Systematic validation of gamma cross sections

New test for brachytherapy

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Systematic test of photon cross sections with respect to NIST data

- CMRP: S. Guatelli and J. Davis

- Swhard: A. Mantero and P. Dondero

Activity within the Geant4 Low Energy Group, in particular S. Incerti, V. Ivanchenko and L. Pandola

Project

- K. Amako et al, IEEE TNS, 52(4), 910-918, 2005.
  - Comparison of
    - Attenuation coefficients
    - Stopping Power and Range of e^-, p and α

    With respect to NIST

- The project is to have systematic regression tests on gamma ray cross sections
  - *trunk/verification/electromagnetic/attenuation*
  - The test are extended to a larger set of materials

Comparison of Geant4 Electromagnetic Physics Models Against the NIST Reference Data

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Abstract—The Geant4 Simulation Toolkit provides an ample set of physics models describing electromagnetic interactions of particles with matter. This paper presents the results of a series of comparisons for the evaluation of Geant4 electromagnetic processes with respect to United States National Institute of Standards and Technologies (NIST) reference data. A statistical analysis was performed to estimate quantitatively the compatibility of Geant4 electromagnetic models with NIST data; the statistical analysis also highlighted the respective strengths of the different Geant4 models.

Index Terms—Geant4, Monte Carlo, NIST, validation.

I. Introduction

GEANT4 is an object oriented toolkit [1] for the simulation of the passage of particles through matter. It offers an ample set of complementary and alternative physics models for electromagnetic and hadronic interactions, based on theory, experimental data or parameterizations.

The validation of Geant4 physics models with respect to authoritative reference data is a critical issue, fundamental to establish the reliability of Geant4-based simulations. This paper is focused on the validation of Geant4 electromagnetic models, with the purpose to evaluate their accuracy and to document their respective strengths. It presents the results of comparisons of Geant4 electromagnetic processes of photons, electrons, protons and α particles with respect to reference data of the United States National Institute of Standards and Technologies (NIST) [2], [3] and of the International Commission on Radiation Units and Measurements (ICRU) [4], [5].

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TABLE I
GEANT4 ELECTROMAGNETIC MODELS IN THIS COMPARISON STUDY

Particle	Geant4 Models in Electromagnetic Packages
Photon	Geant4 Low Energy - EPDL
	Geant4 Low Energy - Penelope
	Geant4 Standard
Electron	Geant4 Low Energy - EEDL
	Geant4 Low Energy - Penelope
	Geant4 Standard
Proton	Geant4 Low Energy - ICRU 49
	Geant4 Low Energy - Ziegler 1985
	Geant4 Low Energy - Ziegler 2000
	Geant4 Standard
α	Geant4 Low Energy - ICRU 49
	Geant4 Low Energy - Ziegler 1977
	Geant4 Standard

The simulation results were produced with Geant4 version 6.2. The Geant4 test process verifies that the accuracy of the physics models will not deteriorate in future versions of the toolkit with respect to the results presented in this paper.

II. Overview of Geant4 Electromagnetic Physics Packages

The Geant4 Simulation Toolkit includes a number of packages to handle the electromagnetic interactions of electrons, muons, positrons, photons, hadrons and ions. Geant4 electromagnetic packages are specialised according to the particle type they manage, or the energy range of the processes they cover.

The physics processes modeled in Geant4 electromagnetic packages include: multiple scattering, ionization, Bremsstrahlung, positron annihilation, photoelectric effect, Compton and Rayleigh scattering, pair production, synchrotron and transition radiation, Cherenkov effect, refraction, reflection, absorption, scintillation, fluorescence, and Auger electron emission [1].

Alternative and complementary models are provided in the various packages for the same process. The Geant4 electromagnetic models studied in this paper are listed in Table I.

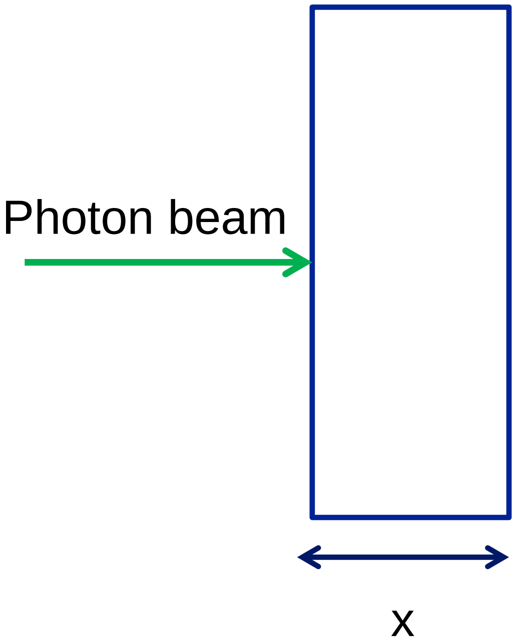
A. *Standard Electromagnetic Package*

The Geant4 Standard electromagnetic package [8] provides a variety of models based on an analytical approach, to describe the interactions of electrons, positrons, photons, charged hadrons and ions in the energy range 1 keV–10 PeV.

Attenuation coeff tests

- Elements: Be (Z=4), C(Z=6), O(Z=8), Z=12, Al (Z=13), Ar (Z=18), Ca (Z=20), Fe(Z=26), Cu(Z=29), Ge (Z=32), Ag (Z=47), Xe (Z=54), Ce(Z=58), Gd (Z=64), W(Z=74), Au (Z=79), Pb (Z=82), Bi (Z=83), U(Z=92)
- Compounds to test: Water, BGO, PMMA, tissue, bone
- New! Materials added for space science applications:mylar, kevlar, polyethylene, polymide, copper, CdZnTe, Fr4, steel, SiC, Si3N4, Iridium (input by P. Dondero and A. Mantero)
- Attenuation coefficients:
  - Total
  - Rayleigh scattering
  - Photoelectric effect
  - Compton scattering
  - Gamma conversion

Simulation set-up



$$N = N_0 e^{-\mu x}$$

- User application
  - Calculate **attenuation coefficients**
  - The cut is fixed 1/10 of the target thickness
  - **Physics lists**:
    - EMStandard_opt0
    - EMStandard_opt3
    - EMStandard_opt4
    - Livermore
    - Penelope

- Same simulation parameters for the alternative physics lists

- Comparison: **% difference**: abs((NIST-Geant4/NIST)*100)

  Ratio

- Regression testing: G4 10.0, 10.1, 10.2.p02

Standard EM physics (option 0)

- Standard Physics List
  - G4PhotoElectricEffect()
  - G4ComptonScattering()
  - G4GammaConversion()

- No Rayleigh scattering

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Standard EM physics, option 3

- G4KleinNishinaModel is used for the Compton scattering simulation
- G4RayleighScattering process is active
  - Default Livermore Rayleigh scattering model
- G4GammaConversion()
- In Geant4 10.2, photoelectric effect by means of Livermore model

Standard EM physics, option 4

- G4RayleighScattering process is active
- G4 Livermore Photoelectric effect
- G4KleinNishinaModel is used above 20 MeV, G4LowEPComptonModel is used below for the Compton scattering simulation.
- G4PenelopeGammaConversion model is used for gamma conversion below 1 GeV.

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EM Livermore Physics List

- Livermore Rayleigh scattering
- G4LivermorePhotoElectricModel for gamma below 1 GeV
- G4LivermoreComptonModel for gamma below 1 GeV
- G4LivermoreGammaConversionModel for gamma below 1 GeV

EM Penelope Physics List

- G4PenelopePhotoElectricModel for gamma below 1 GeV
- G4PenelopeComptonModel for gamma below 1 GeV
- G4PenelopeGammaConversionModel for gamma below 1 GeV
- G4PenelopeRayleighModel
  - Cross section: the same of G4Livermore Rayleigh Model
  - The final state is different

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Summary of the results

- Geant4 10.1
- Reference data of NIST have an uncertainty up to 5%
- The statistical uncertainty of Geant4 results is 3%

Z	Rayl	Photoel	Compton	Conversion	Total
4	Livermore and Penelope: 1 and 1.5 keV, then ok	Livermore: x Penelope: x Std_opt0 and opt3: diff 3 keV <E < 1MeV Std_opt4: x	Livermore: x Std_opt4 : x Penelope: E< ~5 keV Std_opt0 and opt3: E< 6 keV	Livermore:x Penelope: x Std_opt3: x Std_opt4:x	Livermore:x Penelope: x Std_opt0: 4 keV-40 keV Std_opt3: 4 keV-10 keV Std_opt4:x
13	Livermore: 1-8 keV Penelope: 1-8 keV	Livermore: x Penelope: x Std_opt0: x Std_opt3: x Std_opt4: x	Livermore: x Penelope: 1 keV- 10 keV Std_opt3 and opt0: 1keV- 15 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore:x Penelope: x Std_opt0: 15 keV<E< 150 keV Std_opt3: x Std_opt4:x
20	Livermore and Penelope: below 15 keV	Livermore: x Penelope: x Std_opt0 and opt3: 1-3 MeV Std_opt4: x	Livermore: x Penelope: 1 keV- 4 keV Opt0 and opt3: E<10 keV Std_opt4: x	Livermore:x Penelope: x Std_opt3: x Std_opt0:x Std_opt4: x Just first point for penelope, opt0, opt3 and opt4	Livermore: x Penelope: x Std_opt0: 30 keV-200 keV Std_opt3: x Std_opt4: x
26	Livermore and Penelope: below 20 keV	Livermore: x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: E< 8 keV Std_opt3 and opt0: E< 10 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: 40 keV-200keV Std_opt3: x Std_opt4: x
32	Livermore and Penelope: below 40 keV	Livermore: x Penelope: x Std_opt0:x Std_opt3:x Std_opt4: x	Livermore: x Penelope : 1keV< E< 10 keV Std_opt3 and opt0: 1 keV < E< 10 keV Std_opt4: x	Livermore:x Penelope: x Std_opt3: x Std_opt4: x Just first point for penelope, opt0, opt3	Livermore: x Penelope: x Std_opt0: 50 keV – 300 keV Std_opt3: x Std_opt4: x

X: agreement within 5% red: differences > 5 %

Summary 2 – 10.1

green: differences < 5%
red: differences > 5%

Z	Rayl	Photoelectric	Compton	Conversion	Total
47	Livermore: x Penelope: x	Livermore: x Penelope: x Std_opt4: x Std_opt0 and std_ opt3 differences between 5% and 20% for E> ~ 50 MeV	Livermore: x Penelope: E < 8 keV Std_opt0: diff up to 10% E< 5 keV Std_opt3: diff up to 10% E< 5 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: 15 keV-300keV up to 10% Std_opt3: x Std_opt4: x
56	Different	Running more stats	Livermore: x Penelope: E < 10 keV Std_opt0: diff up to 30% E< 10 keV Std_opt3: diff up to 30% E< 10 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Opt0 and opt3: 0.0015 -0.003 keV (up to 7%) opt0: 0.03 -0.4 MeV (up to 7%) Livermore: X Penelope:X Std_opt4:X
64	Different	Running more stats	Livermore: x Penelope: diff up to E< 20 keV std_opt0 and Std_opt3: diff up to 10% E< 20 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Running more stats

Summary 3 – 10.1

green: differences < 5%
red: differences > 5%

Z	Rayl	Photoelectric	Compton	Conversion	Total
74	Different From % to 100% at low energies	Running more stats	Livermore: x Penelope: E < 20 keV Std_opt0: E< 10 keV Std_opt3: E< 10 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: 15 keV-600keV up to 10% Std_opt3:1 keV-10 keV Std_opt4: x
79	Differences between 5 and 10%	Livermore: x Penelope: x Std_opt0: E< 6keV Std_opt3: E < 6 keV Std_opt4: x	Livermore: x Penelope: E < 20 keV Std_opt0: E< 1.5 keV Std_opt3: E< 1.5 keV Std_opt4: x	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x opt0: 1 keV – 600 keV: differences > 5% opt3: 1 keV – 5 keV differences > 5% Std_opt4: x
82	15% difference for all energies	Livermore: x Penelope: x Std_opt0: E< 6keV , up 10% Std_opt3: E < 6 keV , to 10% Std_opt4: x	Livermore: x Penelope: E < 8 keV Std_opt0: E< 8 keV Std_opt3: E< 8 keV Std_opt4: x Running more stats	Livermore:x Penelope: x Std_opt0:x Std_opt3: x Std_opt4: x	Livermore:X Penelope:X Opt0 : E < 600 keV Opt3 E< 6 keV diff up to 10-15% Opt4:X
92	Running more stats	Running more stats	Running more stats	Running more stats	Running more stats

WHARD Cuttin'Edge Technology

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Summary – 4 – 10.1

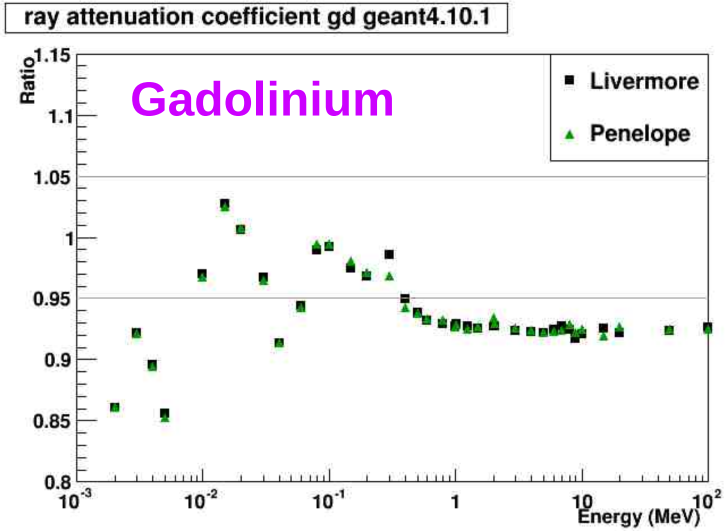
Materials	Rayl	Photoelectric	Compton	Conversion	Total
Water	Livermore: < 5 keV Penelope: < 5 keV	Livermore: x Penelope: x Std_opt0: x Std_opt3: x Std_opt4: x	Livermore: x Penelope: E < 10 keV Std_opt0: E< 10 keV Std_opt3: E< 10 keV Std_opt4: x	Livermore: x Penelope: x Std_opt3: x Std_opt4: x	More statistics Livermore: x Penelope: x Std_opt0: x Std_opt3: x Std_opt4: x
PMMA	Running	Running	Running	Running	Running
BGO	Running livermore	Livermore: x Penelope: x Std_opt0: 1keV – 5keV Std_opt3: 1keV – 5keV Std_opt4: x	Running more stats	Livermore: x Penelope: x Std_opt3: x Std_opt4: x	Livermore: x Penelope: x Std_opt0: 1 keV – 4 keV and 40 keV – 500 keV Std_opt3: 1keV – 5 keV Std_opt4: x
Bone	Running	Running	Running	Running	Running
Soft tissue	Running	Running	Running	Running	Running

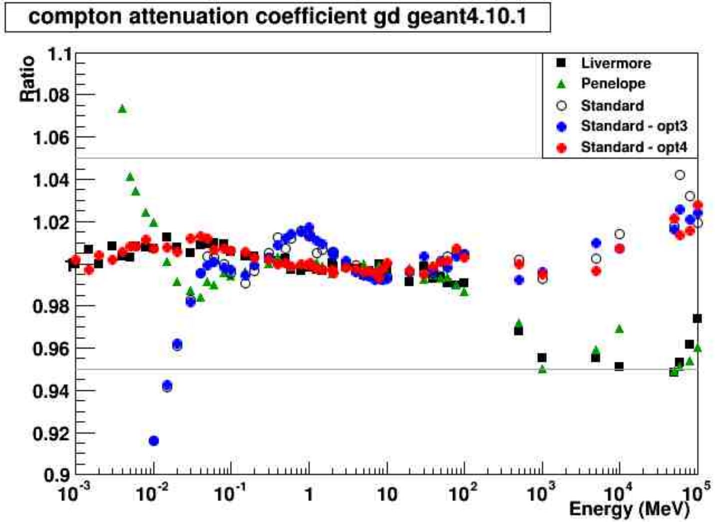
green: differences < 5%

red: differences > 5%

Results

- Overall good agreement (<5%)
- Rayleigh cross sections are different from NIST
- Compton Scattering
  - Penelope, Standard opt0 and 3 have differences below few keV
- Regression test between Geant4 10.0 and 10.1: no differences

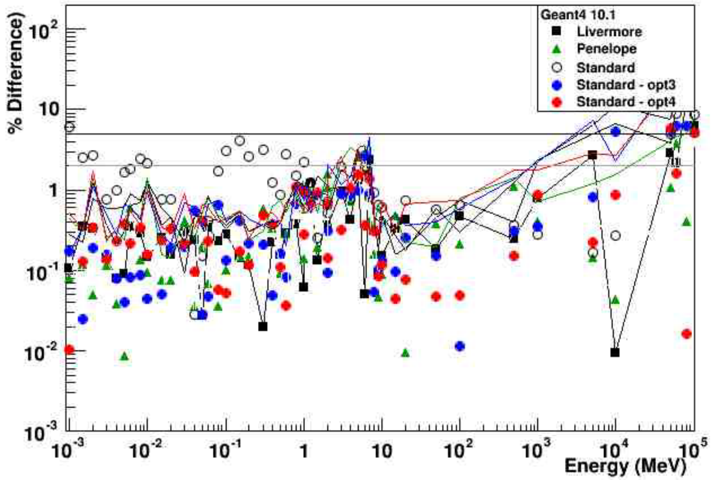




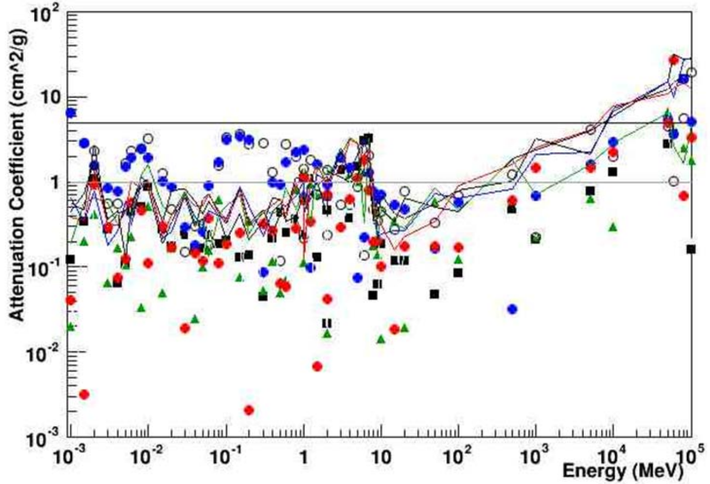
Regression testing

- Geant4 10.2.p02
- By P. Dondero and A. Mantero
- Comparison Geant4 10.1 vs 10.2.p02: EMStandard_option3 has now Livermore photoelectric effect model.

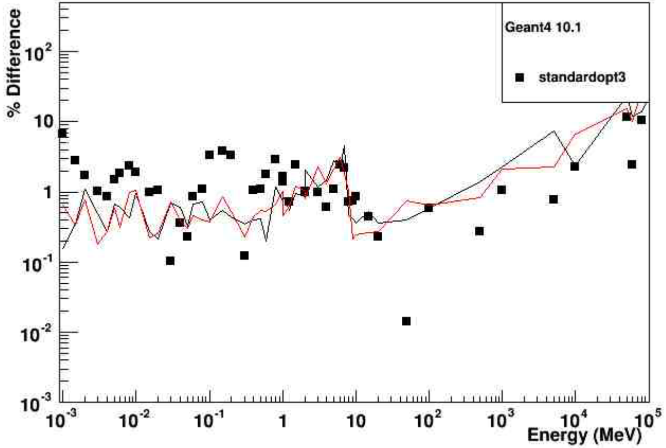
Photoelectric effect, 10.2.p02



Photoelectric effect, 10.1



% Difference between Geant4 10.1 and 10.2.p02



Next step

- Finish the regression testing
- Statistical analysis (Chi-squared)
- Publish

Geant4 validation for Brachytherapy

- Dean Cutajar
  - Centre for Medical Radiation Physics, University of Wollongong, Australia
  - St George Cancer Care Centre, Kogarah, Australia
- Susanna Guatelli
  - Centre for Medical Radiation Physics, University of Wollongong, Australia
- Joel Poder (PhD student)
  - Centre for Medical Radiation Physics, University of Wollongong, Australia
  - Chris O'Brien Lifehouse, Sydney, Australia

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AAPM Task Group 43 Report

- The TG43 report recommends the dose rate for a cylindrical source be expressed in 2D coordinates in terms of separable functions

$$D^{*}(r,\theta) = S_k.\ \lambda.\ [G(r,\theta) / G(r_0,\theta_0)].\ g(r).\ F(r,\theta)$$

Where S_k is the air kerma strength

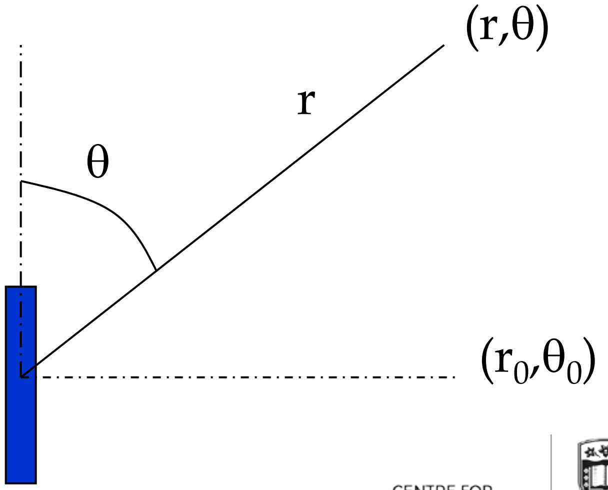
λ is the dose rate constant

$G(r,\theta)$ is the geometry function

$g(r)$ is the radial dose function

$F(r,\theta)$ is the anisotropy function

(r_0,θ_0) is the reference point



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Radial Dose Function

- Takes into account the attenuation of the radiation source through the water medium
- Is one dimensional, based on r only
- Measured along the transverse axis of the source (θ_0 or 90°)
- Is a ratio of the dose deposited at the point of measurement to the dose deposited at the reference point, accounting for the geometry function

$$g(r) = \frac{\dot{D}(r,\theta_0)G(r_0,\theta_0)}{\dot{D}(r_0,\theta_0)G(r,\theta_0)}$$

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Anisotropy Function

- Takes into account the angular distribution of radiation due to the encapsulation of the source
- Is a two dimensional function (r,θ)
- Represented as an angular distribution at individual radial distances
- Is the ratio of the dose at the point of measurement to the dose deposited at 90° for the same radial distance, taking the geometry function into account

$$\mathrm{F}(r,\theta) = \frac{\dot{D}(r,\theta)G(r,\theta_0)}{\dot{D}(r,\theta_0)G(r,\theta)}$$

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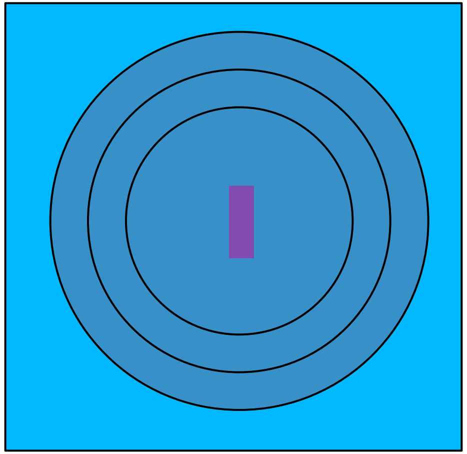
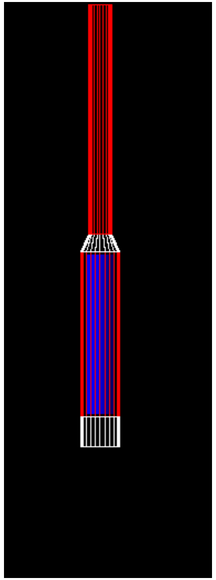
The Geant4 Simulation Model

Flexisource Ir-192 Brachytherapy Source

- Source placed in the centre of an 80x80x80 cm^3 liquid water phantom
- 200 concentric scoring shells surround the source
  - From 1 mm to 20 cm radius
  - Thickness: 0.1mm
- EM Livermore physics list
  - 1 micron cut for secondaries transport
- Energy deposition within a shell
  - Sent to scoring routine
- Radial Dose Function and Anisotropy Function data calculated from the dose deposition





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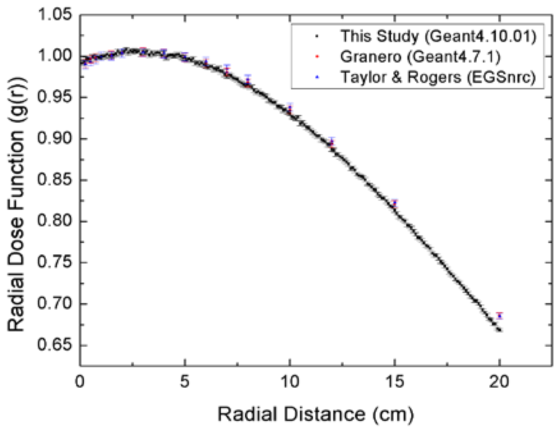
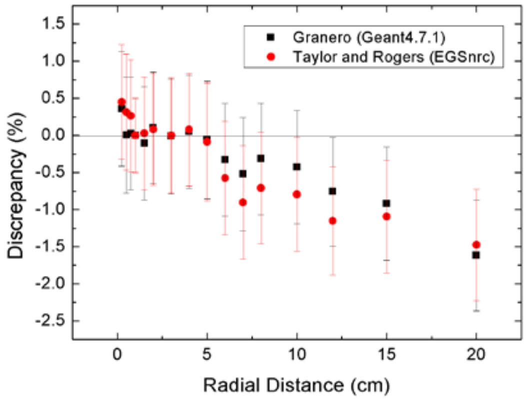
Results: Radial dose function

Geant4 10.1
10^{10} histories

- Agreement to within error up to 10cm radial distance (clinically relevant distances)
- Max discrepancy: 0.7% at 20cm
  - Granero data (2007) used for source consensus data for TG43 based dose planning systems (ESTRO.org)





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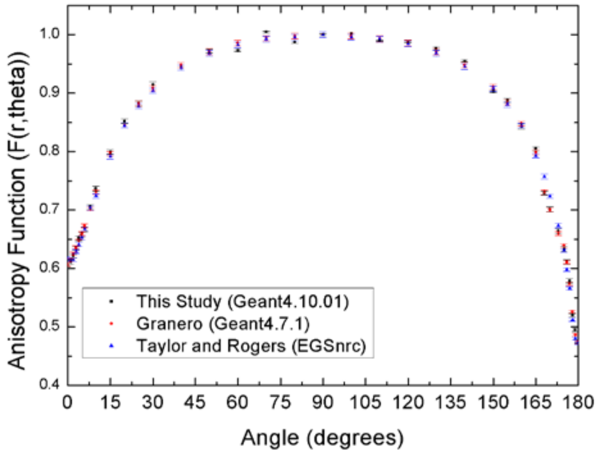
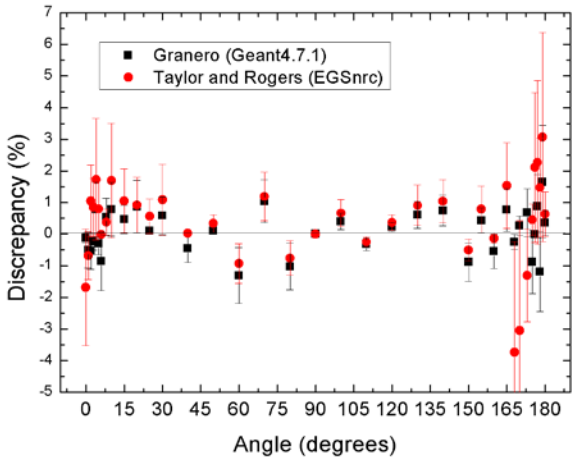
Anisotropy Function data

Geant4 10.1
10^{10} histories

- Generated for 1cm radial distance
- Largest errors at sharp angles (lower statistics)





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Conclusion: next

- Validate also the other physics lists of Geant4
  - Standard option 3, 4, Penelope

- Integrate in the G4 Med Phys Benchmarking

- It will be included in the Brachytherapy Advanced Example

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