Update on the G4-Med project

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On Behalf of the Geant4 Medical Simulation Benchmarking Group

28th Geant4 Collaboration Meeting, 25-29 September, Sapporo, Japan

Outline

- Update on membership
- Maintenance of the tests
- Regression testing results
- New tests
- Perspectives for the future

Members

- Coordinator: S. Guatelli
- Deputy coordinator: P. Arce
- Continuing (42 members, authors of Arce *et al* (2021) Medical Physics, 48 (1)):

P Arce, D Bolst, M-C Bordage, J M C Brown, P Cirrone, M A Cortés-Giraldo, D Cutajar, G Cuttone, L Desorgher, P Dondero, B Faddegon, C Fedon, S Guatelli, S Incerti, V Ivanchenko, D Konstantinov, I Kyriakou, G Latyshev, A Le, Z Li, C Mancini-Terracciano, M Maire, A. Malaroda, A Mantero, C Michelet, M Novak, C Omachi, L Pandola, A Perales, Y Perrot, G Petringa, J M Quesada, J Ramos-Méndez, F Romano, A B Rosenfeld, L G Sarmiento, D Sakata, T Sasaki, I Sechopoulos, E C Simpson, T Toshito, D H Wright

Total number of research entities: 25

Four group meetings per year

- New 12 members:
  - J. Archer (Wollongong University): helping with regression testing and data analysis
  - B. Caccia (Istituto Superiore di Sanita'): external X-ray radiotherapy
  - A. Chacon (ANSTO): in-vivo PET test in carbon ion therapy
  - S. Fattori (INFN): Geant4-DNA tests
  - A. Haga (Tokushima University): hadronic physics tests
  - Z. Li (Bordeaux University): EPICS2017
  - A. Malaroda (Wollongong University): nuclear medicine
  - C. Michelet (Bordeaux University): EPICS2017
  - F. Nicolanti (La Sapienza): Geant4-DNA tests
  - M. Safavi (ANSTO): in-vivo PET test in carbon ion therapy
  - Y. Sato (Tokushima University): hadronic physics tests
  - A. Sciuto (INFN): CATANA radiobiology test

Test repositories

- All tests are in `geant-val` and maintained there
- Aim: to include all tests in the Geant4 rep for an easier maintenance
- Current status – Tests executed in the Geant4 nightly testing:
  - Advanced examples: `brachytherapy`, `hadrontherapy`, `microyz`
  - Extended examples: `TestEm12`, `fanoCavity`
  - G4tests-verification: `attenuation`, `CCCStest`
- 13 tests to be included in the G4tests-verification:
  - Currently working on the e^- backscattering test, then Bragg Peak/GSI
- Comments:
  - Code reviews are often needed
  - Time consuming exercise BUT it helps the maintenance of the codes and a good coding practice
  - This work helps also with the maintenance of the tests in `G4tests-verification`
  - Overall, it is worth to do this effort

Benchmarking activity: updates (1)

- Regression testing between **10.5** (Arce et al (2021), Med. Phys. 48 (1)) and **11.1** for the existing tests
  - Normalised mean square error (NMSE) $NMSE = \frac{\sum_{i=1}^{N_{reg}} |S_i - E_i|^2}{\sum_{i=1}^{N_{reg}} |E_i|^2}$
  - Maximum difference
  - K-S test with p-value (5% significance threshold)
  - Data analysis performed by J. Archer and S. Guatelli, supported by D. Bolst, CMRP, University of Wollongong
- New tests:
  - Geant4-DNA
  - In-vivo PET for hadrontherapy

Ongoing activity
To be documented in paper n. 2

Benchmarking activity: updates (2)

Execution times benchmarking

- Few cases selected for each test
- Benchmark all tested physics lists
- Have enough histories to neglect the initialization phase
- 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

Ongoing activity
To be documented in paper n. 2

Results: EM Physics

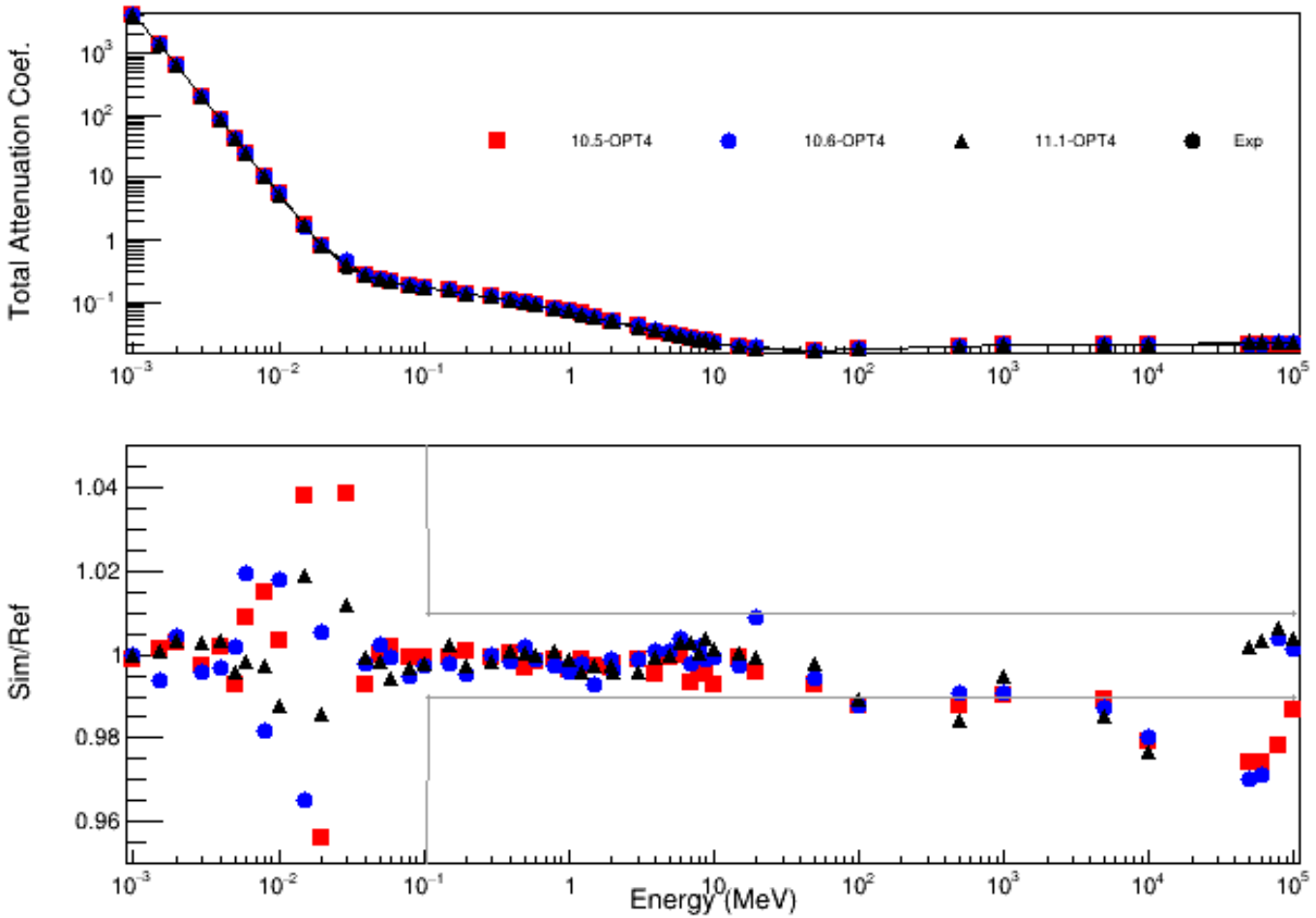
To note: it is work in progress ….

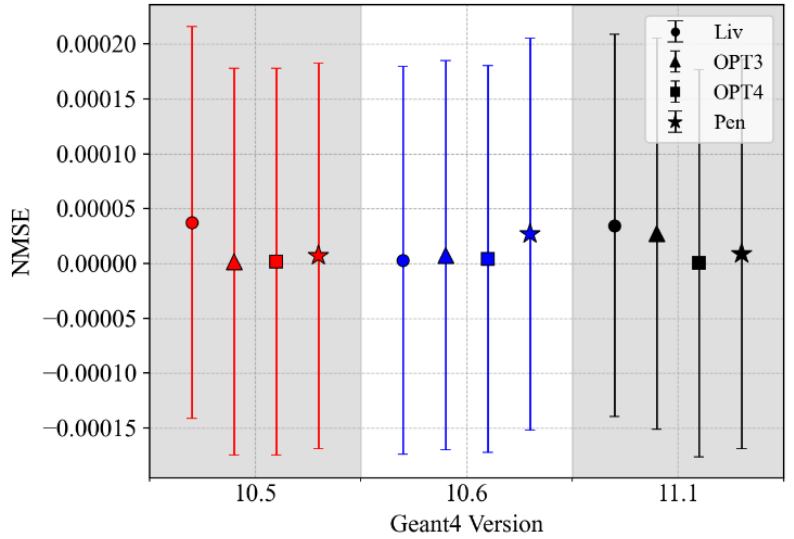
Still to perform an in-depth analysis of the results

Total attenuation coeff. test

Comparison against NIST XCOM

G4 EM Physics list OPT4

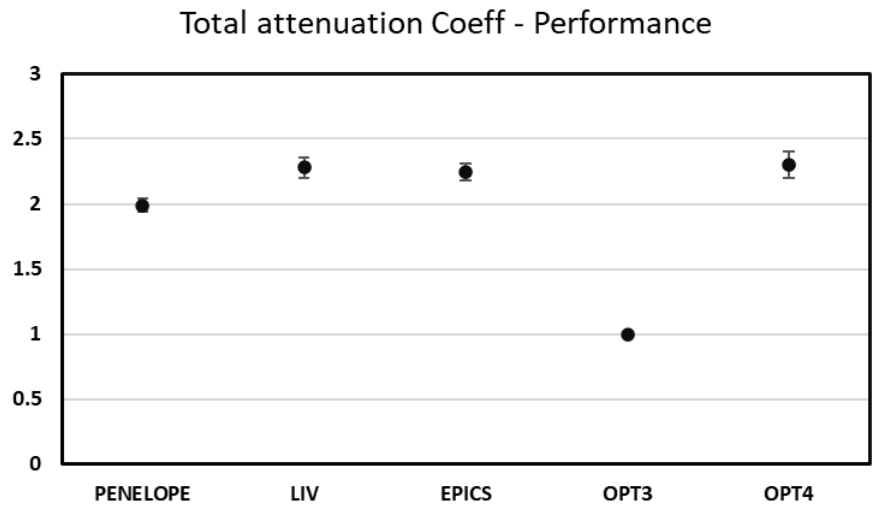




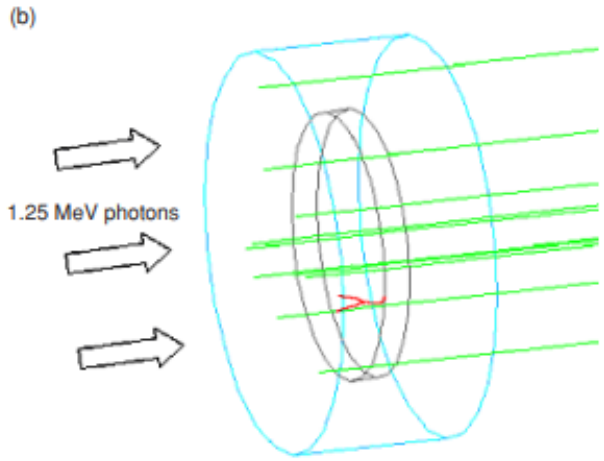
K-S test: p-values above 0.8

All in agreement

EPICS 2017 added

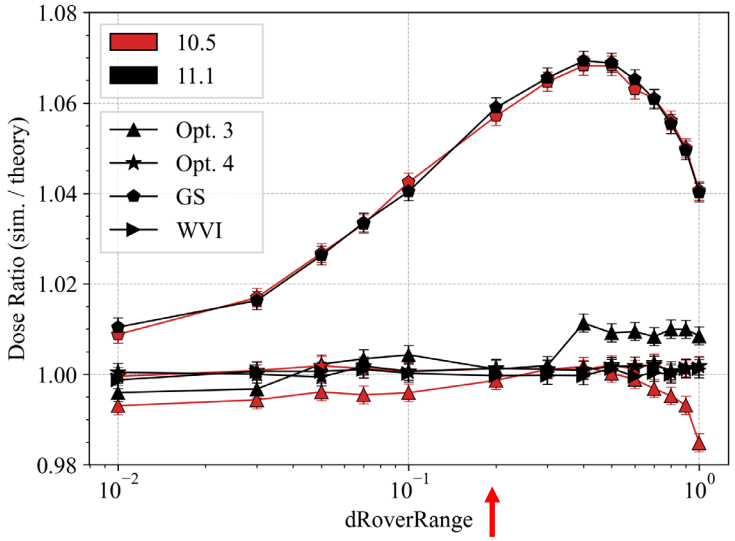


Fano Cavity test

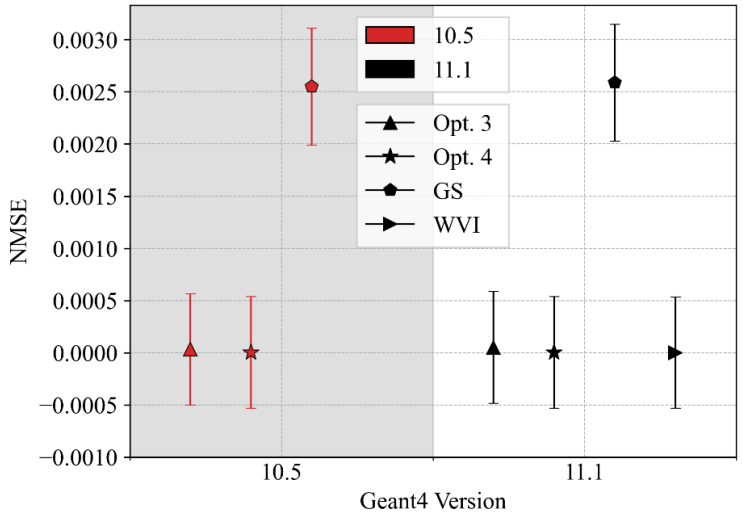


Check that the ratio of the dose deposited in the cavity divided by the beam energy fluence is equal to the mass energy transfer coefficient of the wall material

Single Scattering model still running

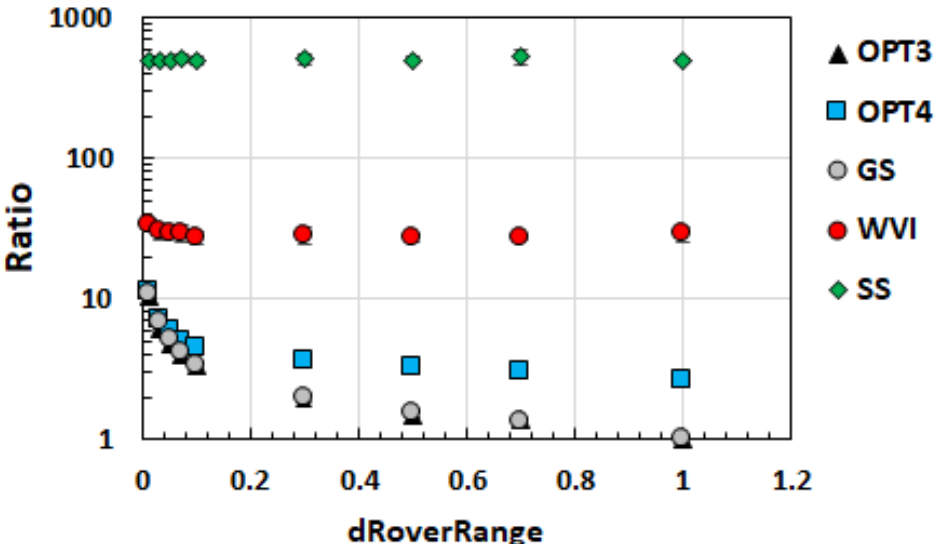


No significant change



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

Computing performance



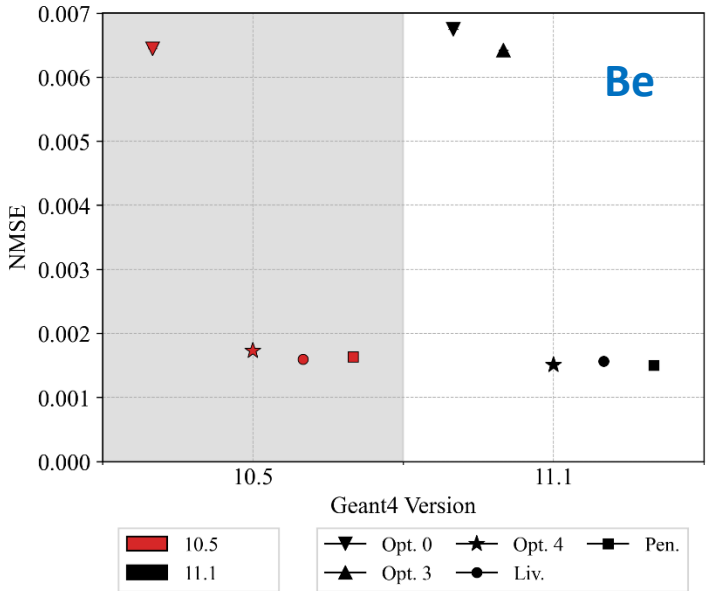
Electron forward scattering

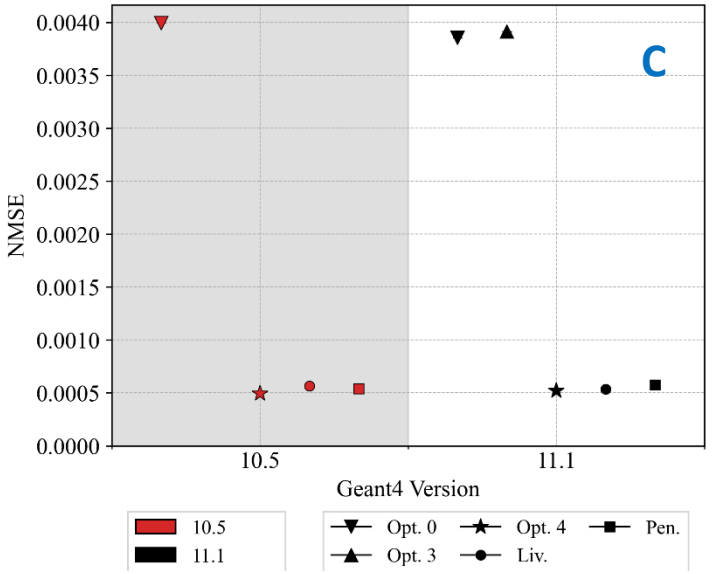
Preliminary results
No significant change

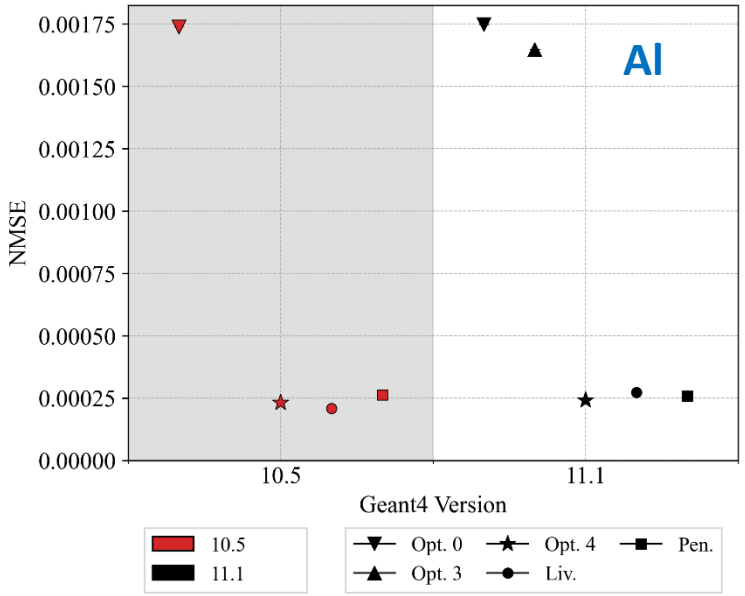
Experimental benchmark of the forward scatter of e^- with energy 13 MeV and 20 MeV

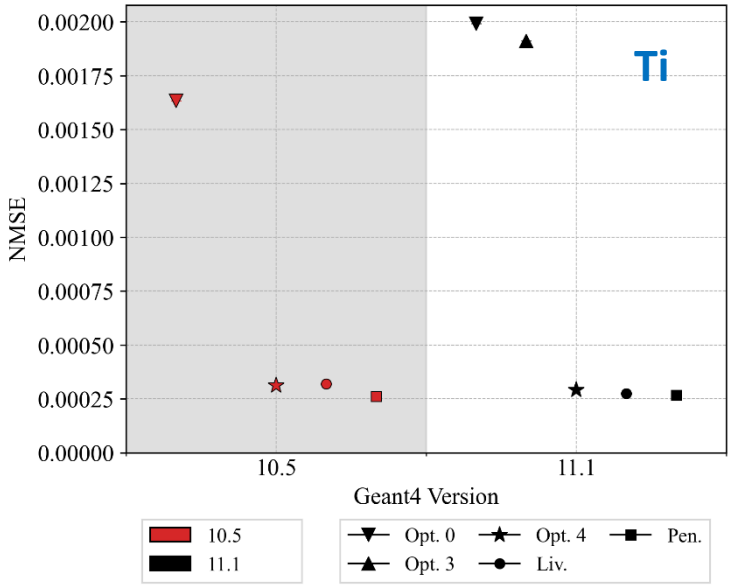
Scattering angle = 2–8 deg

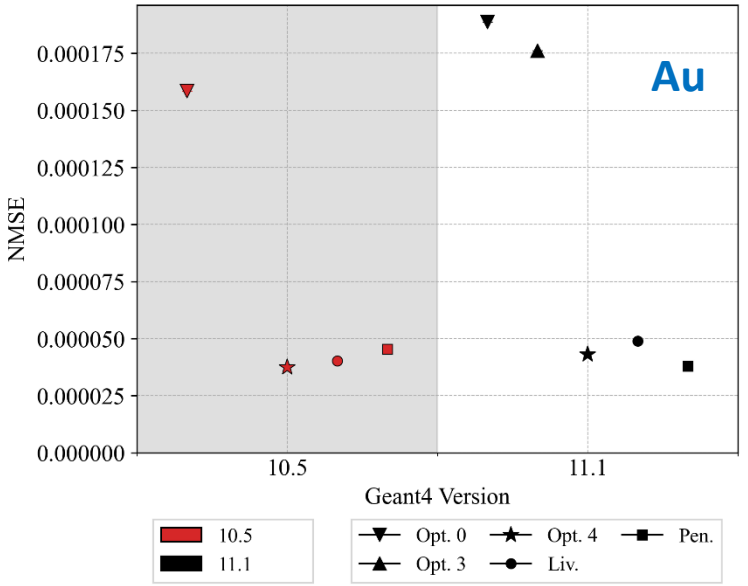
Exp data: Ross C, et al (2008) Medical physics, 35(9):4121–4131







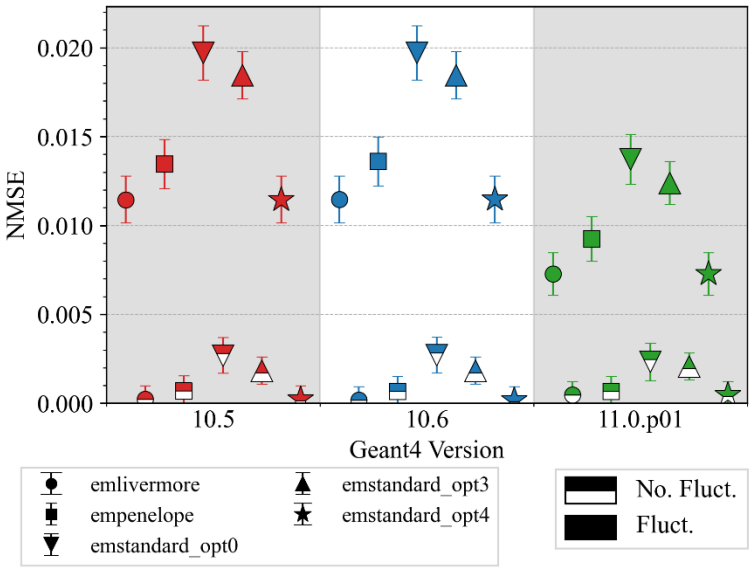




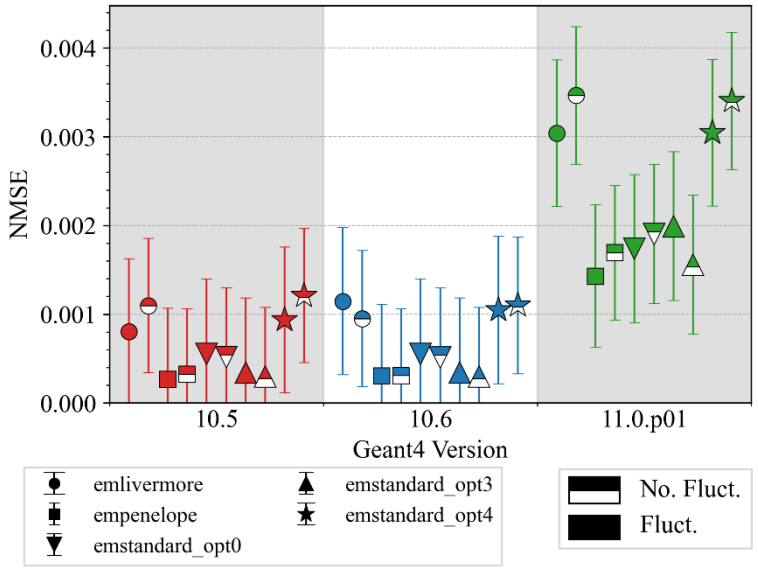
Dose Point Kernel test

Radial energy deposition profiles from an isotropic e^- source in water
Comparison against EGSnrc

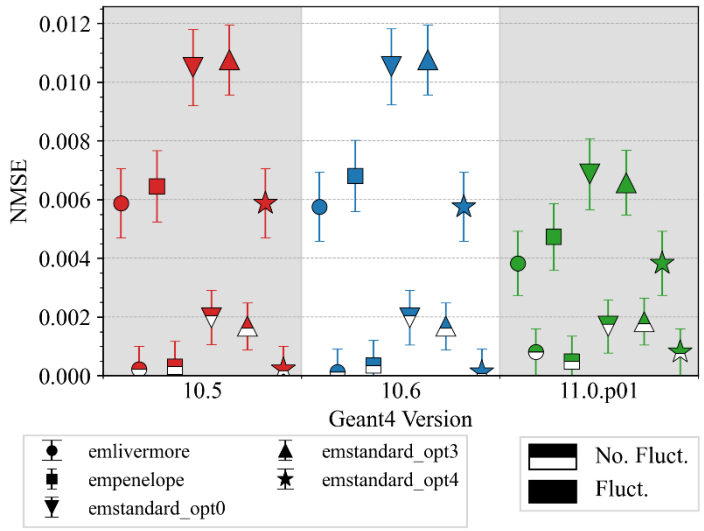
10 keV



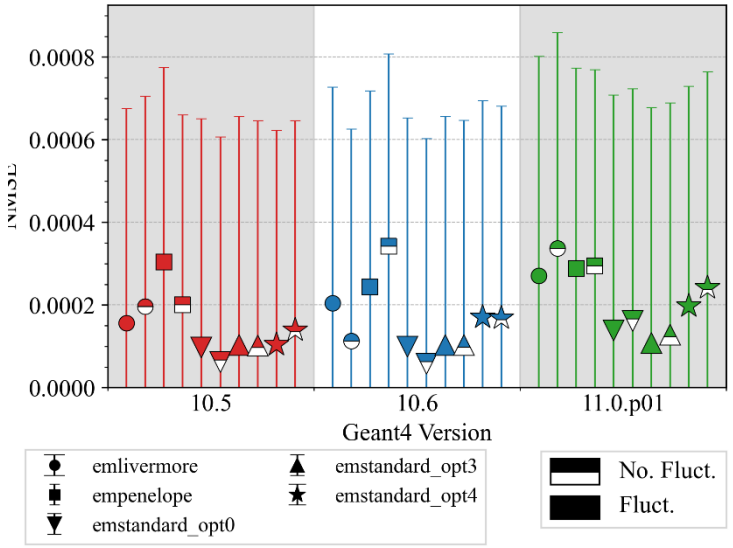
100 keV



15 keV

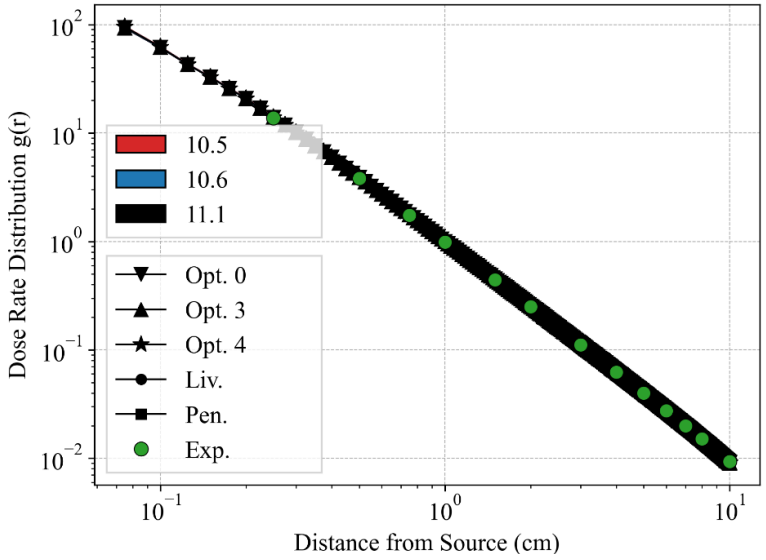


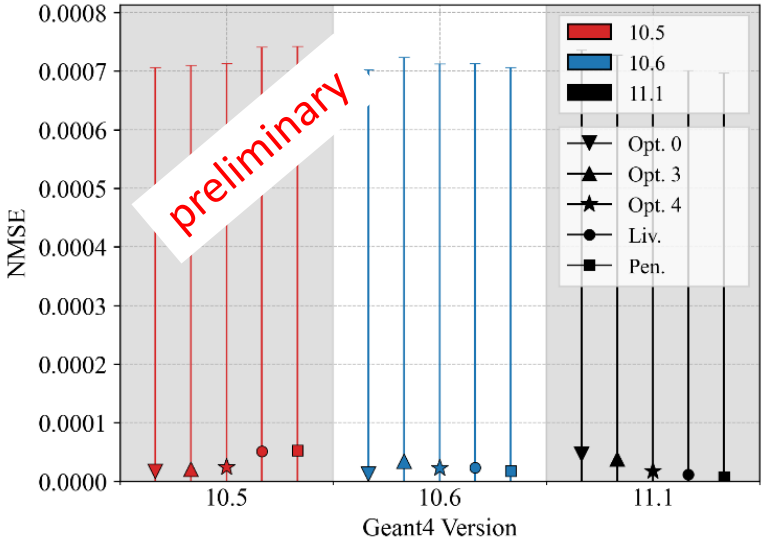
1 MeV



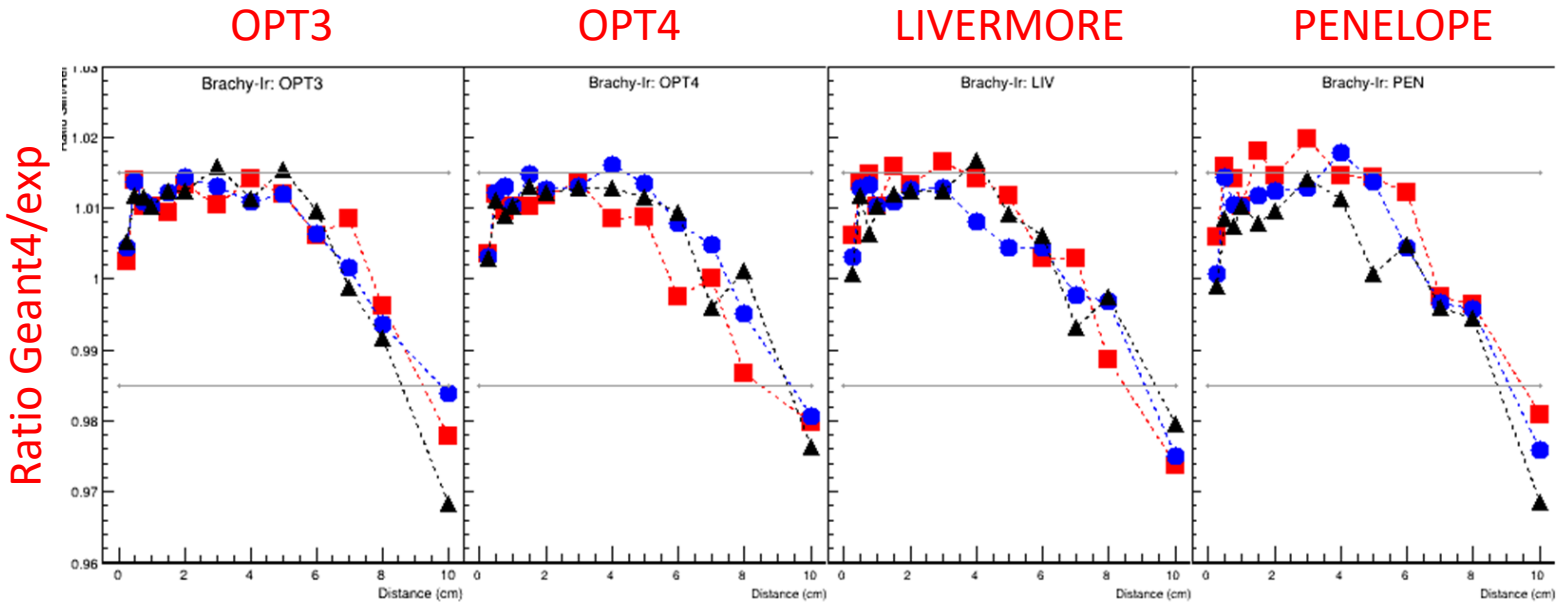
Brachy-Ir source

Calculate dose in water by a Flexisource Ir-192
(Med. Phys 33(12), 2006, 4578-4582)
Reference: Geant4 7.1

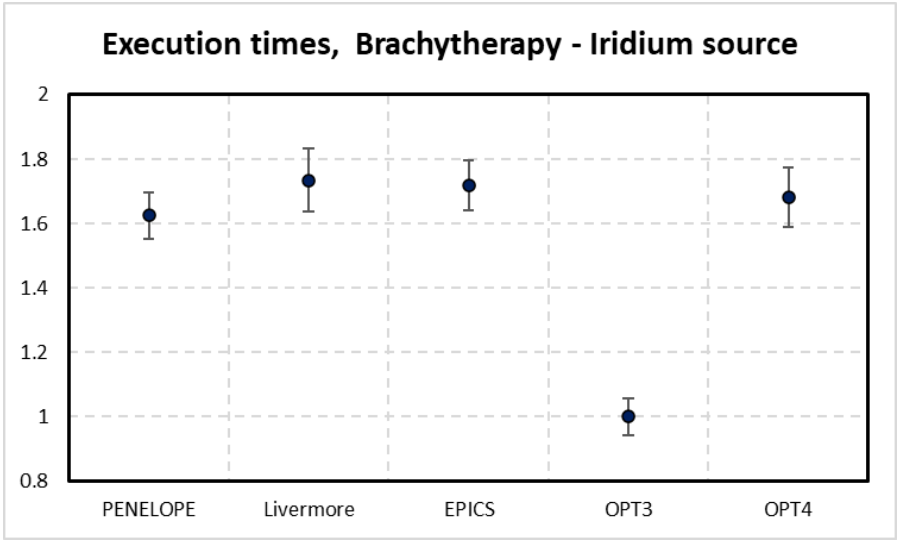




OPT3 OPT4 LIVERMORE PENELOPE

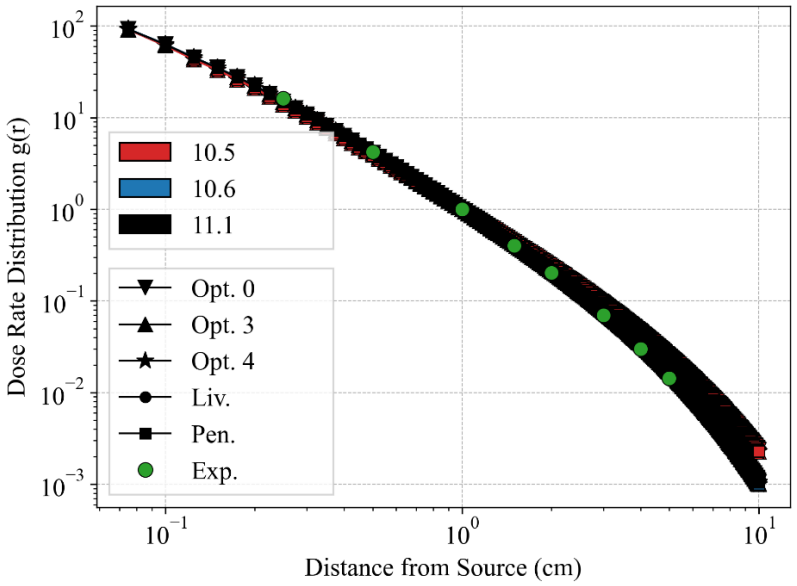


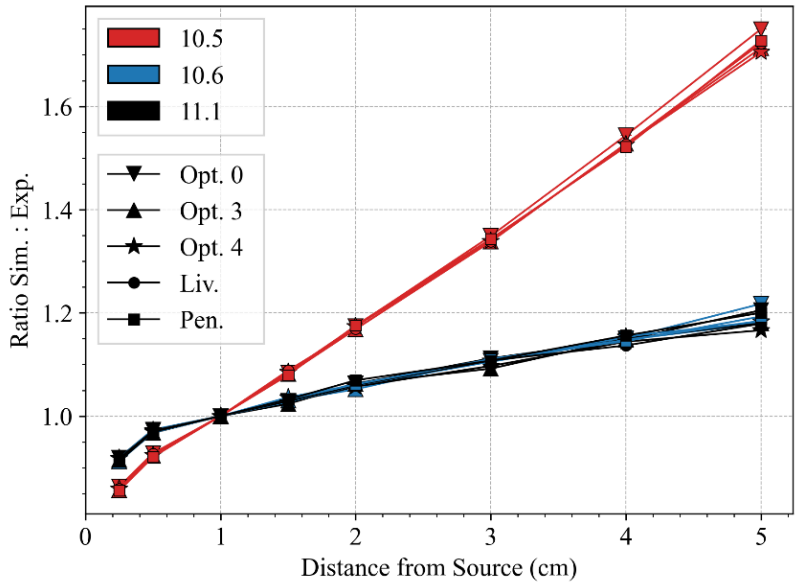
K-S test: p-values ~0.077 for all physics lists, for any Geant4 release

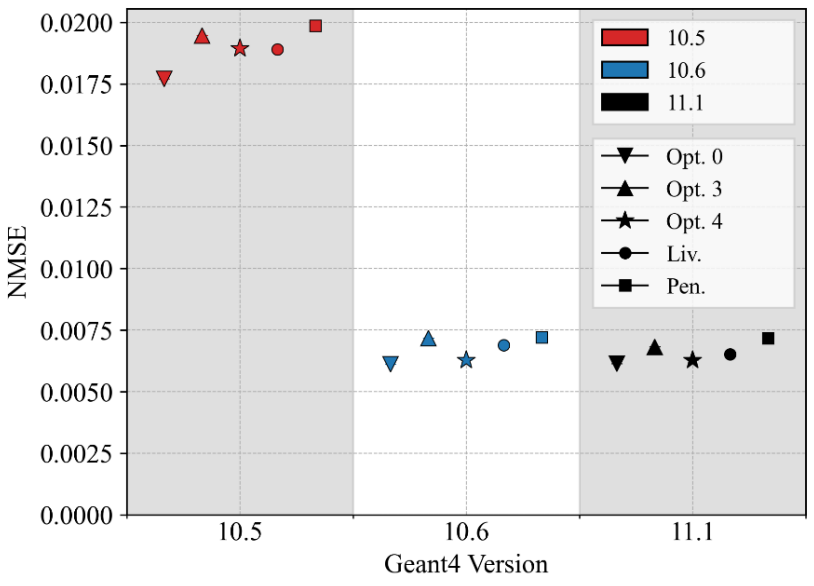


Brachy - Bebig Isoseed I-125, Oncura 6711

Comparison against experimental data



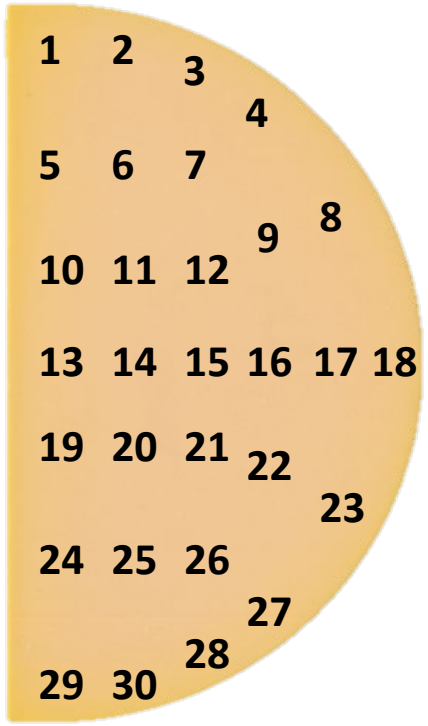


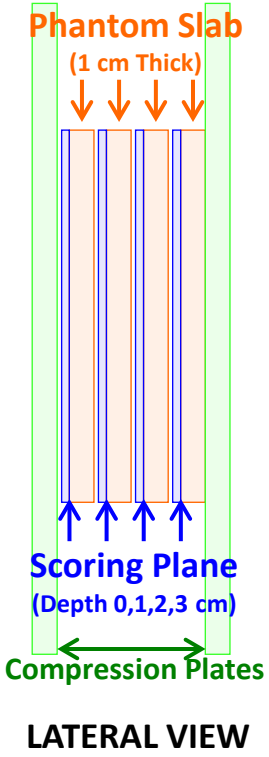


K-S test: p-values ~1 for all physics lists, for any Geant4 release

Improvements in the multiple scattering/energy loss fluctuation? (we still have to understand the details)

Mammography

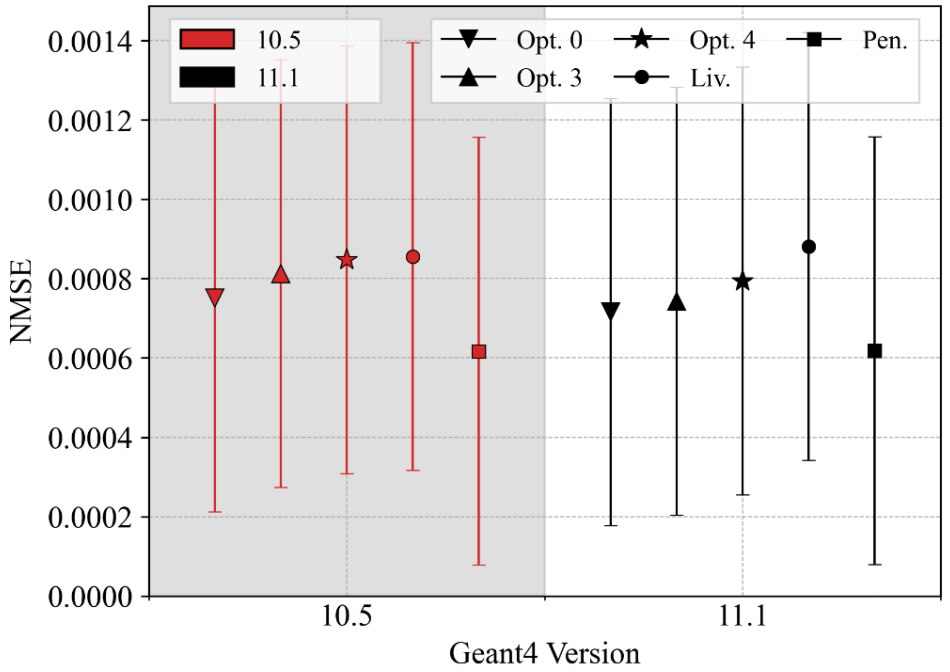


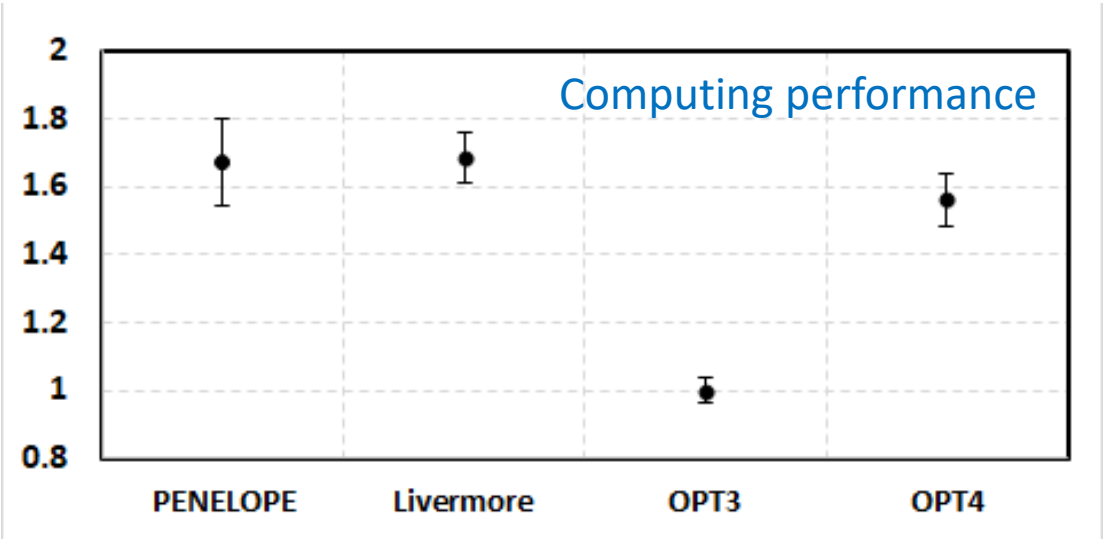


LATERAL VIEW

- 20 keV monoenergetic X-ray beam
- Dose scored in 30 positions at 4 different depths
- Comparison with experimental measurements (TLDs) by C. Fedon et al

No significant change



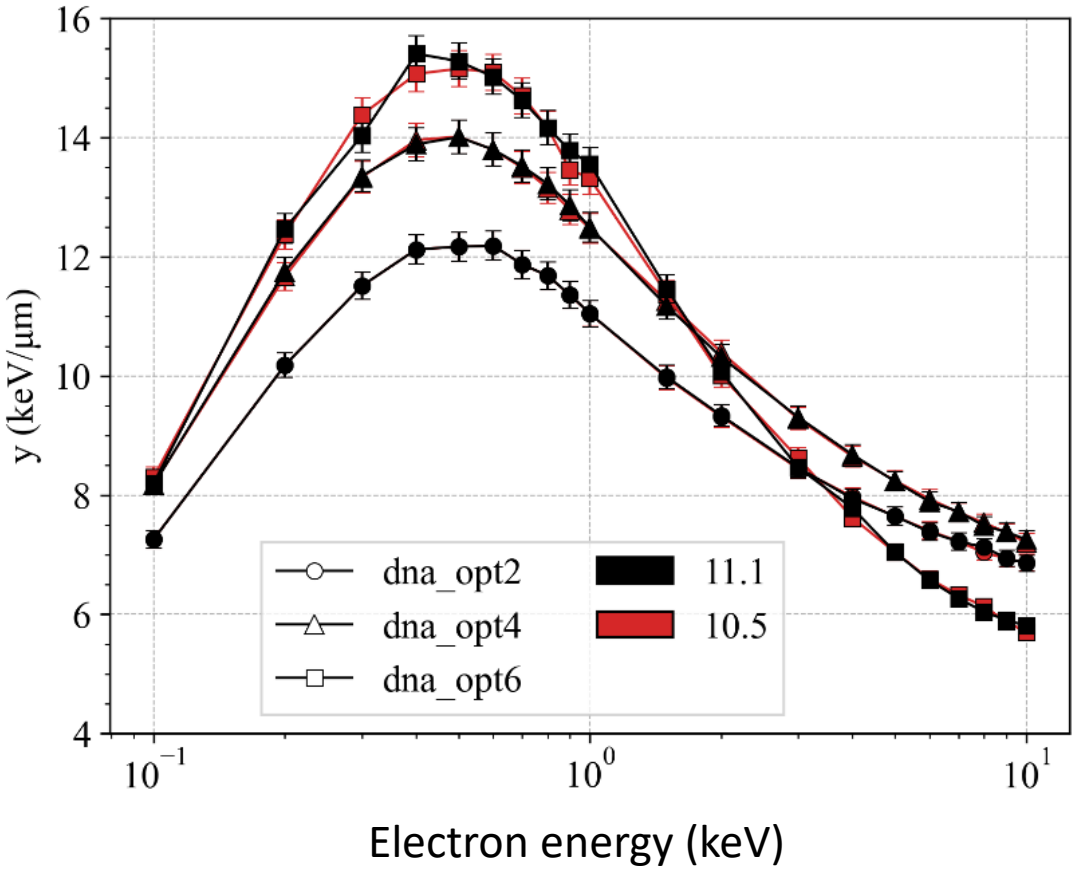


New: Geant4-DNA tests

- Physics tests:
  - Microyz
  - TestEm12 – DPK (running)
  - Geant4-DNA physics list opt2, opt4 and opt6
- Chemistry test:
  - Chem6
  - To do

microyz

Calculation of the lineal energy of monoenergetic e^- in a water sphere with a 10 nm radius



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

Simulation results do not change between 10.5 and 10.6

To do

- Currently:
  - Data analysis of the e^- backscattering test
  - Finalise the execution times for this test

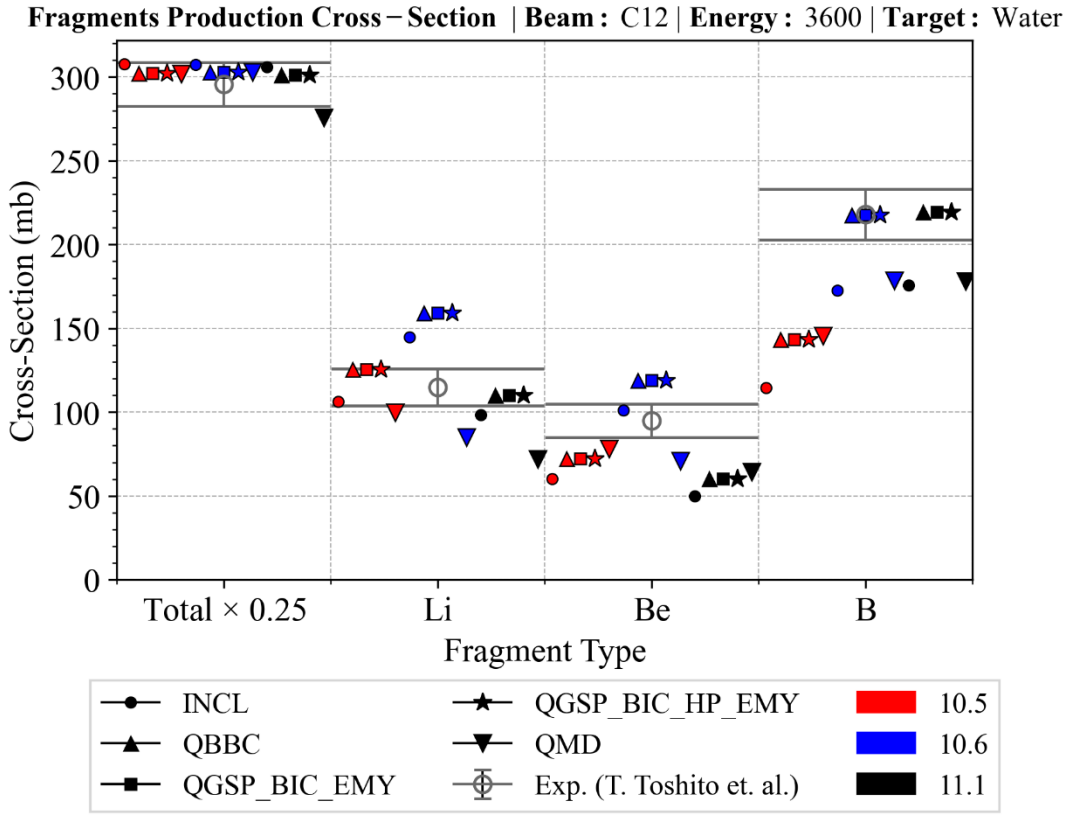
- To do for paper n. 2:
  - Run bremsstrahlung test with 11.1
  - Run `DPK` with Geant4-DNA physics lists with 11.1
  - Run `Chem6` test
  - Finish the execution times benchmarking
  - Discuss the regression testing results

Results: Hadronic physics

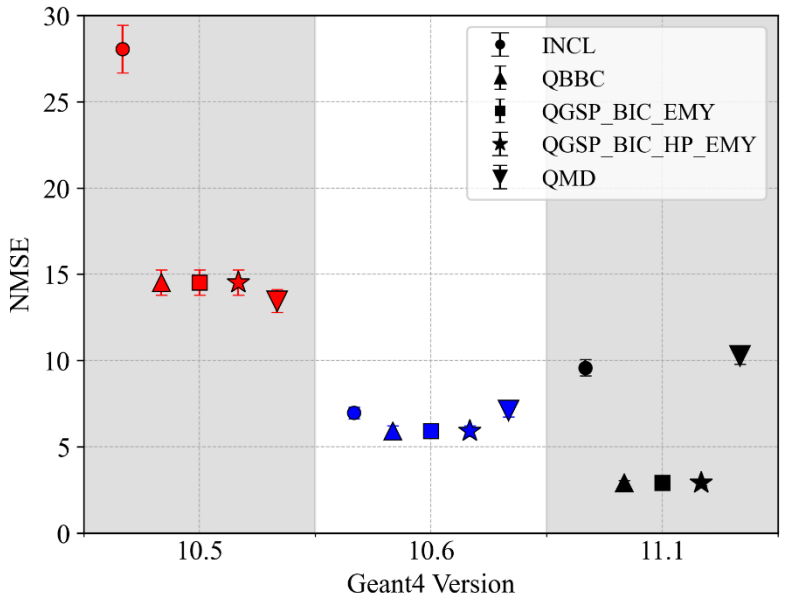
Work in progress ….

CCCSTest: charge changing cross section

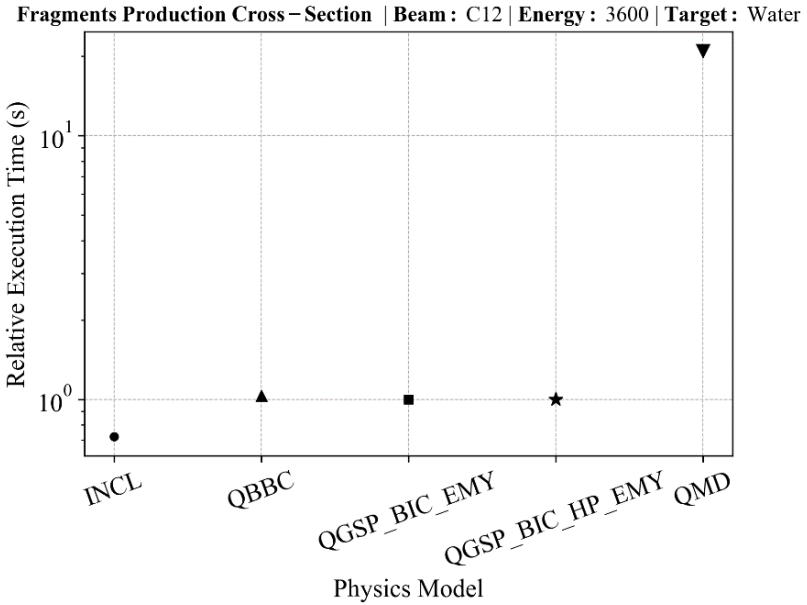
Comparison against experimental measurements by Toshito, T., et al. (2007) Physical Review C, 75 (5):054606



For all fragments (we should break it down for each frag)

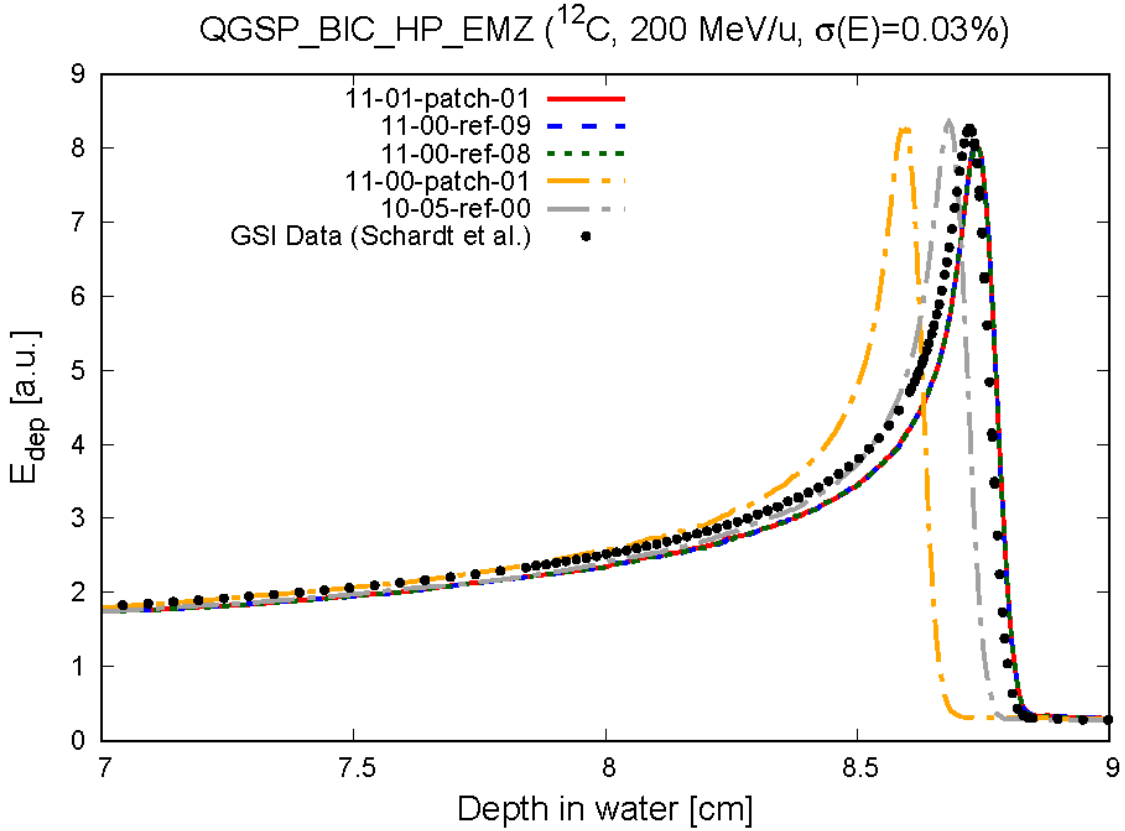


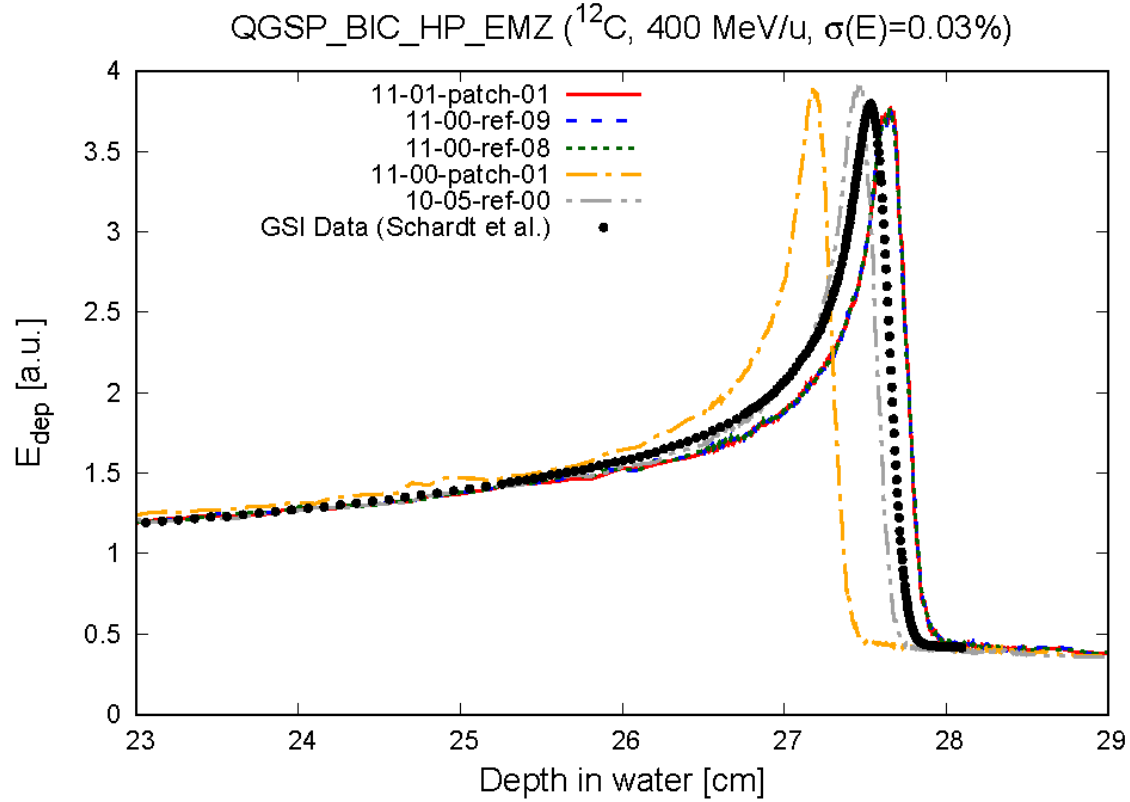
Computational performance test



^{12}C Bragg Peak tests in water

Exp data: Schardt, D, et al. (2007), GSI Scientific Report, vol. 373, 2007



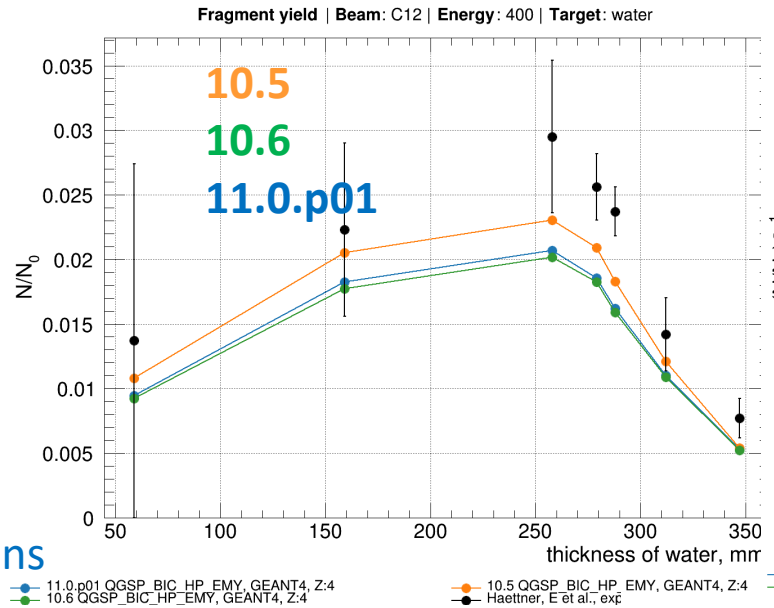


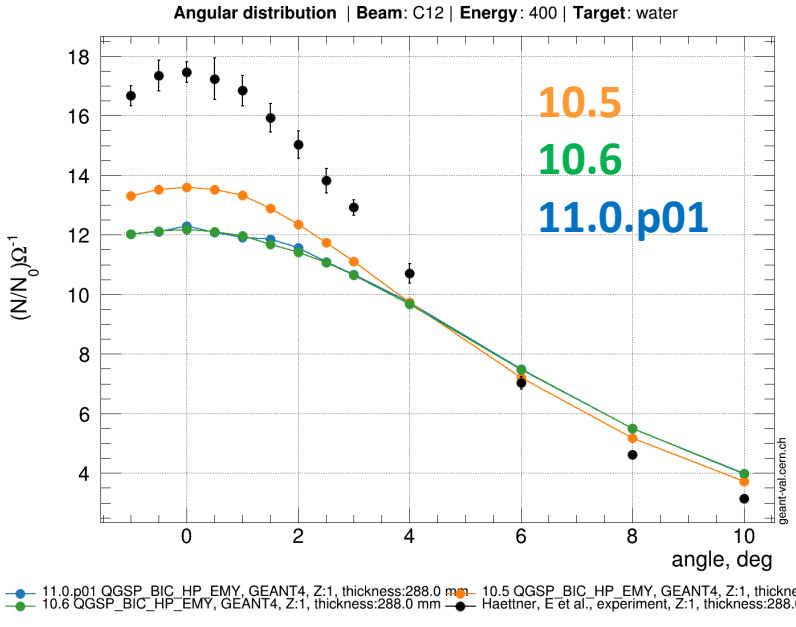
Results and plots by M. Cortes Giraldo

400 MeV/u ^{12}C fragmentation test in water (1)

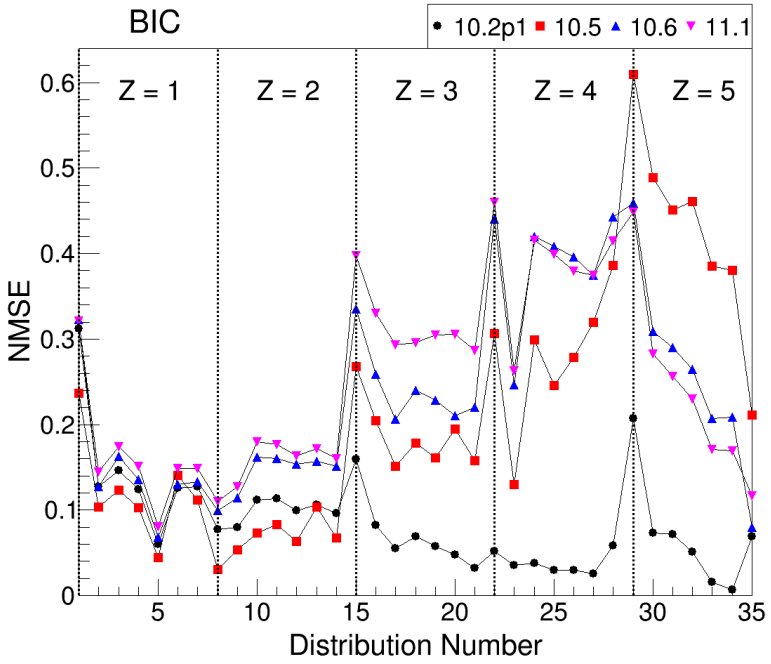
Preliminary analysis by D. Bolst, CMRP, UOW

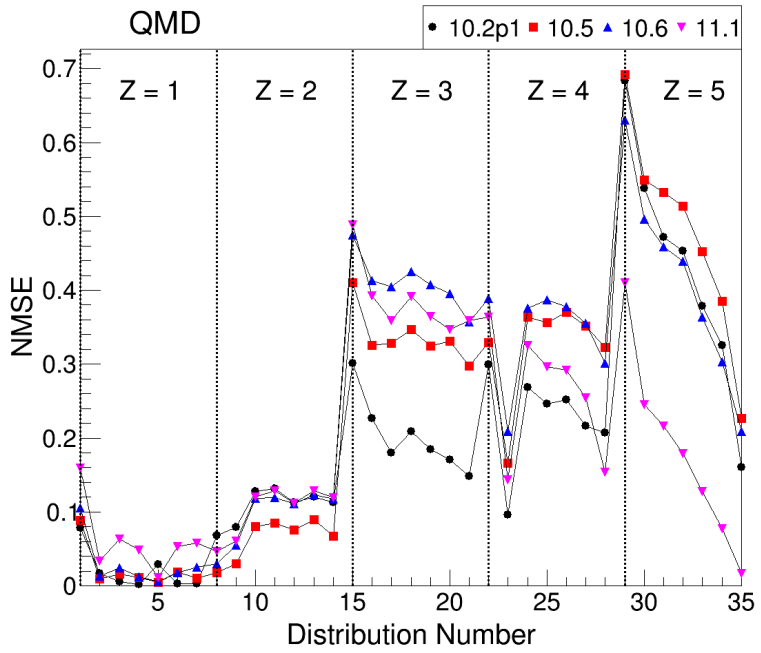
- Results generally change a lot from release to release
  - Yield changes the most, then angular and then energy distributions

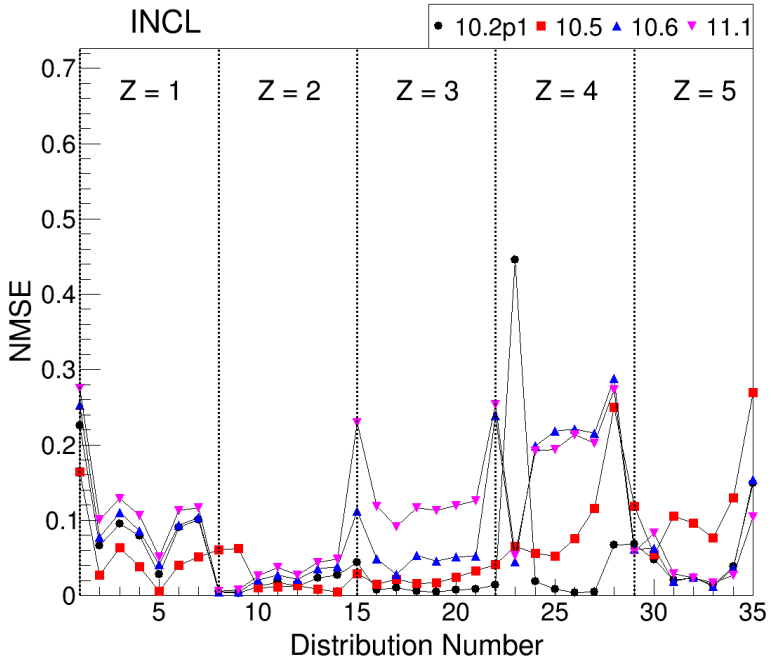




Angular distributions-Comparing all distributions



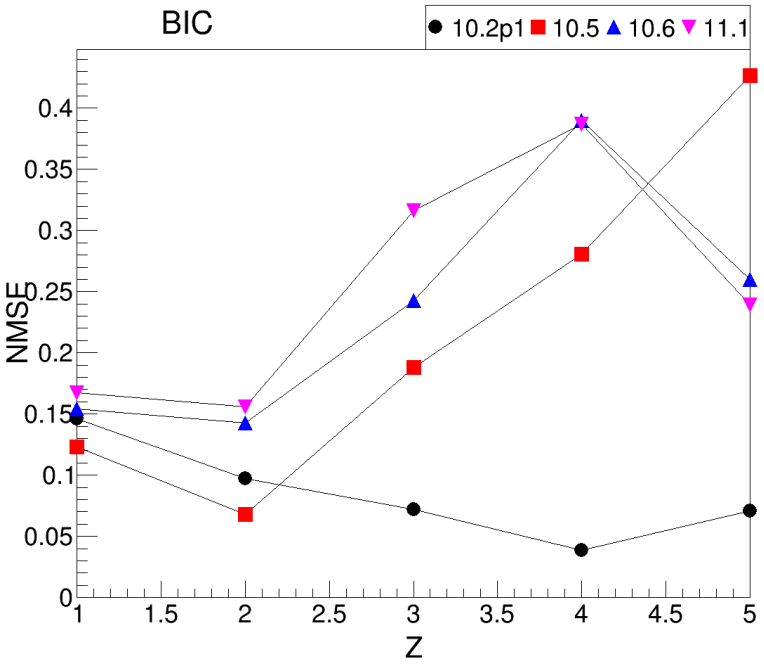


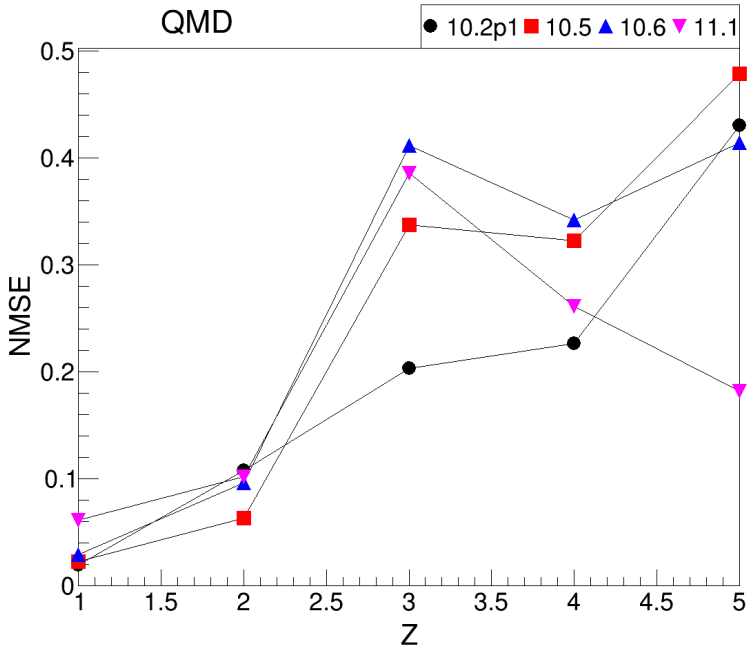


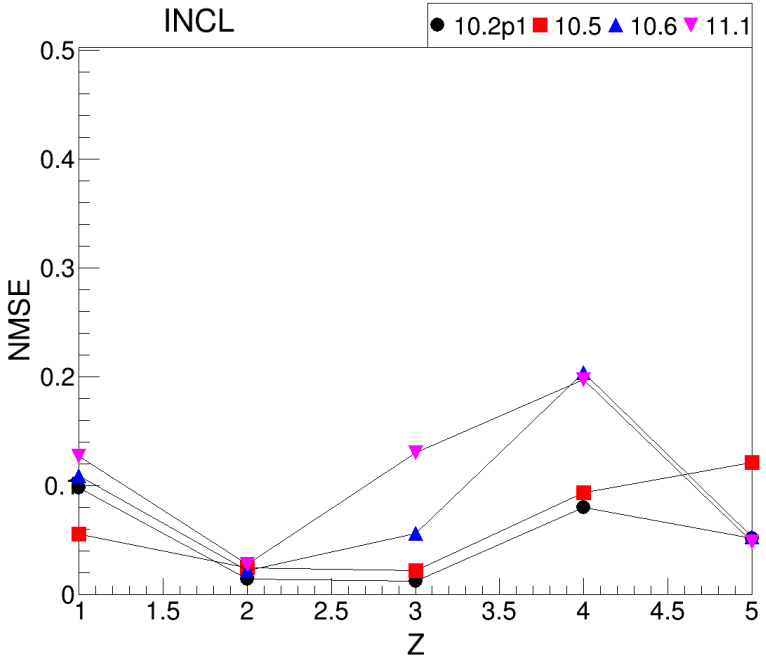
400 MeV/amu ^{12}C fragmentation test in water (2)

Angular distributions-Summary of difference for each Z

10.2 were the golden days of BIC





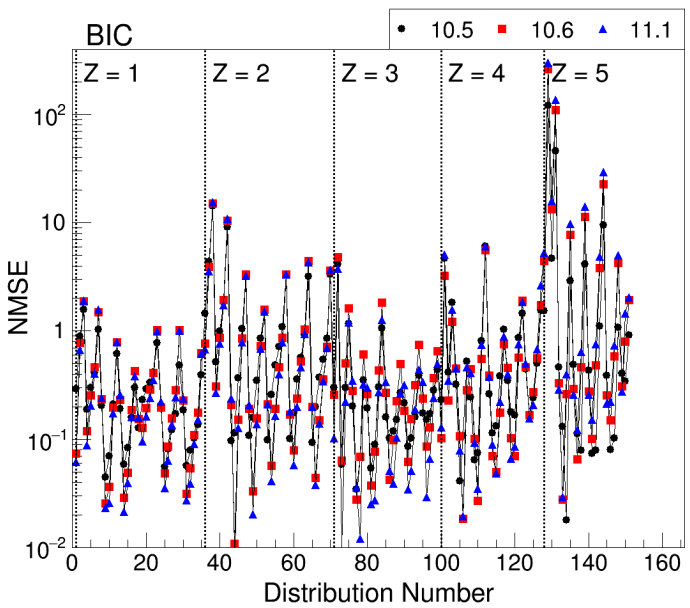


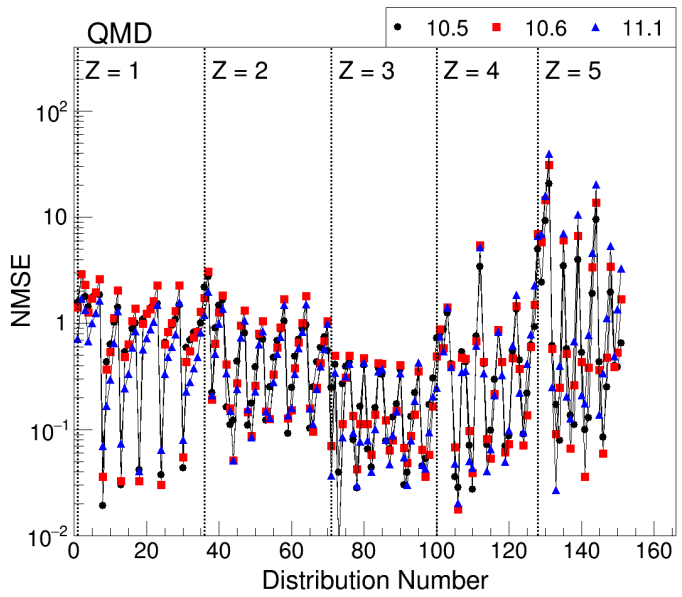
Preliminary analysis by D. Bolst, CMRP, UOW

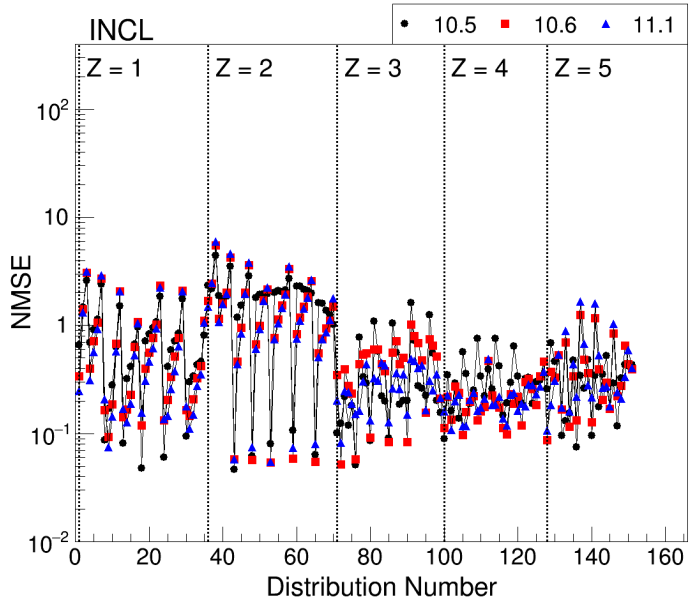
400 MeV/amu ^{12}C fragmentation test in water (3)

Preliminary analysis by D. Bolst, CMRP, UOW

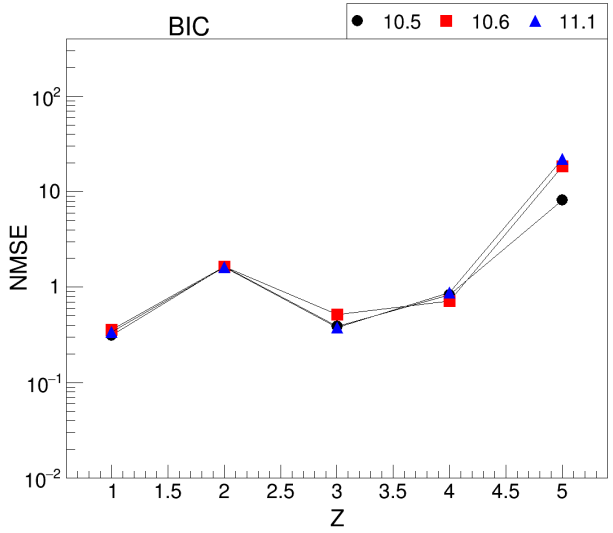
Energy distributions distributions-Comparing all distributions

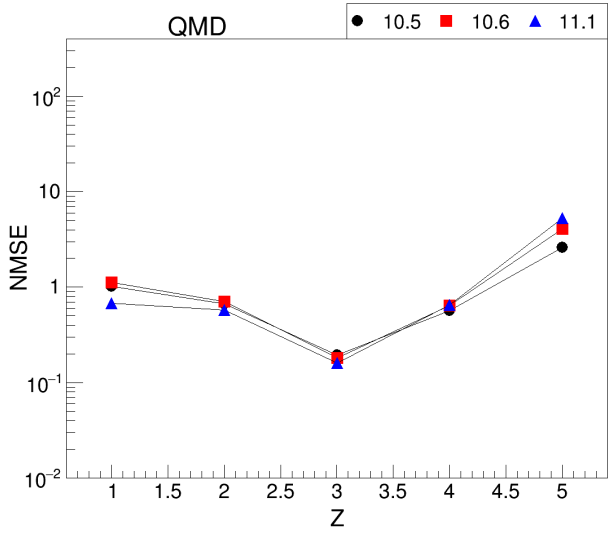


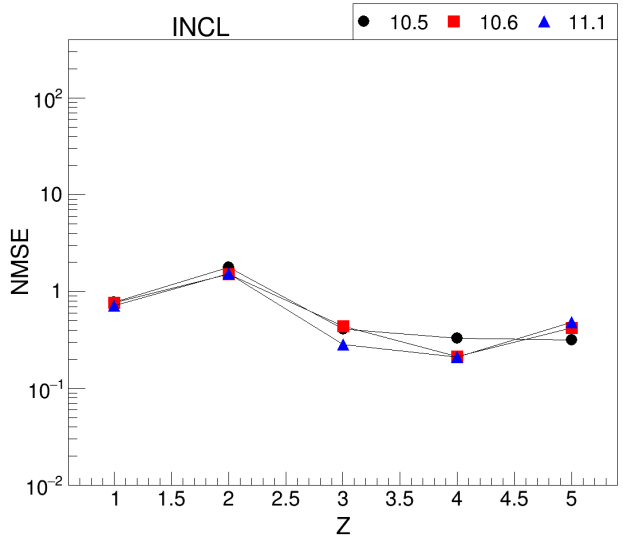




Energy distributions - Summary over Z







Yield and distribution of positron-emitting fragments in heavy ion beam therapy

A. Chacon, M. Safavi et al, ANSTO

BIC,
QMD
INCL

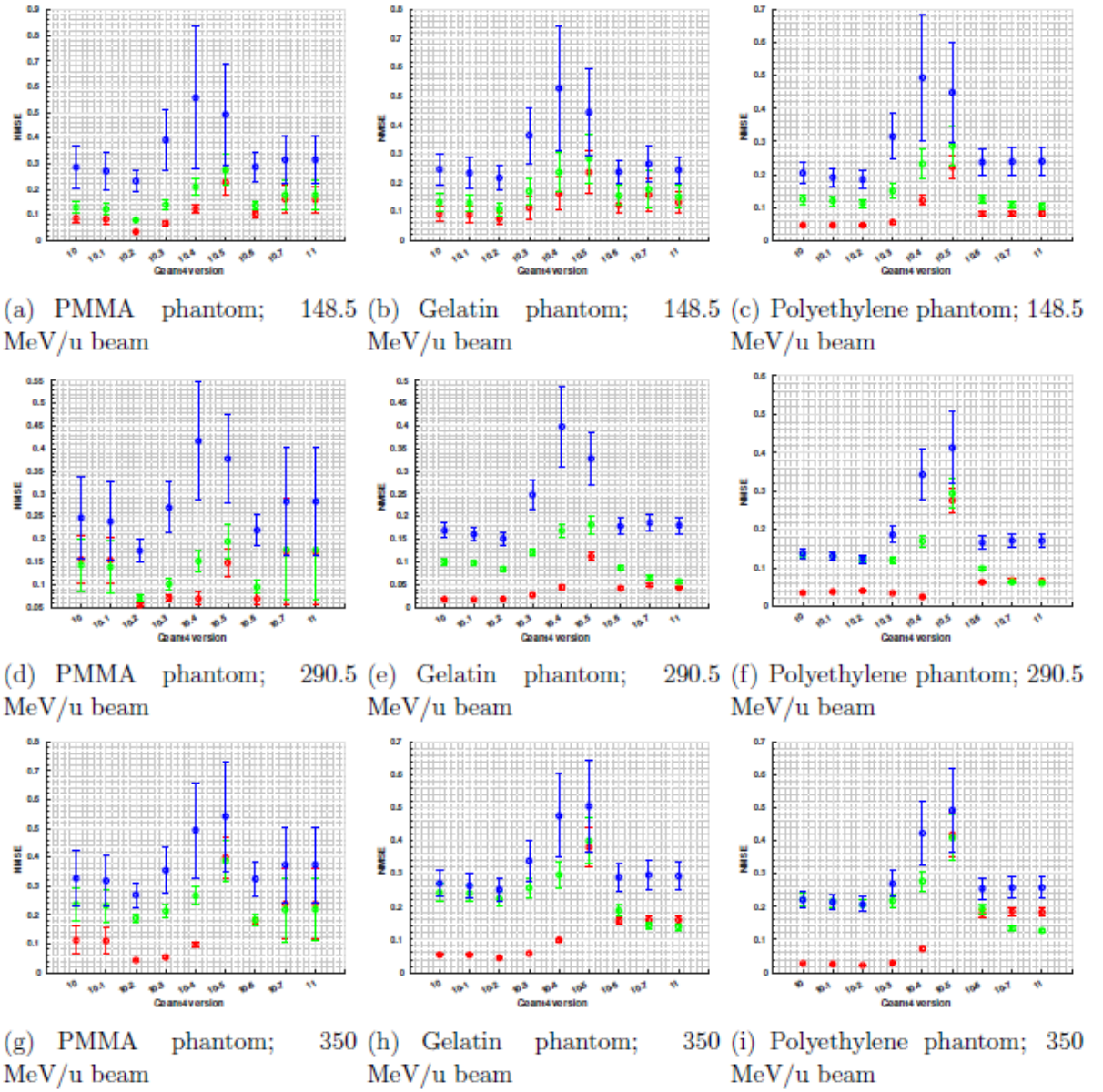
Validation against in-house experimental measurements performed at HIMAC, QST, Chiba, Japan

Table 1: Beam parameters for each ion species and energy. All beams had an energy spread of 0.2 % of the nominal energy; 95% confidence intervals are listed for beam flux.

Ion	Energy (MeV/u)	σ_x (mm)	σ_y (mm)	Beam flux (pps)
^{12}C	148.5	2.77	2.67	$1.8\times10^9 \pm 3.8\times10^7$
^{12}C	290.5	3.08	4.70	$1.8\times10^9 \pm 6.4\times10^7$
^{12}C	350	2.50	2.98	$1.8\times10^9 \pm 4.6\times10^7$
^{16}O	148	2.79	2.89	$1.1\times10^9 \pm 2.8\times10^7$
^{16}O	290	2.60	4.90	$1.1\times10^9 \pm 7.0\times10^7$

normalised mean square error (NMSE)

$$NMSE = \frac{\sum_{i=1}^{N_{reg}} |S_i - E_i|^2}{\sum_{i=1}^{N_{reg}} |E_i|^2}$$



(a) PMMA phantom; 148.5 MeV/u beam (b) Gelatin phantom; 148.5 MeV/u beam (c) Polyethylene phantom; 148.5 MeV/u beam

(d) PMMA phantom; 290.5 MeV/u beam (e) Gelatin phantom; 290.5 MeV/u beam (f) Polyethylene phantom; 290.5 MeV/u beam

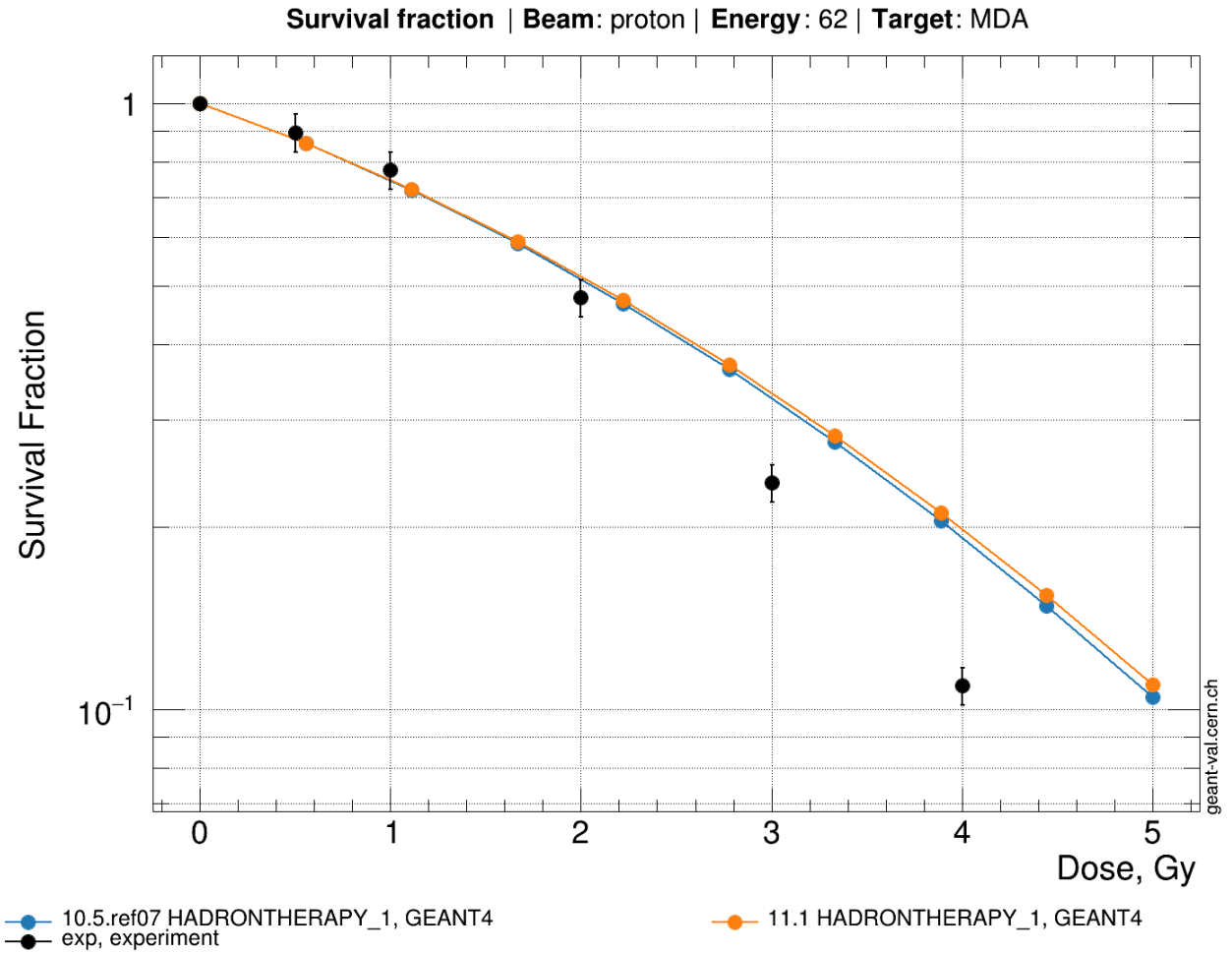
(g) PMMA phantom; 350 MeV/u beam (h) Gelatin phantom; 350 MeV/u beam (i) Polyethylene phantom; 350 MeV/u beam

Figure 5: The NMSE in the build-up and Bragg peak region using carbon beams for *all positron emitting fragments.*

Cell survival - hadrontherapy

Cell line: MDA-MB231 (human breast cancer cell line)

- Calculation of in-vitro cell survival curves and comparison against experimental measurements
- Irradiation at 20 mm depth in water, corresponding to the mid of a clinical 62 MeV modulated clinical proton beam
- Exp data: Petringa et al. 2019, Physica Medica, 58: 72–80



To do

- Currently
  - doing the data analysis for the C-12 fragmentation tests
- Run with 11.1 (for paper n.2)
  - In-vivo PET hadrontherapy tests with 11.1
- Do the data analysis for all hadronic tests (for paper n.2)
- Benchmark the execution times (for paper n.2)
- On the longer term, for both EM and hadronic tests,
  - Include all tests in the Geant4 rep (help is needed)
  - Develop a website to support the Geant4 bio-medical physics community (e.g. examples of Geant4 for bio-medical applications, G4-Med tests, etc)

Tests to include in the future

- Radioactive decay – L. Desorgher et al
- Nuclear medicine tests – A. Malaroda, S. Guatelli et al, help is needed
- Photon energy fluence profile and thick target photon backscatter benchmark - J. Carrasco Hernandez, B. Faddegon and J. Ramos Mendez, UCSF
- Calculation of the wall correction factors, kwall, for two graphite ionization chambers – P. Arce
- Include benchmark against ICRU Report 90: Stopping Powers of electrons (and positrons), protons, α particles and carbon ions for three key materials: graphite, air, and liquid water – Help is needed
- Include total inelastic cross section tests of production of C-10 and C-11 important for carbon ion in-vivo PET and Prompt Gamma imaging- E. Simpson, ANU, help is needed
- Validation of the Medical Linac advanced examples against EURADOS Report 2020-05 – C. Caccia and C. Mancini
- Neutron tests – Help is needed

Final remarks

- To reach the stated goals in a reasonable timeframe, “help is needed” items will be circulated among the G4-Med members
- **`geant-val`**
  - It is important to maintain and further develop this platform
  - It would be useful to have documentation to include tests and run them
  - It would be useful if more people could run the tests on geant-val
  - We have two members of the G4 Medical Simulation Benchmarking Group willing to contribute to `geant-val`
- Let me thank all contributors!