A unified Monte Carlo platform for light transport simulation

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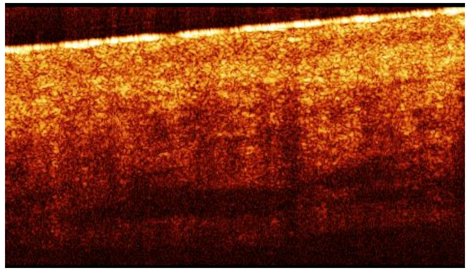
2020 г

Introduction



- Optical diagnostic and treatment modalities are actively introduced into clinical practice.
- Development and improvement of optical imaging techniques requires an effective tool for sophisticated study of light distribution in complex media mimicking biotissues.
- Optical inhomogeneities within tissue and various probing and detector configuration can be reproduced through numerical simulation of light transport in medium.
- The statistical Monte Carlo technique is the most widely used approach providing solutions for complex problems with the required accuracy.

Monte Carlo technique

The Monte Carlo algorithm implementation is based on processing of large number of random photon trajectories for a given sample geometry and irradiation configuration with further statistical analysis of the collected data.

Photon propagation within medium is restricted by a number of rules. The key parameters such as the mean free path, the scattering angle and transmission or reflection at the boundary are probabilistic.

Initializing a photon: set its initial position, direction and statistical weight

Generate a photon step basing on the sampling of the probability for the photon's free path

Check if a photon is in medium

Update photon weight due to absorption as well as photon direction due to scattering event

Repeat while a photon is in medium and weight doesn't too small

Photon's intersection of grid elements contributes to local fluence
(calculations of fluence distribution)

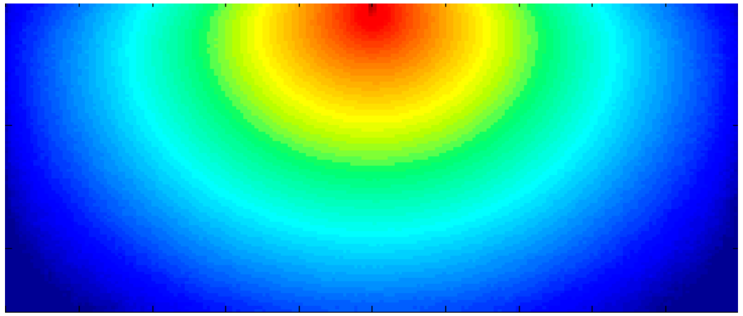
Weight of photon successfully escaped the medium contributes to reflectance/transmittance data
(calculations of reflectance and transmittance coefficients)

A fraction of absorbed weight contributes to absorption in the local grid element
(calculations of absorbed light dose distribution)

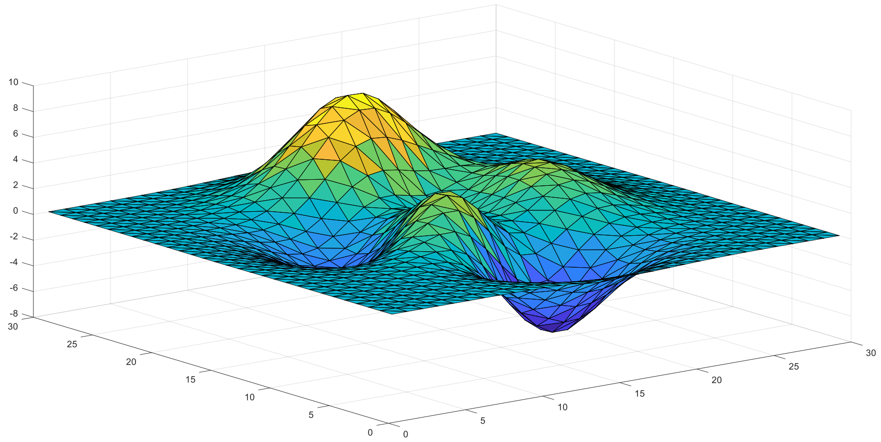
Monte Carlo platform

In this work we present a unified platform for reproducing of simulation of light transport in optically inhomogeneous media using Monte Carlo approach

The simple geometry routine



The complex geometry routine



- plane-layered medium geometry
- simultaneous modification of the entire photon set parameters within an array approach

- triangulation of complex-shaped boundaries within medium
- optimization of the search of photon trajectory intersection with the boundary
- BVH- or KD-trees algorithm for the intersection search

The simple geometry routine

Features:

- MATLAB-based implementation of Monte Carlo algorithm based on the simultaneous processing of a definite number of photons (10^7 photons). The photon parameters are stored as arrays and are transformed in accordance with MC algorithm rules, i.e. 10^7 photons steps are processed at each iteration of the algorithm
- A multi-layered slab medium model with plane boundaries including regions of medium with different optical properties and refractive index

Capabilities:

- Calculation of a three-dimensional distributions of the absorbed energy and optical fluence within the considered tissue
- Calculation of reflectance and transmittance spectra
- Reproducing of fluorescence optical imaging modalities

Calculation of optical fluence from Monte Carlo simulations

Numerical experiment: homogeneous medium with a point source inside

In the light transport theory the basic light characteristics are radiance $L(\boldsymbol{r},\hat{\boldsymbol{s}})$, fluence $\varphi(\boldsymbol{r})$ and flux $\mathbf{S}(\boldsymbol{r})$

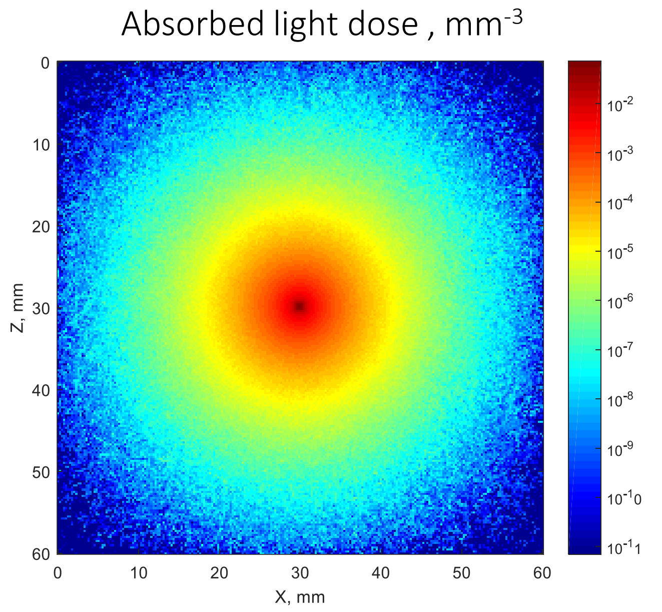
$$\varphi(\boldsymbol{r}) = \int_{4\pi} L(\boldsymbol{r},\hat{\boldsymbol{s}})d\Omega \qquad \mathbf{S}(\boldsymbol{r}) = \int_{4\pi} L(\boldsymbol{r},\hat{\boldsymbol{s}})\hat{\boldsymbol{s}}d\Omega$$

(1)

The **absorbed light dose** (Q, mm^{-3}) map demonstrates the value of absorbed photon weight in the unit volume.

In Monte Carlo simulations, **fluence** can be calculated from the **absorbed light dose** as:

$$\varphi = \frac{Q}{\mu_a}$$

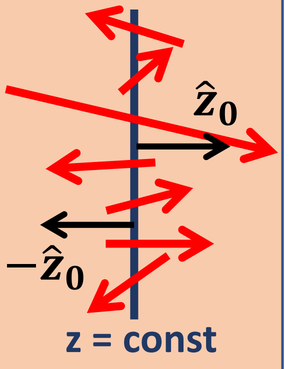


Map is normalized over the total photon number

(2)

In diffusion approximation, **fluence** can also be calculated from **bidirectional integrated flux** through the unit surface in the plane z=const

$$\mathrm{J}(\boldsymbol{r},\hat{\boldsymbol{z}}_0) = \underbrace{\int_{(\hat{\boldsymbol{s}}\cdot\hat{\boldsymbol{z}}_0)\geq 0} L(\boldsymbol{r},\hat{\boldsymbol{s}})(\hat{\boldsymbol{s}}\cdot\hat{\boldsymbol{z}}_0)d\Omega}_{\text{integrated flux in +z direction}} + \underbrace{\int_{(\hat{\boldsymbol{s}}\cdot\hat{\boldsymbol{z}}_0)\leq 0} L(\boldsymbol{r},\hat{\boldsymbol{s}})(\hat{\boldsymbol{s}}\cdot(-\hat{\boldsymbol{z}}_0))d\Omega}_{\text{integrated flux in -z direction}} = \varphi(\boldsymbol{r})/2$$



In Monte Carlo, **bidirectional integrated flux** can be calculated directly

Simulation parameters	
Total photons	1e6
μ_a, mm^{-1}	0.052
μ_s, mm^{-1}	4.74
g	0.8
$X \times Y \times Z, \mathrm{mm}$	$60 \times 60 \times 60$
$dx \times dy \times dz, \mathrm{mm}$	$0.25 \times 0.25 \times 0.25$
Source configuration	Isotropic point source at [30, 30, 30]

Calculation of optical fluence:
Monte Carlo simulations by 2 approaches versus theory

Numerical experiment: homogeneous medium with a point source inside

Theoretical equation for fluence from a point source in diffusion approximation:

$$\varphi(r) = \frac{1}{4\pi D}\exp(-\mu_{eff} r) \qquad D = \frac{1}{3(\mu_a + \mu_s(1-g))} \qquad \mu_{eff} = \sqrt{\mu_a/D}$$

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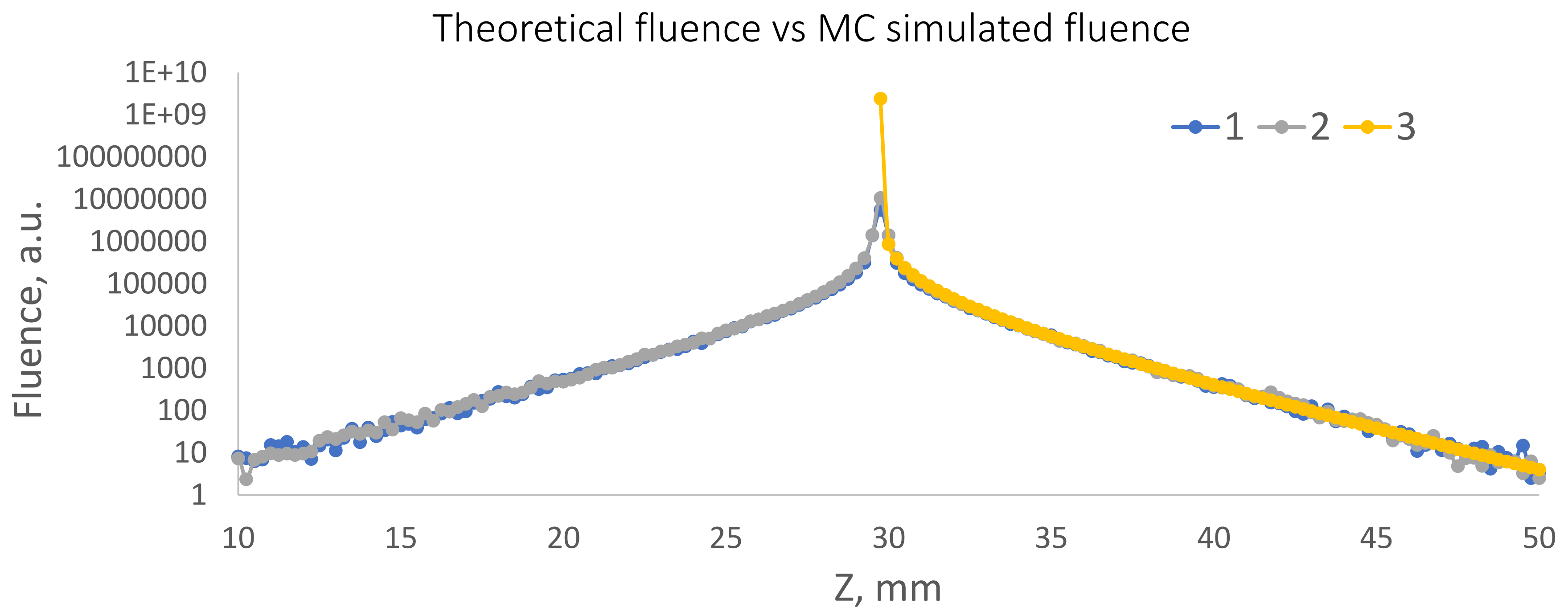


1 – MC using Bidirectional integrated flux

$$\varphi = 2 \cdot J$$

2 – MC using Absorbed light dose

$$\varphi = \frac{Q}{\mu_a}$$

3 – Theory

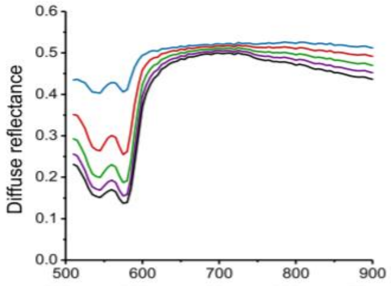
Simulated dependencies are in a good agreement with each other and with the theory

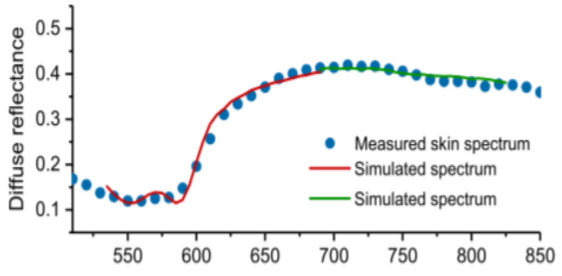
The simple geometry routine: application example

The simple geometry routine provides the capacity for massive simulations with different optical properties allowing to simulate spectral tissue probing and obtain diffuse reflectance spectra that can be used as a training set for Artificial Neural Network based reconstruction of tissue parameters from optical diffuse spectroscopy measurements.

MC modelling of diffuse reflectance spectra for different optical properties → Trained Artificial Neural Network ← Spectroscopic measurements of tissue reflection

Trained Artificial Neural Network ↓ Tissue optical properties





E. Zherebtsov, et al, “Hyperspectral imaging of human skin aided by artificial neural networks,” Biomedical Optics Express 10(7):3545-3559 (2019) DOI:10.1364/BOE.10.003545

The complex geometry routine

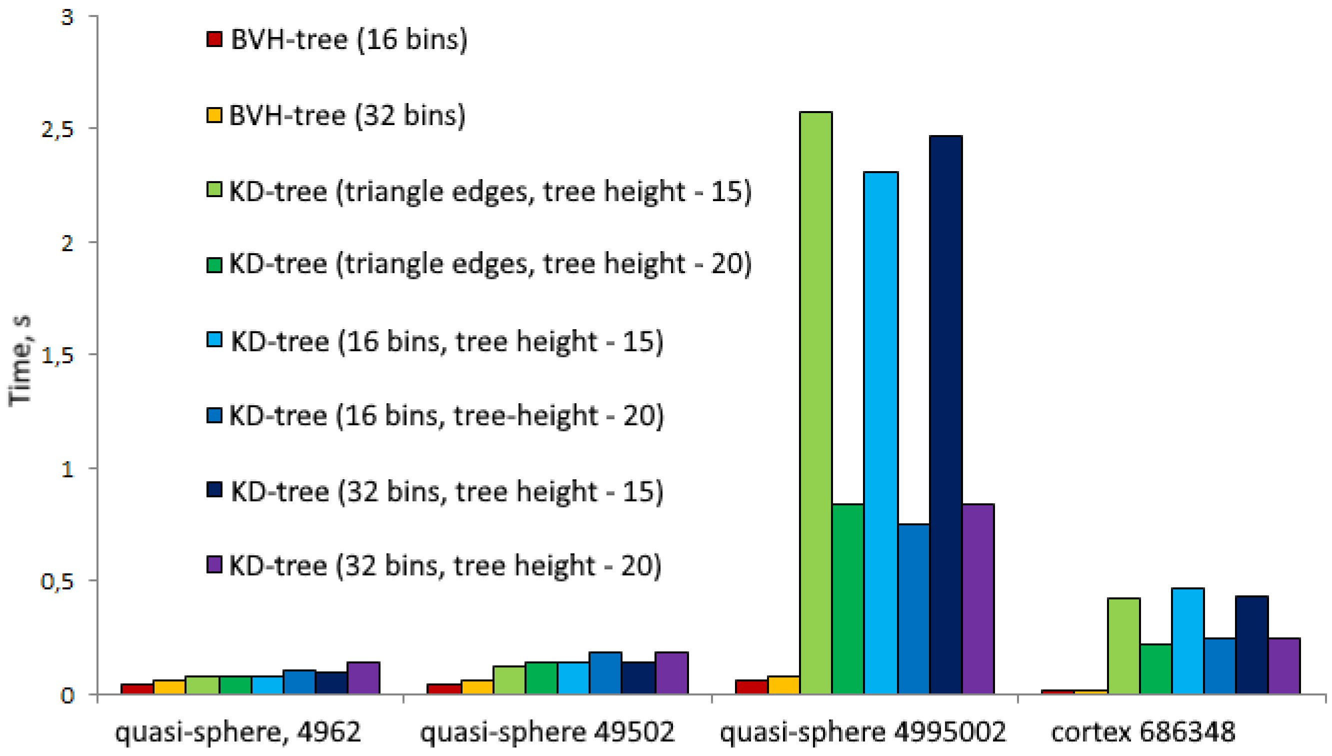
- C++ based routine
- Triangulation of object boundaries within biotissues
- Import of 3D geometry from volumetric diagnostic data (MRI, cryomicroscopy)
- Parallel architecture implementation

Acceleration structure

kd-tree	BVH AABB
Simple and efficient intersection algorithm	The algorithm for finding intersections is more complicated than for a kd-tree
There is no overlap in the space between tree nodes, strictly ordered enumeration of tree leaves in space along the ray during intersection search	The overlaps in the space between nodes are possible, not strictly ordered enumeration of tree leaves in space along the ray during intersection search;
A greater depth of the tree, therefore, more steps when building and finding intersections	Smaller tree depth (compared to kd-trees)
Poorly predictable memory consumption, since one primitive can be in several leaves of the tree at the same time	Predictable memory consumption, since each primitive is located in only one node of the tree.

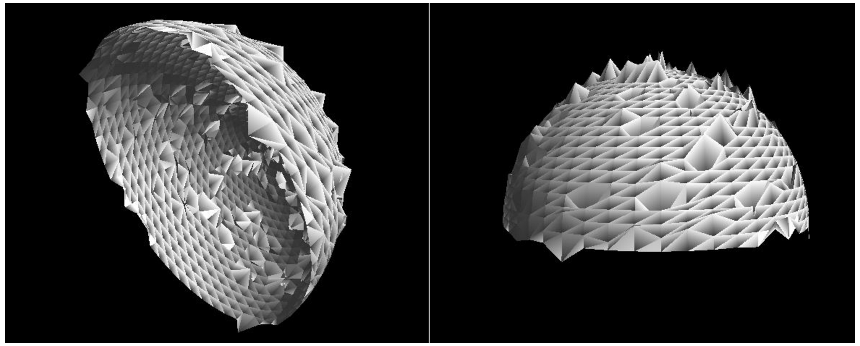
The ray-tracing algorithm in a **kd-tree** is simpler and allows the search to be completed as soon as an intersection with the primitive is found (since there is no overlap between nodes). At the same **BVHs** tend to have shallower depths, and require less memory. Additionally, both of these structures make it possible to effectively use information about the current photon mean free path.

KD-tree vs BVH AABB



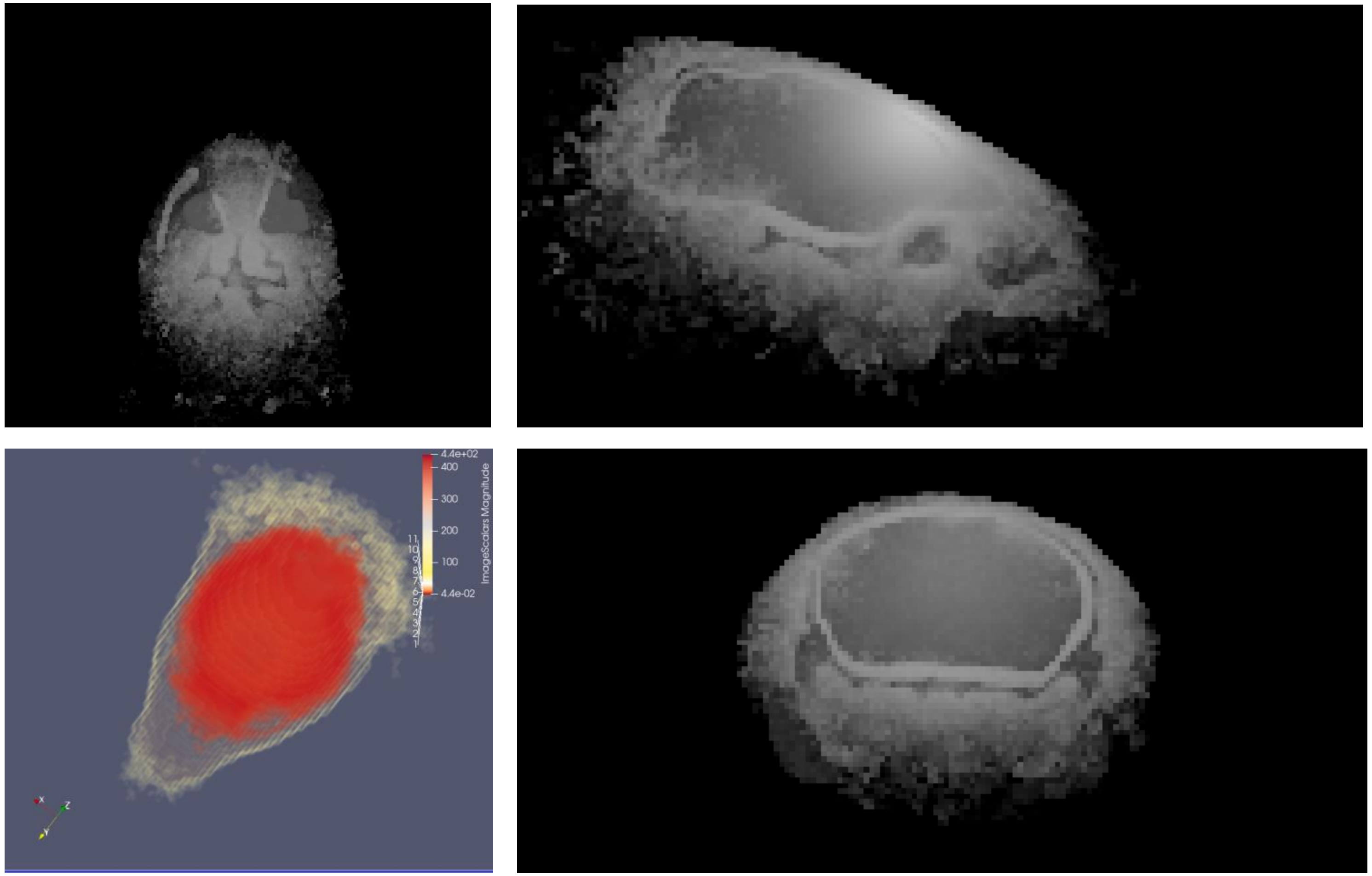
Experiment:

1. Data: a) 5 quasi-spheres, different triangle numbers, b) brain cortex from MRI



2. Intel Core i5 2410M,
2.30 GHz , RAM 4 GB MS Windows 7 x64

Light transport in mouse head: complex geometry simulations



Conclusion

We present a unified platform for reproducing of simulation of light transport in optically inhomogeneous media using Monte Carlo approach featured two routines employed for simulations in simple and complex geometries.

The platform provides a three-dimensional distributions of the absorbed energy and optical fluence within the considered tissue. Different approaches to calculations of these values based on different scale physical principles are considered and compared.

The study is supported by the Russian Governmental Program for World-Class Research Centers (WCRC)

Thank you for your attention!