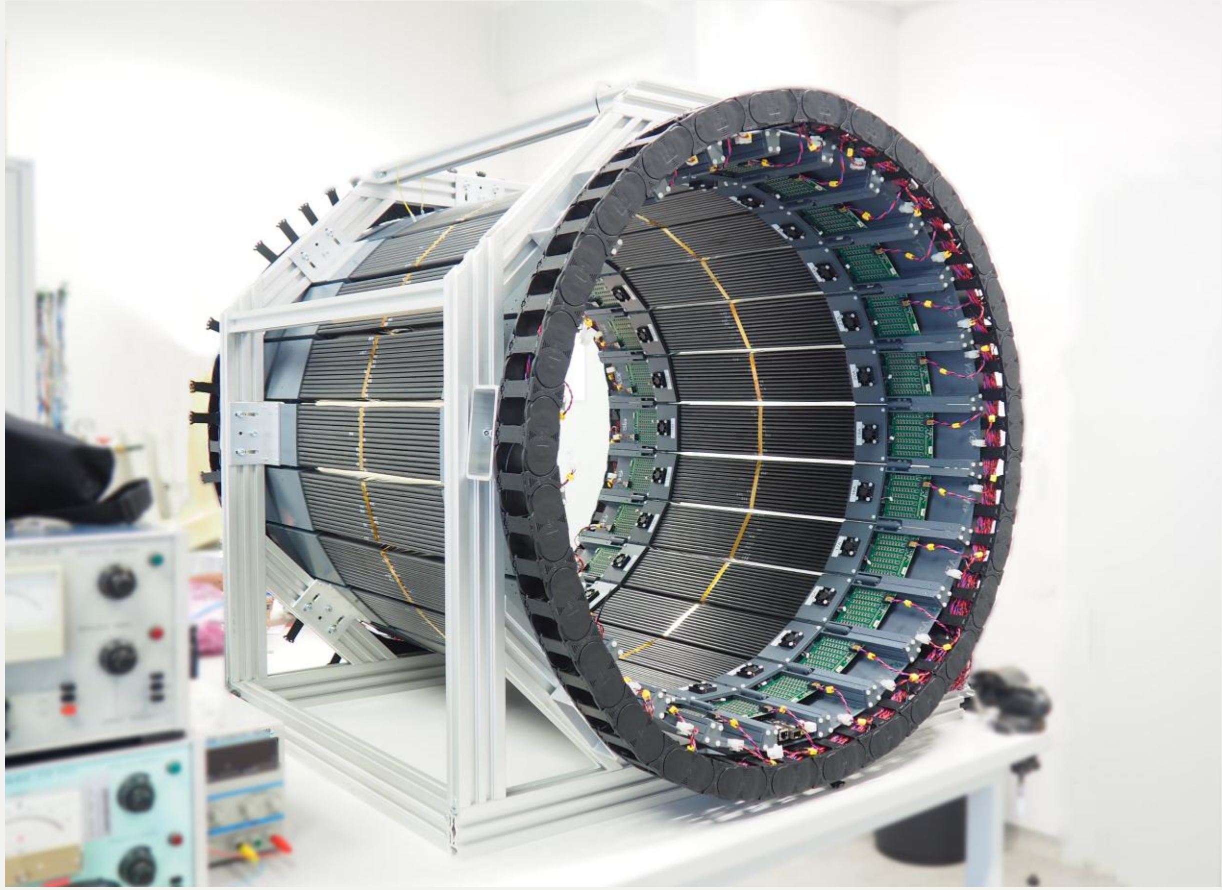
Studies of the absorption parameter $3\gamma/2\gamma$ in positronium decays

Kamila Kasperska on behalf of the J-PET collaboration
Under the supervision of dr hab. Magdalena Skurzok
HPXM Workshop
Frascati, 19.06.2025

J-PET detector



Talk by Magdalena Skurzok, Monday 15:50

- Positron Emission Tomography detector based on plastic scintillators
- Cost-efficient
- Multi-photon detection

- Medical imaging:
  - Total body PET
  - **Positronium Imaging**

- Fundamental physics:
  - Quantum entanglement
  - Discrete symmetries

Positronium imaging

Positron

→ Direct annihilation with an electron 2γ decay

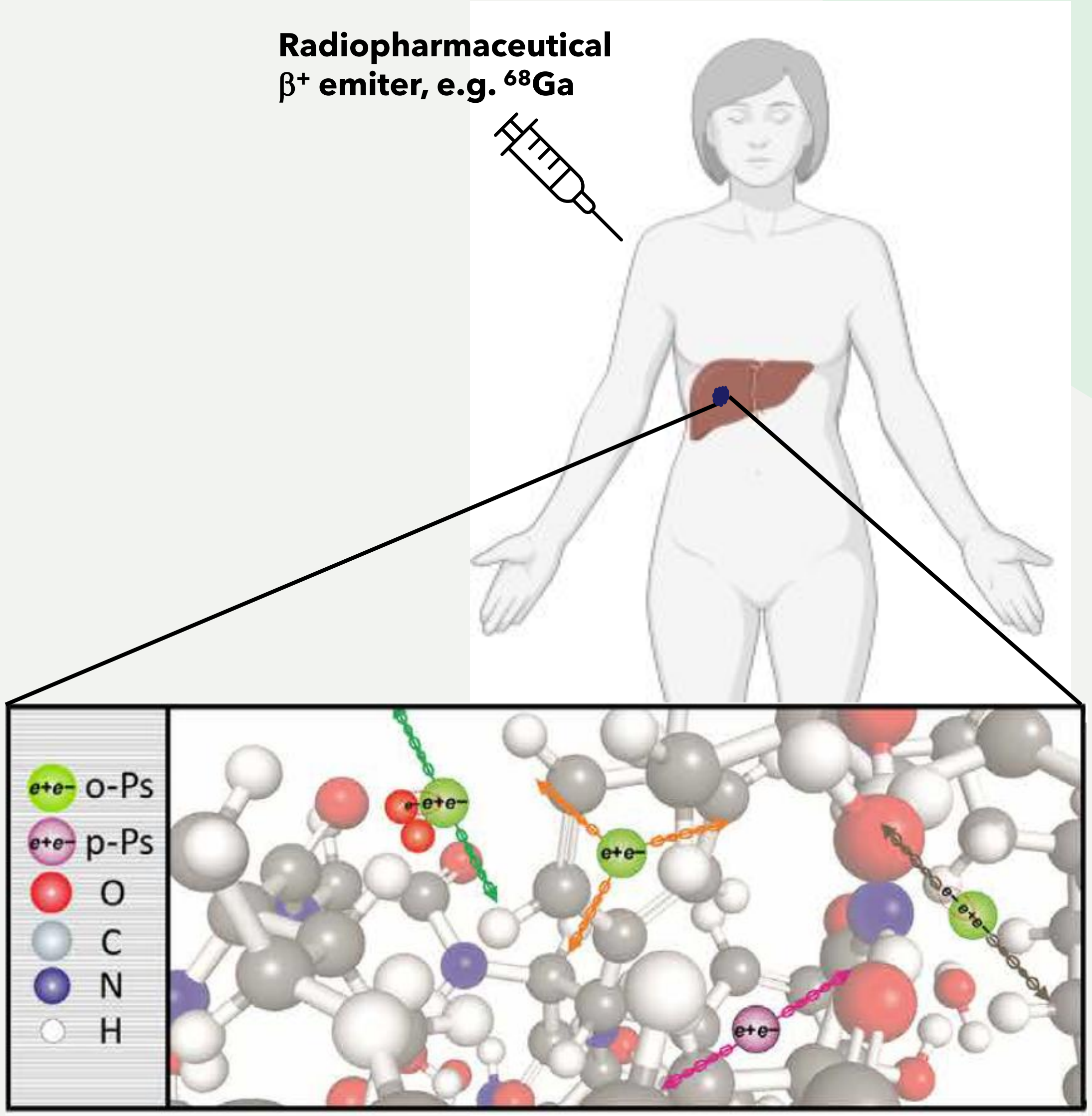
→ Formation of positronium

→ Spin 0 para-positronium 2γ decay

→ Spin 1 ortho-positronium 3γ decay

Volume of free spaces ↘, oxygenation ↗ → oPs lifetime ↘, 3γ fraction ↘

Volume of free spaces ↗, oxygenation ↘ → oPs lifetime ↗, 3γ fraction ↗



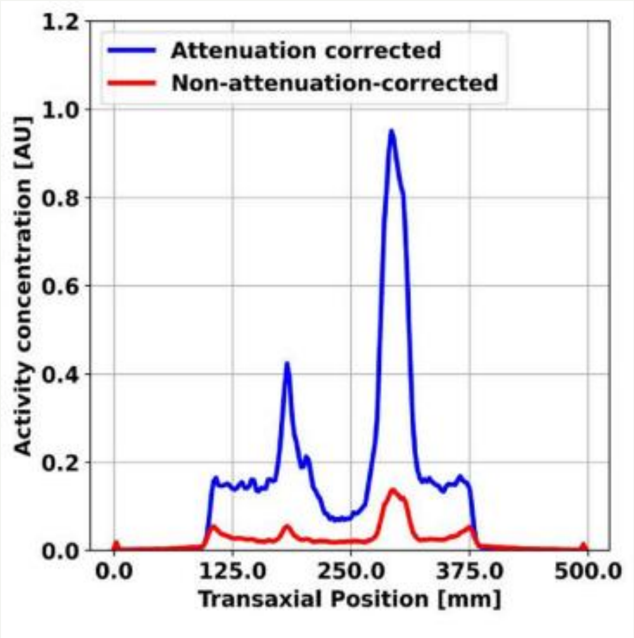
The **3γ/2γ ratio** depends on the tissue's molecular structure.

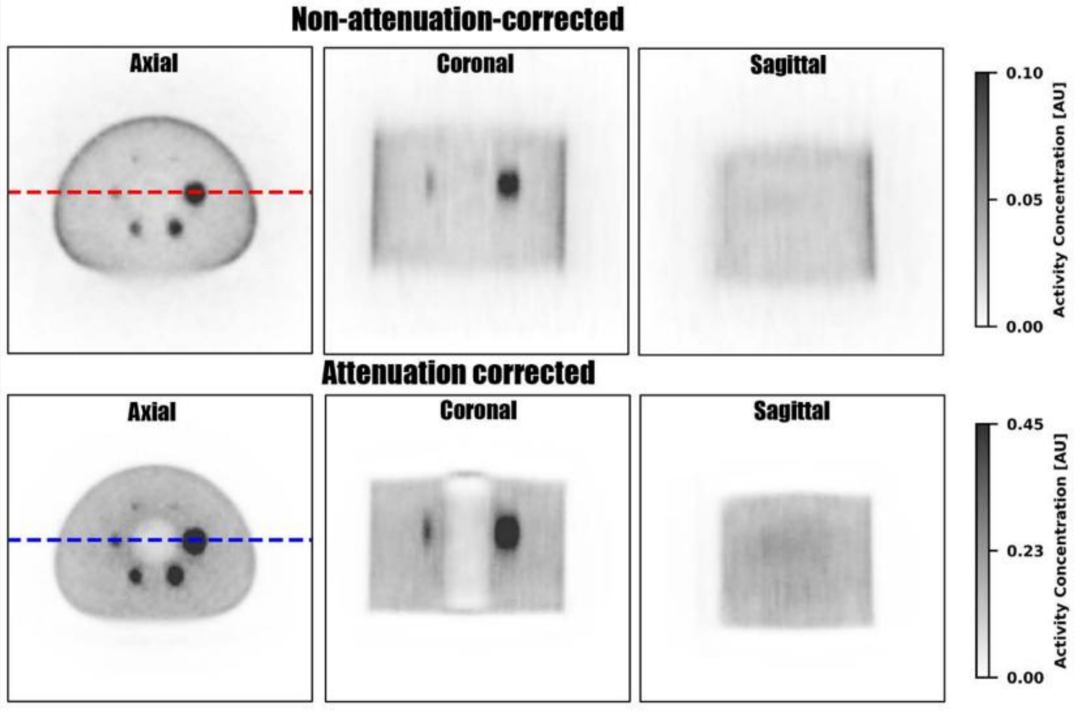
P. Moskal et al. Positronium image of the human brain in vivo, Science Advances 10 (2024)

Absorption correction

Absorption of gamma quanta in tissues → Underestimation of radiopharmaceutical concentration in deeper tissues

- J-PET: CT-based attenuation correction for two-gamma imaging
- Standard attenuation maps – not sufficient for three-gamma imaging





M. Das et al. Development of correction techniques for the J-PET Scanner [Bio-Algorithms and Med-Systems vol. 20 (2024)]

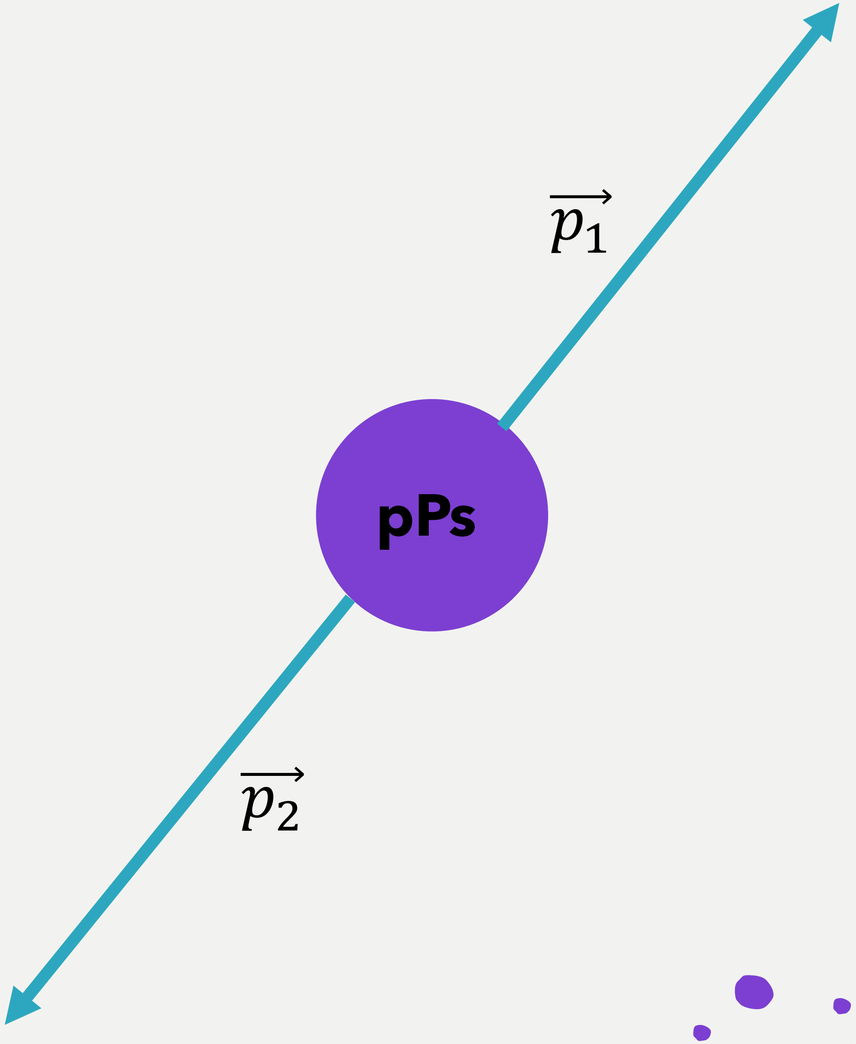
Simulation of pPs decay

Para-positronium – singlet state ${}^{1}S_{0}$

Isotropic decay into 2 back-to-back photons with energies of 511 keV

Decay simulation:

1. Randomizing the direction of $\overrightarrow{p_1}$
2. Assigning the energy of 511 keV
3. Determining the momentum $\overrightarrow{p_2} = -\overrightarrow{p_1}$



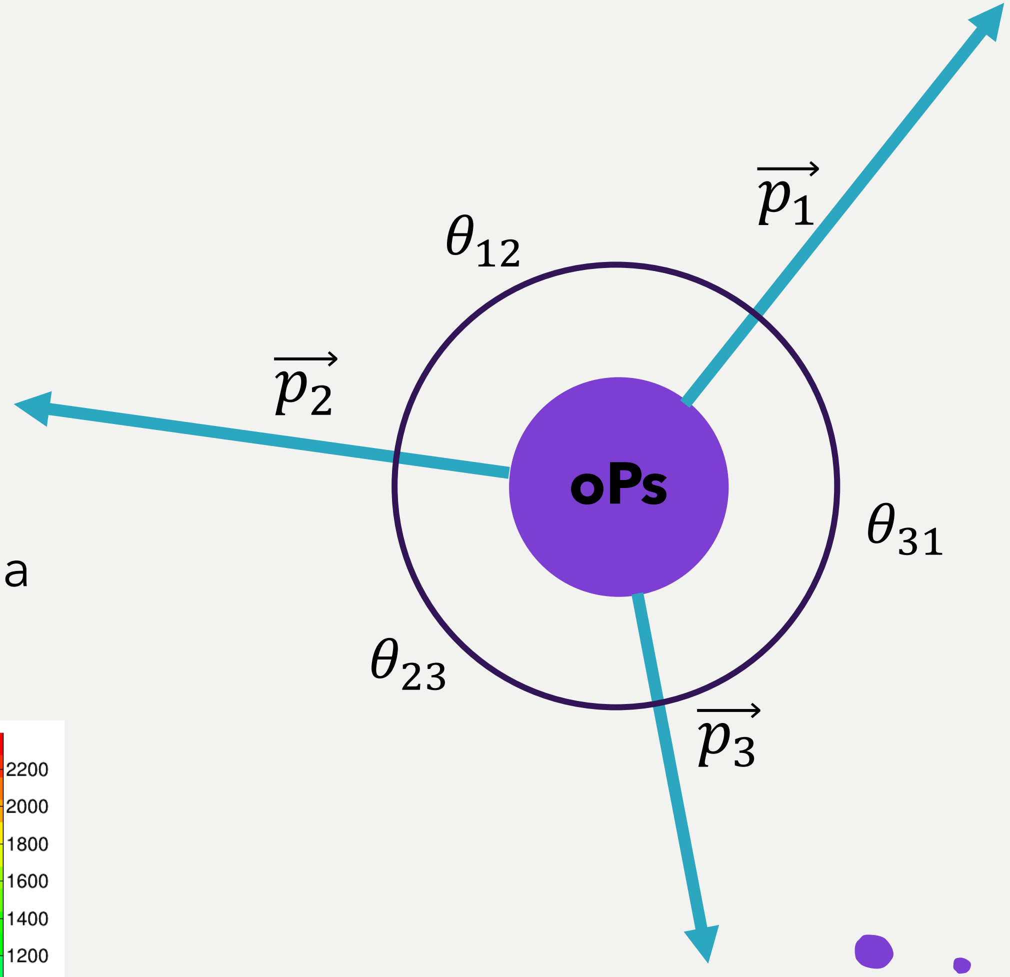
Simulation of oPs decay

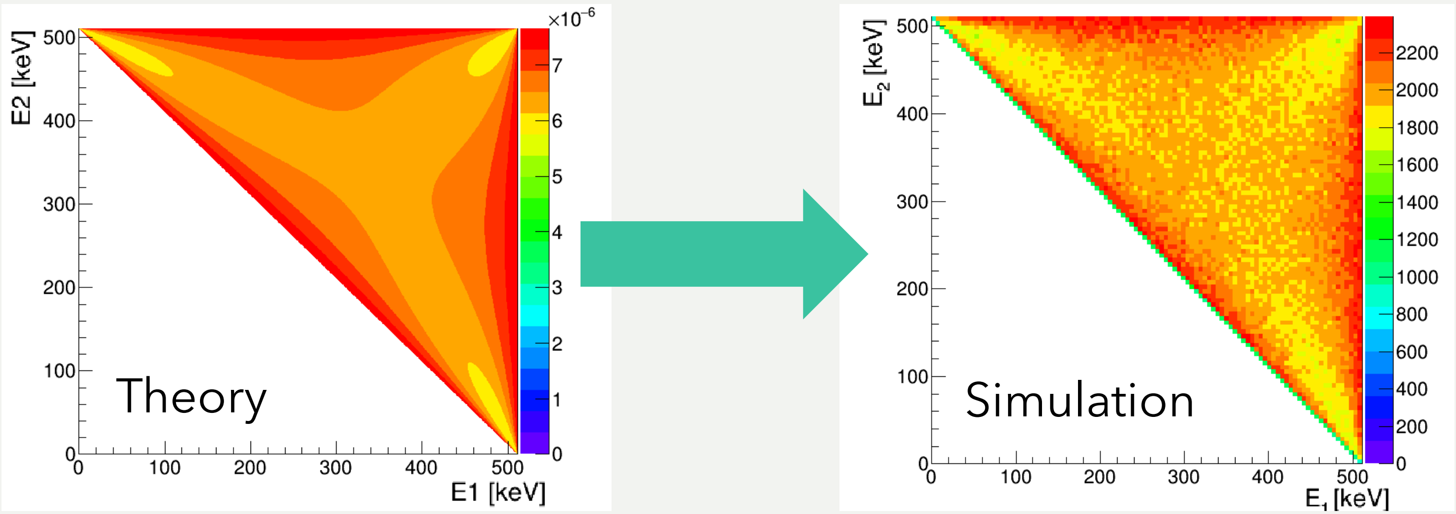
Ortho-positronium – triplet state $^3S_1$

Decay into 3 photons described with the matrix element $M_{oPs\to3\gamma}$:

$$M_{oPs\to3\gamma} = \left(\frac{m_e - E_1}{E_2E_3}\right)^2 + \left(\frac{m_e - E_2}{E_1E_3}\right)^2 + \left(\frac{m_e - E_3}{E_1E_2}\right)^2,$$

where m_e - electron mass, E_1, E_2, E_3 - energies of gamma quanta.





Absorption of gamma quanta in matter

Probability that a photon with energy E_i is **not** absorbed:

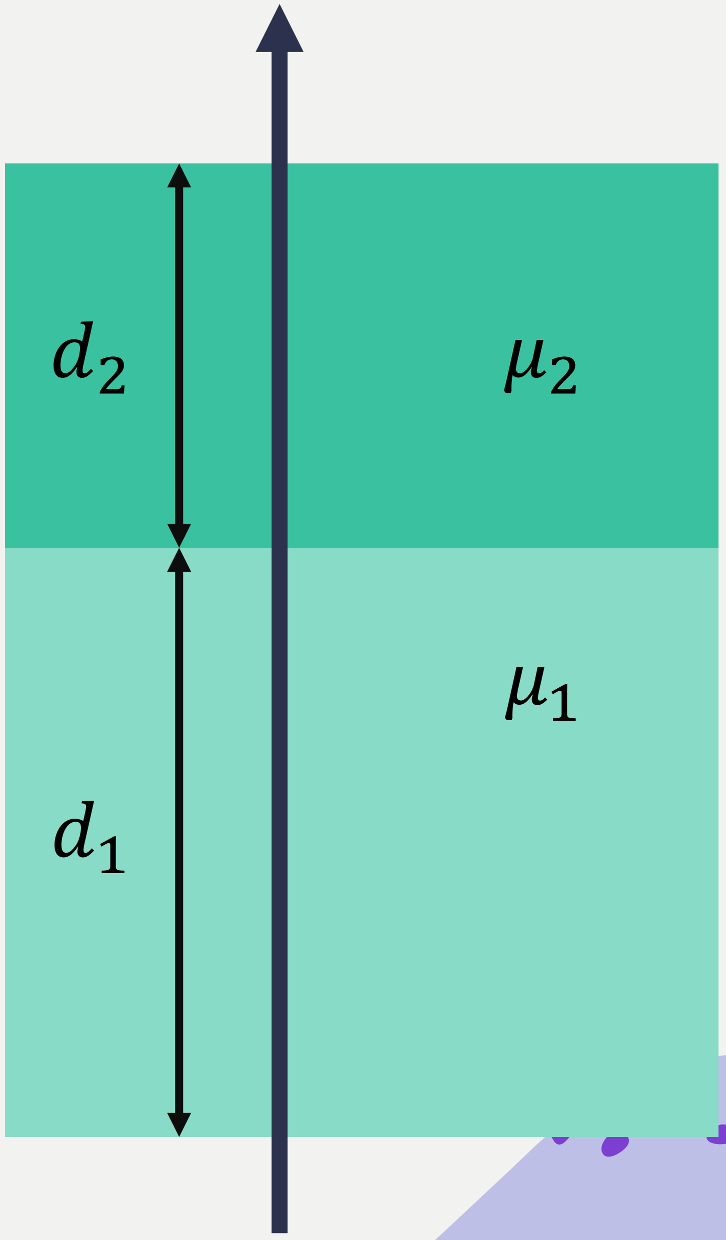
distance

$$P_i = \prod_m e^{-\mu_m(E_i)d_m}$$

linear attenuation coefficient

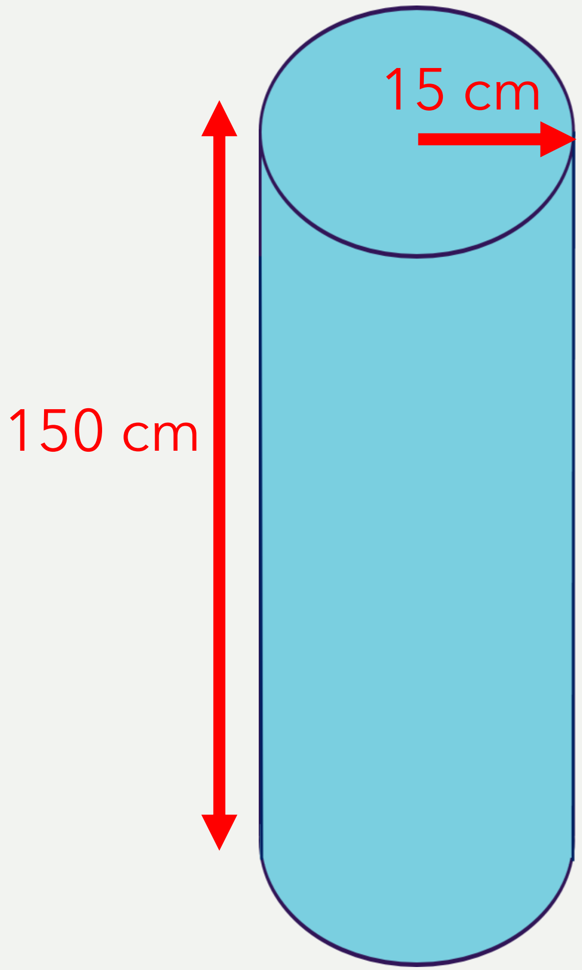
Total probability that **none** of the photons are absorbed:

$$P_{tot} = \prod_i P_i$$

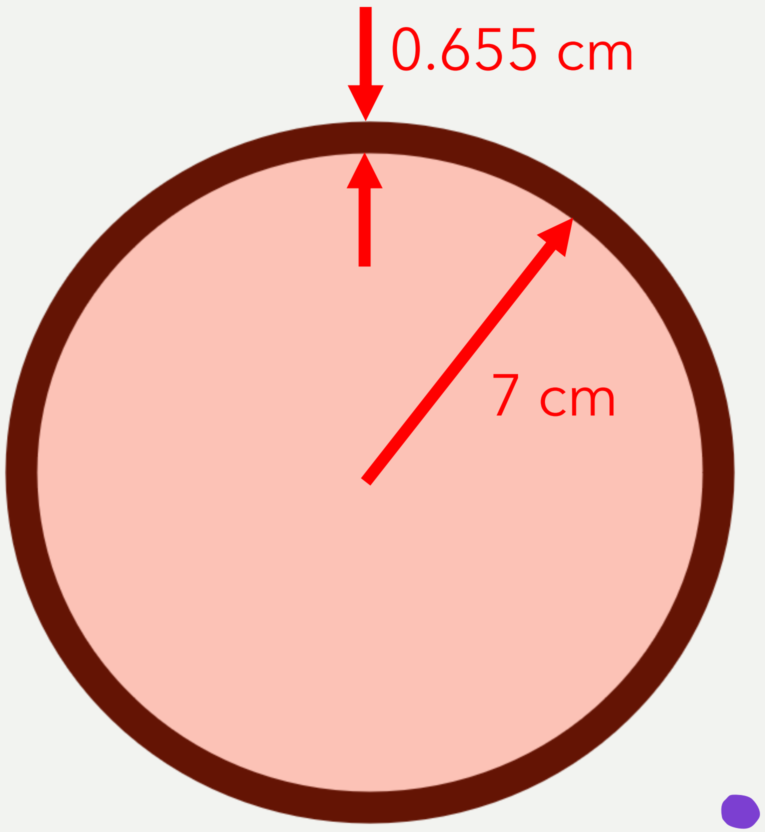


Simplified phantom models

Water sphere



Water cylinder



Brain sphere + layer of bone

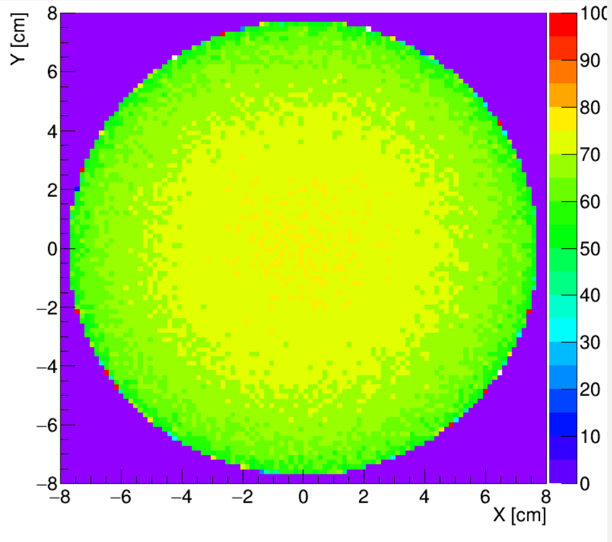
Absorption map – head model

- Percentage of gamma quanta pairs or triplets, from which **at least one** of the photons **reacted** with the model
- Specific to the annihilation point
- 10^7 events

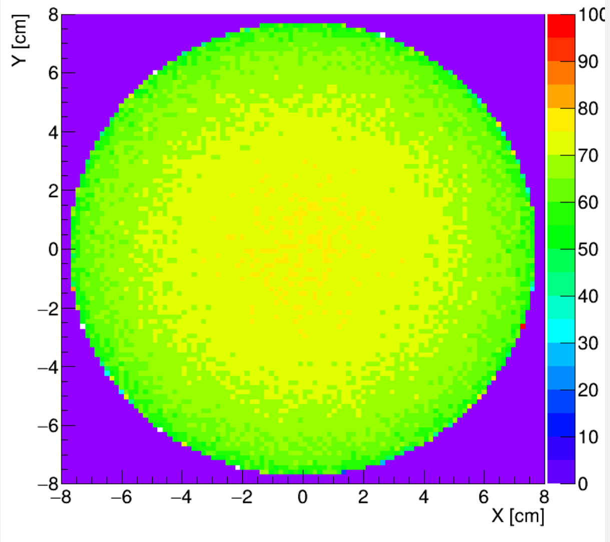
Surviving photon multiplets within the whole model

	Toy MC	GATE
pPs	30.156 ± 0.017%	30.052 ± 0.017%
oPs	11.879 ± 0.011%	11.919 ± 0.011%
$3\gamma/2\gamma$	0.39392 ± 0.00043	0.39392 ± 0.00043

p-Ps → 2γ

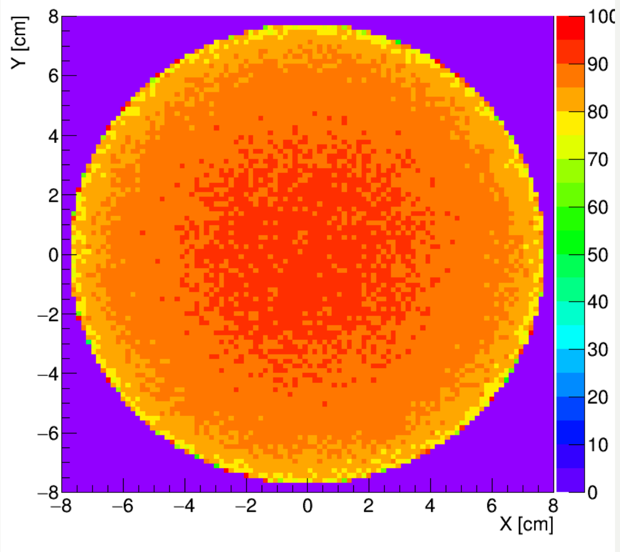


Toy MC

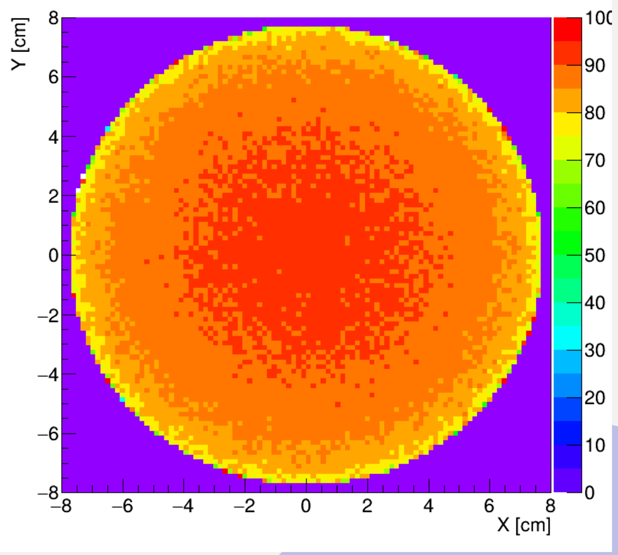


GATE

o-Ps → 3γ



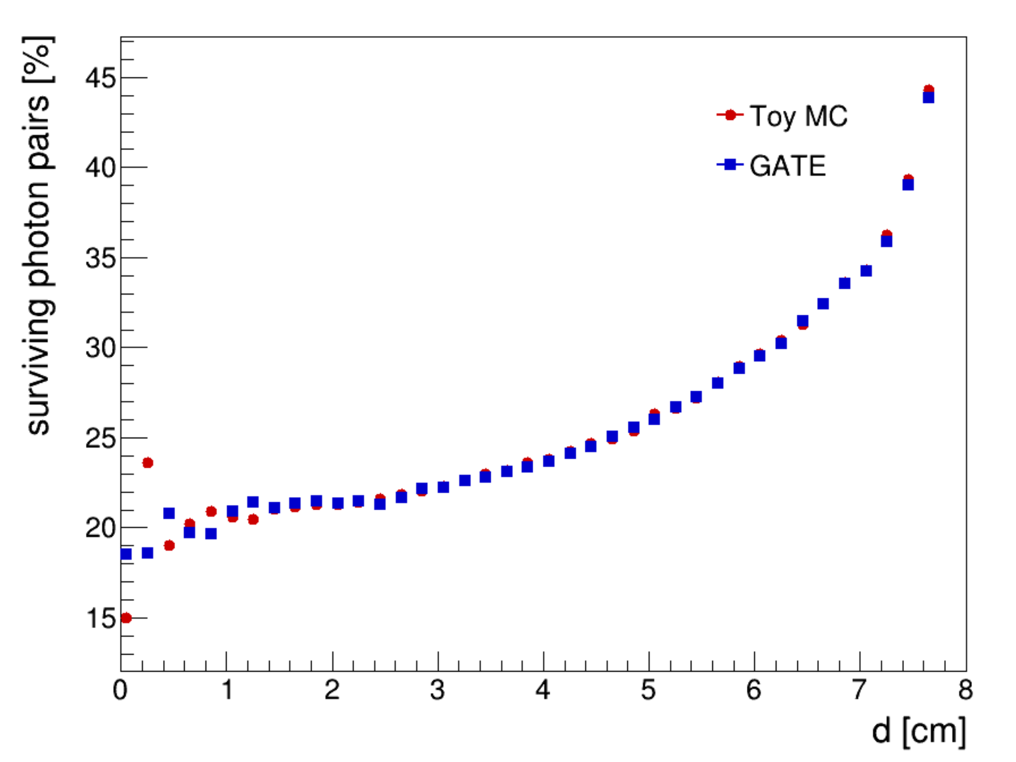
Toy MC



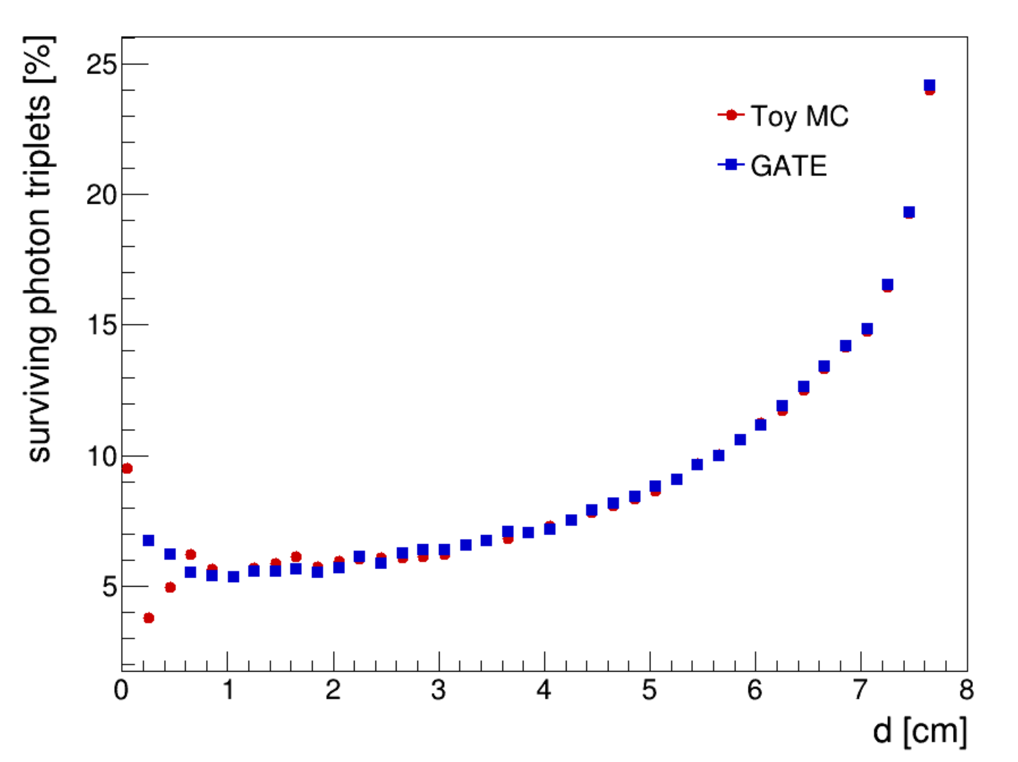
GATE

Dependence of the percentage of surviving photon multiplets on the distance from the center of the head (d)

pPs

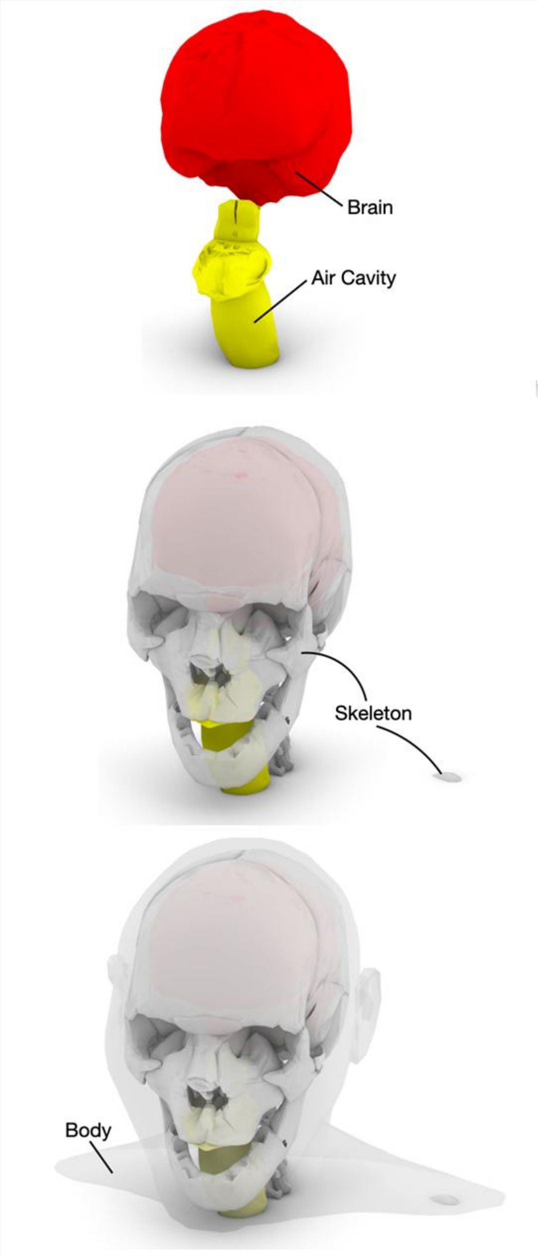


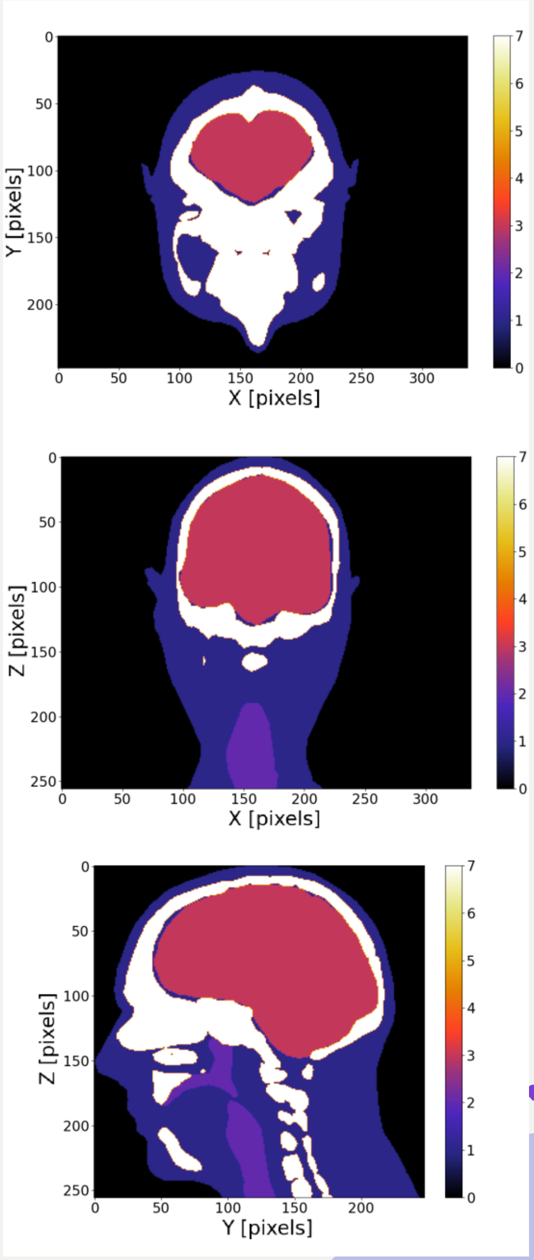
oPs



XCAT human phantom

- Mesh-based XCAT phantom (**mesh50_XCAT**) developed and maintained by Auer Benjamin
- Highly detailed male anatomy for subject in 50th percentile
- Source – voxelized version of the phantom
- Head Only model (computational limitations)

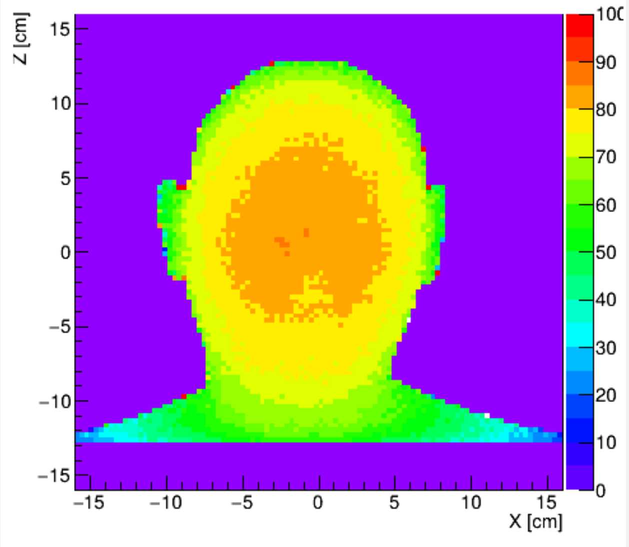


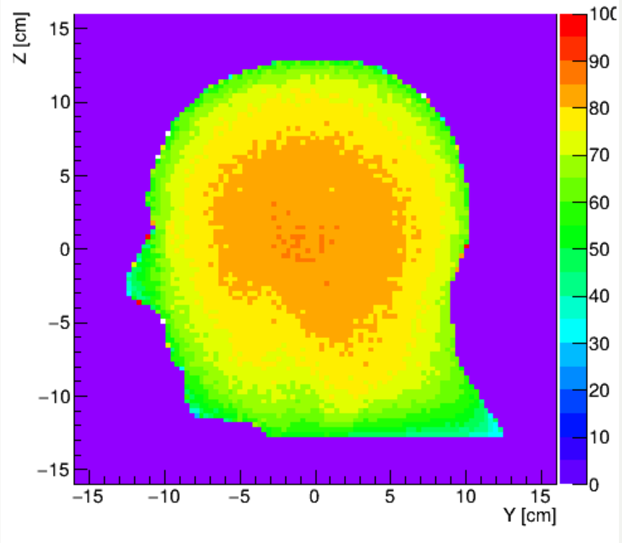


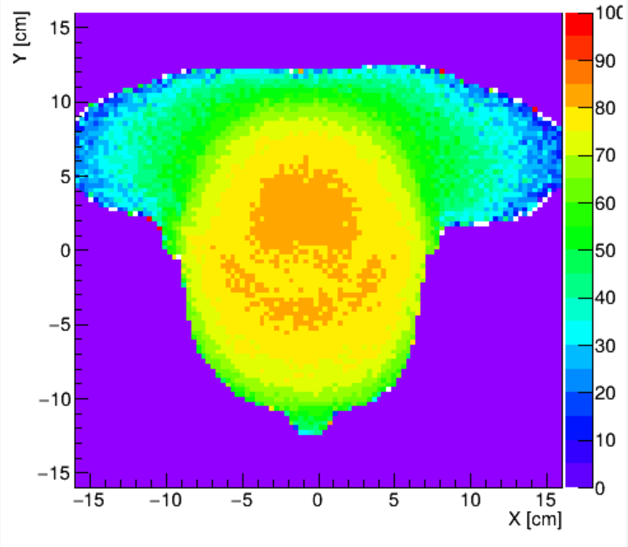
B. Auer et al. [Mesh Modelling of system geometry and anatomy phantoms for realistic GATE simulations and reconstruction](), Physics in Medicine & Biology 68.7 (2023)

XCAT Phantom absorption maps – p-Ps (10^7 events, 24.922 ± 0.016% pairs not absorbed)

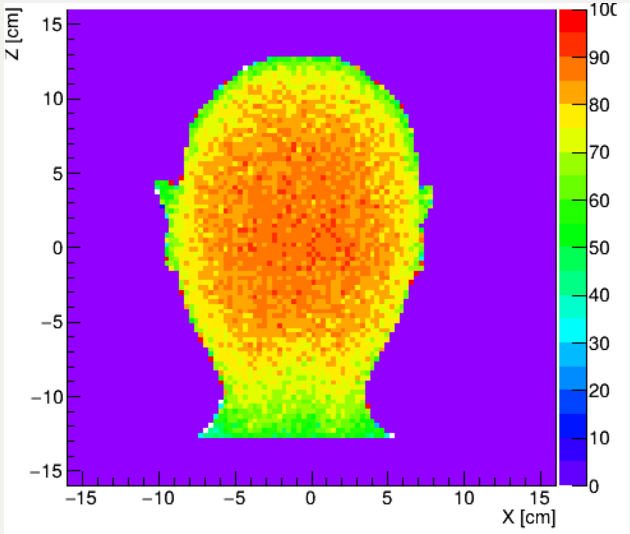
Projection



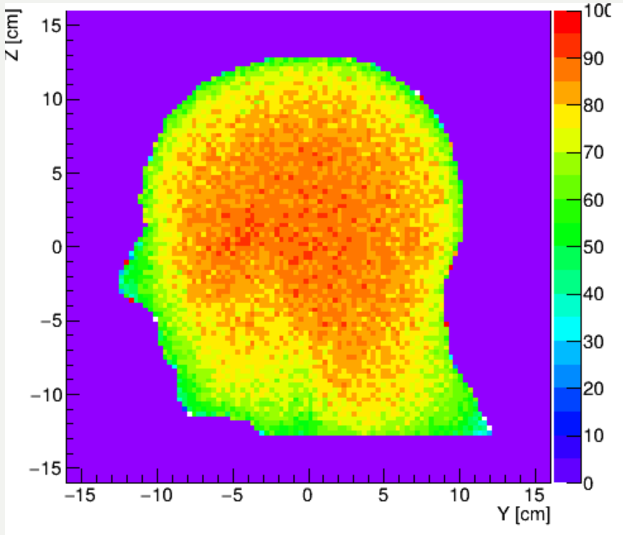




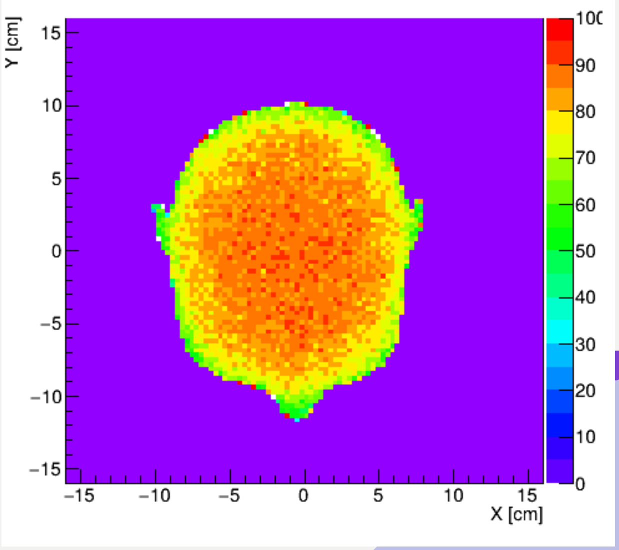
Central slice



Coronal

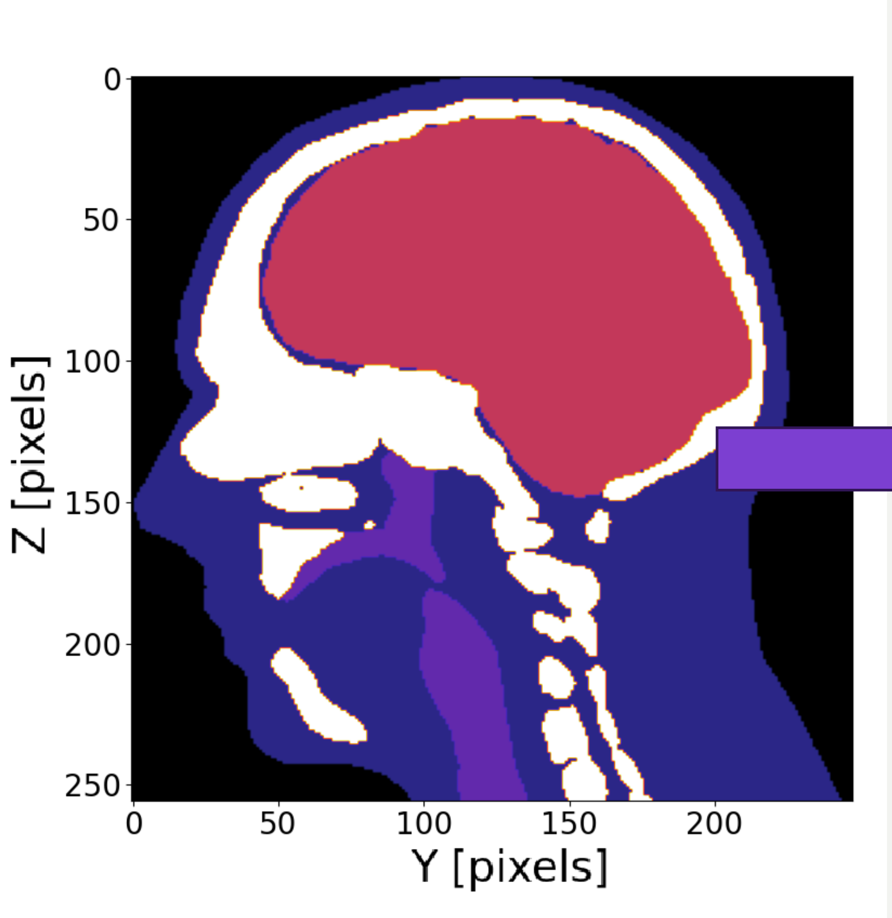


Sagittal

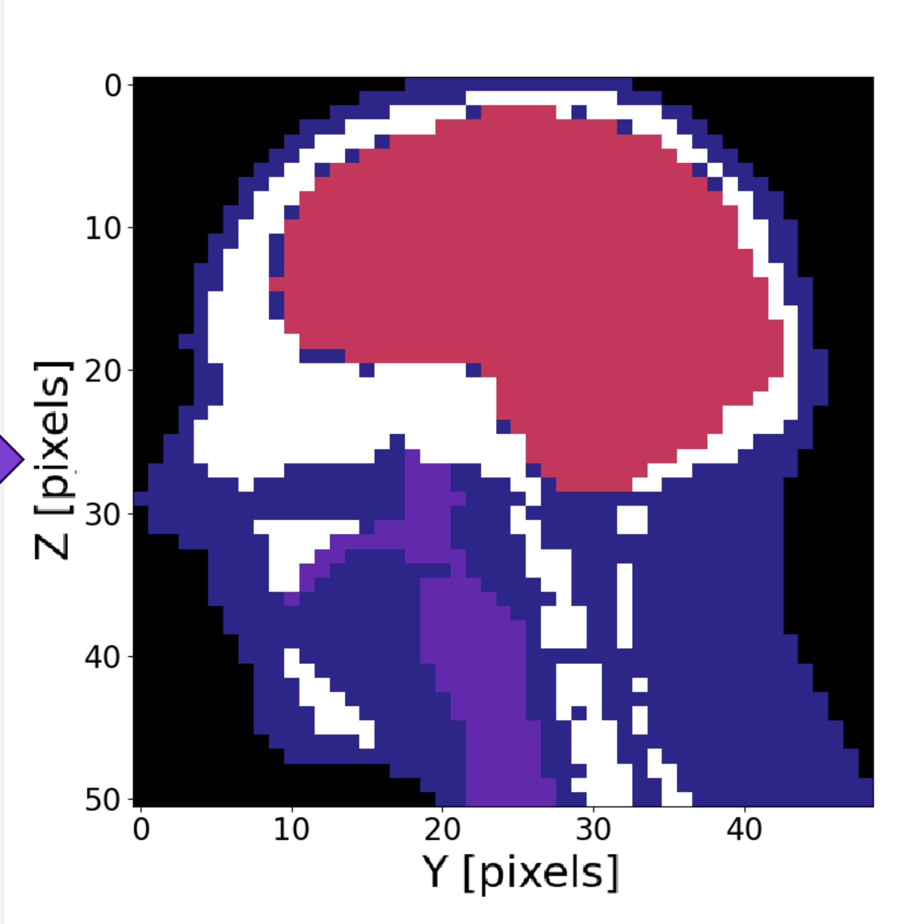


Transverse

oPs source



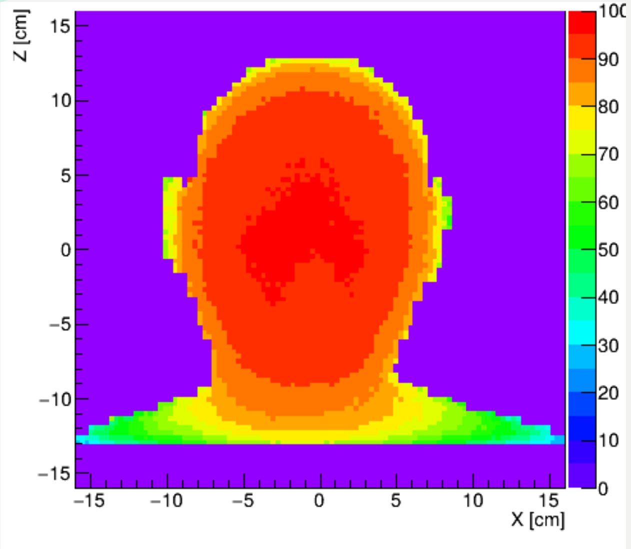
Voxel 1x1x1 mm

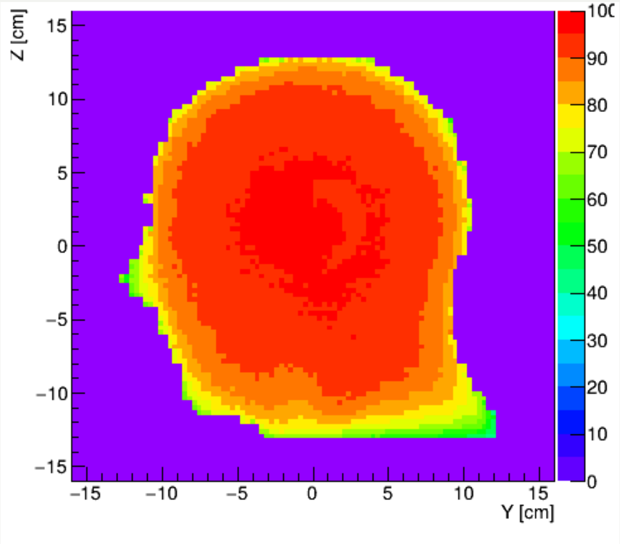


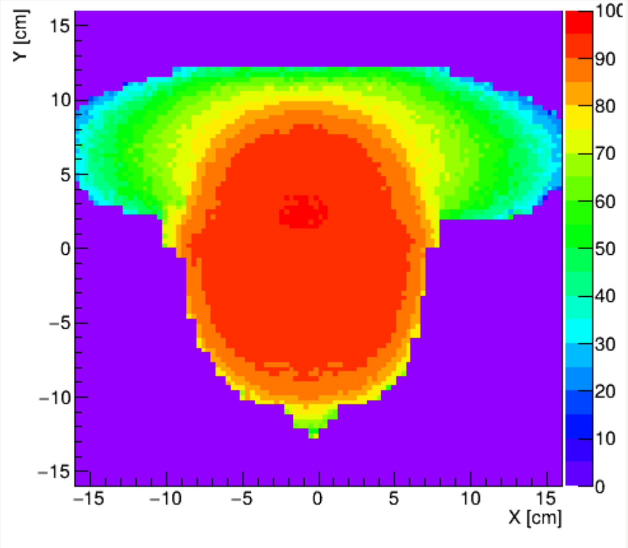
Voxel 5x5x5 mm

XCAT Phantom absorption maps – o-Ps (4.435 · 10^7 events, 10.256 ± 0.010% triplets not absorbed)

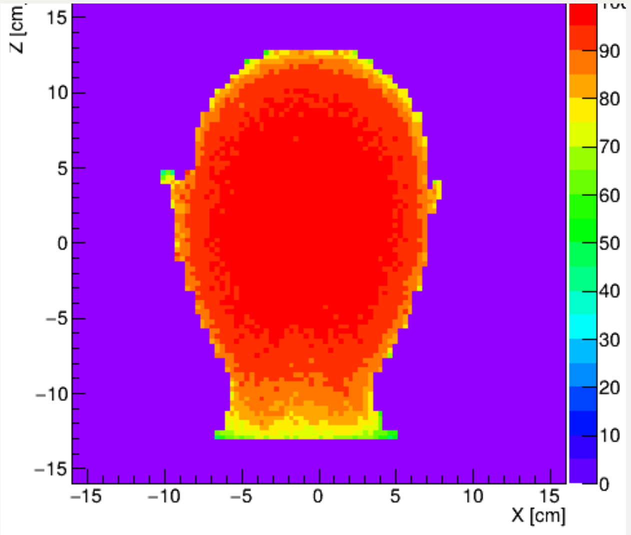
Projection



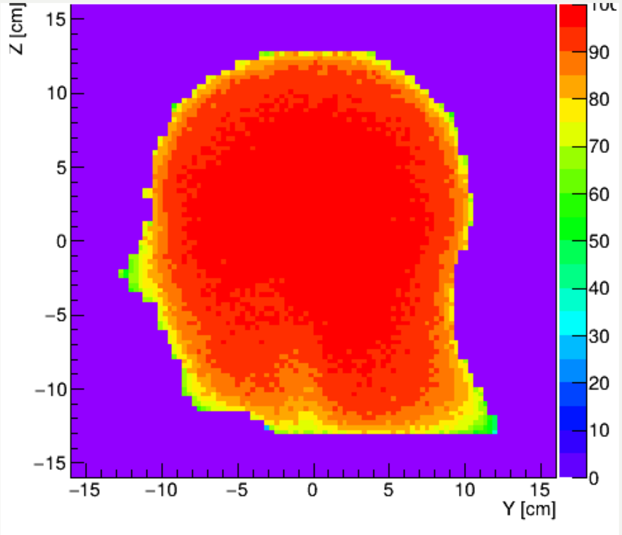




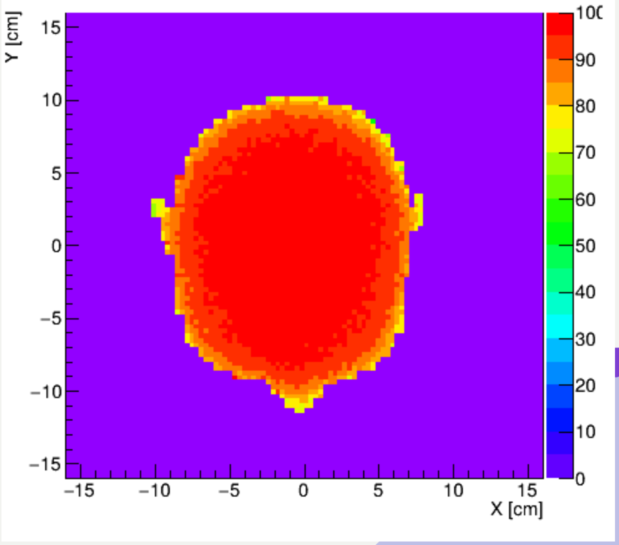
Central slice



Coronal



Sagittal



Transverse

Summary and perspectives

Study of gamma absorption from p-Ps → 2γ and o-Ps → 3γ decays in different phantoms – a foundation for developing attenuation maps required for tomographic image correction

Used custom-developed toy MC simulation and the GATE simulation toolkit to create emission-point-specific absorption maps

According to expectations – absorption of photon triplets significantly higher than that of photon pairs due to their lower energies

What's next?

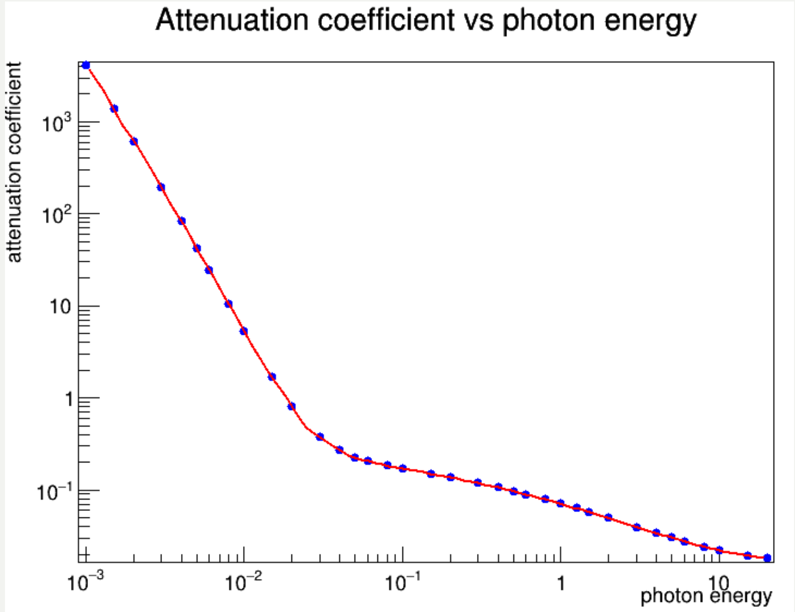
Simulations using whole-body XCAT human phantom

Introducting detector acceptance into the simulation

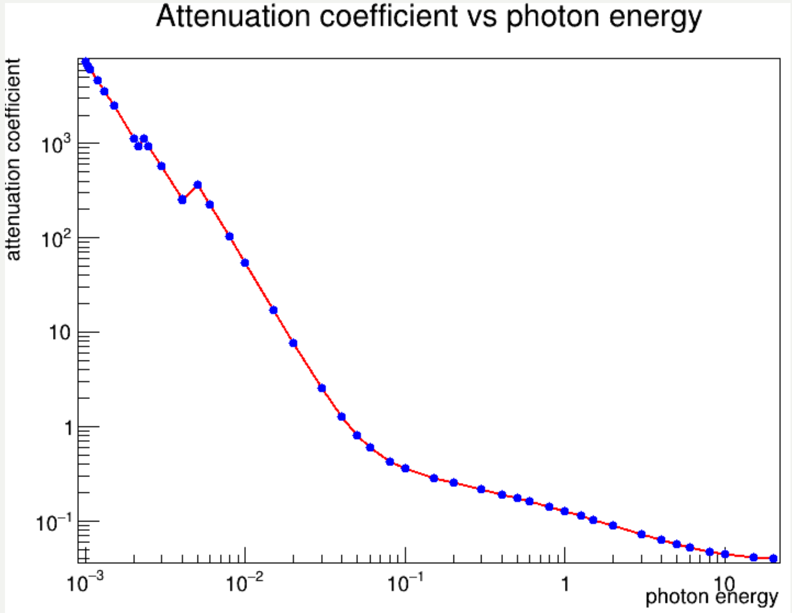
Simulation using a phantom created based on the patient's CT scan

Thank you for your attention!

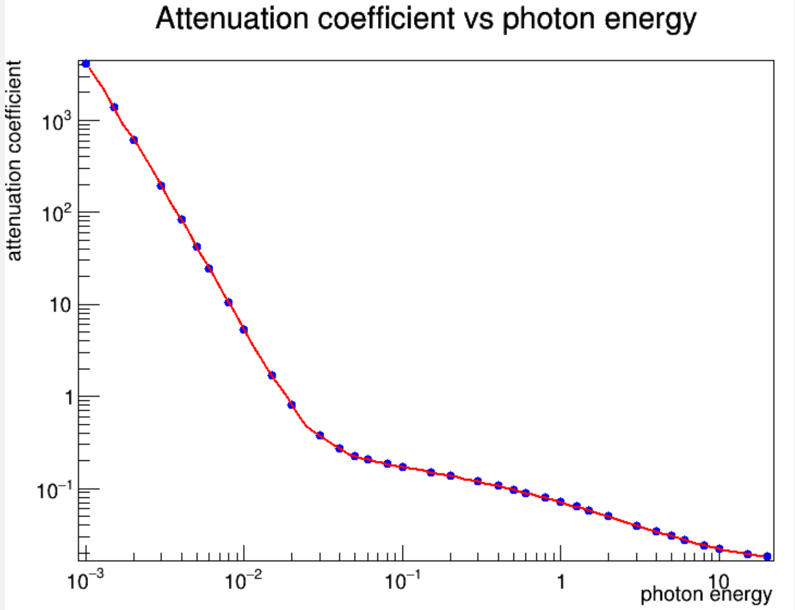
Linear attenuation coefficients for toy MC simulation



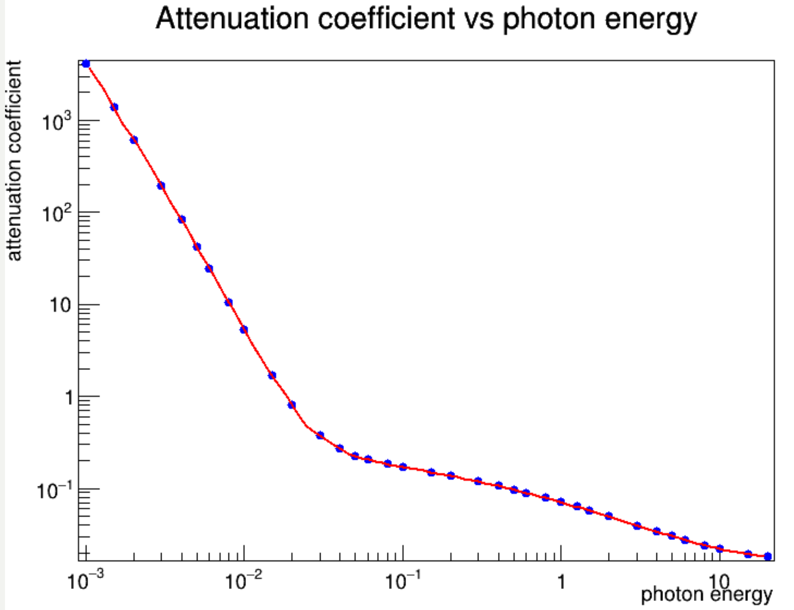
Water



Bone



Brain



Liver

NIST Standard Reference Database 126

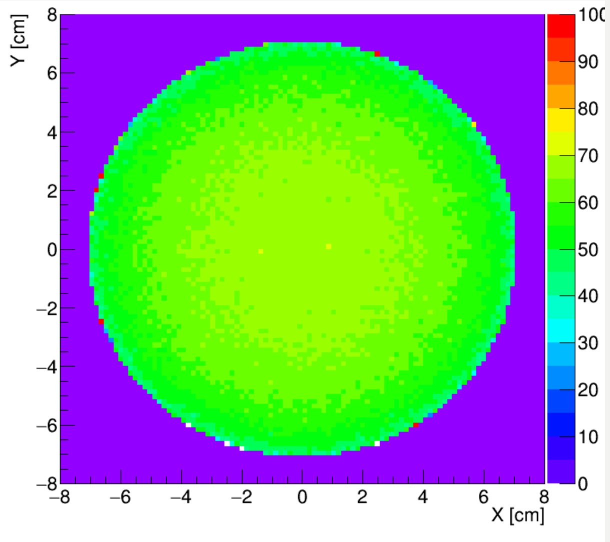
Absorption map – water sphere

- 10^7 events

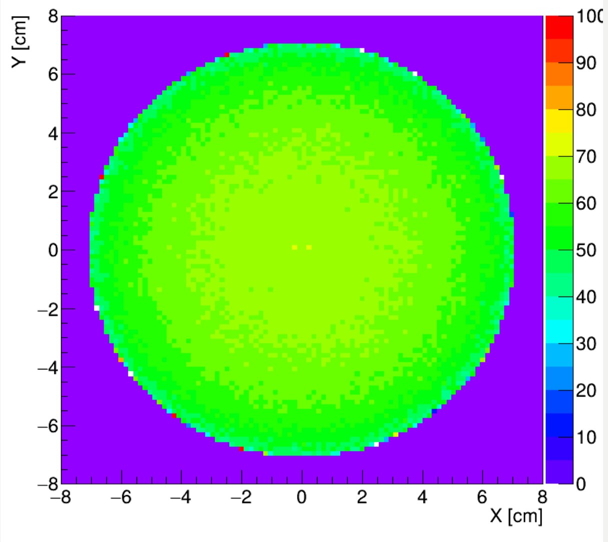
Surviving photon multiplets within the whole model

	Toy MC	GATE
pPs	37.836 ± 0.019%	37.878 ± 0.019%
oPs	18.119 ± 0.013%	18.152 ± 0.013%

p-Ps → 2γ

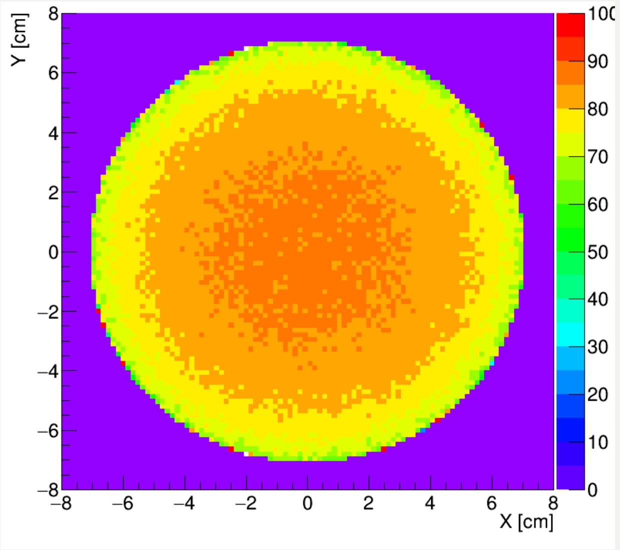


Toy MC

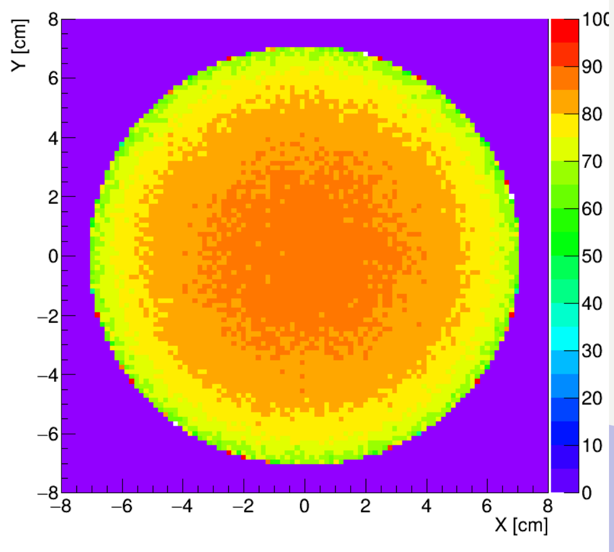


GATE

o-Ps → 3γ



Toy MC



GATE

Absorption map – water cylinder – XY plane

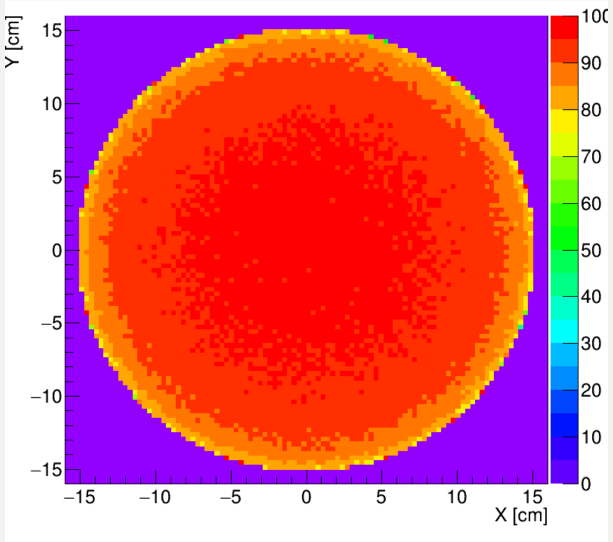
- 10^7 events

Surviving photon multiplets within the whole model

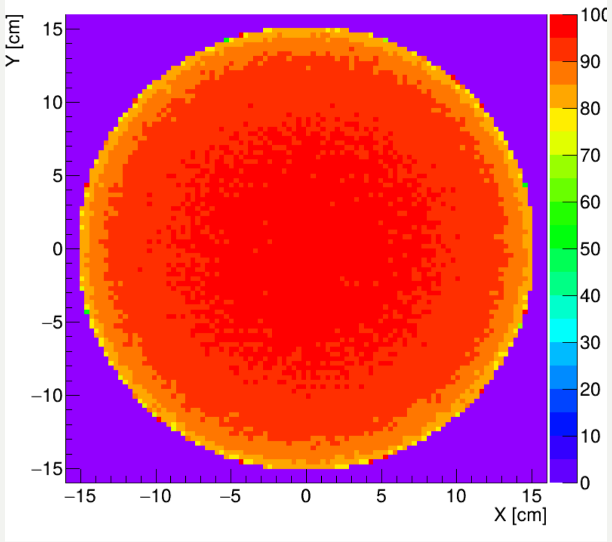
	Toy MC	GATE
pPs	7.6063 ± 0.0087%	7.6176 ± 0.0087%
oPs	1.6403 ± 0.0041%	1.6462 ± 0.0041%

p-Ps → 2γ

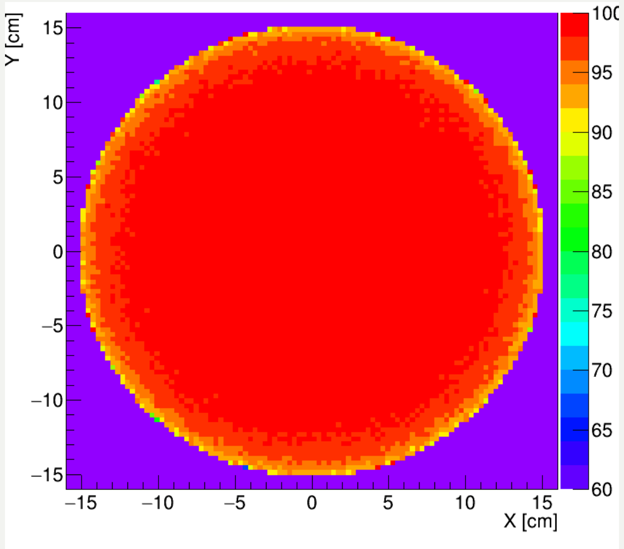
o-Ps → 3γ



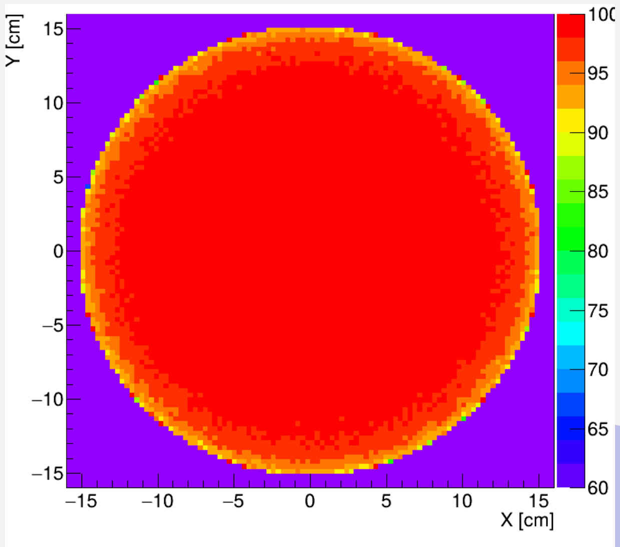
Toy MC



GATE



Toy MC



GATE

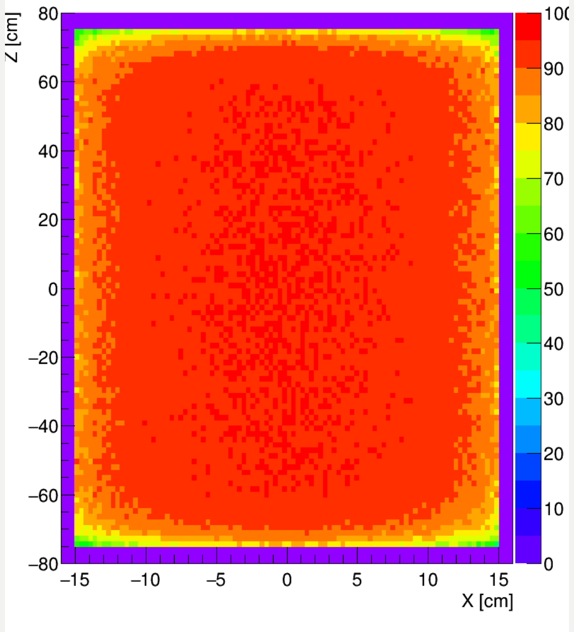
Absorption map – water cylinder – XZ plane

- 10^7 events

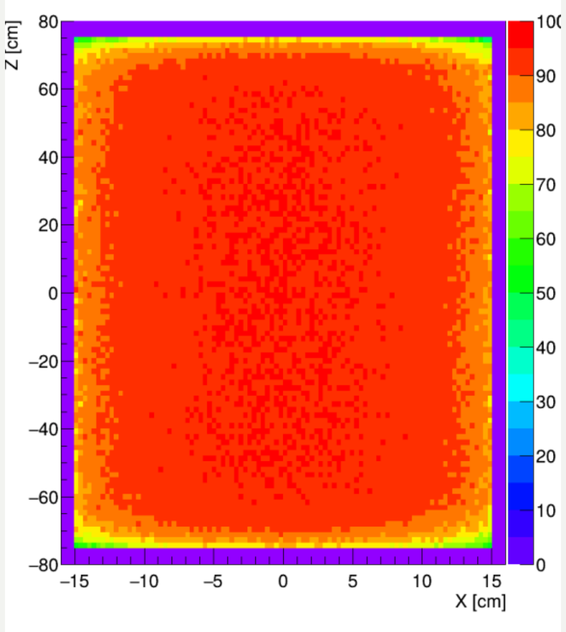
Surviving photon multiplets within the whole model

	Toy MC	GATE
pPs	7.6063 ± 0.0087%	7.6176 ± 0.0087%
oPs	1.6403 ± 0.0041%	1.6462 ± 0.0041%

p-Ps → 2γ

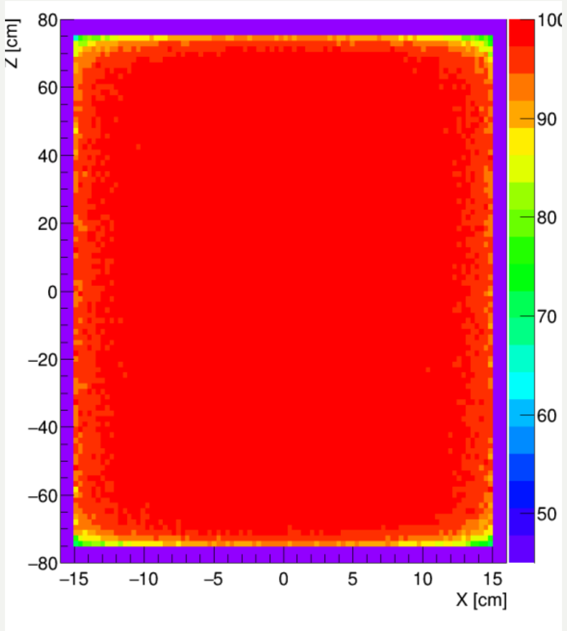


Toy MC

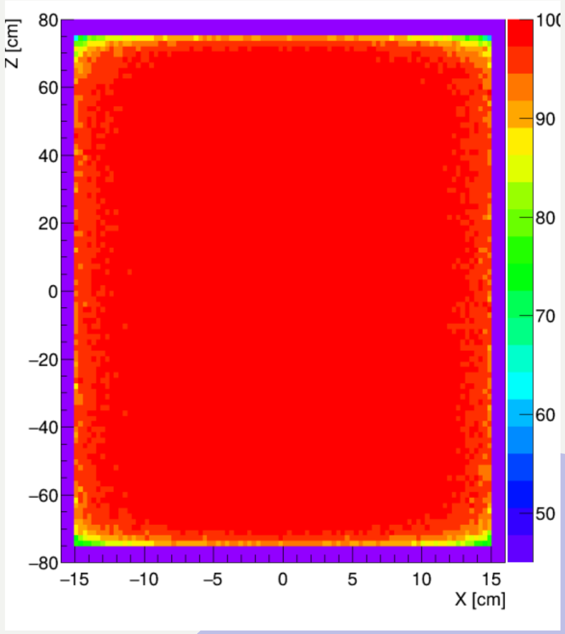


GATE

o-Ps → 3γ

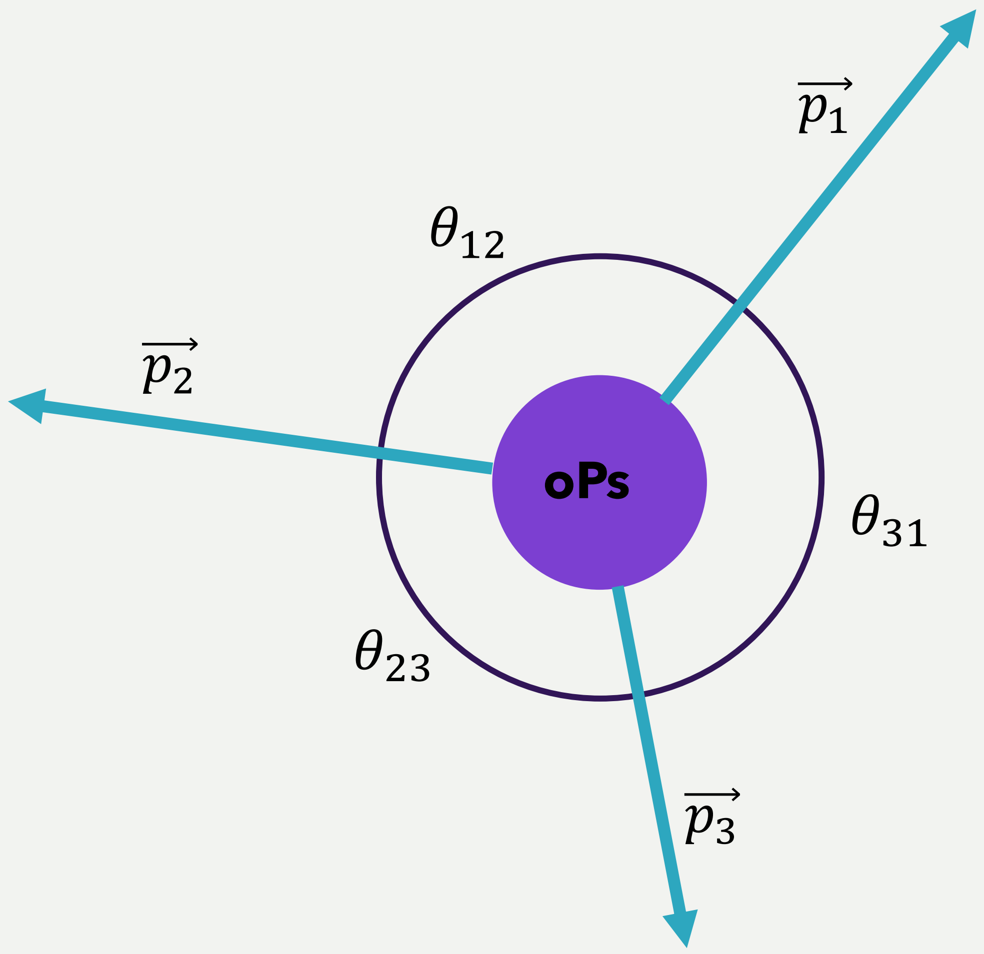


Toy MC



GATE

Simulation of oPs decay



1. Randomizing the energy of photons 1, 2 from the range (0, 511 keV) and assigning:

$$E_3 = M_{Ps} - E_1 - E_2,$$

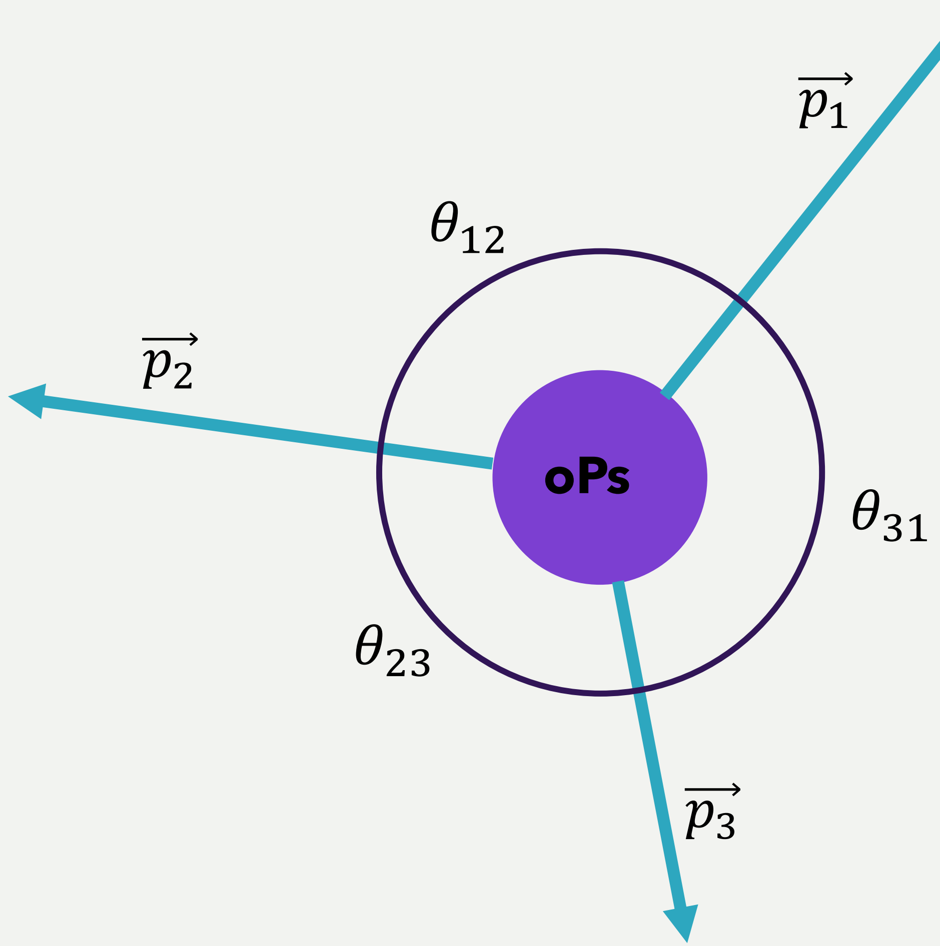
where $M_{Ps} = 1022$ keV - positronium mass.

2. Determination of the angles between momentum vectors in plane:

$$\theta_{12} = \mathrm{acos}\left(\frac{p_3^2 - p_1^2 - p_2^2}{2p_1p_2}\right),$$
$$\theta_{23} = \mathrm{acos}\left(\frac{p_1^2 - p_2^2 - p_3^2}{2p_2p_3}\right),$$
$$\theta_{31} = \mathrm{acos}\left(\frac{p_2^2 - p_1^2 - p_3^2}{2p_1p_3}\right).$$

J. Chhokar, Simulation of Positronium Decays in View of Charge Conjugation Symmetry Test with the J-PET Detector

Simulation of oPs decay



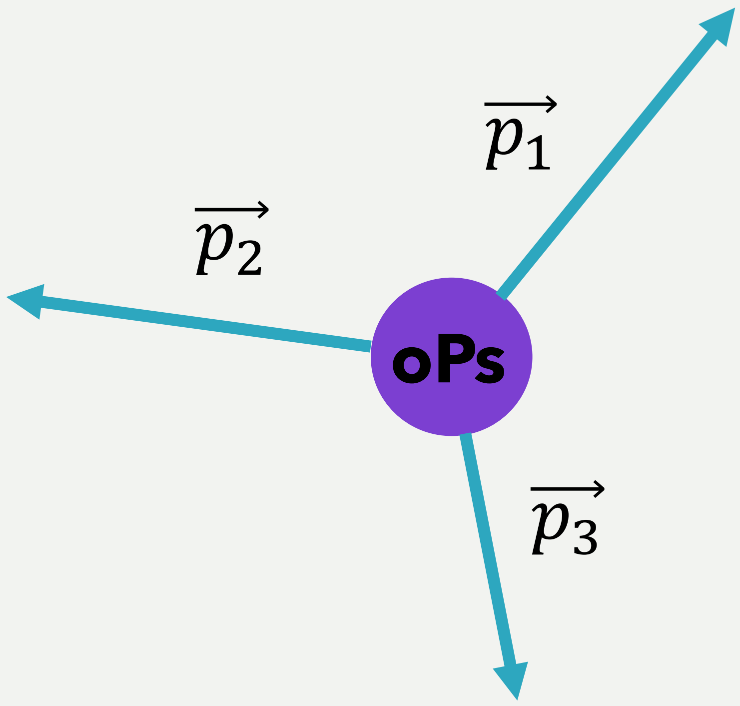
3. Determination of the decay plane:

- Rotating $\vec{p_1}$, $\vec{p_2}$, $\vec{p_3}$ at random angle φ relative to the X axis
- Rotating the decay plane using random rotation matrix (M)

4. Monte Carlo hit and miss simulation with the weight specified by the matrix element:

$$M_{oPs\rightarrow 3\gamma} = \left(\frac{m_e - E_1}{E_2 E_3}\right)^2 + \left(\frac{m_e - E_2}{E_1 E_3}\right)^2 + \left(\frac{m_e - E_3}{E_1 E_2}\right)^2$$

Determination of the decay plane:



Generating random rotation matrix using a method based on uniform sampling of unit quaternions:

- Generating three random variables: u_1, u_2, u_3 from a uniform distribution in range $(0, 1)$.
- Constructing a unit quaternion $q = (x, y, z, w)$ using:

$$x = \sqrt{1 - u_1} \cdot \sin(2\pi u_2),$$

$$y = \sqrt{1 - u_1} \cdot \cos(2\pi u_2),$$

$$z = \sqrt{u_1} \cdot \sin(2\pi u_3),$$

$$w = \sqrt{u_1} \cdot \cos(2\pi u_3).$$

- Defining the rotation matrix M:

$$M = \begin{bmatrix} x^2 - y^2 - z^2 + w^2 & 2(xy - zw) & 2(xz + yw) \\ 2(xy + zw) & -x^2 + y^2 - z^2 + w^2 & 2(yz - xw) \\ 2(xz - yw) & 2(yz + xw) & -x^2 - y^2 + z^2 + w^2 \end{bmatrix}$$