



EuroHPC PL

National Supercomputing Infrastructure for EuroHPC

Quantum simulation and medical imaging platform for PET scanners

Wojciech Krzemień

07.12 2023



NATIONAL CENTRE
FOR NUCLEAR RESEARCH
SWIERK



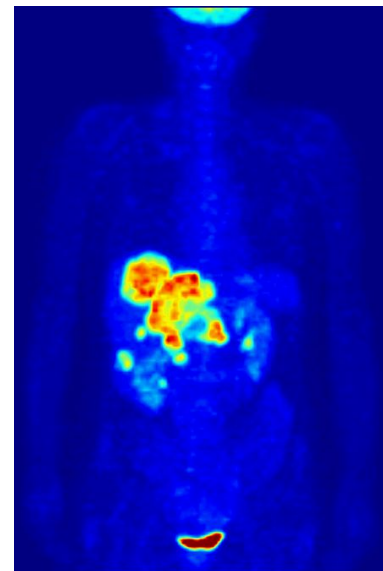
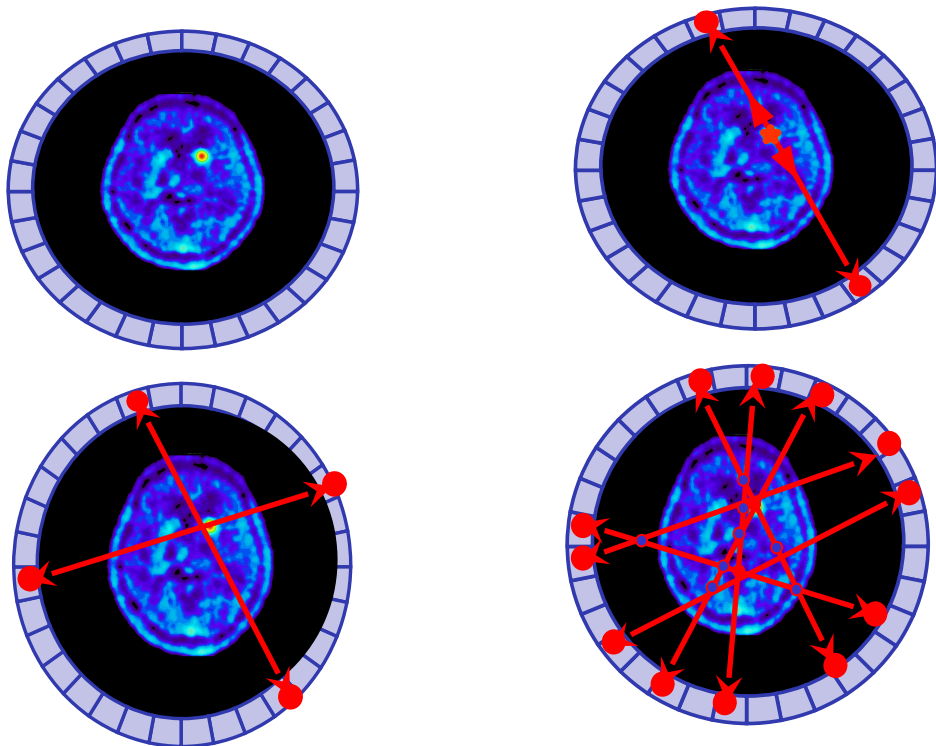
Swierk Computing Centre



- One of the largest research institutes in Poland (1195 employees, incl. 80 prof., 170 PhD, PhD studies: 45 students)
- Scientific achievements: ~ 500 reviewed papers, ~16000 per year (5th/4th position in Poland)
- EU project: success rate ~30 %
- Budget/year : 70M euro
- 124 different projects
- Collaboration with the largest laboratories in the world (CERN, DESY, JPark, FAIR, Julich, ESS, T2K) and many universities
- Maria Reactor



Positron Emission Tomography (PET)



Author: Jens Maus (<http://jens-maus.de/>)
-Own work, Public Domain,



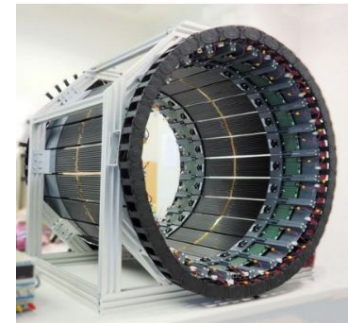
uExplorer



Biograph-Vision Quadra

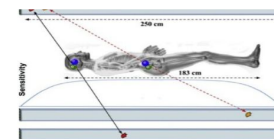


Modular J-PET



Total-body J-PET

- P. Moskal et al. *PET Clinics* 15 (2020) 439
- P. Moskal et al. *Phys. Med. Biol.* 66 (2021) 175015
- J. Baran et al. <http://arxiv.org/abs/2212.02285>



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



<https://www.siemens-healthineers.com/en-us/molecular-imaging/pet-ct/biograph-vision-quadra>

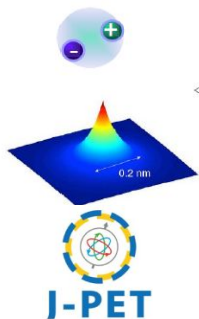
R. Badawi et al.
J Nucl Med. 2019 Mar; 60(3): 299–303.





New techniques and imaging algorithms (multi-photon imaging, quantum imaging, quantum correlations)

Positronium tomography



P. Moskal et al. Nature Reviews Physics 1 (2019) 527

P. Moskal et al. Phys. Med. Biol. 64 (2019) 055017

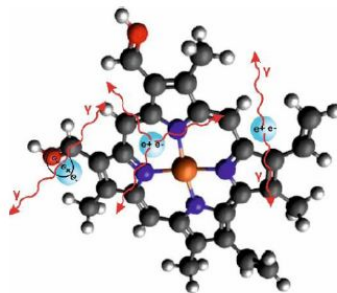
P. Moskal et al. EJNMMI Phys. 7 (2020) 44

P. Moskal et al. Science Advances 7 (2021) eabh4394

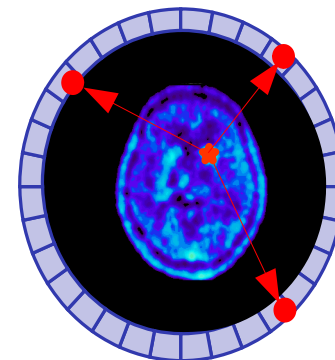
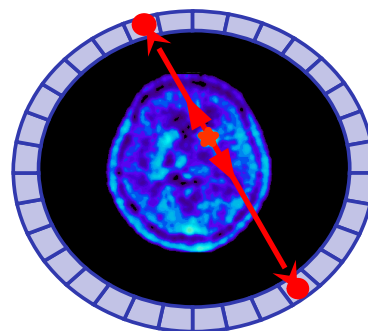
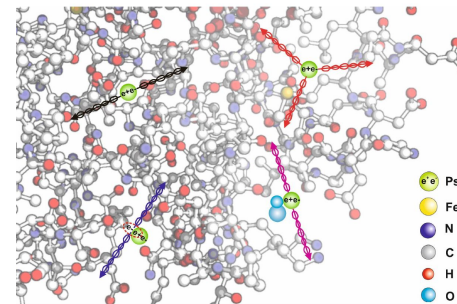
P. Moskal et al. Nature Communications 12 (2021) 5658

S. Bass et al. Rev. Mod. Phys. 95 (2023) 021002

<http://koza.if.uj.edu.pl/publications/pet>



Model of the hemoglobin molecule





Group:

- Wojciech Krzemień
- Konrad Klimaszewski
- Mateusz Bała
- Oleksander Fedoruk
- Lech Raczyński
- Aldona Spirzewska
- Damian Trybek
- Dawid Meleszczuk

Quantum simulations and medical imaging software platform

Common API

Services

Simulators

PET Image Reconstructor

Phantom generator

Quantum emulators/
Quantum computer

Quantum
simulations

Standard
simulations

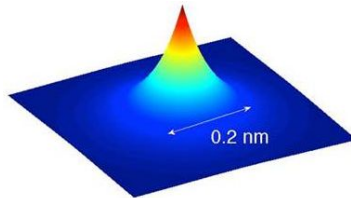
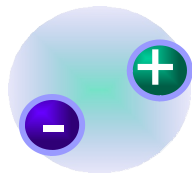
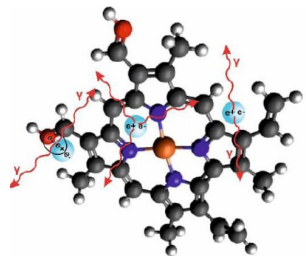
Image
reco.

Quantum
Imaging

GAN
networks

Libraries





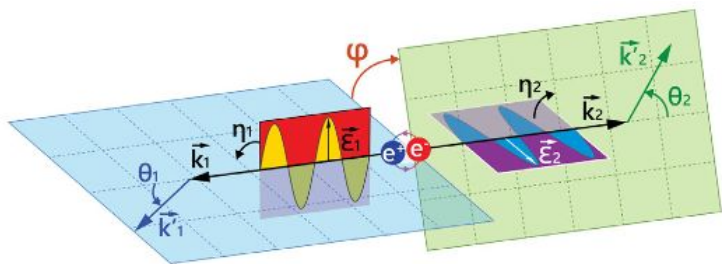
Scientific support:
Prof. B. Hiesmayr, leader of QPW,
University of Vienna

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

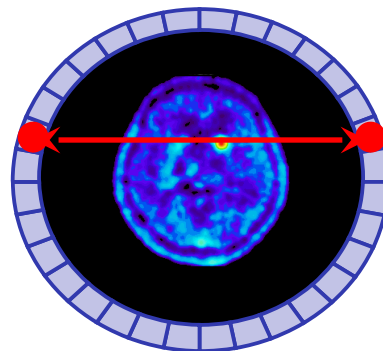
B. C. Hiesmayr, P. Moskal Sci. Rep. 9 (2019) 8166

Physical process simulations (including **quantum** effects) with potential use for the PET tomography applications

Two-photon quantum correlations



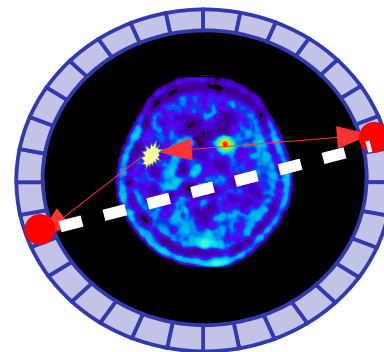
S. Bass et al. Rev. Mod. Phys. 95 (2023) 021002



True events

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

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



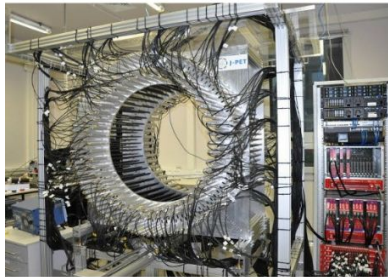
(Noisy) scattered events



Quantum MC simulator

- Geant4 based model with quantum correlations
- Simulations incorporate into platform
- Visualization tools provided as Jupyter-notebooks

Model validation with data taken by the J-PET scanner



Great agreement with data

Input parameters

Define arbitrary two-photon quantum state

OR

Choose one of the predefined states

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|HH\rangle + |VV\rangle)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|RL\rangle + |LR\rangle)$$

$$|\psi_3\rangle = \frac{1}{\sqrt{2}}(|+45^\circ - 45^\circ\rangle + |-45^\circ + 45^\circ\rangle)$$

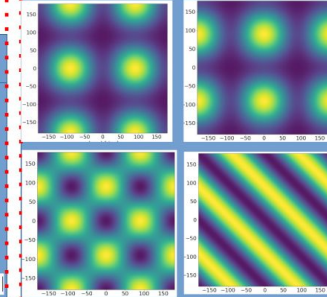
$$|\psi^+\rangle = \frac{1}{\sqrt{2}}(|HV\rangle + |VH\rangle)$$

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}(|HV\rangle - |VH\rangle)$$

$$\rho_{mixed} = \frac{1}{2}(|HV\rangle\langle HV| + \frac{1}{2}|VH\rangle\langle VH|)$$

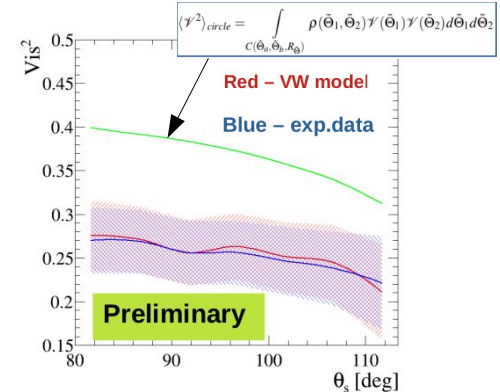
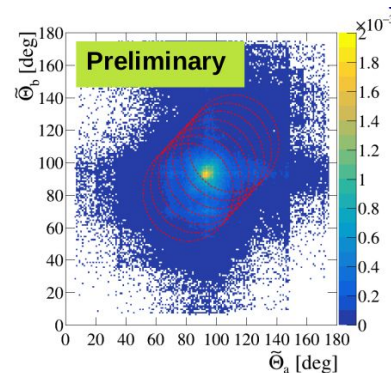
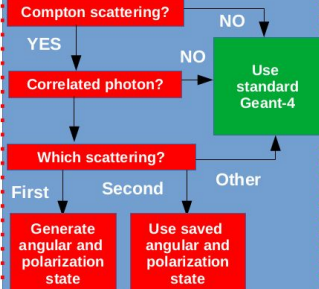
VW model

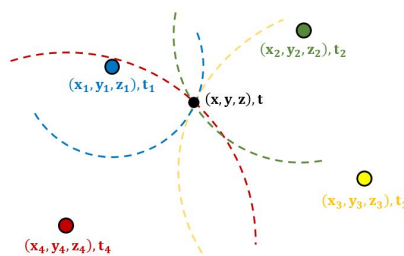
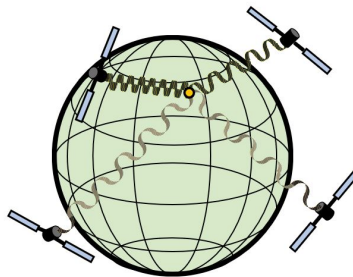
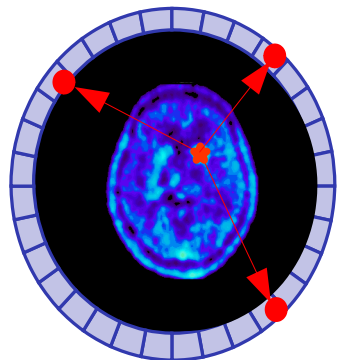
Calculation of the two-photon probability density model



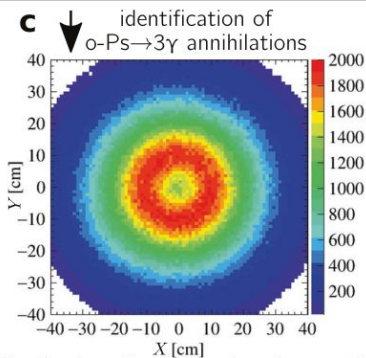
Geant4 simulations

Joint angular and polarization state generation for photon pairs undergoing Compton scattering





A. Gajos et al., NIM A 819 (2016) 54-59

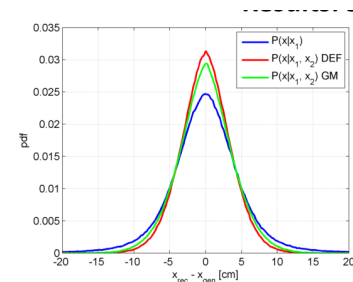
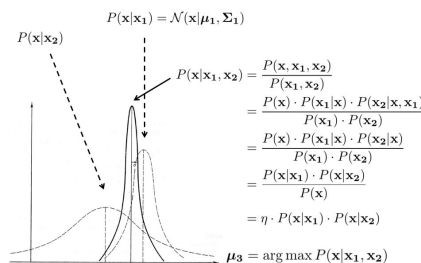


Nature Communications 12 (2021) 5658

Problem → resolution (σ) of about 8 cm

Trilateration “on steroid”

- Set of tools for fast prototyping and algo. comparison
- Three enhanced algorithm implementations
- Jupyter notebook visualizations



**Preliminary results:
resolution improvement at least 2x**



Challenge:

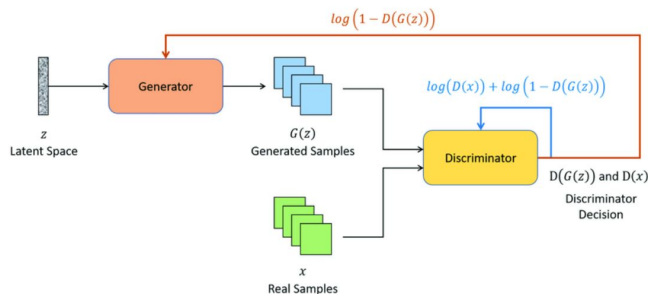
- Small accessibility of the large medical image sets for AI applications e.g. training of deep learning models
- Medical images → sensitive data, privacy issues, limited access due to number of operating facilities

Scientific support:
Dr hab Michał Kruk, SGGW

Proposed solution:

- **Service for generation** of medical pseudo-images using **GAN network models**
- Set of tools in form of the Jupyter notebook scripts that can be run in the batch or interactive mode

Generative Adversarial Networks (GANs)



<https://github.com/junyanz/CycleGAN>

<https://arxiv.org/abs/1406.2661>,

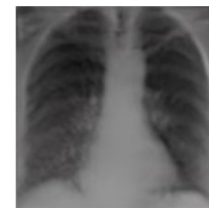
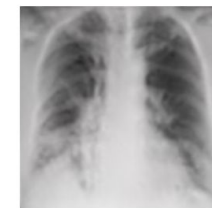
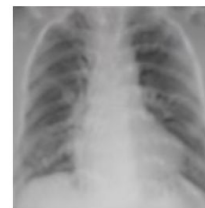
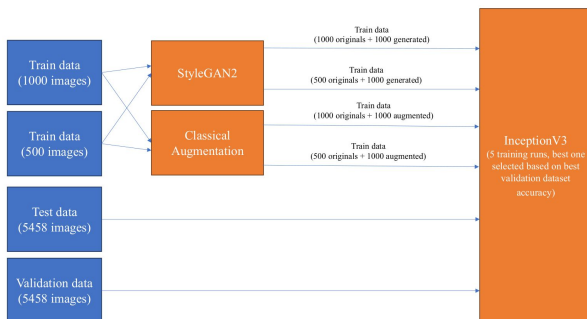
Ian J. Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, Yoshua Bengio



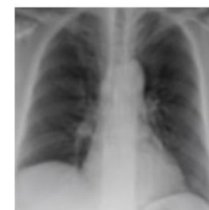
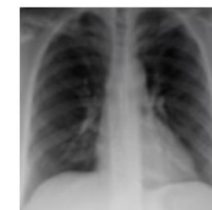


- GAN model trained on COVID-19 dataset:
 - ~3600 Covid-19 images
 - ~10000 healthy images
 - ~6000 lung opacity
 - ~1300 viral pneumonia
- Freschet Inception Distance metric

<https://www.kaggle.com/datasets/tawsifurrahman/covid19-radiography-database>



GAN trained on 1000 images



GAN trained on 500 images

O. Fedoruk et al, accepted for publication "Additional Look into GAN-based Augmentation for Deep Learning COVID-19 Image Classification".

Performance of GAN-based augmentation for deep learning COVID-19 image classification (2023), <https://arxiv.org/abs/2304.09067>

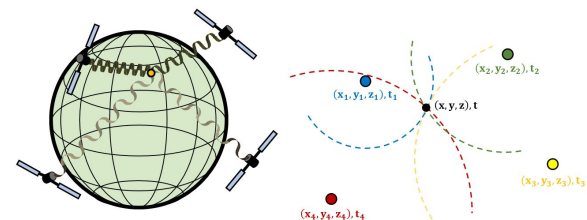
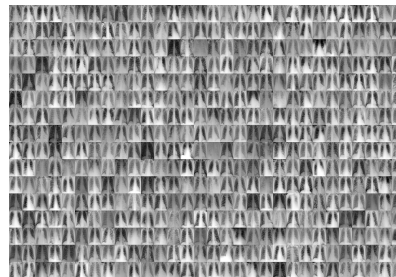
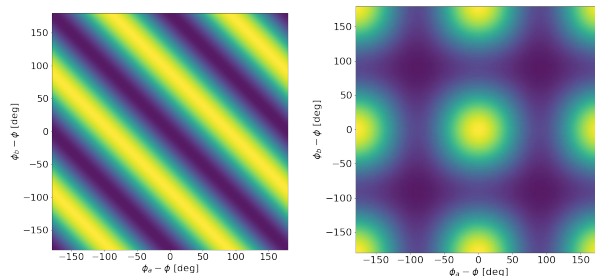
Oleksandr Fedoruk, Konrad Klimaszewski, Aleksander Ogonowski, Rafał Możdżonek





Summary:

- Set of tools and services for scientific community implemented as a platform
- Three main functionalities:
 - **Simulators** → Geant4 Monte Carlo models with quantum correlation included
 - **Phantom generators** → GAN- based service for generation of pseudo medical images for AI support
 - **Image reconstructors** → tools for fast prototyping of multi-photon algorithms





Thank you!

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>