GATE Optical Imaging (SHFJ status report)

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OUTLINE

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Simulation of the visible light fluorescence

Mie Scattering implementation in a standalone code for GPU architecture and validation

Optical Imaging Simulation Using GATE

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On behalf of the OpenGATE collaboration

The Geant4 Application for Emission Tomography (GATE) is an advanced opensource software dedicated to Monte-Carlo (MC) simulations in medical imaging involving photon transportation (positron emission tomography, single photon emission computed tomography, computed tomography) and in particle therapy. In this work, we extend GATE to support simulations of optical imaging such as bioluminescence or fluorescence imaging and validate it against the Monte-Carlo for Multi-Layered media simulation tool.

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Optical imaging simulation using GATE

Vesna Cuplov, Irène Buvat, Mohamed Mesradi, Frédéric Pain and Sébastien Jan.

***Abstract*— The Geant4 Application for Emission Tomography (GATE) is an advanced opensource software dedicated to Monte-Carlo (MC) simulations in medical imaging involving photon transportation (positron emission tomography, single photon emission computed tomography, computed tomography) and in particle therapy. In this work, we extend GATE to support simulations of optical imaging such as bioluminescence or fluorescence imaging and validate it against the Monte-Carlo for Multi-Layered media simulation tool.**

I. Introduction

Monte-Carlo simulations play an increasing role in medical imaging techniques involving radiations (Positron Emission Tomography - PET, Single Photon Emission Computed Tomography - SPECT, and Computed Tomography - CT). For these applications, simulations are used to help design and assess new imaging devices, and to optimize the acquisition and data processing protocols. The GATE ([1], [2]) open-source simulation platform, based on the Geant4 toolkit [3], has been developed since 2002 by the OpenGATE collaboration[1] and is currently widely used by the research community involved in SPECT and PET molecular imaging. In medical imaging, there is also a growing interest for additional molecular imaging modalities, including optical imaging. Indeed, optical imaging is a non-invasive, efficient and low-cost imaging technique allowing real time study of biological processes through 3D images of the light distribution emitted from the surface of small animals or superficial areas in humans. MC simulations involving optical photons are also being used in industry to better understand the light transport features inside or from the surface of an investigated material (silicon thin films, ceramics or even fruits). Other MC software simulating the photon migration in complex 3D shapes exist: the Tetrahedron-based Inhomogeneous Monte-Carlo Optical Simulator [4], the Molecular Optical Simulation Environment [5], the Mesh-based Monte-Carlo [6], and the Monte-Carlo for Multi-Layered media (MCML) [7] software. Yet, there is currently no MC code offering the same flexibility as GATE does for nuclear imaging applications. Given that optical imaging is also a matter of photon transportation, we started to extend GATE so that it can support optical imaging simulations. In this work, we present the simulation of visible or near infra-red light propagation in biological tissues.

II. Methods

A. Physics of optical imaging

When an optical photon travels through a given biological tissue, it can be either absorbed or scattered (Rayleigh or Mie scattering). When it reaches a biological tissue boundary, it can be transmitted and/or reflected. To model these effects in GATE, a set of four parameters has to be defined for each tissue type: a refractive index, the absorption and scattering lengths (L_a and L_s represent the average distance an optical photon can travel in a medium before being absorbed or scattered), and an anisotropy coefficient (g). The inverse of the absorption or scattering length is referred to as the absorption or scattering coefficient (μ_a, μ_s). In inhomogeneous media, reduced scattering coefficients (μ_s') are frequently used. They are defined as follows:

$$L_a = \frac{1}{\mu_a} \quad \text{and} \quad L_s = \frac{(1-g)}{\mu_s'}. \tag{1}$$

Concerning the processes at boundary (reflection and transmission), Geant4 provides a large panel of options to simulate surfaces through another set of parameters including the surface roughness, the reflectivity, the transmittance (in case the medium refractive index is unknown), and the specular and/or diffuse reflection coefficient. The Rayleigh scattering process, which depends on the particle's polarization, is already available in GATE. The Mie scattering has been added. It is significant only when the radius of the scattering object is of order of the photon wavelength. The Mie solution to Maxwell's equations takes the form of an analytical infinite series. A common approximation to this solution is called Henyey-Greenstein. The Henyey-Greenstein model describes the angular distribution of light scattered by small particles. The probability density function is:

$$p(\cos(\theta)) = \frac{1}{2}\frac{1-g^2}{(1+g^2-2g\cos(\theta))^{3/2}}, \tag{2}$$

where θ is the optical photon scattering angle with

$$\int_{-1}^{1} p(\cos(\theta))d\cos(\theta) = 1 \tag{3}$$

and

$$\int_{-1}^{1} p(\cos(\theta))\cos(\theta)d\cos(\theta) = g. \tag{4}$$

Accounting for polarization and momentum is performed using the same approach as for Rayleigh; the new direction of the photon is required to be perpendicular to the new polarization of the photon in such a way that the final direction and the initial and final polarizations are all in one plane.

B. Simulation of the optimal photon fluorescence

One of the most common optical imaging approach is fluorescence spectroscopy. This involves a fluorescent molecule (or probe) which is excited by an external source of light (lamp or laser) and then emits photons at longer wavelengths. When selecting the fluorescent agent for its close affinity with the diseased cells, a region with increased fluorescence emission will represent a diseased tissue. Geant4 already simulates the wavelength shifting (WLS) fibers that are widely used in high energy physics experiments [8]. These fibers absorb λ wavelength light and re-emit a λ' wavelength light. The WLS process was added to the GATE application to enable the simulation of the visible light fluorescence.

[1] www.opengatecollaboration.org

C. Validation of GATE versus MCML

In the MCML code, each layer has its own optical properties of absorption, scattering, anisotropy, and refractive index. The simulation set-up that we used for validating the model implementation in GATE consisted of a rectangular solid BioMimic[2] optical phantom of surface area of 5x5cm^2 and thickness varying from 0.5 to 2mm. Solid BioMimic optical phantoms are made of polyurethane, visible and near infra-red absorbing dyes and titanium dioxide scatterers. They mimic the optical properties of human and animal tissues. We simulated a source emitting unidirectional 530nm wavelength optical photons in a direction perpendicular to the phantom surface. The optical properties of the phantom for two wavelengths of interest in optical imaging are given in Table I. The refractive index was 1.521, the anisotropy 0.62 and the density 1.18 g/cm^3.

wavelength (nm)	μ_a(cm^{-1})	μ_s'(cm^{-1})
530	1.18	8.84
630	1.08	9.54

TABLE I

Optical phantom absorption coefficient and reduced scattering coefficient for two wavelength values.

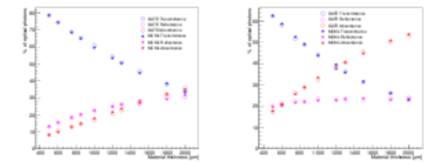
III. Results

For the validation of GATE versus MCML, two cases were studied. Figure 1 shows the percentage of absorbed, transmitted and backscattered optical photons obtained with our BioMimic phantom in the first scenario (a) where only optical absorption and scattering processes were enabled and in the more realistic scenario (b) where optical physics processes at boundaries were added in both simulations. We found an excellent agreement between the two codes. Concerning the WLS process (i.e. fluorescence), Figure 2 shows the GATE simulation of a fluorescence emission spectrum obtained after a Green Fluorescent Protein (GFP) was excited by a 400nm wavelength light. The simulation reproduces the well-known GFP emission spectrum.

IV. Conclusion and Perspectives

In this work, we extended GATE with new features such as the Mie scattering process and the visible light fluorescence so that GATE can support optical imaging simulations. We have validated the optical physics processes of GATE by showing an excellent agreement with MCML. A full simulation set-up for molecular optical imaging (fluorescence and bioluminescence) is currently being implemented: a voxelized phantom including a spherical tumor-like object is excited by an external optical photon beam of wavelength λ and the emitted fluorescent (wavelength λ') photons are detected by a system (i.e. charge coupled device camera) composed of an array of silicon pixel sensors and a photo multiplier tube. 3D images of the light distribution emitted from the phantom will be provided through the GATE software. The validation of this extended version of GATE against real optical imaging data is also planned.

[2] http://www.ino.ca/en-ca/achievements/description/project-p/optical-phantoms.html



a) b)

Fig. 1. Number of absorbed, transmitted and backscattered 530nm wavelength optical photons obtained for the BioMimic optical phantom target of different thicknesses. The left plot concerns the case where only absorption and scattering processes were enabled. The right plot takes into account the optical processes at boundaries.

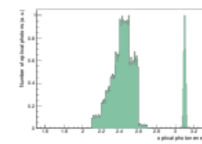


Fig. 2. The GFP emission spectrum simulated with the GATE software. The peak on the right represents the excitation light (400nm).

References

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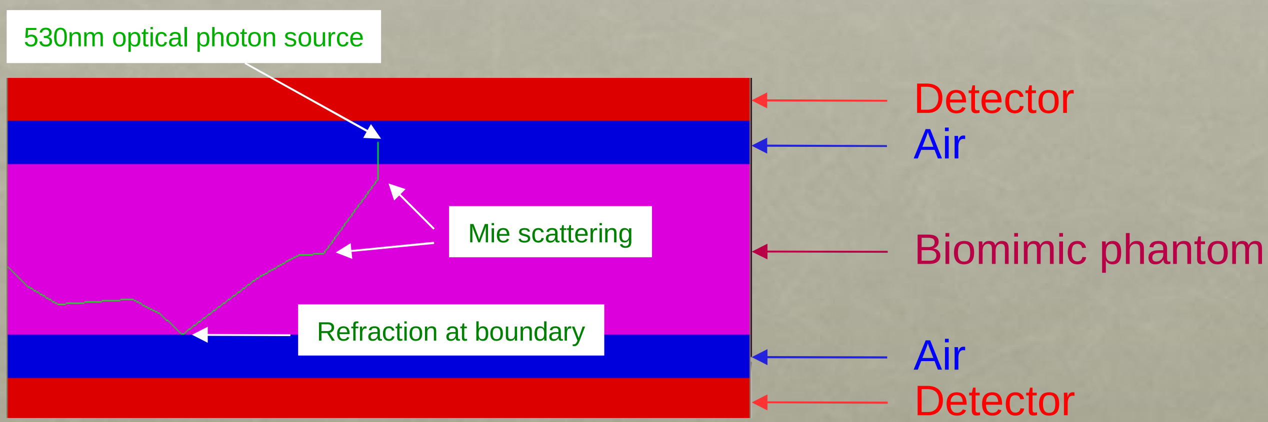
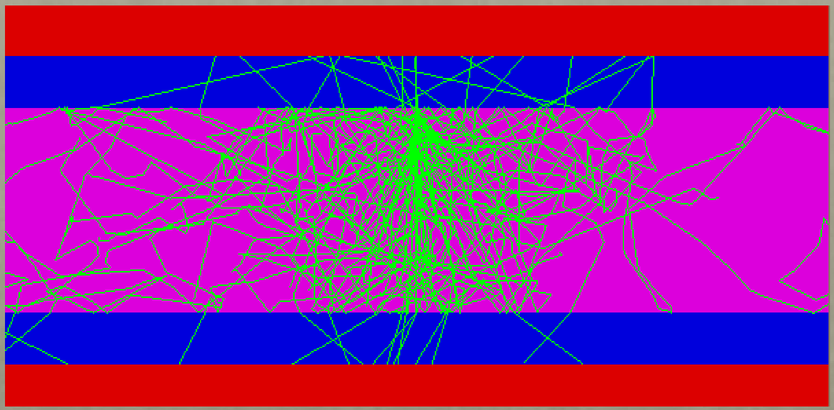
[2] S. Jan *et al.*, *"GATE V6: a major enhancement of the GATE simulation platform enabling modelling of CT and radiotherapy."*, Phys. Med. Biol. 56 (2011) 881-901.
[3] Geant4 Collaboration, *"Geant4: A simulation toolkit"*, Nucl. Instrum. and Methods A506 (2003) 250-303.
[4] H. Shen and G. Wang, *A tetrahedron-based inhomogeneous Monte Carlo optical simulator*, Phys. Med. Biol. 55 (2010) 947-962.
[5] H. Li, J. Tian, F. Zhu, W. Cong, L. V. Wang, E. A. Hoffman and G. Wang, *A mouse optical simulation environment to investigate bioluminescent phenomena in the living mouse with the Monte Carlo method*, Acad. Radiol. (2004) 1029-1038.
[6] Q. Fang, *Mesh-based Monte Carlo method using fast ray-tracing in Plücker coordinates*, Biomed. Opt. Express 1 (2010) 165-175.
[7] L. Wang, S. L. Jacques and L. Zheng, *MCML–Monte Carlo modeling of light transport in multi-layered tissues*, Comput. Methods Programs Biomed. (1995) 131-146.
[8] V. Cavasinni, T. Del Prete, V. Flaminio, E. Mazzoni, C. Roda, G. Usai and I. Vivarelli, *"A method to study light attenuation effects in wavelength shifting fibres"*, Nucl. Instrum. and Methods A517 (2004) 128-138.

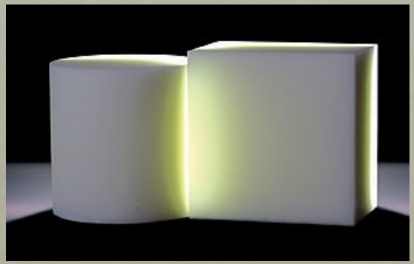
GATE versus MCML

MCML = Monte Carlo for Multi-Layered media





Biomimic optical phantom



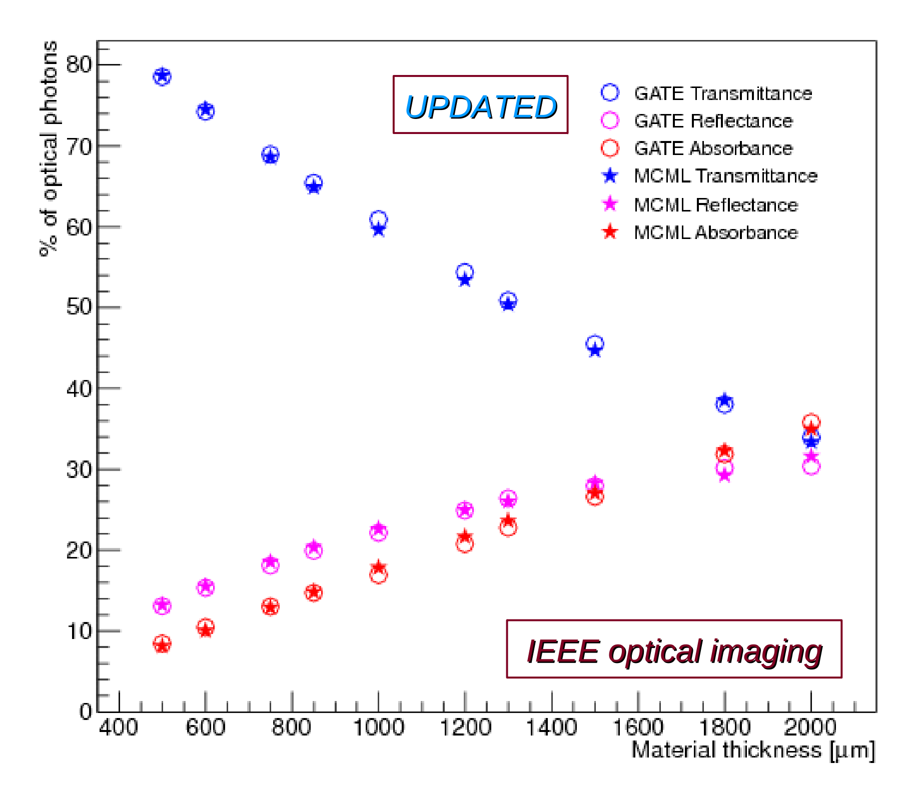
Made of polyurethane, visible and near nfra-red absorbing dyes and titanium dioxide scatterers. They mimic optical properties of human and animal tissues.

wavelength (nm)	μ_a (cm^{-1})	$\mu_s^{'}$ (cm^{-1})
530	1.18	8.84
630	1.08	9.54

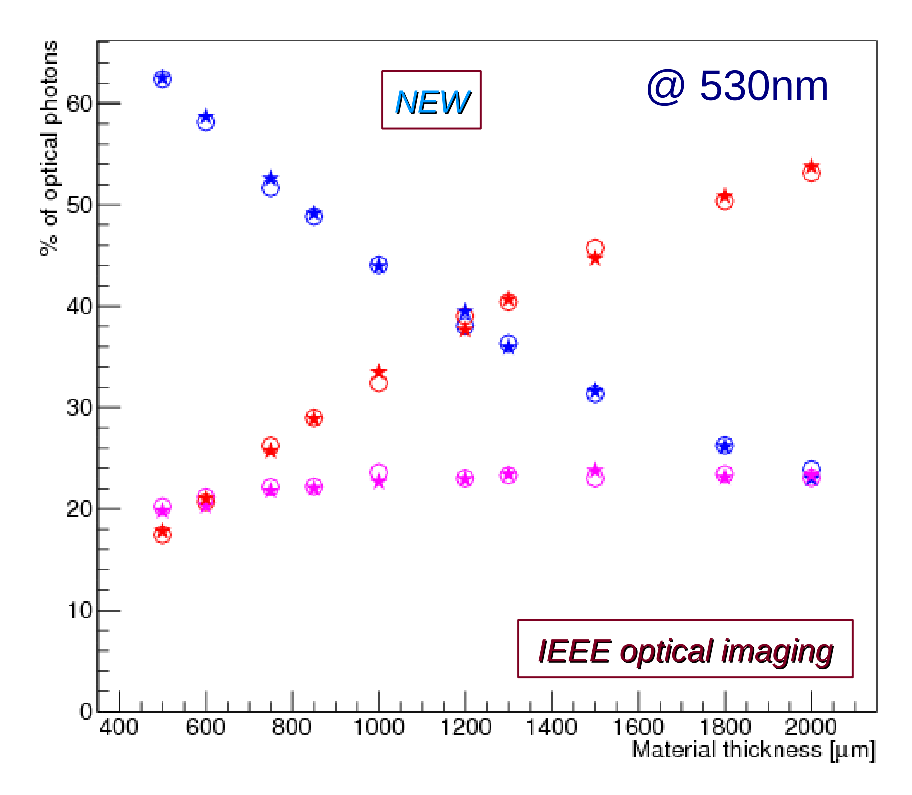
Refractive index = 1.521
Anisotropy = 0.62
Density 1.18 g/cm^3

GATE versus MCML

Bulk absorption + Scattering



Bulk absorption + Scattering + Process at boundary

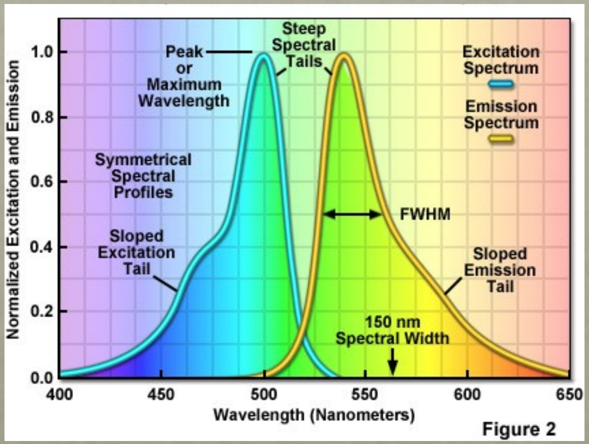


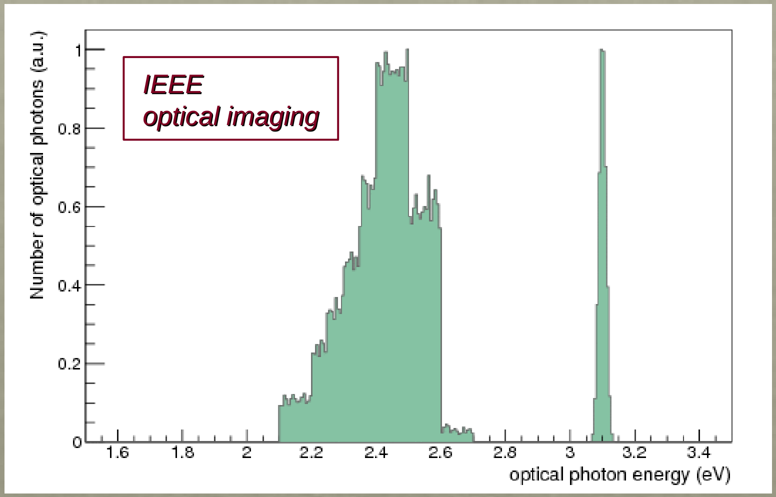
EXCELLENT agreement between the two codes!

Visible Light Fluorescence

One of the most common optical imaging is the fluorescence spectroscopy.

New GATE process : OpticalWLS (WaveLength Shifting: G4OpWLS)





- WLSABSLENGTH
- WLSCOMPONENT
- WLSTIMECONSTANT
- WLSMEANNUMBERPHOTONS

wiki page: Users_Guide_V6.2:Generating_and_tracking_optical_photons

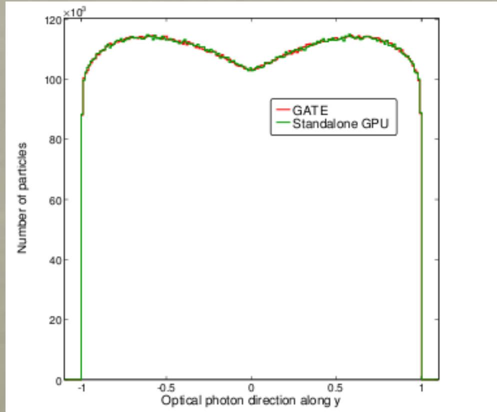
Julien Bert, Hector Perez-Ponce, Sébastien Jan, Ziad El Bitar, Pierre Gueth, Vesna Cuplov, Hocine Chekatt, Didier Benoit, David Sarrut, Yannick Boursier, David Brasse, Irène Buvat, Christian Morel, and Dimitris Visvikis

Mie scattering (standalone cuda code) + validation

D. Application for optical imaging

Optical imaging is an efficient and low-cost imaging technique allowing real time study of biological processes. Several physics processes occur during the optical photon propagation in biological tissues: absorption, scattering, transmission and reflection at tissue boundaries. We extended the standalone GPU framework code by adding the Mie scattering process provided by Geant4. The GPU implementation was validated against GATE simulations running only on CPU.

The simulation set-up that we used consisted of a voxelized phantom made of a water box of $100 \times 100 \times 100$ 4 mm^3 voxels. The water anisotropy and Mie scattering length were set to 0.62 and 6 mm respectively. We simulated an isotropic source of 20.10^6 optical photons of 6 eV located at the center of the water box. After tracking all particles up to the water box boundary, the particles were stored in a phase-space file.

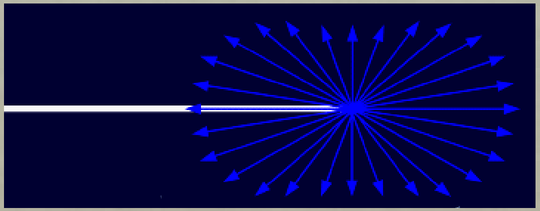


(a)

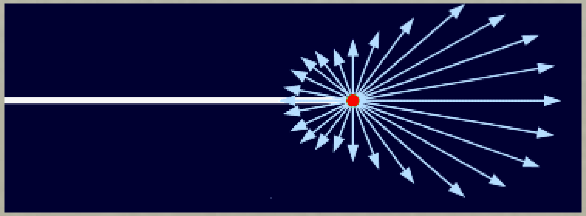
Fig. 2. (a) Simulation of the optical photon direction along the y-axis for the Mie scattering. (b) Simulation of the electron scattering angle as a function of its energy for the electron ionisation effect.

Mie scattering process: *cuda* implementation

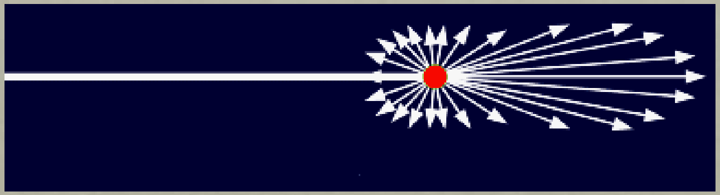
Scattering of light by spherical particles:



Rayleigh scattering



Mie scattering, small particle



Mie scattering, large particle

- A new deflection angle (θ) for the photon propagation is chosen according to the Henyey-Greenstein approximation:

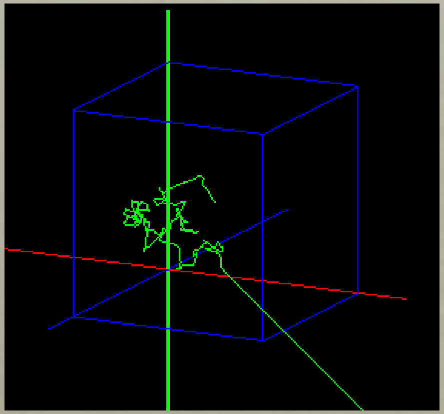
$$p(\cos\theta) = \frac{1 - g^2}{2 \times (1 + g^2 - 2g\cos\theta)^{3/2}}$$

g: anisotropy

- The calculation of the mean free path is done in the woodcock tracing function: -log $\mu(E)$ with $\mu(E) = 1/\sigma(E)$ = scattering length.

wiki page: Users_Guide_V6.2:Generating_and_tracking_optical_photons

Mie scattering Validation: GPU versus GATE-G4



Phantom: voxelized

Water box 100x100x100 voxels of $4mm^3$

Anisotropy set to $g=0.62$

Source: isotropic

Optical photons (6eV)

Positioned at center of the water box (200,200,200)mm

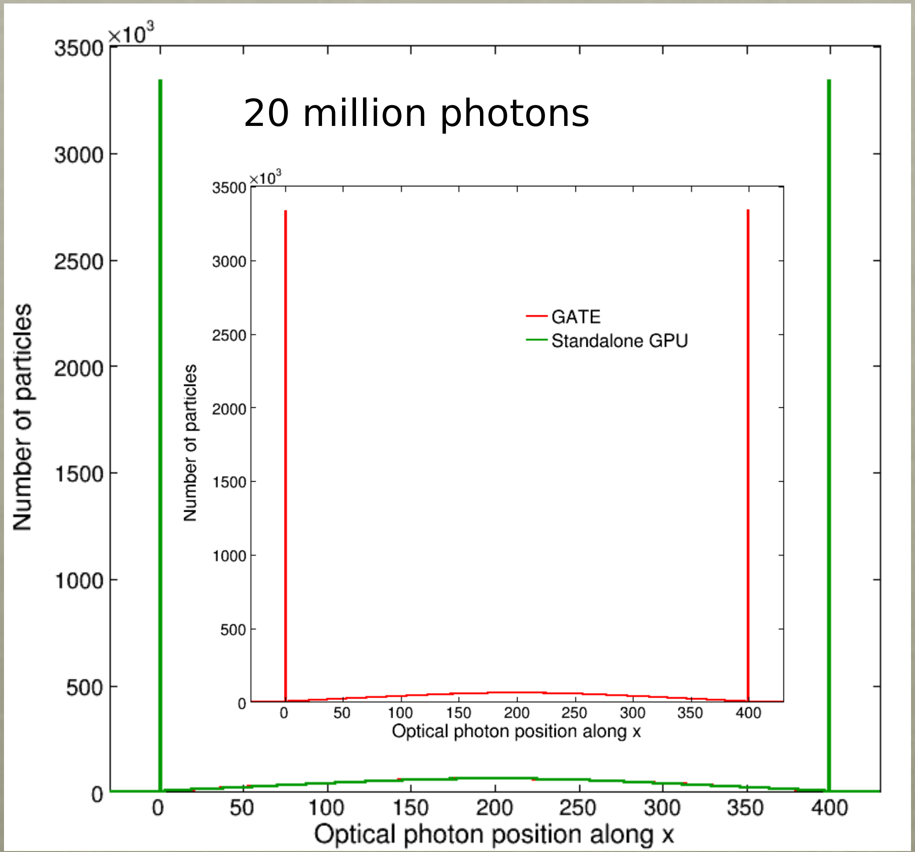
Physics: Mie scattering

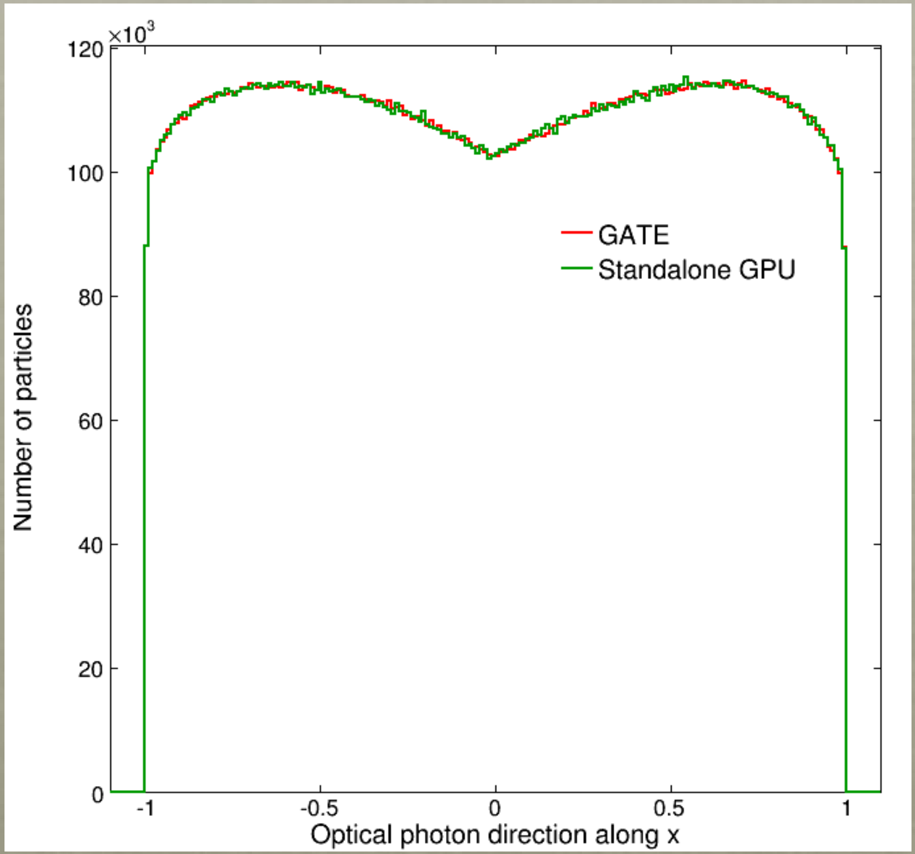
Scattering length set to 6mm

Simulation: 20 million of optical photons were generated

GPU versus GATE-G4

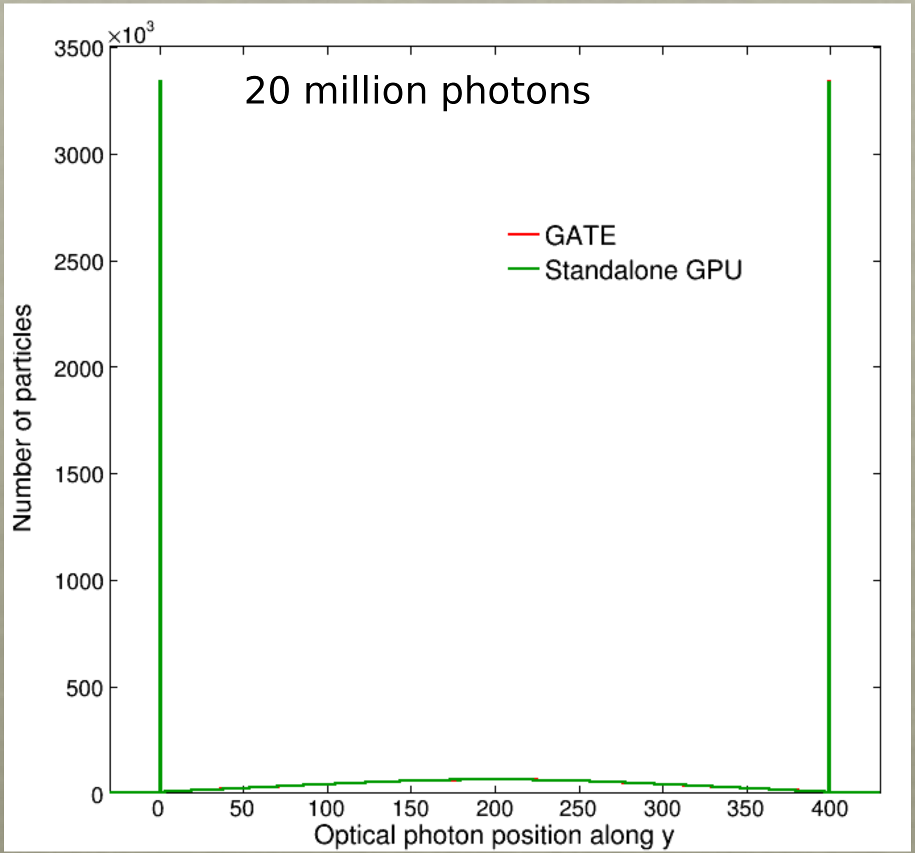
Optical photon position and direction along x-axis

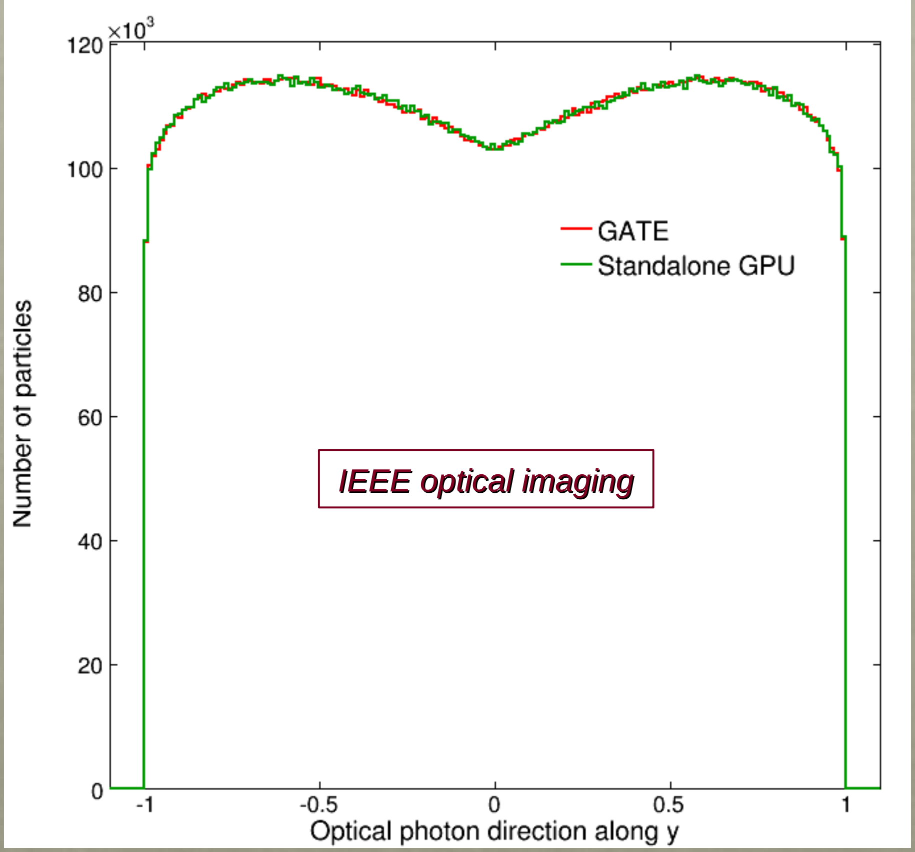




GPU versus GATE-G4

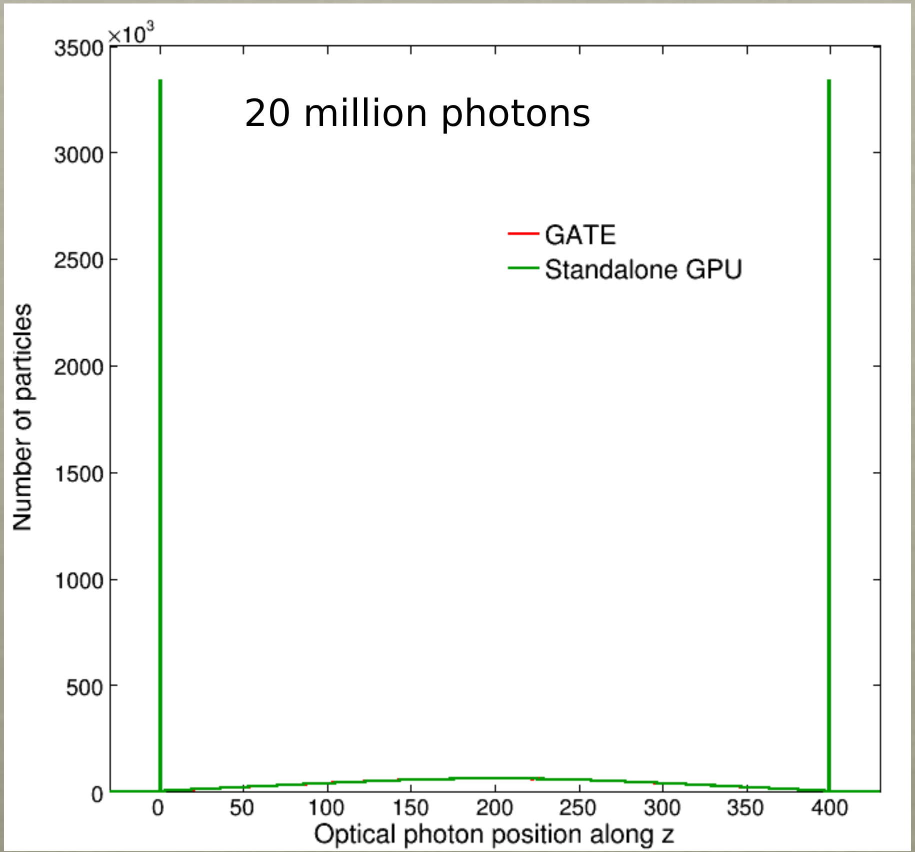
Optical photon position and direction along y-axis

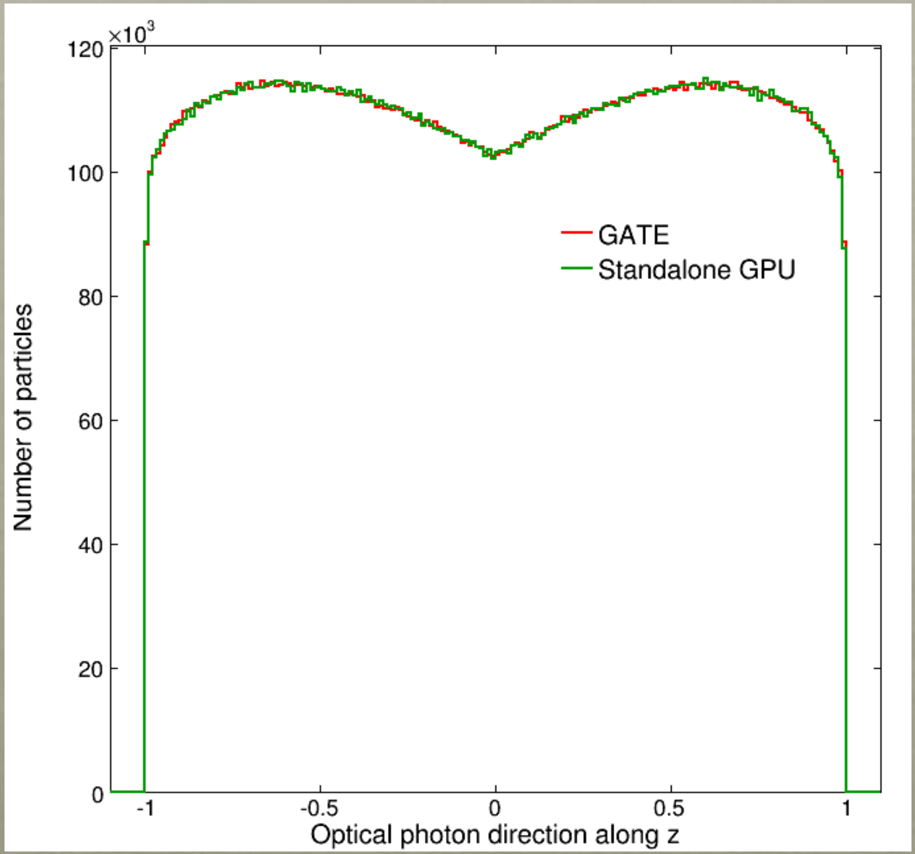




GPU versus GATE-G4

Optical photon position and direction along z-axis





Conclusion and Plans

Validation of GATE against MCML has shown excellent agreement.

GATE is capable of simulating the visible light fluorescence.

The Mie scattering process has been implemented in a *cuda* standalone program and the validation against GATE-CPU has shown excellent results.

A complete fluorescence/bioluminescence optical imaging simulation (GATE-CPU) will be shown *soon*.