Status of ParticleHP models

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Introduction

Geant4 allows to use the information available in **ENDF-6** format data libraries for the transport of low energy neutrons (up to 20 MeV) and charged particles (up to 200 MeV), using the **G4ParticleHP** package.

Originally this package was written for neutrons (G4NeutronHP), but it has been extended → protons, deuterons, tritons, ^{3}He, alphas.

- ENDF-6 format files can contain:
  - ***evaluated*** data: analysis of experiments + theoretical models
  - the **output of a computer code**: TENDL → output of TALYS

- Information inside an ENDF-6 data library:
  - For each isotope in the library:
    - Reaction cross sections
    - Secondary particle yields
    - Energy-angular distributions of secondary particles

Introduction

In this presentation:

- Recent work (2018-2019)
  - New ENDF-6 format data libraries in Geant4 format
  - New verification tests
  - (α,Xn) neutron yields

Improvements in the code

- Future developments

New ENDF-6 format data libraries in Geant4 format

New ENDF-6 format data libraries in Geant4 format

- Evaluated libraries (neutron incident):
  - USA+Canada: **ENDF/B** → ENDF/B-VIII.0, **ENDF/B-VII.1**,ENDF/B-VII.0 … → **G4NDL4.5**
  - NEA (Europe): **JEFF** → JEFF-3.3, JEFF-3.2, JEFF-3.1.2, JEFF-3.1.1 …
  - Japan: **JENDL** → JENDL-4.0, JENDL-3.3
  - Russia: **BROND**, **ROSFOND** → BROND-3.1, ROSFOND-2010 …
  - China: **CENDL** → CENDL-3.1, CENDL-2

- Many of them available for download in Geant4 format from:

  https://www-nds.iaea.org/geant4/

Updated in 2018 → 8 new data libraries; New verification tests

New ENDF-6 format data libraries in Geant4 format

- Evaluated libraries (neutron incident):
  - USA+Canada: **ENDF/B** → ENDF/B-VIII.0, **ENDF/B-VII.1**,ENDF/B-VII.0 …
  - NEA (Europe): **JEFF** → JEFF-3.3, JEFF-3.2, JEFF-3.1.2, JEFF-3.1.1 …
  - Japan: **JENDL** → JENDL-4.0, JENDL-3.3
  - Russia: **BROND**, **ROSFOND** → BROND-3.1, ROSFOND-2010 …
  - China: **CENDL** → CENDL-3.1, CENDL-2

→ **G4NDL4.5**

- Many of them av… …at from:

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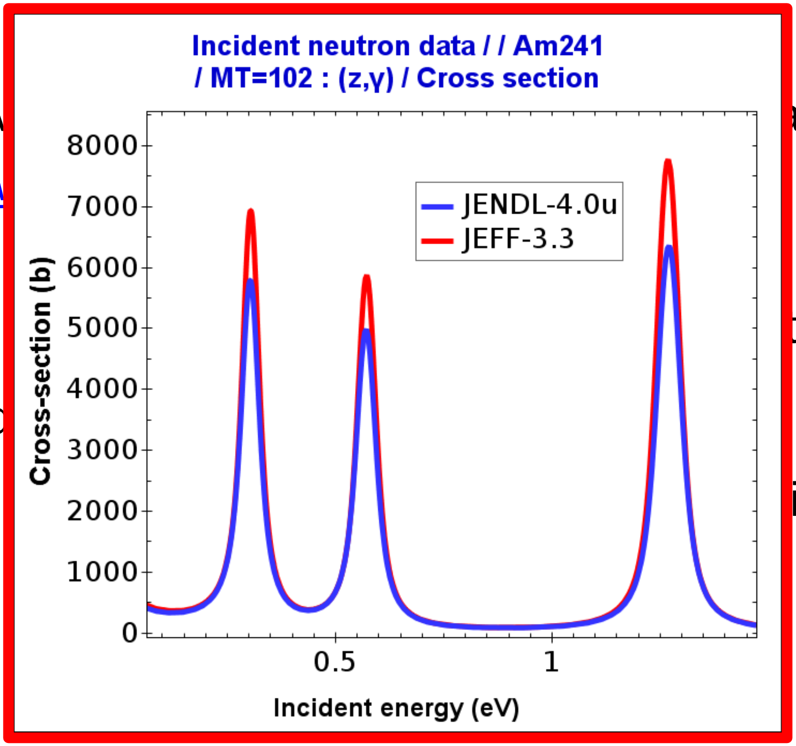


Example of using different libraries

J.L. Taín et al, NIMA 774, 17 (2015)

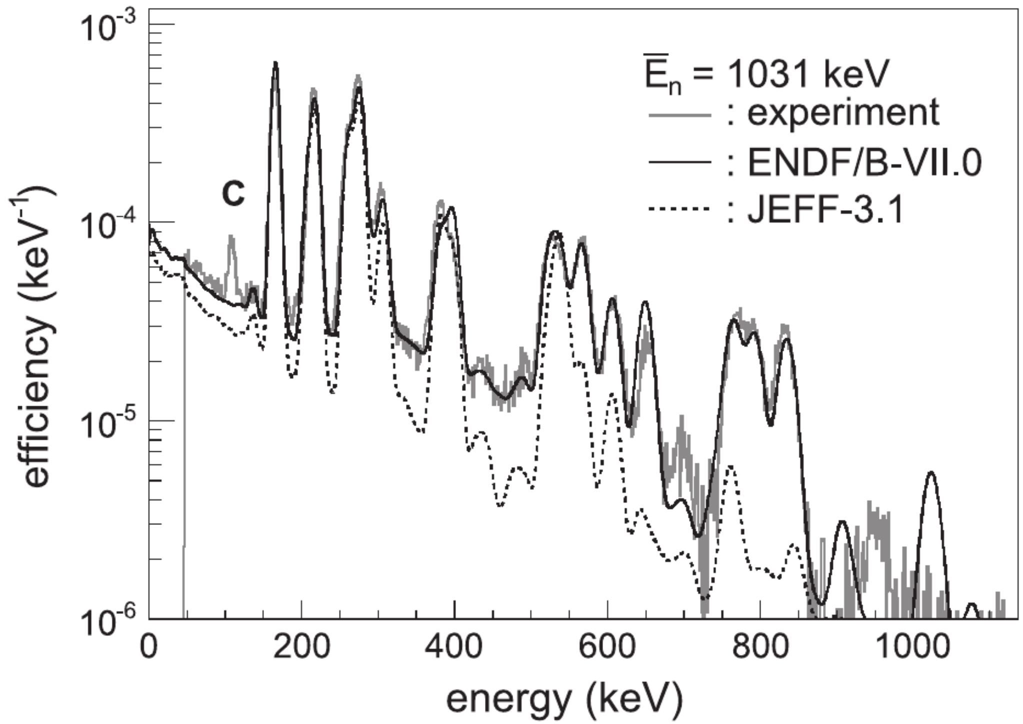
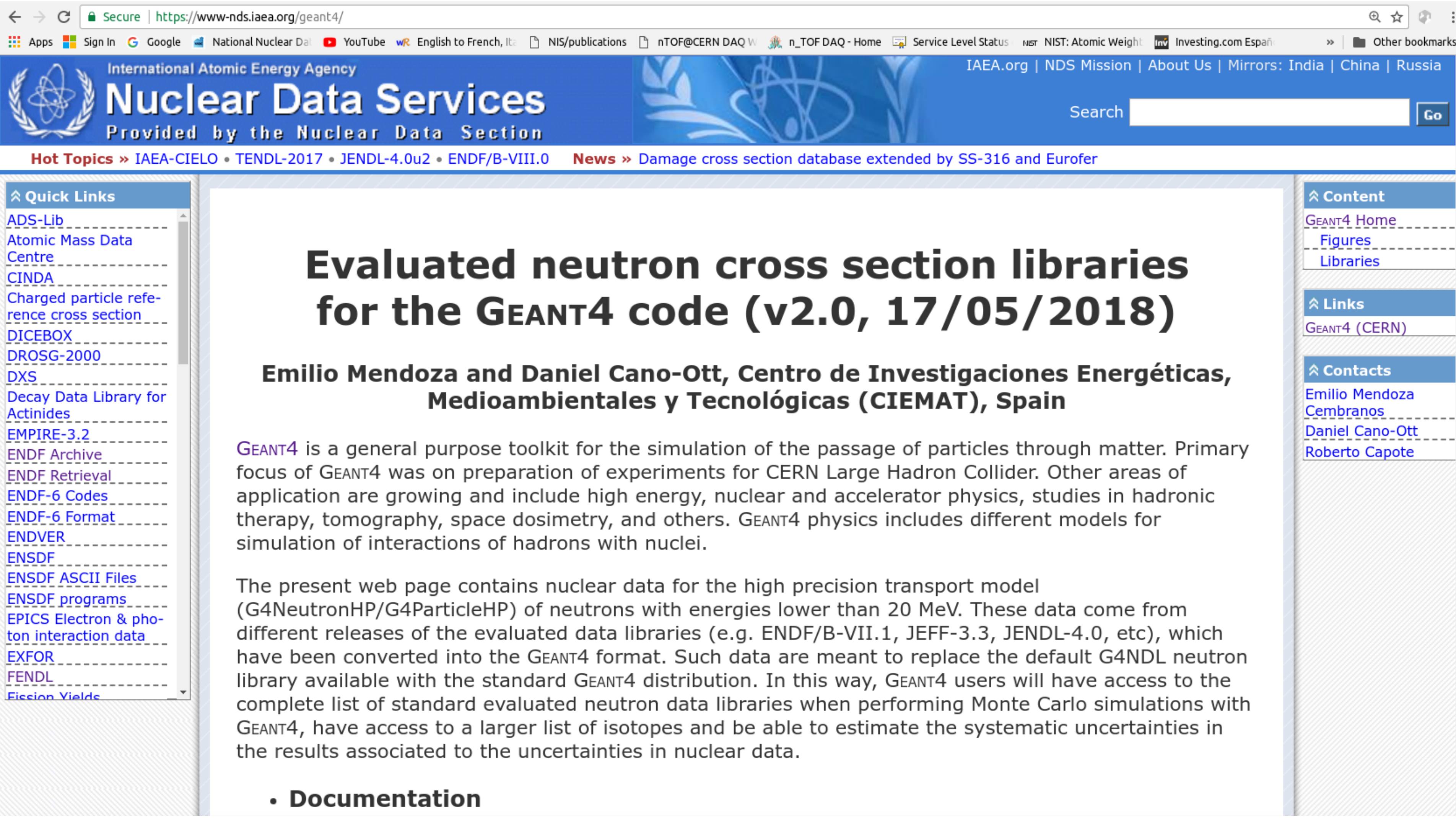


Fig. 6. Comparison of measured and simulated detector response with two different neutron libraries for the distribution with $\overline{E}_n = 1031$ keV. C: contaminant peak.

MC (Geant4) VS experimental response of a $LaBr_3$:Ce detector to 1031 keV neutrons

New ENDF-6 format data libraries in Geant4 format



Secure | https://www-nds.iaea.org/geant4/

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Evaluated neutron cross section libraries for the GEANT4 code (v2.0, 17/05/2018)

Emilio Mendoza and Daniel Cano-Ott, Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT), Spain

GEANT4 is a general purpose toolkit for the simulation of the passage of particles through matter. Primary focus of GEANT4 was on preparation of experiments for CERN Large Hadron Collider. Other areas of application are growing and include high energy, nuclear and accelerator physics, studies in hadronic therapy, tomography, space dosimetry, and others. GEANT4 physics includes different models for simulation of interactions of hadrons with nuclei.

The present web page contains nuclear data for the high precision transport model (G4NeutronHP/G4ParticleHP) of neutrons with energies lower than 20 MeV. These data come from different releases of the evaluated data libraries (e.g. ENDF/B-VII.1, JEFF-3.3, JENDL-4.0, etc), which have been converted into the GEANT4 format. Such data are meant to replace the default G4NDL neutron library available with the standard GEANT4 distribution. In this way, GEANT4 users will have access to the complete list of standard evaluated neutron data libraries when performing Monte Carlo simulations with GEANT4, have access to a larger list of isotopes and be able to estimate the systematic uncertainties in the results associated to the uncertainties in nuclear data.

- **Documentation**

Content: GEANT4 Home, Figures, Libraries

Links: GEANT4 (CERN)

Contacts: Emilio Mendoza Cembranos, Daniel Cano-Ott, Roberto Capote

https://www-nds.iaea.org/geant4/

New ENDF-6 format data libraries in Geant4 format

https://www-nds.iaea.org/geant4/

export G4NEUTRONHPDATA=/[...]/JEFF-3.3

- **Neutron data libraries**

  Neutron data libraries in the G4NDL format for the different evaluated nuclear data libraries:

  - JEFF-3.3 (download the compressed library as JEFF-3.3.tar.gz)
  - JEFF-3.2 (download the compressed library as JEFF-3.2.tar.gz)
  - ENDF/B-VIII.0 (download the compressed library as ENDF-VIII.0.tar.gz)
  - ENDF/B-VII.1 (download the compressed library as ENDF-VII.1.tar.gz)
  - BROND-3.1 (download the compressed library as BROND-3.1.tar.gz)
  - JENDL-4.0u (version 2016/1/6) (download the compressed library as JENDL-4.0u.tar.gz)

  - BROND-2.2 (download the compressed library as BROND-2.2.tar.gz)
  - CENDL-31 (download the compressed library as CENDL-31.tar.gz)
  - ENDF-B/VI.8 (download the compressed library as ENDF-VI8.tar.gz)
  - ENDF-B/VII.0 (download the compressed library as ENDF-VII0.tar.gz)
  - JEFF-3.0 (download the compressed library as JEFF30N.tar.gz)
  - JEFF-3.1 (download the compressed library as JEFF31N.tar.gz)
  - JENDL-3.3 (download the compressed library as JENDL330.tar.gz)
  - JENDL-4.0 (download the compressed library as JENDL-4.0.tar.gz)

  Figures containing energy distributions obtained from Geant4 and MCNP6 simulations of the secondary neutrons, γ-rays, p, d, t, ^{3}He and α as described in **INDC(NDS)-0758**:

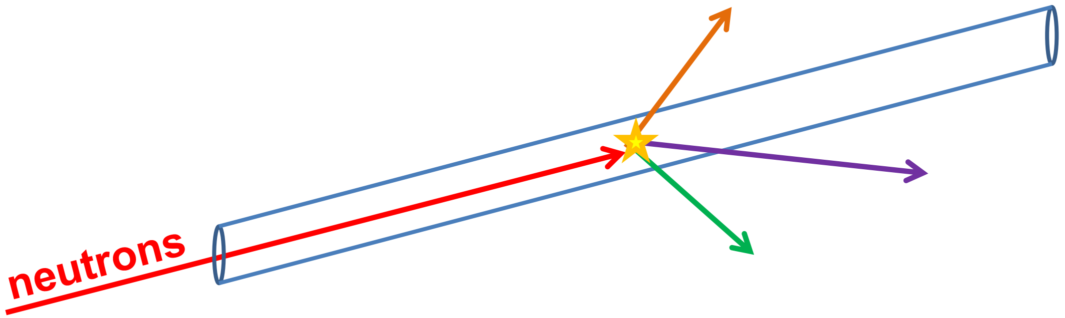
  - JEFF-3.3: figures in PDF format
  - JEFF-3.2: figures in PDF format
  - ENDF/B-VIII.0: figures in PDF format
  - ENDF/B-VII.1: figures in PDF format
  - BROND-3.1: figures in PDF format
  - JENDL-4.0u: figures in PDF format

  Download all the compressed figures as G4_10.04.p01_VS_MCNP6_pdfFiles.tar.gz.

New verification tests

New verification tests

Verification tests have been performed by comparing Geant4 with MCNP



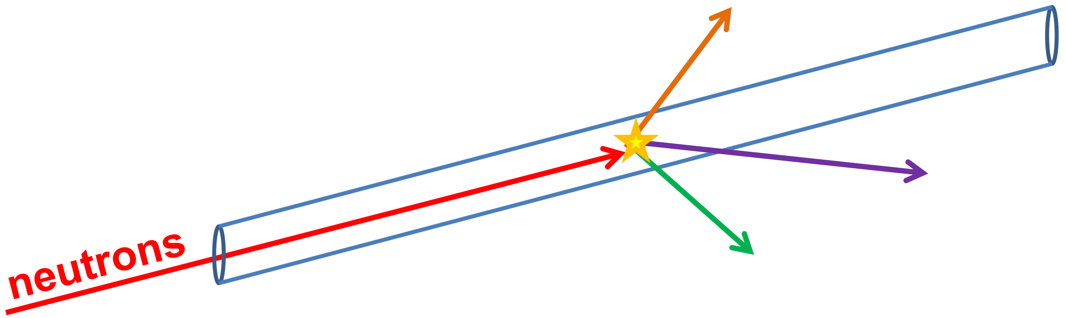
Geometry: 2 m long cylinder with a radius of 1 µm made of an isotopically pure material with density 1 g/cm^3.

Source: neutrons isolethargically distributed with energies ranging from 10^{-10} to 19 MeV impinging on the center of the cylinder along its symmetry axis.

Tallies: energies and angles of the secondary neutrons, γ-rays, protons, deuterons, tritons, ^{3}He and alphas.

New verification tests

Verification tests have been performed by comparing Geant4 with MCNP



Two simulations per isotope and per neutron library: one with Geant4 and other with MCNP6.1

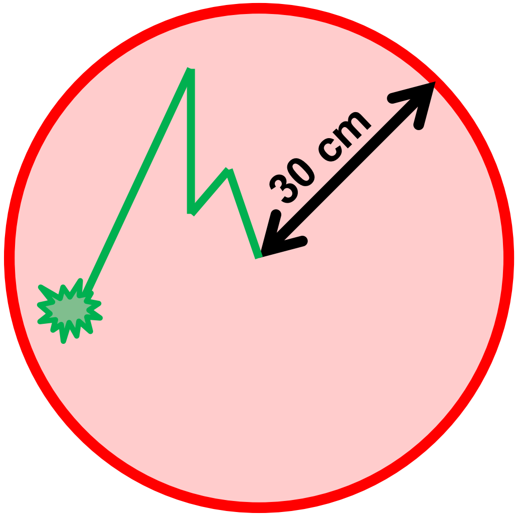
Details of the tests are given in:
E. Mendoza and D. Cano-Ott, *Update of the Evaluated Neutron Cross Section Libraries for the Geant4 Code*, IAEA technical report INDC(NDS)-0758, Vienna, 2018.

Conclusions:

- Good agreement between both codes in the neutron production
- Comparison of charged particle production not straightforward, but available in https://www-nds.iaea.org/geant4/

New verification tests

A new systematic test has been performed (done after some input from Elena Nunnenmann - KIT):



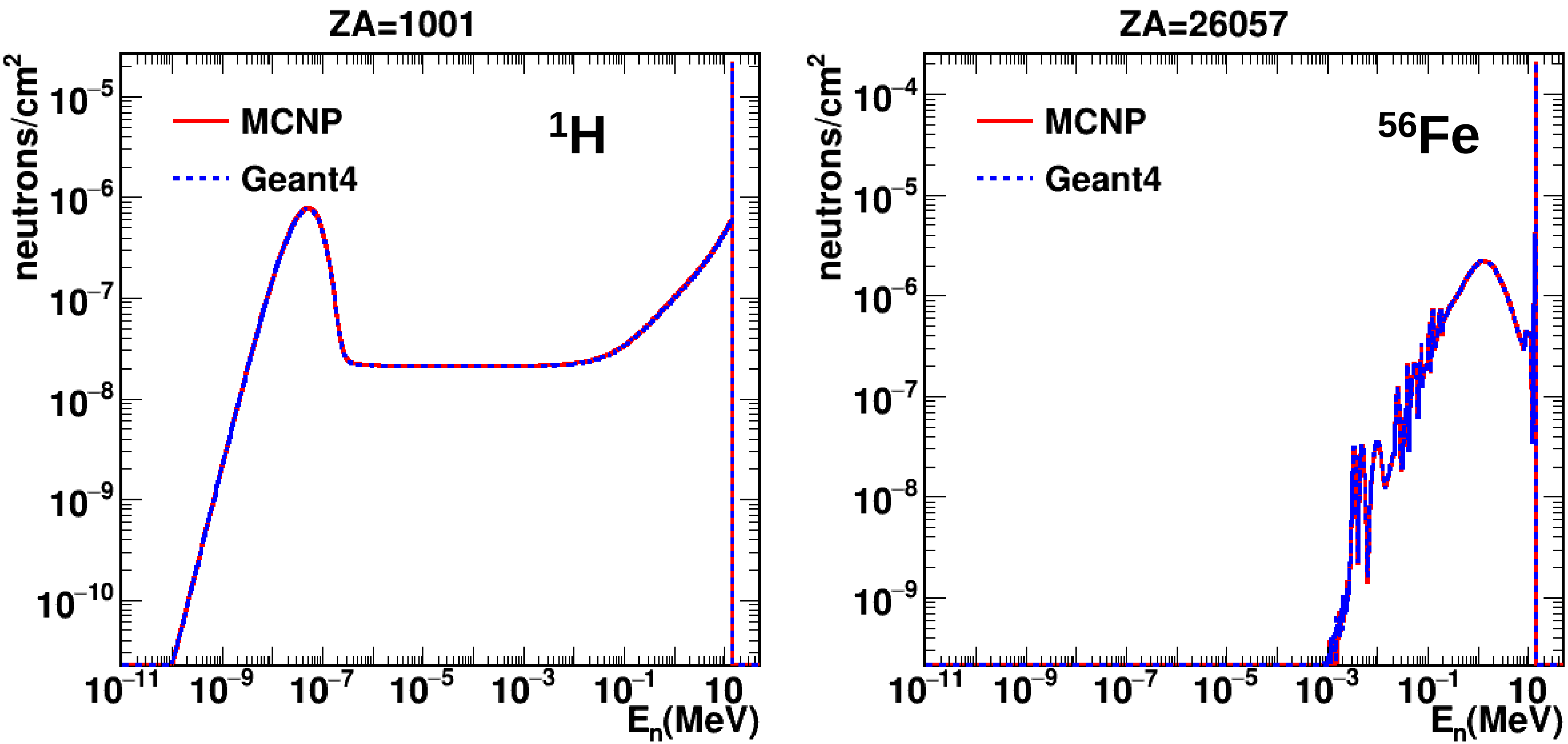
Geometry: 30 cm radius sphere made of an isotopically pure material with density 1 g/cm^3.

Source: 14.1 MeV neutrons from the center of the sphere.

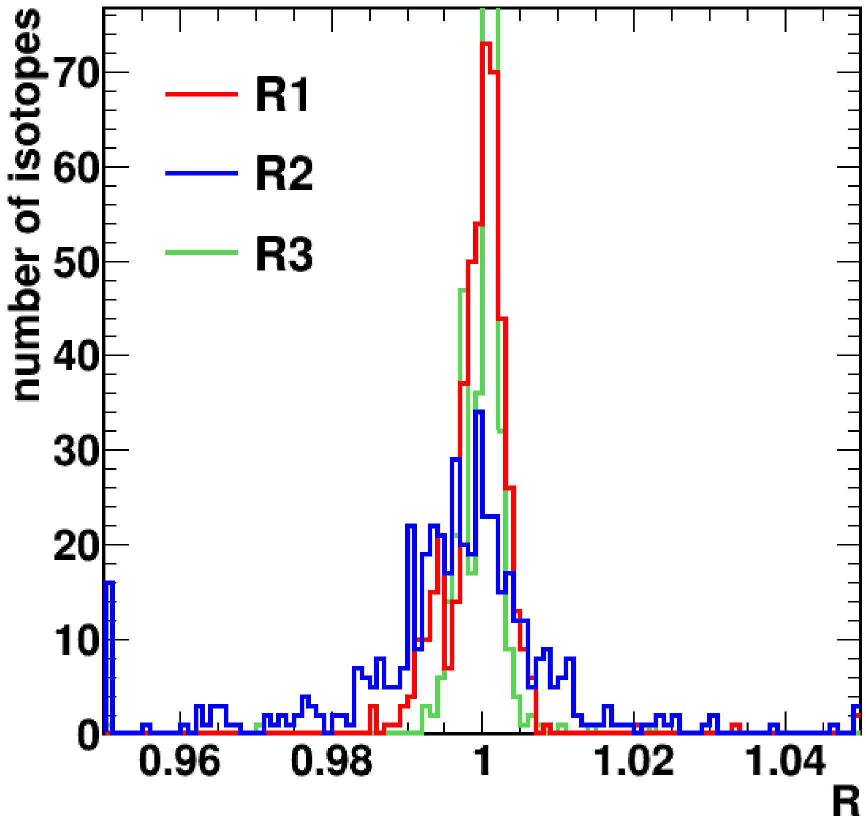
Tallies: neutron flux inside the sphere.

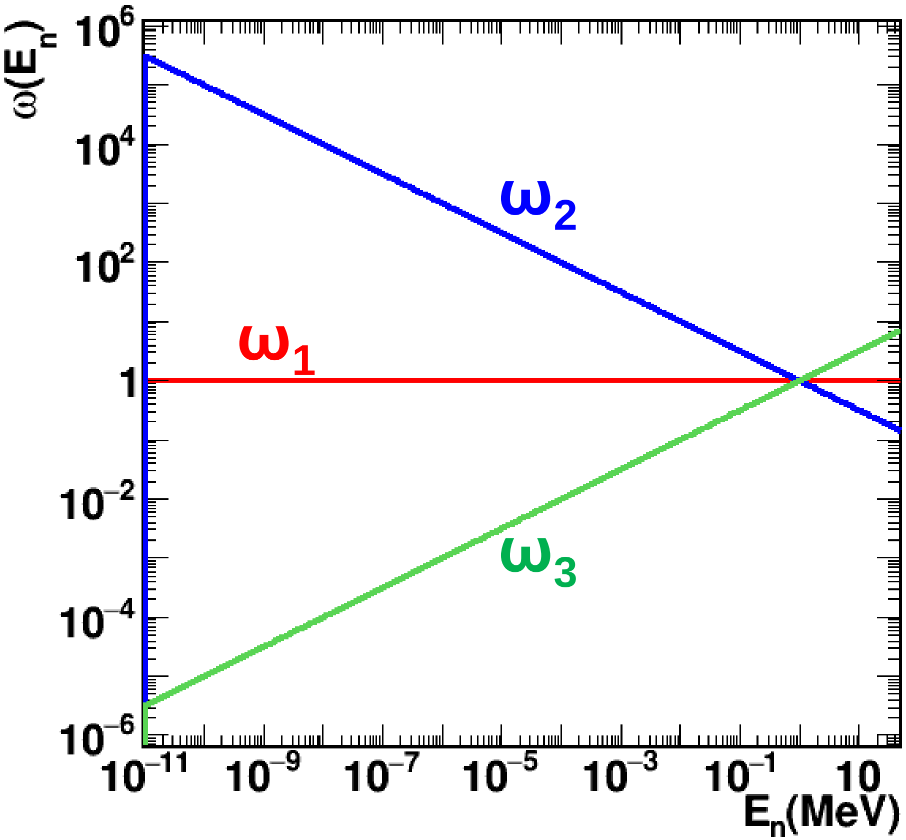
Simulations performed with JEFF-3.3. All isotopes with Z<88 (below Ra).

New verification tests



New verification tests





$C_1 = \int \Phi(E)\, dE$

$C_2 = \int \Phi(E)/\sqrt{E}\, dE$

$C_3 = \int \Phi(E) \cdot \sqrt{E}\, dE$

$R_1 = C_1(MCNP)/C_1(Geant4)$

$R_2 = C_2(MCNP)/C_2(Geant4)$

$R_3 = C_3(MCNP)/C_3(Geant4)$

Neutron production induced by (α,Xn) reactions

Motivation

The simulation of (α,Xn) reactions is required in several fields:

- **Nuclear structure experiments.** Learn about the structure of light nuclei.
- **Nuclear technologies.** α-emitters present in fresh/irradiated nuclear fuels can create a neutron source through (α,Xn) reactions with (light) surrounding nuclei: oxide and carbide fuels, vitrified nuclear waste…
- **Nuclear astrophysics.** Neutron sources in collapsing stars linked to the r-process. E_α below ~1 MeV (around the Gamow peak).
- Neutron background in underground experiments (nuclear astrophysics, **Dark Matter**) due to radiogenic α-decay chains.

For applications, it is necessary to be able to compute **(α,Xn) reaction probabilities**, **particle emission rates** and their associated **energy spectra.**

Can be calculated with the **SOURCES-4C** code: simple geometries and experimental data for a limited number of isotopes.

$$\textbf{Neutrons} \propto \int \boldsymbol{\Phi}(\boldsymbol{E})\,\boldsymbol{\sigma}_{(\boldsymbol{\alpha},\boldsymbol{Xn})}(\boldsymbol{E})\,\boldsymbol{dE}$$

Standard Monte Carlo transport codes: **Geant4**, *MCNP* …

Pros: very detailed geometries,
Cons: large CPU times since EM ion interactions are ~10^6 times more probable than nuclear ones. Model biasing!

Can be calculated independently with Monte Carlo codes like SRIM.

⊗

Can be obtained independently from

a) **Nuclear models** like TALYS and EMPIRE, for a large number of isotopes.
b) **Evaluated cross section files**: cross sections and secondary particles – JENDL and TENDL

NeuCBOT
(SRIM + TALYS)

USD webtool
(SOURCES-4A / EMPIRE)

NEDIS
Similar to SOURCES-4C

Neutron production by α-decay

We have investigated the performance of Geant4 (ParticleHP + (general) biasing + ionization) when simulating the neutron production induced by α-emitters present in the natural decay chains. In particular we have:

- Investigated how to run Geant4 efficiently for this purpose (biasing).
- Verified that the obtained results are consistent with the data used as input (cross sections + energy distributions).
- Evaluated the differences between the existing input data libraries.
- Compared Geant4 with other codes (NeuCBOT, SOURCES, NEDIS, USD) for a few selected cases.

Neutron production by α-decay

After some small modifications to the Geant4 code (already included in the last release), we have verified that it is possible to use Geant4 (ParticleHP + biasing + ionization) to model neutron production induced by alpha decay.

We have translated various ENDF-6 incident alpha data libraries into the G4NDL format. We have performed a comparison between Geant4 using these libraries with other codes and with experimental data.

<u>Advantages of GEANT4 over other codes:</u>

- Complex geometries
- Event generator: gamma rays in coincidence with neutrons.
- Same code for generating and for transporting the neutrons.

Neutron production by α-decay

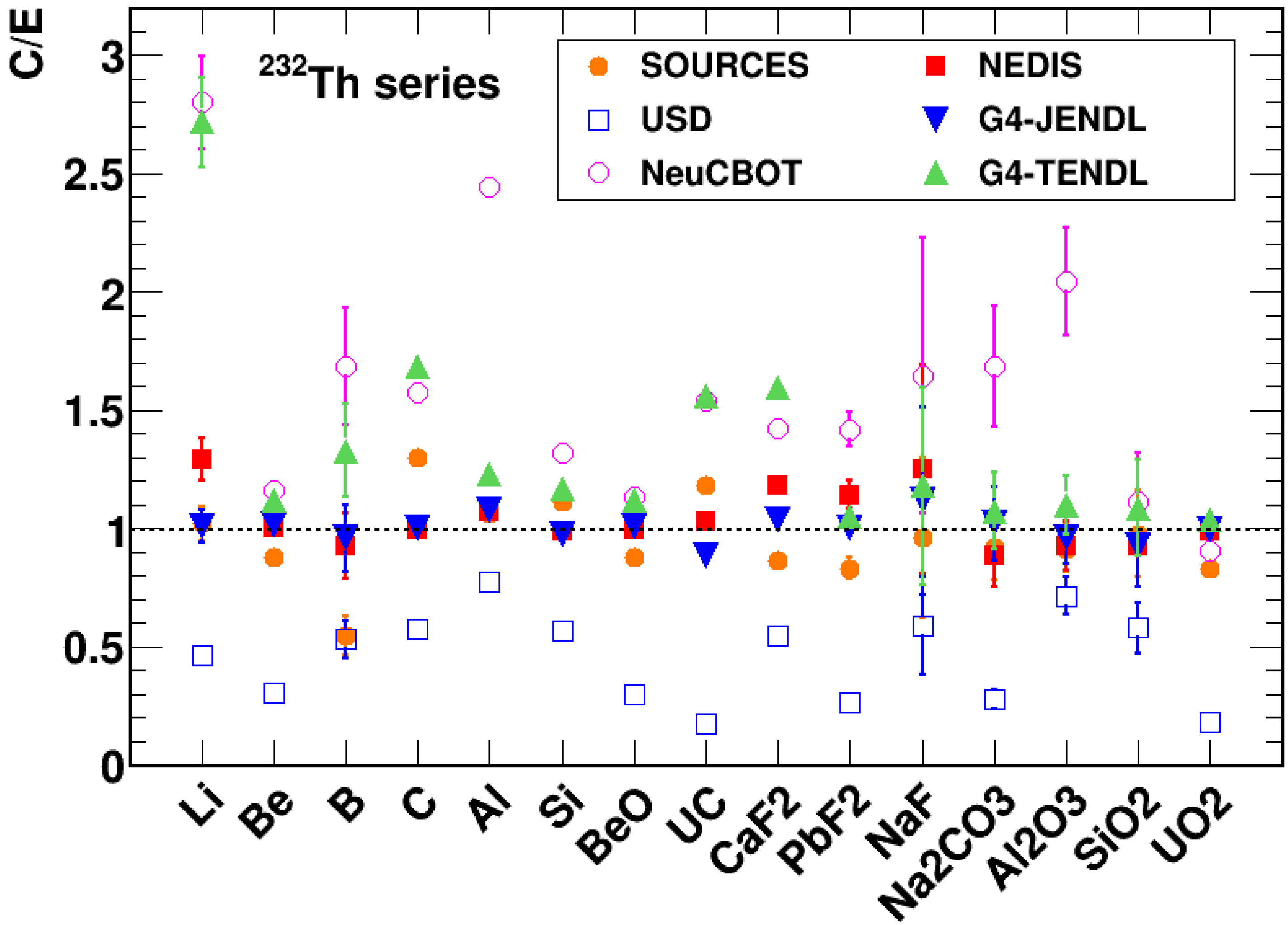
- Paper describing all this work:
  - E. Mendoza et al., Neutron production induced by α-decay with Geant4, arXiv:1906.03903.

- The work has also been presented in:
  - Hadronic group meeting (March 2019).
  - ENSAR2 workshop: GEANT4 in nuclear physics (Madrid, Spain, April 2019).
  - Low Radioactivity Techniques (LRT) workshop (Jaca, Spain, May 2019).

- Neutron yields calculated with Geant4 for dark matter experiments:
  - 16th International Conference on Topics in Astroparticle and Underground Physics (TAUP) (Toyama, Japan, September 2019).

- Worshop: (α,n) Background in Dark Matter Experiments, CIEMAT, Spain, 21-22 November 2019.

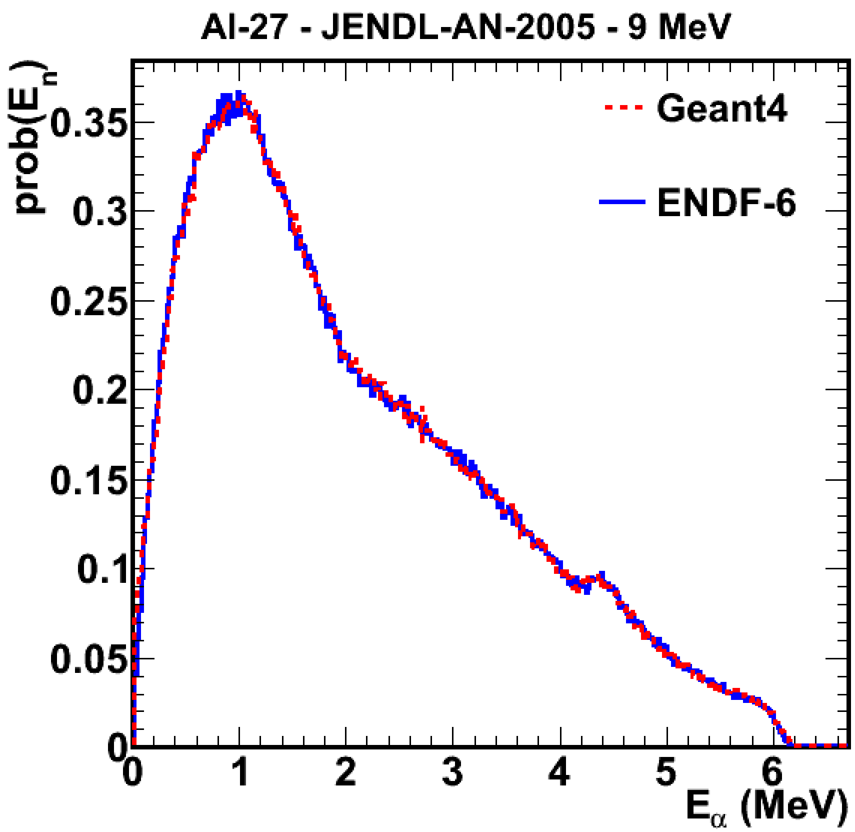
Neutron yields (C/E)

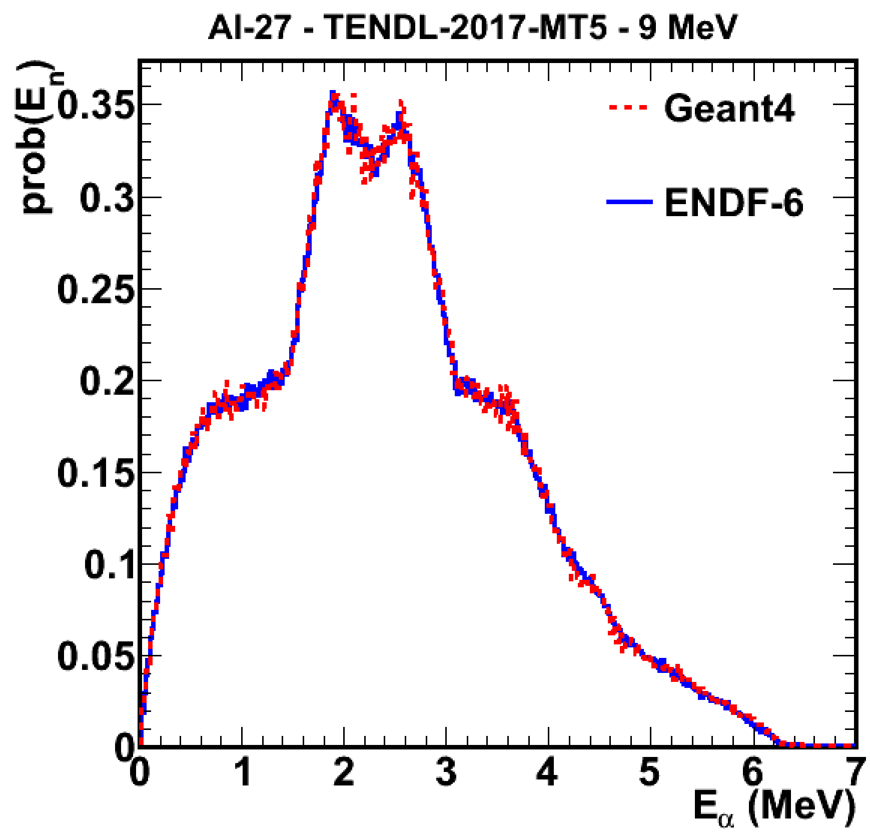


Source: *A. C. Fernandes, A. Kling, G. N. Vlaskin, EPJ Web Conf. 153, 07021 (2017).*

Verification of the neutron energy spectra

In order to verify the the correctness of the neutron energy spectra produced with Geant4 we have compared several spectra sampled by Geant4 with the original data present in the ENDF-6 format files. This has been done for all the TENDL and JENDL nuclear data libraries used later on in the neutron yield calculations.





Future developments

Future developments

1. Energy/momentum conservation: Energy, momentum, baryonic number … are **in general** not conserved event by event. We will try to implement an option which forces ParticleHP to conserve these quantities event by event. Environmental variables will be removed/reduced.

2. Implement a very detailed physics for organic neutron detectors up to 100 – 200 MeV. At present there is a specific model inside ParticleHP for n+^{12}C reactions up to 20 MeV (*A. García et al., NIMA 868, 73 (2017)*). We are trying to extend it to higher energies.

3. Extend the ParticleHP model to higher energies:

- ENDF/HE-VI: n,p incident (4 isotopes, up to 1 GeV).
- JENDL/HE-2007: n,p incident (106 isotopes, up to 3 GeV)

4. Insert into Geant4 the NuDEX code, which generates EM de-excitation cascades by creating full level schemes + BR of a large variety of nuclei. Similar to PhotonEvaporation but with more detail.

Conclusions

During the last year – 2 years:

- Eight new ENDF-6 format data libraries have been translated into the Geant4 format. Detailed consistency checks were performed. The libraries and more info are available at: https://www-nds.iaea.org/geant4/.
- New verification tests have been performed, by comparing ParticleHP with MCNP6.1 isotope by isotope. Some of the results are available at: INDC(NDS)-0758.
- A detailed study concerning the generation of neutrons from α-decays via (α,Xn) reactions have been performed. The results are available at arXiv:1906.03903.

Future developments are in progress