Photon-Counting Computed Tomography and scintillator-based detectors: a simulation analysis with scintillating and reflecting materials currently on the market

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Abstract—During the last decade, Photon-Counting Computed Tomography (PCCT) has been quickly developing and it is expected to revolutionize the X-ray imaging field. Rapid development has also been ongoing in the scintillator and photosensor fields: fast inorganic scintillators have become available on the market and the silicon photomultiplier (SiPM) technology has made substantial progress. Therefore, SiPM-based scintillator detectors may soon be successfully applied in challenging applications like PCCT.

In this work, a simulation framework is developed to evaluate detectors composed of scintillators coupled to SiPMs. The idea is to combine Monte Carlo simulations and a library to generate SiPM signals. Focus is given to six fast inorganic scintillators currently on the market (Ce:LYSO, Ce:LuAP, Pr:LuAG, Ce:LuAG, Ce:GGAG (ceramic), Ce:GAGG (single crystal)) and different TiO$_2$-epoxy mixtures. The main properties of scintillating and reflecting materials to be defined in the simulation database are characterised experimentally. Using a virtual model created within this framework, an analysis of the performance in PCCT of a SiPM-based scintillator detector composed of the considered materials is performed.

Simulated pulses are processed to report on the count-rate capability. Among the studied crystals, Ce:LYSO would enable sustaining the highest rate of interacting X-ray (2.5 Mcps/pixel with 30% of pile-up). Ce:GAGG could also handle a rate $\lesssim$ 1 Mcps/pixel with identical pile-up conditions. Other materials show a slow decay time in their scintillation kinetics, implicating a $< 1$ Mcps/pixel count rate.

A qualitative evaluation of the energy binning efficiency is also accomplished, by defining this parameter as a quality metric for multiclass classification. Scintillators with high light yield and good energy resolution (Ce:LYSO, Ce:GAGG and Ce:GGAG) present the best energy binning performance, as expected. The dependence of this aspect is explored as a function of the pulse processing method used, the crystals size and the pile-up probability. Resulting trends respect predictions, even though for a more quantitative analysis a more in-depth study is required.

Index Terms—photon-counting, scintillators, SiPM, simulation

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I. INTRODUCTION

In X-ray Computed Tomography (CT) field, a breakthrough is expected due to the recent positive results of Photon-Counting Computed Tomography (PCCT) [1]. For decades, CT has been performed using energy-integrating systems. With the photon-counting approach, the number of incoming X-ray is estimated by counting every single particle generating a signal in the detector. This brings many benefits compared to energy-integrating detectors, such as the possibility to discriminate the energy of the incoming particle and the reduction of the electronic noise. In turn, these could boost the imaging task, by improving the contrast-to-noise ratio and opening the possibility of performing material-specific imaging. The energy information, in particular, can be used to assign different weights to X-ray of different energy (“weighting of X-ray”), impacting the contrast and the noise of the reconstructed image of the object. Furthermore, by generating images using X-ray within specific energy ranges, features of the attenuation coefficient of the imaged object dependent on the X-ray energy can be highlighted, allowing the measurement of the composition of the phantom (i.e. “material decompostion”). Finally, a reduction of the required dose deposited to the object to image can be achieved with lower electronics noise [2], [3].

However, several technical challenges have to be tackled to realize the full potential of PCCT. These include X-ray crosstalk and K-escape X-ray, and flux-dependent effects such as pulse pile-up. From a detection system point of view, these translate to stringent requirements. Detectors should be able to sustain X-ray fluence rate up to 100 Mcps/mm$^2$, have an energy resolution that allows to resolve the energy spectrum of incoming X-ray, and be as compact as possible maintaining a fine pixel pitch.

Scintillator-based detectors have not been extensively explored because have characteristics that make it difficult to meet these specifications. Nowadays, the focus of the PCCT community is mainly on room-temperature semiconductors,
or “direct conversion”, detectors because able to generate faster signals, have better energy resolution and be segmented more efficiently [3]. In the past few years, fast inorganic scintillators produced by last trends of R&D have been made available on the market and are ready to be implemented in commercial detection systems. The photosensors field has also seen a rapid development of the silicon photomultiplier technology (SiPM) (also solid-state photomultiplier, SSPM, or multi-pixel photon counter, MPPC). Thanks to the progress in these fields, applications like PCCT where it is required a fast detection response, high gain and compact design are becoming more accessible for SiPM-based scintillation detectors. Hence, “indirect conversion” detectors installing SiPMs may be successfully implemented in PCCT, representing a convenient alternative to semiconductor systems, especially in terms of cost and manufacture.

Experimental tests of photon-counting CT using indirect-conversion detectors have been done for specific applications [4] [5], confirming the advantages of such an approach. An analytical model to evaluate the performance of scintillators coupled to SiPM in PCCT has also been developed, showing that a SiPM-based scintillation detector that competes with direct conversion detectors could be potentially developed [6]. There are no studies that investigate the potential of SiPM-based scintillation detectors in PCCT using Monte Carlo simulations. The development of the simulation framework discussed here offers the possibility to analyse independently single aspects of the detection process, from the detector design to signals processing. Its concept is to integrate Monte Carlo simulations (GATE [7]) and a library to generate SiPM signals (SimSiPM [8]), to fully emulate the main steps involved in an ideal detection system. This will permit performing PCCT-specific analysis using simulated waveforms. Moreover, the compilation of the simulation database with experimental data of state-of-the-art materials on the market will give an indication of the current potentials and limitations of SiPM-based scintillation detectors in PCCT. The objective of this study is thus to develop and validate a simulation framework of a detection system composed of scintillators and SiPMs, with a database including fast scintillators and reflecting materials on the market. This is then used to report on a case study of the performance in PCCT of a SiPM-based scintillation detector with state-of-the-art materials, in terms of rate capability and energy binning efficiency of the X-ray spectrum (i.e. energy resolution).

II. MATERIALS AND METHODS

A. Materials characterization

Scintillators considered in this work are chosen following two principles: availability on the market and favourable scintillation and material properties for fast computed tomography applications. Fast scintillation kinetics and high light yield are desirable to enhance count-rate capability and energy resolution respectively. Moreover, high density and atomic number imply good X-ray detection efficiency, and non-hygroscopicity and radiation hardness permit the usage in compact scintillator arrays exposed to an environment with an intense level of radiation. Six different scintillators that fulfill all or part of these requirements are selected: Ce:LYSO [9], Ce:LuAP [10], Pr:LuAG, Ce:LuAG [11] [12], Ce:GGAG (ceramic), Ce:GAGG (single crystal) [13]. Three 5 mm³ polished samples of each crystal were supplied by Hilger Crystals. To compile the simulation database with realistic values, relevant properties of these crystals are experimentally computed. Measurements are designed and performed to estimate decay time, light yield and energy resolution at 60 keV. The setup used is composed by a 5 series MSO oscilloscope by Tektronix, a fast Hamamatsu PMT (Hamamatsu H6780-06 for LYSO, LuAP and Pr:LuAG or H10721-20 for Ce:LuAG and Gd garnets, in order for the PMT quantum efficiency to match the scintillation emission spectrum) and a ²⁴¹Am source (main emission at 59.5 keV). Scintillator samples are wrapped into PTFE tape and coupled to the PMT using optical grease. Waveforms of 2 µs are digitised and analysed offline to estimate the desired quantities. Integrating the digital signals, the energy spectrum is generated and used to compute the energy resolution and the light yield (Bertolaccini method [14]). The decay time is estimated using waveforms related to the 60 keV peak on the energy spectrum. It is considered X-ray at this energy (60 keV) because within the typical CT energy range, that can extend up to 150/200 keV with an average energy of 50/100 keV, depending on the application. The emission spectrum is also characterised, using a MAYA2000Pro spectrometer by Ocean Optics and a 160 kV X-ray generator. For this measurement, scintillators are not wrapped into any reflector and are dry-coupled to the optical fibre connected to the spectrometer.

Results of the measurements are reported in Table I. Values are coherent with data found in the literature [9]–[13], [15]. All crystals have a 1st decay time that can be considered fast, under 100 ns for most of the materials, and in the order of 150 ns for the ceramic Ce:GGAG. However, the only crystals with zero or low contribution of slow components are Ce:LYSO and the two gadolinium garnets (Ce:GAGG and Ce:GGAG). These materials also have the greatest light yield and energy resolution. Despite having equal chemical formulas, the ceramic and single crystal Gd garnets exhibit different properties. Ceramic garnets are reported to have a greater light yield than single crystals [13]. On the other hand, while the scintillation kinetics of the ceramic sample respect values reported in literature [13], we believe the single crystal result faster because of the presence of co-dopants (Mg²⁺ or Ca²⁺) [15].

Samples of reflecting material produced by mixing several TiO₂ pigments and epoxy resins are also characterised. In an array of mm-size scintillators, mixtures of these materials are solutions adopted to fill the interstices between adjacent crystals. TiO₂ white pigments, in particular, presenting a high reflectance to scintillation photons, enhance the light collection and ensure light confinement between crystals. Epoxy resins, on the other hand, allow for the mixture to be mouldable and efficiently cover the array. A list of the mixtures studied is reported in the legend of Fig. 1, where the binder (standard
The maximum wavelength of the emission spectrum, up to three decay times interpolating the scintillation kinetics, and the energy resolution and light yield measured at 60 keV.

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<tr>
<td>Ce:LYSO</td>
<td>425</td>
<td>44 ± 2 (100 %)</td>
<td>154 ± 12 (7.5 ± 0.3 %)</td>
<td>1405 ± 122 (20.0 ± 0.8 %)</td>
<td>26.4 ± 0.5</td>
<td>25.8 ± 0.7</td>
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<tr>
<td>Ce:LuAP</td>
<td>370</td>
<td>20.8 ± 0.6 (72.5 ± 0.7 %)</td>
<td>165 ± 15 (10.0 ± 0.4 %)</td>
<td>1743 ± 38 (62.4 ± 0.4 %)</td>
<td>39 ± 4</td>
<td>5.3 ± 0.7</td>
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<tr>
<td>Pr:LuAG</td>
<td>310</td>
<td>30 ± 1 (27.5 ± 0.5 %)</td>
<td>1559 ± 47 (58.8 ± 0.5 %)</td>
<td>36.7 ± 0.9 (7.1 ± 0.2 %)</td>
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<tr>
<td>Ce:LuAG</td>
<td>520</td>
<td>73 ± 2 (41.2 ± 0.5 %)</td>
<td>697 ± 15 (18 ± 1 %)</td>
<td>21.3 ± 0.9 (44.5 ± 0.6 %)</td>
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<tr>
<td>Ce:GGAG ceramic</td>
<td>560</td>
<td>173 ± 3 (82 ± 1 %)</td>
<td>139 ± 4 (45 ± 1 %)</td>
<td>564 ± 30 (13 ± 1 %)</td>
<td>23.8 ± 0.2 (30.9 ± 0.2 %)</td>
<td></td>
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<tr>
<td>Ce:GAGG</td>
<td>555</td>
<td>55 ± 1 (41.8 ± 0.8 %)</td>
<td>139 ± 4 (45 ± 1 %)</td>
<td>564 ± 30 (13 ± 1 %)</td>
<td>23.8 ± 0.2 (30.9 ± 0.2 %)</td>
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Table I: Results of the characterization of the six scintillating crystals analysed within this work. From left to right it is reported: the maximum wavelength of the emission spectrum, up to three decay times interpolating the scintillation kinetics, and the energy resolution and light yield measured at 60 keV.

Fig. 1. Reflectance spectra of epoxy - TiO$_2$ pigment combinations. Samples are grouped in the two legends depending on the TiO$_2$ type, rutile or anatase. In there, details of their composition can be found: first the epoxy resin (EP = standard epoxy, CAP = cycloaliphatic) and then the white pigment. Measurements are done using a custom-built setup, in which the light reflected by samples is detected using an integrating sphere and a spectrometer. The emission profiles of LEDs used are plotted on the bottom part of the graph.

Epoxy or cycloaliphatic) and the type of white pigment used are provided. The main difference between the several TiO$_2$ pigments is the crystal structures, either rutile or anatase [16]. Samples were supplied by Hilger Crystals. The most significant optical property to be considered for this study is reflectance, given its impact on light collection efficiency. A custom-built setup is used for its measurement. The setup is designed to estimate the so-called “directional-hemispherical” reflectance [17]. LEDs light is focused to hit the sample at 6° respect to its surface normal. The sample is placed on one port of a Thorlabs integrating sphere, which enables the collection of light reflected over 2π steradians. A MAYA2000Pro spectrometer by Ocean Optics is connected to the integrating sphere and is used to detect reflected light. The estimated reflectance spectra are extracted by comparing the intensity of the light reflected by the sample to the intensity when a PTFE-based reference standard (made of the same material of the integrating sphere) of known reflectance is installed. Multiple LEDs are used (whose emission profile is plotted in Fig. 1). Each of those allows estimating the reflectance in a different wavelength range, depending on their emission. The final reflectance spectra plotted in Fig. 1 are computed by merging results from all the LEDs, and cover a range from 360 to 690 nm. As can be noticed, the main difference is due to the particular type of pigment used. The reflectance of anatase drops at lower wavelengths compared to rutile mixtures [18]. To cover the range of the emission wavelength of the analysed scintillators and be included in the simulation database, data are extended from 360 to 290 nm and from 700 to 900 nm by interpolation.

B. Simulation framework

The simulation framework is developed to emulate the signal generation of a SiPM-based scintillator detector. A virtual model of the detector is created using GATE [7], a Monte Carlo simulation software based on Geant4 [19]. Within this programme, the interaction of X-ray in the scintillator, the consequent generation of scintillation photons and light propagation in the crystal are simulated. The X-ray spectrum included is characteristic of an X-ray generator with tungsten anode and 1 mm thick stainless steel filter, supplied with 160 kV. The virtual model of the detector analysed is composed of a crystal with a cuboid shape. Dimensions are in the order of few mm and the exact geometry is specified when describing the different simulation scenario. The scintillator is surrounded by reflective material and optically coupled to the SiPM. The UNIFIED model [20] is used to define optical interfaces. All surfaces are defined to be ideal Lambertian
diffusers, with “reflectivity” values determined through the experimental characterisation. The index of refraction of the optical coupling media is set to 1.5. When the dimension of the crystal, or “pixel”, of the detector is changed, all three dimensions are equally modified, keeping the cuboid shape.

The SiPM library uses the scintillation photons reaching the SiPM surface to generate SiPM pulses. Each signal is related to a single X-ray interacting in the crystal. It is produced by summing the single microcell discharges within the time window covered by scintillation light. Therefore, the position of photons interaction determines which SiPM microcell is involved and enables the consideration of eventual saturation effects. Finally, arrival times of scintillation photons define the shape of the pulse in the time domain. The main properties of SiPMs can be defined in SimSiPM. In this work, the only parameters which were modified are the “Size” of the SiPM, to be equal to the crystal model used in GATE, as well as “FallTimeFast” and “RecoveryTime”. These describe the fast component of the falling time of the signal generated by single microcells and their recovery time to be able to generate a new discharge, respectively. They are defined with equal values, assuming that microcell discharges are described by a single exponential function. The photodetection efficiency is also set to 30%, constant for all wavelengths. All SiPM secondary effects (gain variation between microcells, crosstalk, and after-pulse) are not activated.

The generated waveforms are then analysed to perform application-specific studies. The spectrum of detected X-ray is produced using the energy information carried by pulses. This is retrieved considering either the maximum value of the pulses (“peaks”) or its “integral”. For PCCT, it is more significant to consider the energy spectrum reconstructed with peaks of the waveforms. In a PCCT detection system, the energy is measured with comparators, that increase the count in a specific energy bin according to the generated pulse height. The possibility of producing pulses affected by pile-up is also included. This is done by defining the pulse duration of the scintillator and SiPM system and the pile-up probability to be considered. Taking these parameters into account, signals affected by pile-up are generated by using scintillation photons related to consecutive X-ray simulated in GATE.

C. Simulation validation

Simulations are validated for aspects that are significant for this work and the photon-counting case study. First, the pulse shape of waveforms generated by the simulation framework is checked against experimental waveforms. This ensures the reliability of the discussion planned on pulse duration and count-rate capability. Secondly, a validation of the simulated energy resolution is achieved. The energy resolution is the primary factor influencing the ability of the detector to discern the energy of the interacting X-ray. Spectra generated by simulated and experimentally acquired waveforms are produced and relative resolutions at 60 keV are compared considering both peaks and integrals of pulses. Experimental data for these benchmarks are acquired with the 5 mm$^3$ crystals coupled to an OnSemi MICROFJ-SMA-60035-GEVB board, and irradiated by the $^{241}$Am source. A virtual model replicating the experimental setup and the specifications of the OnSemi SiPM board is created in the simulation framework and used to generate the simulated waveforms.

D. Case study: photon-counting CT

The developed simulation framework is finally used to study two aspects of SiPM-based scintillator detectors applied to photon-counting CT: count-rate capability and energy binning performance.

1) Count-rate: CT applications require detectors that handle a high rate of events, to reduce the time for a full imaging scan. Pulse duration is the main factor that limits the count-rate capability of a PCCT detector. The longer the pulses, the higher the pile-up. Overimposed signals result as one of greater energy, leading to a miscount of the number of X-ray and to wrong energy discrimination. This increases the image noise and deteriorates the energy resolution. For SiPM-based scintillator detectors, the pulse duration depends on crystals scintillation kinematic and on the SiPM response time. Using the developed simulation framework, the pulses generated by the SiPMs coupled to the considered scintillators are evaluated. The pulse duration is defined as the time for the integral of the pulse to reach 95% of its final value. The virtual detector analysed is composed of a 1 mm$^3$ crystal and SiPM of 1 mm size and 10 µm pitch. For each scintillator analysed, the reflective material that optimises its light collection is used. The impact of the SiPM recovery time is evaluated by changing its value within the SiPM library.

On the other hand, the count-rate capability of a detector depends also on the maximum pile-up accepted to perform satisfactorily the imaging task. The relation between count-rate capability $r$ and pile-up probability $p_{pu}$ is thus analysed. In this case, count-rate capability means the rate of interacting events that produce signals without pile-up for a given pile-up probability $p_{pu}$. The probability of pile-up is defined as the probability that within the specified time of duration of a pulse $t_p$ generated by an event, one or more additional events occur. This is given by $r = -\ln(1 - p_{pu})/t_p$ [21].

2) Energy binning: One of the photon-counting CT core ideas is to be able to use the energy information related to the detected X-ray. This information can be used to assign different weights to X-ray of different energy (improving the signal-to-noise ratio of the reconstructed image) and to perform material-specific imaging of the analysed object. This is usually achieved by dividing the energy spectrum into several bins and assigning each detected event to one of these bins. Within this work, energy binning performance is defined as the ability of the detector to correctly classify the energy of interacting X-ray using the information contained in SiPM pulses. The energy spectrum of X-ray before entering the detector is divided into bins. The energy spectrum generated by pulse processing is then divided using the same bins. An event is properly classified if the energy information estimated by pulse processing is included in the bin that corresponds to the one of
the X-ray primary energy. This approach consents to compare materials taking into account X-ray detection efficiency, which reduces the number of entries in the detected energy spectrum. Additionally, the fraction of partially deposited energy can also be evaluated, as X-ray scattering, K-escape X-ray, alter the comparison between initial and detected energy spectra. Finally, energy resolution and pulse shape are also factors considered within this approach, as they distort the value of the detected energy.

For this case study, the binning of the X-ray energy spectrum is done considering the followings: the X-ray spectrum used in the simulation replicates a 160 kV, ranging from 30 to 160 keV. Focusing on the possible application of PCCT in the security field, it can be interesting to identify materials like platinum and gold, that are non-threats. These have K-edge at \( \sim 80 \text{ keV} \). Therefore, a dedicated bin is defined from 65 to 100 keV. Other two bins include events at lower (from 30 to 64 keV) and higher (from 101 to 160 keV) energies, respectively. A bin from 10 to 29 keV is intended for signals just above the noise levels but related to partial energy deposition in the crystal. Finally, to quantify the pile-up, a bin for estimated energy greater than 160 keV is used. This binning is not optimised for any particular scenario, it is just to make a qualitative case study.

A parameter is introduced to quantify the energy binning efficiency of the detector (\( \varepsilon_{\text{bin}} \)), the Matthews Correlation Coefficient [22] [23]. This coefficient is typically used as a performance metric for binary and multiclass classification tasks in a variety of fields, including particle physics. It provides a versatile tool for quantifying the agreement between predicted and observed outcomes. The performance on binning the X-ray energy in PCCT applications, where the number of bins is limited (five in the case of this analysis), can be thus quantified using this metric. Hence, the energy binning efficiency is based on the definition of a matrix \( C \) such that \( C_{i,j} \) is equal to the number of events whose energy is known to be in bin \( i \) and predicted to be in bin \( j \). For each simulated event, the prediction of the classification is based on the value of the integral or peak of waveforms, while the true value is the energy of the X-ray interacting in the detector. In the case of K bins, the energy binning efficiency \( \varepsilon_{\text{bin}} \) is defined as:

\[
\varepsilon_{\text{bin}} = \frac{c \cdot s - \sum_{k} p_{k} \cdot t_{k}}{\sqrt{(s^{2} - \sum_{k} p_{k}^{2}) \cdot (s^{2} - \sum_{k} t_{k}^{2})}}
\]  

(1)

where:

- \( t_{k} = \sum_{i} C_{i,k} \), number of times that bin \( k \) truly occurred (i.e. interacting X-ray with energy in bin \( k \));
- \( p_{k} = \sum_{i} C_{k,i} \), number of times that bin \( k \) was predicted (i.e. detected events with estimated energy in bin \( k \));
- \( c = \sum_{i} \sum_{j} C_{i,j} \), total number of events correctly predicted;
- \( s = \sum_{i} \sum_{j} C_{i,j} \), total number of events;

This coefficient is 1 when there is a perfect correlation between predicted and true values, whereas it is 0 when there is a random relationship between the two. Therefore, the closer is \( \varepsilon_{\text{bin}} \) to 1, the better the detector can predict the energy of the interacting X-ray and thus correctly perform the classification in bins. For this study, this definition of the energy-binning performance was preferred over other metrics commonly used in nuclear instruments and methods because it allows comparing the energy-binning performance of the considered scintillators and evaluating the SiPM impact using the virtual model developed. It does not require focusing on a specific imaging task and making further assumptions about the array design and the geometry of the setup. It can be seen as a metric for the detector performance that includes more factors than, for example, the estimated energy resolution for a monoenergetic beam. The energy-binning performance is influenced not only by the detector energy resolution but also by other effects (e.g. X-ray crosstalk and K-escape X-ray).

Therefore, this parameter is used, for example, to evaluate the effect of the dimension of the crystal pixel on the energy binning capability of the detector. This is of particular interest because smaller pixel implies a higher spatial resolution and rate capability. On the other hand, this also means more X-ray crosstalk and K-escape X-ray, which deteriorate the energy binning performance. Pile-up also affects the energy binning ability of a photon-counting detector, and its impact can be also assessed using the defined \( \varepsilon_{\text{bin}} \). The higher the pile-up probability, the greater the distortion of the spectrum measured, as already discussed in the count-rate section. The Matthews Correlation Coefficient is thus tested as a parameter to quantify energy binning performance \( \varepsilon_{\text{bin}} \) (or, from another point of view, the spectrum distortion) as a function of pixel size and pile-up probability.

III. RESULTS AND DISCUSSION

A. Simulation validation

A comparison of simulated and experimental waveforms can be seen in Fig. 2. Cases of Ce:LYSO, Pr:LuAG and Ce:GGAG are reported. The “FastTimeFall” and “RecoveryTime” used to model the Onsemi SiPM board is 82 ns, resulted from analysis of dark photon discharges. Simulated and experimental pulses agree with each other. This confirms the coherency of the scintillator decay constants estimated experimentally and included in the simulation database and the reliability of the developed simulation framework for the pulse shape aspect.

Table II shows the result of the validation effectuated for the energy resolution. The comparison between experimental and simulated values is made considering both case where the energy is estimated using peaks and integrals of the waveforms. The energy resolutions estimated using integrals are compatible, especially for the brightest samples (Ce:LYSO, Ce:GAGG and Ce:GGAG). Noise is not perfectly described in the SiPM library, and this might be the cause of the appreciable discrepancy in data related to scintillators that produce less light. Signals are generated by fewer scintillation photons, resulting in a greater contribution of noise on integrals. If peaks are used, the energy resolutions of experimental and simulated data agree partially. For Ce:LYSO, simulated and experimental values are compatible. When considering
Ce:LYSO pulses are the shortest. Single crystal Ce:GAGG is the recovery time of its microcells. As it can be seen in Fig. 3a, analysed as a function of the time constant of the SiPM, i.e. characterization previously performed. The pulse duration is evaluated. The scintillation decay times are defined by the of the analysed scintillators coupled to an ideal SiPM is framework.

B. Case study: photon-counting CT

The following results are obtained for the photon-counting CT case study performed using the developed simulation framework.

1) Count-rate: The pulse duration of a detector composed of the analysed scintillators coupled to an ideal SiPM is evaluated. The scintillation decay times are defined by the characterization previously performed. The pulse duration is analysed as a function of the time constant of the SiPM, i.e. the recovery time of its microcells. As it can be seen in Fig. 3a, Ce:LYSO pulses are the shortest. Single crystal Ce:GAGG is characterised by signals whose length (∼400 ns) is half than the ceramic counterpart (∼1000 ns), reflecting their different scintillation kinetics. Ce:LuAP signals duration is around 2 μs, half of the other lutetium garnets. The pulse duration of a detector with a Ce:LYSO crystal can shorten by 50%, from 300 to 150 ns, if the SiPM recovery time goes from 80 to 10 ns. Focusing on the Gd materials, there is a small influence on the pulse duration, while for the remaining scintillators, the SiPM recovery time does not affect the pulse, given the kinematic is dominated by the slow component.

The time length of signals is directly correlated to the rate capabilities that a detector can sustain. The shorter the pulse, the higher the rate of interacting events that can be handled before pile-up starts to dominate the detection system and degrade its performance. Rate capabilities computed using pulse durations estimated assuming a SiPM recovery time of 10 ns are shown in Fig. 3b, as a function of the pile-up probability. Results are reported in terms of Mcps/pixel, where a pixel is the surface area of crystals composing the scintillator array (1 mm² in this analysis). As expected, Ce:LYSO would enable to sustain the highest rate of interacting X-ray among the studied scintillators: 2.5 Mcps/pixel with 30% pile-up. Ce:GAGG could also handle a rate > 1 Mcps/pixel while the remaining crystals would handle a maximum rate < 0.5 Mcps/pixel. The value of 30% pile-up is taken as the reference value. If demanding to sustain more pile-up, compensation techniques shall be used [2]. As a comparison, state-of-the-art semiconductor detectors, generate pulses that have a duration of ∼35 ns [24]. The input count-rate capability of direct conversion detectors is thus in the order of 10 Mcps/pixel (at 30% pile-up probability), four times greater than Ce:LYSO read out by SiPM.

These results show that to boost the detection rate performance of indirect detectors, scintillation kinetics should be quickened. Most of the considered materials on the market show a slow decay time in their scintillation kinetics. Sup-
Fig. 3. On the left (Fig. 3a), plot of the pulse duration of a SiPM-based detector using the scintillators considered in this work. Pulses are generated using the simulation framework and their duration is defined as the time for the integral to reach 95% of its final value. Pulse duration is plotted as a function of the SiPM recovery time, while the scintillation decay time is evaluated experimentally. On the right (Fig. 3b), assuming a SiPM recovery time of 10 ns, the rate capability achievable by the detector as a function of the pile-up probability is represented.

pression of the slow component in materials like Ce:LuAP and Pr:LuAG could change perspective since they would suddenly become faster than Ce:LYSO. Concurrently, improvements in the SiPM response speed will also have a consistent impact on scintillators whose scintillation decay times are on the same order of magnitude (i.e. < 100 ns).

It is noteworthy that apart from considered scintillators, there are other new promising materials that exhibit potential for enhancing the functionality of a SiPM-based scintillator detector for PCCT in the future. One such example is halide perovskites, available in the form of single crystals or nanocrystals, which shows fast scintillation kinetics in the order of ns or tens of ns. Additionally, there are heterostructure/metascintillators, core-valence luminescence scintillators and loaded plastic scintillators, all of which offer promising options due to their quick scintillation properties. To achieve count-rate capability comparable to direct conversion detectors, bright inorganic scintillators with major fast decay (~ tens of ns) component and minor slow decay components should be thus searched and developed. An ideal scintillator with a single 10 ns decay constant, for example, would generate pulses of a duration of ~40 ns, assuming SiPM with a recharge time of 10 ns.

2) Energy binning: The ability of the detector to generate a signal with an energy information representative of the energy of the interacting X-ray is studied. The energy spectrum of the primary X-ray (true values) and produced by the generated pulses (predicted values) are binned, and a classification is performed. The quality of this energy binning is described by $\varepsilon_{\text{bin}}$, estimated as in Eq. 1. Values of $\varepsilon_{\text{bin}}$ related to SiPM-based detectors using scintillators considered in this work are plotted in Fig. 4. Scintillators with higher light yield and better energy resolution (Ce:LYSO, Ce:GAGG and Ce:GGAG) have the best performance, as expected. $\varepsilon_{\text{bin}}$ is about 0.55, considering an arbitrary 1 mm$^3$ crystal size and no pile-up involved.

To compare this value with semiconductor detectors, they would need to be included in the simulation database, and an equivalent simulation study should be conducted. This is outside the scope of the current work. It is generally expected that direct conversion detectors have better energy binning performance than SiPM-based scintillator detectors. This is because direct conversion detectors provide higher gain when converting the energy deposited and offer a better energy resolution, typically between 5 and 10% at 60 keV, compared to the lower resolution of the considered scintillators (> 20%).

Comparing binning performed using integrals (Fig. 4a) or peaks (Fig. 4b) of waveforms as an indication of the energy of the event, it can be noticed that integrals yield greater $\varepsilon_{\text{bin}}$. This is expected because integrals involve more statistics of scintillation photons, especially if the scintillation kinetics has slow decay components. However, peaks are more suitable for PCCT, given that the read-out of the detector to perform the energy classification would be done using comparators of the signal heights. Focusing on results related to peaks, Ce:LYSO would match up the performance of the brighter Gd garnets, given that its emission is faster and thus more clustered at the beginning of signals.

Another factor that plays an important role in the energy-binning performance of the detection system is the reflector considered to confine the light in the scintillator pixel. All the TiO$_2$-epoxy combinations considered have a reflectance that drops around 400 nm and this affects the light collection of in particular Ce:LuAP and Pr:LuAG (Fig. 1). If considering other reflecting materials, for example, a reflector with properties...
The binning quality is \( \varepsilon_{\text{bin}} \) function of the pile-up probability. In Fig. 4 are included \( \varepsilon_{\text{bin}} \) values for Pr:LuAG and Ce:LuAP related to simulations with crystals wrapped with PTFE as an example.

3) **Energy binning and pixel size:** In applications like PCCT, scintillator arrays composed of crystals of small dimensions imply a higher spatial resolution and rate capability. However, small-size pixels also mean less detection efficiency because of a higher fraction of escaping X-rays due to scattering or fluorescence, and more scattering between pixels and escape X-ray, that deteriorates the energy binning performance. With a lower fraction of X-ray depositing all their energy in the pixel where they interacted, events are more likely to be classified in lower energy bins. Here is evaluated qualitatively the potential of using this simulation framework and the quality parameter selected to study the energy binning performance as a function of this geometry factor. As it can be seen in Fig. 4, \( \varepsilon_{\text{bin}} \) decreases with decreasing size of the pixel. This effect is comparable for the different scintillators, as they all show about 30% \( \varepsilon_{\text{bin}} \) variation from a pixel size of 1.6 to 0.4 mm. Compared to Gd garnets, crystals with lutetium have a higher density and atomic number. Therefore, the effect of the size of pixels is less important given that the scattering is less probable.

4) **Energy binning and pile-up:** Another factor that affects the energy binning ability of a photon-counting detector is pile-up. The higher the pile-up probability, the greater the distortion of the spectrum measured. Nevertheless, the higher the pile-up the detector can sustain, the higher the rate capability, as previously shown. The capacity of this simulation framework to evaluate the impact of pile-up on energy binning is thus explored. Results are illustrated in Fig. 5, related to 1 mm\(^3\) crystal pixels. Already with a 30% pile-up probability, the \( \varepsilon_{\text{bin}} \) falls below a value of 0.3, half of the value without pile-up. This value of \( \varepsilon_{\text{bin}} \) is associated, for example, with a detector without pile-up but with a 50% energy resolution. Fig. 5a and Fig. 5b are related to values of \( \varepsilon_{\text{bin}} \) computed considering integrals and peaks respectively. It is appreciable that in the first case \( \varepsilon_{\text{bin}} \) follows a similar trend for all scintillators. When processing the energy information of signals using peaks, trends are different, as pile-up affects in non-identical ways the two energy estimation methods, especially when the detector has a long pulse duration.

**IV. Conclusion**

Within this work, a simulation framework for SiPM-based scintillator detectors is developed and validated. It is used to tackle a case study to evaluate scintillating and reflecting materials currently on the market for photon-counting computed tomography applications.

In terms of count-rate capability, Ce:LYSO and Ce:GAGG guarantee to sustain the highest rate of interacting X-ray. Considering the energy binning aspect, scintillators with higher light yield and faster scintillation kinetics (Ce:LYSO, Ce:GAGG and Ce:GGAG) present the best performance. A qualitative analysis of the impact of factors like detector geometry and pile-up probability on the energy binning capability is also performed.

The results of the present study evidence that the developed simulation framework, which combines Monte Carlo simulation (GATE) and a SiPM library (SimSiPM), offer the possibility to evaluate the performance of SiPM-based scintillator detectors. Focusing on the PCCT case study, the developed framework was used to study the impact of available on the market whose maturity would allow for immediate commercial usage in this application. It has been shown that Ce:LYSO, Ce:GAGG, and Ce:GGAG are currently the fastest inorganic scintillators on the market, providing the best performance.

However, to enable SiPM-based scintillator detectors to compete with "direct conversion" detectors, they must improve their count-rate and energy binning performance. The highest count-rate capability is achieved using Ce:LYSO: 2.5 Mcps/pixel assuming SiPM with 10 ns recharge time and 30% pile-up probability. This is four times lower than current state-of-the-art PCCT semiconductor detectors under the same pile-up conditions. Focusing on the energy-binning task, Ce:LYSO and the Gd garnets exhibit the best performance. The value of the coefficient appositely introduced to quantify the quality of the energy binning is of 0.55 for a pixel dimension of 1 mm. Future work includes investigating quantitatively the usage of this coefficient and establishing a comparison with the performance of direct conversion detectors.

Exploring new materials with better energy resolution and faster decay time, such as halide perovskites, can significantly improve the performance of SiPM-based scintillator detectors in photon-counting CT applications. However, further research is necessary to explore the utilization of these alternatives. This research should encompass a wide range of factors, including the development of new crystals, and studies on their material and scintillation properties to ensure that PCCT-related requirements outlined in this work are met. Furthermore, to
be a suitable candidate for CT systems, production aspects should also be analysed, to establish large-scale production of scintillators with uniform properties that can be integrated into an array for use in PCCT detection systems. Challenges related to this point are the main reason why hygroscopic materials such as LaBr₃ are not considered in this work, despite already being on the market and exhibiting superior properties for PCCT applications. Maintaining cost-effectiveness is also crucial.

It may also be possible to find an application for PCCT detection systems with less stringent performance requirements, making SiPM-based scintillator detectors using fast inorganic scintillators already on the market considered in this work a competitive option, due to economic and manufacturing convenience compared to direct conversion detectors.

To conclude, the study of SiPM-based scintillator detectors applied in PCCT is just at the beginning and, given the constant development of relevant technologies, it is worth pursuing concurrently to semiconductor detectors.

REFERENCES