GRAY: High Energy Photon Ray Tracer for PET Applications

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Abstract-GRAY (High Energy Photon Ray Tracer) is a Monte-Carlo ray-driven high energy photon transport engine for mainly PET and SPECT applications that supports complex mesh based primitives for source distributions, phantom shapes, and detector geometries. Monte-Carlo modeling is critical for system design evaluation and image reconstruction development. Ray tracing is a technique used in computer graphics to render scenes with realistic light properties. We adapted an open source ray tracing engine to support the physical properties of high energy photon transport. The main project goal of GRAY is to provide a means to import advanced geometrical mesh primitives from graphical CAD programs to create animated vectorial based phantoms and complex detector geometries while preserving physical accuracy and efficient runtime. These phantoms will be able to model complex moving objects targeted towards developing novel image reconstruction algorithms for cardiac, respiratory, and tracer kinetic modeling. Traditionally, complex geometrical phantoms were simulated using a series of discrete voxelized sources that represent the activity source distributions and attenuation media. By using rejection testing, constructive solid geometry can create primitives that are combined using Boolean operations to create complex phantoms. The high energy photon physics modeling of GRAY has been validated against GATE for both runtime performance and accuracy. GRAY runs an order of magnitude faster than GATE with improved geometric modeling capabilities for detectors and sources. To highlight the capabilities of GRAY, a complex mesh phantom of a rat was filled with uniform activity, placed in a high resolution $1mm^3$ small animal box PET scanner, simulated with GRAY, and reconstructed using list-mode 3-D OSEM reconstruction.

Index Terms—Monte-Carlo Simulation, High Energy Photons, Ray Tracing, Positron Emission Tomography, PET

I. INTRODUCTION

ONTE-CARLO simulation of high energy photon transport for Positron Emission tomography (PET) and other nuclear medical imaging technologies is an important tool in understanding the physical processes that govern system design and image reconstruction development [1]. Many different facets of PET and SPECT medical imaging have led to the development of over 11 different Monte-Carlo simulators [2]. Monte-Carlo simulation has been used to design and compare different high performance small animal research scanners [3], [4], for the calculation of the system matrix for image reconstruction [5], for the estimation and removal of

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Compton scatter in image reconstruction [6], [7], and many others not references here. All of these methods use ray tracing to calculate the path of high energy photons through sources and detectors. Ray tracing is the method of storing a photon by its current position and its direction. A ray is cast and the first boundary that intersects the ray is calculated. A wide range of optical and high energy photon physics can be approximated by the relatively simple description of the photon as a ray. Individual simulation of each photon is extremely computationally expensive. Ray tracing methods have been developed that approximate many high energy photon paths together to significantly reduce the number of photons traced [8]. These methods usually reduce either the flexibility of the detector geometry or the accuracy of the photon physics simulated. The current standard for high energy photon Monte-Carlo simulation for PET and SPECT is the extremely powerful GATE toolkit [9], [10] which is built upon Geant4 [11]. GATE is primary focused on providing extremely accurate simulation of many different high energy photon and charge particle transport processes in detectors and source phantoms. The main purpose of this paper is reproduce the same physical accuracy as GATE while using a computer graphics back end. GRAY was based on a freely available

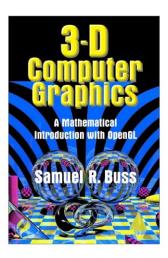


Fig. 1. 3D Computer Graphics: A Mathematical Introduction with OpenGL is an excellent resource for teaching and understanding the mathematics behind computer graphics. GRAY was derived from the excellent free optical ray tracer used in the book by including high energy photon transport.

Ray Tracer described in the book, 3D Computer Graphics: A Mathematical Introduction with OpenGL. (see fig. 1). All of the geometrical primitives of an modern optical ray tracer



Fig. 2. The complete path from source geometry through image reconstruction: Detailed 3-D CAD modeling of a rat phantom (LEFT), import of the vector geometry into GRAY to generate a simulated scan of a uniform distribution of positron decays in a rat placed in a 1mm resolution small animal box LSO-PSAPD PET scanner (MIDDLE), and a volumetric visualization of a reconstruction of the rat using a fully 3-D list-mode OSEM image reconstruction (RIGHT).

are available to GRAY, including parallelpipeds, Bezier (or NURBS) surfaces, and basic triangle meshes. The publically available ray-tracer has an kd-tree based geometrical acceleration structure. Geometrical acceleration structures reduce the number of intersection tests in complex scenes by creating the equivalent of a spatial binary tree. A balanced kd-tree achieves O(log n) increase in the time it takes to compute a single intersection test when there is an increase in n number of geometrical primitives. Therefore, the kd-tree reduces the performance penalty for simulating advanced detectors and complex phantoms. Therefore, the total simulation time grows as O(n log n) with increasing geometrical complexity since high energy photon transport has to perform a linear number of intersection tests to traverse a scene.

II. METHODS

GRAY is a high performance ray tracing engine that is focused on generating high energy photon interactions that were ported from an earlier work [12]. Detectors and Data acquisition are modelled with scripts written in Python language [13]. GRAY was written to incorporate accurate detector and phantom definitions using vectorial or triangle-mesh based primitives. The phantom and detector geometry is then simulated using the high energy photon properties calculated from NIST:XCOM [14] database using a ray-tracer engine.

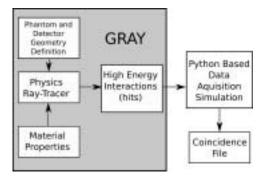


Fig. 3. Input geometry and materials database are simulated using a Ray Tracing Engine. Detector modelling is done with scripts that are written in the Python scripting language.

A. Flexible Geometry Definition

GRAY uses a language based on the neutral file format [15] to input geometry and simulation parameters. The file format allows for arbitrary rotations and positioning of individual geometrical primitives. CAD programs can export their geometry and then simple text parsing can translate the geometry to be imported into GRAY (see fig. 2). There is no distinction between detector geometry or source geometry, and all materials are treated exactly the same.

B. Vectorial Uniform Sources and Phantoms

GATE and other Monte-Carlo simulators, such as SIM-SET [16], represent complex phantoms as a set of voxels. GRAY has been written to use vectorial phantoms while at the same incorporating very flexible and accurate description of detectors. Simulating high energy photon transport in a vectorial phantom is faster than in a voxelized description. For voxel driven transport, many discrete intersection tests must be done on a voxel by voxel basis, which significantly slows down the simulation, while for a vectorial phantom, for most cases only a single intersection test must be performed. High quality vectorial phantoms have been been accurately segmented from high resolution MRI into extremely accurate 4-D phatoms based on NURBS surfaces for small animals [17]. Non-uniform rational B-splines (NURBS) are a vectorial based geometrical primitive that is used for compactly describing smooth, connected surfaces. GRAY can generate a uniform distribution of decays using rejection testing (see fig. 4) within a vectorial mesh and accurately model the high energy absorption and scattering (see fig. 5).

III. RESULTS

The physics of GRAY was validated against GATE [10].

A. Simple Pencil Beam Validation

A simple infinitely narrow pencil beam of 511keV photons were irradiated onto a 3cm and a 100cm thick lutetium-oxyorthosilicate (LSO) infinite panel in both GATE and GRAY to test the implementation of high energy photon absorption

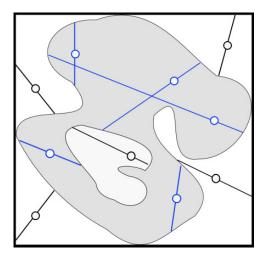


Fig. 4. Constructive solid geometrical sources are generated by taking a uniform random distribution in a bounding rectangle and rejecting or accepting the decay based on a Boolean operation on the inside or an outside intersection test on a set of geometrical primitives. The inside or outside test is determined by casting a ray randomly from the decay and performing an intersection test with the mesh.

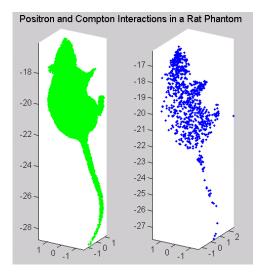
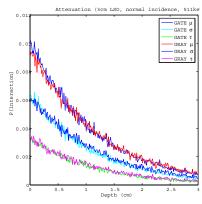
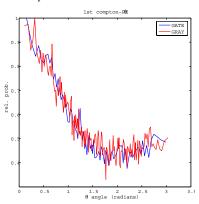


Fig. 5. Uniformly distributed radioactive decays can be generated inside any geometrical primitive. For example, uniformly distributed positron decays are generated (GREEN, LEFT) in a mesh based rat phantom. The phantom is then given the high energy photon transport properties of water. GRAY then models the physics of positron decay and gamma ray transport through the mouse generating physical interactions in the rat phantom (BLUE, RIGHT).

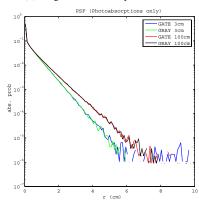
and scatter physics. A histogram of the depth penetration (fig. 6) as a function of summed, photoelectric and Compton interactions was generated. Secondly, the histogram of the radial point spread function of the pencil beam was generated for the 3 cm and 100 cm thick panel. Lastly, the theta angle was compared between the first two interactions for incoherent(Compton) scattering interaction. These three properties capture the most important factors that affect resolution and sensitivity of a PET imaging system. The two Monte-Carlo codes produce statistically identical results for the implementation of inelastic scattering and photoelectric interactions.



(a) Pencil beam absorption for photoelectric and Compton scatter interactions



(b) Angle of first Compton scatter



(c) Pencil beam radial point spread function

Fig. 6. The pencil beam tests validate basic implementation of photon absorption and Compton scattering while ignoring the complications from geometrical factors. Some of the important factors for high energy transport are the absorption, first photon Compton scatter angle, and final point spread blurring function.

B. Geometry of Benchmark

The runtime performance of GRAY was tested using the GATE PET benchmark. The GATE benchmark consists of a 8 panel octagonal ring of a dual LSO-BGO phoswitch detector with two layers of 3.0 mm x 3.8 mm x 15 mm discrete LSO and BGO crystals arranged in a 32 cm x 40 cm panel (see fig. 7. For each panel, five 0.5mm thick, 32 cm long tungsten septa provide scatter reduction, and two 1mm thick lead end shields block randoms from out of field of view activity. The phantom consists of a 70 cm long by 20 cm diameter water cylinder

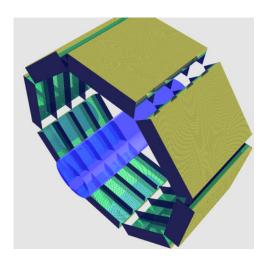


Fig. 7. GRAY has a full optical ray tracer to visualize the PET benchmark geometry.

TABLE I
BENCHMARK RESULTS

| | Total | Single | Coincident | Run |
|------|-----------------|--------------|-------------|-------------|
| | Positron Decays | Events | Events | Time |
| GRAY | $34.08x10^6$ | $13.74x10^6$ | $2.75x10^6$ | 36~min |
| GATE | $34.08x10^6$ | $14.03x10^6$ | $2.76x10^6$ | $371 \ min$ |

that runs down the central axis of the system. Inside the water phantom, are a 100 kBq (2.2 uCi) F-18 and a 100 kBq (2.2uCi) O-15 isotope line sources that are 68 cm in length and offset by 2 cm from the central axis.

C. Benchmark Physics Validation

The physical accuracy and the runtime of the two Monte-Carlo engines were analyzed under exactly the same simulation conditions using an ideal hits parser. GRAY produced statistically equivalent results to GATE for coincident events detected, energy resolution and spatial distribution of events in x, y, z coordinates while performing the same simulation in less time (see Fig. 8 and Table I).

D. Runtime Performance

For the benchmark time test, both simulations had file/io turned off to test the in-memory run time performance and were run on the same Intel Pentium 4 3Ghz PC with 2 GB of RAM running Fedora Core 3 Linux. GRAY was faster than GATE (see Table I) by using a very efficient acceleration structure and simplified code base.

IV. DISCUSSION

This work is an initial validation of the photon physics accuracy of GRAY. We have created an efficient and flexible Monte-Carlo ray tracer for simulation of high energy transport of photons in complex sources and phantoms. The modelling of detectors and data acquisition with energy resolution blurring, dead-time, and light-sharing effects are difficult to generalize to all potential systems and detector technologies. We

have split the modelling of the detector and data acquisition to the domain of another set of simulation tools. We developed a cycle accurate simulator with modelling of the entire electronics chain from detector up through ADC conversion to coincidence pairing and eventually off-line storage [18] for NEC type studies. On the other hand, for the less computationally demanding application of image reconstruction support, we have used much faster, but relatively ideal Python based models.

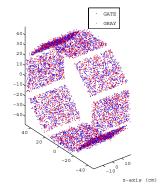
V. FUTURE WORK

Ultra fast and accurate Monte-Carlo simulation has the potential be used as the forward model in iterative image reconstruction algorithms, for system modelling, or as a better scatter estimator. GRAY has been specifically designed so that much faster intersection testers based on GPU hardware can replace the Kd-tree based CPU geometry acceleration structure to achieve another order of magnitude increase in performance. GRAY was also developed to generate realistic scans for 3-D PET detectors. Accurate modelling of Doppler broadening in 3-D semiconductor detectors such as CZT will be added.

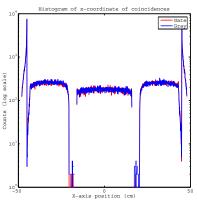
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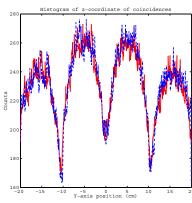
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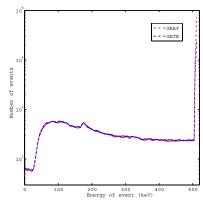
(a) 3-D Scatter plot of coincident events



(b) x-coordinate histogram



(c) z-coordinate histogram



(d) Event energy spectra

Fig. 8. Raw hits files were processed and histogramed to validate the physically accurate of GRAY to GATE when simulating a complex detector. The spatial coordinates and the energy of the events are statistically identical results between the two simulators.