Towards multiphoton imaging @ J-PET

with GATE simulations :-)

Wojciech Krzemień
On behalf of the J-PET collaboration

Gate Scientific Meeting
23.05 2024

UNIWERSYTET JAGIELLOŃSKI W KRAKOWIE

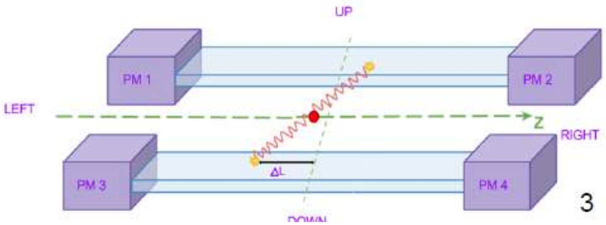
NATIONAL CENTRE FOR NUCLEAR RESEARCH ŚWIERK

Jagiellonian Positron Emission Tomography

J-PET

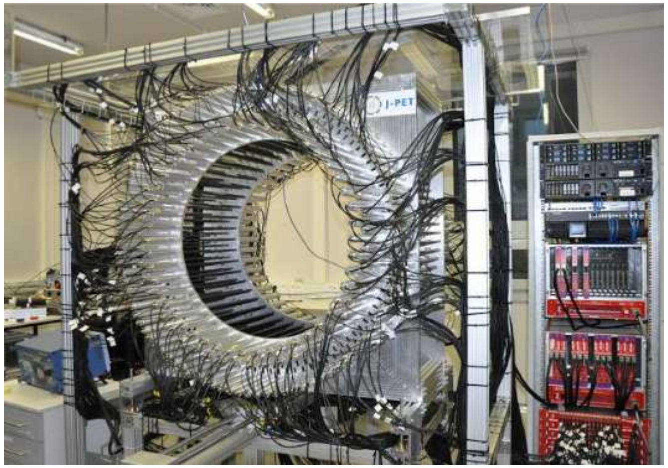
Cost-effective total body solution

$$\Delta l = \frac{(t_2 - t_1) \cdot v}{2} \cong \frac{(t_2 - t_1) \cdot c}{4}$$



$$\Delta x = \frac{(t_l - t_r) \cdot c}{2} \Longrightarrow \Delta x = \frac{\Delta t}{2} \cdot c$$

First prototype



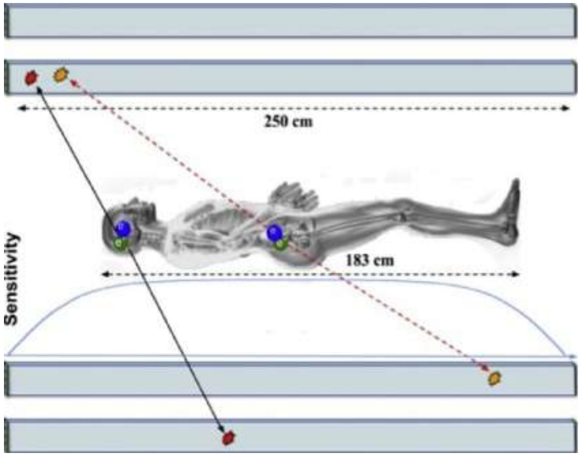
Acta Phys Pol. B 48 (2017) 1567

- 50 cm AFOV
- 192 plastic strips
- Readout → vacuum tube photomultipliers

Modular J-PET

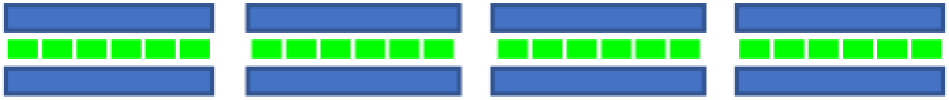
- 50 cm AFOV
- 24 modules x 13 strips
- Readout → silicon photomultipliers matrices

Total-body

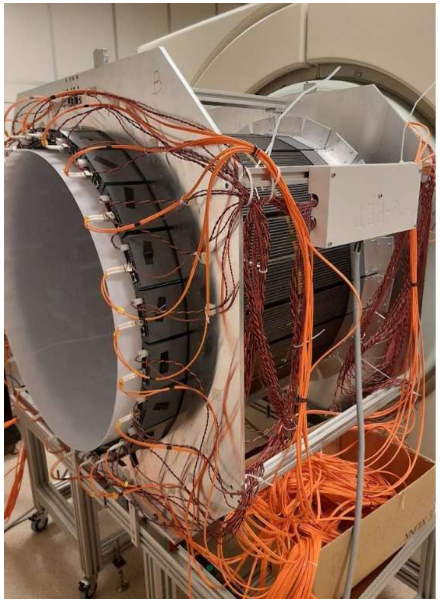


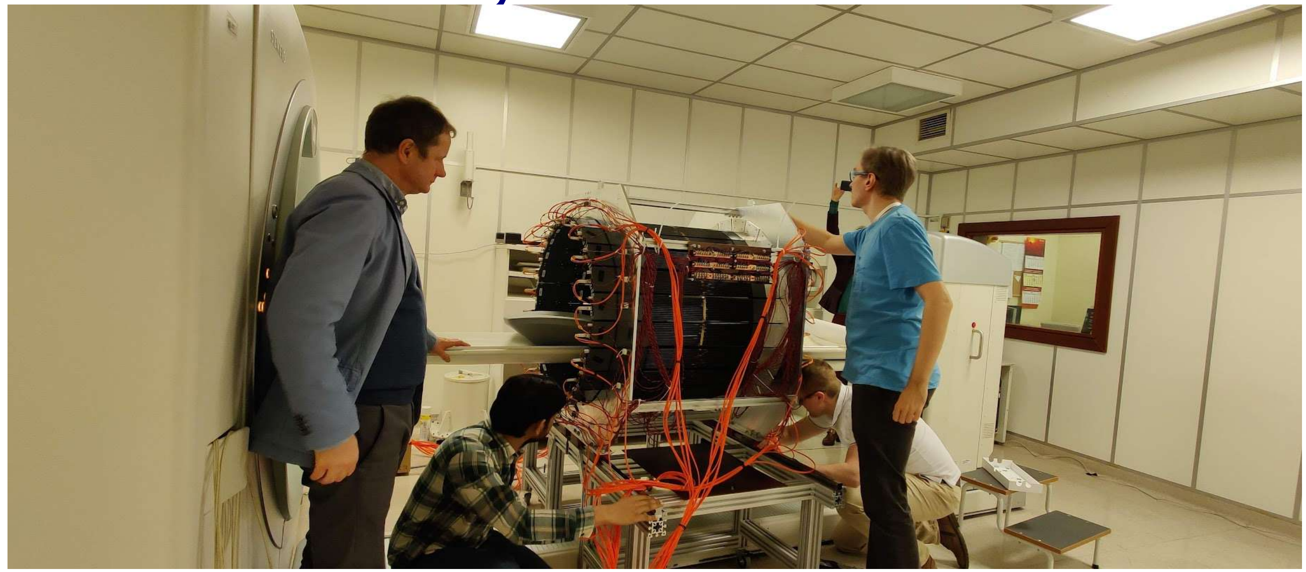
PET Clinics 15 (2020) 439
Phys. Med. Biol. 66 (2021) 175015

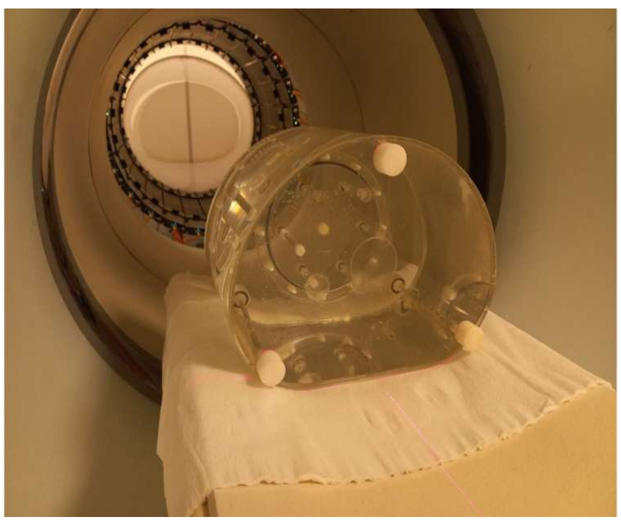
- 250 cm AFOV
- Additional layers of wavelength shifters → better axial resolution

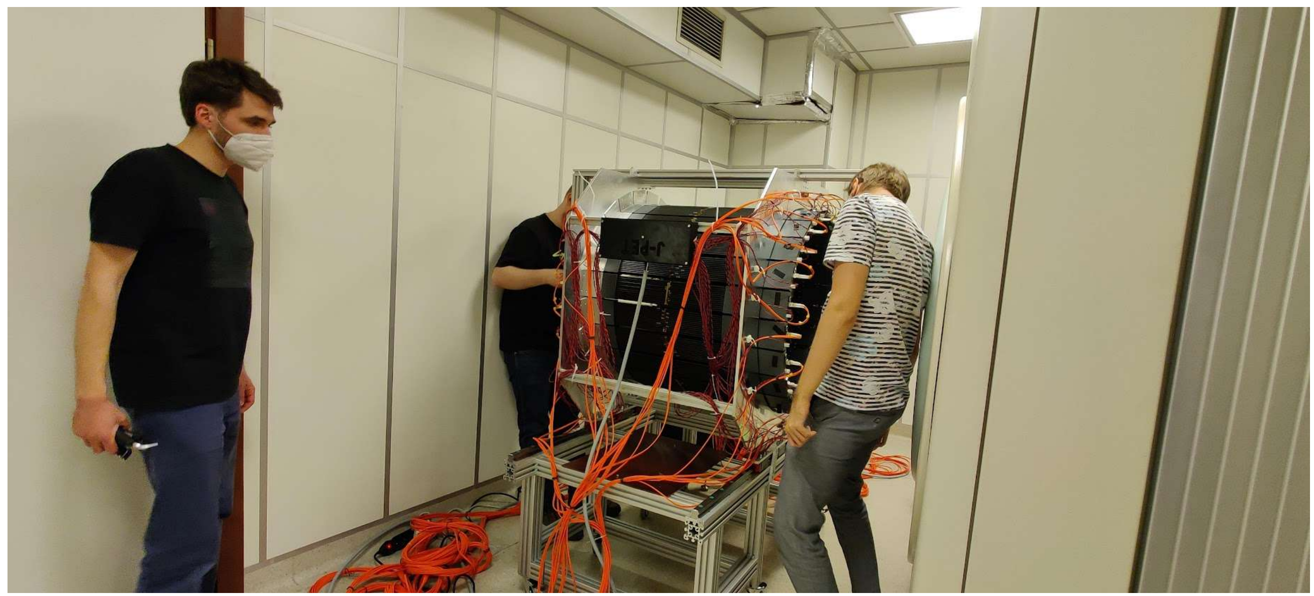


First test measurements with patients @Medical University of Warsaw





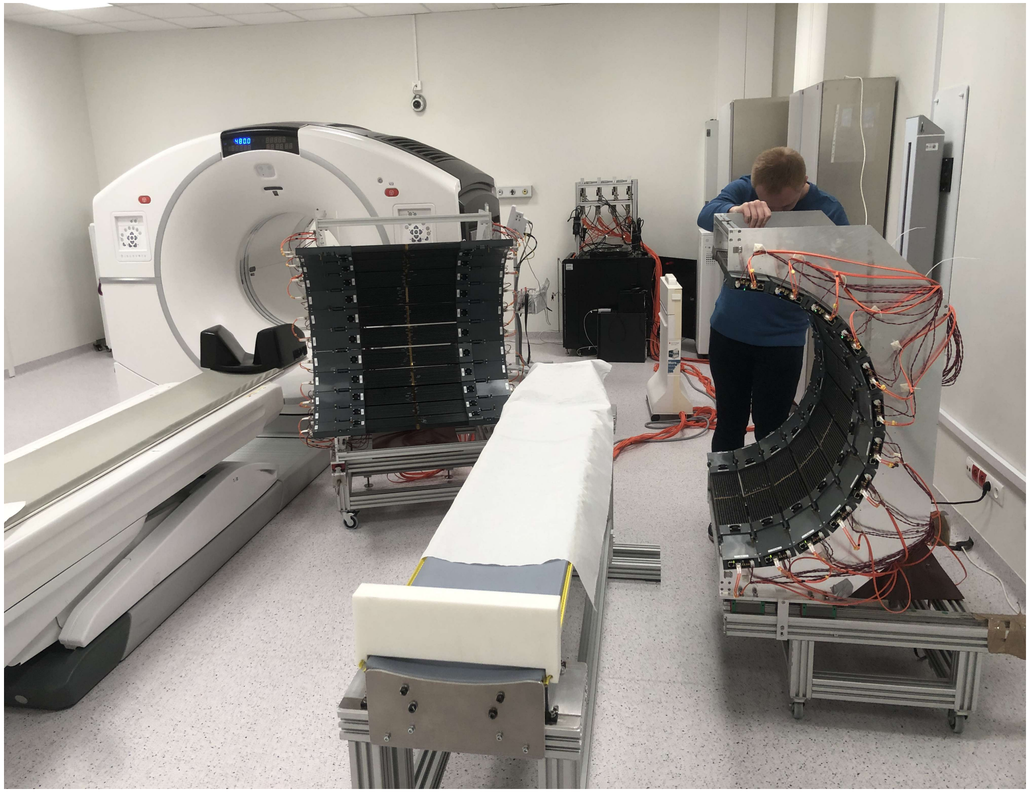




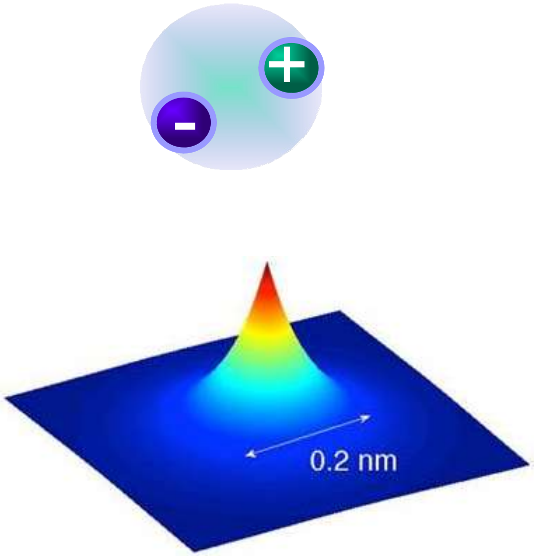
- ^{68}Ga and FDG – phantoms and patients
- data also taken with Biograph Truepoint PET-CT

"First positronium image of the human brain in vivo" P. Moskal et al., medRxiv:2024.02.01.2329902, article submitted.

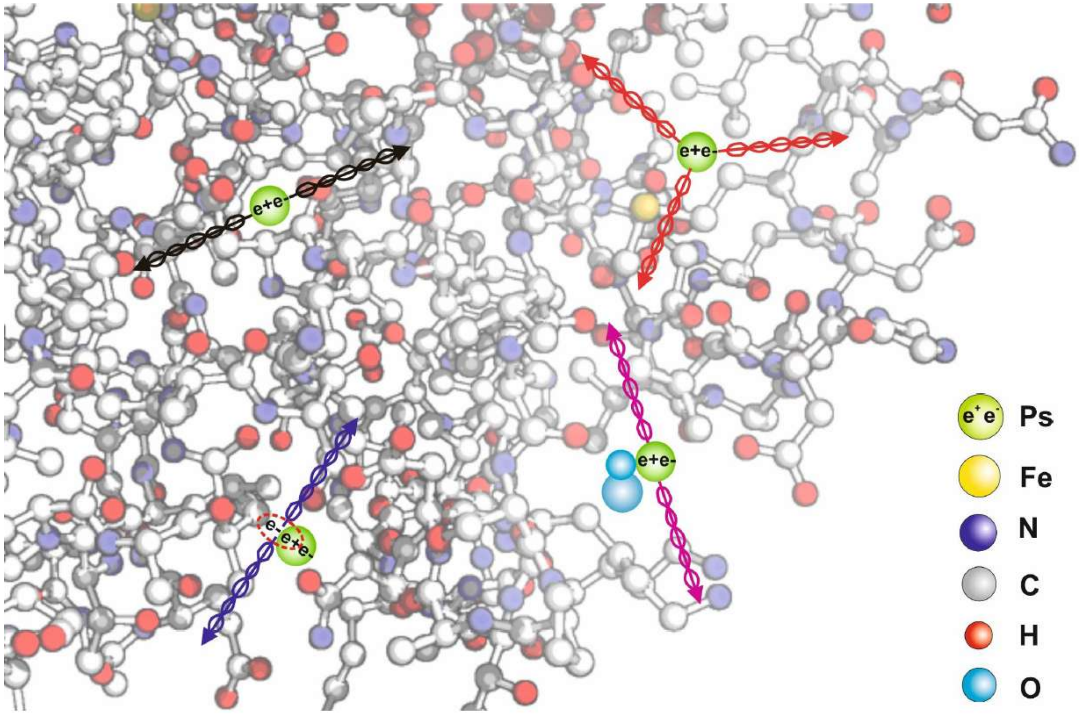
Currently - measurements with patients @University Hospital in Cracow



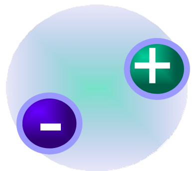
Multi-photon imaging

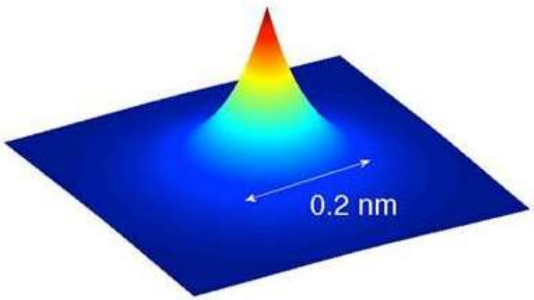


Model of the hemoglobin molecule



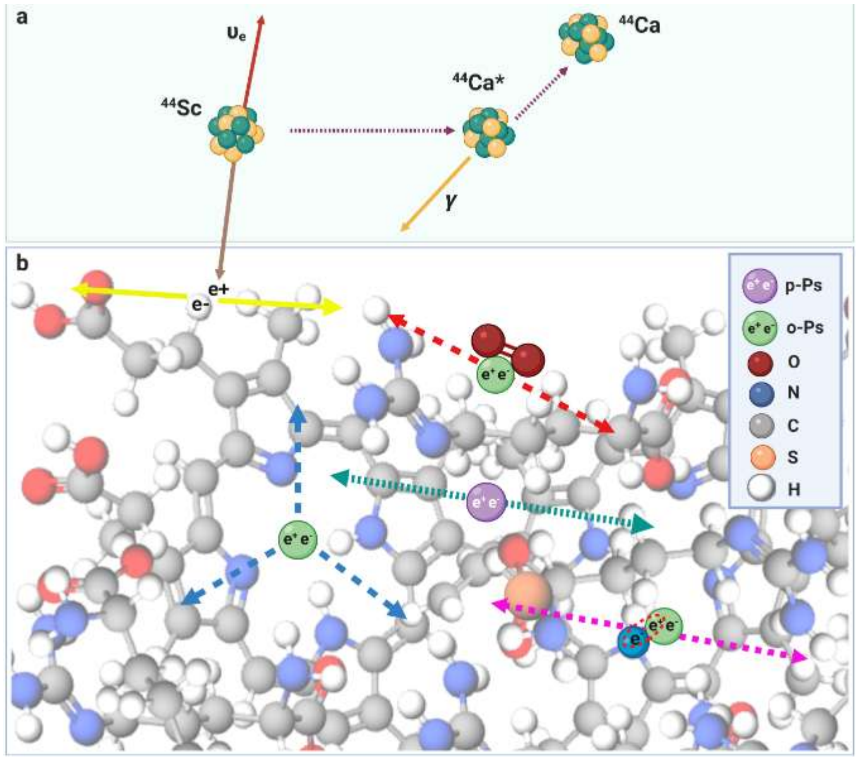
Positronium in PET





Para-positronium:
- **lifetime ~125 ps**
- **two-photon decay**

Ortho-positronium:
- **lifetime ~142 ns**
- **three-photon decay**



Rev. Mod.Phys. S. Bass, S. Mariazzi, P. Moskal, E. Stępień

Fundamental searches with positronium decays @J-PET

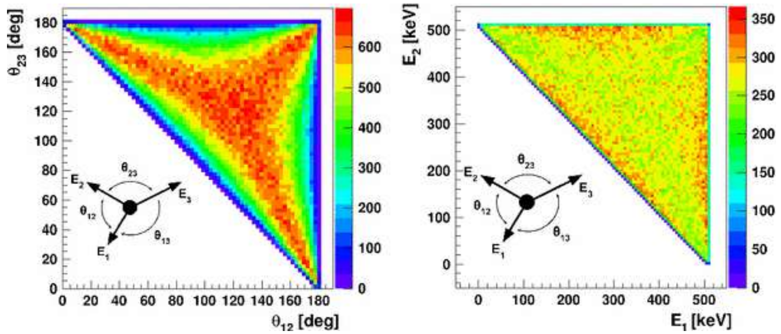
- Study of the CP symmetry:
  P. Moskal, E. Czerwiński, J. Raj et al., Nature Communications 15 (2024) 78

- Testing of CPT symmetry:
  P. Moskal, A. Gajos et al. Nature Communications 12 (2021) 5658

- Study of the forbidden decays (p-Ps -> 3 photons)- conjugation symmetry
  M. Skurzok **Acta. Phys. Polon. A 137 (2020) 134**

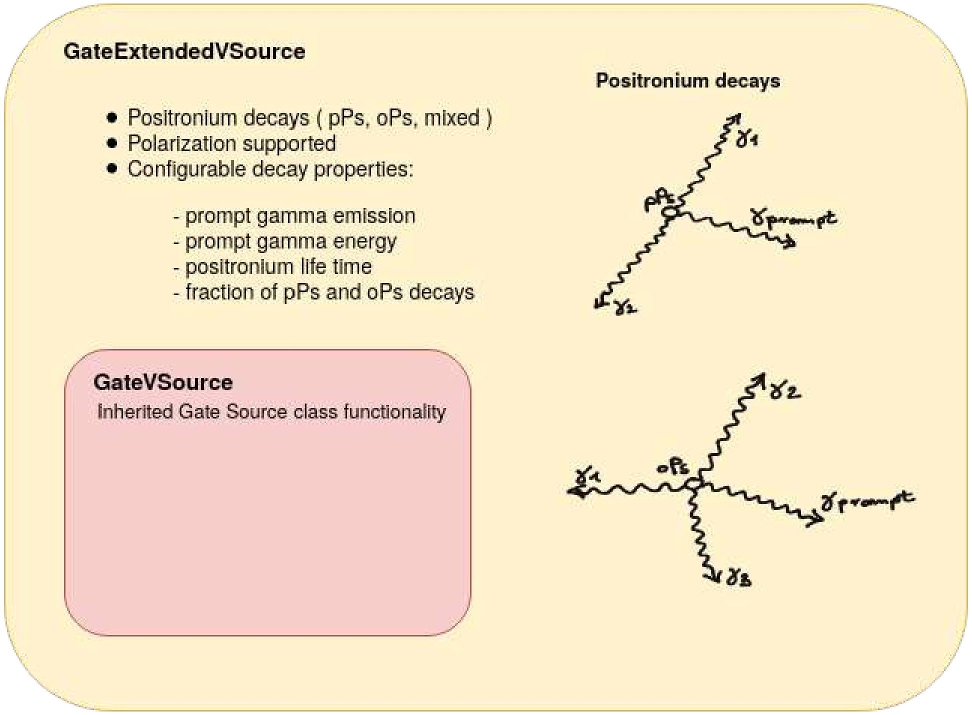
- Invisible decays, dark matter searches, rare decays (ps → 4 photons, ps → 5 photons),
  E. Perez del Rio, P. Tanty, J. Mędrala
  Acta Phys. Polon. A 142(3) (2022) 386-390

- Many more physics topics:
  P. Moskal et al. Acta Phys. Polon. B 47 (2016) 509



Implementation of QED-complient description of
orto-positronium decay

S. Bass et al. Rev. Mod. Phys. 95 (2023) 021002
P. Moskal et al., Phys. Med. Biol. 64 (2019) 055017
P. Moskal et al. Eur. Phys. J. C 78 (2018) 970
D. Kaminska et al., Eur. Phys. J. C (2016) 76:445



Mateusz Bała

available in GATE >= v9.0

Simultanous scans = standard image + lifetime image

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HOME > SCIENCE ADVANCES > VOL. 7, NO. 42 > POSITRONIUM IMAGING WITH THE NOVEL MULTIPHOTON PET SCANNER

Kamil Dulski

RESEARCH ARTICLE | BIOPHYSICS

Positronium imaging with the novel multiphoton PET scanner

PAWEŁ MOSKAL , KAMIL DULSKI , NEHA CHUG, CATALINA CURCEANU, ERYK CZERWIŃSKI , MEYSAM DADGAR, JAN GAJEWSKI , ALEKSANDER GAJOS , GRZEGORZ GRUDZIEŃ , [...] WOJCIECH WIŚLICKI +27 authors Authors Info & Affiliations

SCIENCE ADVANCES • 13 Oct 2021 • Vol 7, Issue 42 • DOI: 10.1126/sciadv.abh4394

Abstract

In vivo assessment of cancer and precise location of altered tissues at initial stages of molecular disorders are important diagnostic challenges. Positronium is copiously formed in the free molecular spaces in the patient's body during positron emission tomography (PET). The positronium properties vary according to the size of inter- and intramolecular voids and the concentration of molecules in them such as, e.g., molecular oxygen, O_2; therefore, positronium imaging may provide information about disease progression during the initial stages of molecular alterations. Current PET systems do not allow acquisition of positronium images. This study presents a new method that enables positronium imaging by simultaneous registration of annihilation photons and deexcitation photons from pharmaceuticals labeled with radionuclides. The first positronium imaging of a phantom built from cardiac myxoma and adipose tissue is demonstrated. It is anticipated that

Abstract
ODUCTION
RESULTS
SCUSSION
METHODS
ledgments
ND NOTES
eLetters

CURRENT ISSUE

Control of lysosomal-mediated cell death by the pH-dependent calcium channel RECS1

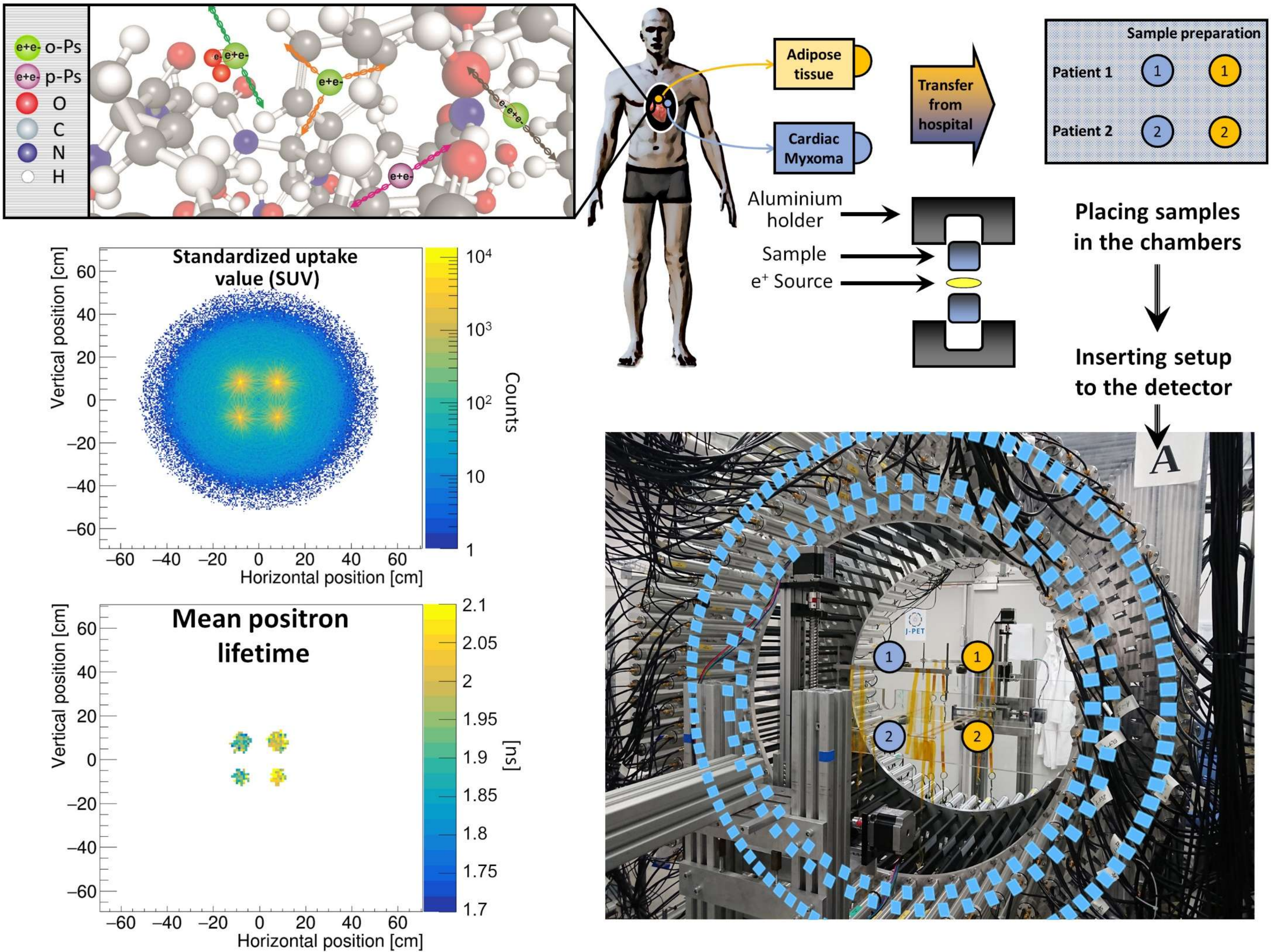
BY PHILIPPE PIHAN, FERNANDA LISBONA, ET AL.

Epitope-preserving magnified analysis of proteome (eMAP)

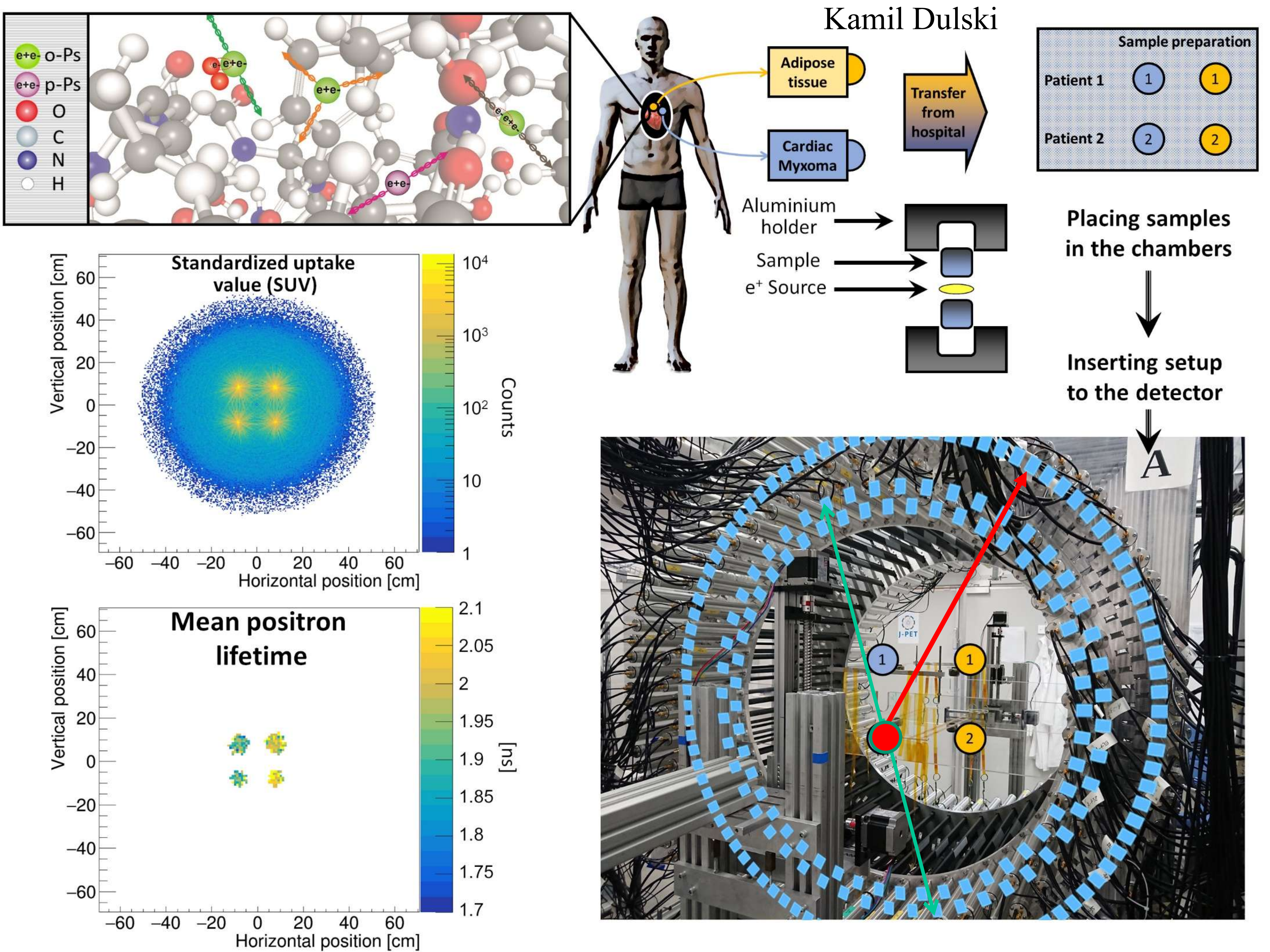
BY JOHA PARK, SARIM KHAN, ET AL.

Speckle-free holography with partially coherent light

Also : Shibuya, K.,et al. Nature Commun Phys 3, 173 (2020).



e+e- o-Ps
e+e- p-Ps
O
C
N
H
Adipose tissue
Cardiac Myxoma
Transfer from hospital
Sample preparation
Patient 1
Patient 2
Aluminium holder
Sample
e+ Source
Placing samples in the chambers
Inserting setup to the detector
Standardized uptake value (SUV)
Vertical position [cm]
Horizontal position [cm]
Counts
Mean positron lifetime
[ns]
J-PET
A



Kamil Dulski
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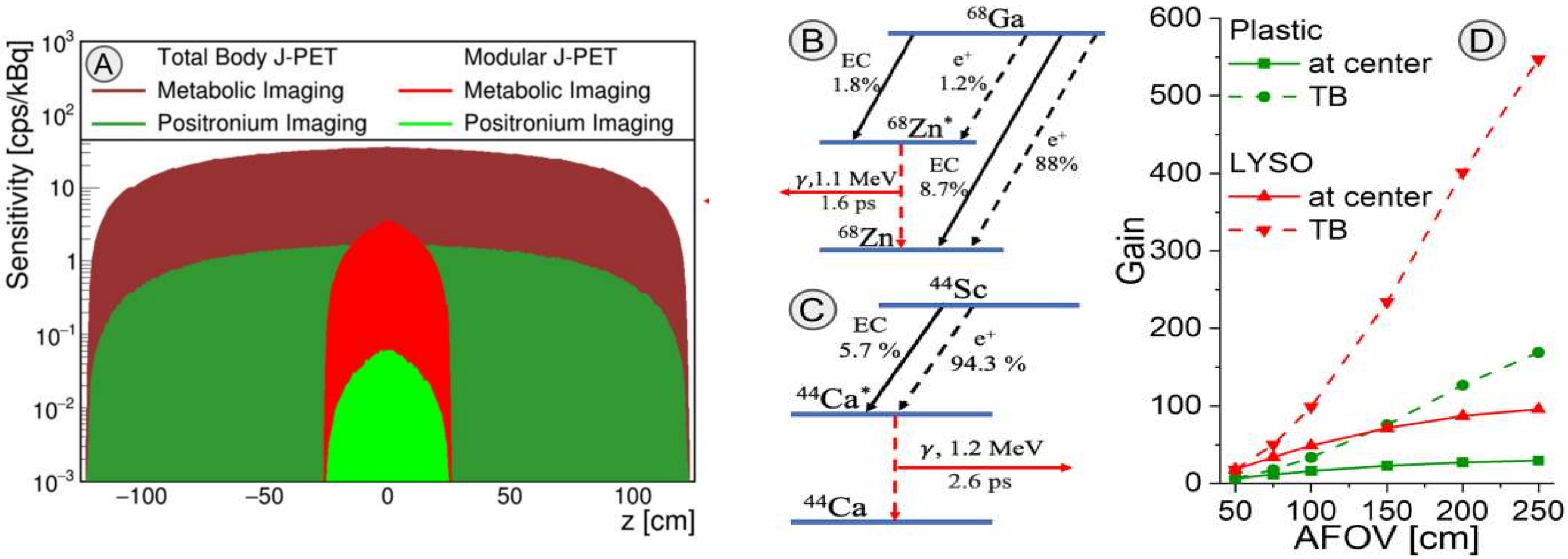
A

Multi-photon tomography challenges



- Efficient (triple) coincidence selection
- New reconstruction algorithms:
  - R. Shopa, K, Dulski Bio-Algorithms and Med-Systems 18(1) (2022) 135-143
  - B. Huang et al., IEEE Transactions on Medical Imaging, doi: 10.1109/TMI.2024.3357659
- Background coincidences (randoms, scatters) reduction

Szymon Parzych

Triple coincidence selection

- Gate version 9.1
- Modified to J-PET needs*
- Further modified due to issues with saving proper scattering statistics for 3^{rd} photon
- Source type: pPs + deexcitation photon (resembling ^{44}Sc)
- Simulation up to the level of Singles
- Personal Coincidence sorter for triple coincidences

*https://github.com/JPETTomography/Gate

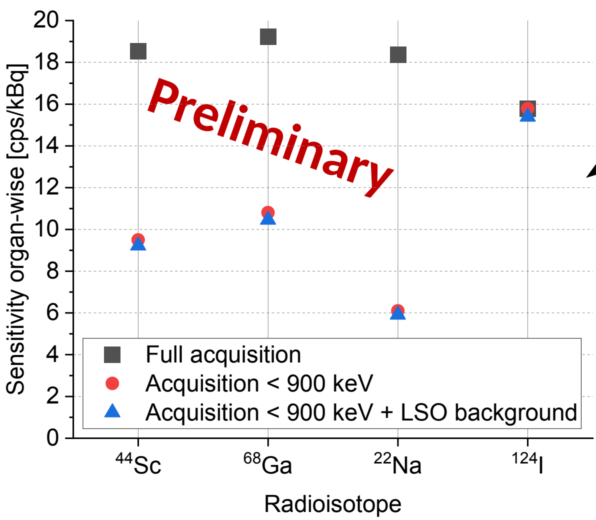
Earlier preliminary results:

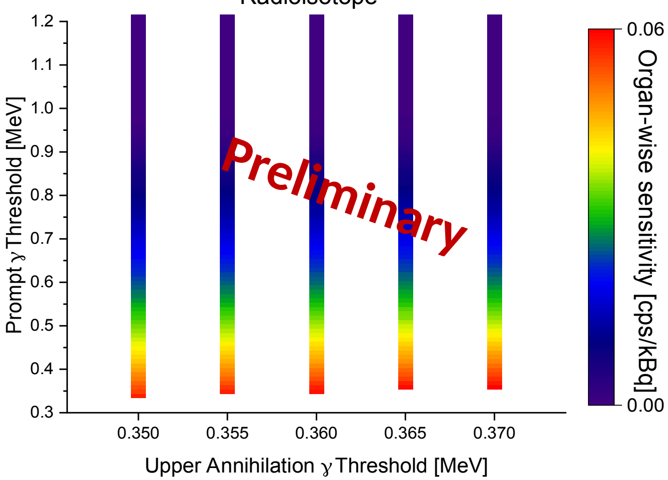
Sz. Parzych et al. Bio-Algorithms and Med-Systems 19 (1) (2023) 80-86

Szymon Parzych

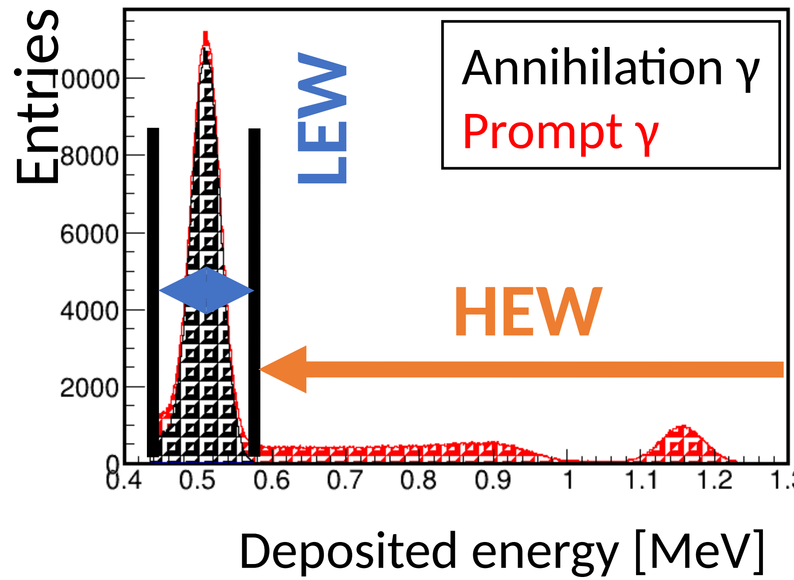
Triple coincidence selection

- Definition: 2 photons from Low Energy Window + 1 photon from High Energy Window
- Possible candidate triples:
  - 2 × Annihilation γ – Annihilation/Prompt γ
  - Annihilation γ + Prompt γ – Annihilation/Prompt γ
  - 2 × Prompt γ – Annihilation/ Prompt γ

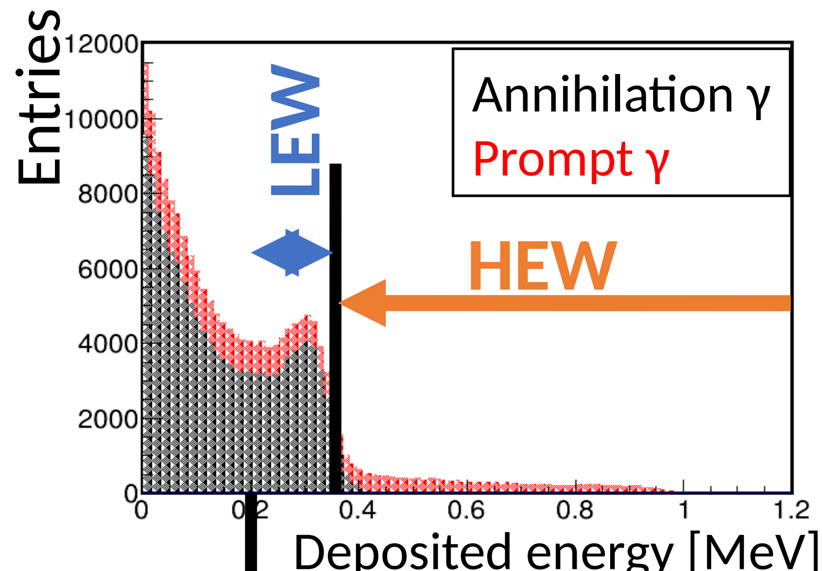




Biograph Vision Quadra

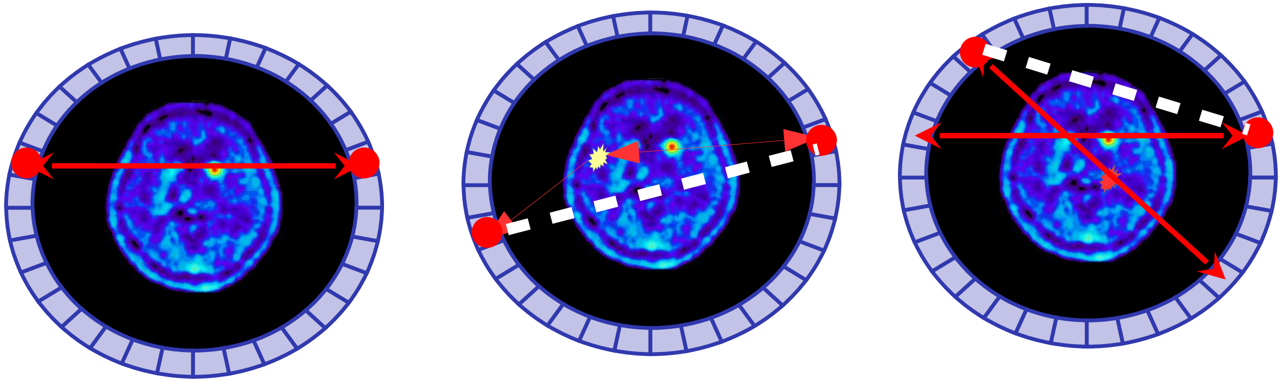


Modular J-PET



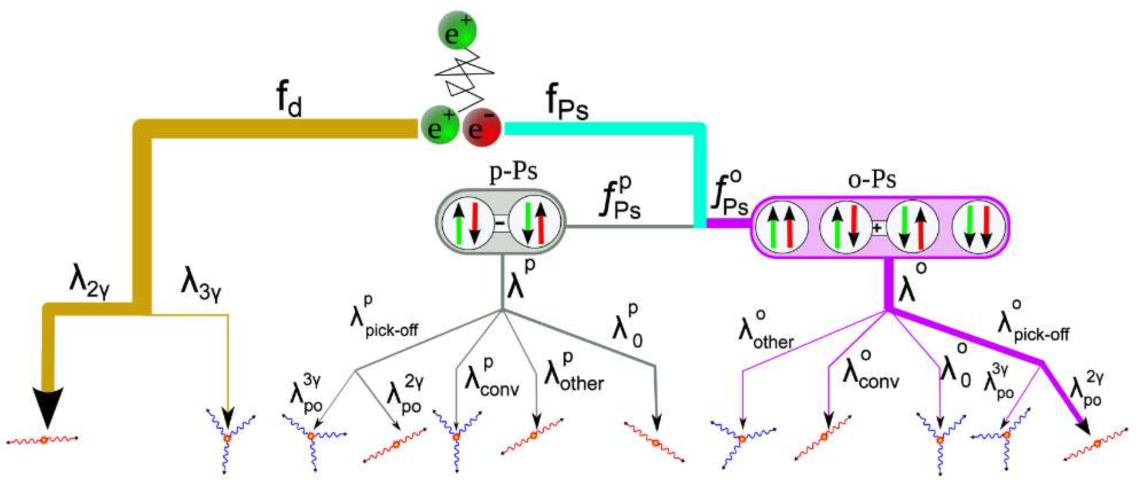
Figures: Exemplary energy spectrum of annihilation + prompt photons; GATE software

Coincidence classes
(multi-photon tomography)

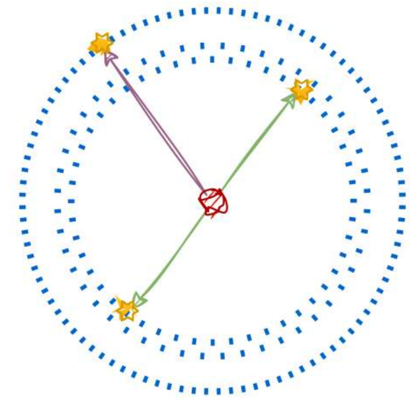


true　　　scatter　　　randoms

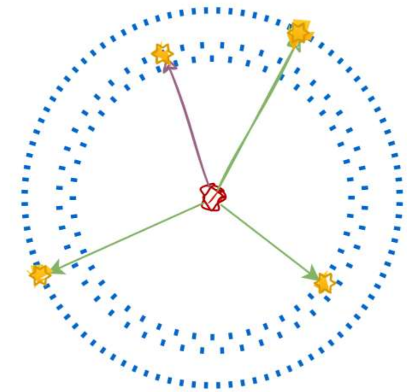
Coincidence classes
(multi-photon tomography)



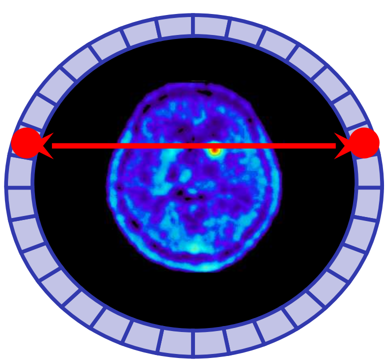
From Rev. Mod.Phys. S. Bass, S. Mariazzi, P. Moskal, E. Stępień
https://arxiv.org/pdf/2302.09246.pdf



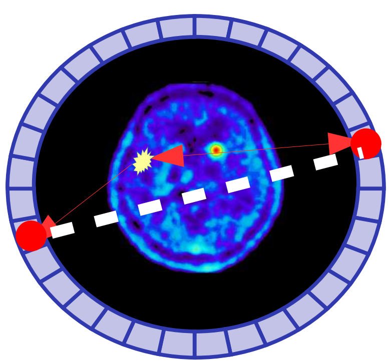
2 annihilation photons + 1 high energy photon



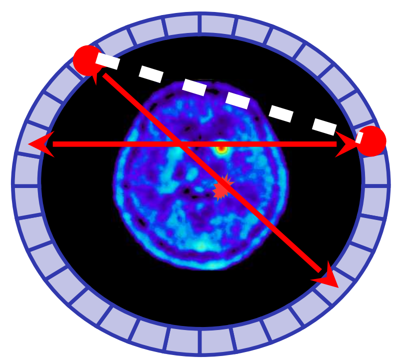
3 annihilation photons + 1 high energy photon



true



scatter

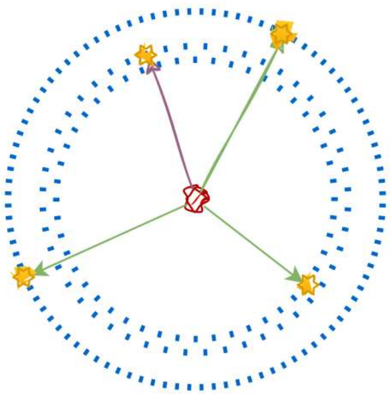


randoms

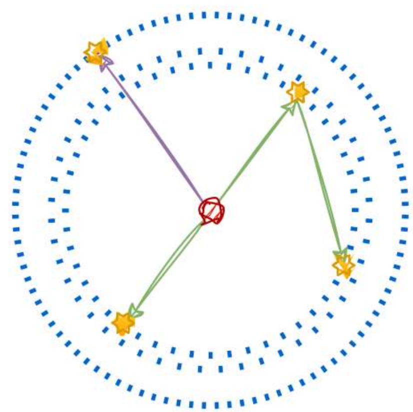
Coincidence classes
(multi-photon tomography)

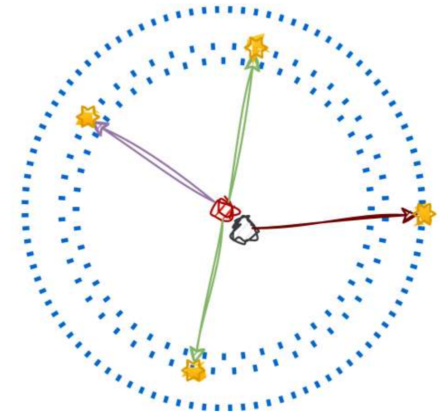
BACKGROUND CASES (JUST EXAMPLES)

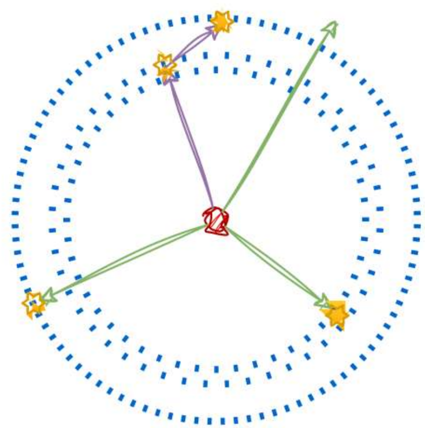
SIGNAL

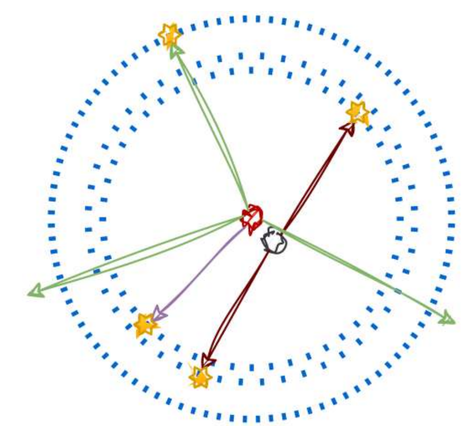


3 annihilation photons + 1 prompt photon









Application of Deep Learning methods for event classification in multi-photon case

Can we apply ML for event selection in view of positronium lifetime tomography?

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RESEARCH ARTICLE | BIOPHYSICS

Positronium imaging with the novel multiphoton PET scanner

PAWEŁ MOSKAL, KAMIL DULSKI, NEHA CHUG, CATALINA CURCEANU, ERYK CZERWIŃSKI, MEYSAM DADGAR, JAN GAJEWSKI, ALEKSANDER GAJOS, GRZEGORZ GRUDZIEŃ, [...] WOJCIECH WIŚLICKI +27 authors Authors Info & Affiliations

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3,485

Abstract | INTRODUCTION | RESULTS | DISCUSSION | METHODS | Acknowledgments | REFERENCES AND NOTES | 0 eLetters

Abstract

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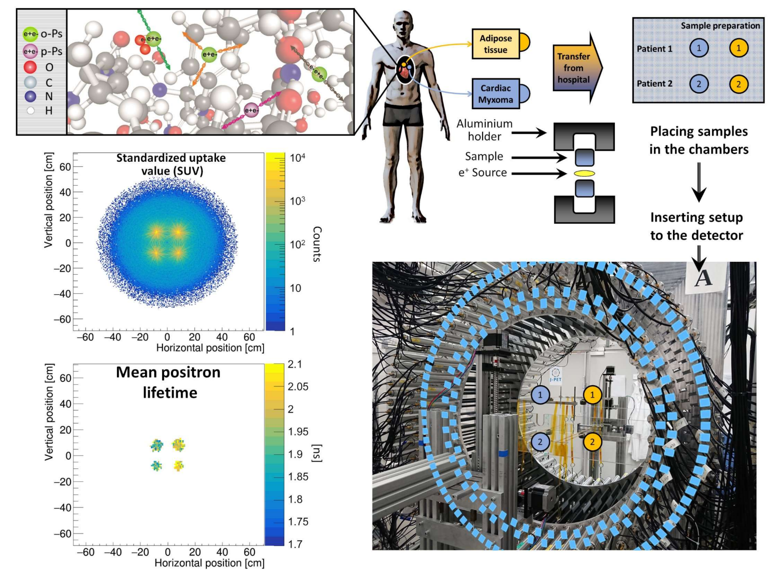
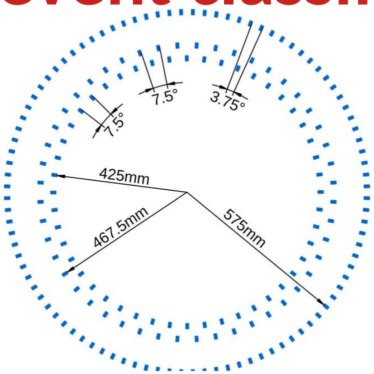
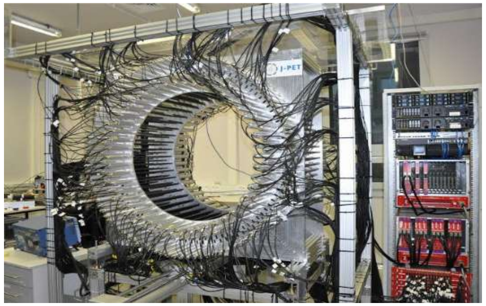
PDF



Damian Trybek

Application of Deep Learning methods for event classification in multi-photon case





Large Barrel geom.

- 50 cm AFOV
- 192 plastic strips
- 3 layers

Acta Phys Pol. B 48 (2017) 1567

Setups:

- Two point sources (0,0,0) cm and shifted (5,0,5) cm
- Small cylinder (R=5cm,L=5cm)
- Positronium lifetime = 2ns

MC Simulation

- Phenomenological time,energy and positional resolution
- Preselection cuts (~17% of background rejected, ~0.6% of signal rejected)
- **S ~ 5 *10^{2}, B ~1.3 *10^{7}**
- Additional signal-only simulations: **10^{5}**

Feedforward Neural Network

PyTorch

Hyperparameter tuning

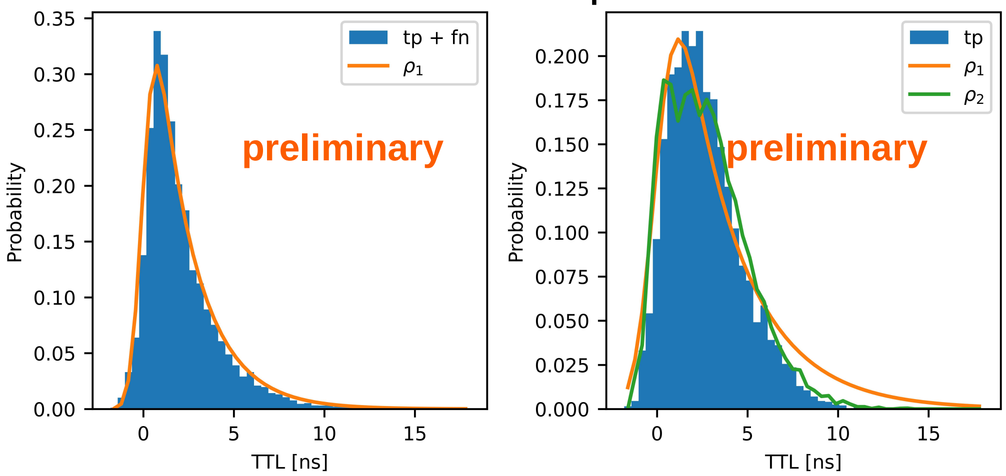
RAY tune

- Optimizer: Adam
- Loss: Customized loss function
- Optimization:Tree-Structure Parzen Estimation
- Feature space: 46 variables

Application of Deep Learning methods for event classification in multi-photon case

Damian Trybek

First setup



$$\rho(t) = \begin{cases} \frac{1}{\tau} exp(-\frac{t}{\tau}), & t \geq 0 \\ 0, & t < 0 \end{cases}$$

$$S(t) = \frac{1}{\sigma\sqrt{2 * \pi}} exp\left(-\frac{t^2}{\sigma_t^2}\right)$$

$$\rho_1(t) = (\rho * S)(t)$$

$$\rho_2(t) = \cdot\rho_1(t) \cdot \text{eff(t)}$$

preliminary

Nominal value 2 ns

TP + FN	ρ_1	τ	$2.163(90)ns$
		σ_t	$0.525(41)ns$
TP	ρ_1	τ	$3.272(216)ns$
		σ_t	$0.918(106)ns$
	ρ_2	τ	$2.024(88)ns$
		σ_t	$0.700(77)ns$

- Comparison with respect to „standard” J-PET selection criteria show 10x improvement in signal to noise terms

Exploiting photons polarization

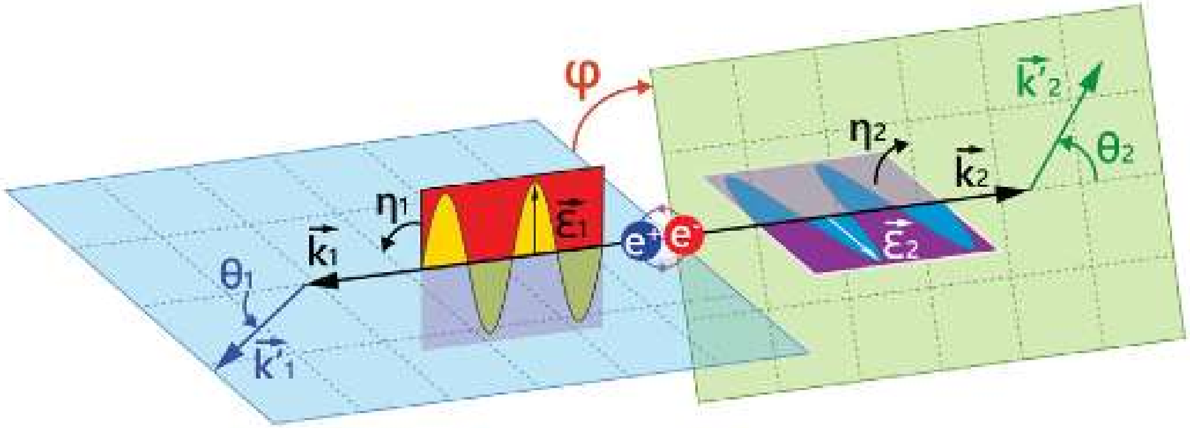
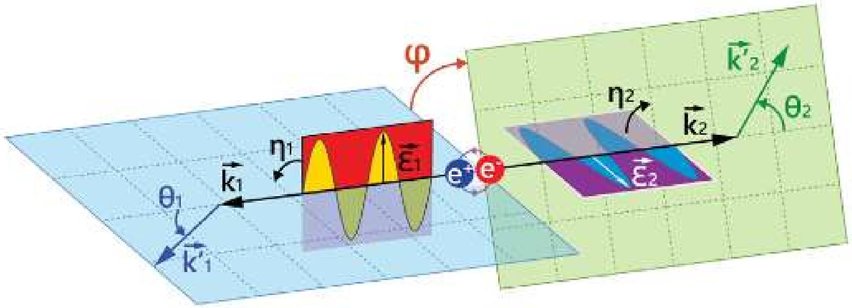
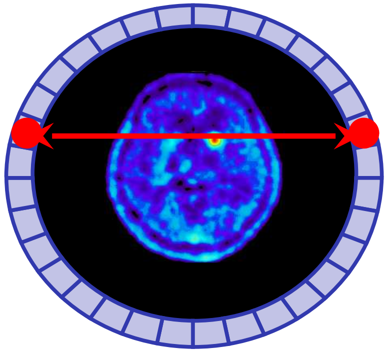


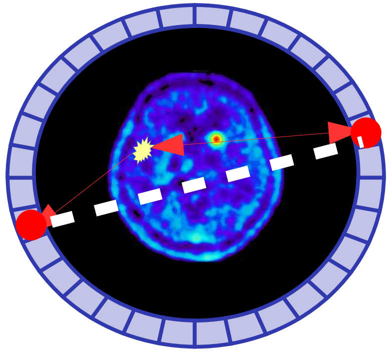
Figure taken from:S. Bass et al. Rev. Mod. Phys. 95 (2023) 021002

Two-photon correlations for PET applications





True events



(Noisy)scattered events

Different modalities (MC estimations):

Kuncic, Z., et al. Instrum. Methods Phys. Res. A 648, S208 (2011)

McNamara, A. et al. Z. Phys. Med. Biol. 59, 7587 (2014)

P. Moskal et al. Eur. Phys. J. C 78, 970 (2018)

Yoshida, E. et al. Phys. Med. Biol. 65, 125013 (2020)

Theory:

B. C. Hiesmayr, P. Moskal Sci. Rep. 7 (2017) 15349

B. C. Hiesmayr, P. Moskal Sci. Rep. 9 (2019) 8166

Experimental results:

D. Watts et al. Nature Communications 12 (2021) 2646

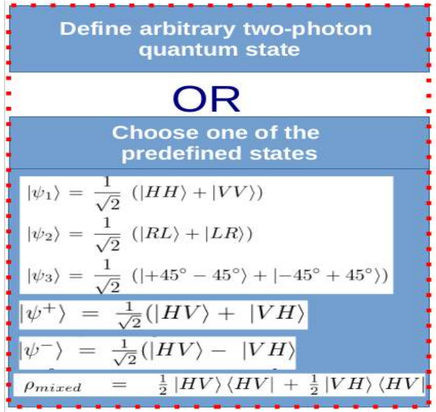
A. Ivaskhin et al. Scientific Reports 13 (2023) 7559

S. Parashari et al. Phys. Lett. B 852 (2024) 138628

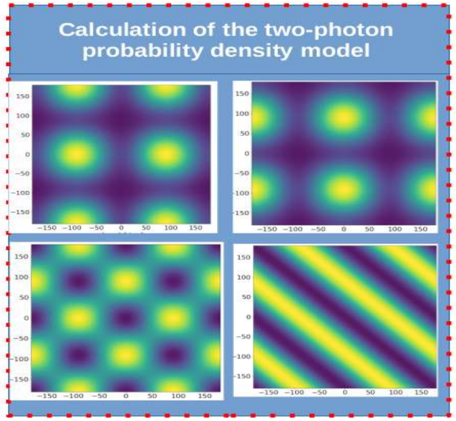
P. Moskal et al., article submitted (2024)

Two-photon correlations for PET applications

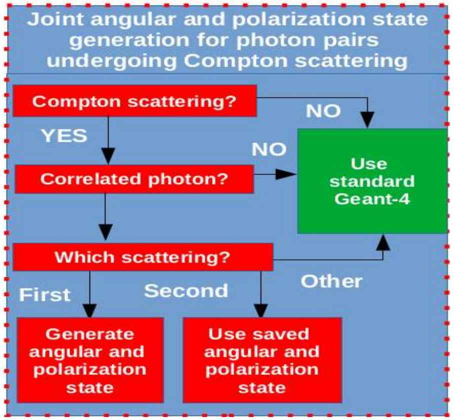
Input parameters



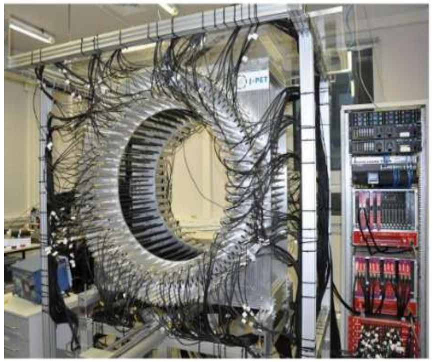
VW model

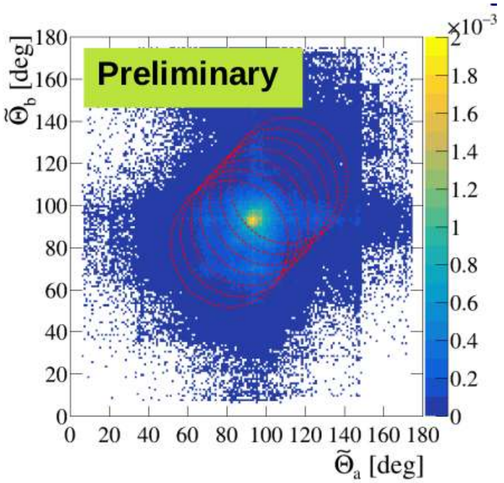


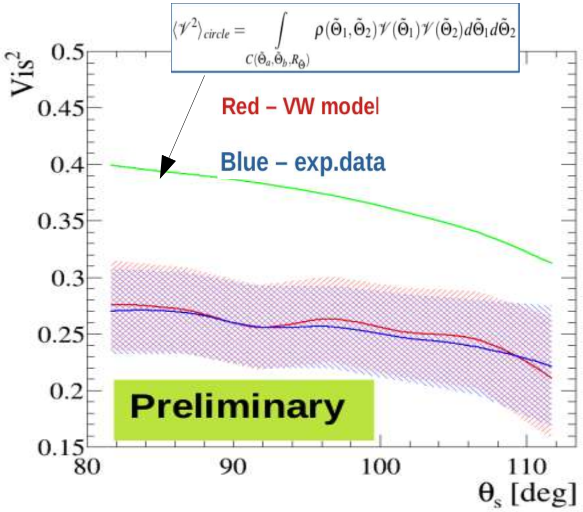
Geant4 simulations



Model validation with data taken by the J-PET scanner







New (multi)scattering formalism:
Hiesmayr, B.C., Krzemień, W. & Bała,M. Sci Rep 14, 9672 (2024)

Other activities

PET imaging toolbox

Aurélien Coussat,
Wojciech Krzemień

- Written in Python
- Currently under (private) development on GitHub
- Collection of tools (initially developed for J-PET) to:
  - Interact with CASToR datafiles
  - Interact with Interfile images
  - Apply some transformations on GATE output files
  - …

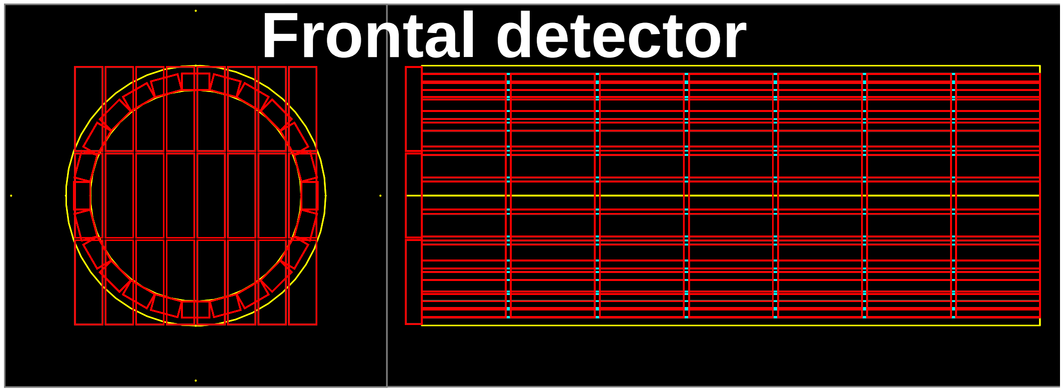
Example use case: Boostrap error estimates for the image quality metrics

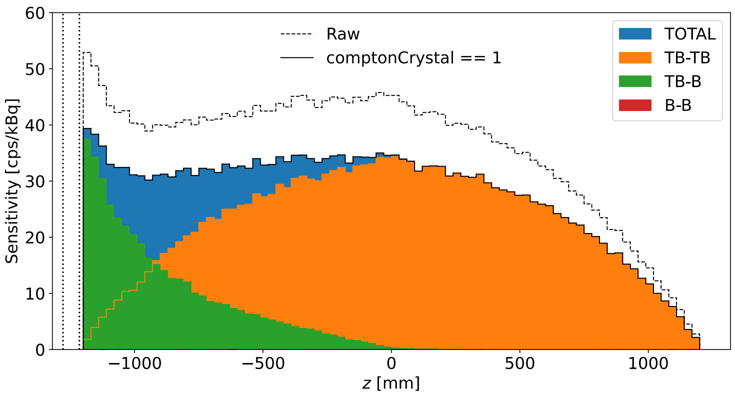
Example use case: MLP/KDE reconstruction of the PET images

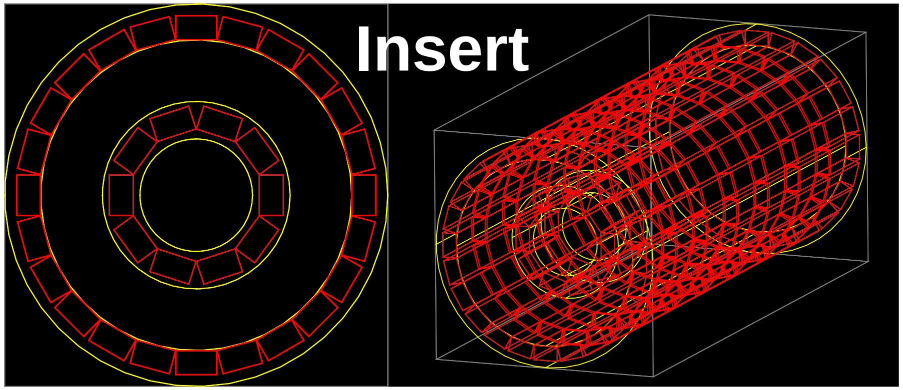
Martin Radler

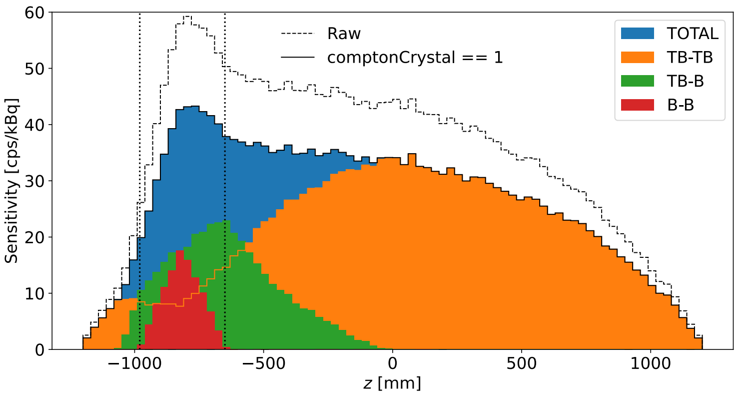
Simulation of multi-detector geometries

Combining the J-PET total body scanner with a second scanner intended for brain imaging





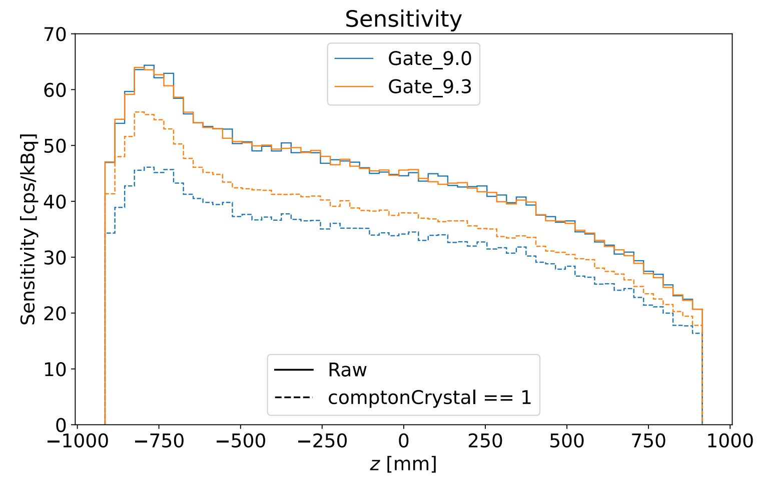




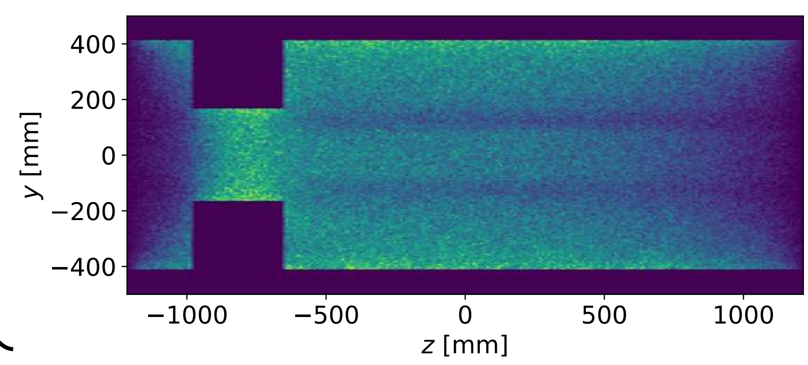
Martin Radler

Issues found in Gate 9.3

- Ambiguity due to hard coded coincidence sorter “Coincidences”
- Compton scatter counts in detector



- MinSectorDifference: Comparing rSectorID from different scanners



2nd International Workshop on Machine Learning and Quantum Computing Applications in Medicine and Physics

WMLQ2024

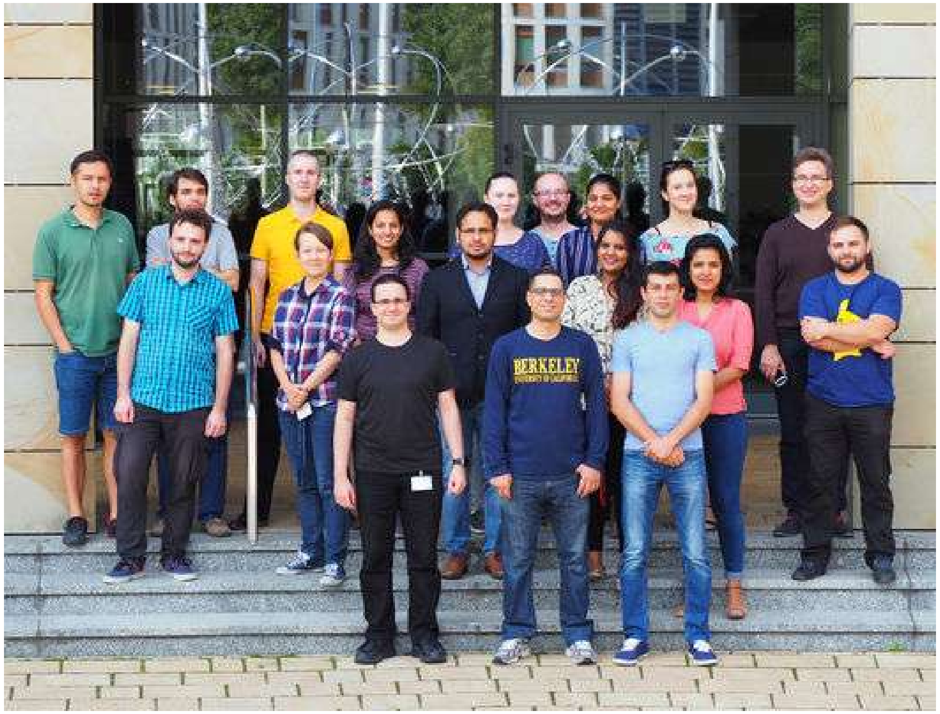
04 to 07 June 2024, Warsaw Poland

https://events.ncbj.gov.pl/event/314/

First edition:

https://events.ncbj.gov.pl/event/141/page/65-home

Thank you for attention

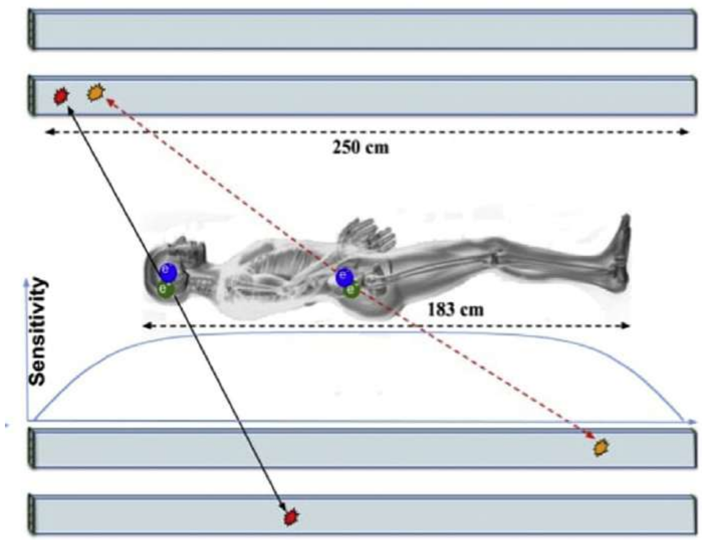


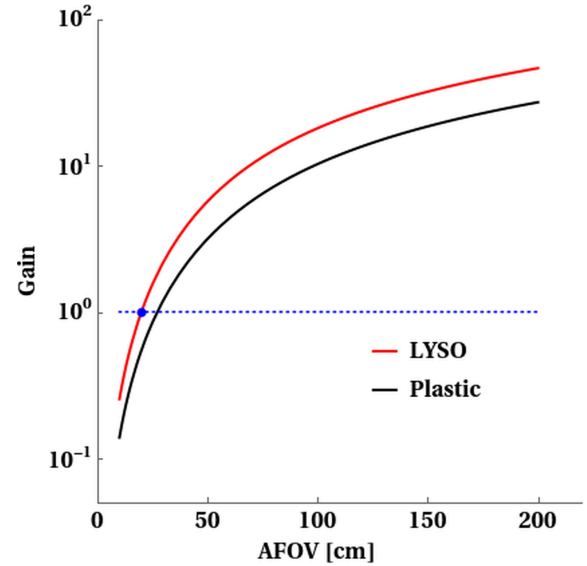
J-PET

More materials available at:

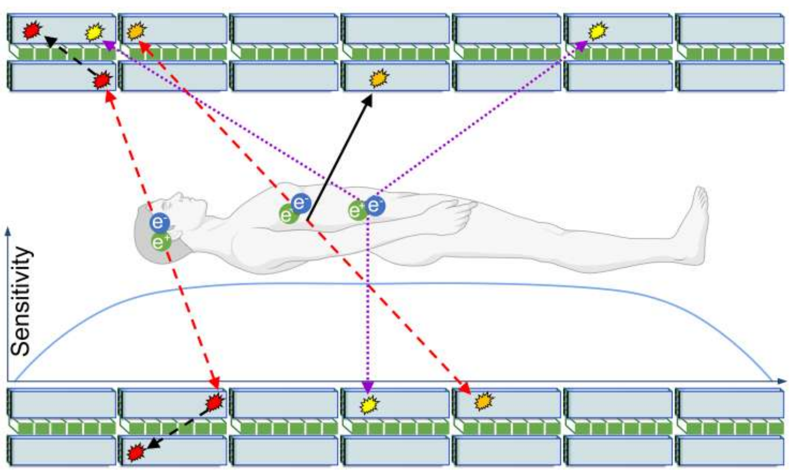
http://koza.if.uj.edu.pl/pet/

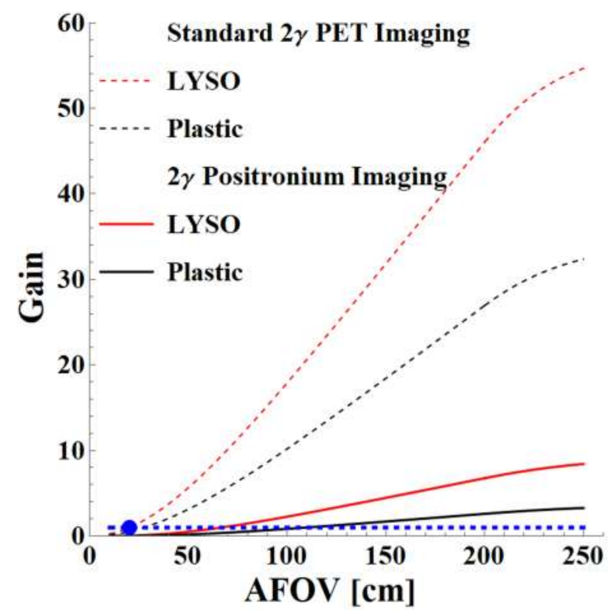
J. Nucl. Med. 60 (2019) 299–303.



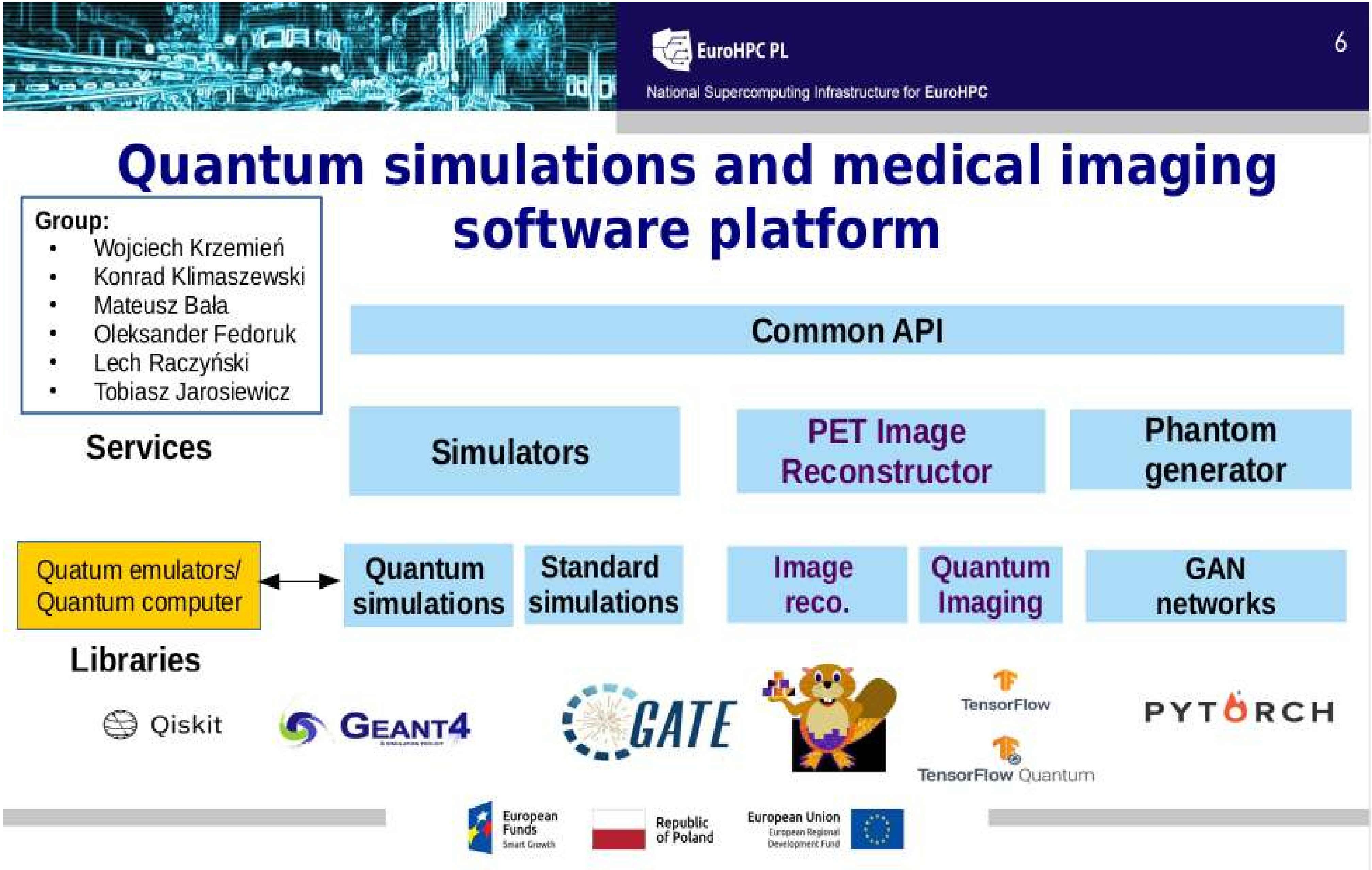


P. Moskal, E. Ł. Stępień,
PET Clinics 15 (2020) 439





Rev. Mod.Phys. (2023) S. Bass, S. Mariazzi, P. Moskal, E. Stępień


EuroHPC PL
National Supercomputing Infrastructure for EuroHPC
6
Quantum simulations and medical imaging software platform
Group:
Wojciech Krzemień
Konrad Klimaszewski
Mateusz Bała
Oleksander Fedoruk
Lech Raczyński
Tobiasz Jarosiewicz
Common API
Services
Simulators
PET Image Reconstructor
Phantom generator
Quatum emulators/ Quantum computer
Quantum simulations
Standard simulations
Image reco.
Quantum Imaging
GAN networks
Libraries
Qiskit
GEANT4
GATE
TensorFlow
TensorFlow Quantum
PYTORCH
European Funds Smart Growth
Republic of Poland
European Union European Regional Development Fund

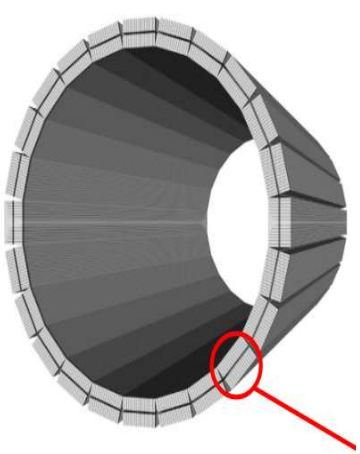
Software for total-body J-PET

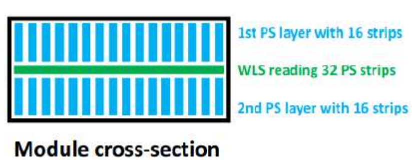
- scatter and random correction for total-body scanners **(see Szymon Parzych talk tomorrow)**
- Normalization corrections (**see A. Coussat's talk this afternoon**)
- point-spread functions
- system matrix parametrization
- Multi-photon + conventional PET reco. algorithms
- **Machine learning techniques for background reduction**
- Various software tools

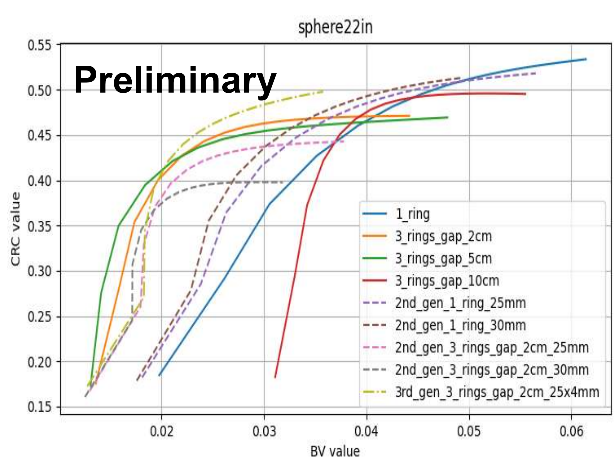
Coordinator: W. Krzemien

- Jakub Baran
- Lech Raczynski
- Szymon Parzych
- Mateusz Bała
- Paweł Kowalski
- Aurelien Coussat
- Damian Trybek

Extensive usage of GATE simulations





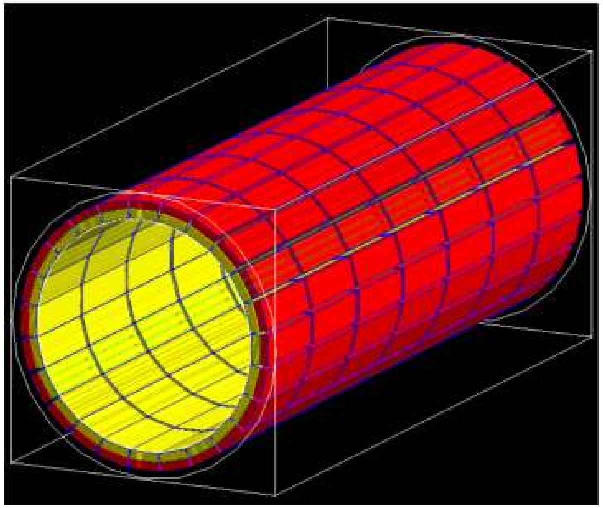


C++

Python

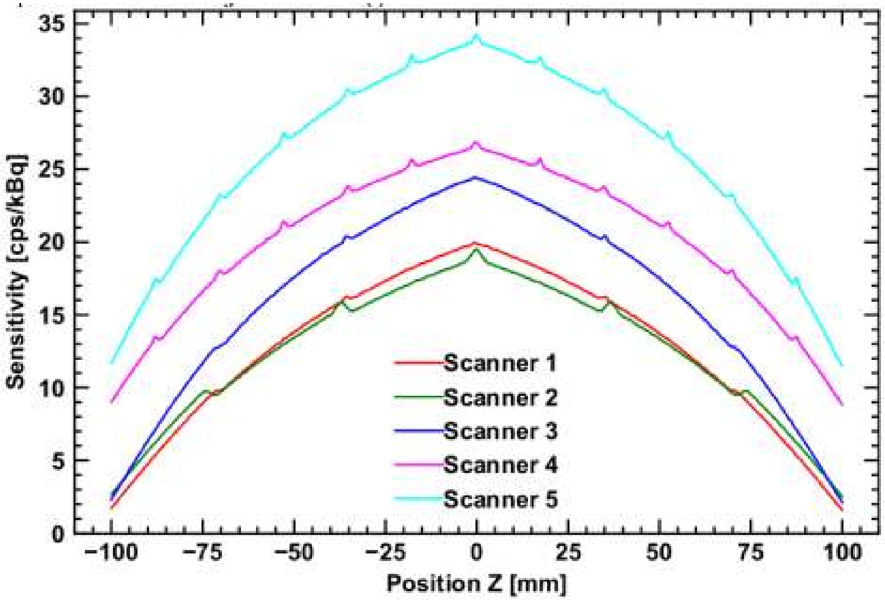
Jakub Baran & Wojciech Krzemień et al.

Total-Body J-PET Geometry Optimization

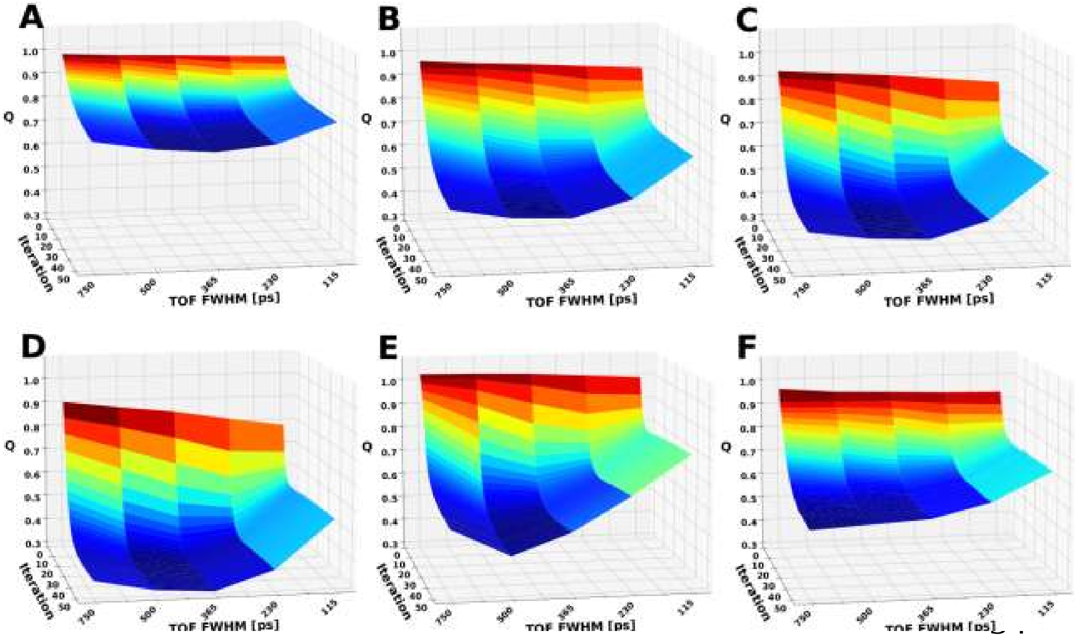


Property	Scanner geometry				
	S1	*S2*	*S3*	*S4*	*S5*
Radius [mm]	506	506	425	414.65	414.65
Axial FOV [mm]	2099.2	2159.2	2099.2	2430	2430
Scintillator length [mm]	686.4	686.4	686.4	330	330
Scintillator cross-section [mm]	25x5.7	25x5.7	25x5.7	25x6.0	30x6.0
No of adjacent rings	3	3	3	7	7
Gap between adjacent rings [mm]	20	50	20	20	20

preliminary Sensitivity

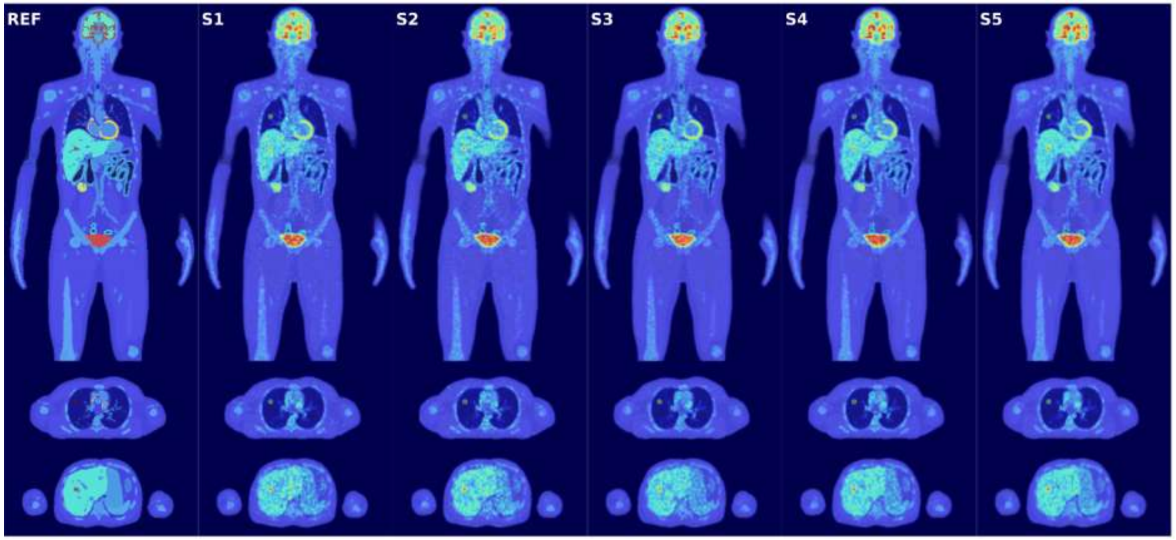


TOF kernel choice



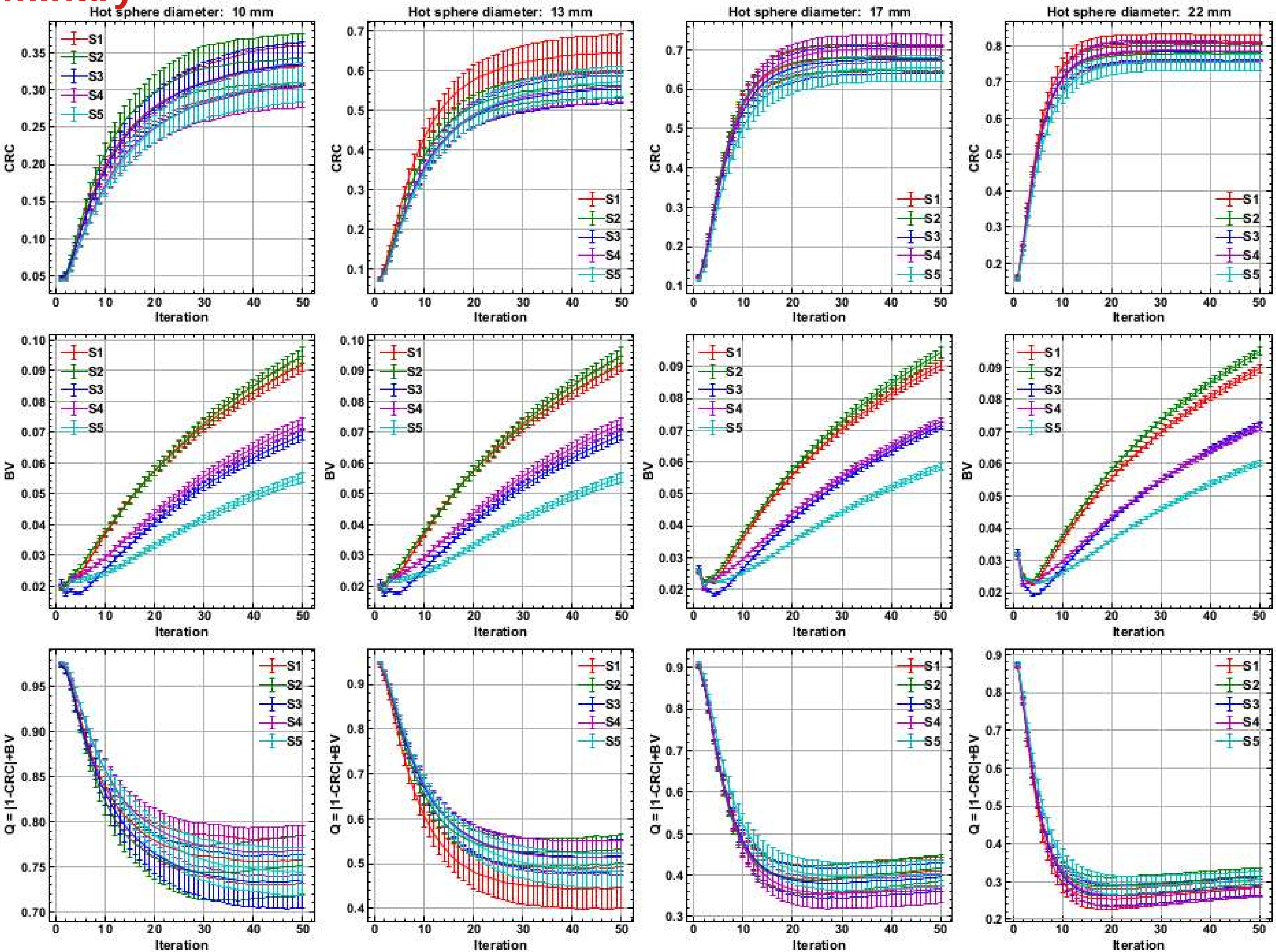
Total-Body J-PET Geometry Optimization – XCAT phantom

preliminary



Total-Body J-PET Geometry Optimization – XCAT phantom

preliminary

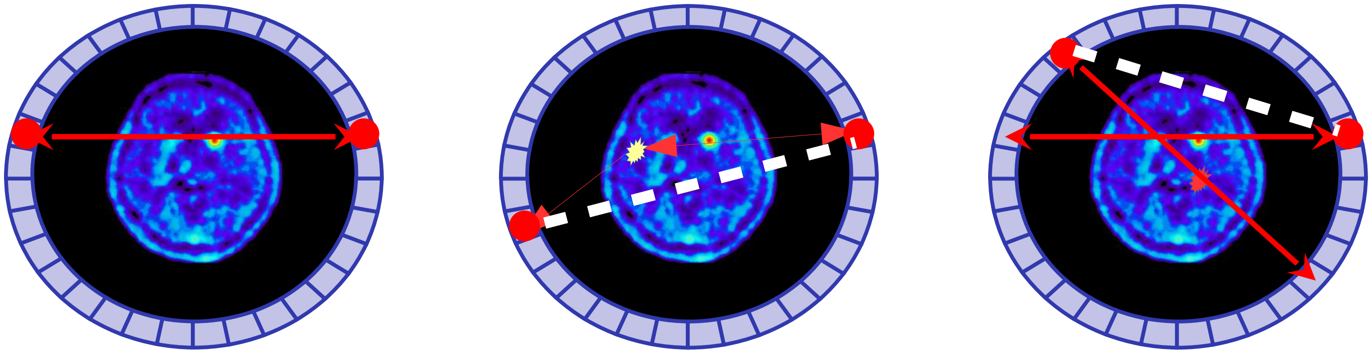


Coincidence classification for total-body J-PET

True events

Scattered events

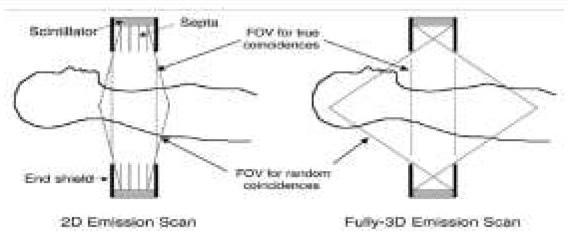
Random events



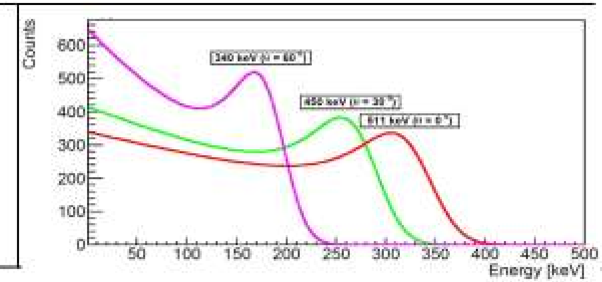
Coincidence classification for total-body J-PET

For total-body J-PET scanner we expect
higher background level from non-genuine coincidences

In J-PET



Multiple scattering in the phantom is not negligible

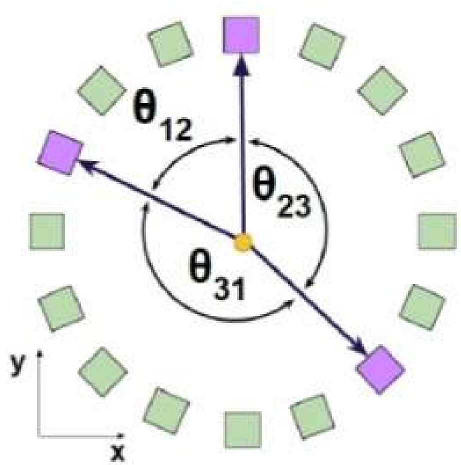


D. Brasse et al. J Nucl Med 2005; 46:859–867

Situation much more complicated for multi-photon coincidences...

- More photons ➡ More combinations
- Less strictly defined geometry
- Photon energies have a distribution

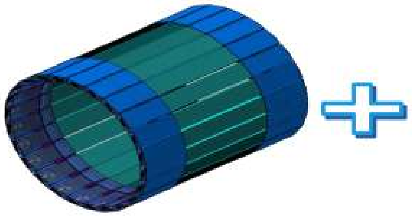
Idea: apply ML techniques to reduce background
(ACCIDENTAL, SCATTER)



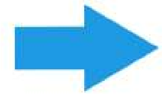
o-Ps → 3γ

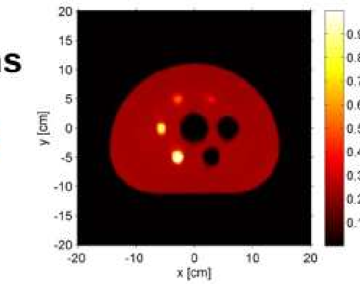
Wojciech Krzemień, Konrad Klimaszewski et al.

Training data generation



Monte Carlo Simulations





Modular J-PET

- 50 cm AFOV
- 24 modules x 13 strips
- 24 x 6 x 500 mm strips

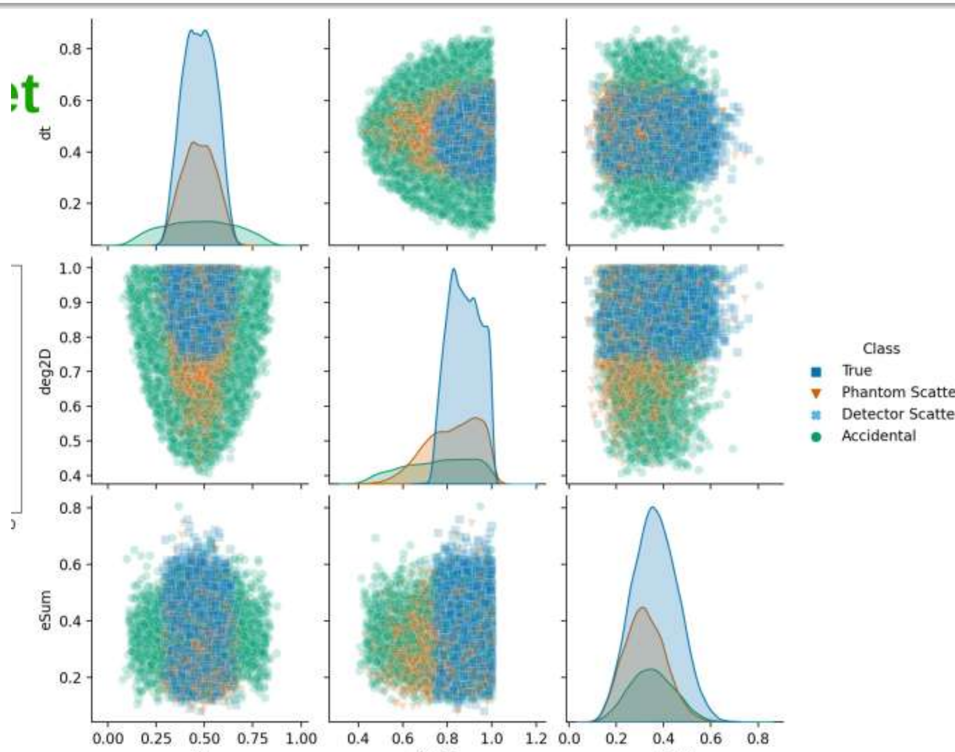
NEMA IEC Phantom

- 4 hot spheres
- 2 cold spheres
- Activity - 59 Mbq
- acquisition time - 500 seconds
- contrast between hot and cold regions – 4:1

GATE MC Simulation

- 30M coincidences
- Phenomenological time, energy and positional resolution
- Geometry cuts → reduce accidental fraction

21



Classificators

- **Feedforward Neural Network**

  Keras + SciKeras + scikit learn

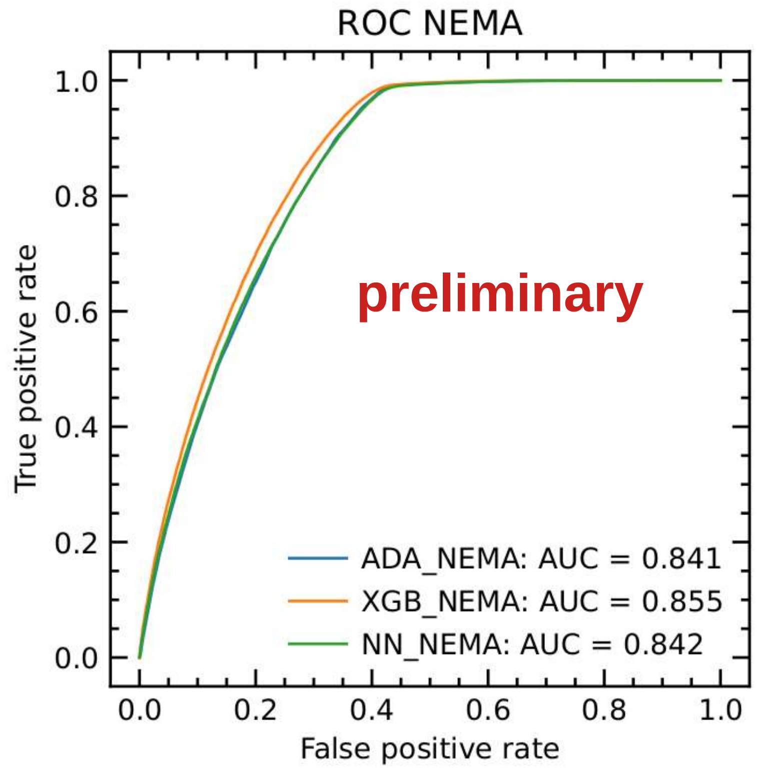
- **ADABoost**

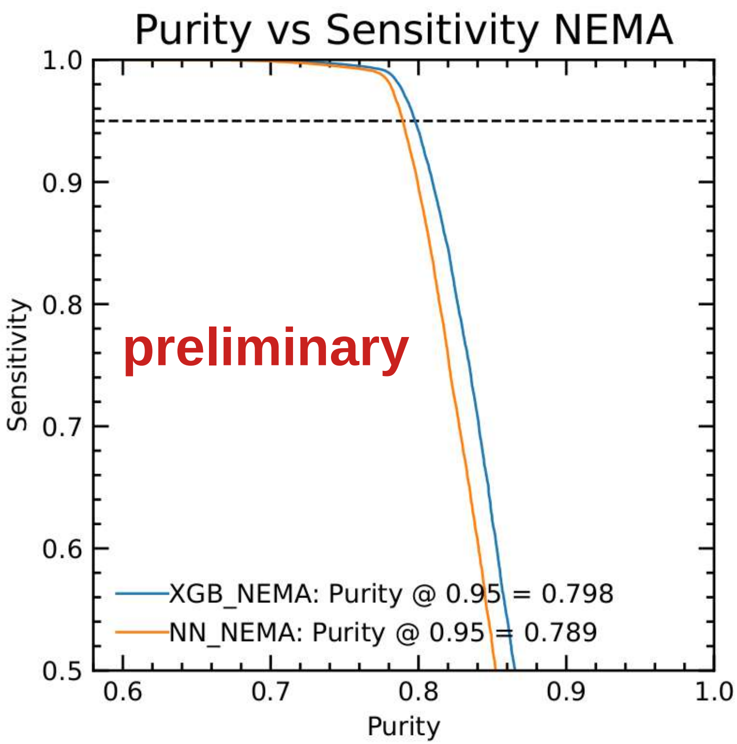
  scikit learn

- **XGBoost**

  dmlc XGBoost + scikit learn

Base line: 65%





Summary 2

- Two applications of ML to data filtering in (J-PET) tomography:
  - reduction of the scatter/random fractions in two-photon case
  - No visible bias observed in reconstructed images

  - First trial to apply ML to multiphoton case
  - S/B ~10x improvement
  - First positronium lifetime spectra obtained

First in the world orthpositronium image of the object

IOP Publishing Phys. Med. Biol. 64 (2019) 055017 (14pp) https://doi.org/10.1088/1361-6560/aafe20

Physics in Medicine & Biology

IPEM Institute of Physics and Engineering in Medicine

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PAPER

Feasibility study of the positronium imaging with the J-PET tomograph

P Moskal[1], D Kisielewska[1], C Curceanu[2], E Czerwiński[1], K Dulski[1], A Gajos[1], M Gorgol[3], B Hiesmayr[4], B Jasińska[3], K Kacprzak[1], Ł Kapłon[1], G Korcyl[1], P Kowalski[5], W Krzemień[6], T Kozik[1], E Kubicz[1], M Mohammed[1,7], Sz Niedźwiecki[1], M Pałka[1], M Pawlik-Niedźwiecka[1], L Raczyński[5], J Raj[1], S Sharma[1], Shivani[1], R Y Shopa[5], M Silarski[1], M Skurzok[1], E Stępień[1], W Wiślicki[5] and B Zgardzińska[3]

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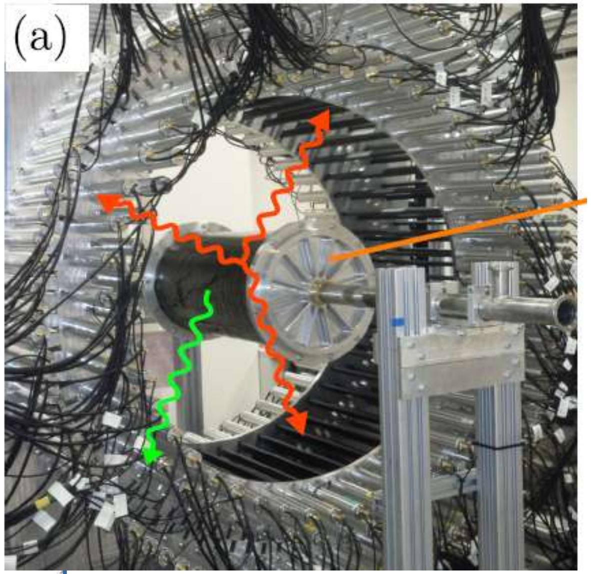
Keywords: positron emission tomography, positronium atom, J-PET

Abstract

A detection system of the conventional PET tomograph is set-up to record data from e^+e^- annihilation into two photons with energy of 511 keV, and it gives information on the density distribution of a radiopharmaceutical in the body of the object. In this paper we explore the possibility of performing the three gamma photons imaging based on ortho-positronium



Article | Open Access | Published: 27 September 2021

Testing CPT symmetry in ortho-positronium decays with positronium annihilation tomography

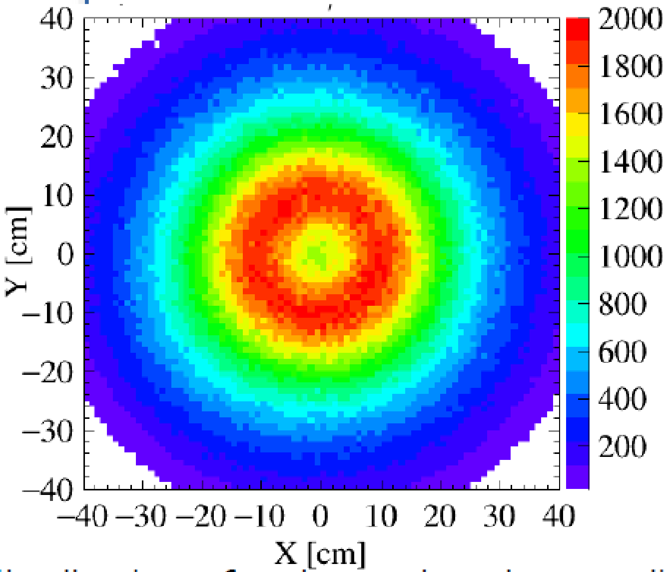
P. Moskal, A. Gajos, [...] W. Wiślicki

Nature Communications 12, Article number: 5658 (2021) | Cite this article

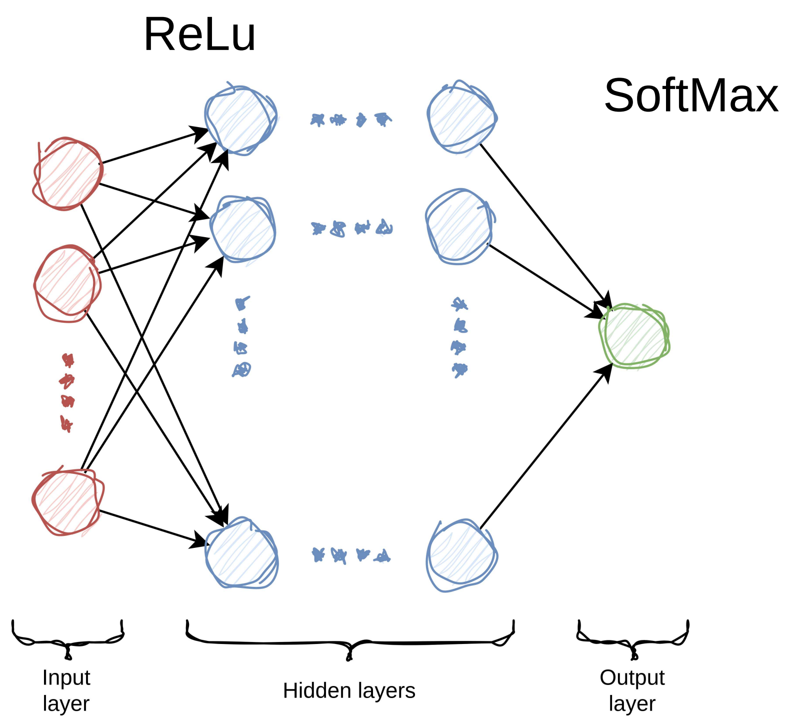
Aleksander Gajos

Abstract

Charged lepton system symmetry under combined charge, parity, and time-reversal transformation (CPT) remains scarcely tested. Despite stringent quantum-electrodynamic limits, discrepancies in predictions for the electron–positron bound state (positronium atom) motivate further investigation, including fundamental symmetry tests. While CPT noninvariance effects could be manifested in non-vanishing angular correlations between final-state photons and spin of annihilating positronium, measurements were previously limited by knowledge of the latter. Here, we demonstrate tomographic reconstruction techniques applied to three-photon annihilations of ortho-positronium atoms to estimate their spin polarisation without magnetic field or polarised positronium source. We use a plastic-scintillator-based positron-emission-tomography scanner to record ortho-



Feedforward Neural Network



- Optimizer: Adam
- Loss: Customized loss function
- Size and number of hidden layers optimized using Cross Validation
- Optimization:Tree-Structure Parzen Estimation
- Input data normalized to (0, 1) range

Training/Validation/Test : 70%/15%/15%

Considered Features

Maximum feature space dimensions 46

- Deposited energies
- spatial hit coordinates
- registration time
- relative distance between hits
- relative time between hits
- total energy sum
- total energy of the annihilation photon candidates
- opening angles between photons after the preliminary vertex reconstruction
- interdetector scatter metric

Aurélien
Coussat

New CASToR toolkits

- `castor-norm`
- Compute direct normalization factors

```
castor-norm \
    -df normalization_scan.Cdh \
    -img normalization_phantom.img \
    -sc Scanner \
    -fout output
```

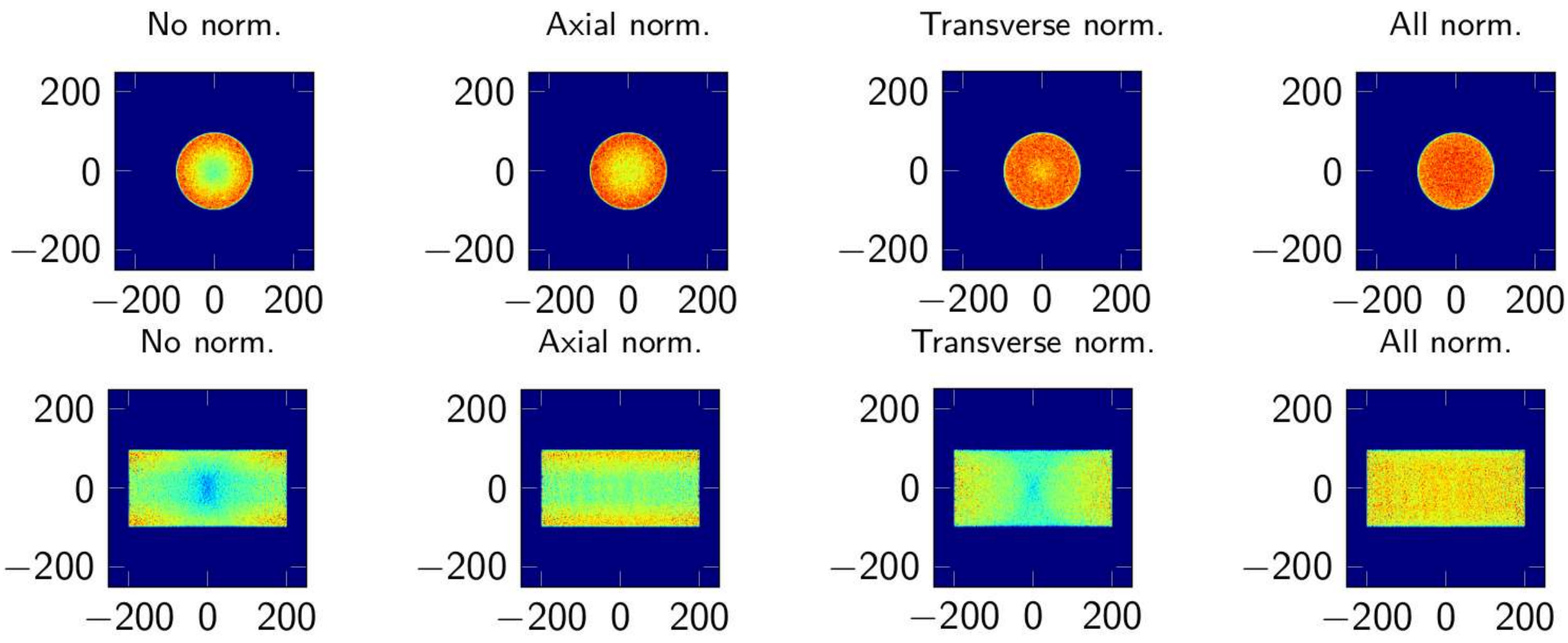
- `castor-datafileMerger`
- Merge several datafiles into one

```
castor-datafileMerger \
    -df input.Cdh \
    -norm with_normalization.Cdh \
    -fout output
```

Aurélien
Coussat

Component-based normalization

- We developed a collection of scripts that compute, from GATE output, component-based normalization factors



Aurélien
Coussat

Decrease efficiency of GATE dataset

- We developed a tool to decrease the efficiency of a GATE dataset, post-simulation, to assess efficiency normalization