Highlight of **Geant4 Physics** from the **25**th Collaboration Meeting

Alberto Ribon
(CERN EP/SFT)

SFT group meeting, 12 October 2020

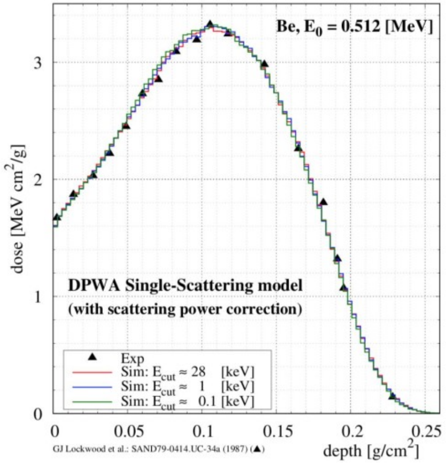
ElectroMagnetic (EM) Physics

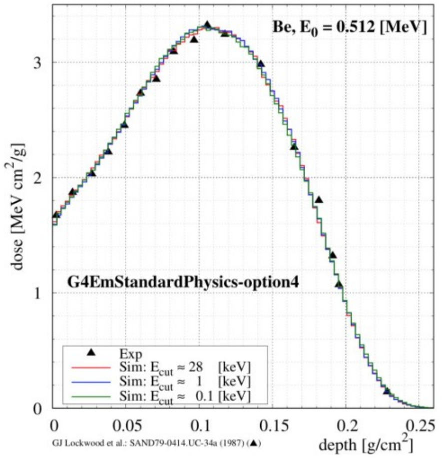
V. Ivanchenko "*Summary on G4 EM Physics*"
Work made by **Mihaly Novak**

The new model:

G4eDPWACoulombScatteringModel

- New model for e-/e+ single Coulomb scattering based on numerical Differential Cross Section (DCS) computed by ELSEPA: Dirac Partial Wave Analysis (DPWA)
  - scattering on the **static-field** of the nucleus **screened** by the atomic electrons
  - using **Fermi charge distribution** of the nucleus and **Dirac-Fock electron densities** of the atoms
  - ***exchange*** (only for e- of course), ***correlation-polarization*** (for E<10 [keV]) were applied on the top of the above ***static-field*** approximation
  - **for electrons** and **positrons** scattering on *free atoms* (described by the above scattering potential) with atomic numbers of **Z = 1-103** and **primary kinetic energies of 10eV - 100MeV**
  - **see more at** https://indico.cern.ch/event/937007/contributions/3937722/attachments/2070119/3475015/MNovak_DPWAElasticModel.pdf
- **NOTE**:
  - ***absorption correction*** **was not included** in the computation (since it's an inelastic channel)
  - most accurate **free atoms DCS**: **accuracy** might be **limited** when **aggregation effects** become **important** (i.e. E < ~keV)
  - the 10 eV low energy limit of the model is only for completeness

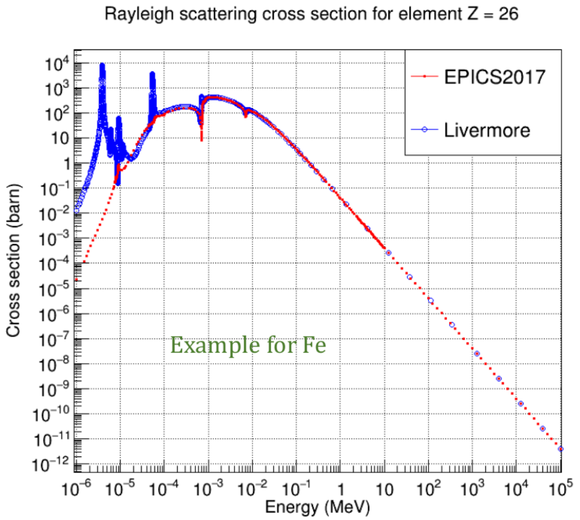




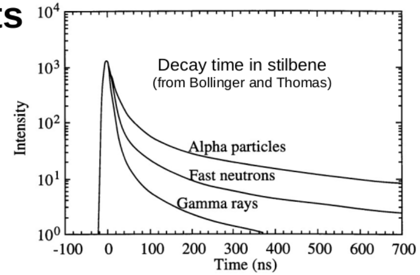
Implementation of EPICS2017 models for photons

Zhuxin Li, Ph.D at CENBG

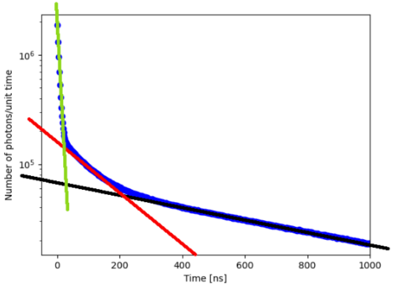
- The "Livermore" low-energy electromagnetic models are currently using the databases of EPDL97/2014
- EPICS2017: Electron Photon Interaction Cross Section library
  - Dermott Cullen https://www-nds.iaea.org/epics/
- Update of data and Livermore model implementations for the following photon-matter interaction processes:
  - 1) Gamma conversion
  - 2) Compton effect
  - 3) Photoelectric effect
  - 4) Rayleigh scattering



New physics: Scintillation time constants



- In <= 10.7, have the choice of fast and slow time constants, with the same yield for all particles; OR particle specific yields, with one time constant
  - Could also write your own physics list!
- In >= 10.7, 3 time constants and particle-specific yields at the same time
  - by users requests
- **Both ways work now**, but the **old way to be deprecated in the next major release**
- In 10.6: material properties SCINTILLATIONYIELD and YIELDRATIO. New method uses SCINTILLATIONYIELD and SCINTILLATIONYIELD[1/2/3].
  - In both methods SCINTILLATIONYIELD gives number of photons (per unit energy).
- Fraction of photons in channel 1 is SCINTILLATIONYIELD1/(SCINTILLATIONYIELD1 + SCINTILLATIONYIELD2 + SCINTILLATIONYIELD3) etc.
- Change material property names from [FAST/SLOW]TIMECONSTANT etc. to SCINTILLATIONTIMECONSTANT[1/2/3] etc.
- Analogous names for particles: PROTONSCINTILLATIONYIELD1 etc.



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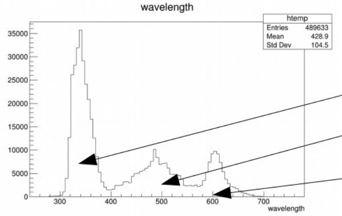
New physics: Two WaveLengthShifting Process

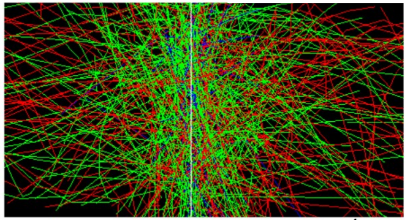
- Process (and slide) by Alex Howard, Imperial College
- Since beta release a simple "clone" of the existing WLS has been included in G4OpticalPhysics constructor
- Cannot convolve the response function as it's a discrete mechanism
  - either WLS-1 or WLS-2 and some transfer from WLS-1 to WLS-2
- Try it with OpNovice2/wls.mac
- Identical interface – append "2":

```
scintCoreMaterialProperties->AddProperty("WLSCOMPONENT",wls1SpecVector);
scintCoreMaterialProperties->AddProperty("WLSCOMPONENT2",wls2SpecVector);
scintCoreMaterialProperties->AddProperty("WLSABSLENGTH",Wls1AbsEnergy,Wls1AbsLength,WLS1_ABS_ENTRIES);
scintCoreMaterialProperties->AddProperty("WLSABSLENGTH2",Wls2AbsEnergy,Wls2AbsLength,WLS2_ABS_ENTRIES);
scintCoreMaterialProperties->AddConstProperty("WLSTIMECONSTANT",Parameters::GetInstance()->WlsDecayTime()*ns);
scintCoreMaterialProperties->AddConstProperty("WLSTIMECONSTANT2",Parameters::GetInstance()->WlsDecayTime()*ns);
```



Generated Photons

Blue: Primary Scintillation
Green: WLS1
Red: WLS2



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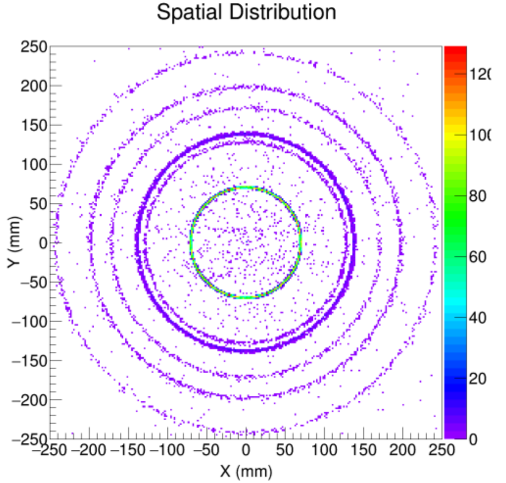
Istituto Nazionale di Fisica Nucleare

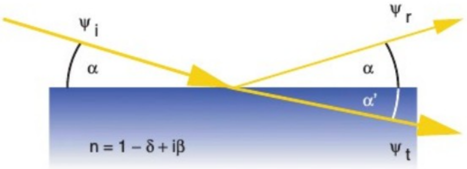
Simple test: diffraction of a **8 keV** X-ray beam from a thin “slab” of a **graphite powder**.



Refinement and extension of photon coherent interaction models with matter

G. Paternò

INFN Sezione di Ferrara, Dipartimento di Fisica e Scienze della Terra, Università di Ferrara

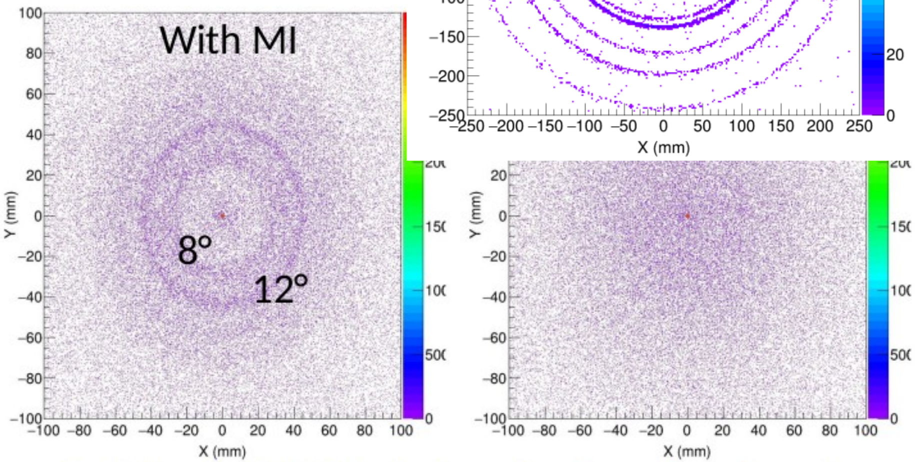


Outline

– Development of interference effects in coherent X-ray scattering model.

– Development of diffraction process in polycrystalline materials.

– Development of refraction/reflection of X-rays.



Scattering of a **20 keV photon beam** in a **human breast** sample

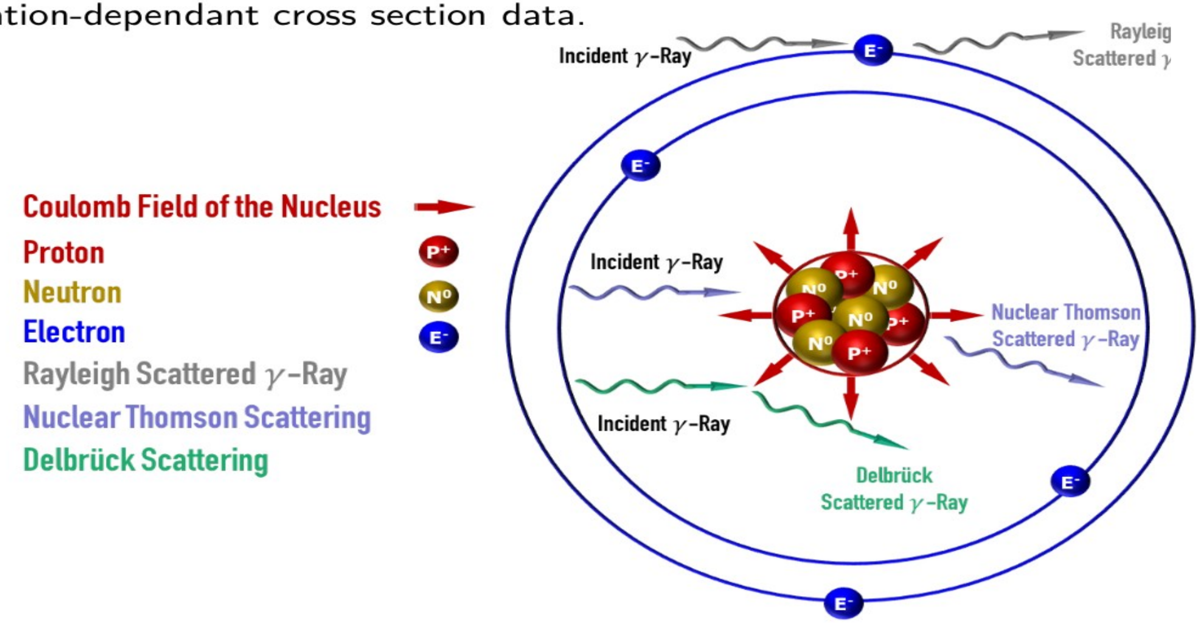
Models for low-energy gamma elastic scattering

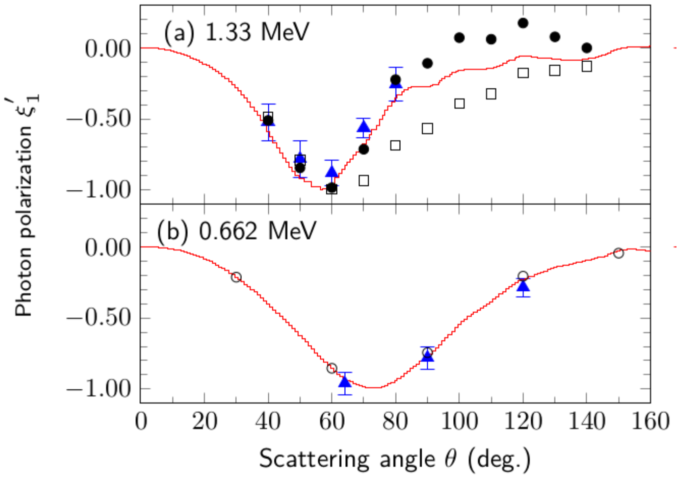
M. Omer[1] & R. Hajima [1,2]

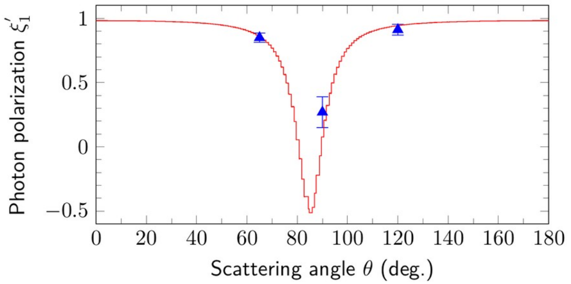
Elastic Scattering of γ-rays

Elastic Scattering should:

- Include all effective contributing scattering processes.
- Superimpose the processes coherently.
- Polarization-dependant cross section data.







Overview of pre-chemical aspects of Geant4-DNA and initial radiological yields

Wook-Geun Shin, Jose Ramos-Mendez, Bruce Faddegon, Chul Hee Min, Sebastien Incerti

Impact of pre-chemical stage on biological damage

- This stage determines the number (and distribution) of chemical species induced by physical interactions at early time (1 ps).
- However, it is still impossible to understand mechanistically femtosecond-scale aspects of pre-chemical stage.
- Thus, the pre-chemical parameters are adjusted for calculating G-values to match experimental data in this study.

Purpose of this study

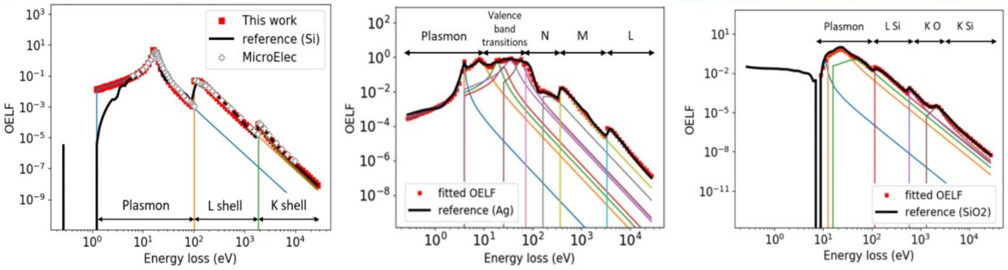
- To find out the optimal pre-chemical model for water radiolysis
- The models used in Geant4-DNA are corrected in order to be consistent with original papers
  1) Electron thermalization model
  2) Physico-chemical interactions
  3) Dissociation channels

GEANT4 MicroElec module 2020 update

Q.Gibaru, P. Caron, C.Inguimbert, M. Raine, D. Lambert

Parallel Session on EM physics

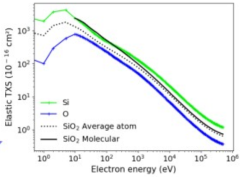
New developments (2)



- **11 materials**

  C, Al, Si, Ti, Ni, Cu, Ge, Ag, W, Kapton and SiO_2
- **2 dielectrics**

  Kapton and SiO_2
- **Low energy limit extended to the work function ~5 eV**



- **ELECTRONS : Elastic cross sections re-calculated following PW formalism using ELSEPA** (1 eV to 500keV)

F. Salvat, A. Jablonski, C.J. Powell, ELSEPA—Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules, Computer Physics Communications. 165 (2005) 157–190.

GEANT4 MicroElec module : current state

MICROELEC :

- Low energy transport module
- [~eV, ~keV] electrons
- > ~50 keV/amu protons & ions
- Based on complex dielectric function (OELF),
- Extended Drude model
- Silicon material
- low energy limit : 16 eV

NEEDs :

- Extending to other materials
- Extending to other applications (≠ microelectronics)
- Improving the reliability specially for protons & ions

Hadronic Physics (HAD)

String Models (FTF & QGS)

- Completed the extension to deal with nuclear interactions of **charm & bottom hadrons**, available in physics lists in 10.7
  - Simple 1-channel, fully-hadronic decays defined for heavy hadrons
    - Applied only for secondary heavy hadrons
  - QGS used above 12 GeV in QGS-based physics lists
- FTF : improved algorithm of string formation
  - To better describe Pt-Xf correlations in NA49 158 GeV/c p-p data
- QGS : improved treatment of anti-baryon interactions
  - In QGS-based physics lists, used QGSP above 12 GeV for : antiproton , antineutron , hyperons and anti-hyperons
- On-going work on neutrino / lepton / gamma - nuclear

HADRONIC PHYSICS AND PHYSICS LIST DESIGN

V. Ivanchenko
CERN & Tomsk State University, Tomsk, Russia

New utilities for hadron physics configuration

- G4HadParticles – returns several lists of particle PDG codes
  - *std::vector<G4int>& G4HadParticles::GetKaons();*
  - *std::vector<G4int>& G4HadParticles::GetHyperons);*
  - *std::vector<G4int>& G4HadParticles::GetAntiHyperons();*
  - ...
- G4HadProcesses – return pointers to hadronic processes per particle and allows adding extra cross section per particle
  - *G4HadronicProcess* G4HadProcesses::FindInelasticProcess(const G4String& partname);*
  - *G4HadronicProcess* G4HadProcesses::FindInelasticProcess(const G4String& partname);*
  - *G4bool G4HadronicProcesses::AddInelasticCrossSection(const G4ParticleDefinition*, G4VCrossSectionDataSet* my_xs);*
  - ......
- G4HadronicBuilder – build standard set of models and cross sections for group of particles
  - *G4HadronicBuilder::BuildHyperonsFTFP_BERT();*
  - *G4HadronicBuilder::BuildBCHadronsFTFP_BERT();*
  - *G4HadronicBuilder::BuildHyperonsQGSP_BERT();*

Variation of hadronic cross sections

- For study of systematic uncertainty due to simulation we may considered following approach:
  - *For hadronic models we propose to use different Physics Lists*
    - FTFP_BERT -> QGSP_BIC, FTFP_INCLXX, or QBBC
  - *For cross sections we may propose to use a factor to vary cross section value*
    - +- 5-10% would be within Geant4 accuracy
- Cross section factors are defined via G4HadronicParameters class:
  - *G4bool ApplyFactorXS() const; // false by default*
  - *G4double XSFactorNucleonInelastic() const ;*
  - *G4double XSFactorNucleonElastic() const ;*
  - *G4double XSFactorPionInelastic() const ;*
  - *G4double XSFactorPionElastic() const ;*
  - *G4double XSFactorHadronInelastic() const ;*
  - *G4double XSFactorHadronElastic() const ;*
  - *G4double XSFactorEM() const ;*
- User must change the flag and set corresponding factor via C++ interface

Recent developments and prospects of ParticleHP

Emilio Mendoza Cembranos, Daniel Cano Ott

CIEMAT

SaG4n: Simulation of (α,xn) reactions with Geant4

We have been investigating the performance of Geant4 in the simulation of **neutrons generated by α-decay**, via (α,xn) reactions.

Motivation:

- Low background experiments. (e.g. dark matter detection).
- Nuclear technology.
- …

We have published a paper → E. Mendoza et al., *Neutron production induced by α-decay with Geant4*, NIMA 960, 163659 (2020)

New neutron library G4NDL4.6

G4NDL4.5 → incident neutron data library used up to Geant4.10.5. It comes mainly from ENDF/B-VII.1.

G4NDL4.6 → incident neutron data library used in Geant4.10.6. It is JEFF-3.3.

Main changes:

ENDF/B → JEFF

Isotopes with Z>92 now available

The main advantage of G4NDL4.6 over G4NDL4.5 is that Geant4 results are closer to MCNP when using JEFF-3.3 than when using any other library, i.e. **the performance of Geant4 seem to be the best when using JEFF-3.3**. A verification study has been

New UI commands to replace environmental variables

There are several options in ParticleHP which are controlled via environmental variables:

G4NEUTRONHP_USE_ONLY_PHOTONEVAPORATION
G4NEUTRONHP_NEGLECT_DOPPLER
G4PHP_NEGLECT_DOPPLER
G4NEUTRONHP_SKIP_MISSING_ISOTOPES
G4NEUTRONHP_PRODUCE_FISSION_FRAGMENTS
G4PHP_USE_NRESP71_MODEL
G4PHP_DO_NOT_ADJUST_FINAL_STATE
G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE
G4NEUTRON_HP_USE_WENDT_FISSION_MODEL

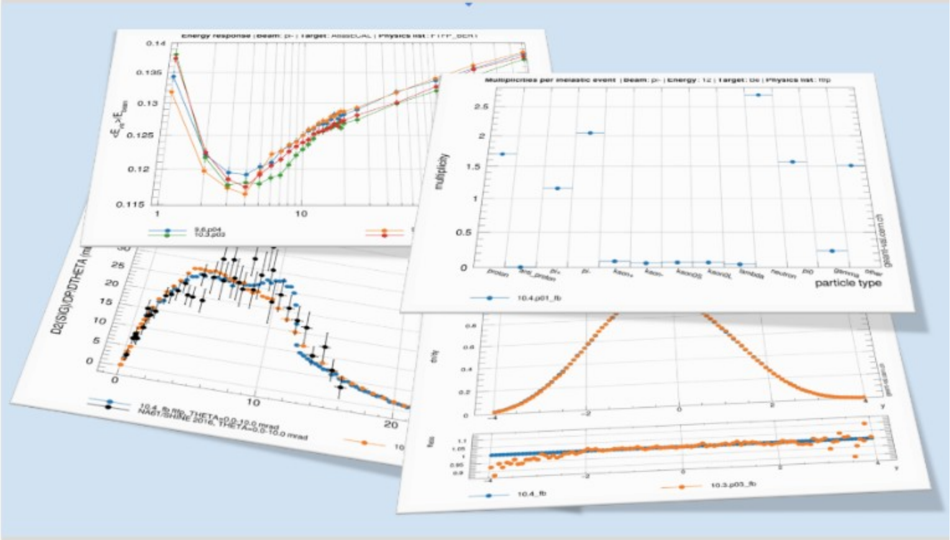
Validation

GEANT-VAL:
VALIDATION WEB APPLICATION

Dmitri Konstantinov — IHEP, Protvino
Grigory Latyshev — IHEP, Protvino

With participation of:
Witold Pokorski, Alberto Ribon, Ivan Razumov, Ioana Ifrim, Luc Feyermuth, Gonzalo De La Cruz, George Lestaris, Hans Wenzel, Julia Yarba.

Virtual Geant4 Collaboration Meeting, 2020



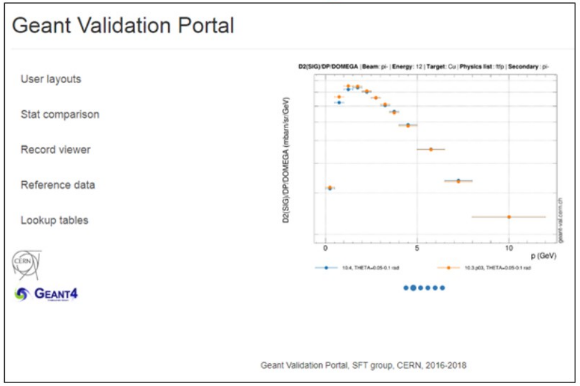
- The official (and now unique) validation tool of Geant4
- Used regularly for hadronic and electromagnetic showers
- Growing number of thin-target tests, for both EM and HAD physics
- Included also a suite of benchmarks relevant for medical physics

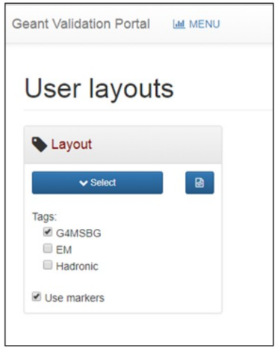
G4_Med, a Geant4 benchmarking tool for medical physics applications: current status and future perspective

S. Guatelli on behalf of the G4-Med Group

P. Arce[1], D. Bolst[2], M-C. Bordage[3], A. Chacon[2], P. Cirrone[4], M.A. Cortes-Giraldo[5], D. Cutajar[2], G. Cuttone[4], L. Desorgher[6],P. Dondero[7], A. Dotti[8], B. Faddegon[9], C. Fedon[10], S. Guatelli[2], S. Incerti[11], V. Ivanchenko[12], D. Konstantinov[13], I. Kyriakou[14], G. Latyshev[13], A. Le[2], C. Mancini-Terracciano[15], A. Mantero[7], M. Maire[16], M. Novak[17], C. Omachi[18], L. Pandola[19], A. Perales[20], Y. Perrot[21], G. Petringa[4], J.M. Quesada[5], J. Ramos-Méndez[9], F. Romano[22], M. Safavi-Naeini[25], D. Sakata[2], L.G. Sarmiento[23], T. Sasaki[24], I. Sechopoulos[10], E. Simpson[26], T. Toshito[18], D. H. Wright[27]

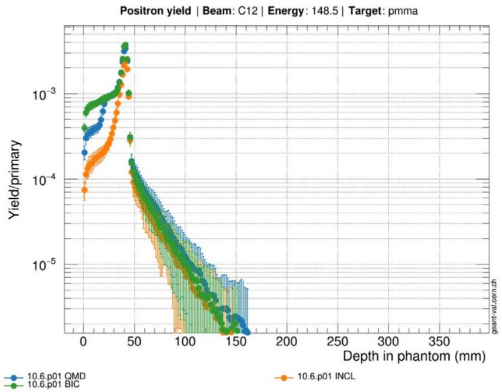
Integration in *geant-val* for Automatized Regression Tests

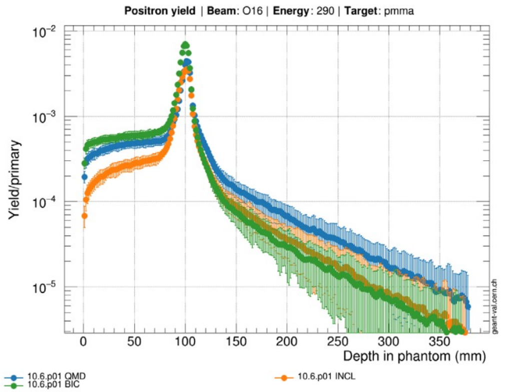




https://geant-val.cern.ch/

Publication: Luc Freyermuth, Dmitri Konstantinov, Grigorii Latyshev, Ivan Razumov, Witold Pokorski, Alberto Ribon
EPJ Web Conf. 214 05002 (2019)
DOI: 10.1051/epjconf/201921405002





G4_Med is integrated in ***geant-val*** to execute regularly automatized regression tests on the CERN computing infrastructure