient’s body with some positron emitter contrast agent [1] injected into it. The 3D image of the contrast agent distribution can be reconstructed from the so called lines of responses (LORs). An LOR is a line along which a pair of annihilation $\gamma$-photons is emitted (opposite to each other). The position of this line is determined from the points of interaction (POIs) of the $\gamma$-photons with PET detector blocks, see figure 1. These blocks are built up from scintillator crystals and photon counters coupled to them. The scintillator material converts $\gamma$-photon energy into optical photons emitted in the UV-visible range. The photon counter records the spatial distribution of optical photons, from which the POI can be determined.

Another quantity that has to be calculated from the PET detector signal is the energy absorbed in the scintillator crystal. This is important in order to separate useful light flashes induced by annihilation $\gamma$-photons from false events generated by other sources of noise: Compton-scattered $\gamma$-photons and self-radiation of the scintillation material. Annihilation $\gamma$-photons have a characteristic
511 keV energy and the energy of the majority of false events is below this value thus they can be effectively filtered based on scintillation energy. The more precisely we measure energy, the less noise is present in the reconstructed image.

Conventional PET detector modules are composed of an array of relatively long and thin scintillator crystals coupled to photomultiplier tubes (PMT). The crystals face the PMTs with their smaller side. In these modules the determination of a POI location means the identification of the given crystal element in which the scintillation occurred [2]. As a consequence, only two of the three spatial POI coordinates can be resolved, the depth of interaction (DOI) — measured in the direction perpendicular to the photon counter’s surface — is lost. The newly developed finely pixelated photon counters [3–6] make it possible to detect the POI in 3D, if a several centimetre thick scintillator crystal slab is coupled to them [7, 8]. The energy and spatial resolution of such modules are more sensitive to changes in POI than the earlier concepts [9, 10]. In addition, dependence on a new parameter, the depth of interaction (DOI) also comes into view.

In summary, the design, optimization, and performance evaluation of slab scintillator-based modules are not straightforward tasks. In order to aid these tasks we developed a precise simulation tool called SCOPE2 [11] using MATLAB programming language [12]. We also proposed a validation method to check the reliability and estimate the precision of the PET detector models [13].

Our aim is to design and characterize a new generation of PET detector modules based on continuous LYSO:Ce scintillator crystals (slabs) and digital silicon photo-multipliers developed in the frame of the SPADnet European project [14]. The concept of the SPADnet sensors is built around single photon avalanche diodes (SPADs) working in Geiger mode [15]. These sensor elements are responsible for the conversion of incoming optical photons (UV and visible) to electric signals (i.e. electron avalanches). Their output is individually digitized and by utilizing CMOS technology, the digital processing circuits are implemented on-chip. This is why we refer to the SPADnet chips as fully digital. The first prototype of the SPADnet sensors is called SPADnet-I (see figure 2).

In this paper we report the results of the performance evaluation of a SPADnet-I based prototype PET detector and conclude on its applicability. Our primary goal is to give an example of PET
detector performance evaluation using SCOPE2 results. Furthermore we show how these results can be used for understanding the effects taking place in a given PET module. Secondly we report on a modification for SCOPE2 that makes it possible to interface with $\gamma$-transport Monte Carlo code, GATE [16]. With this upgraded version not only performance evaluation but precise simulation of full experimental arrangements is made possible. The experimental and simulation results of an electronically collimated $\gamma$-beam [17] arrangement are presented and compared to each other.

2 Simulation methods and algorithms

We developed SCOPE2, a simulation tool to aid the design, optimization and simulation-based performance evaluation of PET detector modules. Our primary aim is to design PET detector modules based on state-of-the-art digital photon-counters — primarily SPADnet sensors — and monolithic scintillator crystals.

The detailed description of SCOPE2 and its validation method was published earlier, see [11, 12]. In the following subsections we give an overview of the PET detector performance evaluation process and the corresponding performance indicators that we use in this paper. POI and energy estimation algorithms required to be able to evaluate the performance of a PET detector are also discussed here.

2.1 Algorithms used with the detector module

The development of POI estimating algorithms is an intensively researched field within the PET community. In this paper the aim is only to demonstrate the PET detector evaluation capability of SCOPE2 so we choose a simple and already known solution for lateral position estimation. Center of gravity (COG) or Anger-method [18] is used to estimate the position of the lateral coordinates ($x$ and $y$ in figure 5) of a scintillation. We denote the $x$ and $y$ directional COG coordinates with $\xi$ and $\eta$ respectively.

To estimate the depth of interaction (DOI, $z$ direction) of scintillations, we calculate the root mean square (RMS) spot size of the light distribution recorded by the photo-sensor. This method was proposed and evaluated by Lerche et al. [19, 20]. The position estimation is based on the fact that the size of the light spot is larger if the POI is farther away from the photon-counter in monolithic scintillators. The size of the spot on the photon-counter is limited by the effect of total
internal reflection (TIR). Light rays incident to the sensor side face of the scintillator under an angle of incidence larger than the angle of TIR are reflected back into the scintillator.

The RMS spot size can be calculated along given directions (x or y) or radially around the COG coordinates. Due to the geometry of our PET detector we decided to evaluate the RMS spot size along y direction using the following formula:

$$\sigma_y = \sqrt{\frac{\sum_k c_k \cdot (\eta - Y_k)^2}{\sum_k c_k}},$$

(2.1)

where $\sigma_y$ is the RMS radius of the light distribution in y direction, $\eta$ is the estimated y position of the given POI, $c_k$ is the number of photon count in the k\textsuperscript{th} pixel, $Y_k$ is the y coordinate of the center of the k\textsuperscript{th} pixel.

A relation needs to be set up to calculate the depth coordinate from the RMS spot size. Lerche et al. proposed a corresponding method, but that is only valid if the relation is linear [20]. In our case this cannot be guaranteed in advance. So at this stage we only investigate the spot size as a potential indicator of DOI (see sections 2.2 and 5.3).

The estimation of the absorbed $\gamma$-photon energy is made by summing the pixel counts from the scintillation ($N_c$). By using a calibration factor or factors the energy can be calculated. In case of the PET detector investigated here, we expect that the calibration factor will depend on the spatial position of the POI. Thus this would require a complex calibration process. Consequently — just like in case of the RMS spot size — we only investigate the statistics of total count as a potential indicator of the absorbed energy and do not perform calibration.

### 2.2 Simulation-based performance evaluation

Performance of monolithic scintillator-based PET detector modules can vary to a great extent with POI [9, 10]. For design and optimization purposes it is crucial to understand what the reason of such variations is and in which region of the detector module it is significant. Evaluation of the PET detector module in our words means the investigation of performance indicators vs. spatial position of POI. These performance indicators are the following:

- energy and spatial resolution
- width of spot size distribution
- bias of position estimation
- spread of energy and spot size estimation.

During the evaluation we calculate these values at the vertices of a 3D grid inside the scintillator (see figure 3). We simulate typically 1000 absorption events of 511 keV $\gamma$-photons at each of these POIs. Resolution, distribution width, bias and spread of the calculated quantities are determined by analyzing their histograms. The calculation method for energy and spatial position are described in section 2.1. Here we discuss the resolution (i.e. distribution width), bias and spread definitions used later on. The formulae are given for an arbitrary performance indicator ($p$), and will be assigned to actual parameters in section 5.
We use two resolution definitions in this investigation. Absolute width of distribution or resolution is defined by the full-width at half-maximum (FWHM, $p_{\text{FWHM}}$) and the full-width at tenth-maximum (FWTM, $p_{\text{FWTM}}$) of the generated histograms. Relative resolution is based on the FWHM of parameter histograms and is defined the following way in percent:

$$\Delta r_p = 100 \cdot \frac{p_{\text{FWHM}}}{\bar{p}}.$$  \hspace{1cm} (2.2)

where $\bar{p}$ is the mean value. To evaluate the bias, we use two definitions depending on the parameter considered. The absolute bias, $\Delta a p$ is given as the absolute difference of the mean estimated ($\bar{p}$) and real value ($p_0$) as defined below.

$$\Delta a p = |\bar{p} - p_0|.$$  \hspace{1cm} (2.3)

The relative spread, $\Delta r p$ is defined in percent as the difference of the estimated mean ($\bar{p}$) and the actual value ($p_0$) normalized, as given below.

$$\Delta r p = 100 \cdot \frac{\bar{p} - p_0}{p_0}.$$ \hspace{1cm} (2.4)

Figure 3. Illustration of POI grid defined inside the investigated PET detector modules. Coordinate system used to define positions in the scintillator is also depicted.

3 Interface to GATE simulations

SCOPE2 was developed to aid the design and performance evaluation of PET detector arrangements. As described in section 2.1 the performance evaluation consists of the estimation of detector performance indicators as a function of spatial position of POI. Consequently the interface and structure of SCOPE2 was developed to handle single $\gamma$-photon absorptions in POIs lying on the vertices of a 3D grid [11].

In order to make the simulation of detector test arrangements possible we modified the photonic simulation block (see figure 4) to be compatible with GATE [16] generated output. This way we can use the POI and absorbed energy values calculated from particle through matter simulations of
GATE. This new element of SCOPE2 is called extended photonic simulation block. It consists of four main steps as depicted in figure 4:

1. The data interface reads the text based results of GATE. This file contains information about the energy deposited by each simulated γ-photon in the scintillator material, the transferred energy ($E_i$), the coordinate of the position of absorption ($x_i$) and the identifier (ID) of the simulated γ-photon ($ε_i$) are stored. The latter information is required to group those absorption events which are related to the same γ-photon emission (see step 3)).

2. 2D probability density function of avalanche events ($ADF$) is generated by geometrical optical simulation for POIs lying on the vertices of a pre-defined 3D grid (see figure 3 and [11]). By using 3D linear interpolation (trilinear interpolation [21]) the $ADF$ of any intermediate point can be approximated.

3. With all this information the photonic simulation block is able to create the distribution of avalanche coordinates for each absorption event in the scintillation list.

4. The role of the scintillation event adder is to merge the avalanche distributions resultant from two or more distinct scintillations (different POI or energy) but related to the same γ-photon emission. The output of the scintillation event adder is a list of avalanche event distributions which correspond to individual γ-photon emissions and is used as input for the electronic simulation block.

A typical example of such an event is a Compton scattered γ-photon inside the scintillator, when the excitations occur at minimum two positions. If the size of the detector is small (several cm) the time difference between such scintillations is very small compared to the time resolution of the photon counter, thus they contribute to the same image on the sensor like they were simultaneous events. The size of the PET detector modules that we want to investigate are all fulfilling the above condition. Consequently, we use the scintillation event adder without applying any further tests on the distance of events with identical IDs.

We have to emphasise that the handling of the time of the arrival of γ-photons in this simulation environment is still simplified. We consider that there is always only one γ-photon impinging into the scintillator within the integration time of the photon-counter. So cases where high count rates are expected or the scintillations due to the self-radiation of the scintillator gives a significant background cannot be modelled without further developments. With this modification SCOPE2 is able to work as an extension of GATE for detailed optical modelling of the PET detectors in complex geometries if the expected count rate is low.

4 Prototype PET detector

Our group formerly published a study [22] where we optimized the photon extraction efficiency of pixelated scintillator arrays. We investigated the effect of the application of specular and diffuse reflectors on the facets of scintillator crystals elements. In the best performing solutions the scintillator faces were covered with a combination of mirror film layers and diffuse reflectors and they were optically coupled to the photo-detector surface. We built up the first version of our
monolithic scintillator based prototype PET detector using these results (see figure 5). In this section we describe the arrangement of the detector module, and provide details on the optical model of system components and the applied materials.

The nominal size of the Saint-Gobain PreLude 420 [23] LYSO:Ce scintillator crystal is $5 \times 20 \times 10 \text{ mm}^3$ in the x, y and z directions respectively. We covered the $\gamma$-side (i.e., the side towards the field of view of the PET system) of the scintillator with mirror film (3M ESR [24]) and the shorter side faces with Toray Lumirror E60L [25] type diffuse reflectors. The diffuse reflectors are optically coupled to the crystal by Visilux V-788 refractive index matching gel. In between the mirror film and the scintillator there is a small (several 100 $\mu$m) air gap. The faces parallel to the $\gamma$–z plane were painted black by using Edding 750 paint marker. With the black paint we intend to eliminate the effect of these side faces so to mimic that the PET detector is infinite in the x direction. We coupled optically two SPADnet-I prototype photon-counters to one of the $5 \times 20 \text{ mm}^2$ faces, but we are only collecting data from one of the sensors due to the limitations of the prototype sensor’s electronics (see figure 5).

The optical model of the SPADnet-I sensor (with cover glass) and LYSO:Ce scintillator (including the scintillation as a light source) are reused in many of our simulations. Their optical properties were investigated in detail previously [26, 27] and the optical models can be found in [11]. The actual geometry of the scintillator crystal is plotted in figure 6a. The optical model of the 3M ESR...
mirror film and the Toray Lumirror E60L diffuse reflector are summarized in table 1 and figure 6b. We validated our simulation model by the UV excitation-based method as described in [13].

<table>
<thead>
<tr>
<th>Component</th>
<th>Parameter name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffuse reflector</td>
<td>Reflectance</td>
<td>95%</td>
</tr>
<tr>
<td>(Toray Lumirror E60L)</td>
<td>Scattering</td>
<td>Lambertian profile</td>
</tr>
<tr>
<td>Specular reflector</td>
<td>Reflectance</td>
<td>see figure 6b</td>
</tr>
<tr>
<td>(3M Vikuiti ESR film)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

5 PET detector performance evaluation

We evaluate the performance of the prototype PET detector module described in section 4. The evaluation is performed as described in section 2, using the results of SCOPE2 simulation tool.

In accordance with these previous sections we simulated 1000 scintillations at POIs defined by a $5 \times 10 \times 10$ (in $x$, $y$ and $z$ direction respectively) element grid inside the scintillator. The reference coordinate system is fixed to one of the corners of the crystal as it is depicted in figure 5. The position of the first POI is $x_0 = 0.49$ mm, $y_0 = 0.5$ mm, $z_0 = -0.41$ mm and the pitch is $\Delta x = \Delta y = -1.0$ mm $\Delta z = 1.0$ mm respectively.

5.1 Absorbed energy estimation

In order to investigate the absorbed energy estimation performance of the PET detector we evaluated the statistics of total counts ($N_t$). We generated a histogram of total counts for each POI with a

Figure 5. Construction of the prototype PET detector module.
bin size of 2 counts and these histograms were fitted with Gaussian functions [28]. The standard deviation ($\sigma_{N}$) and the mean ($\bar{N}_c$) of the Gaussian function was determined from the fit. An example of such a fit is shown on figure 7.

Using the parameters from the fit the relative FWHM resolution ($\Delta_r N_c$) was calculated (see section 2.2).

$$\Delta_r N_c = \frac{N_{\text{FWHM}}}{N_c}$$  \hspace{1cm} (5.1)

The total count averaged over all investigated POIs was also calculated and found to be $N_{c0} = 180.86$ counts. The variation of the relative resolution is depicted in figure 10a as a function of depth (z direction) at 3 representative lateral positions: at the middle of the photon-counter ($x = 2.49\text{ mm}$, $y = 4.5\text{ mm}$), at one of the corners of the scintillator ($x = 0.49\text{ mm}$, $y = 0.5\text{ mm}$) and at the middle of the longer edge ($x = 0.49\text{ mm}$, $y = 4.5\text{ mm}$). We refer to this three representative positions as A, B and C respectively (see figure 8).
Energy resolution averaged over all investigated POIs is 17.8% ± 2.4%. The value of total count varies with the POI. We use the definition of the relative spread to characterize this effect (see section 2.2). The relative bias spread of the total count is defined by the following equation:

\[
\Delta_r N_c = 100 \cdot \frac{N_c - N_{c0}}{N_{c0}},
\]

where \(N_c\) is the average total count from the selected POI, \(N_{c0}\) is the average total count over all investigated POIs. The results are presented in figure 10b and 10c. The mean value of the total count spread is 0 with standard deviation 25.2%.

Figure 10 shows that both the collected photon counts and its resolution vary greatly with spatial position. The energy resolution variation is mainly depth (z direction) dependent with laterally mostly homogenous performance. The absolute scale of the resolution (13%–20%) lags behind the state-of-the-art PET modules [29, 30]. The reason of the poor energy resolution is the relatively small surface of the prototype photon-counter which required the use of relatively narrow (x direction) but thick (z direction) crystal, thus many photons were lost on the side-faces in the x–y plane. The energy resolution could be improved by extending the future PET detector in the x direction. Figure 10c shows the spread of total number of counts collected by the sensor from a given region of the scintillator. As it can be seen the spread of total count varies with the distance from the edges of the sensor. Close to the sensor more photons are collected from those POIs which are closer to the center of the sensor then the ones around the edges. As the POI distance from the sensor gets larger the lateral distribution of photon collection also changes. In larger distances from the sensor, the \(y = 0\) mm side of the scintillator performs better in light extraction. This is due to the diffuse reflector placed on the nearby edge. It helps to save photons that would otherwise escape from the scintillator. If the POIs are in larger distance from the diffuse reflector its effect is less dominant. Additionally larger portion of photons emitted from POIs further away from the reflector impinge to the dummy sensor and thus not considered. This further reduces light collection efficiency closer to the dummy sensor. Also in x direction a slight asymmetry can be observed on figure 10c. The reason for that is the following: the active area of the sensor is slightly smaller than the scintillator and due to geometrical constraints it is not symmetrically placed. This results in photon loss on one side of the module and makes the photon collection asymmetric. The position of the maximum is shifted in different directions close to the sensor and close to the \(\gamma\)-side. This is due to multiple reflections inside the module. It is expected that with a larger detector module and larger sensor the spread can be reduced by lowering the portion of the area affected by the edges.
Not only the edges, but the scintillator crystal facets also have some effect on the photon distribution and thus the energy resolution. In figure 10a, B position the energy resolution changes more than 2% in less than 2 mm depth variation, close to the sensor. This effect can be explained by light transmission through the sensor side, x directional facet of the scintillator (see figure 9). The facet behaves like a prism: it directs the light of the nearby POIs towards the sensor. Photons arriving from more distant \( z \) coordinates reach the facet under larger angle of incidence than the critical angle of total internal reflection (TIR), i.e. 33° for LYSO:Ce. Consequently, for these POIs the facet casts a shadow on the sensor reducing light extraction, which result in worse energy resolution.

A similar but smaller drop in energy resolution can be observed in figure 10a at position B, between \( z = -2 \) mm and 0 mm. The reason for this phenomenon is also TIR, but this time on the black painted, longer side-face of the scintillator. As we reported in [11] the black finish used by us has an effective refractive index of 1.55, so the angle of total internal reflection on this surface is 59°. For larger angles of incidence its reflection is 53 × larger than for smaller ones. By considering the geometry of the scintillator, one can see that photons reach the black side face under smaller angle then its TIR angle, except those originated from the vicinity of the \( \gamma \)-side. This increases photon counts on the sensor and thus improves energy resolution.

**Figure 9.** Transmission of light rays from scintillations at different depths, through the facet of the scintillator crystal. A ray impinges to the facet under larger angle than TIR angle (red) and under smaller angle of incidence (green).

### 5.2 Lateral POI estimation

For the lateral (x–y plane) position estimation algorithm absolute FWHM and FWTM spatial resolutions [31] were determined by generating 2D position histograms for each POIs. The bin size of the histogram was 0.1 mm in both directions. After the normalization of the position histogram their values can be considered as discrete sampling of the probability distribution of the estimated lateral POI. We used 2D linear interpolation between the sampled points to determine the values correspond to FWHM and FWTM of each distribution (one per investigated POI). In 2D these values form a curve around the maximum of the POI histogram. In figure 11 the position histograms with the corresponding FWHM and FWTM curves are plotted for 9 selected POIs.
The absolute FWHM and FWTM resolution (see section 2.2) values were determined in both x and y directions. We define these values in a given direction as the maximum distance between the points of the curve as explained in figure 12. Variation of spatial resolution with depth at our three representative lateral positions is plotted in figure 13a. The values averaged for all investigated POIs are summarized in table 2.

**Table 2.** Average FWHM and FWTM lateral spatial resolution for all investigated POIs in x and y direction for estimated coordinates (COG algorithm).

<table>
<thead>
<tr>
<th>Direction</th>
<th>FWHM Mean</th>
<th>Standard deviation</th>
<th>FWTM Mean</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>0.23 mm</td>
<td>0.03 mm</td>
<td>0.45 mm</td>
<td>0.06 mm</td>
</tr>
<tr>
<td>y</td>
<td>0.45 mm</td>
<td>0.10 mm</td>
<td>0.85 mm</td>
<td>0.18 mm</td>
</tr>
</tbody>
</table>

The mean of the coordinate position histograms was also calculated for all POI. To illustrate the bias of the estimated coordinates we show the typical distortion patterns for POIs at three different depths in figure 13c.

As it can be seen bias has significant variation with depth and lateral position as well. The absolute bias values ($\Delta \xi, \Delta \eta$) were calculated as defined in section 2.2 for x and y direction using the following formulae:

$$\Delta \xi = |x - \bar{\xi}|$$  \hspace{1cm} (5.3)

and

$$\Delta \eta = |y - \bar{\eta}|,$$  \hspace{1cm} (5.4)

where $x$ and $y$ are the lateral coordinates of the POI, $\bar{\xi}$ and $\bar{\eta}$ are the mean of the estimated lateral position coordinates. In order to facilitate its analysis we give the averaged minimum and maximum value as a function of depth. The results are shown in figure 13b.

The resolution of the estimated POIs (COG coordinate resolution) is comparable to similar prototype modules [32], however its value largely depends on the direction of the evaluation. In x direction the resolution is approximately two times better then in y direction. Furthermore, the POI estimation suffers from significant bias so that it deteriorates compression-corrected spatial resolution and thus reconstruction of lateral POI coordinates. The bias of the position estimation varies with lateral position and dominated by barrel type shrinkage. Its average value is comparable in the two investigated directions, but its maximum is larger in y direction for all depths. An approximately $-1$ mm offset can be observed in $\xi$ and $-0.5$ mm $\eta$ directions on figure 13c. The offset in $\xi$ direction can be understood by considering the offset of the sensor’s active area with respect to the scintillator crystal’s symmetry plane as explained in subsection 5.1. This results in photon loss on one side causing an offset in COG position estimation. The shift in $\eta$ direction is the result of the diffuse reflector on the crystal edge at $y = 0$, which can be imagined as a homogenous illumination on the side wall that pulls all COG position estimation towards the $y = 0$ plane.

The bias increases as the POI is getting farther away from the photon-counter. Such behavior can be explained by considering the optical arrangement of the module. If the POI is far from the
Figure 10. Variation of relative FWHM energy (total counts) resolution of total counts as a function of depth $(z)$ at three representative lateral positions. At the middle of the photon-counter (blue), at one corner (red), and at the middle of its longer edge (green) (a). Relative spread of total counts averaged for all POIs with a given $z$ coordinate (bold line), the minimum and maximum from all investigated depths (thin lines) (b). Relative spread of total counts detected by the photon-counter for all POIs in three different depths (c).

In order to make the spatial resolution comparable to PET detectors with minimal bias we calculated the so-called compression-compensated resolution values. This can be done by considering photon-counter the portion of photons directly reaching the sensor is reduced. In other words large part of the beam is truncated by the side-walls of the crystal and the contour of the beam is less well defined on the sensor. This in itself increases the bias. In this configuration some of the faces are covered with reflectors (diffuse and specular). Multiple reflections on these surfaces result in a scattered light background, that depends only slightly on the POI. The contribution of this is more dominant if the total amount of direct photons decreases [34].
Figure 11. 2D position histograms of lateral position estimation (x–y plane) for 9 selected POIs. Three different depths at the middle of the photon counter (A position), at one of its corners (B position) and at the middle of its longer edge. Black and white curves correspond to FWHM and FWTM values respectively.

the local compression ratios of the position estimation in the following way:

\[
\Delta c \xi_{\text{FWHM}} = \frac{\xi_{\text{FWHM}}(x, y)}{r_x(x, y)}, \quad (5.5)
\]

\[
\Delta c \eta_{\text{FWHM}} = \frac{\eta_{\text{FWHM}}(x, y)}{r_y(x, y)}, \quad (5.6)
\]

where \(\xi_{\text{FWHM}}\) and \(\eta_{\text{FWHM}}\) are the non-corrected FWHM spatial resolutions \(r_x\) and \(r_y\) are the local compression ratios, both in x and y direction, respectively. The correction can be defined similarly to FWTM resolution as well. The compression ratios are estimated with the following formulae

\[
r_x = \frac{\partial \hat{\xi}(x, y)}{\partial x}, \quad (5.7)
\]

\[
r_y = \frac{\partial \hat{\eta}(x, y)}{\partial y}. \quad (5.8)
\]
Figure 12. Explanation of the FWHM and FWHM resolution in x direction for the 2D position histograms.

Figure 13. Variation of FWHM spatial resolution of estimated coordinates (COG algorithm) in x and y direction as a function of depth (z) at three representative lateral positions. At the middle of the photon-counter (blue), at one corner (red) and at the middle of its longer edge (green) (a). Average (bold line) minimum and maximum (thin line) absolute bias in x and y direction of position estimation as a function of depth (z) (b). Estimated lateral positions of the investigated POIs at three different depths. Blue dots represent the estimated average position ($\xi$, $\eta$) of the investigated POIs (c).
Unlike non-corrected resolution, the statistics of corrected values is strongly non-symmetrical to the maximum. Consequently, we also report the median of compression-corrected lateral spatial resolution in table 3 besides mean and standard deviation for all investigated POIs.

**Table 3.** Median, mean and standard deviation of compression-corrected FWHM and FWTM lateral spatial resolution for all investigated POIs in x and y direction.

<table>
<thead>
<tr>
<th>Direction</th>
<th>FWHM Median</th>
<th>FWHM Mean</th>
<th>FWHM Standard deviation</th>
<th>FWTM Median</th>
<th>FWTM Mean</th>
<th>FWTM Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>x</td>
<td>3.61 mm</td>
<td>10.90 mm</td>
<td>46.67 mm</td>
<td>6.74 mm</td>
<td>20.48 mm</td>
<td>84.89 mm</td>
</tr>
<tr>
<td>y</td>
<td>2.55 mm</td>
<td>4.90 mm</td>
<td>18.00 mm</td>
<td>4.96 mm</td>
<td>9.32 mm</td>
<td>37.43 mm</td>
</tr>
</tbody>
</table>

The value of mean and standard deviation in table 3 implies that at significant portion of the investigated POIs the compression-corrected spatial resolution is comparable or larger than the size of the detector module. From figure 13 it is clear that the bias is large at the $\gamma$-side of the detector module. From this we can conclude that POIs in the $\gamma$-side half of the module cannot be resolved or effectively decompressed.

5.3 Depth of interaction estimation

The RMS light spot size in y direction is calculated as defined in section 2.2. The histograms were generated for all POIs as in the previous cases. Lerche et al. proposed to model the statistics of spot size by using Gaussian distribution [19]. An example of the spot size distribution and the Gaussian fit is depicted in figure 14a. We report in figure 14b the mean values of $\sigma_y$ for some selected POIs ($\bar{\sigma}_y$) to alleviate the understanding of the spot size distribution and spread results.

Absolute FWHM and FWTM width of the light spot distribution are calculated based on the curve fit. The value of FWHM size are plotted as a function of depth for the three lateral points mentioned earlier (see figure 15a). The FWHM and FWTM distribution sizes were averaged for all POIs and their values are given in table 4.

**Table 4.** Average absolute FWHM and FWTM width of light spot distribution estimation (y direction).

<table>
<thead>
<tr>
<th>Absolute FWHM width of distribution</th>
<th>Absolute FWTM width of distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>Standard deviation</td>
</tr>
<tr>
<td>Mean</td>
<td>1.52 mm</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.27 mm</td>
</tr>
<tr>
<td>Mean</td>
<td>2.77 mm</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.51 mm</td>
</tr>
</tbody>
</table>

The light spot size — just like all the previous parameters — depends on the POI. In order to characterize this we calculate its spread, which is calculated for each depth ($z = \text{const}$) independently by taking the average of $\bar{\sigma}_y$ from all POIs in the given depth as a reference value (see eq. (5.9)–(5.10)):

$$\Delta_y \bar{\sigma}_y (z_i) = 100 \cdot \frac{\bar{\sigma}_y - \sigma_{y0} (z_i)}{\sigma_{y0} (z_i)}, \quad (5.9)$$
Figure 14. Histogram of light spot size at a given POI \((x = 2.49 \text{ mm}, y = 4.5 \text{ mm}, z = -7.41 \text{ mm})\) and the Gaussian function fit (a). Size of the light spot as a function of depth (\(z\) direction) in case of 3 representative points and the mean spot size from each investigated depths (b).

where

\[
\sigma_{y0}(z) = \frac{\sum_{z=\text{const.}} \sigma_y(x_i, y_i, z_i)}{n_{\text{POI}}(z)}.
\]  

(5.10)

Parameters \(x_i, y_i, z_i\) denote coordinates of the investigated POIs, \(n_{\text{POI}}(z)\) is the number of POIs at a given \(z\) coordinate. The minimum and maximum value of the relative spread as a function of depth is reported in figure 15b. The lateral variation of the relative spread is shown for three different depths in figure 15c.

We can separate the behaviour of the light spot size into two regions as a function of depth. In the region \(z < -7 \text{ mm}\) both the value of \(\sigma_y\), the width of its distribution and spread significantly depend on the lateral position. For A and C positions the dependence of the spot size is close to linear. If one compares the FWHM distribution size in figure 15a and depth dependence of spot size in figure 14b the depth resolution for a given lateral position can be determined. For A and C positions the depth resolution falls between approximately 1–2 mm. For \(z > -7 \text{ mm}\) the distribution of \(\sigma_y\) is homogenous over lateral position and depth. The value of \(\sigma_y\) is also homogenous (small spread) in lateral direction, but its value shows very small dependence with depth compared to the size of its distribution. Consequently depth cannot be estimated within this region by using this method in the current detector prototype.

From figure 14b we can conclude that in our prototype PET detector the spot size is not only affected by the total internal reflection on the sensor side surface, because \(\sigma_y(z)\) function is not linear [20]. The side-faces of the scintillator affect the spot shape at the majority of the POIs. In figure 14b at position A and C the trend shows that between \(-10 \text{ mm}\) and \(-7 \text{ mm}\) the spot size in \(y\) direction is not disturbed by the side-faces. But farther from the sensor, the beam’s footprint is larger than the size of the sensor, due to which the spot size is constant in this region. However, at position B the trend is the opposite. The largest spot size is estimated closer to the sensor, but as the distance increases, it converges to the constant value seen at A and C positions.
By comparing the photon distributions (see figure 16) it is apparent that the spot shape is not significantly larger at B position. After further investigations we found that the spot size estimation formula (see eq. (2.1)) is sensitive to the estimation of the y coordinate ($\eta$). If the coordinate estimation bias is comparable to the size of the light distribution then the estimated spot shape size considerably increases. In case of our investigated geometry this occurs for highly non-symmetrical spots around the shorter edges. The same effect explains the relative spread diagrams in figure 15c. The bias grows as the POI moves away from the sensor. Together with that the spot size also increases. Consequently, some positive spread is always expected close to the shorter edges of the crystal.

**Figure 15.** Variation of absolute FWHM width of spot distribution (y direction) estimation as a function of depth ($z$) at three representative lateral positions, at the middle of the photon-counter (blue), at one corner (red) and at the middle of its longer edge (green) (a). Minimum and maximum value of relative spread of the light spot size ($\Delta_r\sigma_y$) as a function of depth ($z$) (b). Lateral variation of light spot size relative spread ($\Delta_r\sigma_y$) from three selected depths ($z$) (c).
5.4 Proposal for an improved arrangement

The primary weaknesses of the investigated PET detector arrangement are the large bias in position estimation and the significant spread in energy and light spot size ($\sigma_y$). We described in the previous subsection that these effects are mainly present because of the edges of the scintillator crystal. Thus, by increasing the size of the detector, the portion of the volume affected by the edge effect can be reduced. Still with this modification, close to the side faces the performance of the detector would be low. Consequently, it is essential to find a scintillator side-face treatment or geometry that reduces the position estimation bias and energy estimation spread.

Based on the previous investigation we propose to apply a light-guide at the edges of the scintillator as depicted in figure 17.

The optical transmittance between the light-guide and the scintillator should grow with increasing distance from the sensor. Such a structure could increase the photon count on the pixels around the edges of the sensor which helps to reduce the bias of lateral POI estimation. By optimizing the coupling profile, the compensation effect can be tuned so that the overall lateral POI bias is minimized. At the same time majority of the photons incident to the side-face are collected so energy spread could also be reduced. The optimization of such a feature is the subject of a subsequent study.

![Figure 16. Averaged light distributions on the photon-counter from POIs at z = -9.41 mm depth at A and B lateral position.](image)

![Figure 17. Concept of using a light-guide with variable light coupling to the scintillator.](image)
6 PET detector exposed to collimated $\gamma$-beam

We prepared an experimental setup in which the prototype PET detector module was excited with an electronically collimated $\gamma$-beam. This setup was simulated as well by taking the advantage of the GATE to SCOPE2 interface described in section 3. The aim of this investigation is to demonstrate how accurate the simulation is if real $\gamma$-excitation is used. In this section we describe the experimental setup and its model and compare the results of the simulation and the measurement.

6.1 Experimental setup

We used the same prototype PET detector construction as we described in figure 5 except that the dummy photon-counter was removed and the active photon-counter was shifted $-1.0$ mm away from the symmetry axis of the scintillator (see figure 18). The face where it was coupled to the crystal was left polished and clear. We used a second $1.5 \times 1.5 \times 10$ mm$^3$ LYSO:Ce crystal (Saint-Gobain PreLude420 [23]) optically coupled to a second SPADnet-I photon counter. This second, smaller detector serves as an electronic collimator. We only recorded an event if a coincidence is detected by the detector pair.

The optical arrangement used on the electronic collimation side of the detector was constructed in the following way: the longer side faces ($1.5 \times 10$ mm$^2$) are covered with 3M ESR mirrors, the smaller $\gamma$-side face ($1.5 \times 1.5$ mm$^2$) with optically coupled Toray Lumirror E60L diffuse reflector. We used a closed $^{22}$Na source to generate annihilation $\gamma$-photons pairs. The source’s activity was $2.07$ MBq at the time of the measurement. The experimental arrangement is depicted in figure 18. With the angle of acceptance of the PET detector and photon-counter integration time (see latter in this section) known, the probability of pile-up can be estimated. We found that it is below 0.05% which is negligible (see section 3).

The parameters of the sensors on both the collimator and detector side were as follows: 25% of the most noisy SPADs were switched off. A single threshold scintillation validation scheme was used, the threshold value was set to 15 counts/bin, with 10 ns time bin lengths. After successful event validation the photon counts were accumulated for 200 ns. The operational voltage of the sensors was set to 14.5 V. The detailed explanation of the sensor settings is described in [11]. The temporal length of the coincidence window of the measurement was 130 ps [33]. The precision of position of the photon-counter with respect to the bulk scintillator block was 0.017 mm in $y$ direction and 0.010 mm in $z$ direction. The positioning error of the components with respect to each other in $x$ and $y$ directions is 0.2 mm, and 2.0 mm in the $z$ direction.

The arrangement depicted in figure 18 was modeled in GATE V6 [16]. The LYSO:Ce scintillator material properties were set by using its stoichiometric ratio: $\text{Lu}_{1.8}\text{Y}_{0.2}\text{SiO}_5$ and density of $7.1$ g/cm$^3$. The self-radiation of the scintillator was not considered. The closed $^{22}$Na source was approximated with a 5 mm diameter 0.2 mm thick cylinder embedded into a 7 mm diameter 2 mm thick PMMA cylinder. This is a simple, but close approximation of the actual geometry of the $^{22}$Na source distribution. Both $\beta^+$ and $1274.5$ keV $\gamma$-photon emission of the source was modeled. We used the Standard processes [35] to model particle-matter interactions.

In SCOPE2 we only simulated the prototype PET detector side of the arrangement. The parameters of the simulation model were the same as described in section 4. The POI grid on which the $ADF$ function database was calculated is the same as for the performance evaluation.
The results of the GATE simulation is fed into SCOPE2 (see section 3, figure 4) and the pixel-wise photon-counter signal was simulated for each scintillation event.

A total of 1393 valid $\gamma$-events were acquired in the measurement and 4271 $\gamma$-photons pairs were simulated by the prototype PET module.

6.2 Comparison of simulation and measurement results

The total count distribution was calculated from the sensor signals for both measurement and simulation and is depicted in figure 19. The number of measured and simulated events was different, so we normalized the area of the histograms to 1000. The bin size of the histogram is 5 counts. The simulated total count spectrum predict the tendencies of the measured one well. The raising section of curve is between 50 and 100 counts, the falling edge is between 200 and 350 counts in both cases. A minor, approximately 10 counts offset can be observed between the curves so that the simulation underestimates the total counts.

The $(\xi, \eta)$ lateral coordinates of the POI were calculated by using Anger-method (see section 2.1). The 2D position histograms of the estimated positions are plotted in figure 20a. The histogram bin size is 0.1 mm in both directions. The position histogram shows the footprint of the $\gamma$-beam.
Figure 19. Total count histogram of collimated $\gamma$-beam experiment from measurement and simulation.

Figure 20. Position histogram generated from estimated lateral $\gamma$-photon absorption position (a). Histogram of light spot size calculated in $y$ direction from simulated and measured events (b).
In section 5.2 we predicted significant distortion (shrinkage) of the flood diagram, the shrinkage is larger in x than in y direction. The same effect can be observed in the footprint of the collimated \( \gamma \)-beam. The real FWHM footprint of the beam is approximately \( 4.4 \times 5.3 \text{ mm}^2 \) estimated from the raw GATE simulation results. (In x direction the \( \gamma \)-beam is limited by the scintillator crystal size.) According to the simulation, this footprint shrunk to approximately \( \frac{1}{10} \) times in x direction and \( \frac{1}{5} \) times in y direction relative to its real size. The peak of the distribution is shifted towards the origin of the coordinate system (bottom left in figure 20a), which effect also coincides with the performance evaluation as it is depicted in figure 13c. The position and the size of the simulated and measured profiles are comparable. There is only an approximately 0.1 mm shift in \( \xi \) direction. A slight asymmetry in the y direction is also visible in both plots.

The distribution of the light spot size (y direction — \( \sigma_y \)) gives an indication on the distribution of \( \gamma \)-absorption as a function of depth (z direction), thus light spot size was also calculated for all measured and simulated light distributions (see eq. (2.1)). The distribution of \( \sigma_y \) values is plotted in figure 20b. The histogram was generated by using 0.5 mm bin size. In figure 14b of section 5.3 the range of \( \sigma_y \) is between 5 mm and 10 mm with significant lateral variation. The vast majority of the samples in the light spot size histogram fall in this range. Still there are some events with \( \sigma_y > 10 \text{ mm} \). Those can be explained by two or more simultaneous scintillation events that occur due to Compton-scattering of the \( \gamma \)-photons. Due to the spatial separation of the scintillations \( \sigma_y \) of such an event will be larger than for a single one.

The asymmetric shape of the light spot distribution can be explained by making some simple considerations. The spot size is larger if the scintillation is farther away from the photon counter surface (smaller z coordinate). If the attenuation of the \( \gamma \)-beam in the scintillator is considered to be exponential, one would expect an asymmetric \( \sigma_y \) distribution with its peak shifted towards the larger spot sizes. These predictions are confirmed by figure 20b. The majority of measured \( \sigma_y \) are between 4 mm and 11 mm with a peak at 9 mm. The simulated curve also shows this behaviour with some differences. The simulated distribution is shifted about 0.5 mm to the left and in the range from 6.5 and 7.5 mm a secondary peak appears at \( \sigma_y = 6.5 \text{ mm} \). Similar but less significant behaviour can be observed in the measured curve.

7 Conclusion

Based on our earlier studies we constructed a prototype PET detector module utilizing the SPADnet-I fully digital photon-counter. We used our formerly validated simulation method to evaluate the performance of this PET module.

During the performance evaluation we found that the prototype PET module has rather poor energy resolution performance (13–20% relative FWHM resolution) which is further degraded by the strong spatial variation of the light collection (spread). The resolution of the lateral POI estimation with COG algorithm is found to be good compared to other prototype PET modules using silicon photon-counters, although large bias of POI estimation far from the sensor degrade the POI resolution and reconstruction significantly. For some POIs the spatial bias is comparable to the full size of the module (4.6 mm in y direction for \( z = -0.41 \text{ mm} \), see figure 13b). The compression-corrected resolution values also confirm that towards \( \gamma \)-side of the module the lateral POI coordinates cannot be resolved. It is presumed that the bias of the position estimation and
spread of the energy estimation would be reduced and thus both energy and spatial resolution would be increased if the lateral size of the detector module were increased. Still close to the crystal sides spread in light collection and bias of position estimation would be present. In order to minimize this effect we proposed an optical solution that we are planning to work out in a subsequent work. The evaluation of the y-direction spot size revealed that the depth estimation is only possible close to the photon-counter surface $z < -7$ mm. Even in that region the lateral position has to be well known due to the variation of the spot size with lateral position. Despite these limitations the algorithm could be sufficient to distinguish between at least the lower ($z < -7$ mm) and upper ($z > -7$ mm) part of the scintillator. With the lateral position estimation bias reduced (see proposed solutions above) this would lead to an improved POI estimation [36].

We reported the results of the measurement and simulation of an arrangement where the prototype PET detector was excited with electronically collimated $\gamma$-beam. We presented that the behavior of the detector model is well understood and predicted by the performance evaluation. By comparing the results of a combined GATE-SCOPE2 simulation to the measurement we found only small differences which could also be easily explained using the previous investigation.

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References


