Recent updates on Geant4 physics validation for ESA AREMBES project

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Introduction

Detailed Geant4 physics validation review and new verification studies performed within the **ESA AREMBES*** project.

Focus on space physics processes of interest for ATHENA

- New dedicated studies
    - Low angle proton scattering (see talk by Valentina Fioretti)
    - Electron backscattering
    - Proton ionization (thanks to Simone Lotti)

- …and detailed review of existent electromagnetic and hadronic models
    - Proton and electron scattering
    - Photon processes
    - Hadronic interactions
    - …

  (lot of inputs taken from Geant4 EM validation results [10])

*The ESA Contract No. 4000116655/16/NL/BW is acknowledged

Electron Backscattering

Backscattering coefficient calculated for

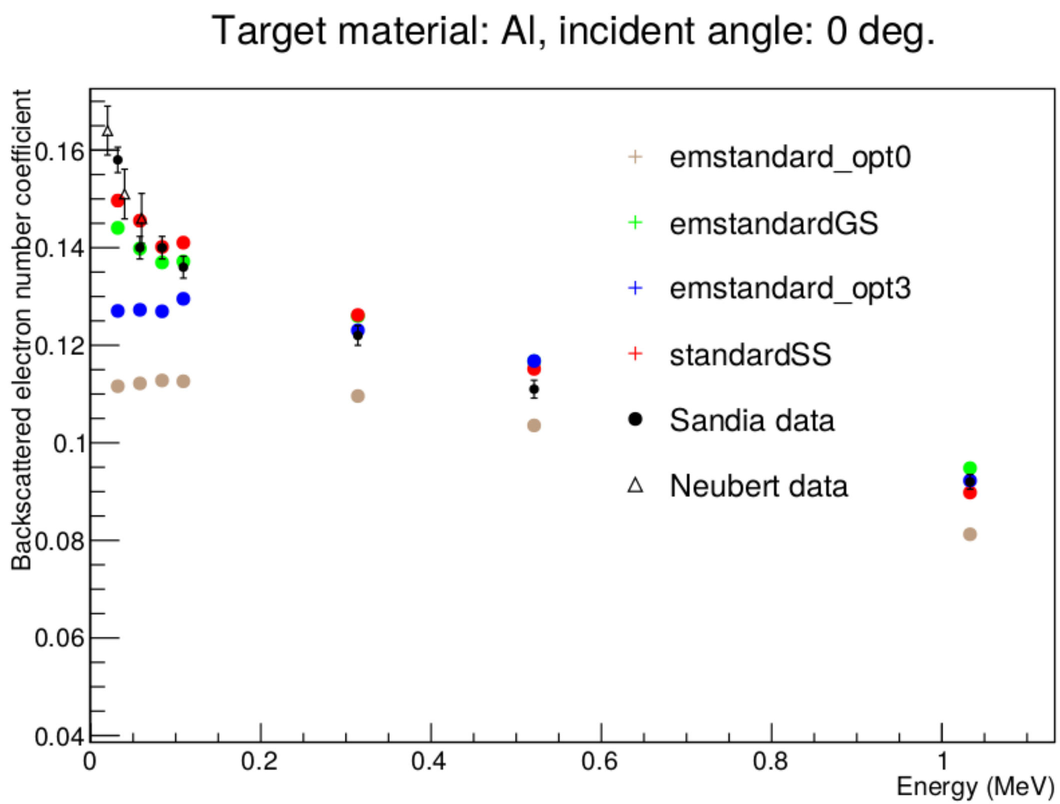
- different beam energies
- several target material
- several incidence angle

NEW

In general **good agreement for all tested combinations!**

Discrepancies in the low energy region among different physics lists.

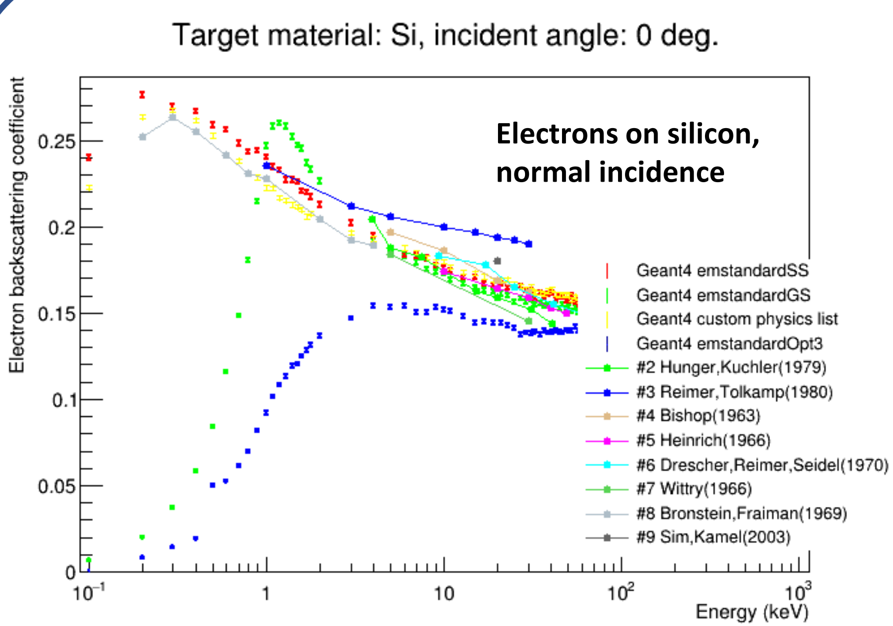
Further studies at low energy for interesting materials (next slide)

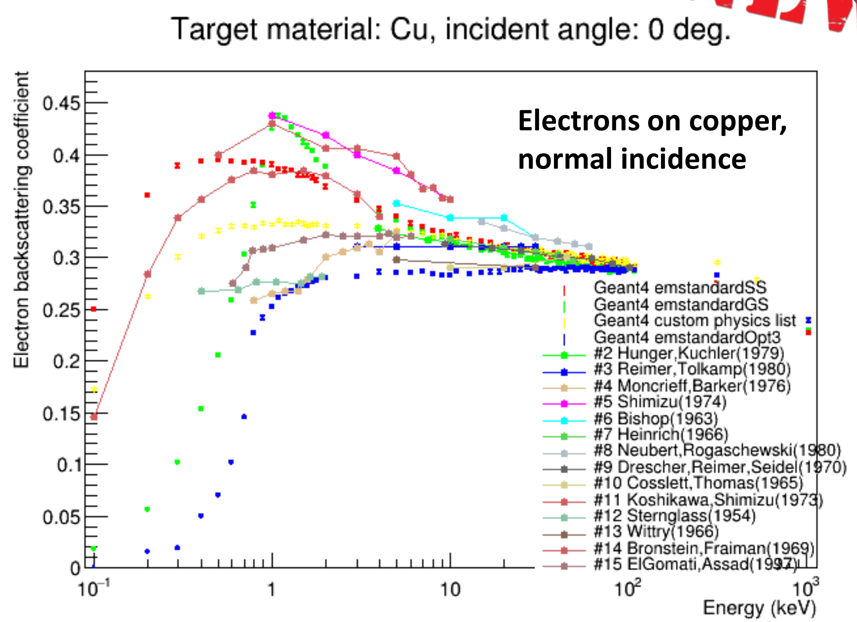


Electron Backscattering

Caveat: **a lot of experimental datasets** (dots with lines), different conditions, energy range, (and reliability?).

- Standard opt0 / opt3 (blue dots) underestimate the coefficient at low energy
- SS very good (red dots)!
- Custom AREMBES physics list (yellow dots) good results (see dedicated talk)





NEW

Simulation in the middle of the experimental spectrum

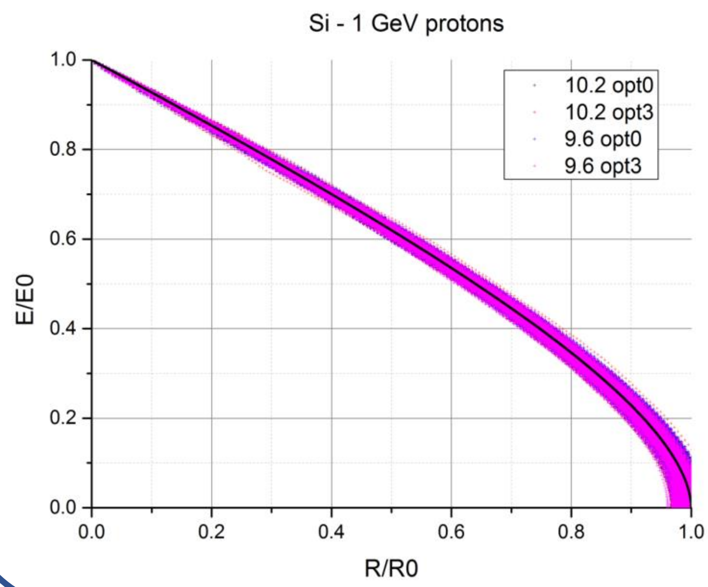
Proton energy deposition tests

Reduced Calibration Curve (RCC) = Projected range VS particle energy [11]

Advantages:

- nearly material independent
- weakly dependent on the initial energy

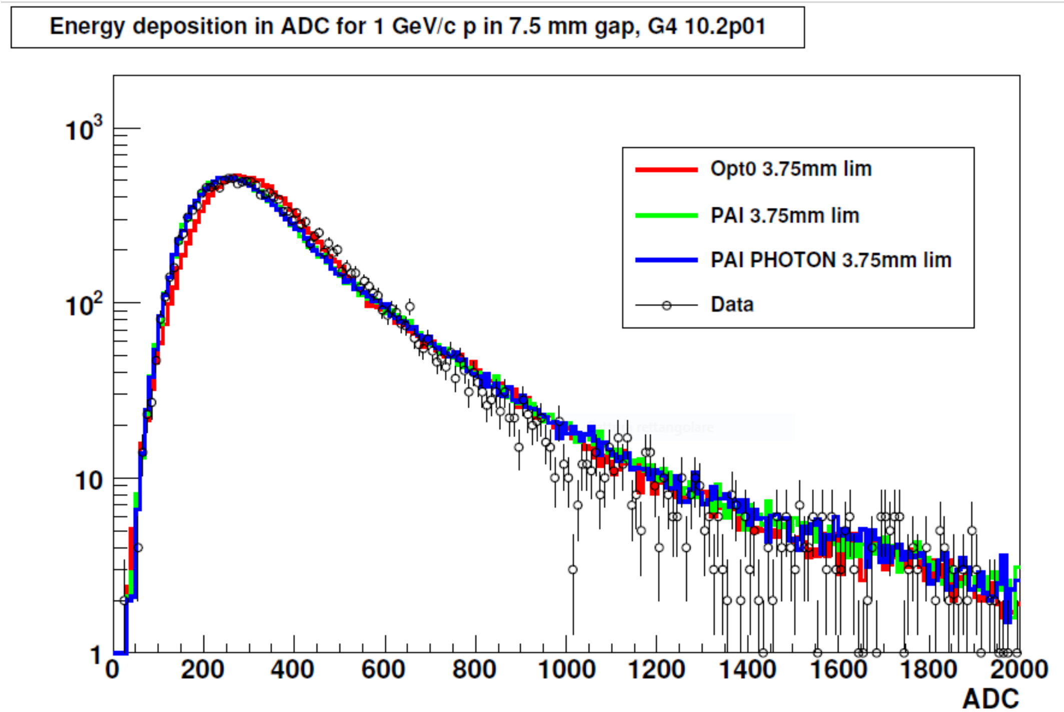
NEW



Proton beams of different energies E_0 impacting to a volume with size $L \geq R_0$, where R_0 is the full projected range expected for a particle of energy E_0, taken from the NIST database.

- ✓ Energy deposition reproduced to ~ percent accuracy by any physics lists
- ✓ Single Scattering provides higher accuracy but more computational times

Proton scattering on thin targets



Energy deposition of 1 GeV/c proton in ALICE TPC test-beam setup

ALICE test beam [1,2] energy deposition data inside TPC gas mixture

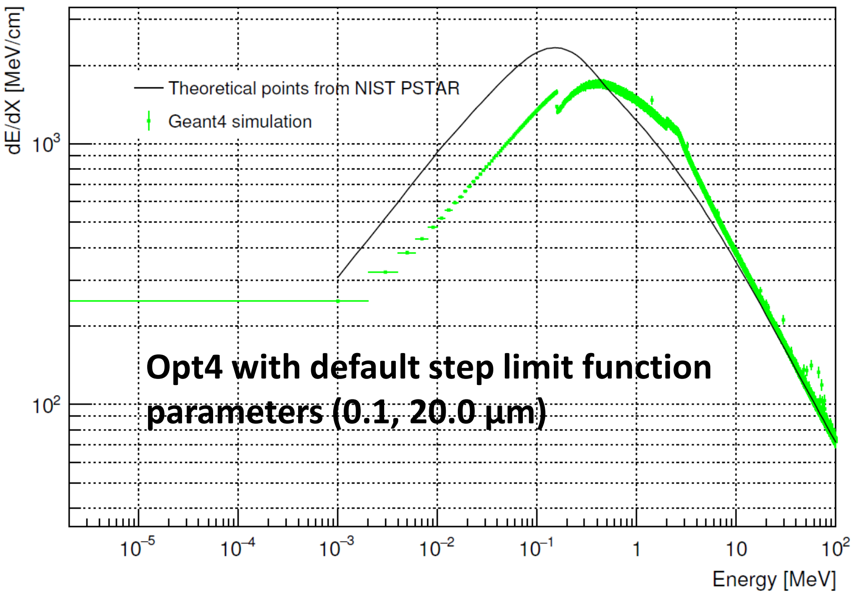
- default model of fluctuations

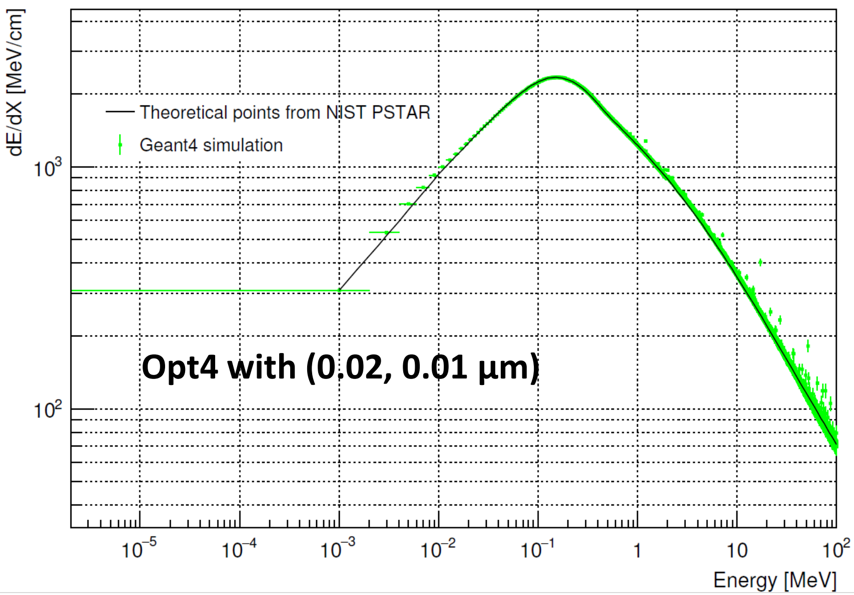
compared with

- two variants of PAI - Photoabsorption Ionization Model- (PAI and PAI Photon)

- For hep applications PAI models are more accurate and may be considered
- For AREMBES, where treatment of low-energy protons is important, PAI models are not applicable…

- for AREMBES, where treatment of low-energy protons is important, PAI models are not applicable…
- …but default model is good enough! (with some step tuning)





1 GeV primary protons in Tungsten compared with NIST PSTAR database

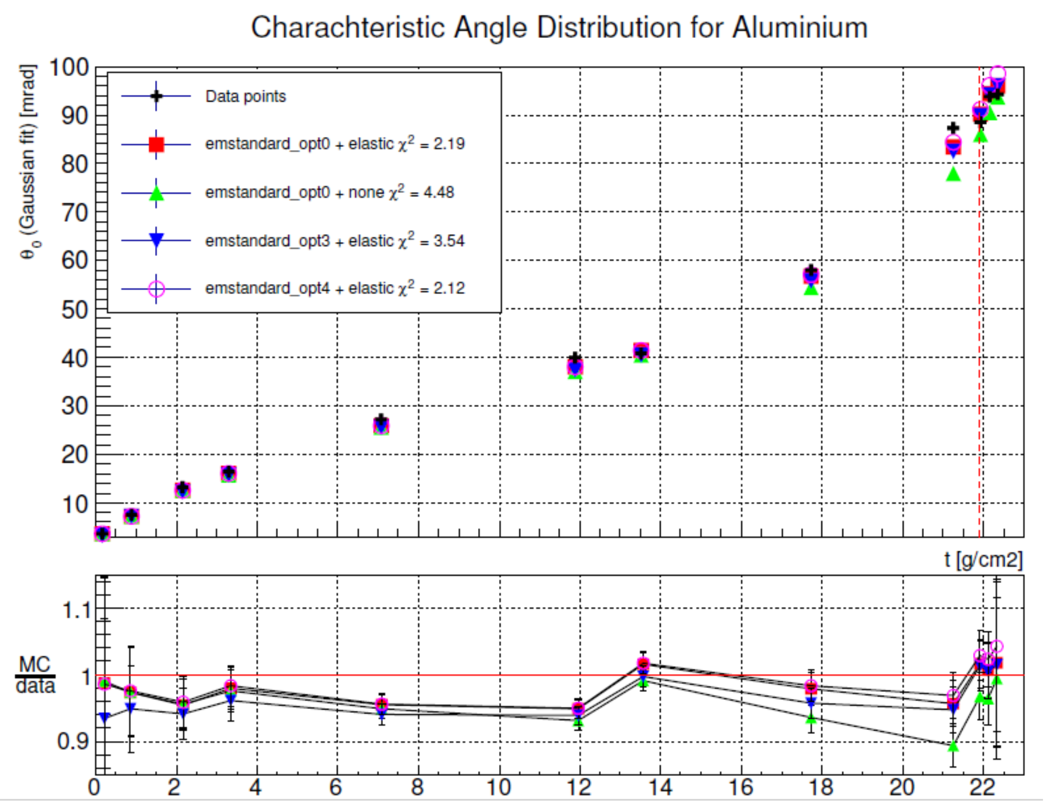
Proton multiple scattering

Proton multiple scattering benchmarks performed regularly by G4 Collaboration (general talk by Vladimir this morning)

- Thin and thick targets
- Different materials
- Different physics lists

Results in general very good!

Results for Aluminum (space shielding) reported in figure.
- Simulations: Geant4 10.3
- Data from [3].



Photon processes validation

Geant4 Collaboration systematically validates photon processes.

Comparison of
- Attenuation coefficients and stopping power
- Compton, Rayleigh, photoelectric, gamma conversion
- Lot of materials (Be, C, O, Al, Ar, Ca, Cu, Fe, Ag, W, Pb,…)

with respect to NIST database.

Comparison of Geant4 Electromagnetic Physics Models Against the NIST Reference Data

Katsuya Amako, Susanna Guatelli, Vladimir N. Ivanchenko, Michel Maire, Barbara Mascialino, Koichi Murakami, Petteri Nieminen, Luciano Pandola, Sandra Parlati, Maria Grazia Pia, Michela Piergentili, Takashi Sasaki, and Laszlo Urban

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 electrons 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.

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Reference: [8] + S. Guatelli contribution [9]

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Photon processes validation

Geant4 Collaboration systematically validates photon processes.

- Test with 10.2 completed
- Added to the G4 regression test suite (thanks to A. Dotti, SLAC)
- Test with 10.3 ongoing

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Best: opt4 and Livermore physics lists.

Extend to space materials: mylar, kevlar, polyethylene, polymide, copper, CdZnTe, Fr4, steel, SiC, Si3N4, Iridium...(inputs are welcomed!)

Other EM models

Several other Geant4 models tested

- Originally with Geant4 10.2
- Started to update results to 10.3
- Firsts conclusions are coherent

Bremsstrahlung
Atomic relaxation and PIXE
Auger effect
…

No time to speak about all, but in general good status.

No changes with respect to the default physics will be suggested for ATHENA.

Hadron-nuclear interactions

The Geant4 Collaboration periodically performs comprehensive tests on all hadronic interactions (general talk by Dennis this morning).

Proton inelastic interactions with atomic nuclei provide secondary

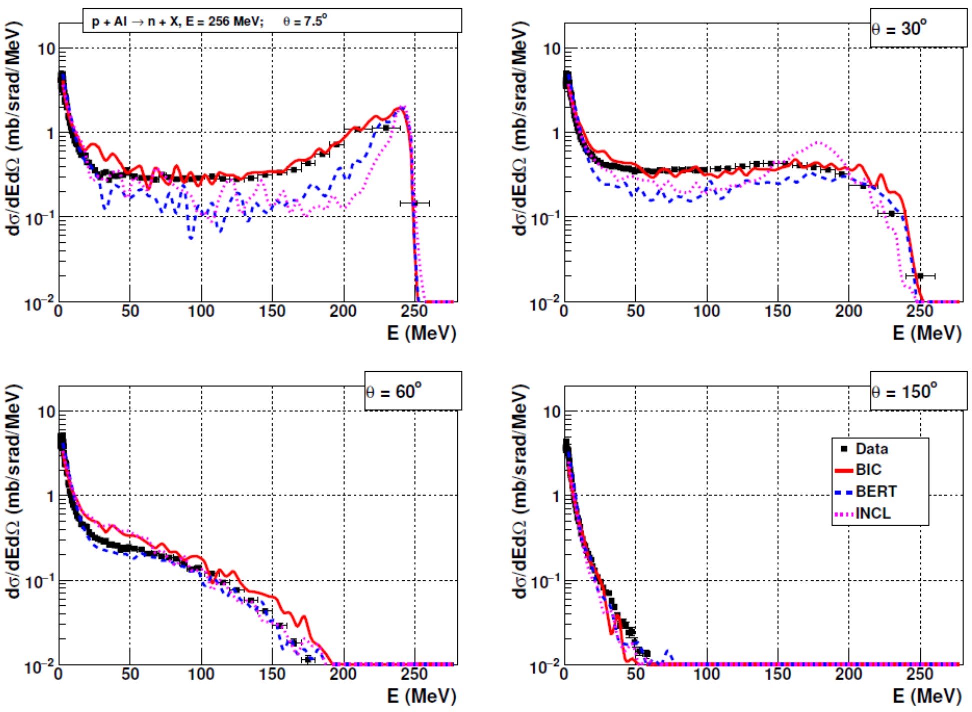
- Neutron
- Protons
- Light and heavy fragments

→ radiative damage of sensitive elements of space missions (ATHENA)

- Slow charged fragments are stopped near production point
- Neutrons penetrate for long distances
    - Radiation damage far from the production point
    - An accurate simulation of secondary neutrons is necessary
    - Validation performed using double differential cross section of neutron production by protons in various targets and different energies.

Hadron-nuclear interactions

Selected results of Geant4 hadronic testing suite [4] for neutron double differential production cross section by protons in Al (interesting for the interaction with shielding).



- Simulations with Geant4 10.3
- Data from [5]

Different cascade models:

- Binary (BIC)
- Bertini (BERT)
- INCL++ (INCL)

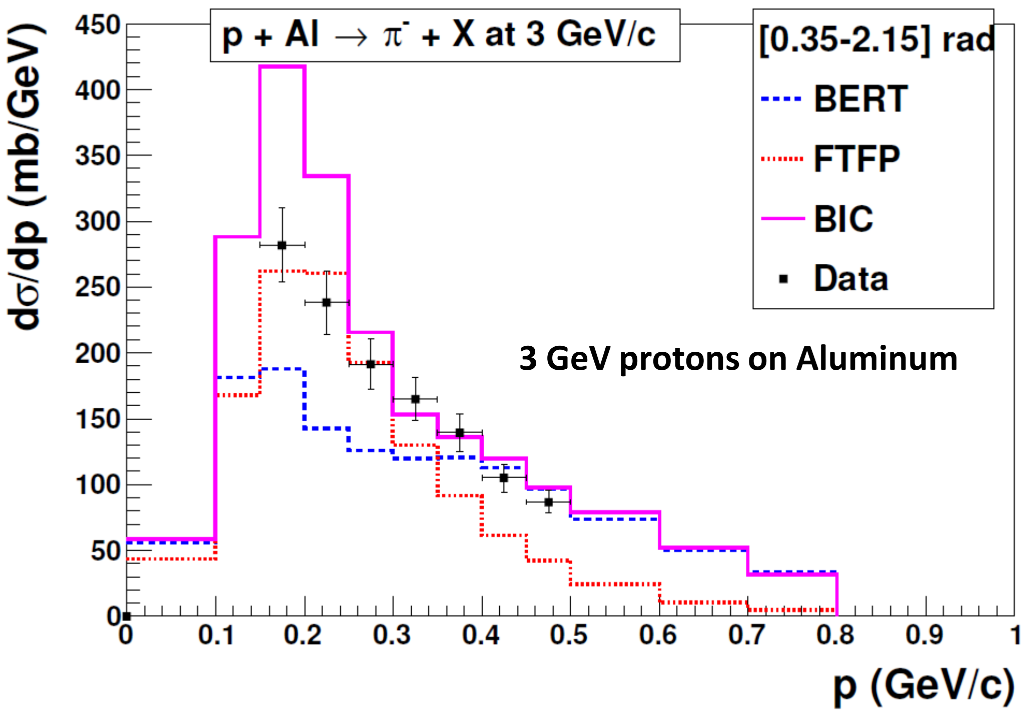
Below 1 GeV BIC provides more accurate predictions (especially for the forward direction).

At higher energy and angles BERT and INCL become competitive.

Hadron-nuclear interactions

For higher beam energy a dataset from the CERN HARP experiment is available [6]. This allows to compare physics performance of Geant4 cascade and string models.

Only a selection of the available validation results is reported (protons on Al target).



Different cascade models:

- Binary (BIC)
- Bertini (BERT)
- FTFP (INCL)

BIC is close to the data whereas BERT and FTFP slightly underestimate the pion yield.

- Simulations with Geant4 10.3
- Data from [6]

QBBC physics list

QBBC [7] is the reference hadronic physics list for space applications

- Main hadronic models:
    - BERT (below 3-5 GeV)
    - FTFP (above 3-5 GeV)
    - BIC for primary proton and neutron interactions with nuclei below 1.5 GeV
- Derived QBBC_EMZ where opt4 is used instead of standard EM

From the AREMBES WP3 and WP4 review and new results QBBC is confirmed to be the best combination of hadronic models in Geant4 10.3 for ATHENA (and maybe for space applications more in general).

Conclusions

To address **radiative effects** in space missions both an accurate simulation of **electromagnetic** and **hadronic physics** is needed.

Detailed studies on the Geant4 physics processes have been performed for the AREMBES simulation framework.

- Mostly updated to Geant4 10.3
- At now no different conclusions between 10.2 and 10.3

1) EM sector: single scattering and opt4 physics lists are actually the best choice

- Low energy and angle proton scattering
- Electron scattering
- Energy deposition
- Photon processes

A combination of SS+opt4 physics lists could be the best approach for ATHENA (see dedicated talk).

2) Hadronic sector: QBBC physics list is the best choice

- Best combination of cascades and string models

Conclusions (2)

This is not the end of the work…

- AREMBES project is ongoing
- New Geant4 releases will be available

That means updates, continuous validation and review by the Geant4 Collaboration…

…and obviously feedbacks!

- Feedbacks from developers on new/updated models
- Feedbacks from users on needs or issues

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9. Susanna Guatelli et al., Geant4 21st Collaboration Meeting, Ferrara, 2016 https://agenda.infn.it/contributionDisplay.py?contribId=67&sessionId=10&confId=11196

10. Geant4 Electromagnetic Validation Repository, http://geant4.web.cern.ch/geant4/results/EmVali/verification3.php

11. Comparison of the GEANT4 releases 8.2 and 9.2 in terms of a pCT reduced calibration curve. DOI:10.1109/NSSMIC.2010.5874220

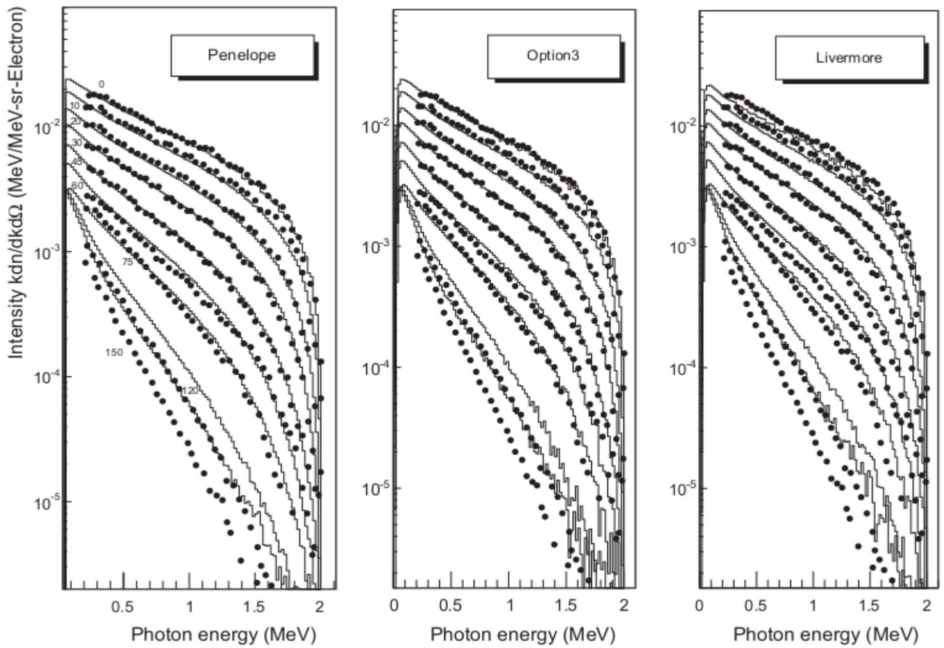
Backup

Bremsstrahlung

In general good agreement.

Best results for:

- Incidence angles below 75°
- Energies above the MeV
- Low Z (better agreement for Al than Fe)



Discrepancies for backward-emitted photons

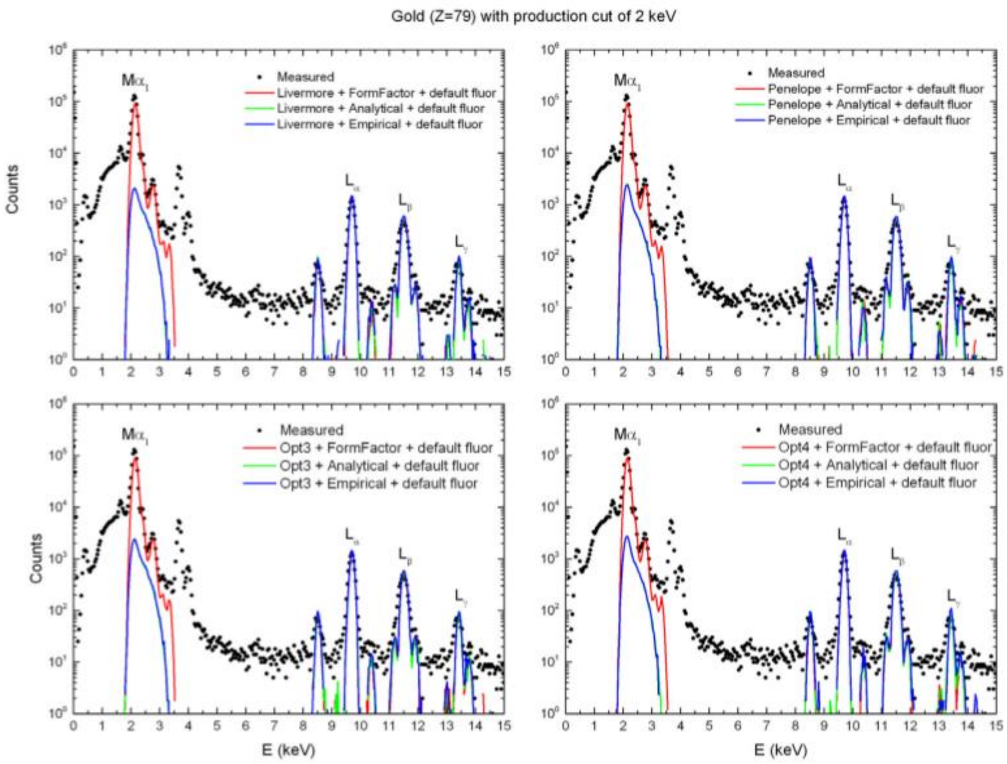
Best: Penelope

Just below:
Emstandard_option3
Livermore

PIXE

Good description of the peaks for both

- Energy
- Normalization



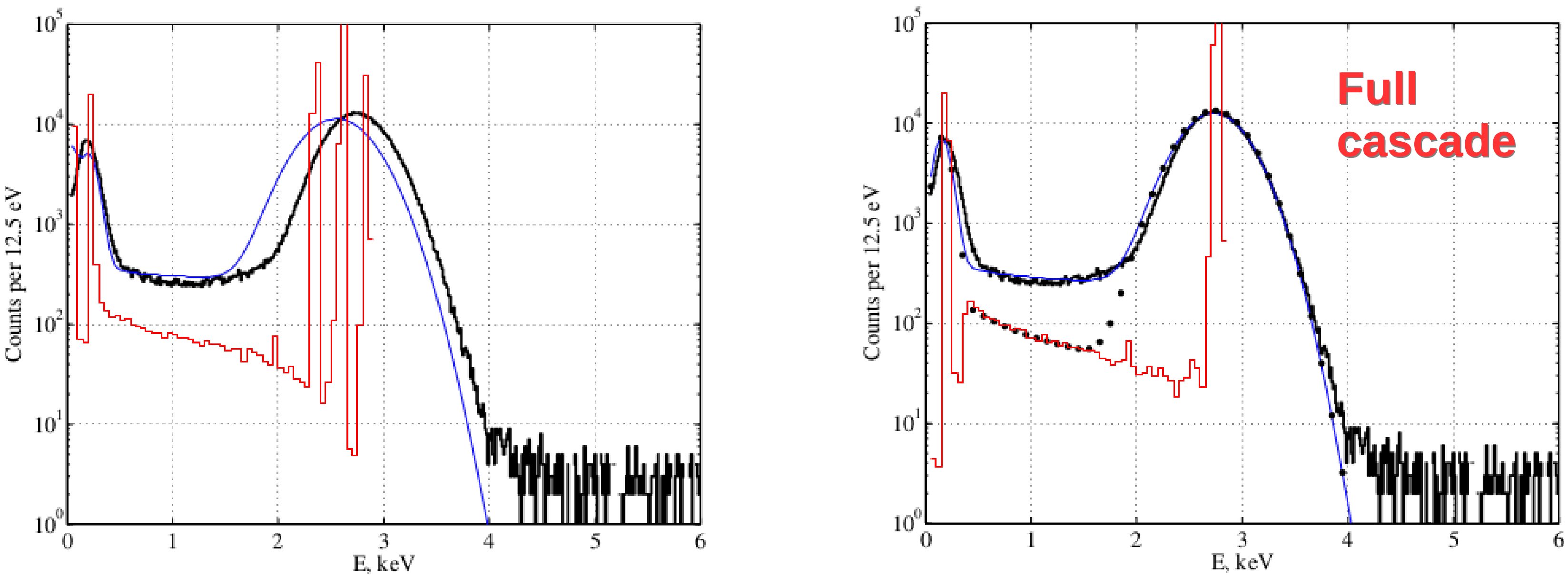
Three sets of alternative ionization cross section models for the K, L and M atomic shells.

Use standard model + FormFactor for M shells.

Auger

Atomic de-excitation by default doesn't simulate the complete Auger deexcitation chain.

- Improve the peak precision: simulate the complete Auger cascade.
- CONS: time consuming!



Radioactive decays

Data driven technique using the ENSDF. Systematic validation ongoing, comparing Geant4 w.r.t. NUDAT2 and DDEP databases for:

- Gamma rays
- X-rays
- Electron internal conversion
- Auger electrons
- Alpha emission

Additional results on AREMBES materials kindly provided by L. Desorgher. Thanks!

Gamma rays are simulated very well

X-ray sand Auger emissions depend on the particular nuclei case (but not a relevant problem for ATHENA).

The hadronic world