1 **A Hybrid Monte Carlo Model for the Energy Response Functions of X-ray Photon Counting**
2 **Detectors**

3 Dufan Wu^{a,b}, Xiaofei Xu^{a,b}, Li Zhang^{a,b}, Sen Wang^{a,b}

4 ^aKey Laboratory of Particle & Radiation Imaging (Tsinghua University), Ministry of Education, China

5 ^bDepartment of Engineering Physics, Tsinghua University, Beijing 100084, China

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7 **Corresponding author:** Li Zhang, Department of Engineering Physics, Tsinghua University, Beijing,
8 100084, China; Tel: +86-13910686306; E-mail: zli@mail.tsinghua.edu.cn.

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10 **Abstract**

11 In photon counting computed tomography (CT), it is vital to know the energy response functions
12 of the detector for noise estimation and system optimization. Empirical methods lack flexibility and
13 Monte Carlo simulations require too much knowledge of the detector. In this paper, we proposed a
14 hybrid Monte Carlo model for the energy response functions of photon counting detectors in X-ray
15 medical applications. GEANT4 was used to model the energy deposition of X-rays in the detector.
16 Then numerical models were used to describe the process of charge sharing, anti-charge sharing and
17 spectral broadening, which were too complicated to be included in the Monte Carlo model. Several free
18 parameters were introduced in the numerical models, and they could be calibrated from experimental
19 measurements such as X-ray fluorescence from metal elements. The method was used to model the
20 energy response function of an XCounter Flite X1 photon counting detector. The parameters of the
21 model were calibrated with fluorescence measurements. The model was further tested against measured
22 spectrums of a VJ X-ray source to validate its feasibility and accuracy.

Key Words: photon counting detector, modeling, computed tomography, X-ray imaging

1. Introduction

In recent years, with the development of single photon counting pixel detectors, spectral computed tomography (CT) has been of great research interest in X-ray imaging [1]. With the capability of discriminating incident photons' energy, spectral CT is able to achieve better material discrimination and quantitative K-edge imaging [2]. In order to minimize reconstruction noise, the thresholds of the photon counting detector have to be optimized according to the imaging tasks. Instead of an exhaustive search, the reconstruction noise level could be calculated and optimized with the knowledge of imaging object, X-ray source spectrum and energy response functions [3][4]. While the first two can be easily modeled with adequate accuracy in most cases, the modeling of energy response functions of photon counting detectors is more complicated due to various non-ideal effects such as charge sharing, K-escaping and pulse pileup [1]. The pileup model has been thoroughly discussed by Taguchi et al. [5], and it would not cause serious spectrum distortion under low photon flux. The main scope of this paper is to model the energy responses without pulse pileup, with enough accuracy for noise estimation and optimization. The modeled spectrums could also be used as initial values for spectrum estimation, e.g. with measurements of staircases and expectation maximization [6]. However, it was not our goal to directly use the spectrums in reconstruction.

Several methods have been proposed for the modeling of energy response functions. Nilsson et al. simulated the charge transportation with Monte Carlo simulation for Si and GaAs detectors [7][8]. They also derived an analytical formula for charge spread with the diffusion equation in normally depleted detectors. The Monte Carlo approach was complicated because it needed to deal with the transportation of particle groups. Furthermore, it required the knowledge of the bias voltage of the

detector, which is sometimes unavailable for end-users.

Schlomka et al. measured the energy response functions of a CdTe detector with a synchrotron source [2]. Energy up to 65keV was measured and the response functions were fitted with an empirical model, which consisted of two Gaussian peaks and a plateau. The model was extrapolated up to 130keV and K-edge imaging was successfully achieved with the calculated spectrums. Ponchut used a similar approach to model the response function of a Medipix2 detector with 300um Si [9]. Empirical models can be accurate as long as incident ray is near monochromatic and the charge sharing effect does not cause significant spectral distortions. The extrapolation accuracy of the models also varies under different circumstances.

Uher et al. used a Gaussian function to describe the spread of charges, and fitted the energy response functions of a 300um Si based Medipix2 detector with X-ray fluorescence [10]. Campbell and Das did a similar work with some minor improvement, and further used the response functions for spectral restoration [11]. The Gaussian model combined the advantage of the flexibility of Monte Carlo simulation and the simplicity of empirical fitting. Instead of monochromatic sources such as synchrotrons or isotopes, it used the X-ray fluorescence as the calibration source, which is easier to be implemented. The problem of the Gaussian model is that it could not take the K-escaping peaks into consideration due to characteristic X-ray in the detector, thus it does not apply to CdTe or CdZnTe detectors.

In this paper, we proposed a novel method for the modeling of the energy response functions, where Monte Carlo simulation was combined with a numerical Gaussian model. GEANT4 [12] was used to simulate the interaction between photons and the detector, such as energy deposition, scattering and fluorescence. The charge transportation and spread were described with the Gaussian

spread model, and anti-charge sharing logics were also included in the model. The spectral broadening was modeled by spectral convolution with shift variant Gaussian kernels. The free parameters in the numerical model were decided by measuring spectrums of X-ray fluorescence from metal elements, where the differential evolution algorithm [13] was used for the fitting.

The paper is organized as follows: In the next section, the model will be described in detail, including the energy deposition, charge transportation, anti-charge sharing and the spectral broadening. In the third section, it will be shown how to determine the free parameters in the model with X-ray fluorescence spectrums. These two sections are the main contributions of this paper. The fourth section will show experimental results of an XCounter Flite X1 detector, whose main parameters are listed in table 1 [14]. Results from both fluorescence and X-ray source validation experiments will be shown to verify the feasibility of the proposed model. The last section is discussion and conclusion.

Table 1. Main parameters of the XCounter Flite X1 detector [14]

Parameter	Value
Material	CdTe
Thickness	750um
Pixel size	100×100um ²
Resolution	1536×128
Number of thresholds	2
Cover	500um carbon fiber

2. Modeling

2.1 Energy deposition

GEANT4 was used to simulate the energy deposition of the photons in the detector. Photons

with monochromatic energy distribution were generated and irradiated the detector in a small area. All the energy deposition incidents were recorded for each photon and its secondary particles. The recorded information included the index of the photon, the amount of energy deposited in the detector, and the coordinates of interaction. The required information in this step was the materials and thicknesses of the detector and its covers, which were acquired from the detector manufacturer.

2.2 Charge transportation

The holes and electrons generated in the semiconductor will spread due to repulsion and diffusion during their drifting towards the electrodes. Nilsson et al. derived the spread deviation for normally depleted semiconductors with diffusion equations [8]. For over depletion, which is more common in semiconductor detectors, Kim et al. gave an approximate formula to express the spread of charges [15]. The charge distribution was Gaussian with the standard deviation of

$$\sigma = \sqrt{\frac{2k_B T D d}{eV}} \quad (1)$$

where k_B is the Boltzmann constant, T is the temperature in Kelvin unit, D is the thickness of detector, d is the drifting distance, e is the charge of electron, and V is the bias voltage.

To further simplify the model, it was assumed that the collected charges for each pixel were induced by the majority carriers at the end of drifting [16]. For example, for CdTe detectors, we assumed that the collected charges for each pixel equal to the number of electrons that reached it.

Equation (1) could be further written as:

$$\sigma = \sigma_0 \sqrt{\frac{d}{D}} = \sigma_0 \sqrt{\frac{D-z}{D}} \quad (2)$$

where z is the depth of energy deposition, and σ_0 is a parameter to be decided, which means the charge spread deviation at the surface of the detector. For applications in medical imaging and security inspection (10keV – 200keV), the initial size of the charge clouds could be neglected [15].

Fig. 1. Demonstration of charge sharing calculation.

Figure 1 demonstrates the calculation of charge sharing. For each energy deposition incident (the black dot), the integrals of the 2-dimensional Gaussian function were calculated in each pixel in its 9-pixel neighborhood (the grey blocks). The integrals were calculated by calculating the integrals along two directions separately. The 1-dimensional Gaussian integral was calculated using the Gaussian error function $\text{erf}()$ [17], which had a rapid approximation as shown in appendix A.

For all the energy deposition incidents with the same photon index, the charges for all the relevant pixels were accumulated and stored for further processing. It should be noticed that because the charge transportation model was applied to individual energy absorption event instead of the whole absorption process of a photon, the 9-pixel neighborhood was sufficient for most detectors, because the amount of charges would be too small (less than 0.3%) 2 pixels away [18]. However, if the pixel size was too small compared to the spread of charges, the size of the neighborhood should be further enlarged.

2.3 Anti-charge sharing

Anti-charge sharing circuits sum the charges that are generated simultaneously in adjacent pixels and reassign them to one pixel [18][19]. Several possible anti-charge sharing strategies are available for pixel detectors, including 4-pixel, 5-pixel and 9-pixel. The strategy T was considered as a

parameter in our model which needed to be decided, because sometimes end-users do not know the exact anti-charge sharing tactics employed by the manufacturer.

Fig. 2. Possible anti-charge sharing strategies, from left to right: 4-pixel, 5-pixel, and 9-pixel.

Figure 2 demonstrates the strategies that were included in our model. The 4-pixel strategy was adopted in Medipix3 [18]. Its logic was realized as follows in our model: The charges were stored at the corners of the pixels. For each corner, the charges from its 4 adjacent pixels were summed. Then for each pixel, only the corner with the largest sum of charges would be kept.

The 5-pixel and 9-pixel logics were much simpler: first the charges of all the 5-pixel or 9-pixel neighborhoods were summed and stored in each one's central pixel, then the pixels that were local maximum in 5-pixel or 9-pixel neighborhood kept their charges.

In our modeling, for a photon that hits the detector, the indices of all the relevant pixels and the total deposited charges were recorded with the charge transportation model in section 2.2. The anti-charge sharing model dealt with this recorded information and reassigned the deposited charges. It was possible that the relevant region was larger than 9 pixels, and our model would process the pixels in a sequential order.

After anti-charge sharing logics, the collected energy of the pixels were built into a histogram (spectrum), whose x axis was energy and y axis was number of pixels in each energy bin.

2.4 Spectral broadening

The number of the electron-hole pairs generated for each energy deposition incident follows Gaussian distribution whose variance is proportional to the deposited energy. Furthermore, electronics noise and ballistic deficit will also degrade the energy resolution of the detector [27]. Instead of randomly disturbing the amount of charges generated before charge transportation, the spectral broadening was approximated by shift variant Gaussian convolution of the spectrum after anti-charge sharing. The approximation was for the sake of computational acceleration and fitting stability. The variation of the Gaussian kernel was linearly proportional to the energy E :

$$\sigma_e^2 = k_e E \quad (3)$$

where k_e is a parameter to be decided in the model. It should be noticed that in photon counting detectors, the main factors that lead to energy resolution degradation is not necessarily the statistical fluctuation. However, as it will be shown in the experimental results, (3) was a reasonable choice for the spectral broadening model which compromised between the model precision and model robustness. The final energy response function is the spectrum divided by the number of photons.

2.5 Thresholds mapping

The thresholds of the detector were set through software interface and digital analog converter (DAC). We assumed a linear relationship between the thresholds and the corresponding energy E :

$$E = k_{th} \times TH + b_{th} \quad (4)$$

where TH is a threshold set through the software interface, k_{th} and b_{th} are two parameters to be fitted.

We conclude the 5 parameters to be decided here: the charge spread deviation σ_0 , the anti-charge sharing strategy T , the spectral broadening factor k_e , and the thresholds mapping

coefficients k_{th} and b_{th} . In the following section, it will be introduced how to fit the 5 free parameters with X-ray fluorescence spectrums.

3 Fitting of the key parameters

3.1 X-ray fluorescence experiment

The X-ray fluorescence experiment could be carried out by irradiating samples which contain metal elements with common X-ray sources. With simple collimations, it could be guaranteed that most of the photons that reach the detector were X-ray fluorescence, whose spectrum consisted of a few monochromatic characteristic spectral lines. Characteristic X-ray up to 85keV could be produced with common stable metal elements. The stability and precision of the model fitting would increase if more kinds of elements were used. The detailed experiment configuration of our system will be introduced in section 4.1.

3.2 GEANT4 simulation

The GEANT4 simulation proposed in section 2 has to be adjusted for the fitting task. Instead of using monochromatic incident ray which directly irradiated the detector, a system was setup to approximate the fluorescence experiment. The sample was made of metal simple substances and was irradiated with collimated polychromatic source, whose spectrum was generated by simulations such as SpekCalc [20]. The recording of the energy deposition information and following process were the same with section 2.

3.3 Parameter fitting

Assume M samples were used for fluorescence measurement, denote the spectrums with and without anti-charge sharing as $R_0^{(m)}(TH)$ and $R_{0AC}^{(m)}(TH)$, where m stood for the m th sample. Each spectrum was normalized so that the area under curve equaled to 1. The peak positions of $R_{0AC}^{(m)}(TH)$

was fitted to the corresponding $K\alpha_1$ peaks, and the fitting results, k_{th0} and b_{th0} would be used later as initial values.

The parameter σ_0 was fitted with $R_0^{(m)}(TH)$. Several possible values of σ_0 were selected, and for each σ_0 , fluorescence spectrums were generated with GEANT4 and charge transportation model. The results before spectral broadening were denoted as $R_1^{(m)}(E; \sigma_0)$. Spectrums with different m were then fitted to $R_0^{(m)}(E)$ individually:

$$k_{th}^{(m)}, b_{th}^{(m)}, \sigma_e^{(m)}, A^{(m)} = \arg \min \int \left[R_0^{(m)}(TH) - A^{(m)} R_2^{(m)}(k_{th}^{(m)} \times TH + b_{th}^{(m)}; \sigma_e^{(m)}) \right] dTH \quad (5)$$

$$R_2^{(m)}(E; \sigma_e^{(m)}) = \int R_1^{(m)}(E'; \sigma_0) \frac{1}{\sqrt{2\pi}\sigma_e^{(m)}} \exp\left(-\frac{(E-E')^2}{2(\sigma_e^{(m)})^2}\right) dE' \quad (6)$$

Note that it was assumed that the spectral broadening parameter $\sigma_e^{(m)}$ did not change with energy for individual samples m in this step. Differential evolution (DE) algorithm was employed to solve (5). An initial range has to be given for the algorithm to work: $k_{th}^{(m)} \in [0.95, 1.05] \times k_{th0}$, $b_{th}^{(m)} \in [0.95, 1.05] \times b_{th0}$, and $\sigma_e^{(m)} \in [1\text{keV}, 5\text{keV}]$. $A^{(m)}$ was determined during fitting with least squares algorithm. The range of $\sigma_e^{(m)}$ was decided empirically, but one advantage of DE algorithm is that the initial range does not constrain the final solution. DE algorithm will be briefly introduced in appendix B.

After individual fitting, $\sigma_e^{(m)}$ was further used to fit the initial value of k_e according to (3). Let

$$R_3^{(m)}(E; \sigma_0, k_e) = \int R_1^{(m)}(E'; \sigma_0) \frac{1}{\sqrt{2\pi}k_e E} \exp\left(-\frac{(E-E')^2}{2(k_e E)^2}\right) dE' \quad (7)$$

The rest of the parameters were fitted by

$$k_{th}, b_{th}, k_e, A^{(m)} = \arg \min \sum_m \int \left[R_0^{(m)}(TH) - A^{(m)} R_3^{(m)}(k_{th} \times TH + b_{th}; \sigma_0, k_e) \right]^2 dTH \quad (8)$$

The selection of initial ranges for all the variables was the same as the previous step.

A few σ_0 were tested and fitted, and the final σ_0 was selected as the one which gave the

minimum fitting error in (8). The range of σ_0 had to be selected empirically or with a few tests. The above steps were repeated with spectrums that had anti-charge sharing, where σ_0 was fixed to the fitted value, and the rest of the parameters were fitted for each anti-charge sharing strategy T . The T which gave the minimum fitting error was selected as the anti-charge sharing strategy. The corresponding parameters σ_0 , k_{thAC} , b_{thAC} , and k_{eAC} were taken as the parameters for the model.

4 Experiments

4.1 X-ray Fluorescence configurations

The fluorescence experiment was carried out with metal simple substances or compounds. Most of the samples were in the form of powder except for Pt which was in the form of small foils. The intensities of spectral lines were slightly different in different compounds of the same metal elements, but it could be safely ignored because we did not need a very precise response function.

The samples were sealed in plastic bags and irradiated by a VJ X-ray source with 160kVp voltage, 3mA current and 2mm additional Al filters. The X-ray was collimated to the sample by a lead brick with a small cylindrical hole which was approximately 50mm thick and 5mm in diameter. There was no object behind the sample in 3m.

The XCounter Flite X1 detector was placed by the side of the source and the sample, so that it could avoid the bremsstrahlung ray and receive the fluorescence ray. No collimator was added in front of the detector and the entire detector could receive the fluorescence ray in our experiment. To remove background scattering, a background spectrum was measured with no sample installed and subtracted from the fluorescence spectrums.

The spectrums were acquired with dual thresholds scan, where the high and low thresholds of the detector kept a distance of 1 (approximately 4keV) and increased with a step of 0.5, from

approximately 12keV to 110keV. We didn't use a smaller interval due to the precision of the detector's DAC. The spectrum for each sample was calculated by difference of the high and low thresholds data and taking the mean of all the pixels. Pixel inconsistency was not considered in our energy response function calibration. The acquisition time for each step was 2s. Each sample was acquired with both anti-charge sharing on and off under the same conditions.

As for the GEANT4 simulation, the source spectrum was generated by SpekCalc and sampled with 1keV interval from 16keV to 160keV. 1×10^5 photons were simulated for each energy sample. The recorded spectrums were also sampled in 1keV interval.

The experiment system is shown in figure 2, and the samples are listed in table 2 with their corresponding $K\alpha_1$ and $K\beta_1$ peaks [21].

Table 2. The samples used in the fluorescence experiment [21]

Chemical formula	$K\alpha_1$ (keV)	$K\beta_1$ (keV)
La_2O_3	33.4	37.8
CeO_2	34.7	39.2
$\text{Nd}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$	37.3	42.3
Gd_2O_3	43.0	48.6
Er_2O_3	49.1	55.6
W	59.3	67.2
Pt (small foils)	66.8	75.7
Pb	74.9	84.9

Fig. 3. The experiment system for X-ray fluorescence. Left: a photo of the system; Right: the geometric configuration, where the green area stands for the area that the fluorescence rays could reach.

4.2 X-ray source spectrum experiment configurations

The acquired fluorescence spectrums were used for the parameter fitting, thus they could not be used for the validation of the fitted energy response functions. For the validation task, the detector was directly irradiated by the X-ray source and spectrums were taken. The source operated with 3 different voltages (80kVp, 100kVp and 120KVp) and 2 different additional filters (2mm Al and 0.03mm Ta), which made 6 different spectrums. The anti-charge sharing was on while the rest of the configurations were mostly the same as in section 4.1. The only difference was that to avoid counter saturation, the source operated with 0.5mA current and the acquisition time for each threshold step was 0.33s.

The theoretical results were calculated by convolving the SpekCalc spectrums with the simulated energy response functions:

$$S_{TH}(E) = \int R(E; E') S_0(E') dE' \quad (9)$$

where $R(E; E')$ stands for the intensity of energy response function at energy E with incident photon at energy E' , $S_0(E)$ is the simulated source spectrum. $S_{TH}(E)$ was normalized and

compared to the acquired source spectrums.

4.3 X-ray Fluorescence results

4.3.1 Thresholds-energy fitting with $K\alpha_1$ peaks

The spectrums with anti-charge sharing on were up sampled by a factor of 10 by spline interpolation, and the $K\alpha_1$ peaks were located at the local maximum of the full energy peaks. The fitting result between the measured $K\alpha_1$ peaks and the theoretical peak positions is shown in figure 4. The linear correlation coefficient was 0.9998. The result indicated that linear relationship assumption (4) was reasonable.

Fig. 4. The threshold-energy fitting result with the $K\alpha_1$ peaks.

4.3.2 σ_e^2 fitting results

The fitting results of σ_e^2 from individual fluorescence spectrums are shown in figure 5. The results showed that the assumption (3) was reasonable for the relationship between spectral broadening and incident photon energy.

Fig. 5. The fitting results of σ_e^2 . The red dots are the σ_e^2 fitted from individual fluorescence spectrums, the blue lines are the fitting results according to (3). From left to right are the results of no anti-charge sharing, 4-pixel, and 5-pixel, respectively.

4.3.3 Fitting results with anti-charge sharing off

σ_0 from 10um to 25um with 1um interval were used to simulate fluorescence spectrums. The fitting errors for measured spectrums without anti-charge sharing are shown in figure 6. It could be seen that $\sigma_0 = 15$ um gave the minimum fitting error, which was taken as the charge spread deviation in our model.

Fig. 6. The fitting errors with different σ_0 for measured spectrums without anti-charge sharing.

Fig. 7. The fitting results for all the fluorescence spectrums with anti-charge sharing off.

Figure 7 shows the fitting results for all the fluorescence spectrums. It could be seen that the model recovered most of the features of the spectrums. There were noticeable errors at the K-escape peaks for Pt and Pb, where the measured escape peaks were lower than the modeled ones. One possible explanation was the difference between the practical fluorescence cross section of CdTe compound and the theoretical ones of Cd and Te used in the GEANT4 simulation [28].

4.3.4 Fitting results with anti-charge sharing on

The fitting errors with different anti-charge sharing strategy T are shown in figure 8. It could be seen that 4-pixel and 5-pixel strategies gave quite similar errors, and further investigation would be made with the X-ray source spectrum measurement.

Fig. 8. The fitting errors with different anti-charge sharing strategies for the spectrums with anti-charge sharing on.

The fitting results for all the measured spectrums with anti-charge sharing on are shown in figure 9 and 10, for 4-pixel and 5-pixel strategies respectively. It could be seen that while most features of the spectrums have been recovered, there were noticeable errors at the k-escape peaks. It should be due to the same reason that led to the errors at the k-escape peaks in section 4.3.3.

It could be also noticed that the measured data was obvious larger than the modeled spectrums near 20keV for W, Pt and Pb, which was not so obvious for elements with low atomic number. One possible reason was that the anti-charge sharing model in our study was not exactly the same with the real case. For La, Ce, and Nd, the full peak was not far from 20keV and the errors were suppressed by it. For Gd and Er, the k-escape peaks overlapped with the characteristics peaks near 20keV, which also greatly reduced the fitting errors. However, for most medical X-ray imaging applications where the energy near 20keV was not concerned, the proposed model could still be useful despite of the errors.

There was no significant difference between the results of 4-pixel and 5-pixel anti-charge sharing strategies. Decisions have to be made with further experiments.

Fig. 9. The fitting results for all the fluorescence spectrums with 4-pixel anti-charge sharing.

Fig. 10. The fitting results for all the fluorescence spectrums with 5-pixel anti-charge sharing.

4.3.5 Fitting results of the other parameters

Figure 11 demonstrates the fitting results of the other parameters. It could be seen that there was no noticeable error between the 4-pixel and 5-pixel anti-charge sharing strategies. But the parameters for spectrums modeled with anti-charge sharing on and off were different. It was due to noise level difference and model errors.

Fig. 11. The threshold-energy relationship (left) and the spectral broadening (right).

4.3.6 X-ray spectrum validation results

The validation results are shown in figure 12. It could be seen that the 4-pixel recovered most of the features of the measured spectrum. The 4-pixel results also fitted better than the 5-pixel results. The results showed that 4-pixel anti-charge sharing should be selected in the model for our detector, and the model was precise enough to predict the scanned spectrum, which indicated that it had enough precision for noise estimation and thresholds optimization.

Fig. 12. The X-ray spectrum validation results: top row is with 2mm Al filter, bottom row is with 0.03mm Ta filter. From left to right, the source voltage was 80kVp, 100kVp and 120kVp for each column.

5 Discussion and conclusion

This paper proposed a hybrid Monte Carlo model for X-ray pixel photon counting detector, and the corresponding calibration methods with X-ray fluorescence. The model consisted of 4 steps: GEANT4 simulation of energy deposition, Gaussian model of charge transportation and sharing, anti-charge sharing logics, and shift-variant Gaussian convolution for spectral broadening. There were 5 free parameters to be determined in the model: charge spread deviation σ_0 , anti-charge sharing strategy T , spectral broadening coefficient k_e , and the threshold-energy mapping coefficients k_{th} and

b_{th} . Fluorescence spectrums of metal elements were taken via thresholds scans, and the free parameters were fitted via DE algorithm. The results with X-ray source spectrums showed the precision of the method.

The advantage of the proposed method was its flexibility. It could be applied to the calibration for most photon counting detectors at the energy range of medical applications. The only challenge was to determine the range of σ_0 , which required a few trials. The drawback of the proposed method was lack of high precision. The modeled spectrums were biased from the measured ones, especially near the k-escape peaks. However, since our goal was noise estimation with continuous X-ray sources, the precision of the proposed model should be enough.

The complexity in the physics of pixel photon counting detectors made it very hard to be modeled precisely. Several factors were ignored in our model, including trapping effect [22], electronics noise, pixel inconsistency, etc. It should be noticed that the error of the proposed model increased at higher energies, and errors were seen mostly at the k-escape peaks and characteristics peaks. One possible reason was the difference of fluorescence cross sections between theoretical values and practical values. Furthermore, in anti-charge sharing mode, there was also noticeable increase of fitting errors, which could be due to the difference between modeled and on-chip logics.

Further work includes using the modeled energy response functions for noise optimization with Cramer-Rao lower bound [23]. We will also try to combine the response functions with empirical calibration methods for spectral calibration, and then apply it to reconstruction.

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Appendix A. Fast calculation of Gaussian Integrals [17]

The Gaussian integrals were calculated as

$$\int_a^b \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx = \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right) \quad (10)$$

where

$$\Phi(x) = \frac{1}{2} \left[1 + \operatorname{erf}\left(\frac{x}{\sqrt{2}}\right) \right] \quad (11)$$

$\operatorname{erf}()$ is the error function, which could be approximated as shown in algorithm 1.

Table 3. Fast approximation of $\operatorname{erf}()$

Algorithm 1. Fast approximation of $\operatorname{erf}(x)$

Define constants:

$$a_1 = 0.254829592, a_2 = -0.284496736, a_3 = 1.421413741, a_4 = -1.453152027, a_5 = 1.061405429,$$

$$p = 0.3275911;$$

Calculate:

$$t = 1 / (1 + p|x|);$$

$$y = 1 - (((((a_5 t + a_4) t + a_3) t + a_2) t + a_1) t) \times \exp(-x^2);$$

Output $\operatorname{sign}(x) \times y$

where $\operatorname{sign}(x)$ is 1 when x is larger or equal to 1, otherwise it is -1.

Appendix B. Brief introduction to differential evolution algorithm [13]

The DE algorithm was proposed by Storn and Price in 1997. Same as simulated annealing [24]

and genetic algorithms [25], DE is a kind of global optimization algorithms, which has large

possibility of converging to global minimum rather than local minimum for non-convex problems. It

was designed for problems with continuous variables. It does not require derivative of the object

function, so it suits for problems with complex object functions and not too much variables. The basic outline of the DE algorithm is described in algorithm 2. The open-sourced code from Berkeley was used in our work [26].

Table 4. Basic outline of DE algorithm[13]

Algorithm 2. Basic outline of DE algorithm to solve $\mathbf{x} = \text{argmin } f(\mathbf{x})$

- 1 Generate initial values $\mathbf{x}_{i,0}$ randomly in certain ranges, where $i = 1, 2, \dots, NP$;
- 2 For generations $G = 1 : N_G$, repeat step 3-5: (N_G is the number of iterations)
- 3 **Mutation:** $\mathbf{v}_{i,G+1} = \mathbf{x}_{i,G} + F(\mathbf{x}_{r_2,G} - \mathbf{x}_{r_3,G})$ for each i . F is a constant and $F \in [0, 2]$. r_1, r_2, r_3 are three different random values from set $\{1, 2, \dots, NP\}$;

- 4 **Crossing:** Let

$$u_{ij,G+1} = \begin{cases} v_{ij,G+1}, & \text{randb}(j) \leq CR \text{ or } j = mbr(i) \\ x_{ij,G}, & \text{otherwise} \end{cases}$$

where CR is a constant and $CR \in (0, 1]$, $\text{randb}(j)$ is a uniformly distributed random number between $[0, 1]$, $mbr(i)$ is a randomly chosen number in the set $\{1, 2, \dots, J\}$, and J is the dimension of variables.

- 5 **Choosing:** for each i ,

$$\mathbf{x}_{i,G+1} = \begin{cases} \mathbf{u}_{i,G+1}, & f(\mathbf{u}_{i,G+1}) \leq f(\mathbf{x}_{i,G+1}) \\ \mathbf{x}_{i,G}, & f(\mathbf{u}_{i,G+1}) > f(\mathbf{x}_{i,G+1}) \end{cases}$$

In algorithm 2, larger population NP led to more stable solutions but longer computation time. Normally $NP \geq 7J$. Larger F led to faster convergence but less stable solutions, and it was chosen as 0.85 in our work. CR followed the same trend and it was chosen as 0.9. Appropriate choice of initial ranges would also speed up convergence, but the results were not necessarily constrained in the initial ranges. The iteration number N_G was 100 in our work.

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