Published in final edited form as:

Med Phys. 2021 June ; 48(6): 2800–2808. doi:10.1002/mp.14863.

Technical Note: Standalone application to generate custom reflectance Look-Up Table for advanced optical Monte Carlo simulation in GATE/Geant4

Carlotta Trigila^{a)},

Department of Biomedical Engineering, University of California Davis, Davis, CA, USA

Eshani Moghe,

Department of Biomedical Engineering, University of California Davis, Davis, CA, USA

Emilie Roncali

Department of Biomedical Engineering, University of California Davis, Davis, CA, USA,

Department of Radiology, University of California Davis, Davis, CA, USA

Abstract

Purpose: The need for high-fidelity modeling of radiation detectors to perform reliable detector performance optimization using Monte Carlo simulations requires to accurately simulate the light transport in the scintillator and the light collection by the photodetector. In this work, we implement our well-validated crystal reflectance model computed from three-dimensional (3D) crystal surface measurement in a standalone open-source application to allow researchers to generate fully customized crystal reflectance look-up-tables (LUTs) to be used in optical Monte Carlo simulation.

Methods: The LUTDavisModel application can be installed in a few minutes on Windows, macOS, and Linux, using 26 MB of space. MATLAB Runtime is required and is automatically installed with the application. The core algorithm has been previously validated experimentally and implemented in GATE v8.0. The standalone is divided into five panels, each of which performing a specific task: generate LUTs from a combination of surface type, scintillator, and coupling medium available in the database (such as LSO or BGO) or custom; compute LUTs with the reflectors available and custom coupling thickness; create a mixture of coupling media to account for possible defects in the optical coupling; plot precomputed LUTs for visual comparison. Tooltips and errors/warnings facilitate the navigation. The reported computational times were obtained with an Intel Core i7 MacBook Pro.

Results: LUTs can be generated with computational time ranging from a few minutes to several hours depending on the selected surface, sampling, and computational power. A longer time is needed when using rough surfaces and thick coupling media (hundreds of μm) due to increased photon tracking.

^{a)} Author to whom correspondence should be addressed. ctrigila@ucdavis.edu.

SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of the article.

Conclusions: We developed a user-friendly standalone application to generate LUTs that can be used inside GATE Monte Carlo simulations. It can be easily downloaded, installed, and used. Future optimizations will expand the database, decrease the computational time through greater parallelization, and include the generation of LUTs to study Cerenkov photons transport.

Keywords

GATE; light transport model; Monte Carlo optical simulations; scintillation detectors; surface finish

1. INTRODUCTION

Optimizing scintillation-based gamma-ray detectors is of great interest in nuclear medicine and high energy physics and often uses optical Monte Carlo simulation. In the development of positron emission tomography (PET) detectors, improving the overall performance requires a deep understanding of the light transport in the scintillator and the light collection by the photodetector.¹ Accurately modeling them is thus critical for achieving high performance, mainly when the design incorporates depth-of-interaction (DOI) encoding or time-of-flight information.^{2,3} In this context, simulation software that can precisely predict the behavior and impact of each of the components influencing the photon transport prior to detection is needed to study potential design improvements.⁴ Variations in the scintillator intrinsic properties, geometry, and surface finish can strongly affect the behavior of scintillation photons at the crystal sides and consequently their detection.^{5–7}

To perform those simulations, open-source simulation toolkits as Geant4⁸ and GATE⁹ can be used. In previous works, we developed a look-up-table (LUT) model of crystals reflectance computed from a 3D measurement of crystal surface to address significant deficiencies in the optical modeling capabilities of GATE.^{9–13} The algorithm computes the reflectance, transmittance, and angular distribution of reflected and transmitted rays as a function of incidence angle (from 0° to 90°) starting from a surface sample. The LUT computation includes the reflector, the coupling medium, and the photon tracking between the two interfaces. This algorithm allows for more accurate modeling of photon interactions with crystal surfaces with or without a reflector than previously proposed models such as the UNIFIED¹³ and the experimental approach of Janecek and Moses.¹⁴

The Davis LUT model has been validated against experimental data and implemented in GATE v8.0 and subsequent versions.¹⁵ GATE now includes LUTs for rough and polished lutetium oxyorthosilicate (LSO) crystal surfaces without reflector, with a Lambertian reflector (e.g., Teflon tape), and an air- and grease-coupled specular reflector (ESR). While these LUTs allow performing light transport simulations that showed good agreement with experimental data,^{10,11} the demand for higher-fidelity detector modeling to optimize the detector performance requires the computation of more customized LUTs.

We implemented our reflectance model in a standalone graphical interface to generate GATE LUTs from users' customized surface, crystal, and coupling medium or from the database's samples. A set of reflectors is included together with the possibility to generate LUTs with and without a reflector. The reflector and photodetector are coupled to the crystal through

a medium (typically air, glue, or optical grease). The attenuation in the coupling is set to zero. To model imperfections in the coupling medium, “mixed” LUTs can be computed with a coupling medium composed of both air and glue/optical grease to represent poor optical coupling between the crystal and the photodetector or deficiencies in the crystal-reflector coupling. These LUTs will make optical MC simulations more realistic by considering possible sources of light loss.

In this work, we present the standalone and its main features. It is a user-friendly tool for researchers to generate LUTs for their custom scintillator-coupling-reflector configuration that can then be used in GATE optical Monte Carlo simulations. This will allow users to predict the light transport in a scintillation crystal with an accurate description of their setup and detector design, as an alternative to using the existing LUTs. This tool aims to address the need for users to carry out optical Monte Carlo simulations with high fidelity to optimize their original design and explore many configurations flexibly and independently.

2. MATERIALS AND METHODS

2.A. LUT Davis Model standalone download and technical information

Created with App Designer (MATLAB 2019b) and packaged with MATLAB Compiler™ (MATLAB 2019b), the LUT Davis Model Standalone can be installed and used on Windows, macOS, and Linux independently of MATLAB based on MATLAB Runtime. The installers for the three operating systems can be download together with the standalone User’s Guide from several sources.^{16,17} The guide contains a detailed description of the app functionalities together with a description of the installation procedure. It takes a few seconds if MATLAB Runtime is already installed. If not, it goes up to a maximum of 30 min since it will automatically include the MATLAB Runtime installation. In its first version, the standalone size is 26 MB. The Standalone source code will also be available on GitHub as part of the open-GATE collaboration source code.

2.B. LUT Davis Model structure

A detailed description of the algorithm implemented in the standalone app, its experimental validation, and GATE implementation can be found in our previous works.^{10,11,15}

Briefly, the LUT Davis algorithm computes the reflection and transmission probabilities and the photons’ angular distributions as a function of incidence angles (from 0° to 90°) of 3D crystal surfaces scanned with atomic force microscopy (AFM), coupled to a reflector through a coupling medium. The scintillator-coupling-reflector LUT is computed in two steps. First, the *scintillator-coupling* reflectance and transmittance LUTs are computed using a scintillator defined by its topography, emission spectrum, and index of refraction as a function of the wavelength and a coupling medium defined by its index of refraction. The scintillator-coupling-reflector reflectance and transmittance LUTs (also named *reflector LUTs*) are computed using the transmitted photons’ information stored in the transmittance LUT. Each reflector is defined by its reflectance and angular distribution of reflection. In this way, multiple reflectors LUTs can be tested using the same scintillator-coupling LUTs. This leads to an important computational time gain if multiple reflectors are tested. Mixed

LUTs can be generated from two precomputed scintillator-coupling LUTs or reflector LUTs to account for possible coupling medium inhomogeneities.

Following the algorithm functionalities, the standalone has been divided into five panels: “Generate Scintillator-coupling LUTs” to generate the scintillator-coupling LUTs; “Generate Reflector LUTs” to include the reflector in the LUT computation; “Generate Mixed LUTs” to generate the mixture of coupling media in the interface between the crystal surface and the reflector or photodetector; “Compare LUTs” to plot and compare already computed LUTs and “Merge existing LUTs” to merge and create LUTs from several non-completed computations. Each panel is further described.

The LUTs computational times were obtained with a Mac-Book Pro (Apple Inc.) with macOS Catalina, a 2GHz, Intel Core i7 quad-core processor, and an 8 GB, 1600 MHz DDR3 memory).

2.B.1. Scintillator-coupling LUTs computation: Generate Scintillator-coupling LUTs panel—Figure 1 shows the standalone first panel. It allows the scintillator-coupling LUT generation (bottom subpanel) after defining the surface (top-left subpanel), the crystal, and the coupling medium (top-right subpanel). The user can choose between a surface and a scintillator available in the standalone database or use customized ones. Table I contains the details about the database and the files needed to use customized surfaces/scintillator. The database scintillators’ emission spectra and refractive indices as a function of the wavelengths are plotted in Fig. S1. More details about the “.txt” needed to use a customized scintillator can be found in the User’s Guide. While choosing a scintillator from the database, a user can customize its index of refraction. The emission spectrum and the index of refraction can be plotted together.

The index of refraction of the coupling medium must also be defined. Fresnel equations can be computed and plotted to visualize a photon’s probability of being reflected or transmitted by a flat surface.

In Fig. 1, a polished bismuth germanate (BGO) crystal was selected with air as a coupling medium (polished-BGO-air configuration).

After specifying the output directory, the user can run a test (*Run Test*) and/or run the complete LUT (*Run LUT*) computation using the corresponding *play* buttons (Fig. 1 bottom subpanel). The computation can be paused or stopped when needed using the corresponding *stop* and *play* buttons. The *Run Test* functionality consists of running the LUT algorithm using low statistics in terms of incident photon angular distribution (from 0° to 90°, each 5°). Test LUTs could provide insight on the reflectance and transmittance dependency with the incident angle for selected configurations. It can also give an estimate of the total computation time. The *Run LUT* functionality allows running the scintillator-coupling LUTs computation after defining the “Angles Specifications.” If “*All Angles*” is selected, the complete LUT computation is performed (from 0° to 90°, each 1°). If “*Specific Angle*” is selected, only a few select angles, defined by the user in the corresponding input boxes, are computed. This partial computation is helpful to analyze specific incident angles or if

the “All Angles” computation is stopped before completion (either by a manual interruption through the stop command, or an unexpected computer shut down or issue with high overall CPU usage). In all cases, users can compute only the remaining polar angles (values from 0° to 90° are needed) and then use the *Merge existing LUTs* panel, as described in subsection 2.B.4.

Green progress bars help visualize the status of the computation of the algorithm. Once finished, the reflectance and transmittance can be plotted using the *plot* buttons and superimposed to Fresnel equations. Log “.txt” files with a summary of the parameters used are always automatically saved in the output directory.

The results of several LUTs computations will be shown in Section 3.A.

2.B.2. Reflector LUTs computation: Generate Reflector LUTs panel—LUTs with a reflector can be generated using the standalone second panel (Fig. S2). First, the user has to upload a previously computed scintillator-coupling LUT, whose characteristics are automatically summarized in a table. The coupling medium thickness must be set in μm , with a value greater than the coupling thickness minimum value. It is defined as the distance between the mean and minimum surface elevation. The mean elevation is the mean value between the surface maximum and minimum elevation. The coupling thickness minimum value is automatically displayed in the coupling thickness edit field (Fig. S3).

Then, the reflector should be chosen from the database (see Table I). Its reflectivity can be manually adjusted through a scaling factor (default value 1) to study its effect on the light output, for example, or to model a deterioration of the reflector efficiency such as Teflon impregnated with grease. More information about the reflectors’ reflectivity spectra can be found in our previous work.¹¹

After defining the output directory, the LUT computation can be started (paused or stopped), and the results can be plotted using the *plot* button. Both 1 and 10 μm thicknesses are tested in scintillator-coupling configurations coupled with Teflon, as shown in the results Section 3.B.

2.B.3. Mixed LUTs computation: Generate Mixed LUTs panel—LUTs with an inhomogeneous coupling medium, for example, composed of a mixture of air and grease, can be generated from two existing LUTs. This can be done by randomly selecting the optical photon fate through the reflectance and angular distributions based on the fraction of each material in the coupling medium. It implies that the two media are spatially arranged within the coupling in a random fashion. Mixed LUTs can only be computed if the two LUTs are compatible, that is, if they differ only in the coupling medium. For example, using two scintillator-coupling LUTs computed with air and grease (e.g., polished-BGO-air and polished-BGO-grease), the mixed LUTs allow simulating grease coupling with some air inhomogeneities (e.g., air bubbles in the photodetector–crystal interface). While using two reflector LUTs, one can consider the case in which an amount of optical grease, pushed away from the photodetector–crystal face, fills space between the crystal and the reflector, thus causing the interface to be far from an ideal crystal-air one. It can be done using the

third panel of the standalone (Fig. S4) by uploading two LUTs, choosing the output folder, choosing the mixture percentage (a single value or a range of values), and running the computation with the corresponding button. The results can then be visualized using the *plot* button.

2.B.4. Compare LUTs and Merge existing LUTs: The last two panels—The fourth panel allows superimposing the reflectance and transmittance curves of existing LUTs for qualitative comparison. The last panel gives the possibility to merge multiple incomplete computations of the same configuration once all polar angles are available (values from 0° to 90° are needed) and after checking their compatibility (same surface, scintillator, coupling). For example, it can be used if an *All Angles* computation crashed and a *Specific Angles* computation with the missing angles was performed. Panels are shown in Figs. S5 and S6, respectively.

3. RESULTS

3.A. Scintillator-coupling GATE LUTs

Figure 2 shows the first panel bottom subpanel with the results of several LUTs computations performed with the polished-BGO-air configuration (as previously shown in Fig. 1). While performing a complete simulation [Fig. 2(a)] with *All Angles* as “Angles Specification,” GATE LUTs are available. Two GATE LUTs (.dat format) are saved in the output folder: one data file contains the reflection probabilities and the other the reflection directions. As shown in Fig. 2(b), while running a test (“Test LUT”) and a partial computation (“Run LUT,” from 20° to 35° as *Specific Angles*), GATEs LUTs are not available due to the low statistics used and the absence of some incident angles (values from 0° to 90° are needed for a complete computation). Examples of a polished-BGO-grease and rough-BGO-air complete LUTs computations are shown in Fig. S7.

The simulations’ computational times are summarized in Table II.

3.B. Reflector LUTs

Figure 3 shows the reflector LUTs computation performed with the complete polished-BGO-air precomputed LUT [shown in Fig. 1 and Fig. 2(a)] coupled with a 1- μm -thick air coupling to Teflon (polished-BGO-1 μm Air-Teflon). Since we used an *All Angles* scintillator-coupling LUTs, the light in the summary table is green (Fig. 3 top-left subpanel) indicating that the reflector GATE data files will be available. The results obtained with the polished-BGO-air LUT and a 10 μm coupling (polished-BGO-10 μm Air-Teflon configuration), with the polished-BGO-grease and a 1 μm coupling (polished-BGO-1 μm Grease-Teflon), and with rough-BGO-air and a 10 μm coupling (rough-BGO-10 μm Air-Teflon), all coupled to Teflon, are shown in supporting Fig. S8. See Table II for computational times. It is important to note that a scintillator-coupling LUT obtained with a test or a partial computation can be used as input (e.g., configurations 2 and 3, Table II) to perform a Reflector LUT computation, but GATE LUTs will not be available if incomplete. It will be indicated by a yellow light in the summary table (and not green as shown in Fig. 3 top-left subpanel).

3.C. Air-Grease mixed LUTs

Mixed LUTs are generated from the polished-BGO-air and polished-BGO-grease precompiled LUTs [shown in Fig. 2(a) and Fig. S7, respectively]. The air-grease ratio was sampled from 0% to 10%, each 1%, to simulate the case of a grease coupling containing some air bubbles, as shown in Fig. 4. At the end of the computation, GATE data files are available. See Table II for computational times.

3.D. Compare LUTs

The visual comparison of the reflectance and transmittance of the polished-BGO-air, polished-BGO-grease, polished-BGO-9% air-81% grease, and polished-BGO-1 μ mGrease-Teflon configurations is performed using the standalone fourth panel and can be visualized in Fig. S9.

3.E. Merge existing partial LUTs

Three scintillator-coupling LUTs of the same configuration (polished-BGO-air) are generated with various ranges of “Specific Angles” (from 0° to 20°; from 20° to 60°; from 60° to 90°) and are merged to generate GATE LUTs, using the last panel of the app. The merging procedure is shown in detail in Fig. S10.

4. DISCUSSION

The LUTDavisModel Standalone provides a fast and user-friendly method to generate customized LUTs to model radiation detector optical interfaces in GATE optical Monte Carlo simulations. Fully customized LUTs represent the first step toward high-fidelity modeling of light transport inside a detector. They allow working on advanced and unique applications with users meeting their simulation needs, such as modeling crystal bars segmented using subsurface laser engraving.¹⁸

The standalone functionalities are schematically shown in Fig. 5 and described in detail in File S11. Its schematic structure, tooltips, and warning/error alerts help the users handily run a complete LUT computation.

Although the computational time depends on the used computer processor, several qualitative observations can be pointed out from Table II. For the same crystal-coupling pair, the use of a rough surface increases the computational time compared to a polished one (e.g., BGO-air, configurations 1 and 5 without reflector, or configurations 7 and 9 with Teflon, Table II). It is due to an increased number of multiple reflections/transmissions for each processed photon. Second, for the same surface-crystal pair (polished-BGO), increasing the coupling medium index of refraction (e.g., from air = 1 to grease = 1.5, configurations 1 and 4, Table II) does not affect the scintillator-coupling LUT computational time. Instead, it affects the reflector LUTs (e.g., configurations 6 and 8 for the same coupling thickness). Indeed, when BGO is coupled to air, the critical angle is 26°. Thus a lower number of transmitted photons are processed to model the reflector effect than BGO coupled to grease (critical angle of 44°). Moreover, increasing the coupling medium thickness increases the computational time. When the coupling thickness (e.g., 100 μ m) and

the 3D scanned surface's dimensions (e.g., $90 \times 90 \mu\text{m}^2$, Table I) are comparable, a photon reflected by the reflector typically travels in the coupling until it reaches the 3D surface boundaries. A larger surface is needed to enable the tracking over the necessary distance and is created through stitching: the initial surface is vertically and horizontally flipped and then concatenated. Consequently, the algorithm tracks over greater path lengths in the medium, causing a computational time increase. As shown in Table II, the computational time does not increase linearly with the thickness. Consequently, simulating greater thicknesses (e.g., hundreds of microns, like that of common tapes) could lead to computational time in the order of weeks. To overcome this issue, future versions will include the possibility to heavily use parallel computing. Computing different incidence angles can readily be done on different computer processors independently. The users will be able to choose the number of processors available. Furthermore, the definition of the coupling attenuation length will be added to model nontransparent media (e.g., thicker coupling medium).

As shown, the app allows to generate mixed LUTs and decrease the reflector's reflectivity using a scaling factor. These features open the possibility to simulate suboptimal optical configurations (e.g., deterioration of the reflector efficiency such as Teflon impregnated with grease or air bubbles in the photodetector–crystal interface). It can be done in GATE by building a specific geometry with these LUTs only on the surfaces of interest (e.g., in the crystal–photodetector face or the crystal's borders close to the photodetector face). In future work, we will use the mixed LUTs to understand the effect of suboptimal optical photodetector–crystal and reflector–crystal couplings on detectors' light collection.

In recent years, great attention has been given to prompt Cerenkov photons to improve coincidence timing resolution measurement, in which variation of the photon travel time within the crystal becomes critical.^{19–23} Cerenkov LUTs can be computed with the LUTDavisModel algorithm for a given material using its index of refraction as a function of the wavelength and can be used within GATE.^{4,24} The standalone's next release will allow the generation of Cerenkov LUTs for both scintillation and nonscintillation materials. It will be followed by GATE modifications to enable users to simultaneously study scintillation and Cerenkov photons transport in the material using their specific LUTs.

5. CONCLUSION

In this work, we presented the LUTDavisModel standalone, an application to generate fully customized crystal reflectance LUTs to be used in optical Monte Carlo simulation. We suggest referring to the Standalone User's Guide to understand how to use the generated data files inside GATE.^{16,17} Although customized surface and scintillator can be used, the app database will be expanded gradually to give users the possibility to test several materials easily. Moreover, new reflectors will be made available, such as retroreflectors and Lumirror (Toray). The next release will support Cerenkov photon LUTs generation due to the great interest in Cerenkov photons tracking.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

ACKNOWLEDGMENTS

This work was supported by NIH grant R01EB027130. C. Trigila and E. Moghe are with the Department of Biomedical Engineering, University of California Davis, Davis, CA 95616, USA. E. Roncali is with the Department of Biomedical Engineering and the Department of Radiology, University of California Davis, Davis, CA 95616, USA. The authors thank M. Stockhoff and S. Cherry for the initial developments of the LUTDavis model that led to the implementation of this standalone app.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES

1. Lecoq P. Pushing the limits in time-of-flight PET imaging. *IEEE Trans Radiat Plasma Med Sci.* 2017;1:473–485.
2. Gundacker S, Auffray E, Frisch B, et al. Time of flight positron emission tomography towards 100ps resolution with L (Y) SO: an experimental and theoretical analysis. *J Instrum.* 2013;8:P07014.
3. Berg E, Roncali E, Cherry S. Optimizing light transport in scintillation crystals for time-of-flight PET: an experimental and optical Monte Carlo simulation study. *Biomed Opt Express.* 2015;6:2220–2230. [PubMed: 26114040]
4. Roncali E, Kwon S II, Jan S, et al. Cerenkov light transport in scintillation crystals explained: realistic simulation with GATE. *Biomed Phys Eng Expr.* 2019;5:035033.
5. Huber JS, Moses WW, Andreaco MS, et al. Geometry and surface treatment dependence of the light collection from LSO crystals. *Nucl Instrum Methods Phys Res Sect A.* 1999;437:374–380.
6. Kilimchuk IV, Tarasov VA, Vlasova ID. Study of light collection as a function of scintillator surface roughness. *Radiat Meas.* 2010;45:383–385.
7. Gundacker S, Knapitsch A, Auffray E, et al. Time resolution deterioration with increasing crystal length in a TOF-PET system. *Nucl Instrum Methods Phys Res Sect A.* 2014;737:92–100.
8. Agostinelli S, Allison J, Amako K, et al. GEANT4—a simulation toolkit. *Nucl Instrum Methods Phys Res Sect A.* 2003;506:250–303.
9. Jan S, Santin G, Strul D, et al. GATE: a simulation toolkit for PET and SPECT. *Phys Med Biol.* 2004;49:4543. [PubMed: 15552416]
10. Roncali E, Cherry S. Simulation of light transport in scintillators based on 3D characterization of crystal surfaces. *Phys Med Biol.* 2013;58:2185–2198. [PubMed: 23475145]
11. Roncali E, Stockhoff M, Cherry S. An integrated model of scintillator-reflector properties for advanced simulations of optical transport. *Phys Med Biol.* 2017;62:4811. [PubMed: 28398905]
12. Nayar SK, Ikeuchi K, Kanade T. Surface reflection: physical and geometrical perspectives. *IEEE Trans Pattern Anal Mach Intell.* 1991;13:611–634.
13. Levin A, Moisan C. A more physical approach to model the surface treatment of scintillation counters and its implementation into DETECT. *IEEE Nucl Sci Symp Conf Record.* 1996;2:702–706.
14. Janecek M, Moses WW. Simulating scintillator light collection using measured optical reflectance. *IEEE Trans Nucl Sci.* 2010;57:964–970.
15. Stockhoff M, Jan S, Dubois A, et al. Advanced optical simulation of scintillation detectors in GATE V8.0: first implementation of a reflectance model based on measured data. *Phys Med Biol.* 2017;62:L1. [PubMed: 28452339]
16. OpenGATE Collaboration. Documentation. <http://www.opengatecollaboration.org/>. Accessed December 15, 2020.
17. Roncali lab website. Documentation. <https://roncalilab.engineering.ucdavis.edu>. Accessed December 15, 2020.

18. Ogata Y, Ohnishi T, Moriya T, et al. GPU-based optical propagation simulator of a laser-processed crystal block for the X'tal cube PET detector. *Radiol Phys Technol.* 2014;7:35–42. [PubMed: 23896989]
19. Lecoq P. New approaches to improve timing resolution in scintillators. *IEEE Trans Nucl Sci.* 2012;59:2313–2318.
20. Korpar S, Dolenc R, Križan P, et al. Study of TOF PET using Cherenkov light. *Nucl Instrum Methods Phys Res Sect A.* 2011;654:532–538.
21. Ota R, Nakajima K, Ogawa I, et al. Coincidence time resolution of 30 ps FWHM using a pair of Cherenkov-radiator-integrated MCP-PMTs. *Phys Med Biol.* 2019;64:07LT01.
22. Cates JW, Levin CS. Electronics method to advance the coincidence time resolution with bismuth germanate. *Phys Med Biol.* 2019;64:175016. [PubMed: 31300623]
23. Kratochwil N, Gundacker S, Lecoq P, et al. Pushing Cherenkov PET with BGO via coincidence time resolution classification and correction. *Phys Med Biol.* 2020;65:115004. [PubMed: 32268304]
24. Arino-Estrada G, Mitchell GS, Kwon SI, et al. Towards time-of-flight PET with a semiconductor detector. *Phys Med Biol.* 2018;63:04LT01.

Fig. 1. First panel of the LUTDavisModel Standalone. The Menu on the left corner gives users information about the standalone version and how to contact the developers. The user can move from one panel to the other from the top panel bar. Warnings/error alerts facilitate the navigation within the standalone. Most components have tooltips, as shown here for the “Plot Fresnel Equation” button.

Fig. 2.

Bottom subpanel of the “Generate Scintillator-coupling LUTs” panel. (a) Results of a complete simulation, obtained by setting the “Angles Specification” at “All Angles”. Note that a “Run Test” was started and stopped before the “Run LUT.” (b) Results of a “Run Test” and a “Specific Angles” (from 20° to 35°) computation. In all cases, the results are plotted and superimposed to Fresnel equations. Simulations performed with a polished surface (polished-BGO-air configuration) closely match Fresnel equations.

Fig. 3.
Standalone panel to create reflector LUTs. The green lamp in the summary table indicates that the reflector GATE “.dat” files will be available using the chosen scintillator-coupling LUT.

Fig. 4.

Standalone panel to create Mixed LUTs, which can be generated from two precomputed scintillator-coupling or reflector LUTs that have to differ only in the index of refraction. Parameters are automatically summarized in a summary table: the first has air (1) and the second has grease (1.5), but the rest is identical. A green light indicates that GATE LUTs are available.

Fig. 5.
Standalone schematic flow. Refer to Fig. S11 for more details.

Table I.

LUTDavisModel Standalone database and information needed to use customized surfaces and scintillators. Scintillators in the database: Lutetium oxyorthosilicate (LSO), bismuth germanate (BGO), lanthanum bromide (LaBr₃), yttrium aluminum garnet (YAG), and yttrium gallium garnet (YGG).

Database		Custom
Type	Characteristics	Information needed
Surface	Polished	- “.txt” file with a 2D array of the surface heights
	Rough	- surface X dimension in μm
Database		Custom
Name	Properties	Information needed
Scintillator	LSO	- Scintillator name
	BGO	- Index of refraction as a function of the wavelength as a 2×N matrix saved in a .txt file
	LaBr ₃	- “.txt” file with the emission spectrum distribution
	YAG	
	YGG	
Coupling medium	Examples: air (1), optical grease (1.57), glass (1.5), generic glue (1.5), MeltMountTM (1.582), TiO ₂ (1.61)	
Reflector	Specular reflector (ESR), Lambertian reflector (AceTeflon4L), Teflon materials (PTFE) with several layers (two, four, and eight layers)	

Table II.

Review of the computational time needed to compute several configurations, without and with a reflector, computed from the first and second panel, respectively. Notice that a reflector LUT computation (e.g., Polished-BGO-1 μm Air-Teflon, configuration 6) is performed using a scintillator-coupling LUT (Polished-BGO-Air, configuration 1) as input.

Configurations	Setting	Panel	Time	Fig.
1 Polished-BGO-air	"Run LUT" with "All Angles"	1	10 h40	2(a)
2 Polished-BGO-air	"Run Test"	1	5 min	2(b)
3 Polished-BGO-air	"Run LUT" with "Specific Angles"	1	1 h20	2(b)
4 Polished-BGO-grease	"Run LUT" with "All Angles"	1	10 h30	S7(a)
5 Rough-BGO-air	"Run LUT" with "All Angles"	1	43 h	S7(b)
6 Polished-BGO-1 μm Air-Teflon	"Run LUT" using Config. 1	2	2 h	3
7 Polished-BGO-10 μm Air-Teflon	"Run LUT" using Config. 1	2	12 h	S8(a)
8 Polished-BGO-1 μm Grease-Teflon	"Run LUT" using Config. 4	2	5 h	S8(b)
9 Rough-BGO-10 μm Air-Teflon	"Run LUT" using Config. 5	2	29 h	S8(c)
10 Mixed Polished-BGO-air/grease LUTs	"Run LUT" using Config. 1 and Config. 4	3	6 min	4