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

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On behalf of the Geant4 Medical Simulation Benchmarking Group

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The Geant4 Medical Simulation Benchmarking Group

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

- Created in 2014
- <u>Coordination Team since 2018:</u>
 - Coordinator: Susanna Guatelli (Univ. Wollongong, Australia)
 - Deputy-coordinator: Pedro Arce (CIEMAT, Spain)
- 58 researchers; 33 institutions from 12 different countries



Health

Nepean Blue Mountains Local Health District

Motivation & Goals

• G4-Med project:

- 23 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

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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.

G4-Med tests: Update

- 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 ¹²C fragmentation
 - Charge-changing cross sections for 300 MeV/u ¹²C 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 ¹²C ion beam in water

Green: tests included since 2021 (since Paper I)

Regression testing: Geant4 10.5 (paper #1) and 11.1

- Difference for both release is within $3\sigma_{ref}$ with the reference data -> no change
- If the difference for at least one release is > $3\sigma_{ref}$ -> analysis with three metrics:
 - Mean Relative Error (MRE), Normalised Mean Absolute Error (NMAE) and maximum difference between simulated and reference data

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

- 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/

Backscattering test

- 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)

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 × 2.5 mm² e⁻ source with an ad-hoc energy spectrum peaked at 9 MeV, provided by the manifacturer (SIT Sordina)





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 released where the *RangeFactor* in Opt3 is back to 0.04 and step limitation algorithm from *SafetyPlus* to *DistanceToBoundary*

Electron FLASH radiotherapy test (2)

- 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

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



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MV X-ray radiotherapy test



Continued

In the first 10 cm of water phantom for the longitudinal profiles, differences against Option4 are about 1% for Livermore, between 6% and 10% for Option3, and between 15% and 16% for Penelope.

Not normalised distributions



Hadrontherapy test

- 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

$$y = \frac{\varepsilon_s}{\overline{l}}$$
 $\overline{y}_F = \int_0^\infty y f(y) dy$,

 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.

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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 IonBragg Curves

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

QGSP_BIC_HP for hadronic physics

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



- 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 ¹²C ions with E < 250 MeV/u .
- In the case of 400 MeV/u ¹²C, the difference of R₈₂ is ~ 1 mm with Geant4 11.1 and 0.85 mm with Geant4 10.5.

A pencil beam is generated just inside 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⁻	DNA-OPT2	1
	DNA-OPT4	1.62 ± 0.09
	DNA-OPT6	0.76± 0.04
	OPT3	(5 ± 1)·10 ⁻⁴
	OPT4/LIV/PEN	~ (10 ±2)·10 ⁻⁴

	EM physics	Ratio to OPT3
1 MeV e⁻	OPT3	1
	OPT4/LIV	2.5 ± 0.2
	PENELOPE	3.9 ± 0.3

2.30 GHz Intel Xeon E5--2650v3

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- Apptainer (formerly Singularity) is a container system (compatible with Docker images and files)
- Largely available on scientific computing clusters, eg: <u>https://confluence.infn.it/display/TD/Singularity+in+batch+jobs</u> <u>https://batchdocs.web.cern.ch/containers/singularity.html</u>
- With a few commands it's possible to run a Geant4 application regardless of the environment (even without installing Geant4)
- Example: <u>https://github.com/carlomt/container-medical_linac</u>
- The container is built via GitHub CI and hosted on ORAS (<u>https://oras.land/</u>)

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Download the container image
apptainer pull oras://ghcr.io/carlomt/container-medical_linac:latest

• Create a folder for the Geant4 datasets and download them mkdir ./g4datasets

apptainer exec --bind ./g4datasets:/opt/geant4/data containermedical_linac_latest.sif /opt/geant4/bin/geant4-config --install-datasets

Download a macro

wget https://raw.githubusercontent.com/carlomt/containermedical_linac/main/testrun.mac

• Launch the simulation apptainer exec --bind ./g4datasets:/opt/geant4/data containermedical_linac_latest.sif run testrun.mac



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Summary of achievements of 2023/2024 and next steps

Achievements since the last Geant4 Collaboration Meeting:

- Full analysis of the tests results (Geant4 10.5 and 11.2)
 - Paper on Medical Physics currently under review
- Fully automatised analysis system has been developed
- Development of containers for running Geant4 tests
 - This will facilitate the execution of the tests
- Geant4 11.2.1 has been released to solve the problems of the multiple scattering in G4 EM Constructor Opt3

Next steps:

- Finalise the Medical Physics paper (to be submitted next week)
- Create a git rep for the tests
- Run the tests on supercomputing facilities
- Run the tests with Geant4 11.3
- Analyse the results of the tests



Tests to add

- Radioactive decay Pico Sarmiento et al
- Nuclear medicine tests A. Malaroda, S. Guatelli et al, help needed
- Neutron cross sections S. MacLeod and help needed
- 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 – M. A. Cortés-Giraldo, help 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 needed
- Add tests in applications scenarios not currently covered, e.g. Calculation of S-values, for internal dosimetry – help needed



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
 - Add new test
 - Accelerate the system from the execution of the tests to plotting and analysis

Acknowledgement: the Geant4 Medical Simulation Benchmarking Group.

200 Zoom Meeting 0 III View W Andrew Chacor Susanna Guate Chris Whit **Pedro Arce** 🔏 Pedro Arce Jay Archer Some G4MSBG members in one of the many Zoom meetings



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)
 - New extended relativistic version up to MeV energies will be released soon (Kyriakou et al., Front. Phys. 2022, 9:711317)
- 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)

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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 Δt) 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 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.



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	Livernore					PENELOPE
scattering and	(EPICS2017) Li et al. 59					
photoelectric						
effect						
Compton	G4K leinN ishi	na		G4Low EPC ompton Model	PENELOPE	
scattering	Model			for $E < 20 MeV$	(EPICS2017) Li et al. ⁵⁹	
				Brown et al. 62 ,		
	4K leinNishina for $E > 20 MeV$					
Gamma	G4BetheHeitler5DModel $G4Livermore5DModel$				PENELOPE	
conversion	Bernard ⁶⁰ , ⁶¹				Li et al. 59	
e^- and e^+	Standard			PINELOPE for $E < 100 \text{ keV}$,	Livermore for $E < 100 \text{ keV}$	PENELOPE
ionisation				Standard for $E > 100 \text{ keV}$	Standard for $E > 100 \text{ keV}$	
e^- and e^+	Geant4 Standard			eV,	PENELOPE	
bremsstrahlung	Model		G4 elremsstrahlung RelModel for $E > 1 GeV$			
e ⁺ annihilation	$G4 eplus To 2 Gamma OKVIM odel^{56}$		Standard			PENELOPE
e^- and e^+	Urban model	Urban	Not Goudsmit-Saunderson model (Incerti et al. ⁶³)			
multiple	for $E < 1$ MeV,	model	available for $E < 100 \text{ MeV}$			
scattering	Wentzel model		Wentzel model for $E > 100 \text{ MeV}$			
	for $E > 1 MeV$					
Coulomb	on	off				
scattering						
Bremsstrahlung	Modified Tsai	2BS	Modified Tsai 2BS		PENELOPE	
angular						
distribution						

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Refer to the Geant4 physics reference manual **25**

Snapshot of the G4EM constructors (Geant4 11.1) (2)

- Geant4 11.1, In Opt3
 - the rangeFactor has been changed from 0.04 to 0.03
 - Step limitation algorithm for multiple scattering from *DistanceToBoundary* to *safetyPlus* (similar to the other constructors)

Step limit:
$$L = \min \{F_R \cdot \max(R, \lambda), F_s \cdot s, D/F_G\}.$$

 F_R : range factor

- *F*_G: geometry factor,
- $F_s = 0.3$ (safety factor), fixed.
- R(T): particle range where T is kinetic energy,
- $\lambda(T)$: inverse transport cross section [12, 13],
- S: geometrical safety s
- D: distance to a geometrical boundary
- UseSafety, F_R = 0.04, F_G is ignored, default;
- UseDistanceToBoundary, $F_R = 0.04$, $F_G = 2.5$

Geant4 EM parameter		Opt3	Opt4	SS	GS	WVI
			Livermore			
			Penelope			
Minimum	a energy (eV)	10.	100.	100.	100.	10.
Lowest electr	on energy (keV)	0.1	0.1	0.01	1.	0.1
Number of	bins per decade	20	20	7	7	20
Mott c	corrections	on	on	on	off	on
dRov	dRoverRange		0.2	0.2	0.2	0.2
for e	$$ and e^+					
finalRange for	e^{-} and e^{+} (mm)	0.1	0.01	1.	1.	0.1
dRov	verRange	0.2	0.1	0.2	0.2	0.2
for muons	and hadrons					
finalRa	ange (mm)	0.05	0.05	0.1	0.1	0.5
for muons	and hadrons					
Skin for	$r e^-$ and e^+	1	3	1	1	1
Rang	ge factor	0.03	0.08	0.04	0.06	0.04
for e	$-$ and e^+					
Range factor		0.2	0.2	0.2	0.2	0.2
for muons and hadrons						
Msc Ste	pLimitType	$fUseSafetyPlus^{*}$ $fUseSafety$		ety		
Fluo	rescence	on				
and A	Auger e ⁻					
PIXE modelling		off	off	on	off	off

Ivantchenko et al (2010) Journal of Physics: Conference Series 219, 032045 doi:10.1088/1742-6596/219/3/032045



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, ²H, ³H, α and ³He 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 +

G

- **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 $A \le 18$.

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