J-PET Monte Carlo simulation with the Geant4 package

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on behalf of the J-PET Collaboration

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Frascati
Monte Carlo simulation is a support for...

- creating the calibration and reconstruction methods
  - additional reconstruction method of radiopharmaceutic position

- searching for the physics beyond the Standard Model:
  - discrete symmetries violation
  - extra dimensions
  - dark matter
  - a new light vector gauge boson

- creating the diagnostic methods in medicine
  - morphometric imaging

Tools available on the market:
- Geant (general purpose)
- Gate (PET and SPET)
- Fred (Ion beam therapy)
- EGSnrc (it models the propagation of $\gamma$, $e^-$ and $e^+$ through matter)
- many more ...
J-PET detector

For details see a talk by P. Moskal on Monday
Event types

Emitted positrons

- Free positron annihilation
  - 2γ
  - 3γ

Formation of positronium

- para-positronium
  - 2γ self annihilation
  - 2γ pick-off annihilation

- ortho-positronium
  - 3γ self annihilation
  - 2γ pick-off annihilation

Effective yield of 3γ decay:
- In most non-metallic materials (e.g. water) is of the order of 0.5%.
- Although in some cases, as for example fine powders of alkaline oxides, can reach 20% or greater.

Literature:

<table>
<thead>
<tr>
<th>Material</th>
<th>No Ps formed(^1)</th>
<th>Water(^1)</th>
<th>IC3100(^2)</th>
<th>XAD-4(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(f_{3\gamma} = \sigma_{3\gamma}/\sigma_{2\gamma})</td>
<td>0.27%</td>
<td>0.52%</td>
<td>16.9%</td>
<td>28.9%</td>
</tr>
</tbody>
</table>

Program architecture and simulated geometry

- code available at GitHub
  https://github.com/JPETTomography/J-PET-geant4.git
- required packages: geant.10.4, root6, cadmesh, cmake
- physics list:
  G4EmLivermorePolarizedPhysics
  (Livermore physics models with polarized photon models)
- the Monte Carlo simulations account for:
  - angular and energy distributions of gamma quanta originating from direct or ortho-positronium annihilation,
  - Compton interactions of emitted gamma quanta in the detector built from plastic scintillators,
  - determination of gamma quanta hit-position and hit-time in the detector with experimentally determined resolutions,
  - multiple scattering and accidental coincidences,
Event classification

Goal: distinguish between following categories:

- $2\gamma$
- $3\gamma$
- prompt $\gamma$
- phantom scatterings
- detector scatterings

### Hit energy

![Hit energy chart](image)

### Hit X position

![Hit X position chart](image)

### Hit Y position

![Hit Y position chart](image)

### Hit Z position

![Hit Z position chart](image)

### Hit time

![Hit time chart](image)
Machine Learning classifier

- MC for run6
  - large annihilation chamber
  - prompt from the center
- variables for each hit:
  - deposited energy,
  - registration time
  - position coordinates
- used Long Short Term Memory (LSTM) layer
- the series of hits is fed into network
Learning process

Training Loss and Accuracy

- **loss**: this score is minimized and a perfect cross-entropy value is 0
- **accuracy**: to judge the performance of model \( \frac{\text{correctly classified events}}{\text{all events}} \)
Classifiers - run6 (3γ: 0.3%)

- loss 29.1 %
  - this score is minimized and a perfect cross-entropy value is 0
- accuracy 90.6%
  - to judge the performance of model \( \frac{\text{correctly classified events}}{\text{all events}} \)
Classifiers - run6 (3\(\gamma\): 40%)

- loss 37.2%
  - this score is minimized and a perfect cross-entropy value is 0
- accuracy 84.3%
  - to judge the performance of model \(\frac{\text{correctly classified events}}{\text{all events}}\)
Summary

- J-PET-Geant4 is a Monte Carlo simulation program designed for the J-PET detector created in Geant4 toolkit.
- Software is maintained within public repositories on GitHub: https://github.com/JPETTomography
- Many contributing members
Thank you for your attention
Back to back events

- simulated two 511 keV back to back gamma quanta
- $\equiv$ emitted gamma quanta interact via Compton scattering
- $\Downarrow$ Sensitivity map in $x - y$ plane in the central part of the detector. Figure is made in a transverse view of the detector with 0.5 mm $\times$ 0.5 mm bin size.

o-Ps → 3γ annihilation

- simulated two 511 keV back to back gamma quanta
- emitted gamma quanta interact via Compton scattering
- Sensitivity map in x − y plane in the central part of the detector. Figure is made in a transverse view of the detector with 0.5 mm × 0.5 mm bin size.
Studies of discrete symmetries

<table>
<thead>
<tr>
<th>Operator</th>
<th>C</th>
<th>P</th>
<th>T</th>
<th>CP</th>
<th>CPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\vec{S} \cdot \vec{k}_1 \times \vec{k}_2$</td>
<td>+</td>
<td>+</td>
<td>−</td>
<td>+</td>
<td>−</td>
</tr>
</tbody>
</table>

$C_{CPT} = 0.0026 \pm 0.0031$ (for $\vec{S} \cdot \vec{k}_1 \times \vec{k}_2$)  

$\text{SM: } 10^{-9} - 10^{-10}$  
effects of final state interaction  
(W. Bernreuther et al., Z. Phys. C 41 (1988) 143)

Observable: $A = \frac{N(\alpha) - N(\alpha + 180)}{N(\alpha) + N(\alpha + 180)}$
Application example - $\mathcal{CPT}$ violation parameter

- $C_{CPT} = 0.0026 \pm 0.0031$ (for $\vec{S} \cdot \vec{k}_1 \times \vec{k}_2$) (P.A. Vetter et al., Phys. Rev. Lett. 91 (2003) 263401)

- Dependency between number of reconstructed o-Ps→3$\gamma$ events and the amplitude of $\mathcal{CPT}$ violating asymmetry uncertainty (red line). Plot is made assuming detection parameters as in Gammashpere detector. Result obtained by Vetter and Freedman is denoted by black square.

- $R_{o-Ps \rightarrow 3\gamma} = A \cdot f_{o-Ps \rightarrow 3\gamma} \cdot \epsilon_{det}(th) \cdot \epsilon_{ana}$,
  - $A$ - source activity
  - $f_{o-Ps \rightarrow 3\gamma}$ - fraction of o-Ps→3$\gamma$ annihilation
  - $\epsilon_{det}(th)$ - detection efficiency
  - $\epsilon_{ana}$ - analysis efficiency

- XAD-4 (10MBq, th=50keV):
  $R_{o-Ps \rightarrow 3\gamma} = 25$ events/s
  $\approx 1.5 \times 10^7$ events/week

- around 1.5 year of measurement is required to improve the previous result by an order of magnitude
Integration with J-PET Analysis Framework

- J-PET Framework is the analysis environment written in C++ for the low- and high-level data processing.
- provides adjusting of Geant MC output in framework structures (hit level)
- user can process MC in the same manner as collected data