

# G4-Med, a Geant4 benchmarking for bio-medical physics applications

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***On behalf of the Geant4 Medical Simulation Benchmarking Group***

**ICCR 2024, XX<sup>th</sup> International Conference on the use of Computers in Radiation therapy,  
8 - 11 July 2024, Lyon, France**



# Geant4 Medical Simulation Benchmarking Group

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# The Geant4 Medical Simulation Benchmarking Group

<https://twiki.cern.ch/twiki/bin/view/Geant4/G4MSBG>

- Created in 2014
- Coordination Team since 2018:**
  - Coordinator:** Susanna Guatelli (Univ. Wollongong, Australia)
  - Deputy-coordinator:** Pedro Arce (CIEMAT, Spain)
- 57 researchers; 32 institutions from 12 different countries



Health  
Nepean Blue Mountains  
Local Health District



Radboudumc  
university medical center



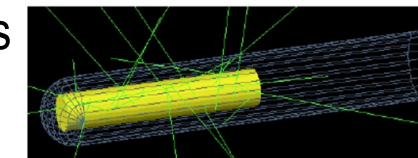
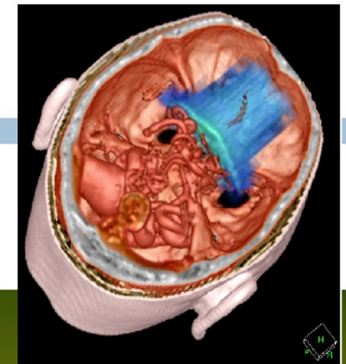
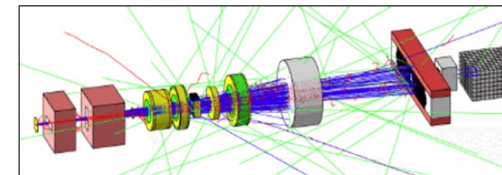
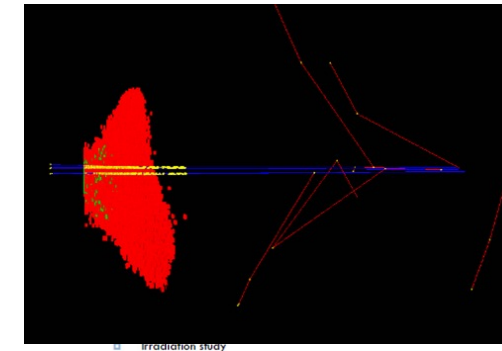
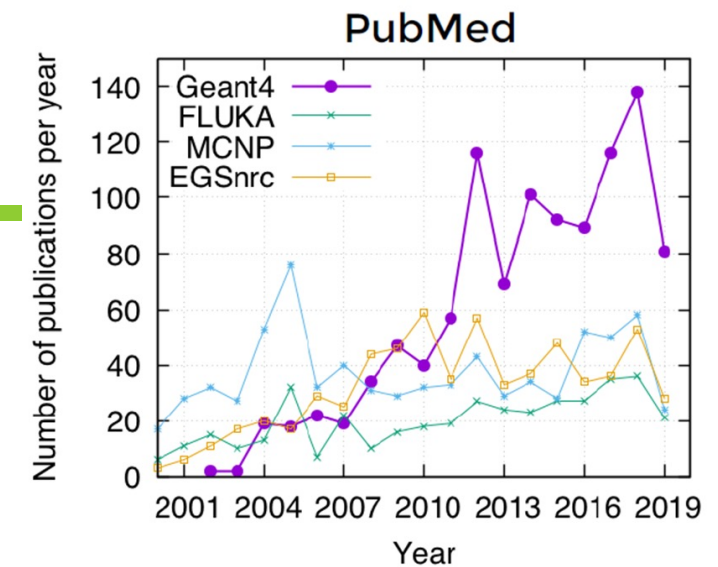
SAPIENZA  
UNIVERSITÀ DI ROMA



UNIVERSITY  
OF WOLLONGONG  
AUSTRALIA



- General purpose MC code modelling particle transport and interactions in matter
  - Developed and maintained by a large international Collaboration (> 100 members),
- Applications in medical physics, including:
  - Verification of clinical TPS
  - Development of detectors
  - Dosimetry
  - Imaging (e.g PET, SPECT, CT)
  - Radiopharmaceutical production
  - Radiation protection
- Dosimetry, micro-dosimetry to DNA damage
- It can be used stand-alone or via GAMOS, GATE and TOPAS
- Beta release in July, public release per year (December), eventual patches



# Motivation & Goals

- **G4-Med project:**

- 22 tests to benchmark Geant4 pre-built physics lists for bio-medical physics applications.
  - Against reference data and experimental measurements.
- Executed for regression tests.
  - **geant-val** @ CERN
  - Some in Geant4 **nightly** tests.

- **Goals:**

- Provide physics list recommendations.
- Monitor physics capability of Geant4.
- **New:** track computational execution time

- **Webpage:**

<https://twiki.cern.ch/twiki/bin/view/Geant4/G4MSBG>



Results with Geant4 10.5, Arce et al (2021),  
Medical Physics, 48 (1), pp:19-56 (paper #1)

## MEDICAL PHYSICS


The International Journal of Medical Physics Research and Practice




Research Article | [Full Access](#)

### Report on G4-Med, a Geant4 benchmarking system for medical physics applications developed by the Geant4 Medical Simulation Benchmarking Group

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, A. Dotti, B. Faddegon, C. Fedon, S. Guatelli , S. Incerti ... See all authors 

First published: 11 May 2020 | <https://doi.org/10.1002/mp.14226> | Citations: 102

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### Abstract

#### Background

Geant4 is a Monte Carlo code extensively used in medical physics for a wide range of applications, such as dosimetry, micro- and nanodosimetry, imaging, radiation protection, and nuclear medicine. Geant4 is continuously evolving, so it is crucial to have a system that benchmarks this Monte Carlo code for medical physics against reference data and to perform regression testing.

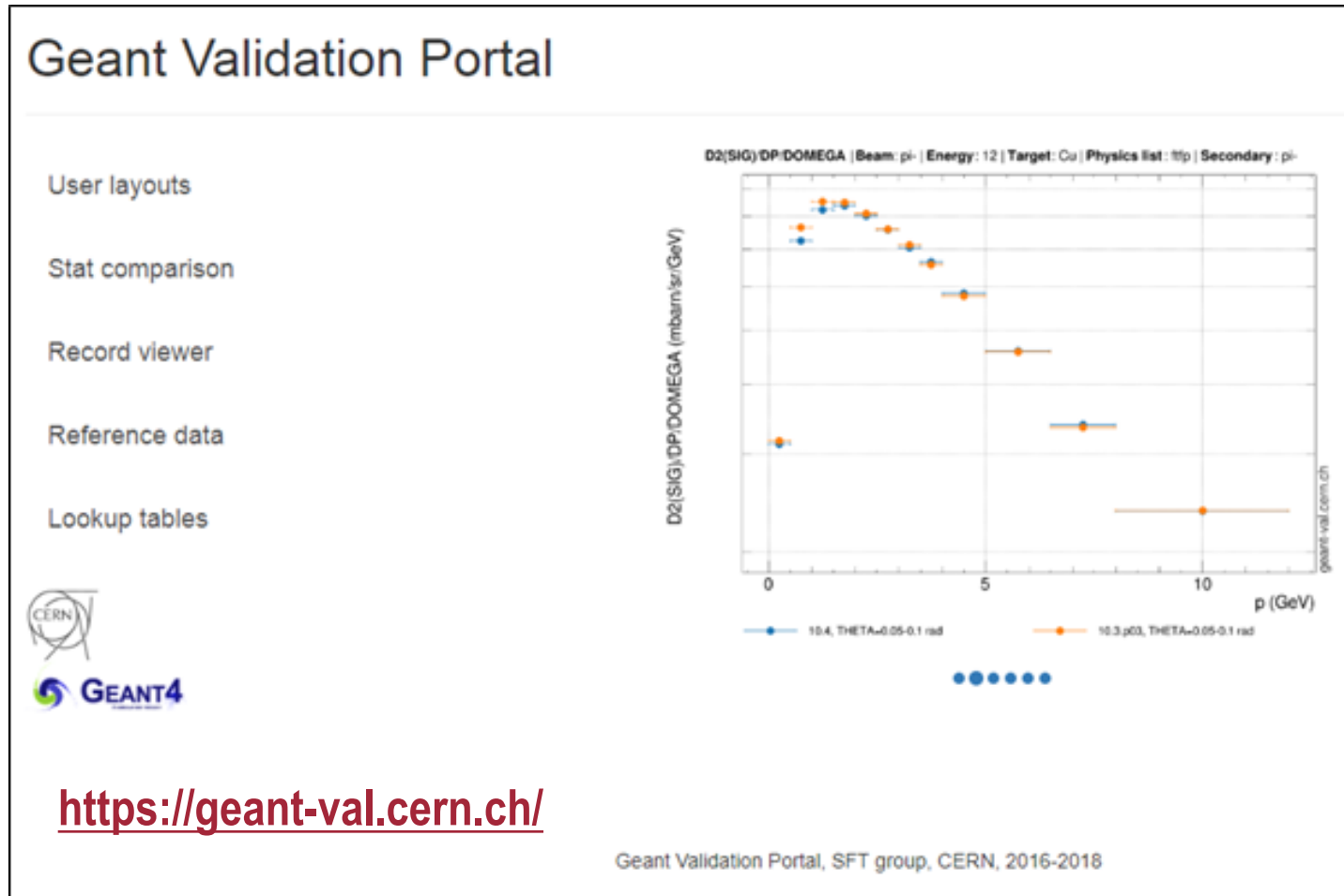
#### Aims

To respond to these needs, we developed *G4-Med*, a benchmarking and regression testing system of Geant4 for medical physics.



# How to access the results of the tests

## Regression tests on the CERN computing infrastructure



- Results with **Geant4 10.5** documented in Arce et al (2021), Medical Physics, 48 (1), pp:19-56 ([Paper #1](#))
- Results with **Geant4 10.5, 10.6 and 11.1** in geant-val
- Now running **Geant4 11.2.1**

# G4-Med tests

- Geant4-DNA tests:
  - Low dose energy electron Dose Point Kernels
  - Microdosimetry
  - Chemistry
- EM physics tests
  - Brachytherapy (Ir-192 and I-125)
  - Electron FLASH radiotherapy
  - MV X-ray radiotherapy test
  - Photon attenuation coeff
  - Electron electronic stopping power
  - Electron backscattering
  - 13 MeV electron forward scattering
  - Bremsstrahlung from thick targets
  - Fano cavity
  - Monoenergetic x-ray internal breast dosimetry
- Hadronic nuclear cross section tests
  - Nucleus-nucleus hadronic inelastic scattering cross sections
  - 62 MeV/u  $^{12}\text{C}$  fragmentation
  - Charge-changing cross sections for 300 MeV/u  $^{12}\text{C}$  ions
- EM + hadronic physics tests
  - 62 MeV proton beam test (cell survival modelling and averaged LET track)
  - In-vivo PET for carbon ion therapy
  - 67.5 MeV proton Bragg curves in water
  - Light Ion Bragg Peak curves
  - Neutron yield of 113 MeV and 256 MeV protons and 290 MeV/u carbon ions
  - Fragmentation test of a 400 MeV/u  $^{12}\text{C}$  ion beam in water

Green: tests included since 2021

# Regression testing: methodology

- Regression testing between Geant4 10.5 (paper #1) and 11.1 for the existing tests:
  - Mean Relative Error (MRE), Normalised Mean Absolute Error (NMAE) and maximum difference between simulated and reference data

$$\text{MRE} = \sum_{i=1}^n \frac{|S_i - R_i|}{R_i} \quad \text{NMAE} \equiv \frac{\frac{1}{n} \sum_i |S_i - R_i|}{\frac{1}{n} \sum_i R_i} = \frac{\sum_i |S_i - R_i|}{\sum_i R_i}.$$

- Data analysis performed by J. Archer, with the support of C. White, @ CMRP, University of Wollongong (Australia).
- Results available at <https://g4-med.docs.cern.ch/>



# Geant4-DNA tests: new

## Tests: Low energy $e^-$ dose point kernels and microdosimetry

- **Geant4-DNA physics list Option 2**
  - Based on the dielectric theory for electron ionisation and excitation
- **Geant4-DNA physics list Option 4**
  - Based on the dielectric theory for ionisation and excitation
  - More accurate electron cross sections at lower energies ([Kyriakou et al 2016, Journal of Applied Physics, 119\(19\):194902](#))
- **Geant4-DNA physics list Option 6**
  - Re-engineering of CPA100 for electrons ([Terrissol and Baudre, Radiation Protection Dosimetry, 1990, 31\(1-4\), 175-177](#)).
  - Binary Encounter model Bethe formalism for ionisation ([Kim & Rudd, Physical Review A, 1994, 50\(5\):3954-67](#); [Bordage et al Physica Medica 2016, 32\(12\):1833-40](#)).
  - Dielectric theory for electron excitation
- Same proton, H, He and its charge states, ions physics processes (see [Incerti et al, Medical Physics, 2018, 45:e722-e739](#))

## Test on chemical stage: **chem\_option3** chemistry constructor

- **Step-by-Step approach (SBS)** ([Karamitros et al, 2011, Prog. in Nucl. Sci. and Tech., 2:503](#))
  - Transport of chemical species in discrete steps (or time steps  $\Delta t$ ) through Brownian motion until a chemical encounter defines a reaction
- **IRT** ([Ramos-Méndez et al, 2020, Medical Physics, 47\(11\):5919-30](#))
  - Calculation of chemical reaction probability
  - Reaction times can be sampled for every potential pair of reactants.
  - Reactions are then modelled sequentially, starting with those with the shortest reaction time.
  - Products of chemical reactions may undergo further reactions
- **IRT-sync** ([Tran et al, 2021, Medical Physics, 48\(2\):890-901](#))
  - It uses as the time step the randomly sampled time given by the IRT model until the next expected reaction.
  - After each time step, it is necessary to synchronise the time and position of all diffusing species
  - + access to spatial-temporal information at certain times, for all chemical species, which can then be coupled with information about geometry and boundaries.

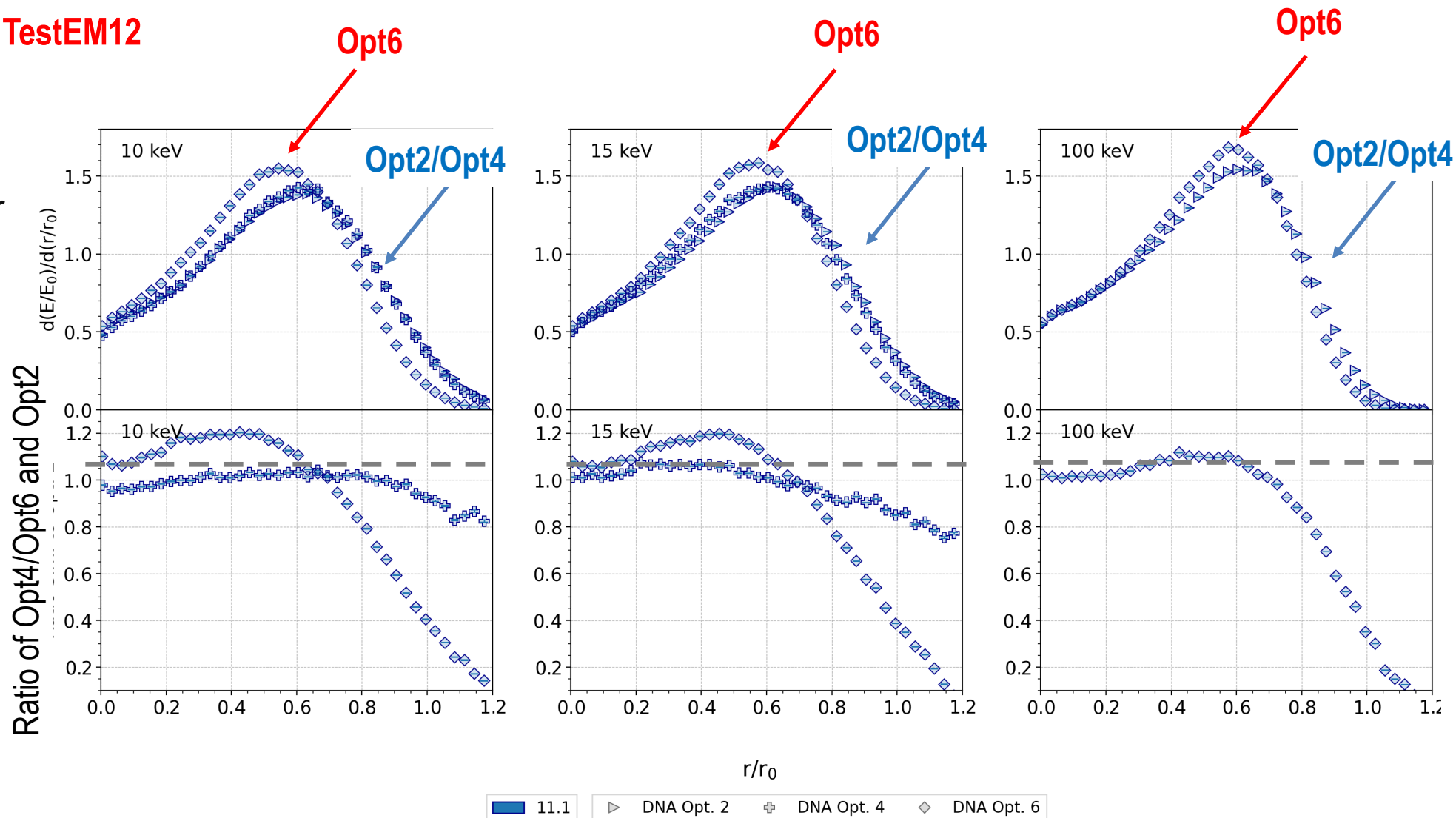
# Geant4-DNA (new) : Low energy dose point kernels test – Geant4 11.1

## Geant4 extended example TestEM12

Dose point kernel test

Radial energy deposition for  
an isotropic source of  
electrons

Regression testing



# Snapshot of the G4EM constructors (Geant4 11.1) (1)

- G4EmStandardPhysics\_option3 (“**OPT3**”), G4EmStandardPhysics\_option4 (“**OPT4**”), G4EmLivermorePhysics (“**LIVERMORE**”), G4EmPenelopePhysics (“**PENELOPE**”) and G4EMStandard\_SS (“**SS**”)

Geant4	WVI	Opt3	SS	Opt4	Livermore	Penelope
Rayleigh scattering and photoelectric effect	Livermore (EPICS2017) Li et al. <sup>59</sup>					PENELOPE
Compton scattering	G4KleinNishina Model		G4LowEPComptonModel for E < 20 MeV Brown et al. <sup>62</sup> , G4KleinNishina for E >20 MeV		Livermore (EPICS2017) Li et al. <sup>59</sup>	PENELOPE
Gamma conversion	G4BetheHeitler5DModel Bernard <sup>60 61</sup>				G4Livermore5DModel Li et al. <sup>59</sup>	PENELOPE
e <sup>-</sup> and e <sup>+</sup> ionisation	Standard		PENELOPE for E < 100 keV, Standard for E > 100 keV		Livermore for E < 100 keV Standard for E > 100 keV	PENELOPE
e <sup>-</sup> and e <sup>+</sup> bremsstrahlung	Geant4 Standard Model	G4SeltzerBergerModel for E < 1 GeV, G4eBremsstrahlungRelModel for E > 1 GeV				PENELOPE
e <sup>+</sup> annihilation	G4eplusTo2GammaOKVIModel <sup>56</sup>	Standard				PENELOPE
e <sup>-</sup> and e <sup>+</sup> multiple scattering	Urban model for E < 1 MeV, Wentzel model for E > 1 MeV	Urban model	Not available	Goudsmit-Saunderson model (Incerti et al. <sup>63</sup> ) for E < 100 MeV Wentzel model for E > 100 MeV		
Coulomb scattering	on	off	on			
Bremsstrahlung angular distribution	Modified Tsai	2BS	Modified Tsai	2BS		PENELOPE

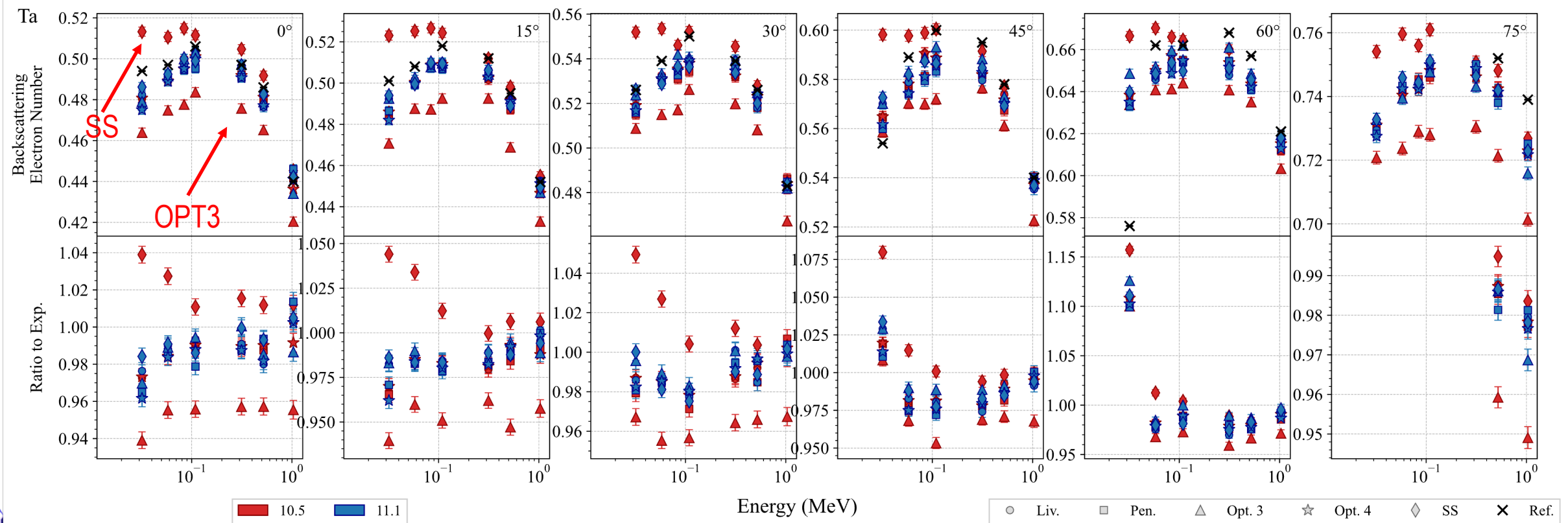
# Geant4 EM Physics constructors: changes between Geant4 10.5 and 11.1

- Multiple scattering parameters in Opt3 changes in Geant4 11.1
  - RangeFactor has been changed from 0.04 to 0.03
  - Step limitation algorithm for multiple scattering from *DistanceToBoundary* to *safetyPlus*
- Since Geant4 11.1, the [Livermore physics processes](#) use by default the newly introduced [EPICS2017](#) (Electron–Photon Interaction Cross Sections) data libraries to describe Rayleigh scattering, photoelectric effect, Compton scattering and gamma conversion processes ([Li, Z, et al. \(2022\) Physica Medica, 95:94–115](#)).
- The [G4BetheHeitler5DModel](#) ([D. Bernard \(2013\) NIM A. 2013;729:765–780 and 2018; 899:85–93](#)), has become the default model to describe gamma conversion in Opt3 and Opt4, substituting the Standard model.
- In Geant4 11.1, in Opt4, the Penelope model substitutes the Livermore model to describe the ionisation process of electrons with energy below 100 keV.
- Proton ionisation: in Geant4 11.1 [adoption of ICRU90 data for water, air, graphite](#). For the other materials, NIST PSTAR data are used if available. If not, ICRU49 is used.
- In Geant4 11.1, new ionization model for ions heavier than Helium, the [G4LindhardSorensenIonModel](#) for energies above 2MeV/amu, while, for lower energies, ICRU73 and ICRU90 data are used.

# Backscattering test

by P. Dondero, R. Stanzani and A. Mantero,  
SWHARD, Genova, Italy

- Calculation of the fraction of electrons backscattered by a target
- Comparison against Sandia Lab experimental data (Lockwood et al. Technical Report, Sandia Labs., 1980 and 1981)
- Geant4 11.1 provides a clear improvement for the Geant4 EM constructors Opt3 and SS for high Z materials (Mo, Ta, U)





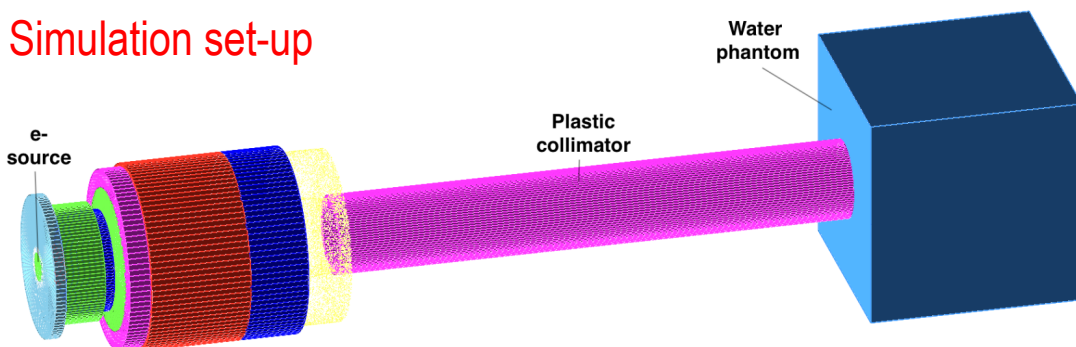
# Electron FLASH radiotherapy test (1): new

by F. Romano & G. Miluzzo (INFN Catania), and J. H Pensavalle  
(Azienda Ospedaliero Universitaria Pisa)

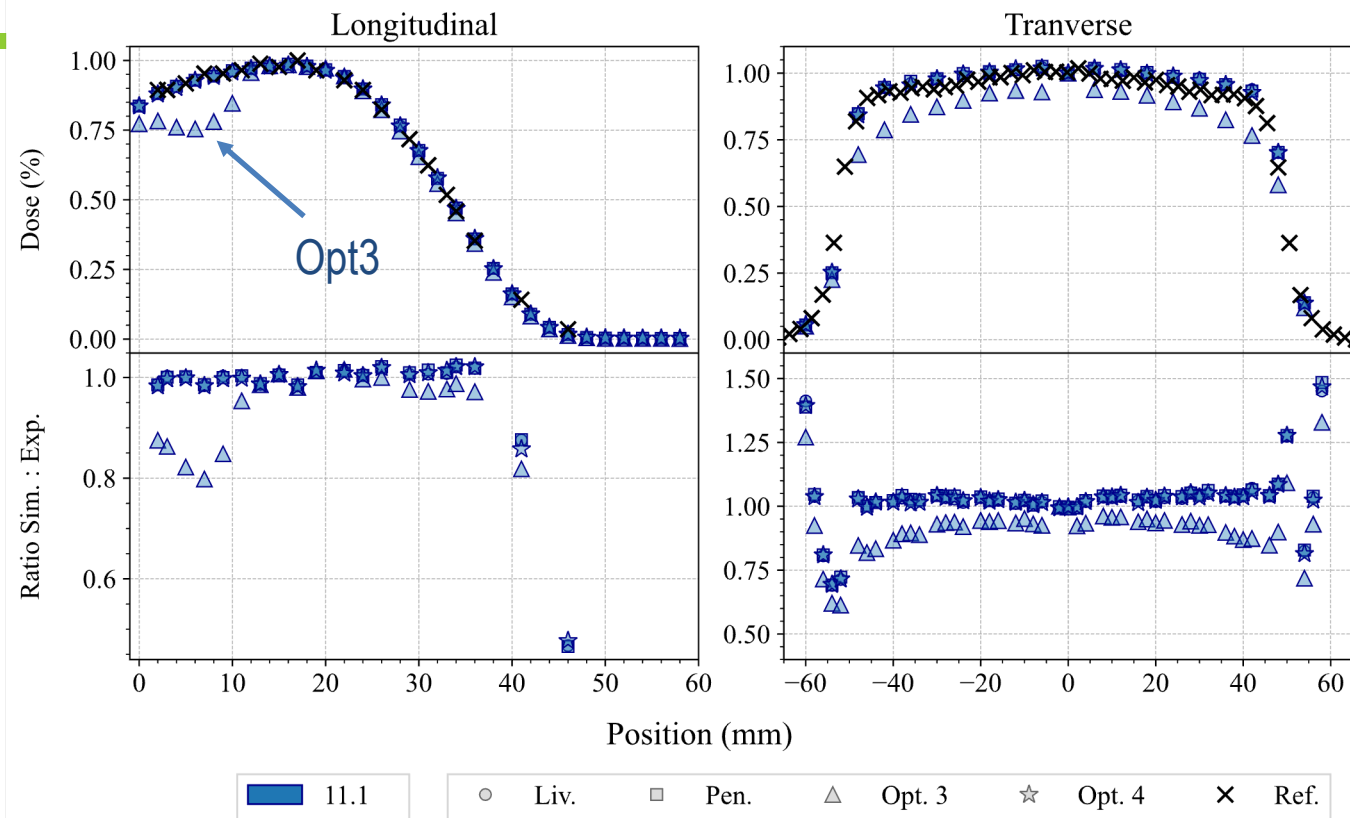
## Geant4 advanced example eFLASHradiotherapy

- Model of a Triode Electron Gun Equipped ElectronFlash Linac, manufactured by Sordina Iort Technologies S.p.A.
  - Installed at the CPFR (Centro Pisano Flash Radiotherapy) in Pisa, Italy
- a  $2.5 \times 2.5 \text{ mm}^2$   $e^-$  source with an ad-hoc energy spectrum peaked at 9 MeV, provided by the manufacturer (SIT Sordina)

## Simulation set-up



Geant4 11.1



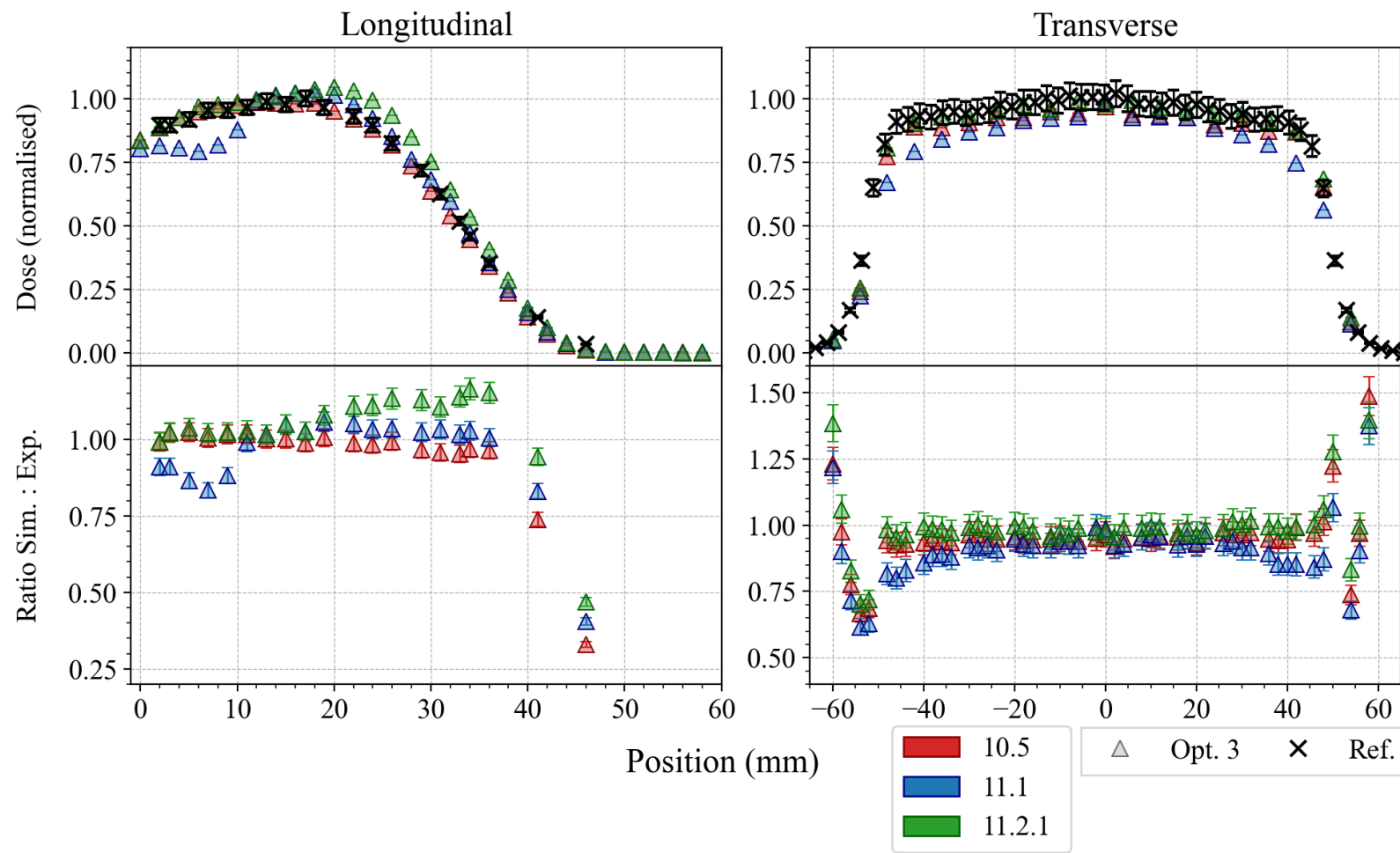
Geant4 EM Standard Physics Option 3: *RangeFactor* in Geant4 11.1 is 0.03.

Based on these results, [Geant4 patch 11.2.1](#), has been recently released where the *RangeFactor* in Opt3 is back to 0.04.



# Electron FLASH radiotherapy test (2): new

- Geant4 11.1: multiple scattering parameters were changed in Opt3
- Reverted back to parameters of Geant4 10.5 in Geant4 11.2.1

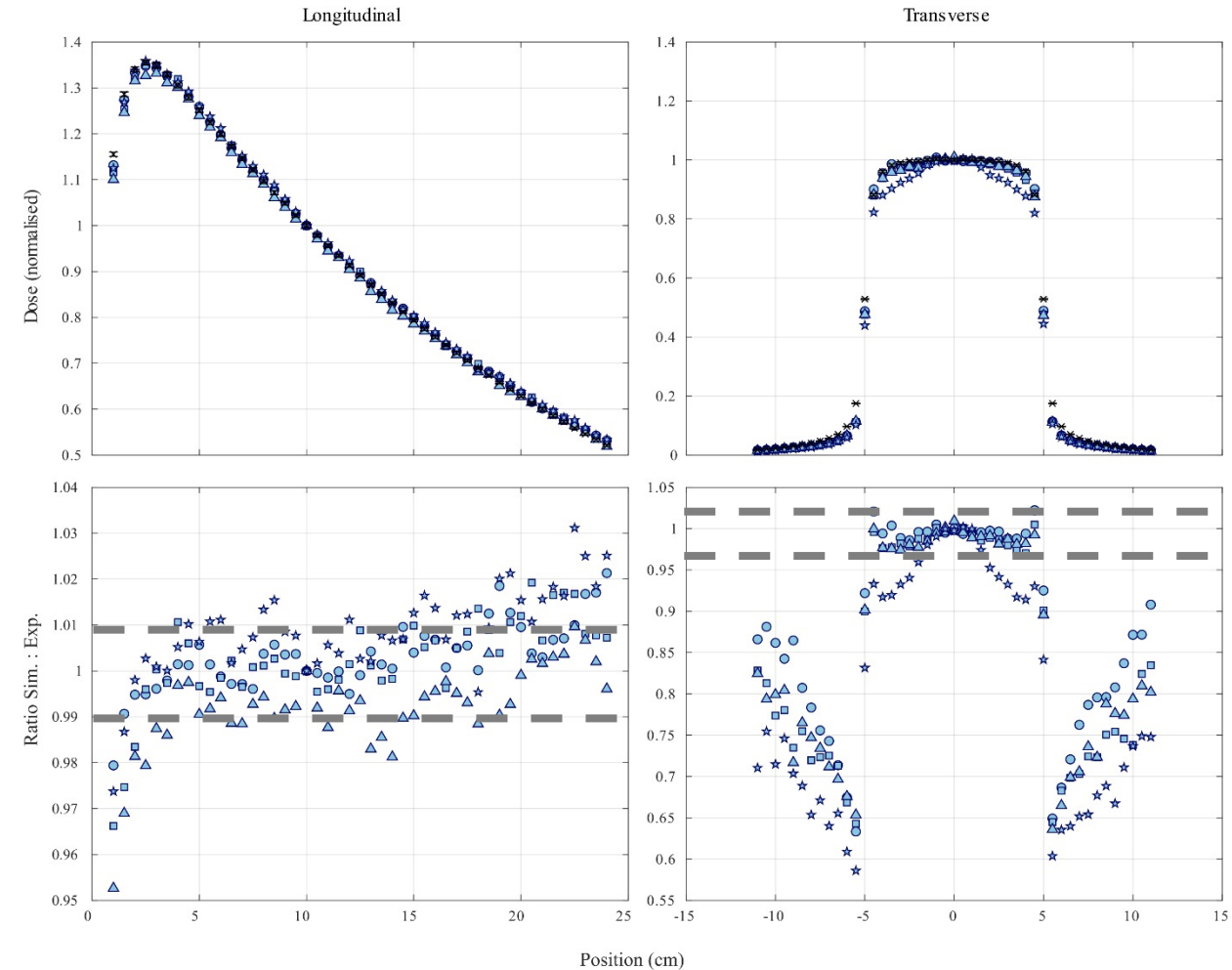
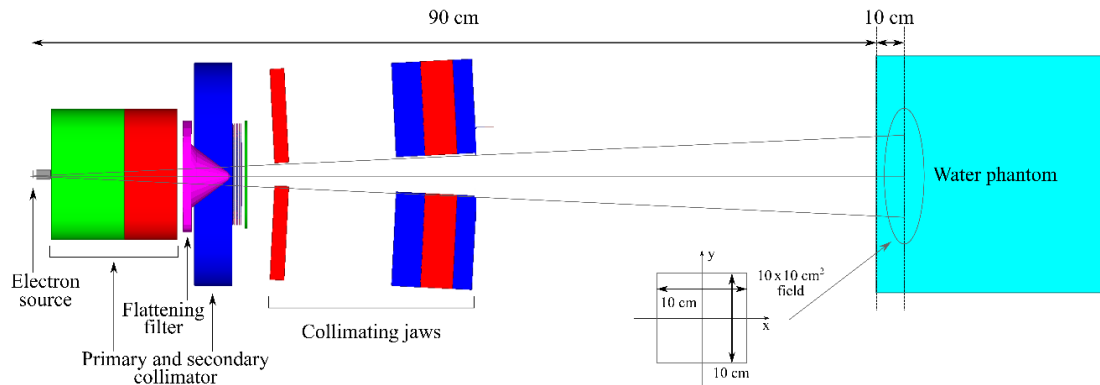


# MV X-ray radiotherapy test: new

By B. Caccia and S. Pozzi (Istituto Superiore di Sanita', Rome, Italy)  
and C. Mancini-Terracciano (La Sapienza, Rome, Italy)

- Geant4 advanced example medical\_linac
- Model of a GE Saturne 43 linear accelerator (EURADOS Report Caccia et al, 2020-05)
- 3D dose in a water phantom

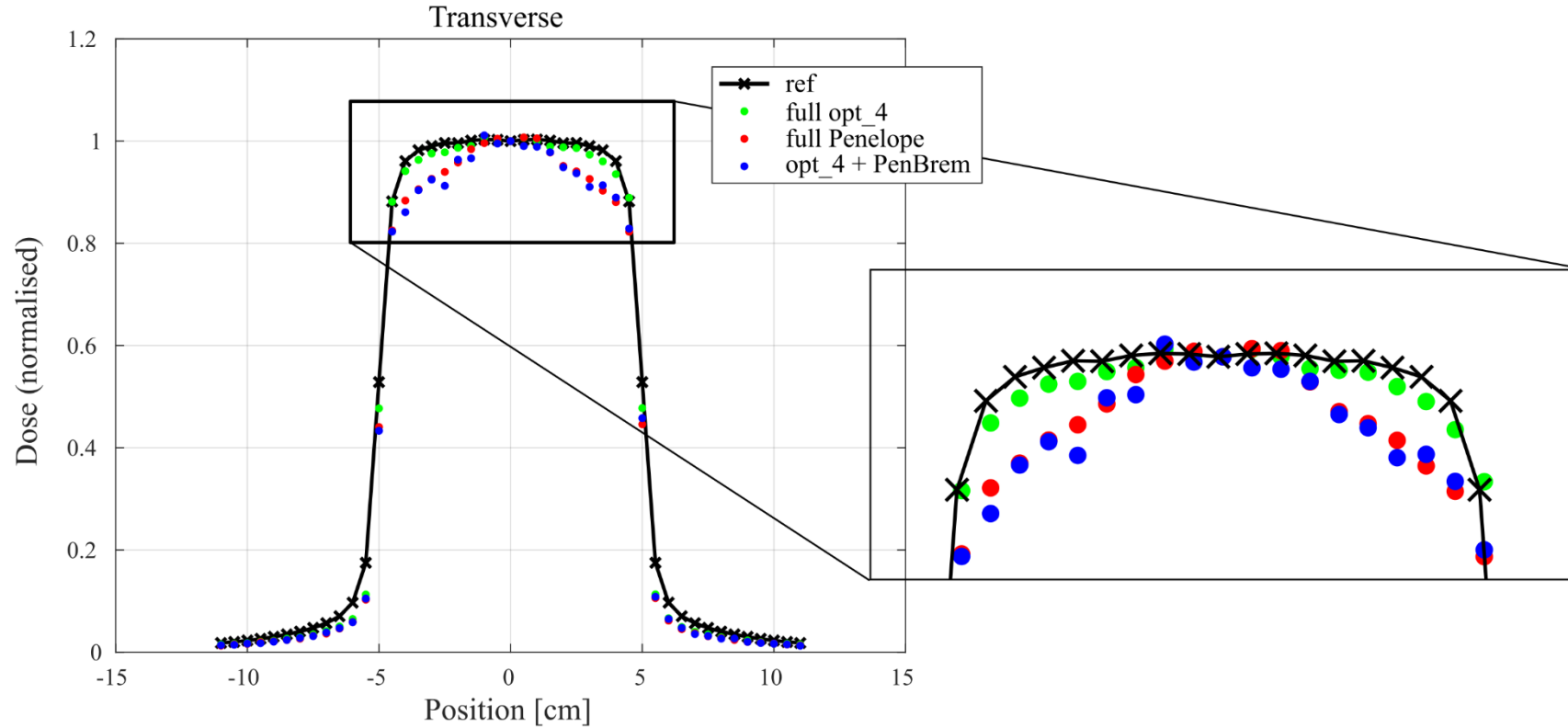
## Simulation set-up



— — ■ Uncertainty affecting the exp data

■ 11.1    ● Opt. 3    ■ Opt. 4    ▲ Liv.    ★ Pen.    ✕ Ref.

# MV X-ray radiotherapy test: new



- The Geant4 Penelope Bremsstrahlung process seems to have problems
- This is now under investigation

# Geant4 Physics Lists Tested: EM + Hadronic

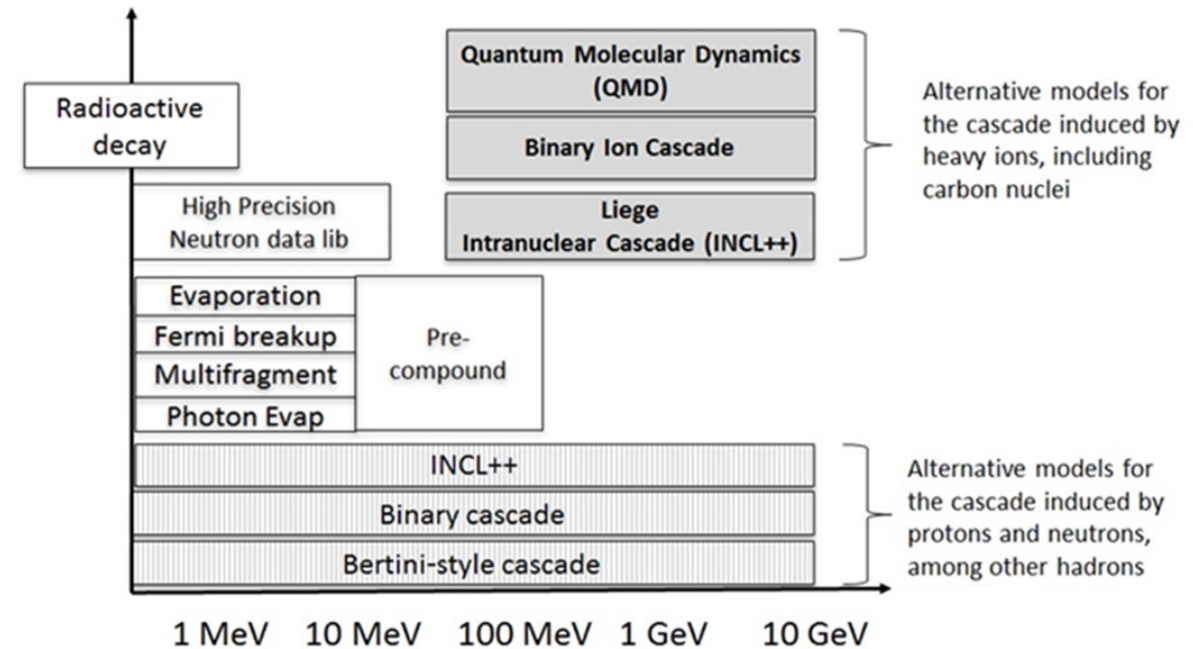
## For proton therapy:

- **QGSP\_BIC\_HP**
  - High Precision data libraries for neutrons with energy < 20 MeV
- **QGSP\_BIC\_AIHHP**
  - Physics model that uses TALYS-based Evaluated Nuclear Data Library (TENDL). TENDL is based on experimental and calculated results of TALYS nuclear model code to produce a nuclear data library for p, n,  $^2\text{H}$ ,  $^3\text{H}$ ,  $\alpha$  and  $^3\text{He}$  for energies below 200 MeV
- **QGSP\_BERT\_HP**
  - High Precision data libraries for neutrons with energy < 20 MeV

## For carbon ion therapy:

### QGSP\_BIC\_HP +

- **G4IonBinaryCascade** - LightIonBinaryCascade model (BIC).
- **G4IonQMDPhysics** - Quantum Molecular Dynamics (QMD) model.
- **G4IonINCLXXPhysics** - Liège Intranuclear-Cascade model (INCL).



## Fragmentation models

- **BIC:** Interaction between a projectile and a single nucleon of the target nucleus interacting in the overlap region as Gaussian wave function
- **QMD:** All nucleons of the target and projectile, each with their own wave function;
- **INCL:** Nucleons as a free Fermi gas in a static potential well. Targets and projectiles with  $A \leq 18$ .

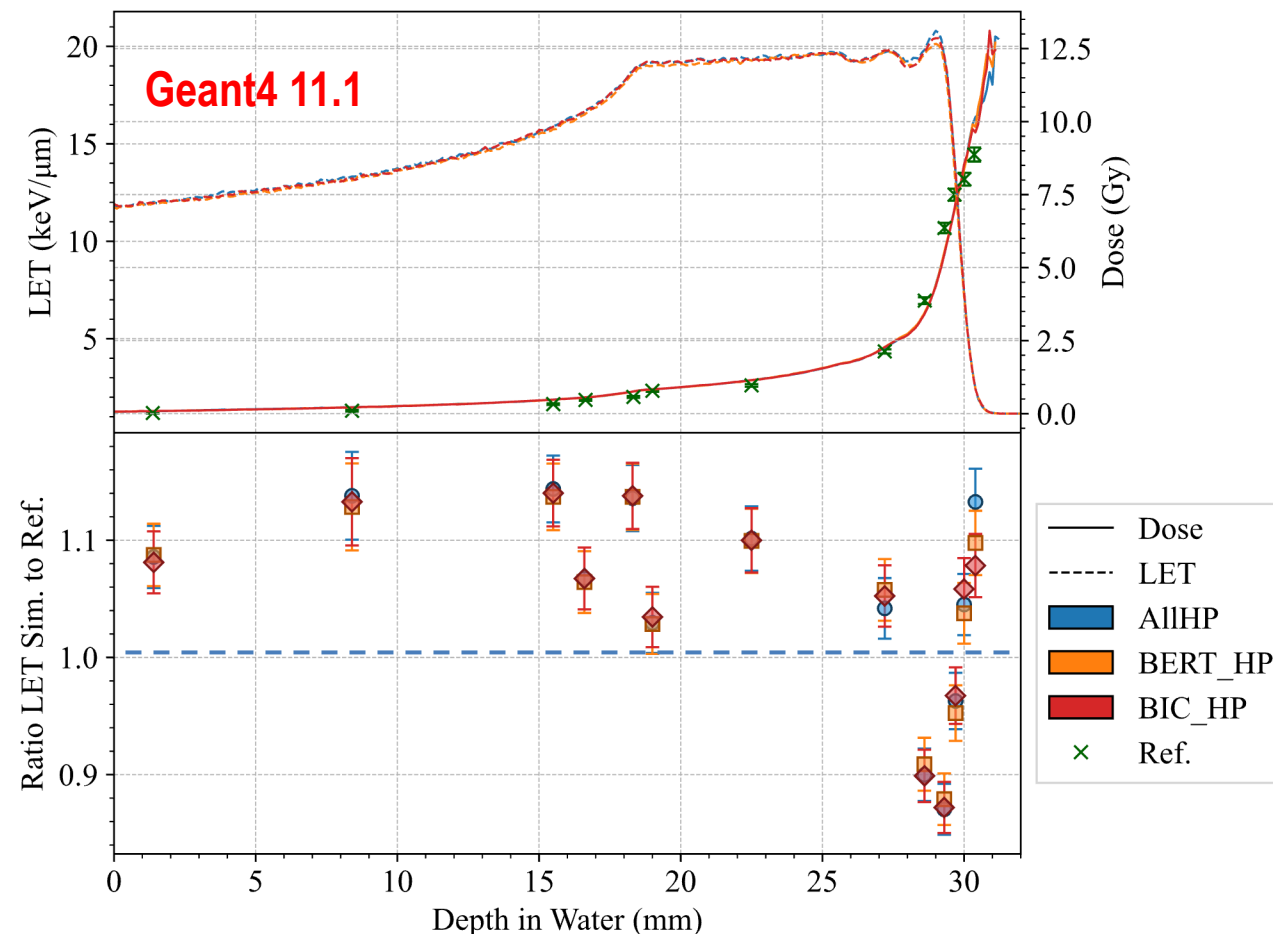
# Improvements in Geant4 hadronic physics for medical applications (between Geant5 10.5 and 11.1)

- Consistency improvements, clean-up and optimization of the code have been performed
- Improvements in nuclear data libraries
  - [G4PARTICLEXS1.1](#) in Geant4 10.5 -> [G4PARTICLEXS.4.0](#) (Geant4 11.0 and used also in Geant4 11.1)
    - more accurate fusion cross-sections and inelastic cross-sections for n, p, light ions and gamma
  - The [former G4PhotoNuclearCrossSection](#) has been substituted by [IAEA evaluated photo-nuclear data library](#), which covers the energy range 0 —130 MeV, for 219 isotopes.
  - [G4NDL.4.7](#) (released with Geant4 version 11.1), [incorporates new neutron cross-sections and final states obtained from JEFF-3.3 data library](#), including new materials for the simulation of thermal neutrons (vs. G4NDL.4.5 present in version 10.5).
  - [G4TENDL.1.4](#), released with Geant4 11.0, uses ENDF/B-VIII.0 and TENDL-2019 libraries (vs. G4TENDL.1.3.2 in Geant4 10.5, which used ENDF/B740 VII.1 and TENDL-2014 libraries).
- Changes in the modelling of the [de-excitation channels in the Fermi Break-Up model](#): Many more reaction channels are now considered

- **Geant4 advanced example hadrontherapy**
- Model the INFN-LNS "CATANA" clinical proton therapy beamline designed for treating ocular melanomas using 62 MeV proton beams
- Track-average LET is compared against  $y_F$  values (ICRU Report 36), derived from experimental microdosimetric spectra acquired at different depths in water along the SOBP

$$y = \frac{\varepsilon_S}{\bar{l}} \quad \bar{y}_F = \int_0^\infty y f(y) dy,$$

- Exp data obtained using the MicroPlus probe detector (Tran T et al, Applied Sciences. 2022;12(1): 2076-3417)  
 $L_i$ = electronic stopping power



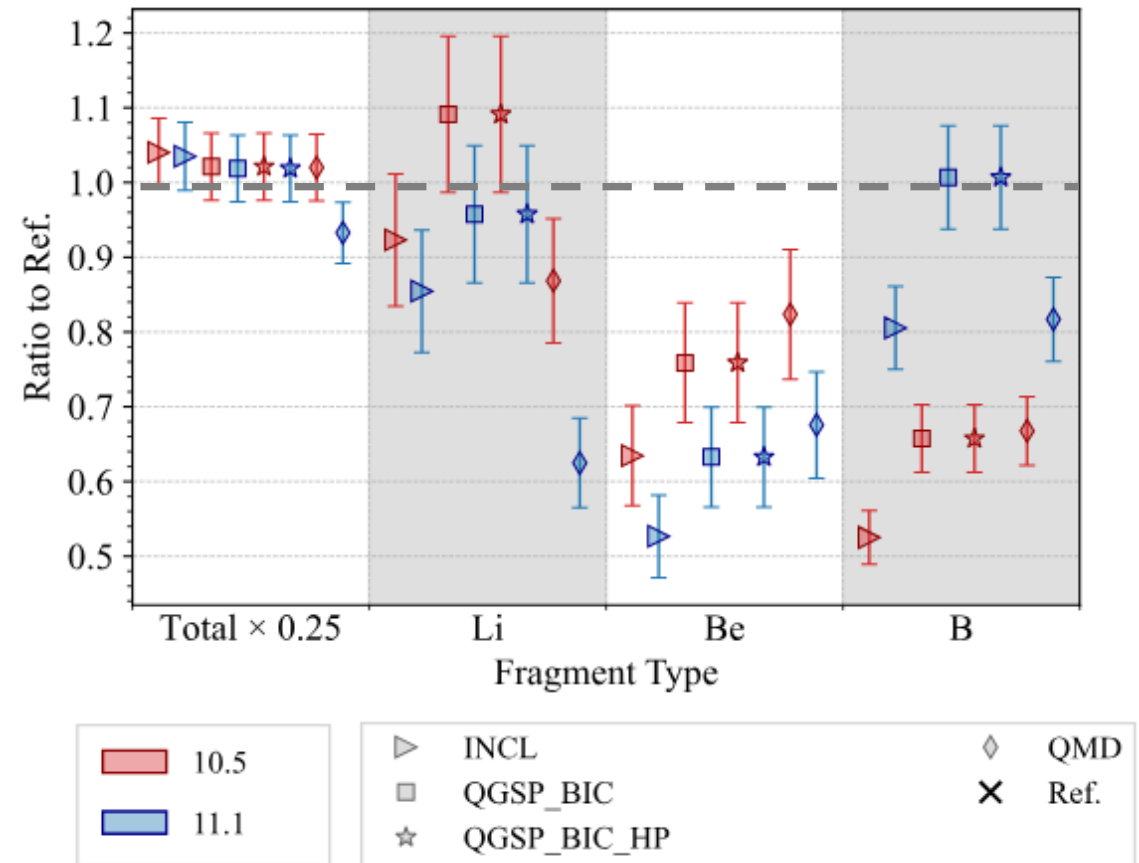
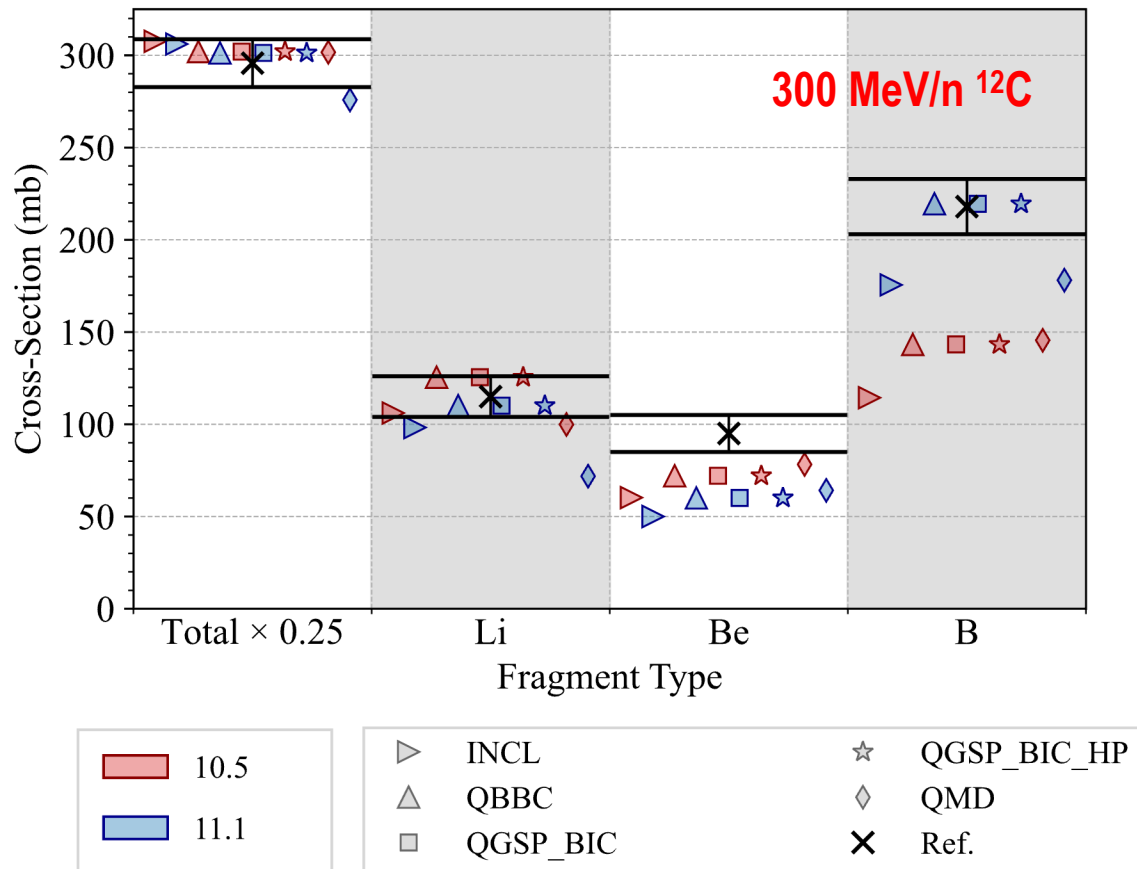
Track-averaged LET

$$\bar{L}_T = \frac{\sum_{i=1}^N L_i l_i}{\sum_{i=1}^N l_i} \quad \bar{L}_T^{Total} = \frac{\sum_{j=1}^n [\sum_{i=1}^N L_i l_i]_j}{\sum_{j=1}^n [\sum_{i=1}^N l_i]_j}$$



# Charge Changing Cross Section (CCCS) By C. Omachi, T. Toshito (Nagoya PTC), T. Sasaki (KEK)

Ref. data: Toshito T, et al (2007) *Phys Rev C*, 75(5): 054606.



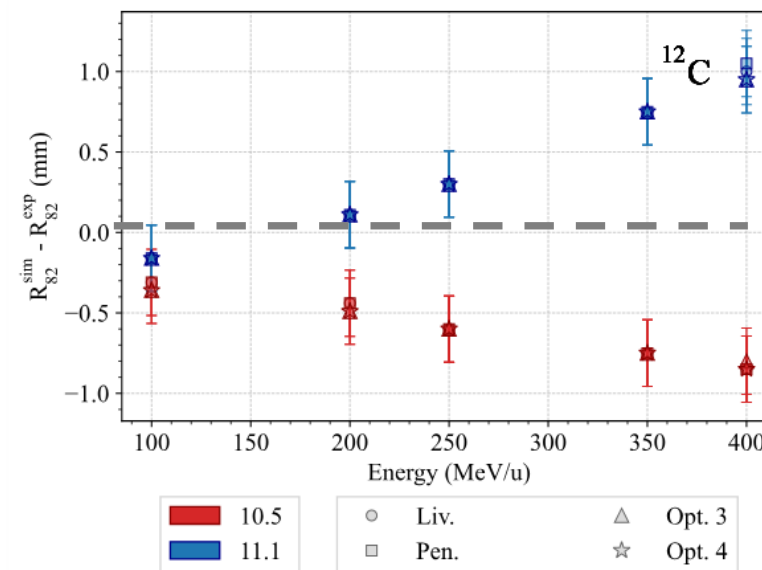
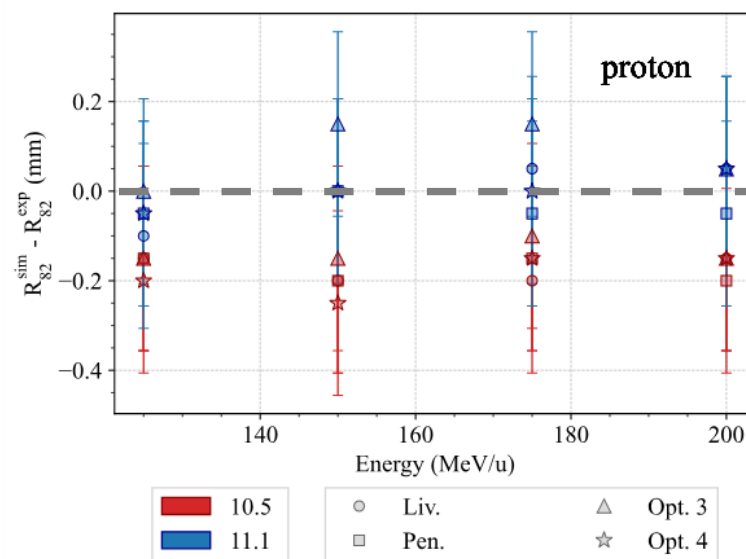
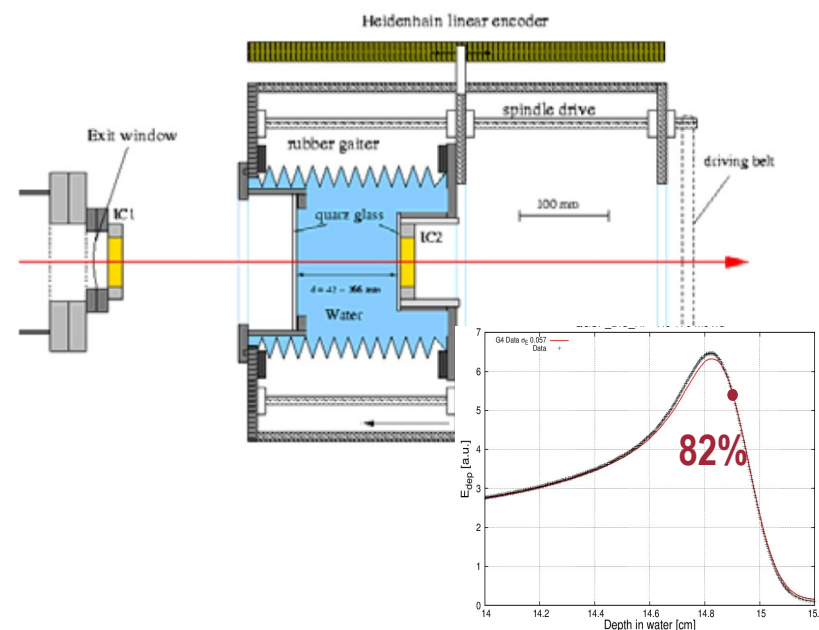
The observed differences in the results are ascribed to differences between Geant4 10.5 and 11.1 in the modelling of the de-excitation channels in the Fermi Break-Up model

# Light Ion Bragg Curves

By M A Cortés-Giraldo, A. Perales and J. M. Quesada, Sevilla University, Spain

Ref. Data: D. Schardt et al., GSI Report 2008-1

QGSP\_BIC\_HP for hadronic physics



- Initial energy spread adjusted from experimental Bragg curves.
- Simplified geometry model for simulation
  - Depths of 82% distal dose are compared.

- Improvement in the calculation of the position of the Bragg Peak of approximately 0.2 mm for incident protons in Geant4 11.1
- Geant4 11.1 produces  $R_{82}$  closer to the reference data for  $^{12}\text{C}$  ions with  $E < 250$  MeV/u.
- In the case of 400 MeV/u  $^{12}\text{C}$ , the difference of  $R_{82}$  is  $\sim 1$  mm with Geant4 11.1 and 0.85 mm with Geant4 10.5.

# In-vivo PET Positron-emitting fragments in heavy ion beam therapy: new

By A. Chacon (former ANSTO), S. Guatelli (UOW), M. Safavi (ANSTO)

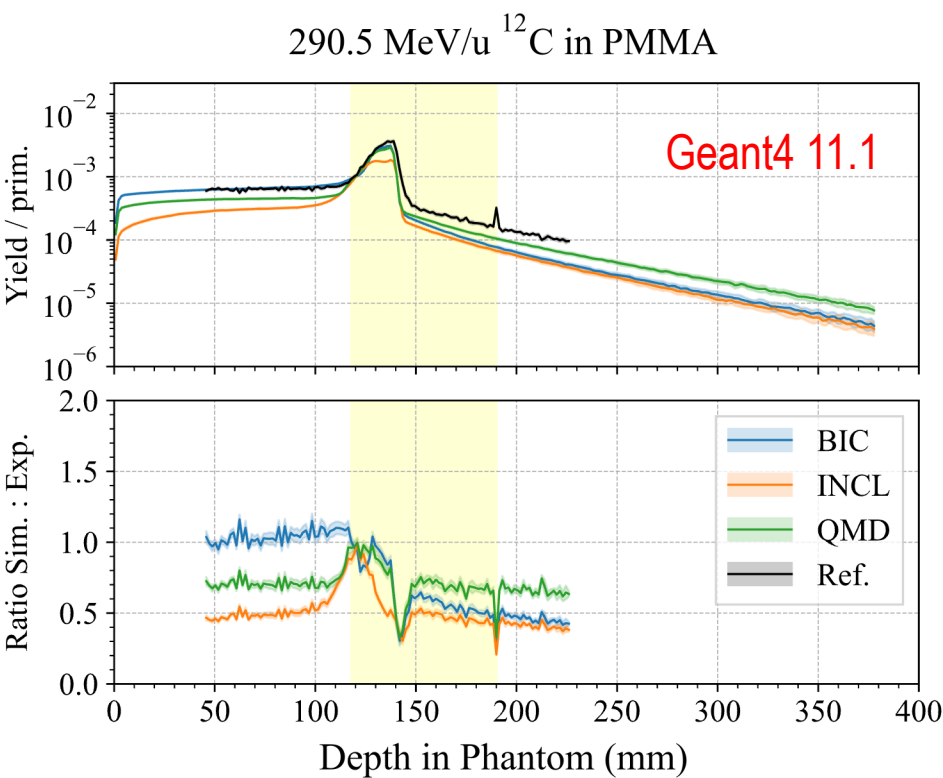
Validation against in-house experimental measurements performed at HIMAC. QST. Chiba (Japan)

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)	$\sigma_x$ (mm)	$\sigma_y$ (mm)	Beam flux (pps)
$^{12}\text{C}$	148.5	2.77	2.67	$1.8 \times 10^9 \pm 3.8 \times 10^7$
$^{12}\text{C}$	290.5	3.08	4.70	$1.8 \times 10^9 \pm 6.4 \times 10^7$
$^{12}\text{C}$	350	2.50	2.98	$1.8 \times 10^9 \pm 4.6 \times 10^7$
$^{16}\text{O}$	148	2.79	2.89	$1.1 \times 10^9 \pm 2.8 \times 10^7$
$^{16}\text{O}$	290	2.60	4.90	$1.1 \times 10^9 \pm 7.0 \times 10^7$

Gelatine, PMMA and polyethylene phantoms

Exp data and simulation details in: Chacon et al (2019), Physics in Medicine & Biology, 64(15):155014.



- The BIC provides an overall better agreement for the entrance and Bragg Peak region, while the QMD outperforms the BIC in the distal region (tail).

# Execution times test: **new**

By D. Bolst, CMRP, University of Wollongong, Australia

Some results - Geant4 11.1

- A pencil beam is generated on the surface of a 30 cm water cube.
- No particle track information or other quantities (for example, energy deposition) are retrieved or stored by the simulation.
- The execution time from the start of the first event to the end of the last event is retrieved.
- Among Geant4-DNA physics lists, Geant4-DNA OPT6 is the fastest
- Among the EM condensed history approaches, OPT3 is the fastest
- For protontherapy, QGSP\_BIC\_HP\_AllHP is about 8 times faster than QGSP\_BIC\_HP and QGSP\_BERT\_HP
- For heavy ion therapy, QMD is 3.5 times slower than BIC and INCL

	EM physics	Ratio to DNA-OPT2
10 keV e <sup>-</sup>	DNA-OPT2	1
	DNA-OPT4	$1.62 \pm 0.09$
	DNA-OPT6	$0.76 \pm 0.04$
	OPT3	$(5 \pm 1) \cdot 10^{-4}$
	OPT4/LIV/PEN	$\sim (10 \pm 2) \cdot 10^{-4}$

	EM physics	Ratio to OPT3
1 MeV e <sup>-</sup>	OPT3	1
	OPT4/LIV	$2.5 \pm 0.2$
	PENELOPE	$3.9 \pm 0.3$

2.30 GHz Intel Xeon E5--2650v3

# Summary and Conclusions

- We recommend to use **G4EMStandard\_Physics\_option4** and **QGSP\_BIC\_HP**
- The **G4-Med tests** have proved
  - To **monitor** how changes in the Geant4 physics component translate in physical quantities of interest;
  - To **support** significantly the development of the Geant4 physics component.
- The next steps are to
  - **Accelerate the system**
  - Add test on **radioactive decay**
  - Modelling of **ionization chambers**.
  - Add more tests on **hadronic physics**
  - Add tests in applications scenarios not currently covered, e.g. Calculation of **S-values**, for internal dosimetry.

Acknowledgement: the Geant4 Medical Simulation Benchmarking Group.

