Medical and bio science User Requirements

23rd Geant4 Collaboration Meeting,
Lund University, 27th-31st August 018

Pedro Arce Dubois
Medical Applications Unit, CIEMAT, Madrid, Spain

Outline

- Status of 2017 User Requirements
- New User Requirements
- Summary of fulfillment of User Requirements
- A few personal comments

Review of the Medical Physics UR presented by S. Guatelli at the 22nd Geant4 Workshop

Validate the microdosimetric performance of Geant4-DNA physics models for liquid water

Originator: Ioanna Kyriakou, University of Ioannina

Status: in progress (I. Kyriakou)

- Validated the microdosimetric spectra of monoenergetic low-energy electrons in spheres of 2-300nm : J: Appl. Phys. 122, 024303 (2017)

Geometry: Develop a DNA string volume

Originator: S. Meylan (ISRN), U. Vimont (LJK), S. Incerti (U. Bordeaux,CNRS), I. Clairand (ISRN), C. Villagrasa, (ISRN) / A. McNamara (MGH)

Status: in progress by ISRN as an independent code (DNAFabric)

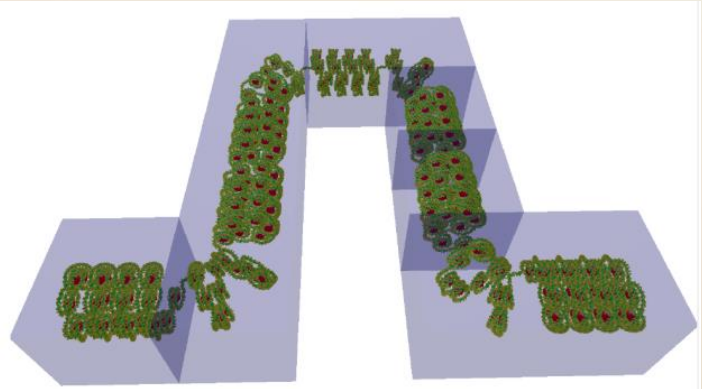
Double strand breaks (DSBs) calculations for protons at different energies in a human cell

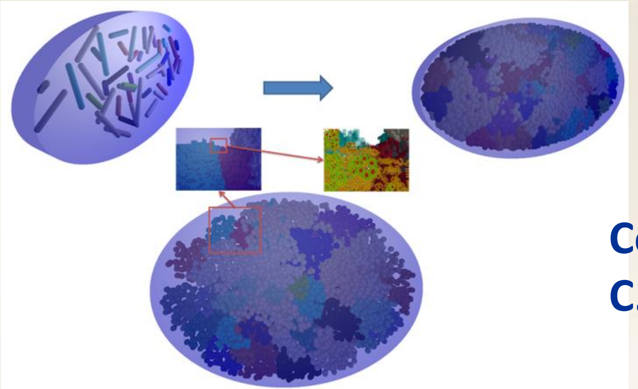
Originator: S. Meylan and C. Villagrasa (IRSN, France)

Status: published results based on Geant4-DNA (10.1). Upgrade to 10.4 and publication of a new user example in progress (H.Tran, IRSN)

Simulation of early DNA damage after the irradiation of a fibroblast cell nucleus using Geant4-DNA. Meylan S. et al. Scientific reports. 2017;7(1):11923

- **DNA cellular geometry generated with DNAFabric :** C++ software : generation, modification and 3D geometries of DNA model that can be exported to Geant4. **Comput. Phys. Comm. 204 (2016) 159**
- **Physical stage + chemical stage combined** in these calculations within the same DNA geometry
- DNA **clustered damage scoring** made using **DBScan** Algorithm





Courtesy of C. Villagrasa (ISRN)

2017 User Requirements

Validate the Geant4-DNA chemistry w.r.t. experimental measurements

Originator: Eva Bezak, University of South Australia, Australia

Status: In progress (on-going activity by the group of E. Bezak)

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

Status: some comparisons by S. Incerti

2017 User Requirements

UR37: Definition of irradiation profile w.r.t. time for radiation therapy

Originator: Laurent Desorgher, CHUV

Status: partially fulfilled in G4RadioactiveDecay. Biasing mode recently improved by Dennis

See talk by L. Desorgher at session 5A, Wed. 9.00 "Radioactive Decay Model: Status and Plans"

Develop ad-hoc track structure physics models for nanomaterials

– Graphite, gold, platinum, gadolinium, iodine, iron and iron oxide

Originator: from papers, conferences, …

Status: gold done, others open

See talk by D. Sakata at session 1A, Mon. 14.00 "Models for simulation of Gold nanoparticles"

2017 User Requirements

Modelling Synchrotron radiation

Originator: S. Guatelli, M. Cameron, A. Dipuglia, M. Lerch, CMRP

Status: in progress

G4SynchrotronRadiation seems to underestimate the production of synchrotron radiation by a 3 GeV electron beam (B= 1-3 T).

- Shown by comparison against existing analytical model and in-house experimental measurements done at the Australian Synchrotron
- Important for Microbeam Radiation Therapy, imaging applications and also High Energy Physics applications

See talk by S. Guatelli at session 1A, Mon 14.00 "Validation of the Geant4 EM physics for modelling high energy synchrotron beamlines"

2017 User Requirements

Validation for X-ray radiotherapy treatments

Non electronic equilibrium / at the interface between different media / high spatial resolution

Originator: S. Guatelli, CMRP, UOW

Status: in progress

Proceeded with non-equilibrium but still not at the interface between different materials

2017 User Requirements

Validation of bremsstrahlung process for targets used in radiotherapy (such as tungsten), energy range: 6-15 MeV

Originator: B. Caccia, Istituto Superiore di Sanita', Rome, Italy

Status: validation up to 2.8 MeV

- Detailed validation for beams between 10 and 30 MeV (Faddegon et al.)
- No data found 3-10 MeV (which is very interesting for medical physics)

JOURNAL OF APPLIED PHYSICS VOLUME 39, NUMBER 6 MAY 1968

Bremsstrahlung Produced in Thick Aluminum and Iron Targets by 0.5 to 2.8 MeV Electrons*

W. E. DANCE, D. H. RESTER, B. J. FARMER, AND J. H. JOHNSON
LTV Research Center, Ling-Temco-Vought, Incorporated, Dallas, Texas
AND
L. L. BAGGERLY
LTV Research Center, Dallas, Texas and Texas Christian University, Fort Worth, Texas
(Received 21 December 1967)

Data from Dance et al. (0.5 – 2.8 MeV)

Nuclear Instruments and Methods in Physics Research B56/57 (1991) 327–329
North-Holland

Angular dependence of thick-target bremsstrahlung

R. Ambrose [1], D.L. Kahler, H.E. Lehtihet and C.A. Quarles
Department of Physics, Texas Christian University, Fort Worth, TX 76129, USA

Data from Ambrose et al. (70 keV)

Material	Energy (MeV)	Data (MeV/electron) (±11%)	Simulation/data		
			Option3	Livermore	Penelope
Forward ($\theta < \pi/2$)					
Al	0.5	$8.80 \cdot 10^{-4}$	0.99	1.00	1.01
Al	1.0	$4.45 \cdot 10^{-3}$	0.70	0.90	0.93
Al	2.0	$1.65 \cdot 10^{-2}$	1.00	1.02	0.99
Al	2.8	$3.52 \cdot 10^{-2}$	0.98	1.00	0.97
Fe	0.5	$1.41 \cdot 10^{-3}$	1.27	1.24	1.23
Fe	1.0	$7.94 \cdot 10^{-3}$	0.83	0.93	0.91
Fe	2.0	$2.99 \cdot 10^{-2}$	0.90	1.04	1.01
Fe	2.8	$6.05 \cdot 10^{-2}$	0.99	1.03	1.00
X^2 ($\nu = 8$)			18.2	9.8	6.3
All space ($\theta < \pi$)					
Al	0.5	$1.15 \cdot 10^{-3}$	1.16	1.18	1.16
Al	1.0	$5.20 \cdot 10^{-3}$	0.81	1.06	1.08
Al	2.0	$1.78 \cdot 10^{-3}$	1.11	1.15	1.11
Al	2.8	$3.98 \cdot 10^{-2}$	0.99	1.03	0.99
Fe	0.5	$2.08 \cdot 10^{-3}$	1.34	1.37	1.35
Fe	1.0	$1.03 \cdot 10^{-2}$	0.94	1.10	1.08
Fe	2.0	$3.65 \cdot 10^{-2}$	0.99	1.15	1.13
Fe	2.8	$7.52 \cdot 10^{-2}$	1.05	1.09	1.05
X^2 ($\nu = 8$)			21.9	26.7	19.7
X^2 w/o Fe 0.5 MeV ($\nu = 7$)			7.9	9.8	5.4

Nuclear Instruments and Methods in Physics Research B 350 (2015) 41–48

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

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Validation of the GEANT4 simulation of bremsstrahlung from thick targets below 3 MeV

CrossMark

L. Pandola [a,b,*], C. Andenna [c], B. Caccia [d]

[a] INFN, Laboratori Nazionali del Sud, Via Santa Sofia 62, I-95125 Catania, Italy
[b] INFN, Gran Sasso Science Institute, Viale Francesco Crispi 7, I-67100 L'Aquila, Italy
[c] INAIL, Dipartimento Innovazioni Tecnologiche e Sicurezza degli Impianti, Prodotti ed Insediamenti Antropici, Via Alessandria 220, I-00198 Roma, Italy
[d] Dipartimento Tecnologie e Salute, Istituto Superiore di Sanità and INFN, Gruppo Collegato dell'Istituto Superiore di Sanità, Viale Regina Elena 299, I-00161 Roma, Italy

Courtesy of B. Caccia (I.S.S, Rome)

2017 User Requirements

Validation of carbon ion therapy physics

Originator:S. Guatelli and D. Bolst, CMRP, UOW

Status: in progress

- The nuclear cross sections in different versions of Geant4 are seen to change results drastically for medical physics applications relevant to ion therapy (thick targets with primary energies of ~100-400 MeV/u)
  - Fragments yield: important for dosimetry (verification of TPS) and in-vivo range verification techniques (production of β^+ emitters)
  - E.g. from 10.2 to 10.3/10.4 almost doubled the difference between simulation and experiment for certain fragments
- It would be very beneficial to the medical physics community if there were a “Medical Physics” cross section option in Geant4 as it was in 10.2

See talk by S. Guatelli at session 5A, Wed 9.00 “Hadron Therapy validation”

2017 User Requirements

BNCT and Fast Neutron Therapy

Validate neutron physics and activation against experimental measurements

Originator: S. Guatelli

Status: in progress

- Waiting for the reactor data from the KURRI facility in Japan
- Analysing FNT experimental measurements at the iThemba facility in South Africa

Modeling of x-ray optics for Microbeam Radiation Therapy

Relevant for the Synchrotron Radiation community

Originator: Elke Braeuer-Krisch, ESRF

Status: open

2017 User Requirements

UR-34: Tallying of the ambient dose equivalent

Originator: Laurent Desorger

Status: to be implemented in September 2018

UR-35: Calculation of the dose H*(10) resulting from radioactive decay at different time windows

Originator: Laurent Desorger

Status: to be implemented in September 2018

New Requirements

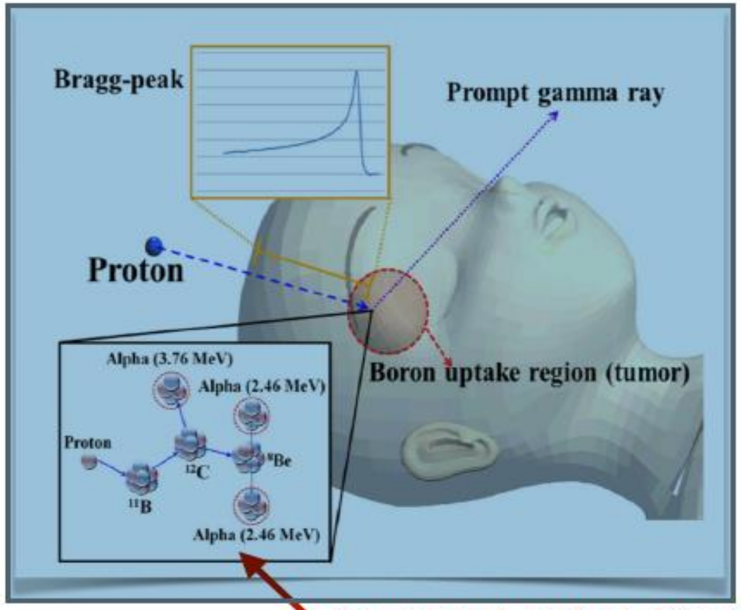
Exact estimation of alpha and other secondary particles for proton therapy energies

Improvement/test of AllHP physics for the case of interest in hadrontherapy

Originator: Giada Petringa, Pablo Cirrone, Giacomo Cuttone (LNS)

Status: in progress

the idea is to investigate the possibility to treat patient by using protontherapy and 11B atoms injected into the tumor



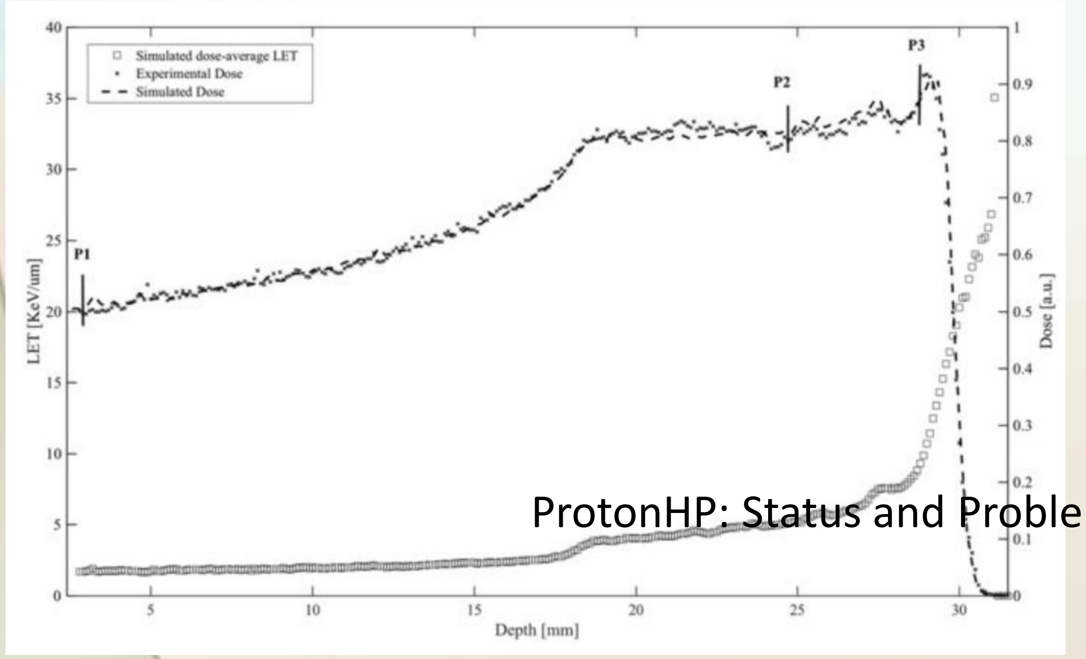
the incident protons trigger a nuclear fusion reaction by the

First in-vitro experiment at LNS:

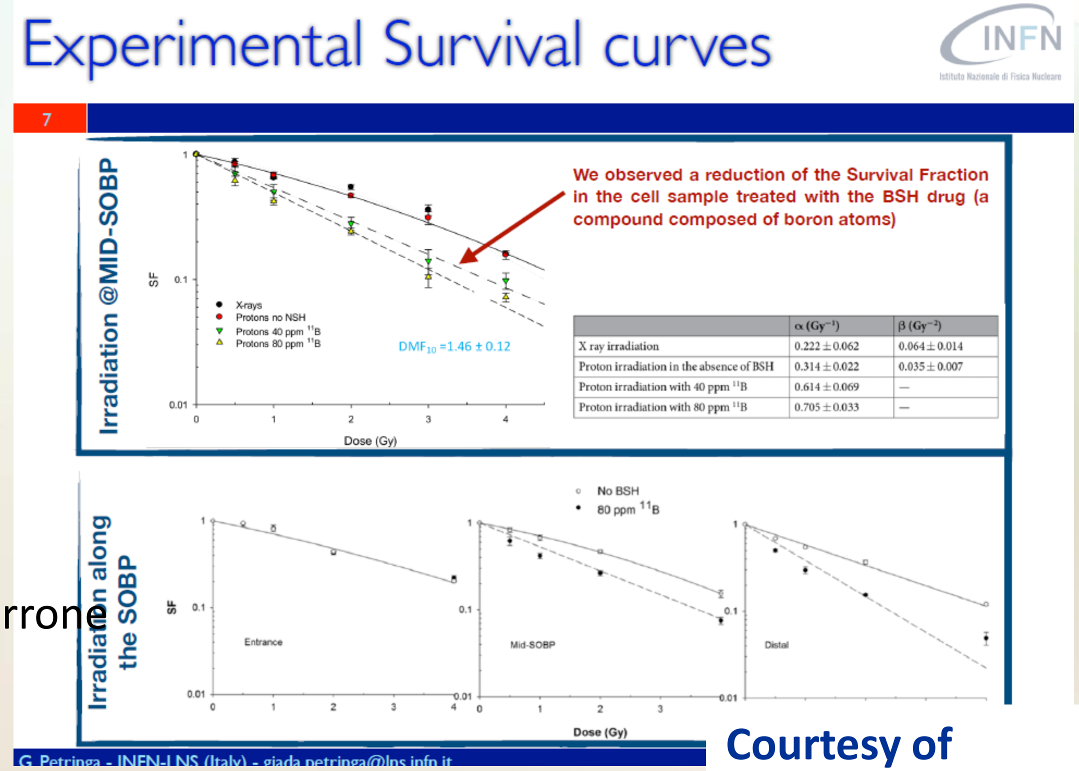
G.A.P. Cirrone, et al. Scientific Reports, vol 8: 1141 (2018)

Courtesy of G. Petringa (LNS)

Irradiated prostate cancer cell line DU145 at three different positions along the Spread-Out Bragg Peak. We measured the clonogenic survival and chromosomal aberrations and **we found an effect that could be related to the alpha particles emitted**



ProtonHP: Status and Problems - Pablo Cirrone



	α (Gy^{-1})	β (Gy^{-2})
X ray irradiation	0.222 ± 0.062	0.064 ± 0.014
Proton irradiation in the absence of BSH	0.314 ± 0.022	0.035 ± 0.007
Proton irradiation with 40 ppm ^{11}B	0.614 ± 0.069	—
Proton irradiation with 80 ppm ^{11}B	0.705 ± 0.033	—

Courtesy of G. Petringa (LNS)

See talk by P. Cirrone. session 8A, Fri 9.00 "ProtonHP: Status and Problems"

New Requirements

Introduction of models to calculate RBE directly inside Geant4

Originator: Giada Petringa, Pablo Cirrone, Giacomo Cuttone (LNS)

Status: in progress

For more than four years LNS is working in the coupling between radiobiological models (able to calculate cell damage from ionising radiation) and a Geant4 simulation

This has been introduced in the Hadrontherapy example

But Giada is proposing a new dedicated extended example on this

The idea is to move the algorithms for the RBE calculation inside the Geant4 kernel in the next year.

New Requirements

Adding a user interface that helps the users to build their own geometry, which allows also to visualize what you are doing, interactively debug, etc....

Originator: Valentina Giacometti

Status: open

Having a model of a generic CT scanner or linac

If the model of a generic CT scanner or linac could be included, a doctor would maybe consider using Geant4 for research purposes.

Originator: Valentina Giacometti

Status: open (linac already available in example “medical_linac”)

New Requirements

MT version of classes to interact with IAEAphsp files

Originator: Miguel Cortés Giraldo, Univ. Sevilla

Status: open

Proton transport models for Geant4-DNA above 100 MeV

Originator: A. Carabe (Univ. Pennsilvania), Miguel Cortés Giraldo (Univ. Sevilla)

Status: on progress (Damián Domínguez)

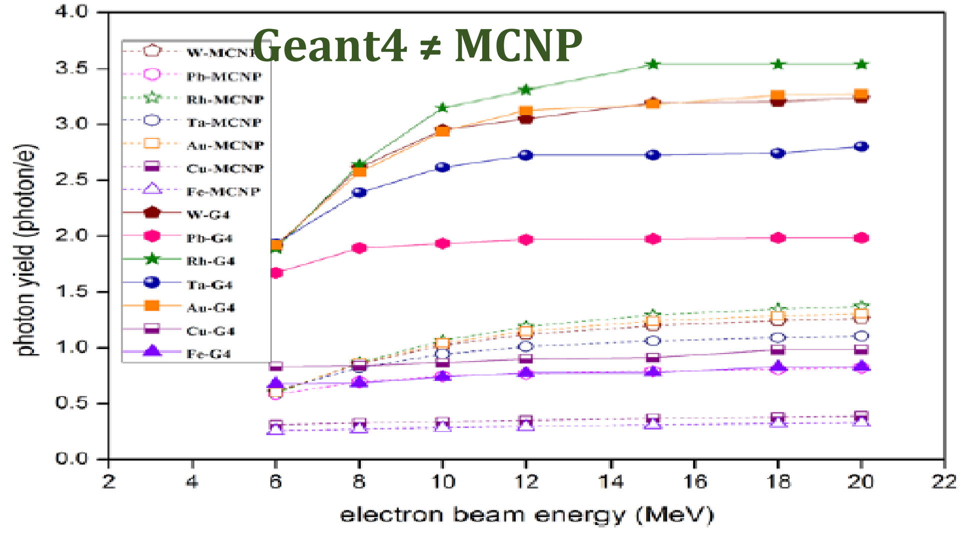
New Requirements

Validation of photoneutron production in radiotherapy linacs

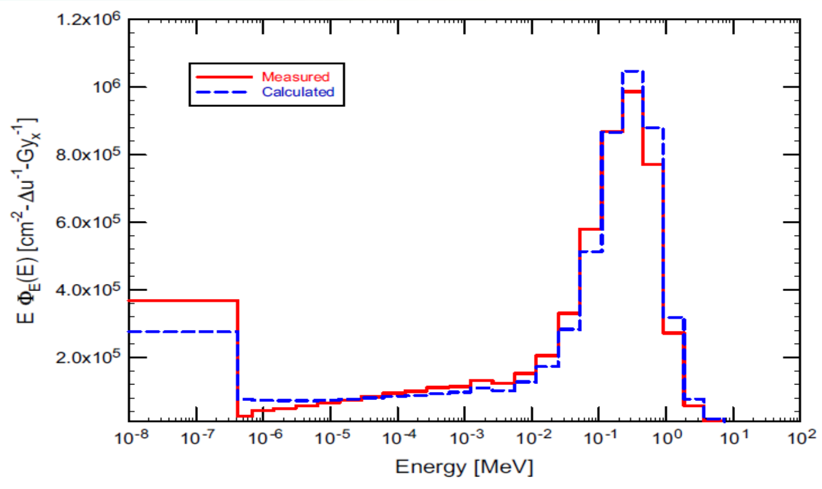
Originator: Miguel Cortés Giraldo, Univ. Sevilla

Status: open

Geant4 ≠ MCNP



and MCNP seems to be right



Isn't this model implemented?

Nuclear Instruments and Methods in Physics Research B 358 (2015) 194–200

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BEAM INTERACTIONS WITH MATERIALS AND ATOMS

A data-based photonuclear reaction model for GEANT4

Jae Won Shin

Department of Physics, Soongsil University, Seoul 156-743, Republic of Korea

Courtesy of M. Cortés-Giraldo (Univ. Sevilla)

Summary of UR fulfillment

	Open	In progress	Ended (or almost)	New ‘18	In Geant4 URT
2017	8	7	0	-	4
2018	3	10	2	7	4

Some personal comments

Geant4 Medical Users is a very well established community:

- ➢ + 200 publications in 2018

but it is a very disperse one

☹ Difficult collaboration

☹ Difficult to find resources to improve Geant4 performance in this field

☹ Not a good communication with Geant4 Collaboration

Should we revive the Geant4 Medical User Organizations?

A perpetual user requirement of the Geant4 Medical Users:

Get an optimal physics list for each simulation field

(Electromagnetic physics lists of V. Ivantchenko are a big step forward)

People uses a best guess physics list, without optimizing it or checking different options

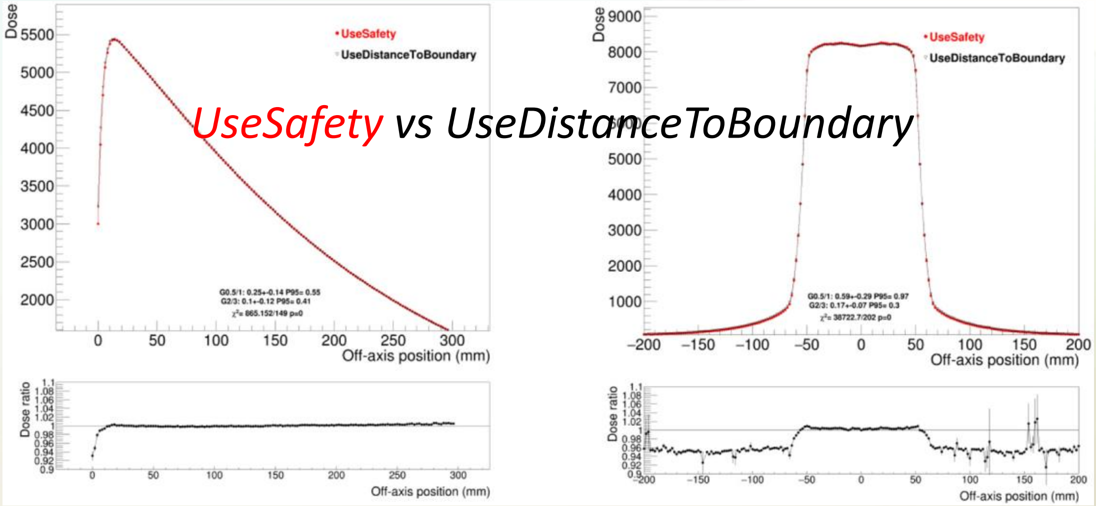
Optimized physics for gamma radiation therapy

P. Arce and J.I. Lagares. Phys. Med. Biol. 63 (3), (2018), 23 pp.

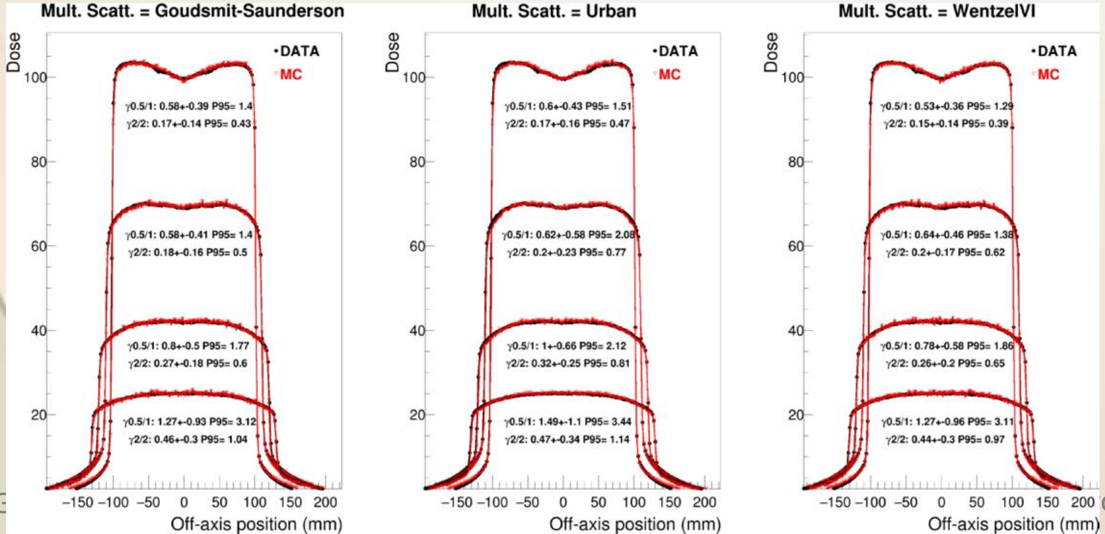
✓ **Optimization of production thresholds and user limits**

✓ **Optimization of EM physics parameters:**

- *lowKinE*
- *mscStepLimit*
- *RangeFactor*
- *RoverRange/FinalRange*
- *binsDecade*
- *linLossLimit*



UseSafety vs *UseDistanceToBoundary*

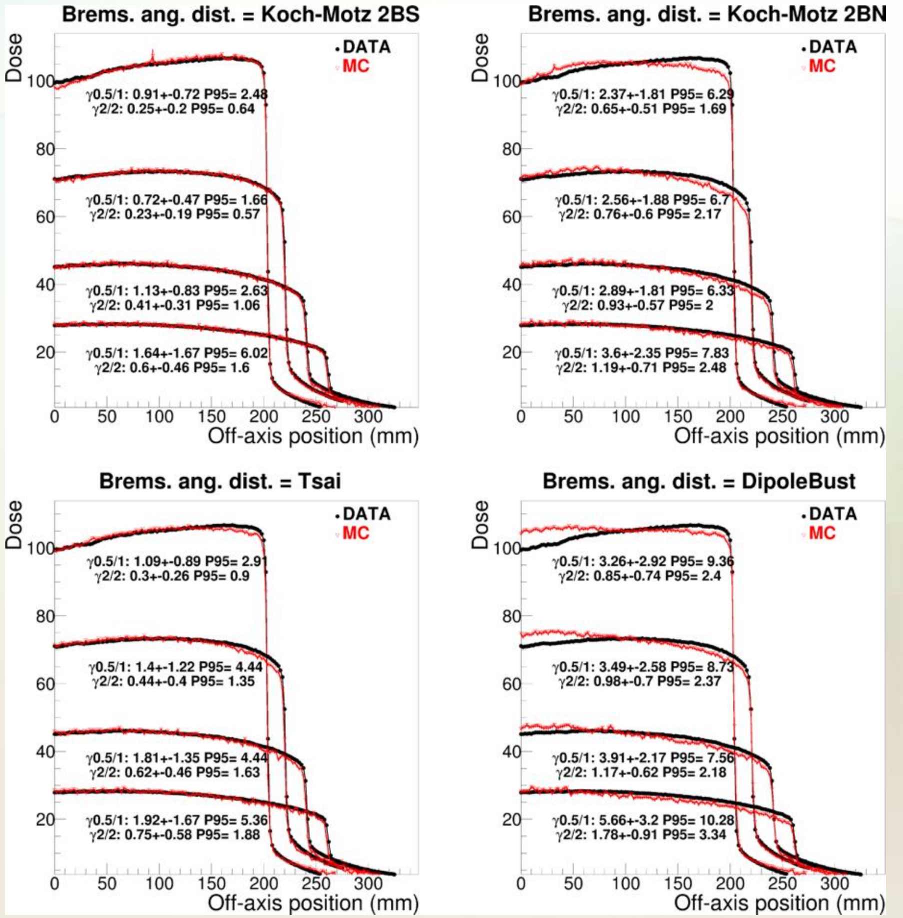


Multiple scattering algorithms

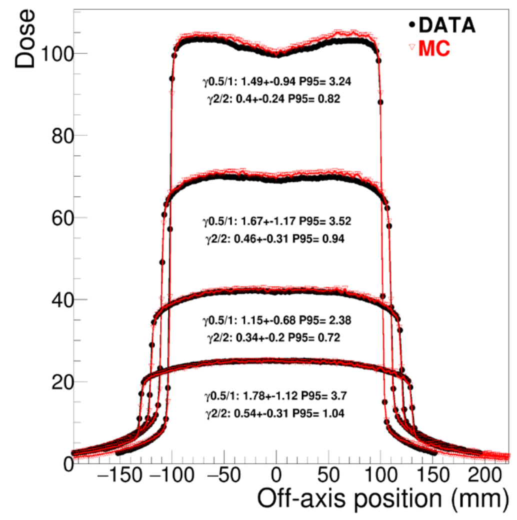
Optimized physics for gamma radiation therapy

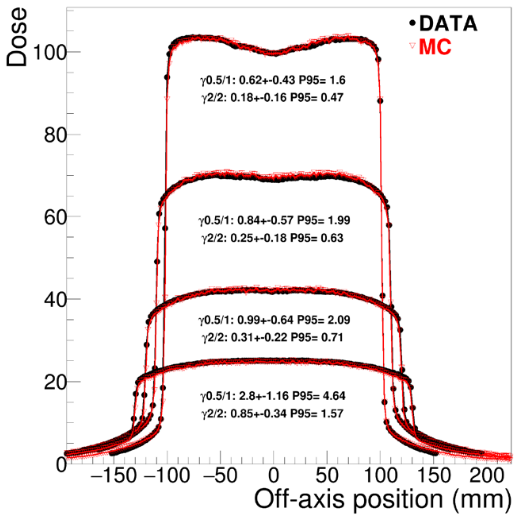
P. Arce and J.I. Lagares. Phys. Med. Biol. 63 (3), (2018), 23 pp

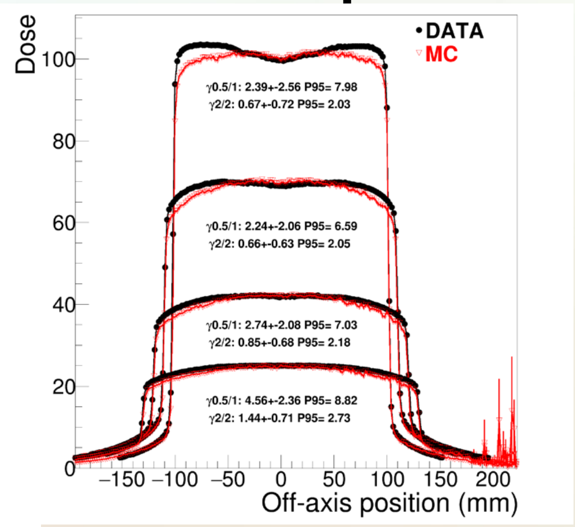
✓ **Bremsstrahlung angular models**



Standard **Livermore** **Penelope**







✓**And several optimization techniques: X 525 speed improvement**

➢**Repetition with an accelerator of a different brand (2 energies) in progress**

Geant4 Medical Simulation Benchmarking Group

A joint effort of several Geant4 developers to:

- identify benchmarks of medical simulation that are based on high quality experimental or theoretical data for simple source and geometry set-ups
- prepare these benchmarks for routine regression testing
- determine when action needs to be taken and work with the developers to determine what that action should be

X-ray imaging
Bremsstrahlung from thick targets
Gamma attenuation
Electron stopping power
Electron backscatter
Electron forward scatter
Low energy isotropic electron kernels

Fano cavity
Brachytherapy validation
Proton Bragg curves
Neutron yield from protons
Light ion Bragg curves
Carbon-12 Bragg peak fragmentation