

# NeutronHP Development and Plans

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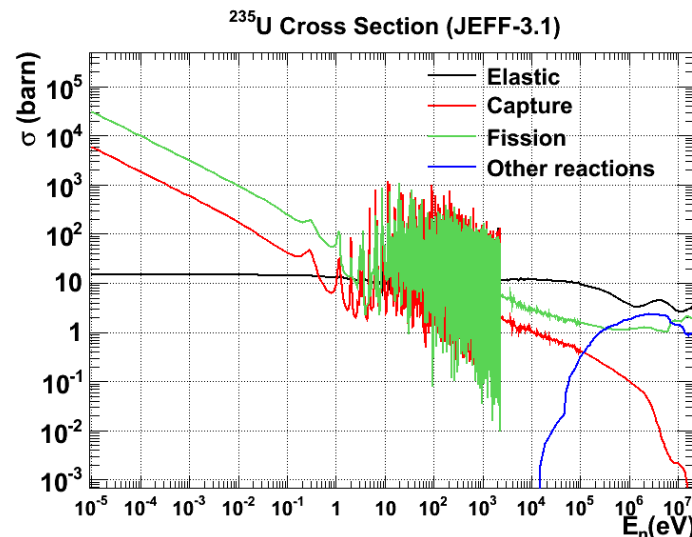
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Emilio Mendoza Cembranos  
GEANT4 collaboration meeting – Sevilla, Sept. 2013

# What is NeutronHP?

- Nuclear models fail at predicting with reasonably accuracy the neutron physics of low energy neutrons (<20 MeV).
- All physical quantities relevant for an accurate modeling of nuclear reactions in Monte Carlo simulations need to be provided as a database (cross section, energy-angle of secondary particles, ...).
- These data bases are called **E**valuated **N**uclear **D**ata **F**iles, written in a specific format called **ENDF-6**.
- GEANT4 uses the G4NDL (G4 Neutron Data Library), which is constructed from the information available in the ENDF-6 format libraries, written in a different format.
- NeutronHP is the GEANT4 package which simulates the low energy neutrons, according to the information available in the G4NDL.



# What have we (CIEMAT) done?

- “Translated” 8 different ENDF-6 format libraries into the G4NDL format.
- Improvement of the NeutronHP code.
- Validation of the NeutronHP code and the G4NDL libraries.



# New G4NDL libraries

**ENDF-6**



**G4NDL**

**USA**

ENDF/B-VII.1  
ENDF/B-VII.0  
ENDF/B-VI.8

G4NDL-4.1/4.2  
G4NDL-4.0

**EUROPE**

JEFF-3.1.2  
JEFF-3.1  
JEFF-3.0

**JAPAN**

JENDL-4.0  
JENDL-3.3

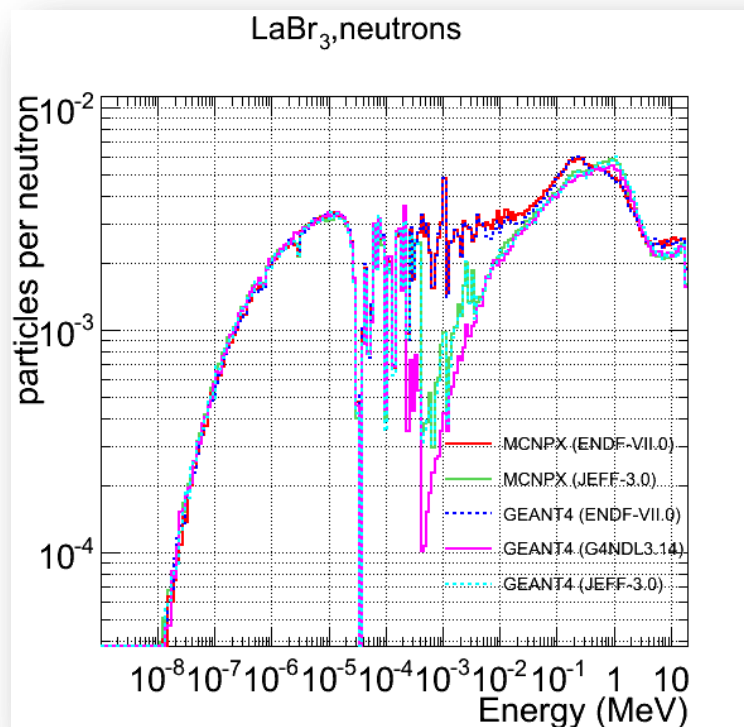
**CHINA**

CENDL-3.1

**RUSSIA**

ROSFOND-2010  
BROND-2.2

...



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# New G4NDL libraries

[www-nds.iaea.org/geant4/](http://www-nds.iaea.org/geant4/)

The screenshot shows a web browser window displaying the GEANT4 Libraries page. The page header includes the International Atomic Energy Agency (IAEA) logo and the text "Nuclear Data Services". The main content area features a large heading: "New evaluated neutron cross section libraries for the GEANT4 code". Below this, the authors are listed as Emilio Mendoza and Daniel Cano-Ott from CIEMAT, Spain. The text explains that Geant4 is a general purpose toolkit for simulating particle passage through matter, and that the new libraries (e.g., ENDF/B\_VII.0, JEFF-3.1, JENDL-4.0) are meant to replace the default G4NDL library. It also mentions that these new libraries provide access to a larger list of isotopes and systematic uncertainties. The page includes sections for "Documentation" and "Installation of new Geant4 source code", with sub-sections for installing new classes with Geant4 versions 4.9.2, 4.9.3, 4.9.4, and 4.9.5. A sidebar on the left lists various nuclear data services, and a sidebar on the right provides navigation links and contact information.

## New evaluated neutron cross section libraries for the GEANT4 code

**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) of neutrons with energies lower than 20 MeV. These data come from recent releases of the evaluated data libraries (e.g. ENDF/B\_VII.0, JEFF-3.1, 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**
  - Please [READ THE DETAILED INSTRUCTIONS](#) carefully before starting the installation of the new source code and the neutron data libraries. You will be modifying a standard release of the Geant4 source code and its performance can be affected severely in case of an incorrect installation. The installation procedure will consist mainly in two steps:
    - **Installation of new Geant4 source code**, necessary for the performing simulations with the new libraries.
    - **Installation of the Geant4 neutron data libraries**. Please notice that the format of the new data libraries IS NOT compatible with G4NDL3.14 and earlier versions.
- **Installation of new Geant4 source code**
  - **I. Installation of the new Geant4 classes with the Geant4 versions 4.9.2, 4.9.3 and 4.9.4**

The new classes provided should replace the already existing Geant4 classes with the SAME names. Geant4 will have to be recompiled afterwards. The new classes and the data libraries have been tested with the geant4.9.2, geant4.9.3 and geant4.9.4. No test has been performed with earlier versions of the Geant4 simulation package and therefore its use is not recommended.

**IMPORTANT:** after the replacement of the classes, the G4NDL3.14 and earlier versions of it will no longer be usable!
  - **II. Installation of the new Geant4 classes with Geant4 version 4.9.5**

**REPLACE** only the G4NeutronHPCaptureFS.cc class when running geant4.9.5 (release 0). Geant4 will have to be recompiled afterwards. The geant4.9.5 version was expected to be fully compatible with the neutron data libraries distributed in this webpage. However, a bug has been detected in the official release, making necessary the replacement of that source file. It is expected that the bug will be corrected in future releases; thus no further modification of the source code will be necessary.

# New G4NDL libraries

GEANT4 Libraries - Google Chrome

GEANT4 Libraries

www-nds.iaea.org/geant4/

hotmail Google Rebellion YouTube - Broa... National Nucl... T-2 Nuclear Inf... Diccionarios de... IAEA Nuclear D... Other Bookmarks

- **Installation of new Geant4 source code**
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- **Installation of the new neutron data libraries**

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

  - 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 for every distribution (partial cross sections, energy and angular distributions of secondaries...) sampled with the GEANT4 classes and generated the "viewr" program of NJOY code. The figures have been compiled in postscript and there exists one for each isotope in each library processed.

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

*The authors would appreciate that their work is acknowledged properly. Please cite:*  
**E. Mendoza, D. Cano-Ott, C. Guerrero, and R. Capote, IAEA technical report INDC(NDS)-0612, Vienna, 2012. Data available online at <http://www-nds.iaea.org/geant4>.**

**Please read our [DISCLAIMER!](#)**

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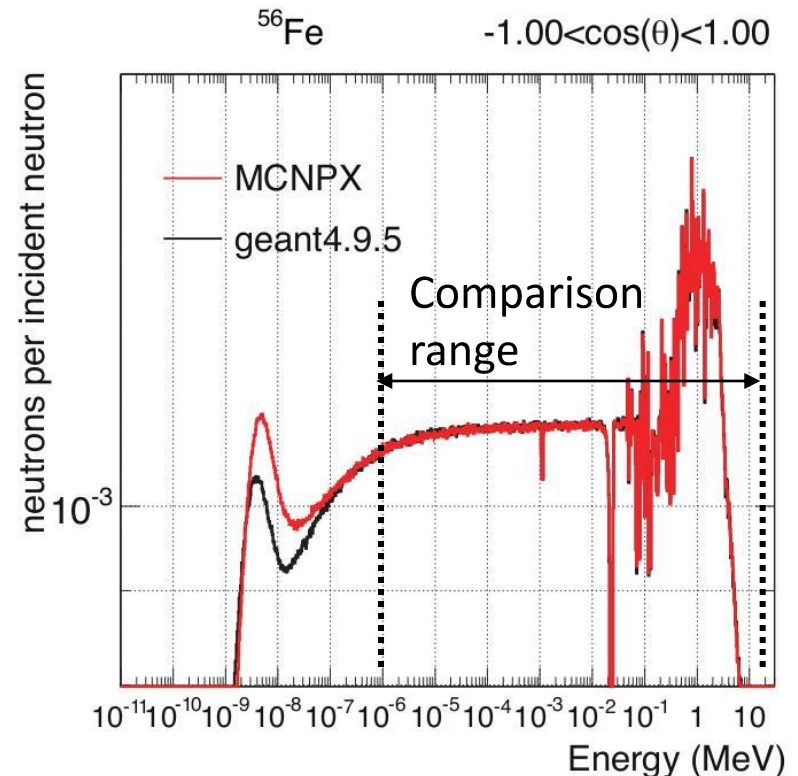
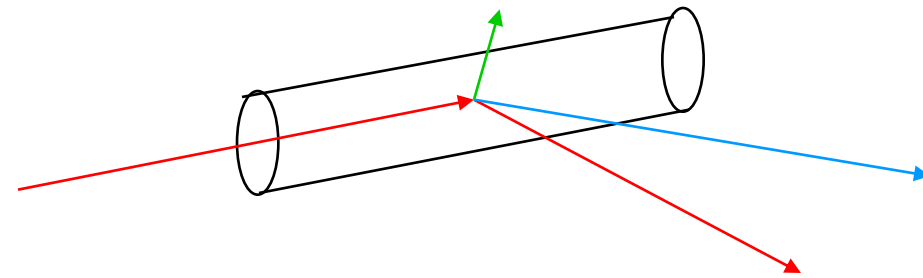
# Improvements and validation

## VALIDATION STRATEGY

Monte Carlo simulations with Geant4 and MCNPX of the interactions with a thin 200 cm long cylinder with negligible radius with the same neutron energy spectrum (isoethargic in the  $1e-10 - 19$  MeV energy range). Every secondary particle goes out of the cylinder after the first interaction. The energy and angle of secondary particles are histogrammed. This method allows to compare not only the energy and angle of secondary neutrons and gammas, but also the energy and angle of other secondary charged particles (p,d,t, $^3\text{He}$ , $\alpha$ ).

With these simple MC results it is easy to:

- See the differences between the different libraries.
- See the differences between both codes (detect bugs in GEANT4).



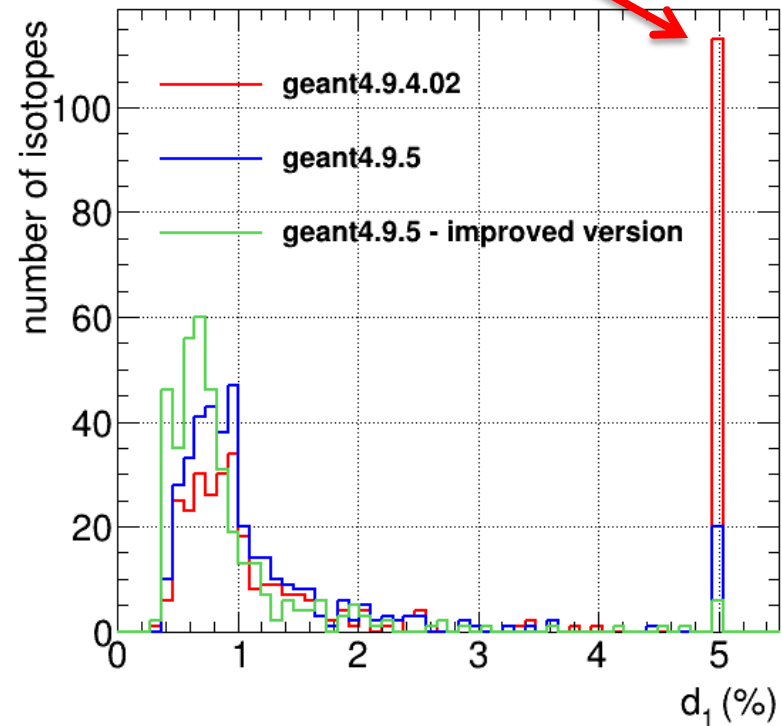
# Improvements and validation

The validation of the code has been performed with the ENDF/B-VII.0 library, by simulating  $1e8$  neutrons per isotope (383 isotopes). Only the energy spectra ( $>1eV$ ) of the outgoing neutrons have been compared, integrating over all angles.

The following variable has been defined to compare between the GEANT4 and the MCNPX results:

$$d_1 = 1/n * \sum |x_1 - x_2| / x_1$$

Isotopes with  $d_1 > 5\%$  are stored here





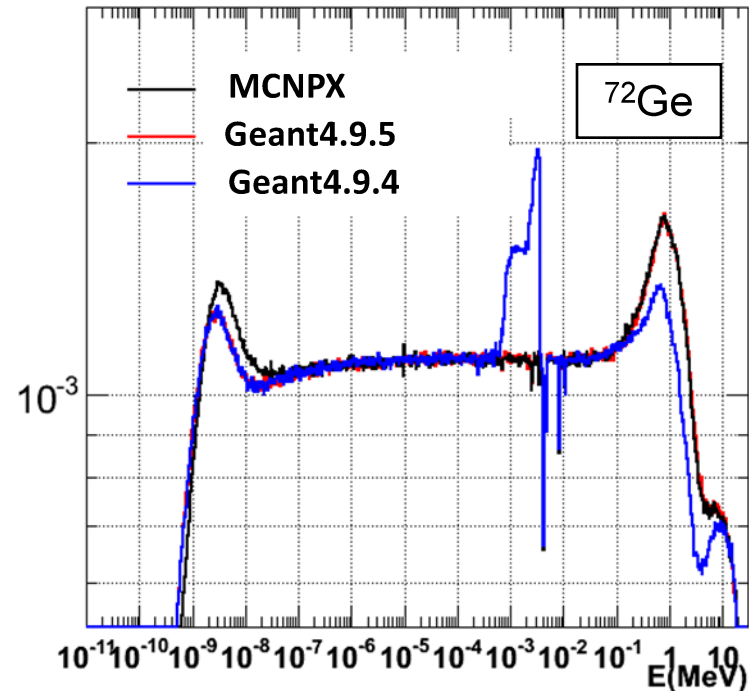
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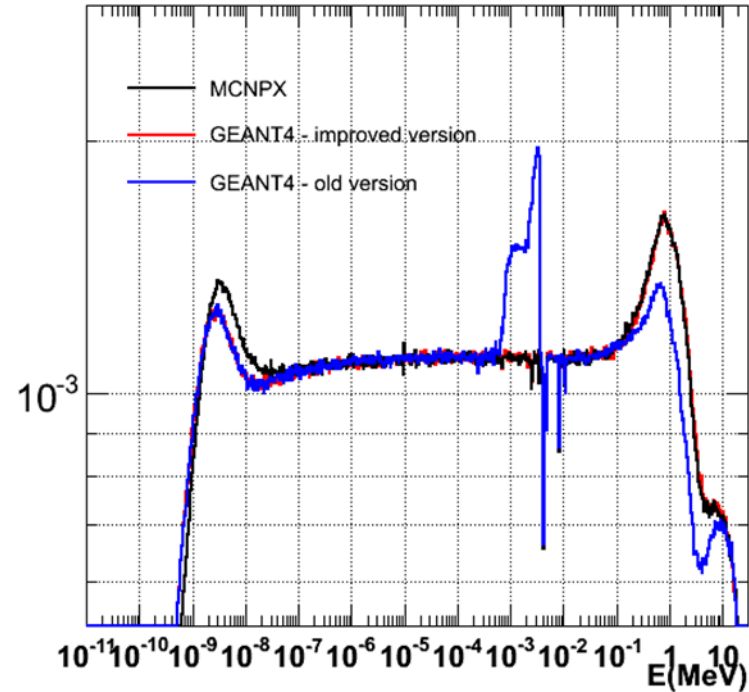
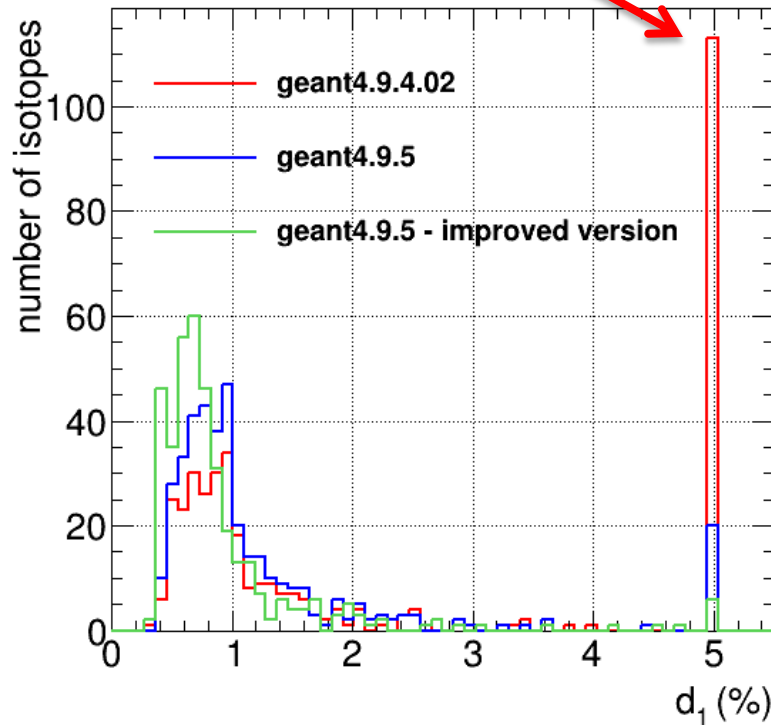
ZA=32072 , neutron ,  $-1.00 < \cos(\theta) < 1.00$



# Improvements and validation

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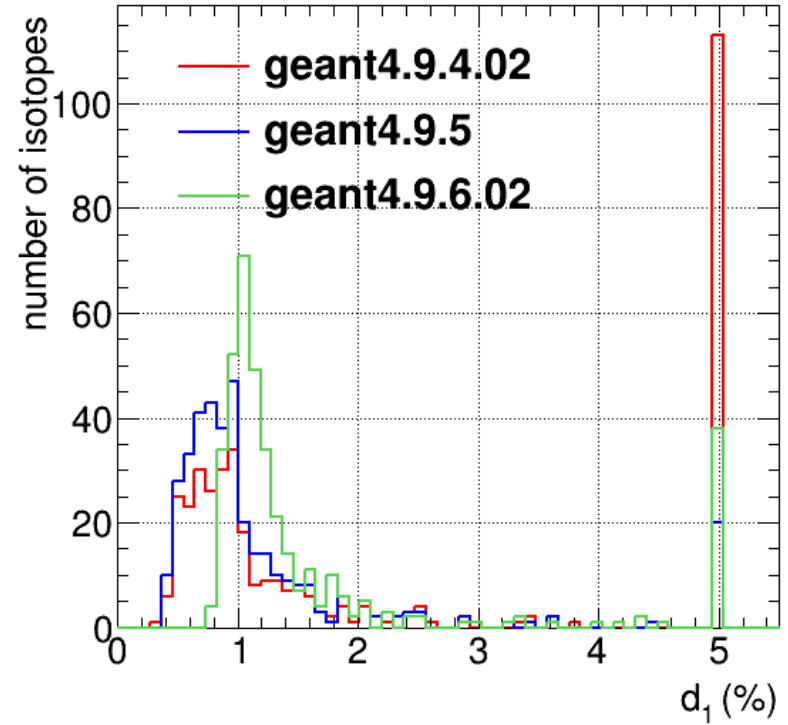
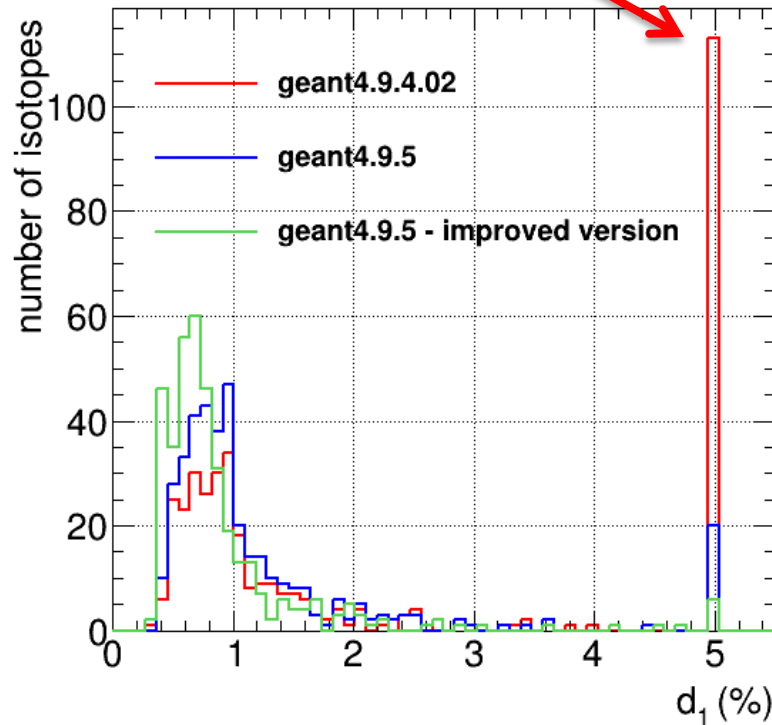
ZA=32072 , neutron ,  $-1.00 < \cos(\theta) < 1.00$



|                | geant4.9.5  | improved geant4.9.5  |
|----------------|---|--|
| $5\% \leq d_1$ | $^{124}\text{Xe}$ , $^{148}\text{Pm}$ , $^{152,156}\text{Eu}$ ,<br>$^{230}\text{Th}$ , $^{232}\text{Pa}$ , $^{236,238}\text{Np}$ ,<br>$^{236}\text{Pu}$ , $^{241,242,243,244}\text{Am}$ ,<br>$^{247}\text{Cm}$ , $^{250}\text{Bk}$ , $^{249,254}\text{Cf}$ ,<br>$^{254,255}\text{Es}$ , $^{255}\text{Fm}$ | $^{148}\text{Pm}$ , $^{156}\text{Eu}$ , $^{230}\text{Th}$ ,<br>$^{241,242,243}\text{Am}$ |

# Improvements and validation

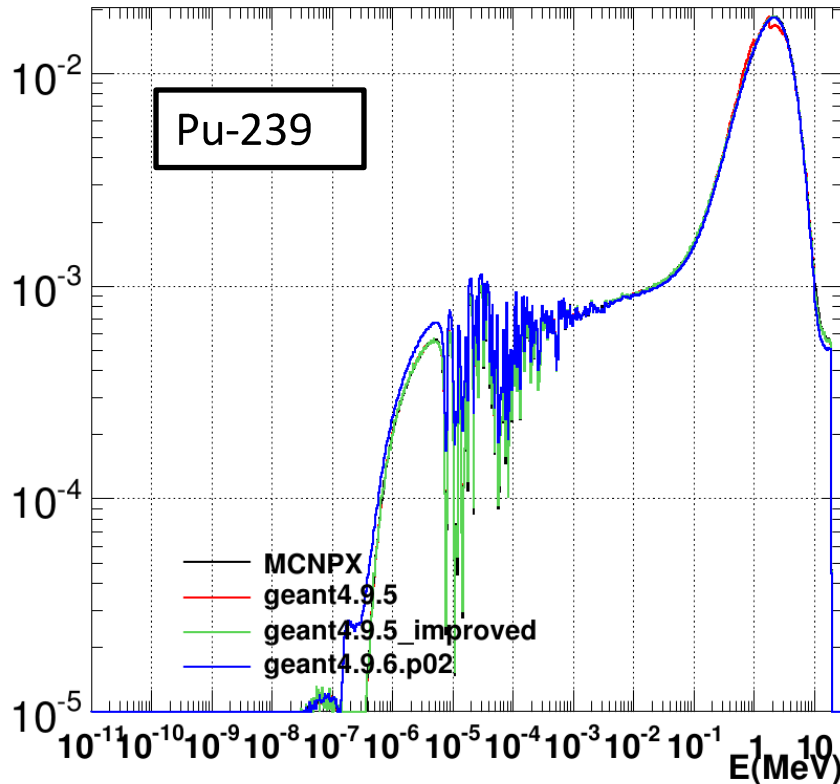
Isotopes with  $d_1 > 5\%$  are stored here



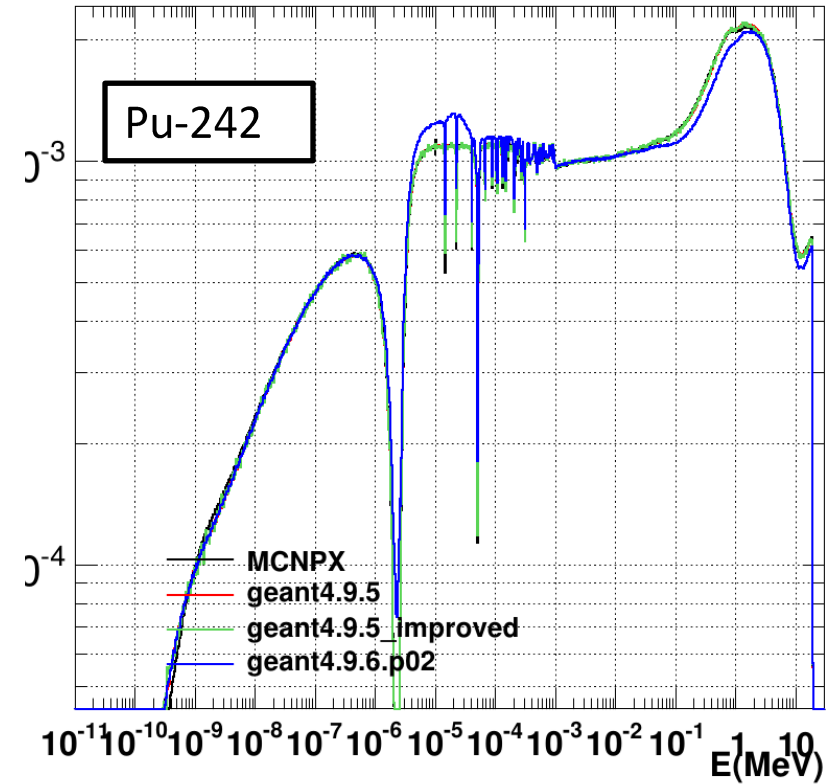
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|----------------|---|--|
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# Improvements and validation

ZA=94239 , neutron ,  $-1.00 < \cos(\theta) < 1.00$



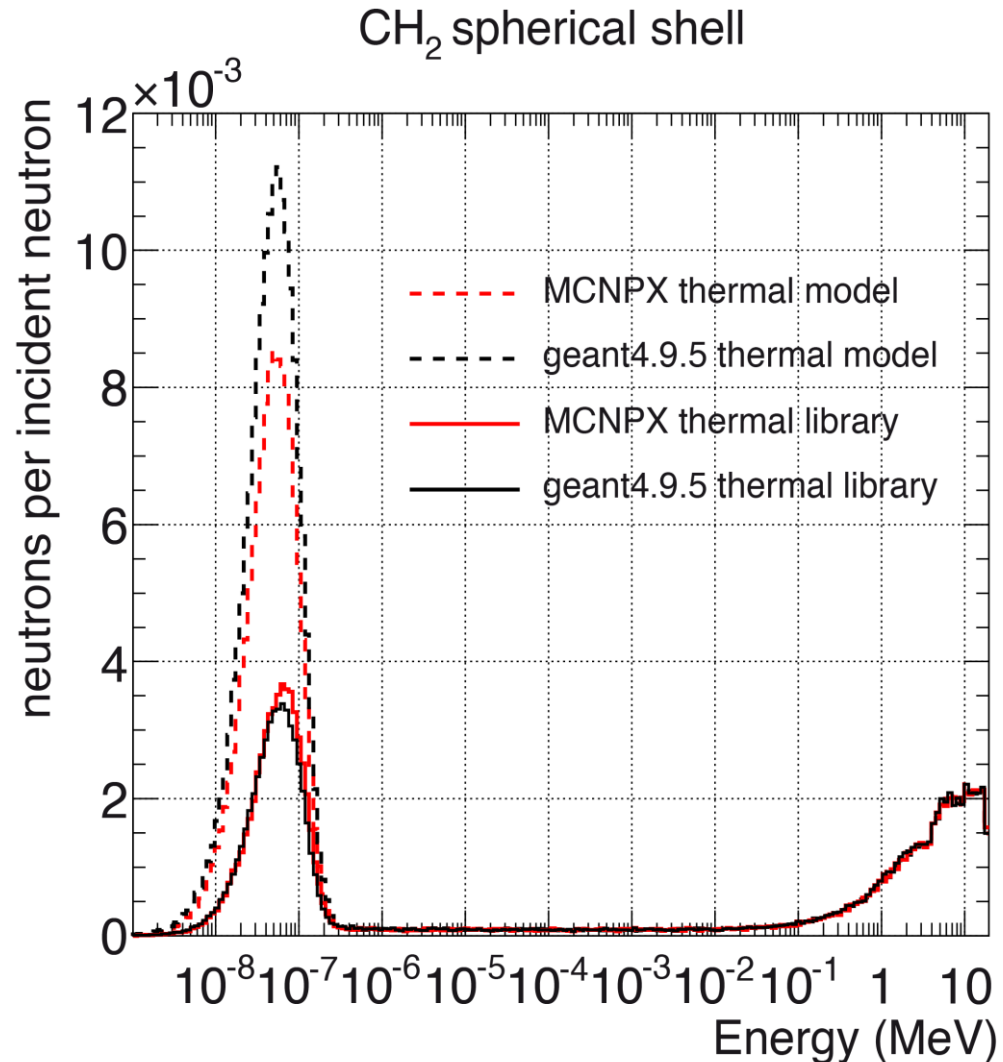
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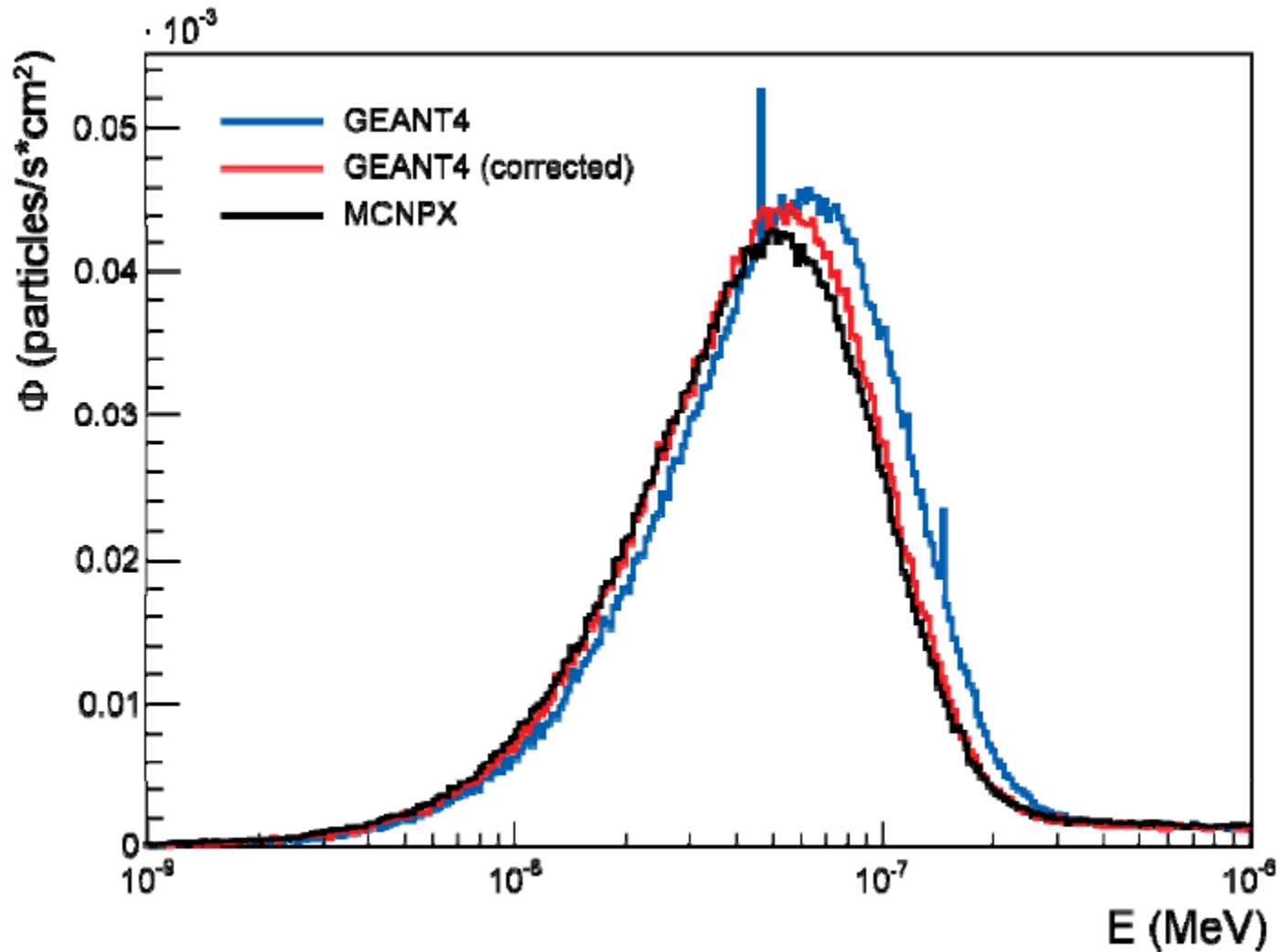
# Other recent improvements: thermal libraries

The interaction of thermal neutrons ( $E_n = 0.025$  eV) with matter needs to be treated in detail as a function of the temperature of the material for obtaining accurate results from Monte Carlo simulations. Such a treatment is important for a wide range of applications: neutron shielding problems – polyethylene or water–, neutron detectors, dosimetry ...

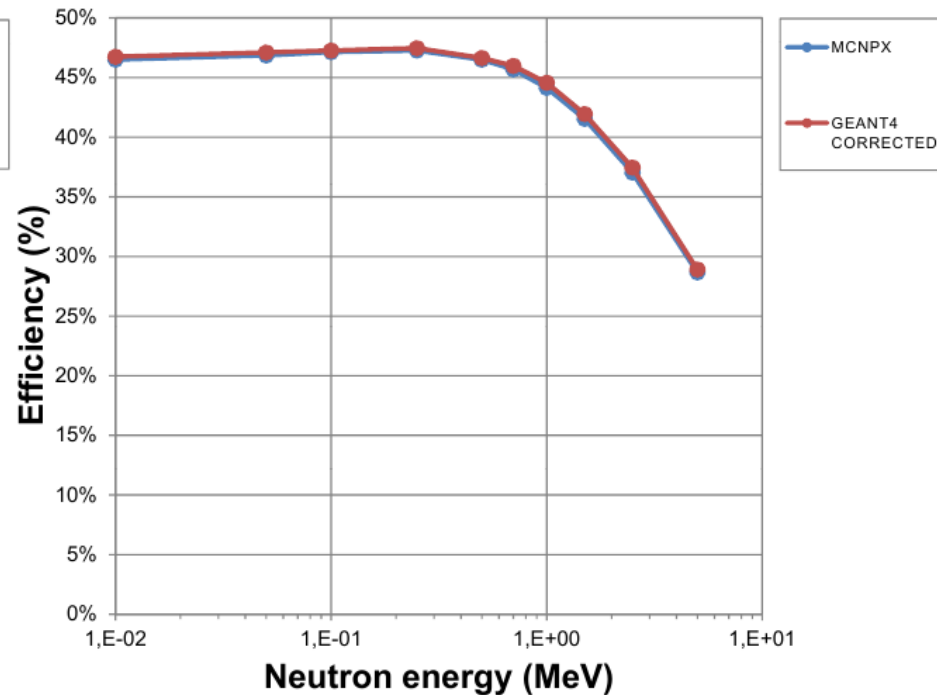
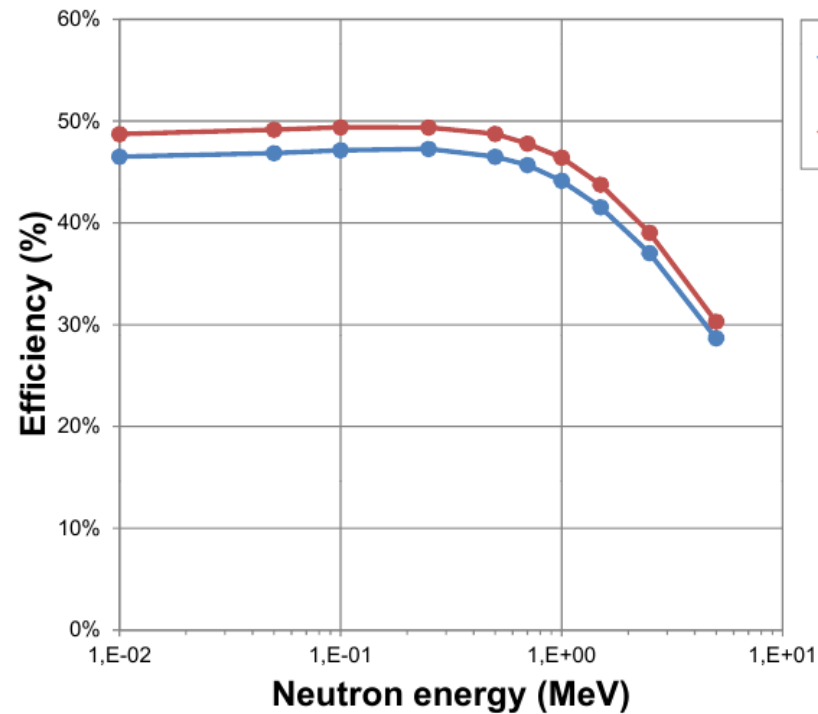
The most accurate/reliable results are obtained by using the thermal neutron data libraries for materials delivered together with the evaluated data libraries.



# Other recent improvements: thermal libraries



# Other recent improvements: thermal libraries



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# Future Work

1. **URGENT:** Correct the new bugs introduced in the geant4.9.6 release.
2. Validation and maintenance of the rest of the libraries.
3. Validation including the angular distribution of the outgoing neutrons.
4. Study the neutron transport at low energies without thermal libraries.
5. Unresolved resonance treatment.
6. Charged particle production.

