Computing performance: bio-medical applications

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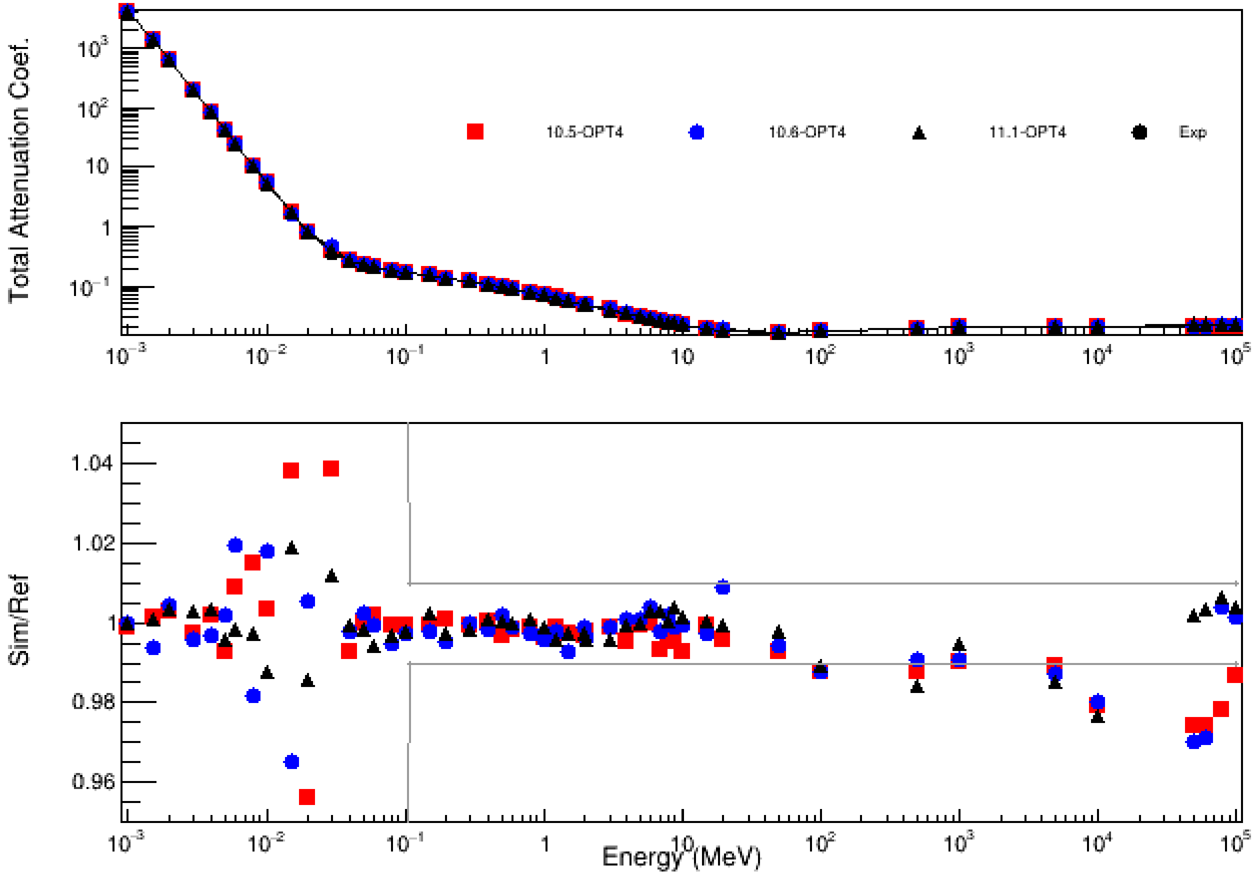
Computing performance benchmarking

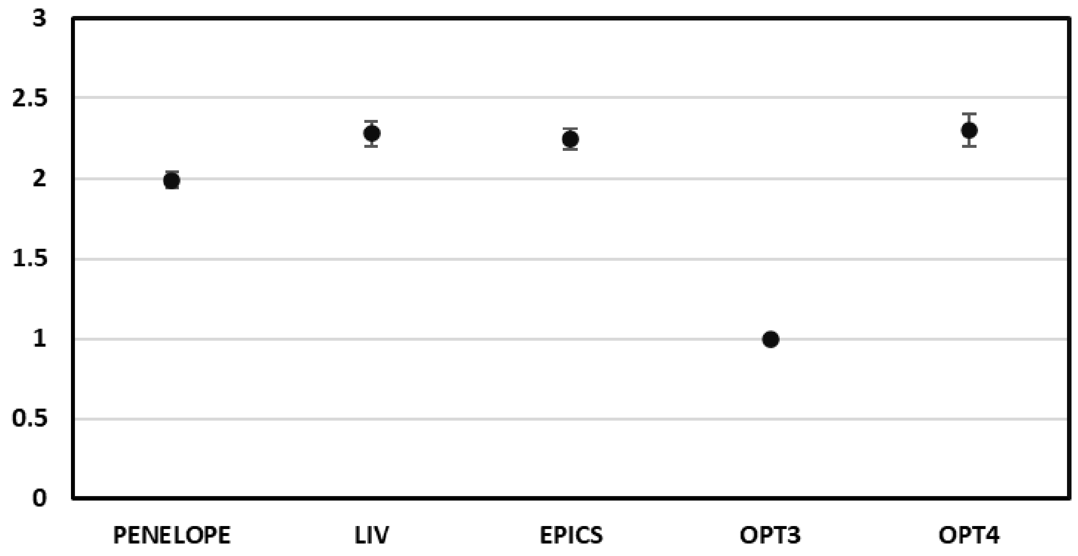
- We are currently performing some tests within the G4-Med project
  - Please see talk S. Guatelli, The G4-Med project: status update, in Plenary 7, Wednesday the 27th Sept, 16:30
- Few cases selected for each test
- Benchmark all the tested physics lists
- Execution in sequential mode, on a dedicated local cluster at the University of Wollongong
- Relate the execution times to a physics list used as a reference
  - EMStandardPhysics option 3
  - G4-DNA physics list option 2
- Done with Geant4 11.1

Total attenuation coeff. test in water

G4 EM Physics list OPT4



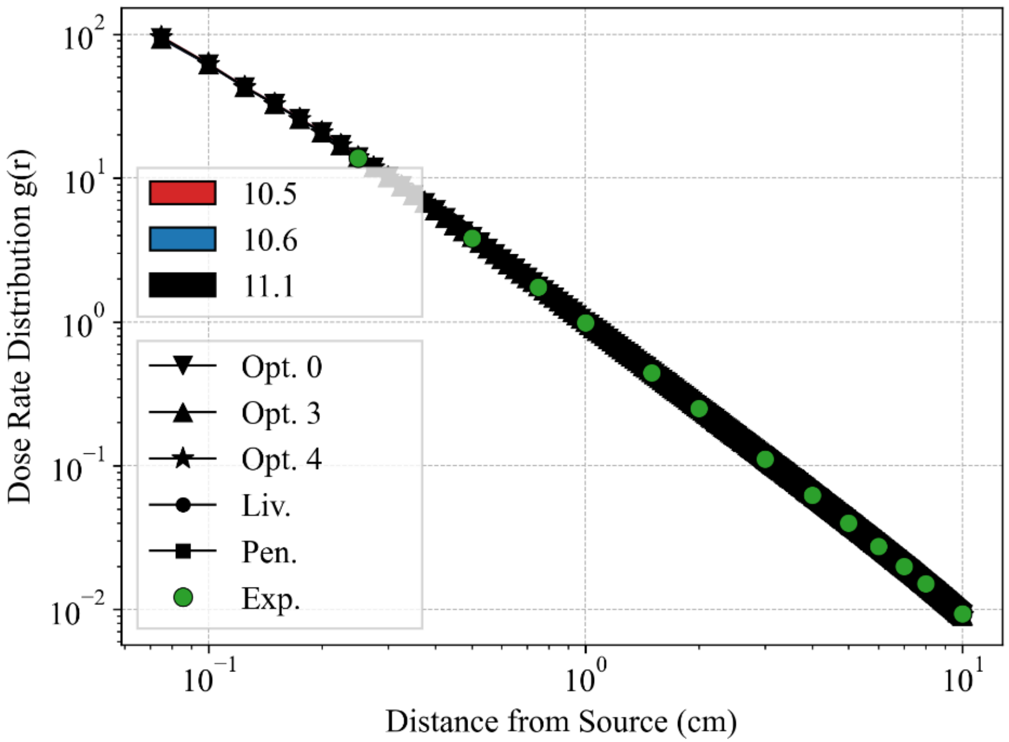
Computing performance test

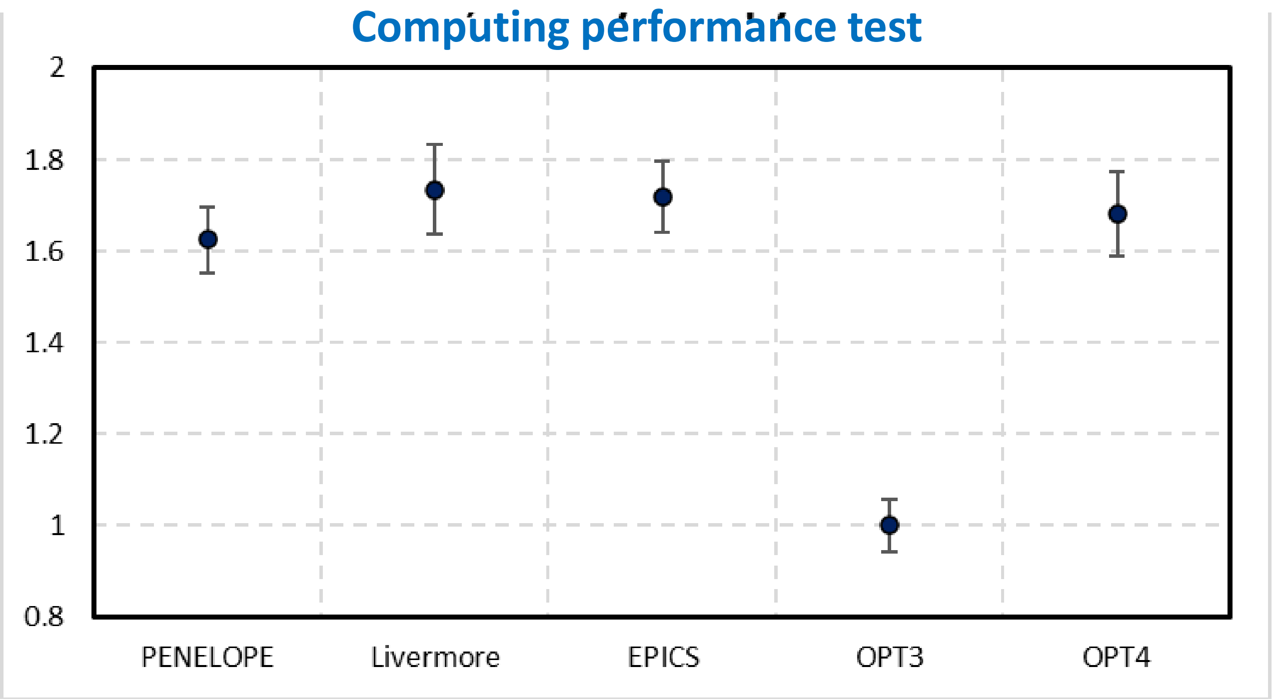


Brachytherapy test

- Calculate dose in water by a Flexisource Ir-192 (Med. Phys 33(12), 2006, 4578-4582)

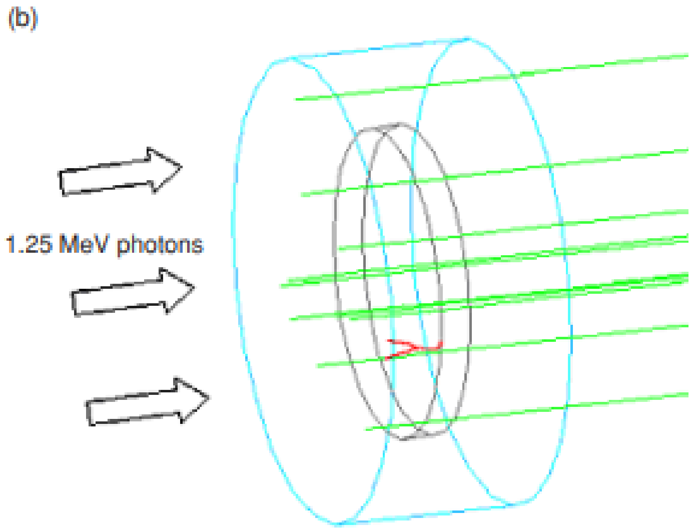
Flexisource Ir-192

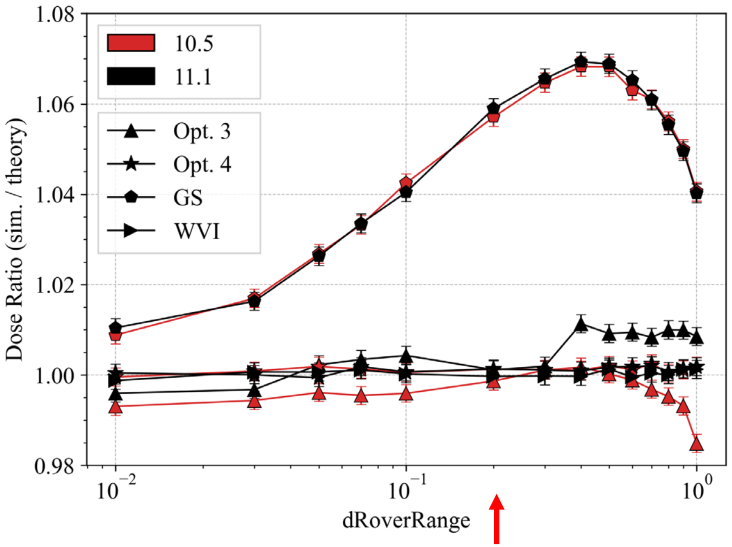




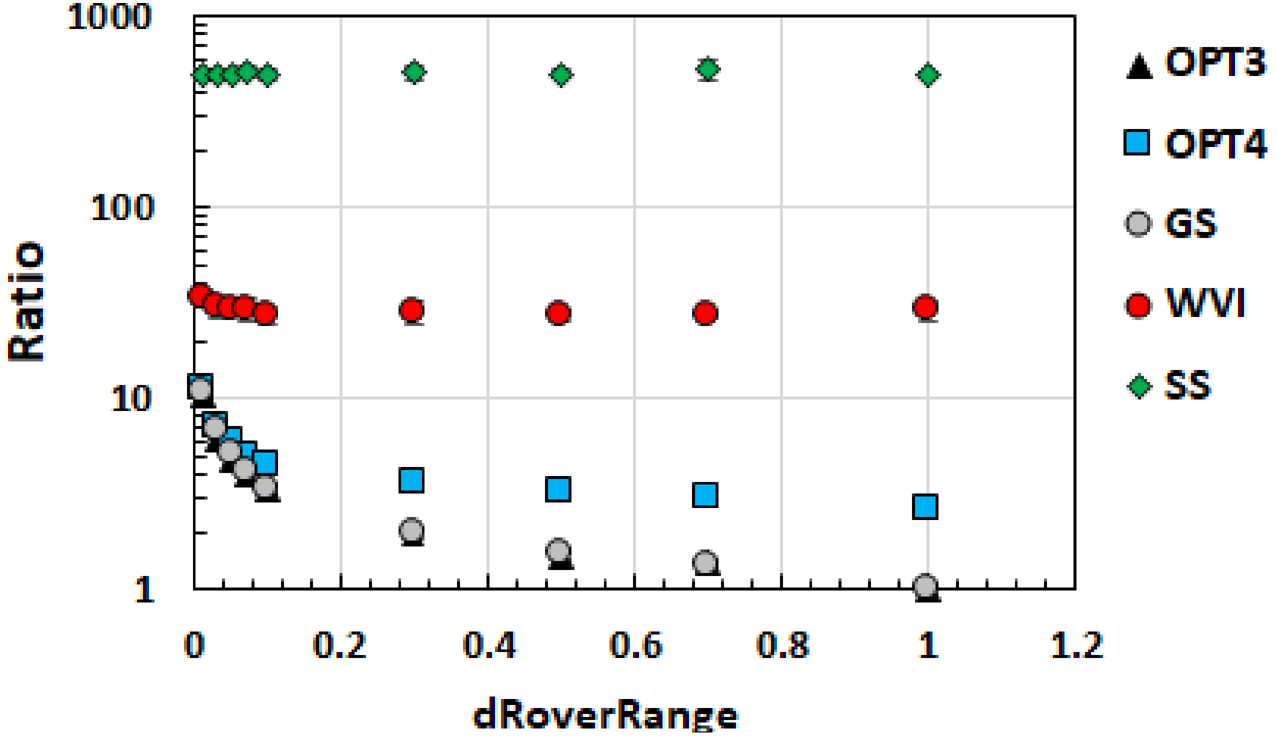
Fano Cavity test

Check that the ratio of the dose deposited in the cavity divided by the beam energy fluence is equal to the mass energy transfer coefficient of the wall material



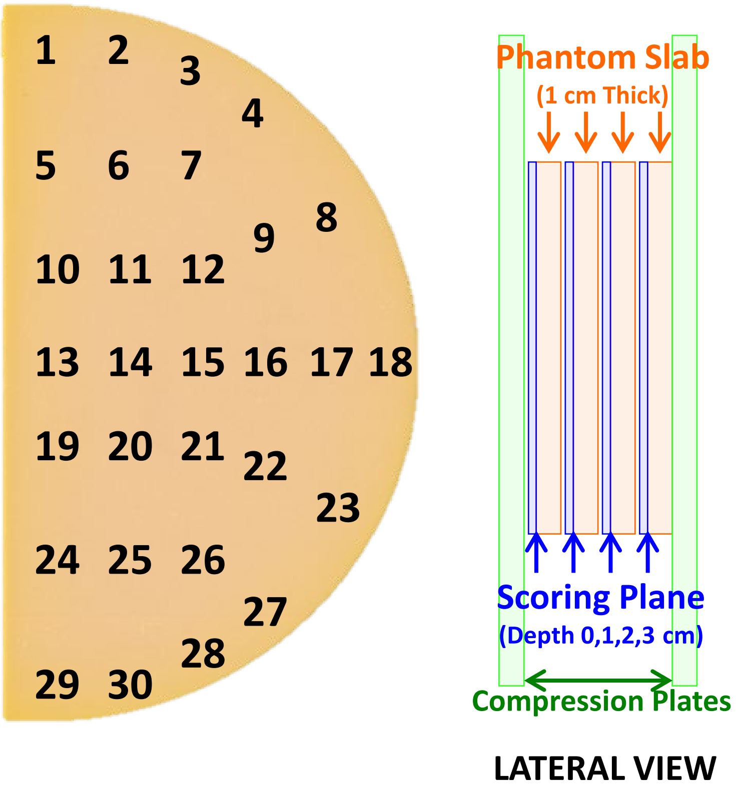


Computing performance test

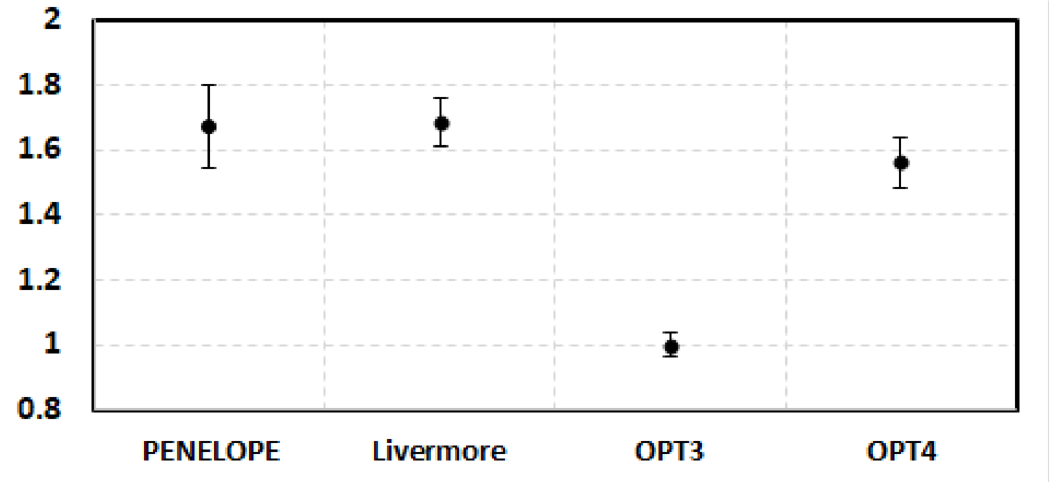


`WVI` is about 30 times and `SS` about 500 times slower than `G4EMStandardPhysics_option3`

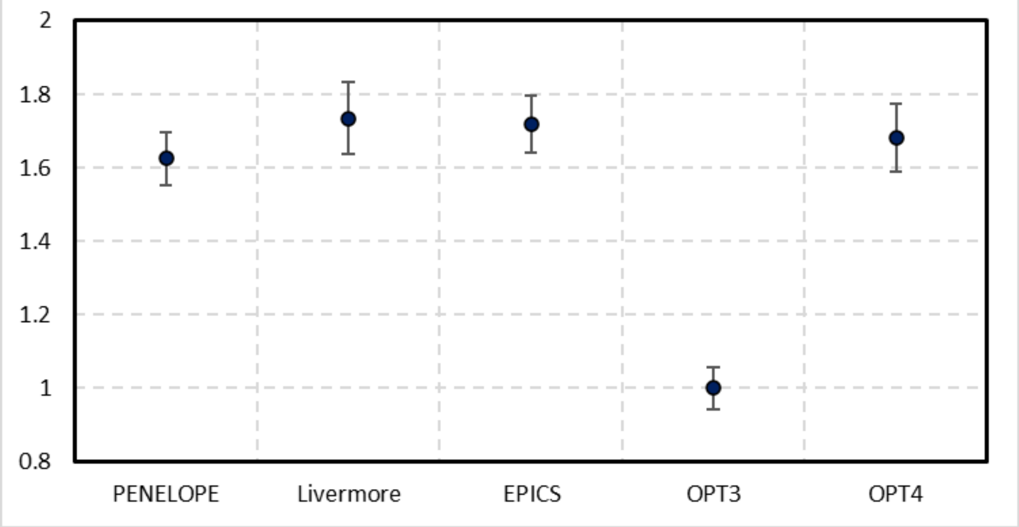
Mammography test



Computing performance test - Mammography



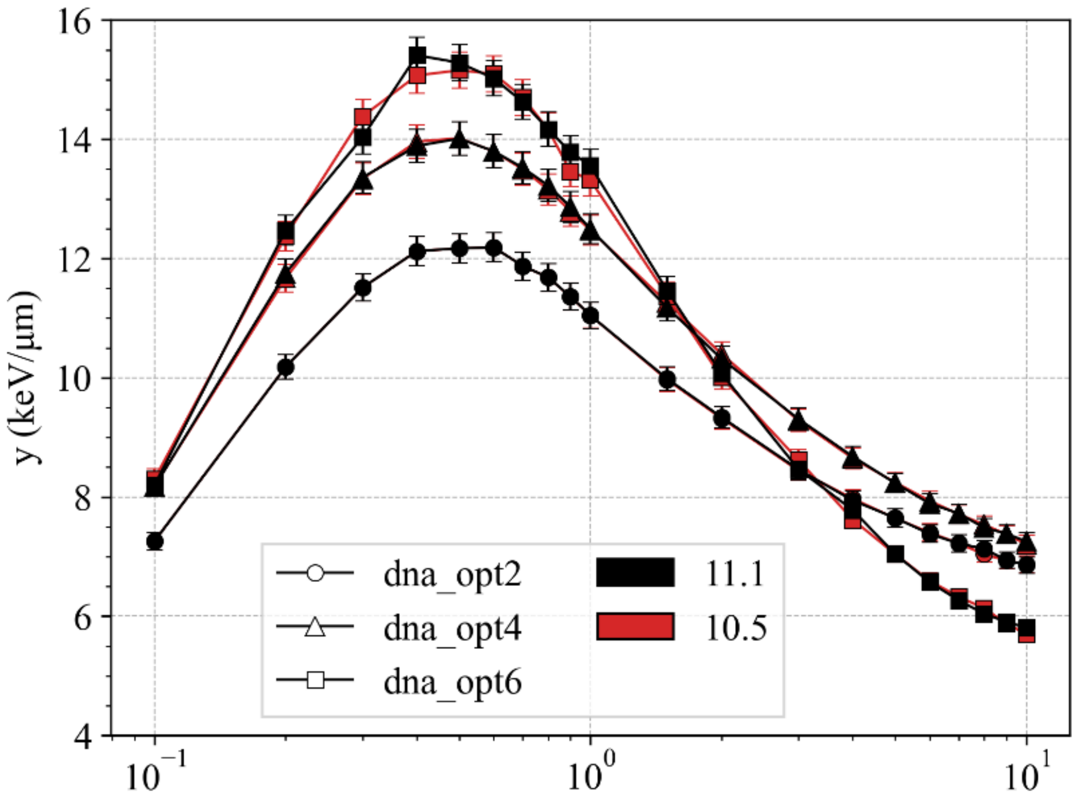
Computing performance test - Brachy



- Monoenergetic 20 KeV X-rays
- Dose scored in 30 positions at 4 different depths
- Comparison with experimental data (TLDs)

microyz

Microdosimetric spectra due to monoenergetic electrons in a 10 nm radius water sphere



Electron Energy (keV)

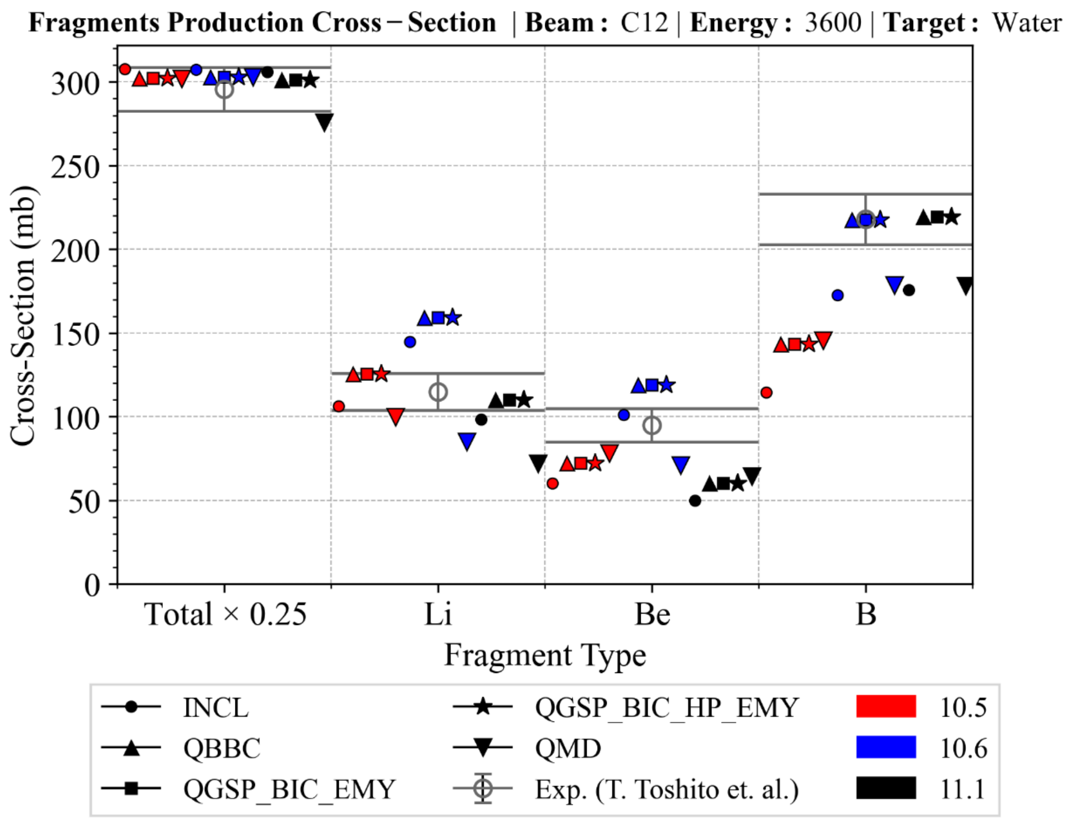
Computing performance test

G4DNA-OPT2 as reference

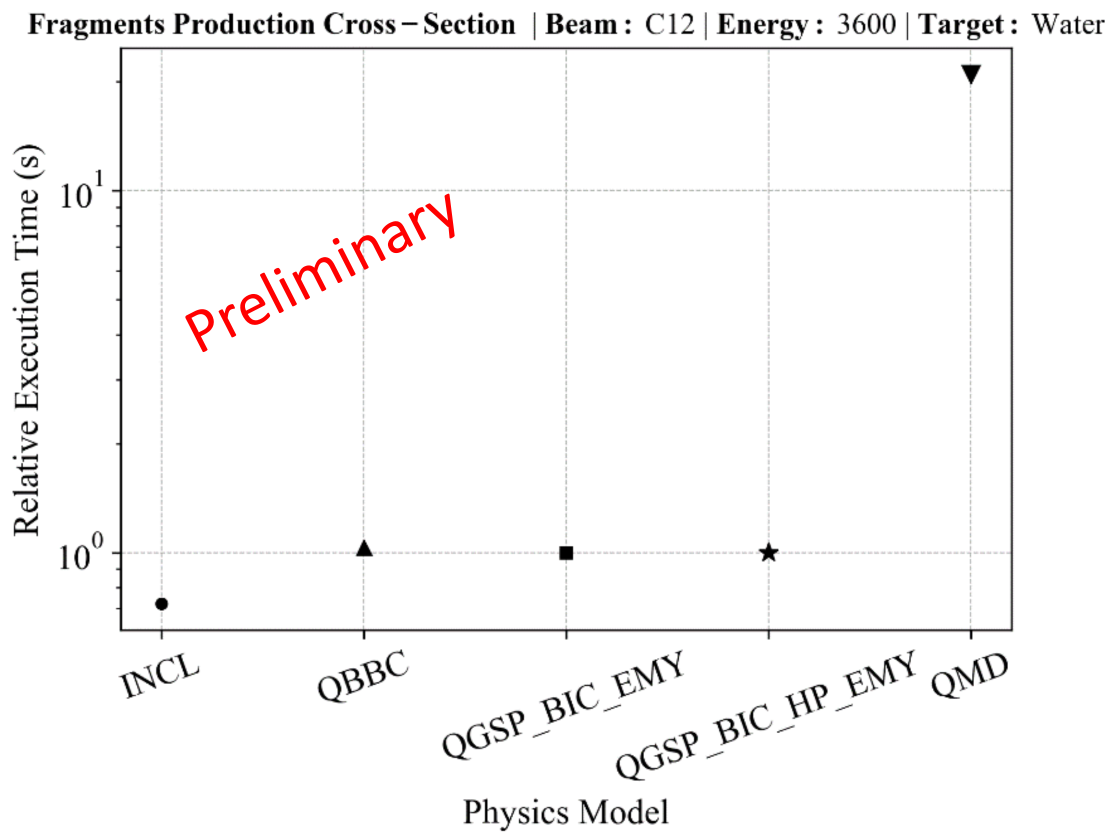
Preliminary results (to be confirmed)

Electron energy	G4DNA-OPT4	G4DNA-OPT6
1 keV	2	1.84
10 keV	1.45	1.85

CCCSTest: charge changing cross section



Computing performance test



Notes

- Physical accuracy is paramount
  - Usually, it is deemed acceptable to sacrifice computational performance to achieve better physics accuracy
- Nevertheless, computational performance becomes important in pre-clinical (calculation of the dose in the target) and clinical settings (verification of TPSs)
  - Use of local clusters and supercomputing facilities
  - Increasing the use of Machine Learning solutions

Fast dose calculations for Microbeam Radiation Therapy

- Forward planning dose prediction with:
  - Geant4: ~15 h/ CPU [Dipuglia et al (2019), Scientific Reports, 9:17696]
  - *HybridDC*: ~30 minutes [M. Donzelli, et al (2018)PMB, 63:45013]

  →Bottleneck for treatment plan dose engines
- Train a Machine Learning solution with Geant4-calculated 3D dose maps to predict doses

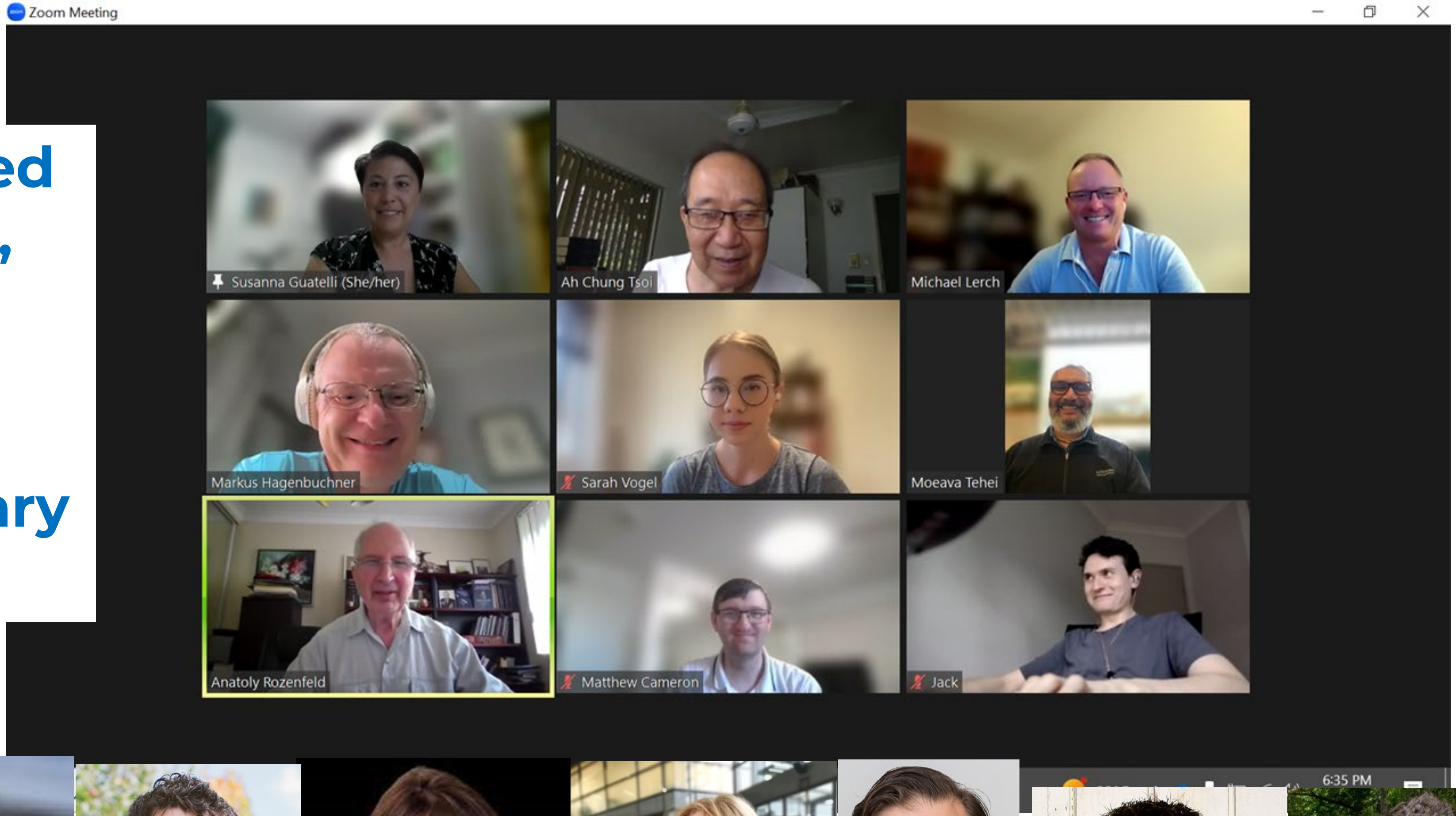
PhD student Florian Mentzel thesis: Microbeams – quick and dirty

Publications:

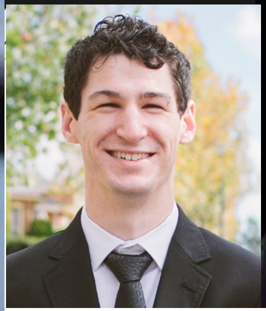
- Mentzel et al (2022) Medical Physics, 49(5): 3389
- Mentzel et al (2022) Medical Physics, 49(12): 7791
- Mentzel et al (2023) Cancers, 15 (7), art. no. 2137

Research based at the CMRP, UOW

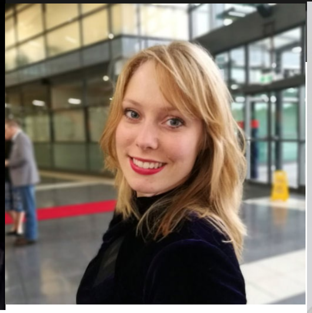
Our multidisciplinary team!




F. Mentzel


M. Barnes


S. Corde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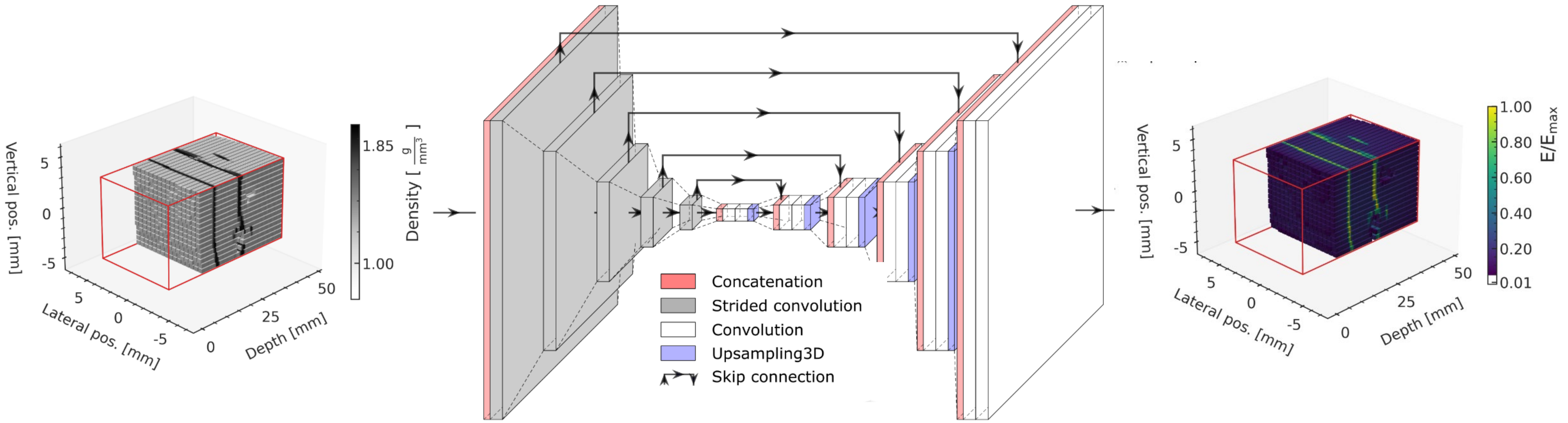
Fast dose predictions with machine learning (ML)

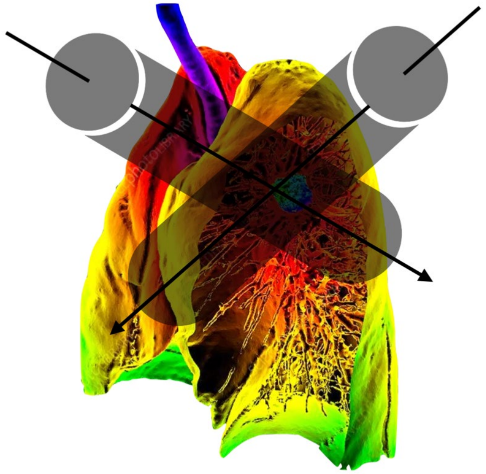
- Our data: **3D density matrix -> 3D energy deposition** matrix
- **Adapted 3D U-Net** [Ö. Çiçek, et al. MICCAI, LNCS, 9901:424–432, 2016]
  - Training (fitting process): very slow **(~ days/ weeks)**
  - Execution: very fast **(~ 0.1 second in our case)**
  - Tensorflow v2.2
- We use **Geant4 simulations to train, validate and test** the 3D U-Net

Results

- In the entire volume:
  - Over 98% of voxels have < 10% dose deviation
    - Deviations mainly scattered around bone-water interfaces
- In the tumor:
  - ΔD < 3% for more than 96% voxels
- Speeding factor of the ML-based dose engine vs Geant4 : **10^6** considering 1 computing unit



Deep Learning in medical MC simulations

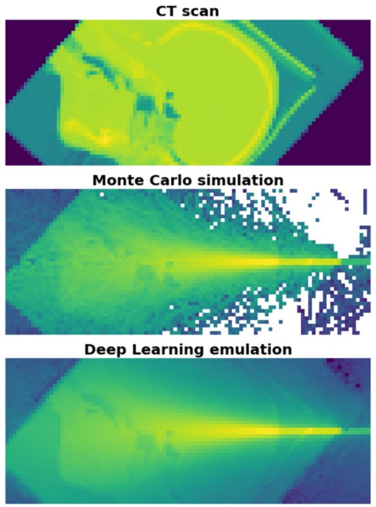


Cylindrical shaped scorers around the beam

- Work by L. Arsini[1], B. Caccia[2], A. Ciardiello[1], S. Giagu[1], C. Mancini Terracciano[1]

[1]La Sapienza, Rome, Italy, [2]Istituto Superiore di Sanita', Rome, Italy

- DL algorithms could be trained to emulate MC simulations or to emulate physics models (or part of them)
- A Graph Neural Network has been developed
  - to use whatever (a-priori decided) geometry to emulate the energy deposition of a beam in a voxelized geometry
  - and emulate BLOB (QMD as a preliminary test)
  - References:
    - A. Ciardiello et al. Preliminary results in using Deep Learning to emulate BLOB, a nuclear interaction model. Phys. Med. 70 (2020)
    - L. Arsini et al. Nearest Neighbours Graph Variational AutoEncoder. Alg. 16(3) (2023)
  - For details see L. Arsini's presentation, Parallel 3A, Tuesday 26th September



That’s all, thank you