

# 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

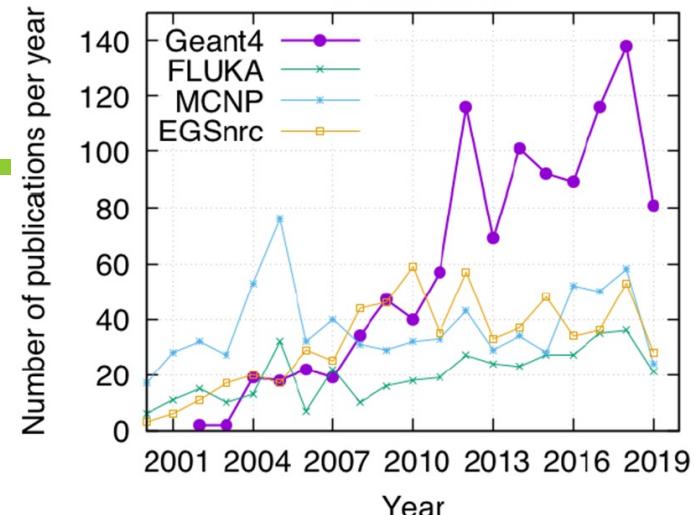
- Created in 2014
- Coordination Team since 2018:
  - **Coordinator:** Susanna Guatelli (Univ. Wollongong, Australia)
  - **Deputy-coordinator:** Pedro Arce (CIEMAT, Spain)
- 57 researchers; 32 institutions from 12 different countries

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

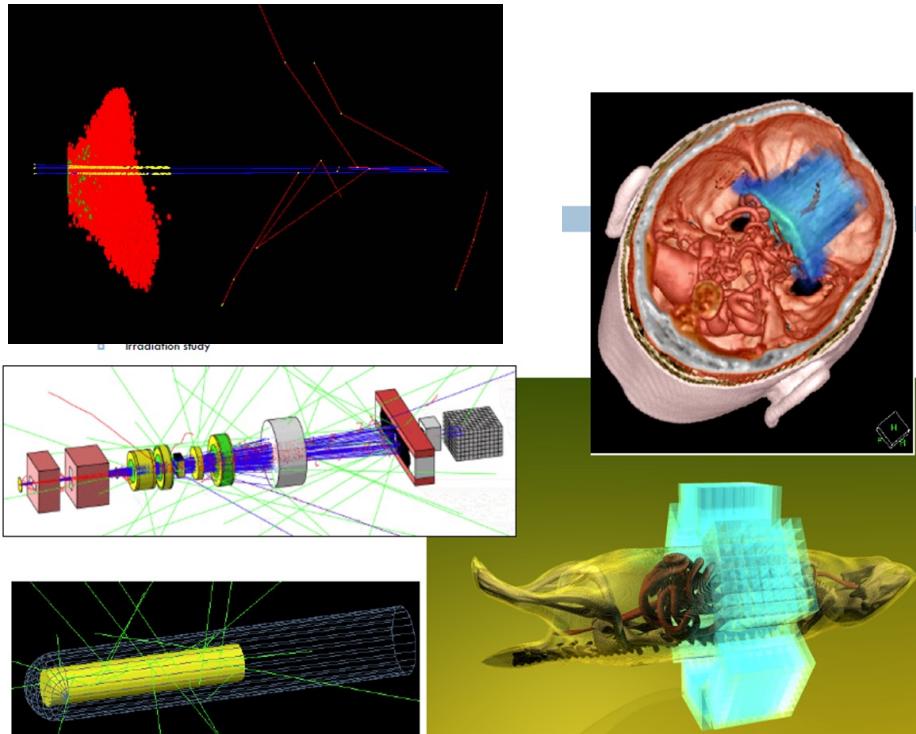


# Geant4 [www.geant4.org](http://www.geant4.org)

- 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



Courtesy of Carlo Mancini,  
Sapienza, Rome, Italy



# 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

## Geant Validation Portal

User layouts

Stat comparison

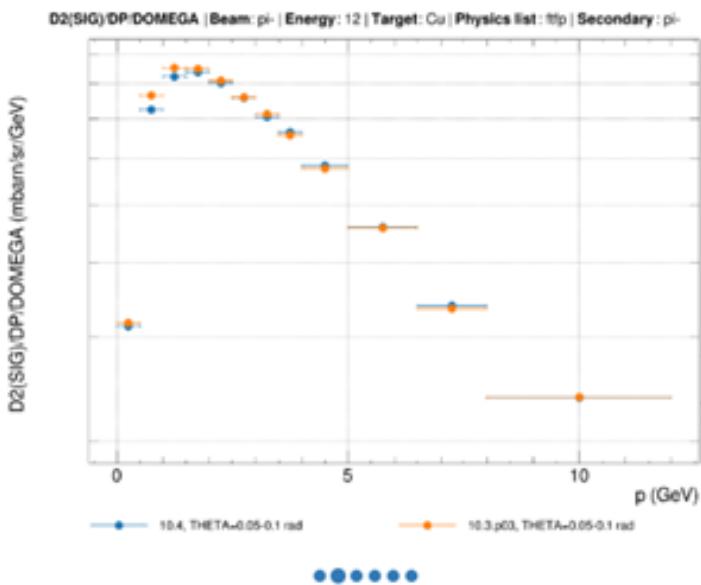
Record viewer

Reference data

Lookup tables



GEANT4



<https://geant-val.cern.ch/>

Geant Validation Portal, SFT group, CERN, 2016-2018

- 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<sup>-</sup> 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.

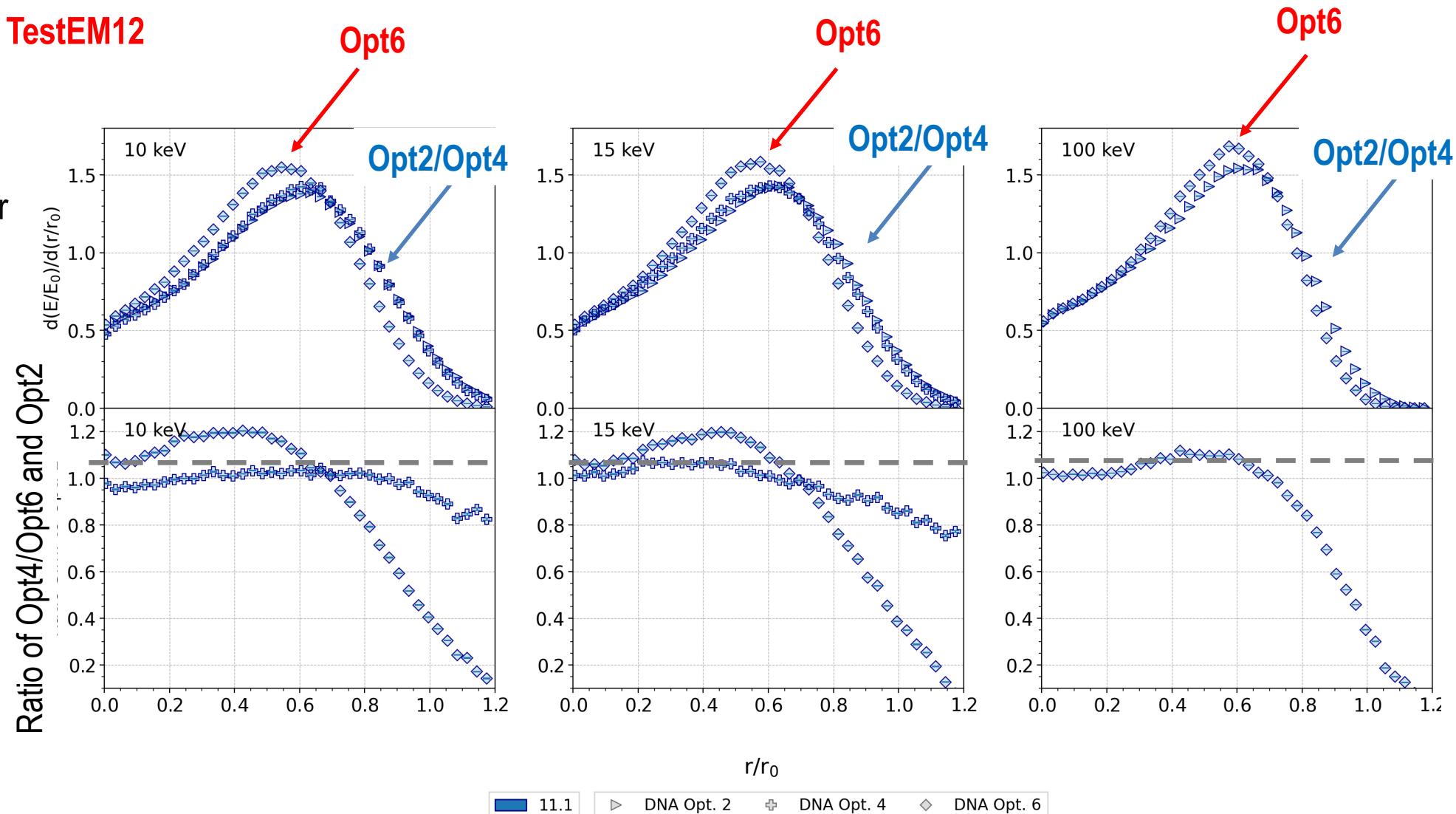
# Geant4-DNA (new) : Low energy dose point kernels test – Geant4 11.1

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

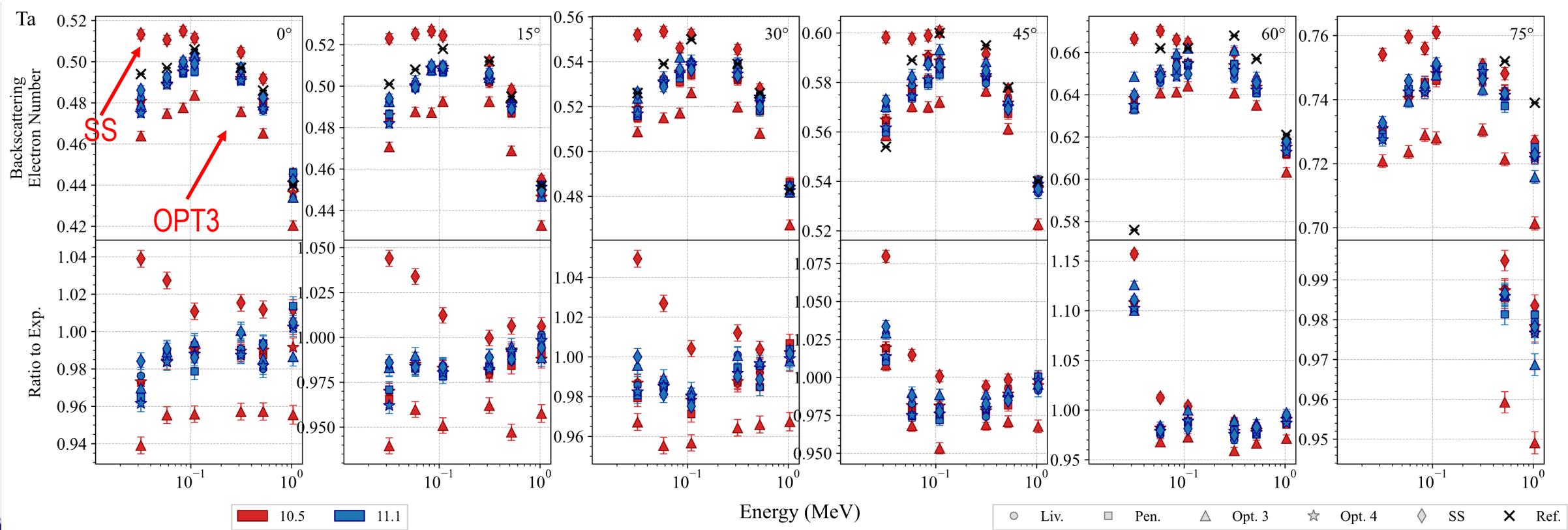
# Geant4 EM Physics constructors: changes between Geant4 10.5 and 11.1

- 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)



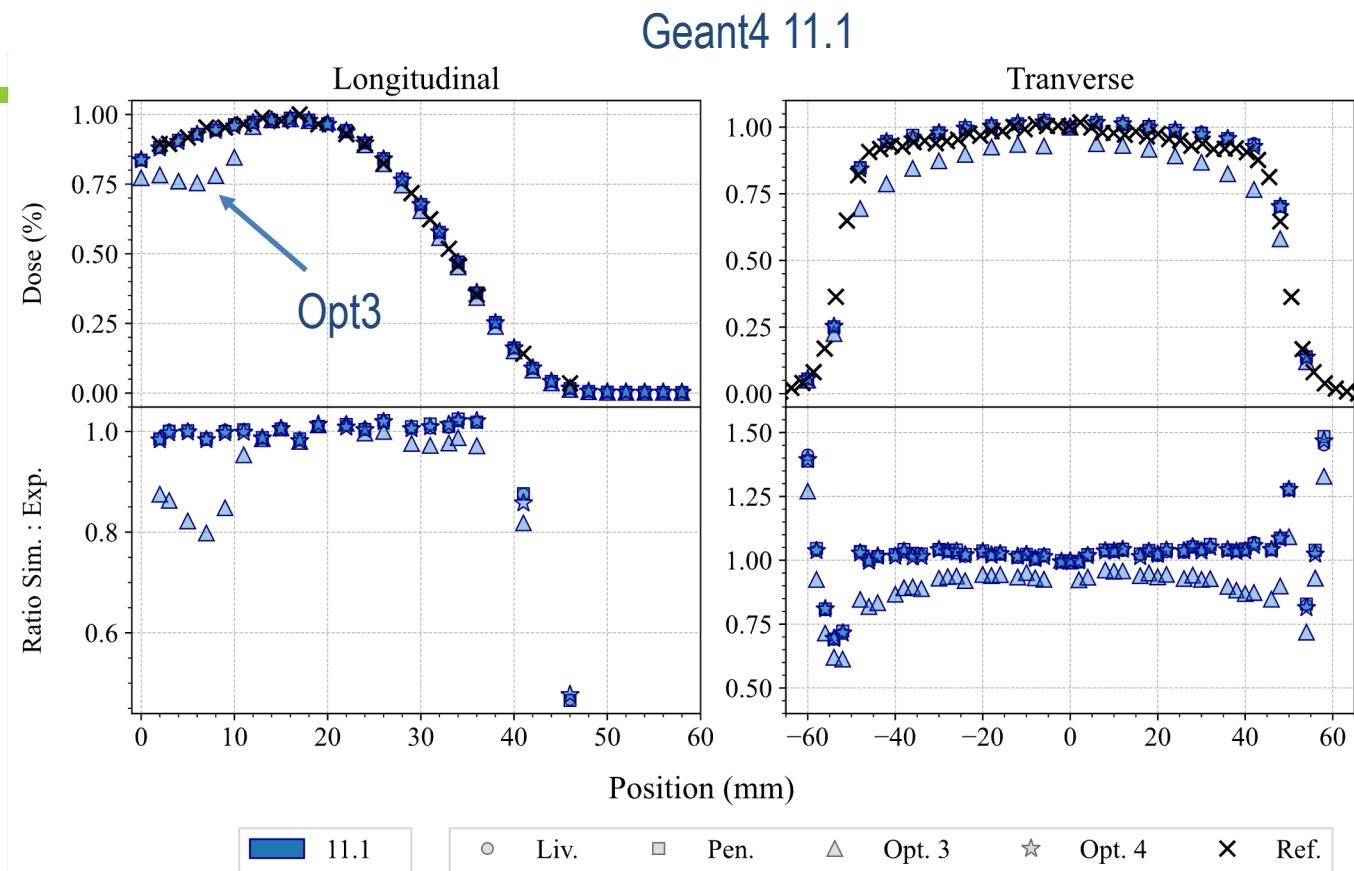
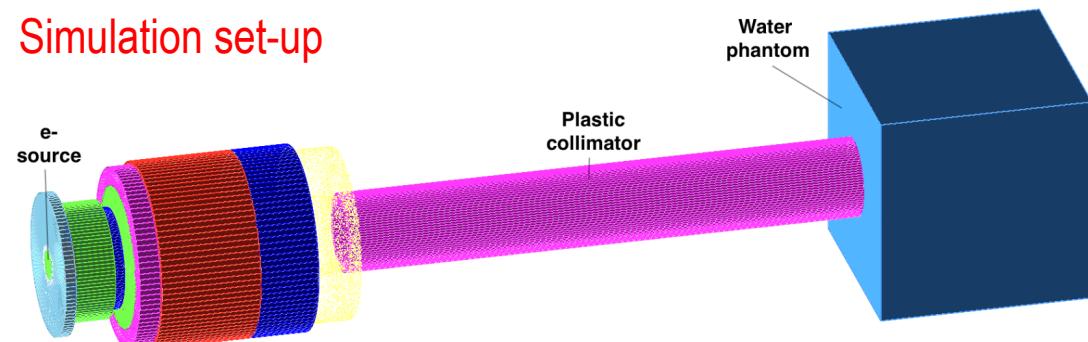
# Electron FLASH radiotherapy test (1): new

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

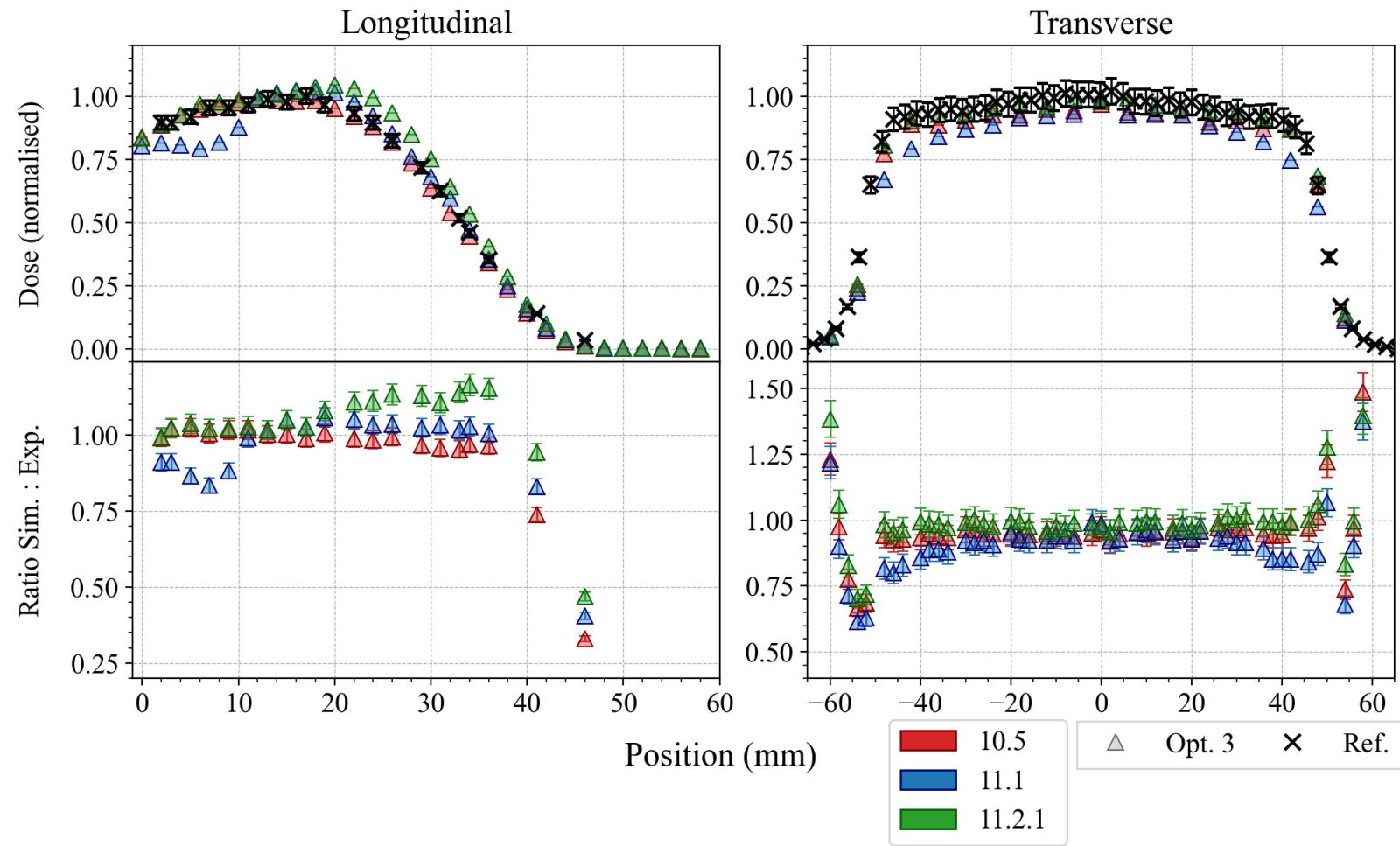


Geant4 EM Standard Physics Option 3: *RangeFactor* in Geant4 11.1 is 0.03.

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

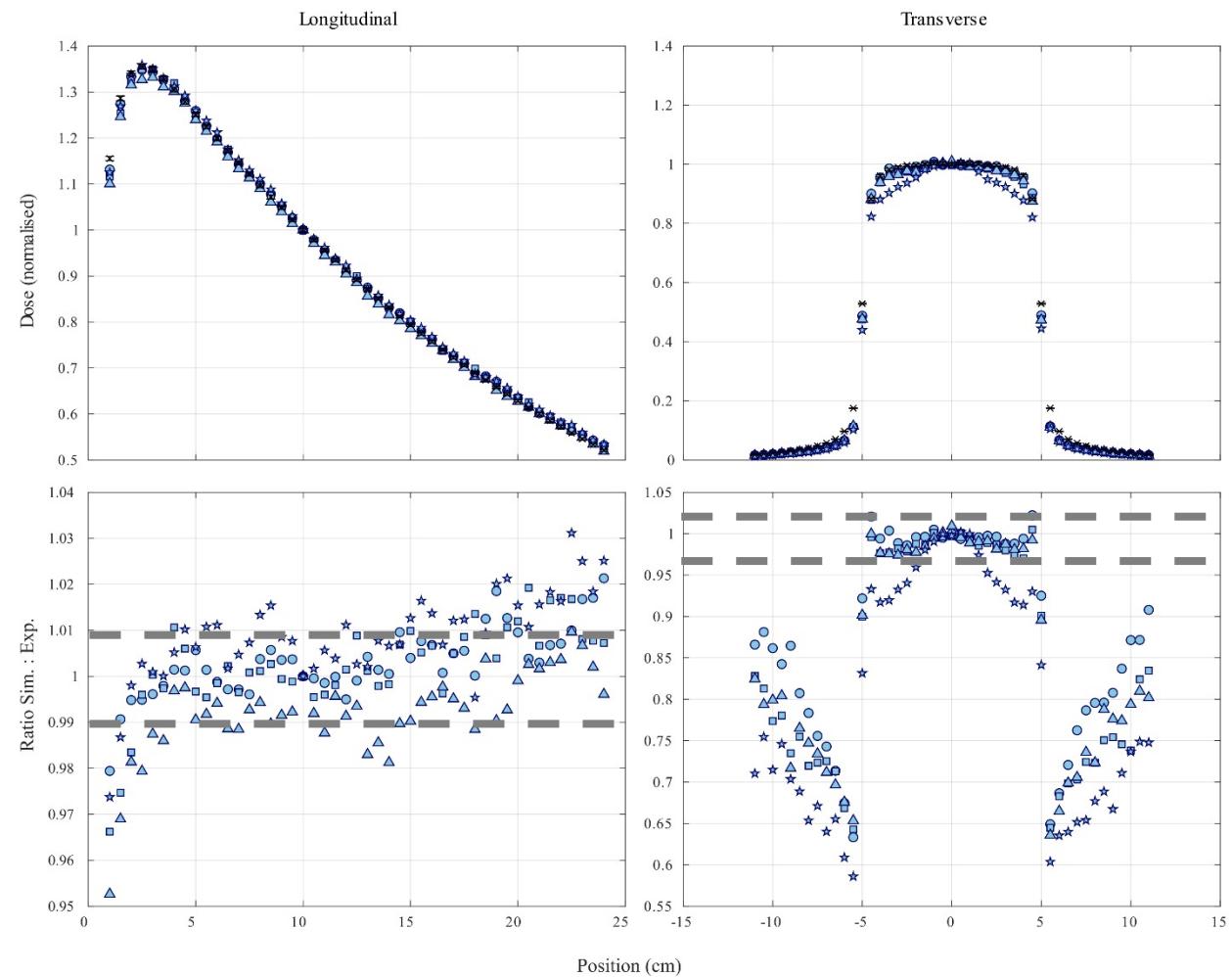
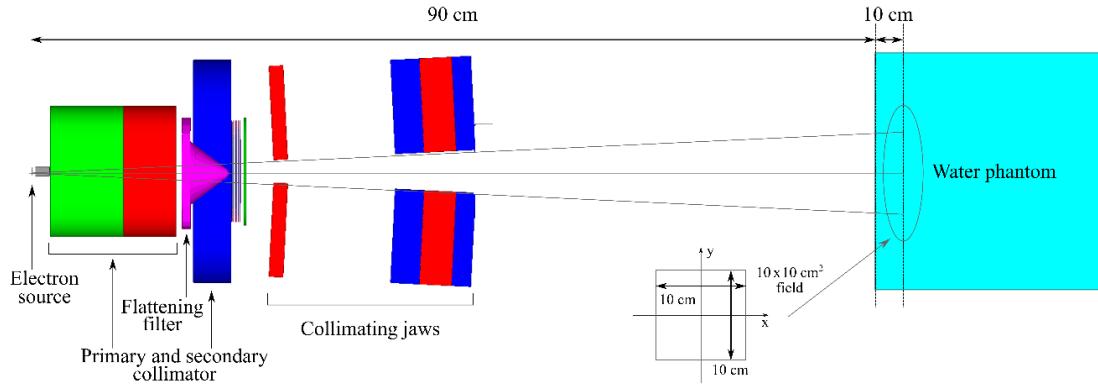


# MV X-ray radiotherapy test: new

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

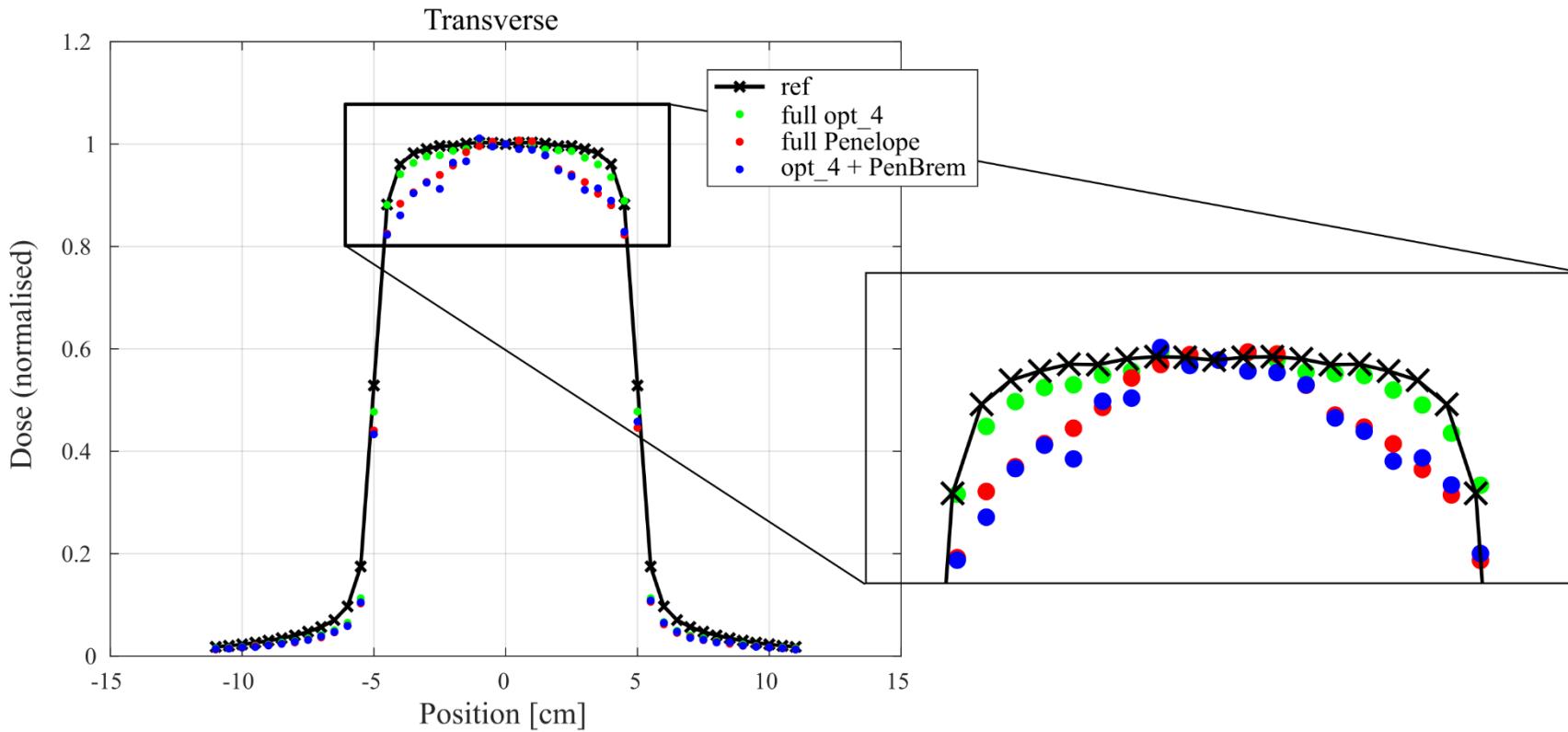
- Geant4 advanced example medical\_linac
- Model of a GE Saturne 43 linear accelerator (EURADOS Report Caccia et al, 2020-05)
- 3D dose in a water phantom

## Simulation set-up



— — — Uncertainty affecting the exp data

# 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

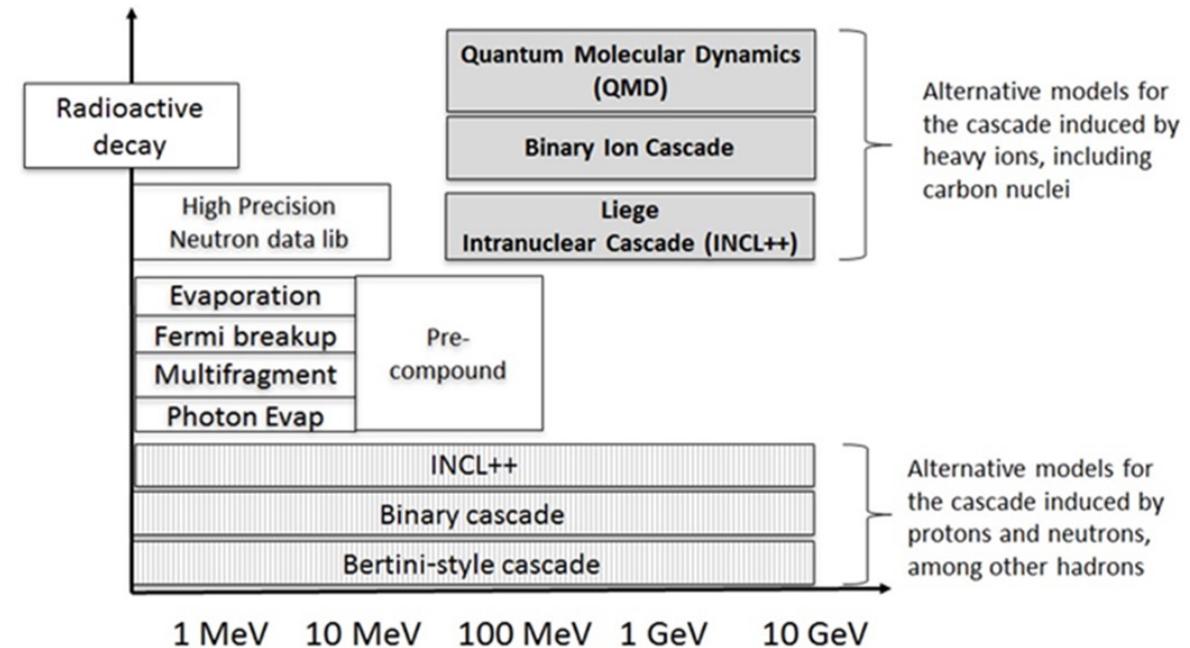
## For proton therapy:

- **QGSP\_BIC\_HP**
  - High Precision data libraries for neutrons with energy  $< 20$  MeV
- **QGSP\_BIC\_AIIHP**
  - 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)

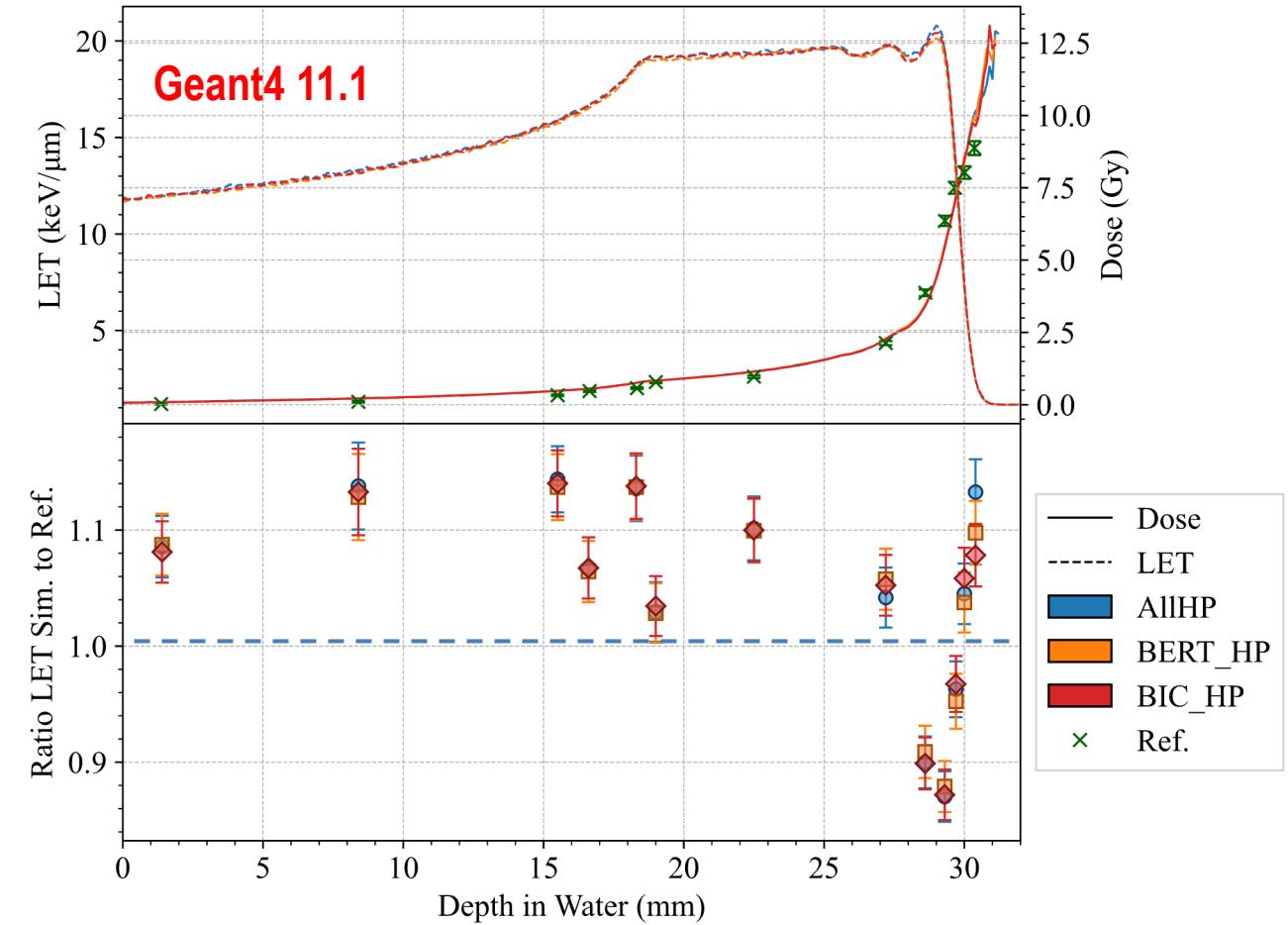
- Consistency improvements, clean-up and optimization of the code have been performed
- Improvements in nuclear data libraries
  - [G4PARTICLEXS1.1](#) in Geant4 10.5 -> [G4PARTICLEXS.4.0](#) (Geant4 11.0 and used also in Geant4 11.1)
    - more accurate fusion cross-sections and inelastic cross-sections 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

# Hadrontherapy test: new

By P. Cirrone, G. Petringa, S. Fattori and A. Sciuto, LNS, INFN, Catania, Italy

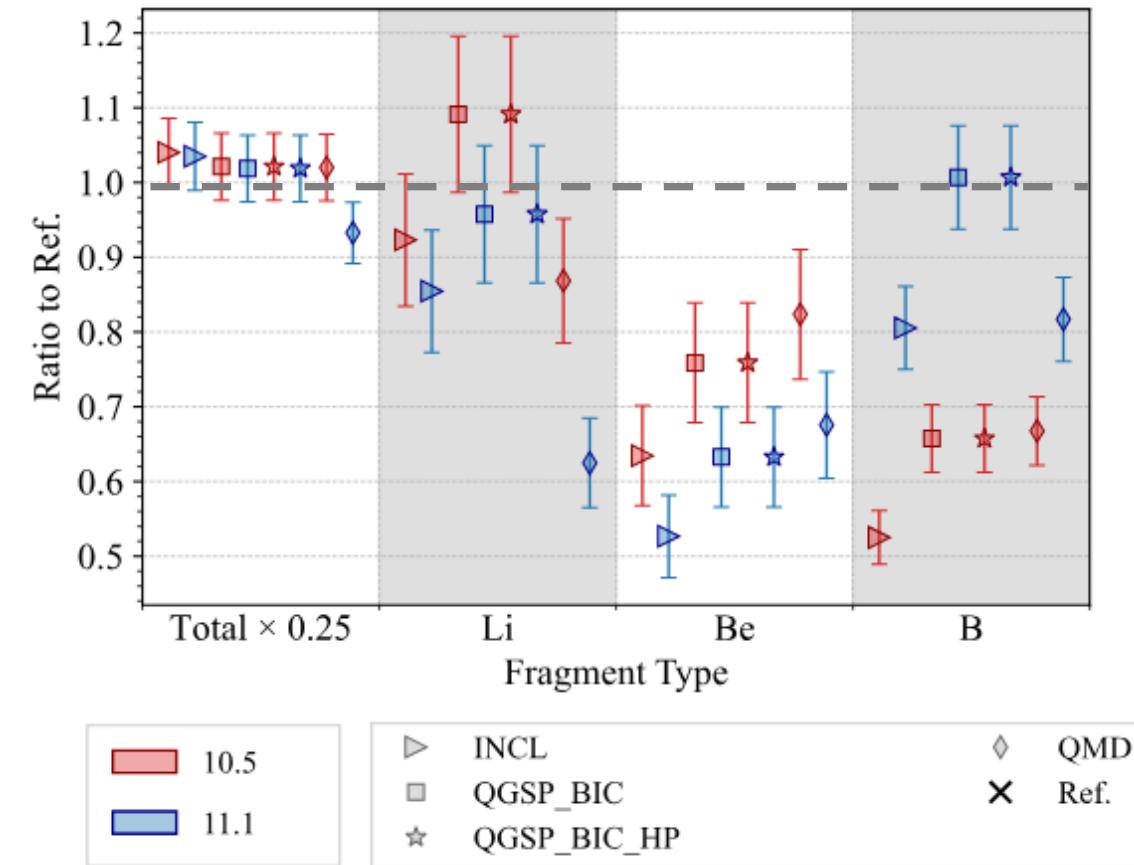
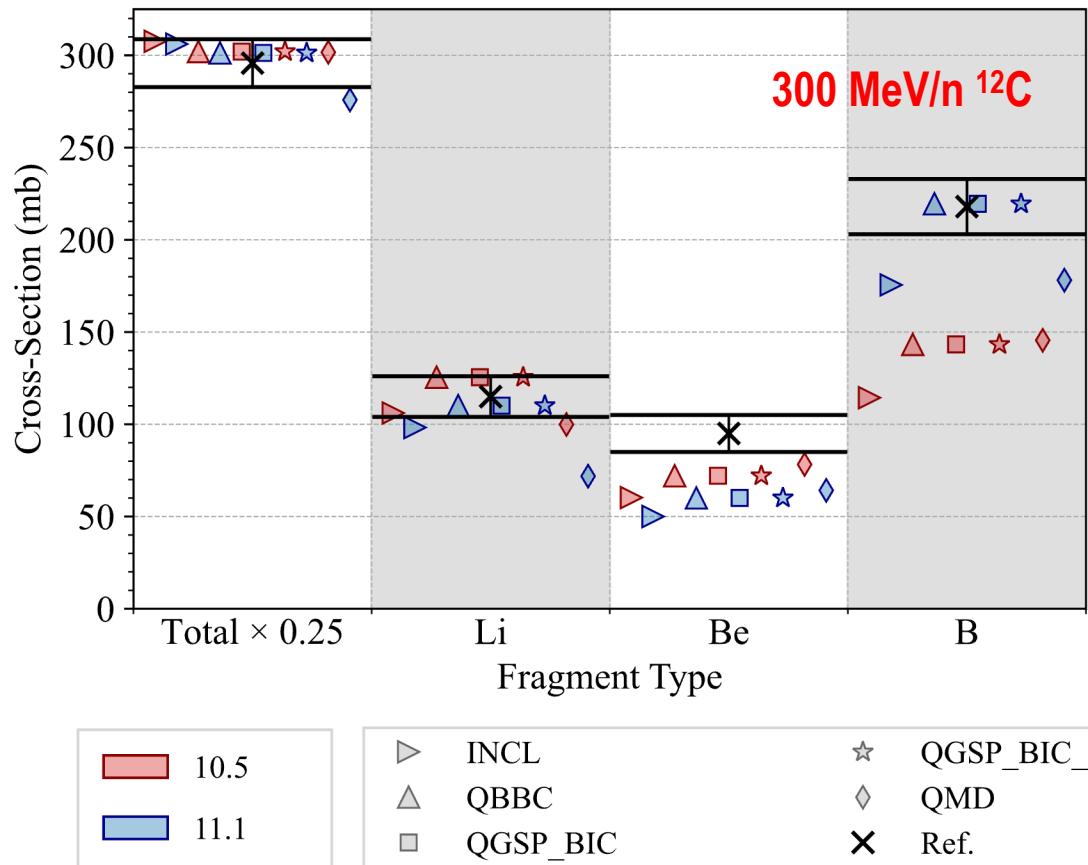
- **Geant4 advanced example hadrontherapy**
- Model the INFN-LNS "CATANA" clinical proton therapy beamline designed for treating ocular melanomas using 62 MeV proton beams
- **Track-average LET is compared against  $y_F$  values** (ICRU Report 36), derived from experimental microdosimetric spectra acquired at different depths in water along the SOBP
- $$y = \frac{\varepsilon_s}{l} \quad \bar{y}_F = \int_0^{\infty} y f(y) dy,$$
- Exp data obtained using the MicroPlus probe detector (Tran T et al, Applied Sciences. 2022;12(1): 2076-3417)  
 $l_i$  = electronic stopping power

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



# 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.

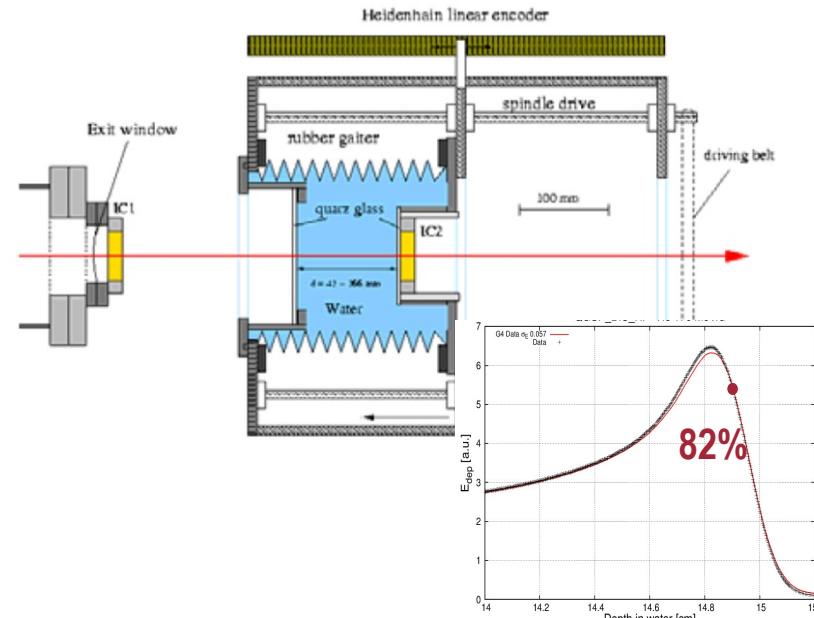


The observed differences in the results are ascribed to differences between Geant4 10.5 and 11.1 in the modelling of the de-excitation channels in the Fermi Break-Up model

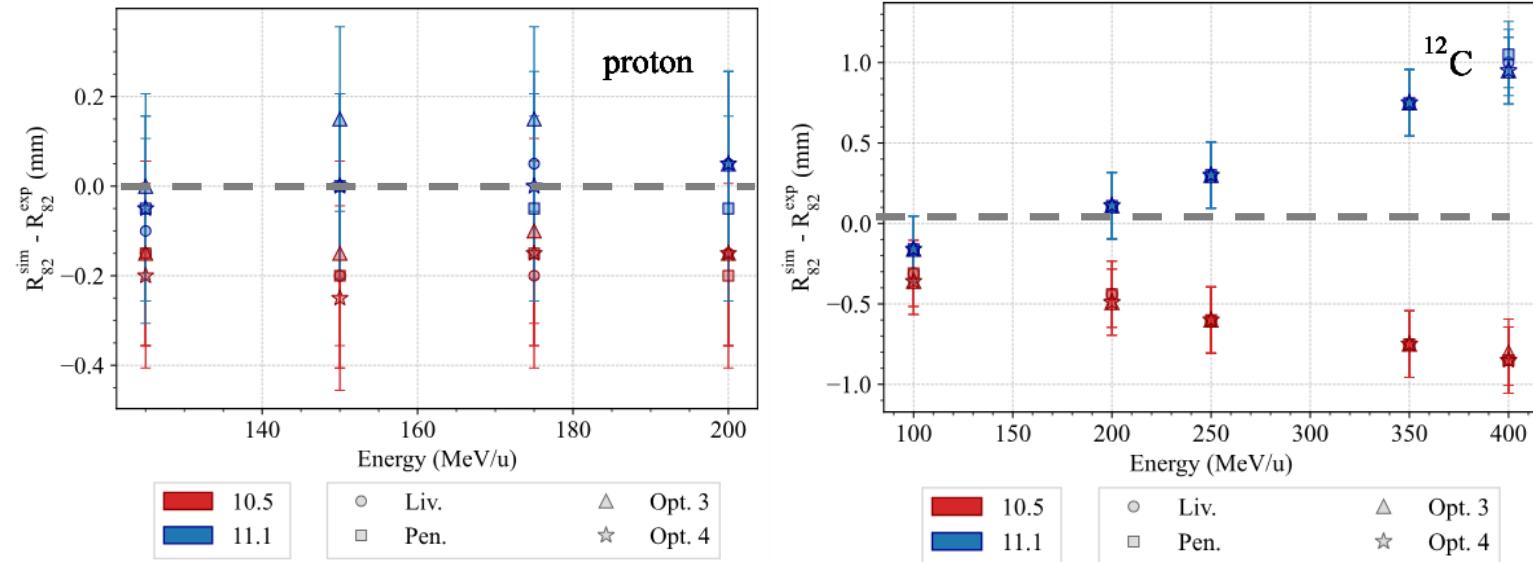
# Light Ion Bragg Curves

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<sub>82</sub> closer to the reference data for <sup>12</sup>C ions with E < 250 MeV/u .
- In the case of 400 MeV/u <sup>12</sup>C, the difference of R<sub>82</sub> is ~ 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)

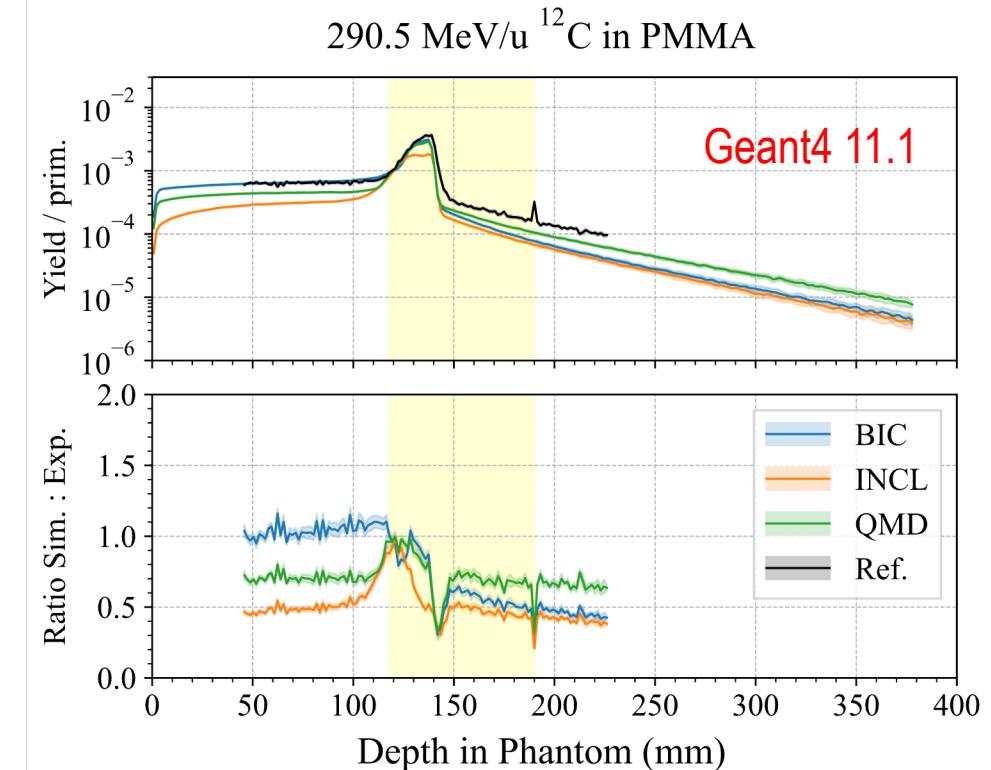
Validation against in-house experimental measurements performed at HIMAC. QST. Chiba (Japan)

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

- 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

Some results - Geant4 11.1

|                       | 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 | $\sim (10 \pm 2) \cdot 10^{-4}$ |

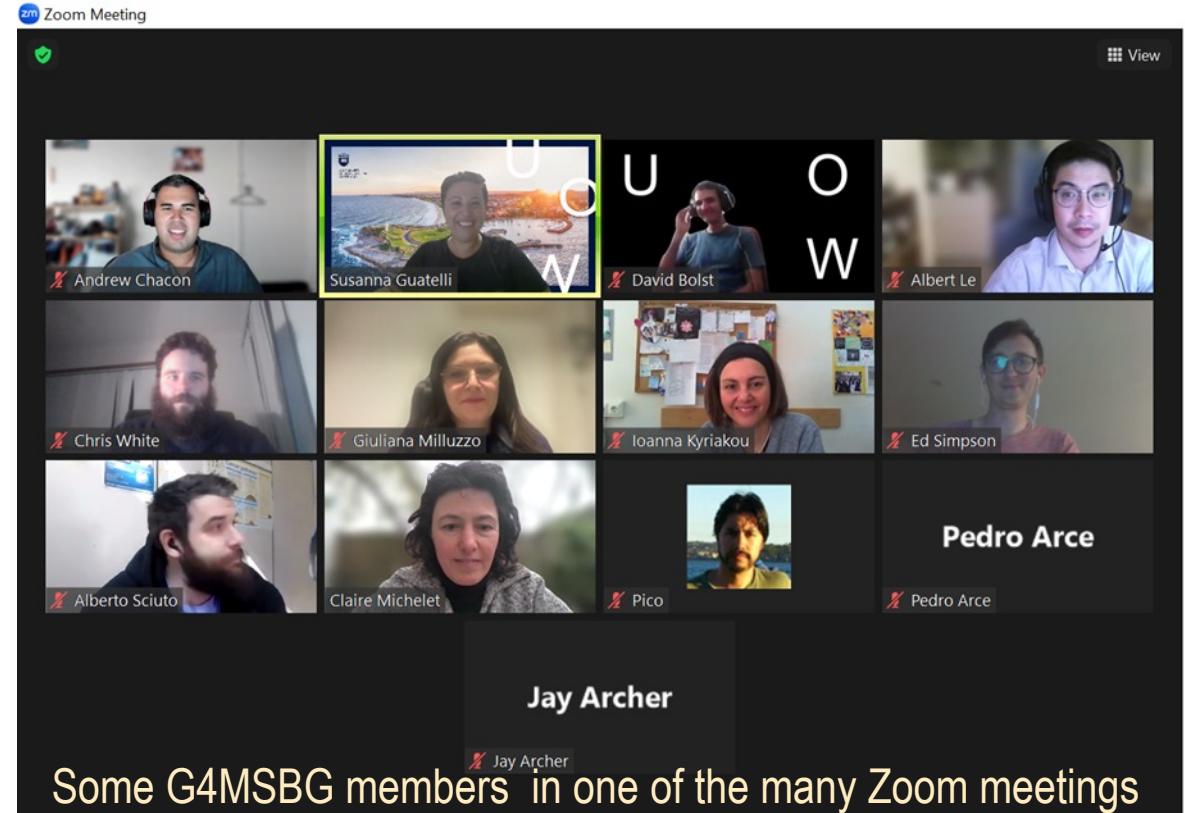
|                      | EM physics | Ratio to OPT3 |
|----------------------|------------|---------------|
| 1 MeV e <sup>-</sup> | OPT3       | 1             |
|                      | OPT4/LIV   | $2.5 \pm 0.2$ |
|                      | PENELOPE   | $3.9 \pm 0.3$ |

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.



Some G4MSBG members in one of the many Zoom meetings

