Update of the evaluated neutron cross section libraries for the Geant4 code

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Evaluated libraries in Geant4

For the transport of low energy neutrons in Geant4 it is possible to the G4NeutronHP/G4ParticleHP model, which rely in evaluated data libraries containing the same information as in the ENDF-6 format libraries but written in a different format: G4NDL.

The G4NDL library distributed by Geant4 together with the code is, at this moment, G4NDL4.5, which:

- Corresponds to ENDF/B-VII.1 for most of the nuclei, but not for all.
- Contains 363 nuclei instead of the 423 nuclei in ENDF/B-VII.1. In particular, there are no data for isotopes with Z>92.

In order to have more flexibility when performing Monte Carlo simulations we developed a tool for transforming any ENDF-6 format evaluated neutron cross section library into the G4NDL format. Eight different releases of the ENDF, JEFF, JENDL, CENDL and BROND libraries were translated into the G4NDL format and distributed by the IAEA nuclear data service: https://www-nds.iaea.org/geant4/. Now this list has been updated with six new releases:

Older releases: JEFF-3.1, JEFF-3.0, ENDF/B-VII.0, ENDF/B-VI.8, CENDL-3.1, BROND-2.2, JENDL-4.0, JENDL-3.3.
New releases: JEFF-3.3, JEFF-3.2, ENDF/B-VIII.0, ENDF/B-VII.1, BROND-3.1 and JENDL-4.0u (version 2016/1/6).

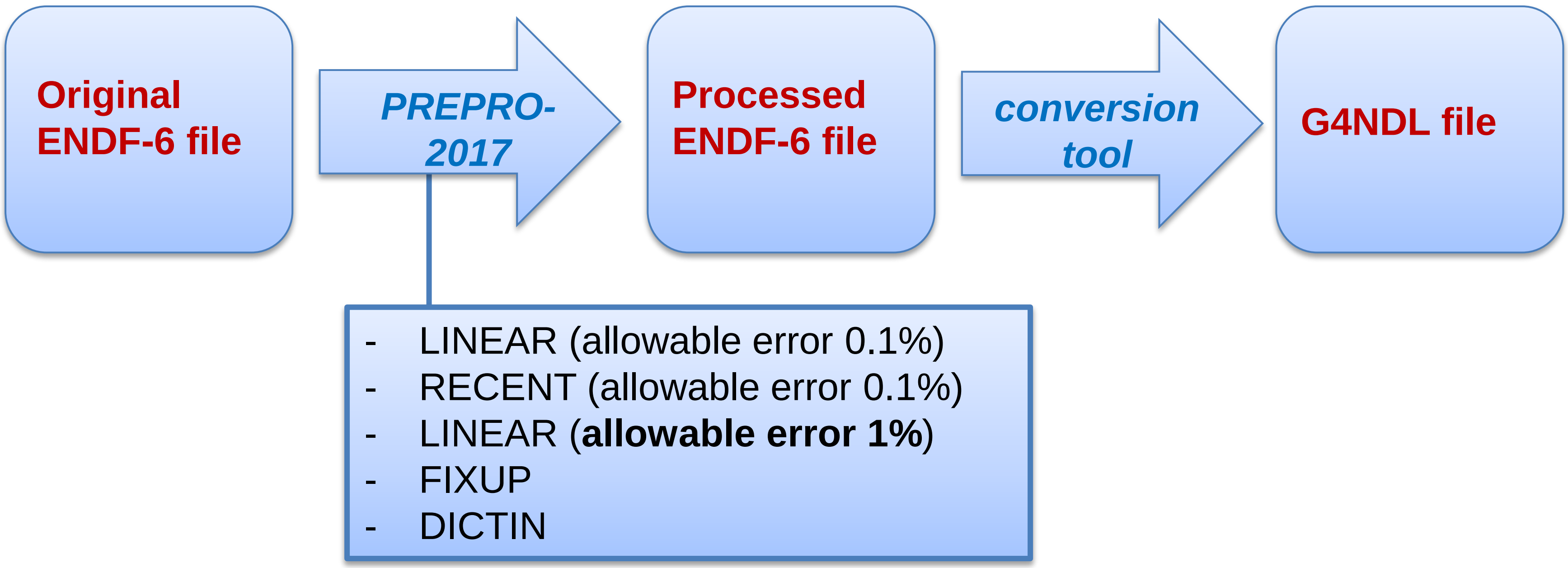
Production of the data libraries

The G4NDL format contain, in general, the same values as the ENDF-6 format written in a different format, but:

1 - Not all the information of the ENDF-6 files can be written in G4NDL format (covariances, decay data, some reaction channels …).

2 - Cross section must appear as pointwise-linear interpolable data tables, at 0 K temperature. The Doppler broadening is done "on flight".

Due to (2) we first processed the original ENDF-6 data files with PREPRO-2017:



Difficulties in the conversion process

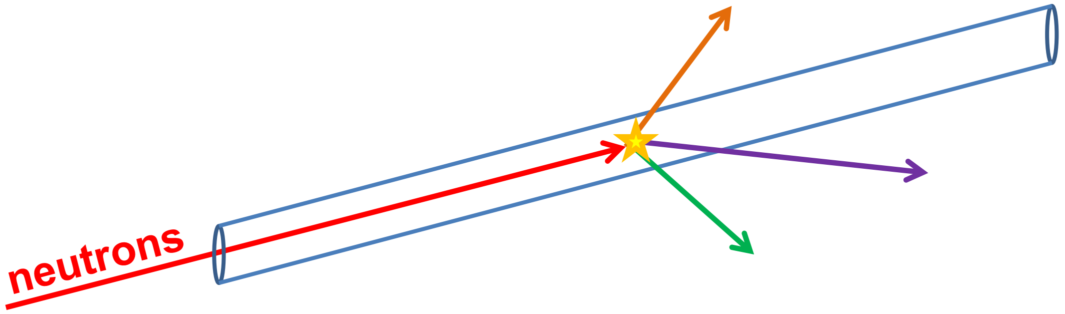
In JEFF-3.3:

- **^{9}Be**: secondary neutrons of reaction (n,2n) is described with reaction types MT=875 to MT=891 instead of MT=16. GEANT4 is not able to read such data in this format so **reaction (n,2n) has been replaced with the (n,2n) from JEFF-3.0**, which uses MT=16.

- **^{232}Th, ^{231,233}Pa: MF=6 data (product energy-angle distributions) for MT=18 (fission) has been converted to MF=4,5,12,14,15** with the PREPRO SIXPAK program before the translation into the G4NDL format, since Geant4 is not able to read such data in MF=6 format.

Comparison with MCNP6

We have verified the integrity of the new G4NDL libraries by performing identical simulations with GEANT4 and MCNP6. These simulations are the ones described in *E. Mendoza et al., IEEE Trans. Nucl. Science 61, 2357 (2014)* (Section III.B.1).



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.

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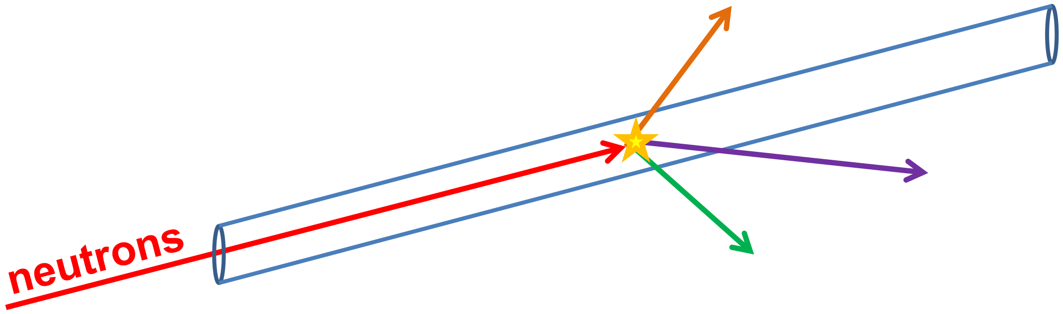


Two simulations per isotope and per neutron library: one with Geant4 and other with MCNP6.1

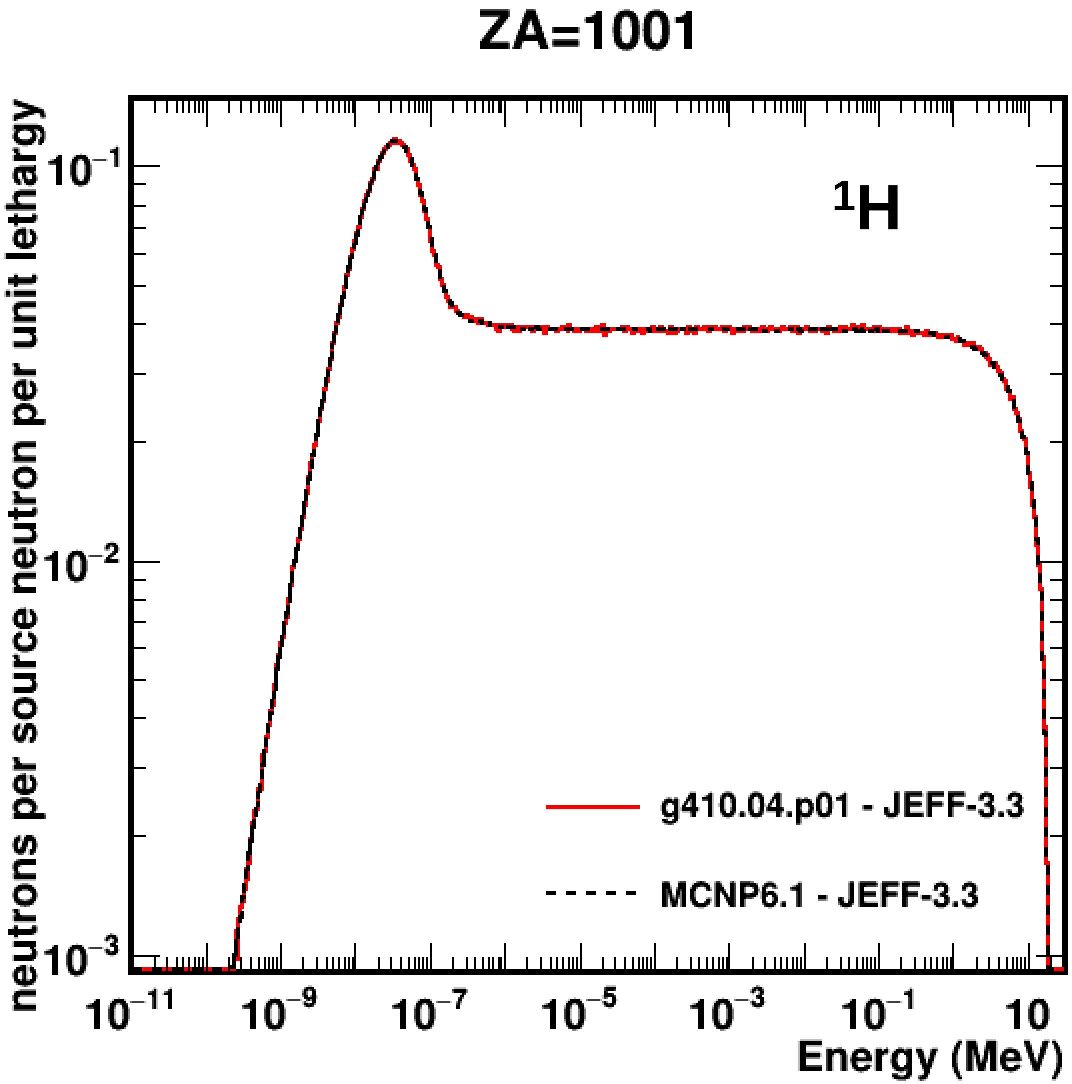
Geant4:

- 10^7 source neutrons
- version geant4.10.04.p01
- with the environmental variable "G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE"

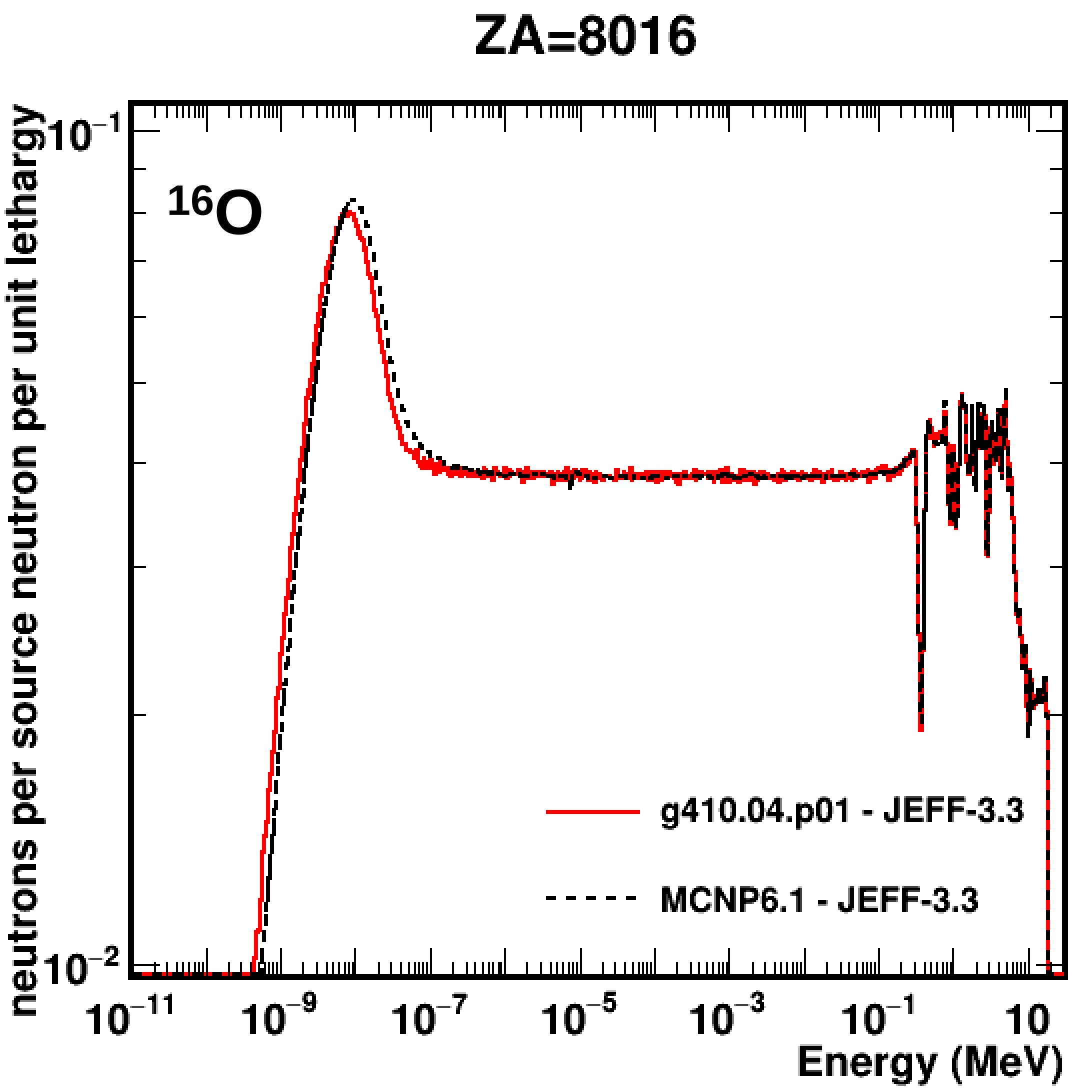
MCNP6.1:

- 10^8 source neutrons
- the unresolved resonance range probability table treatment was turned off

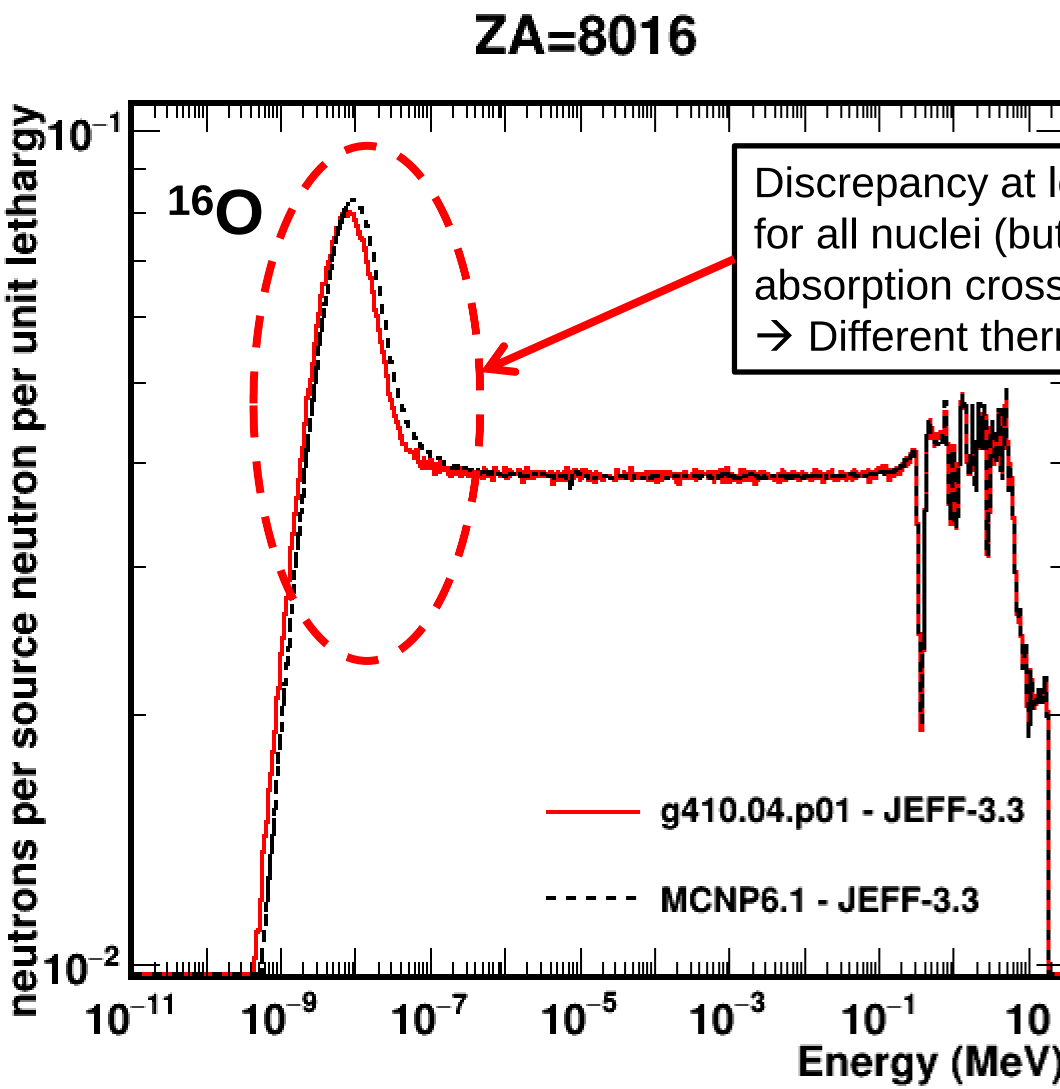
Energies of the secondary neutrons



Energies of the secondary neutrons

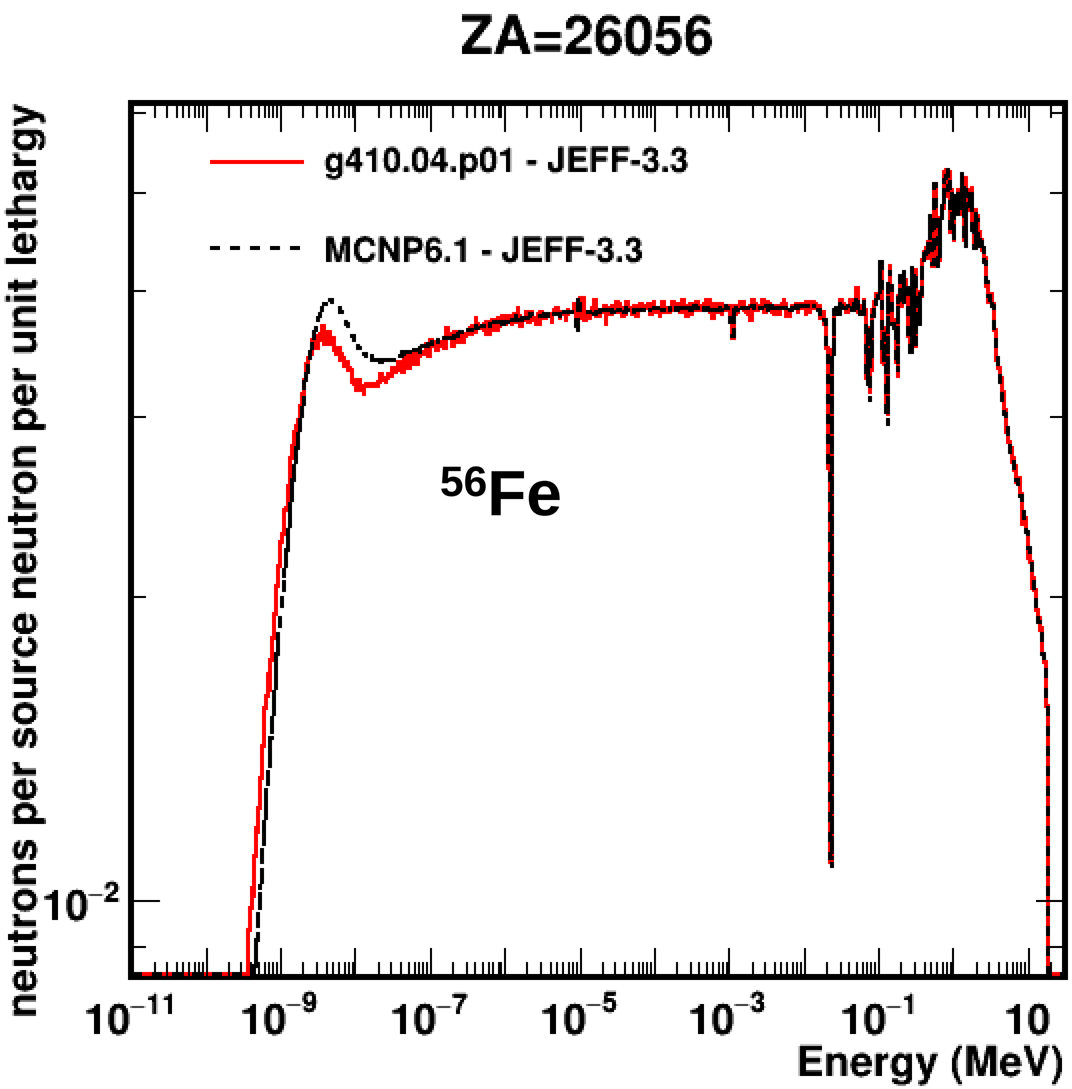


Energies of the secondary neutrons

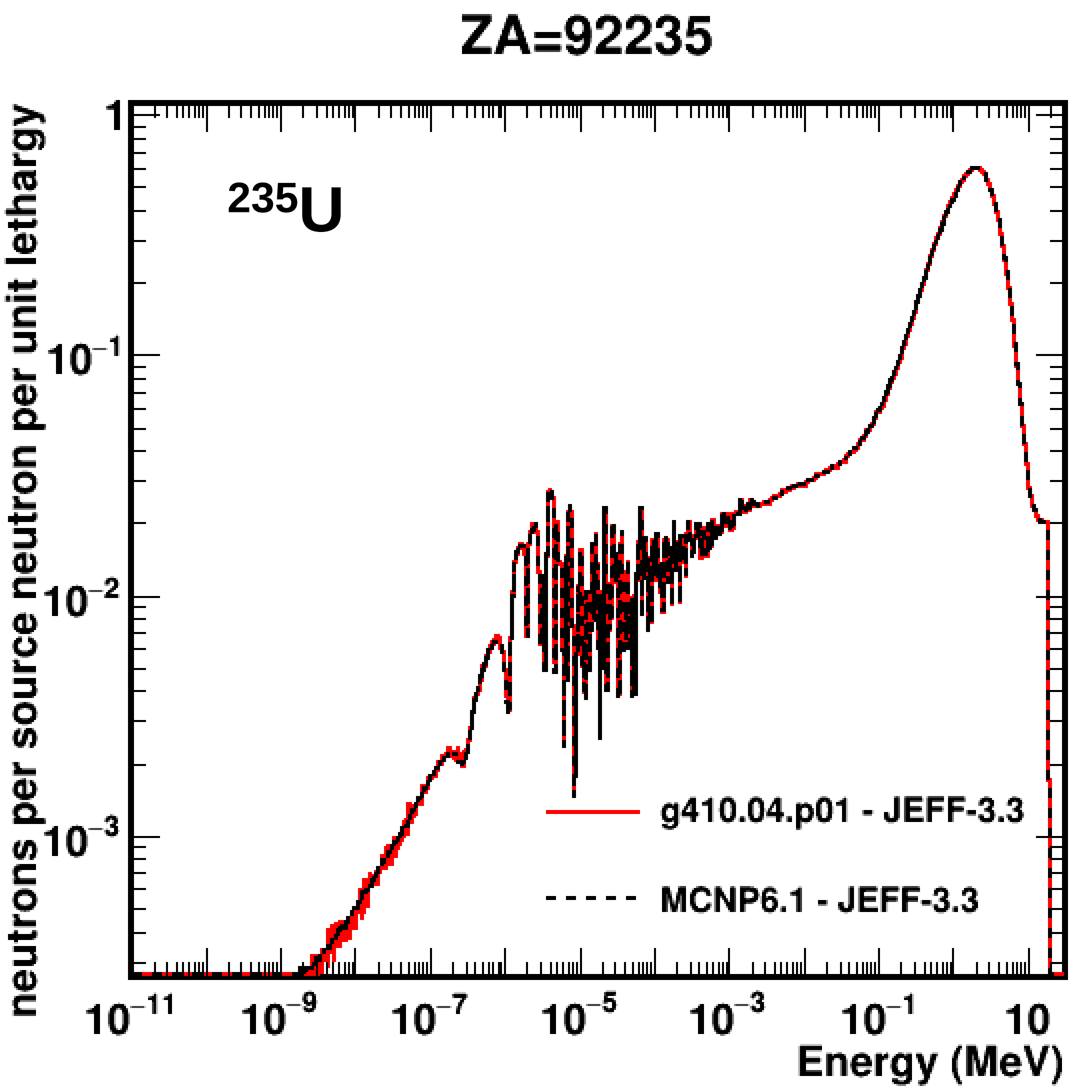


Discrepancy at low neutron energies for all nuclei (but ^{1}H) with low absorption cross sections.
→ Different thermal treatment.

Energies of the secondary neutrons



Energies of the secondary neutrons



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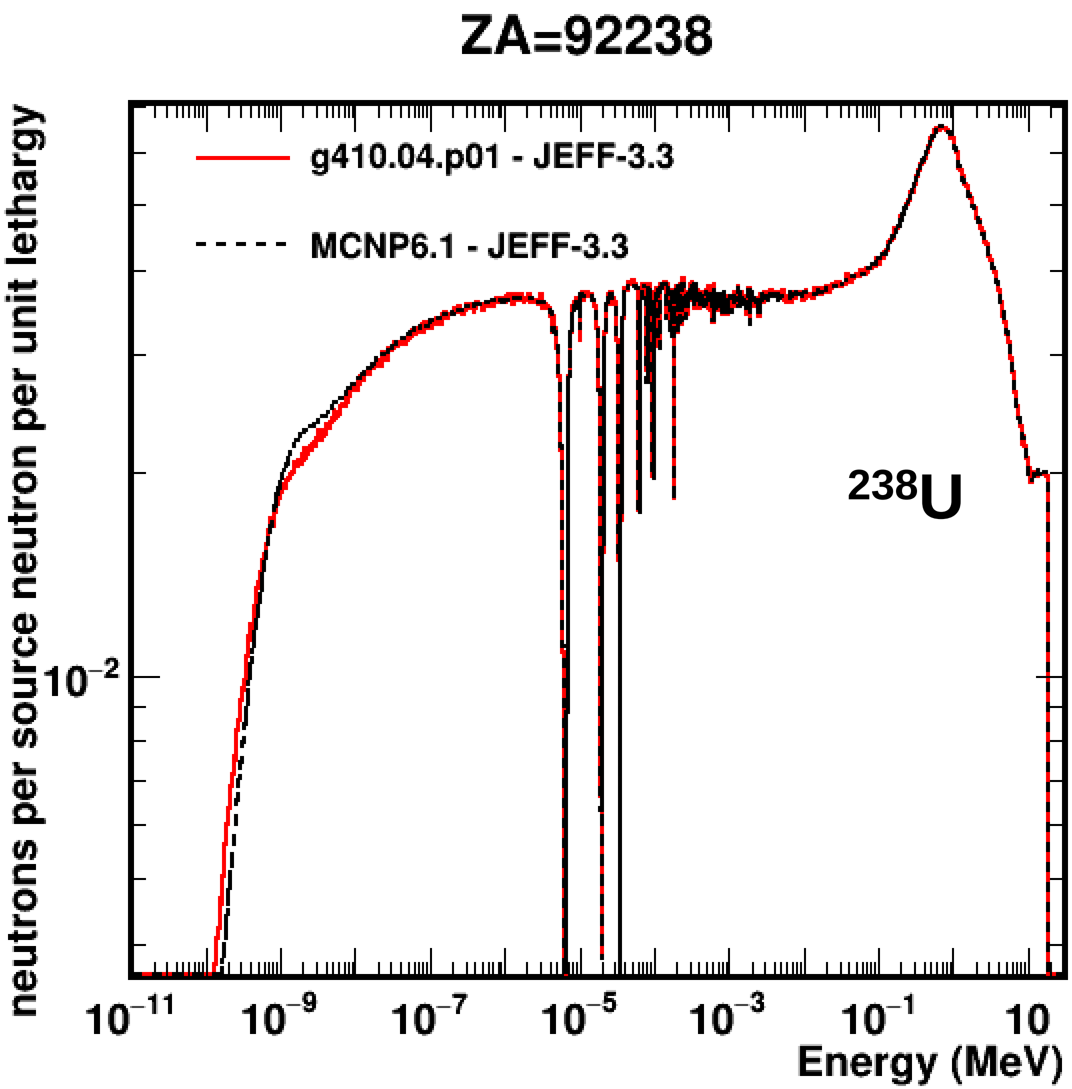
Energies of the secondary neutrons



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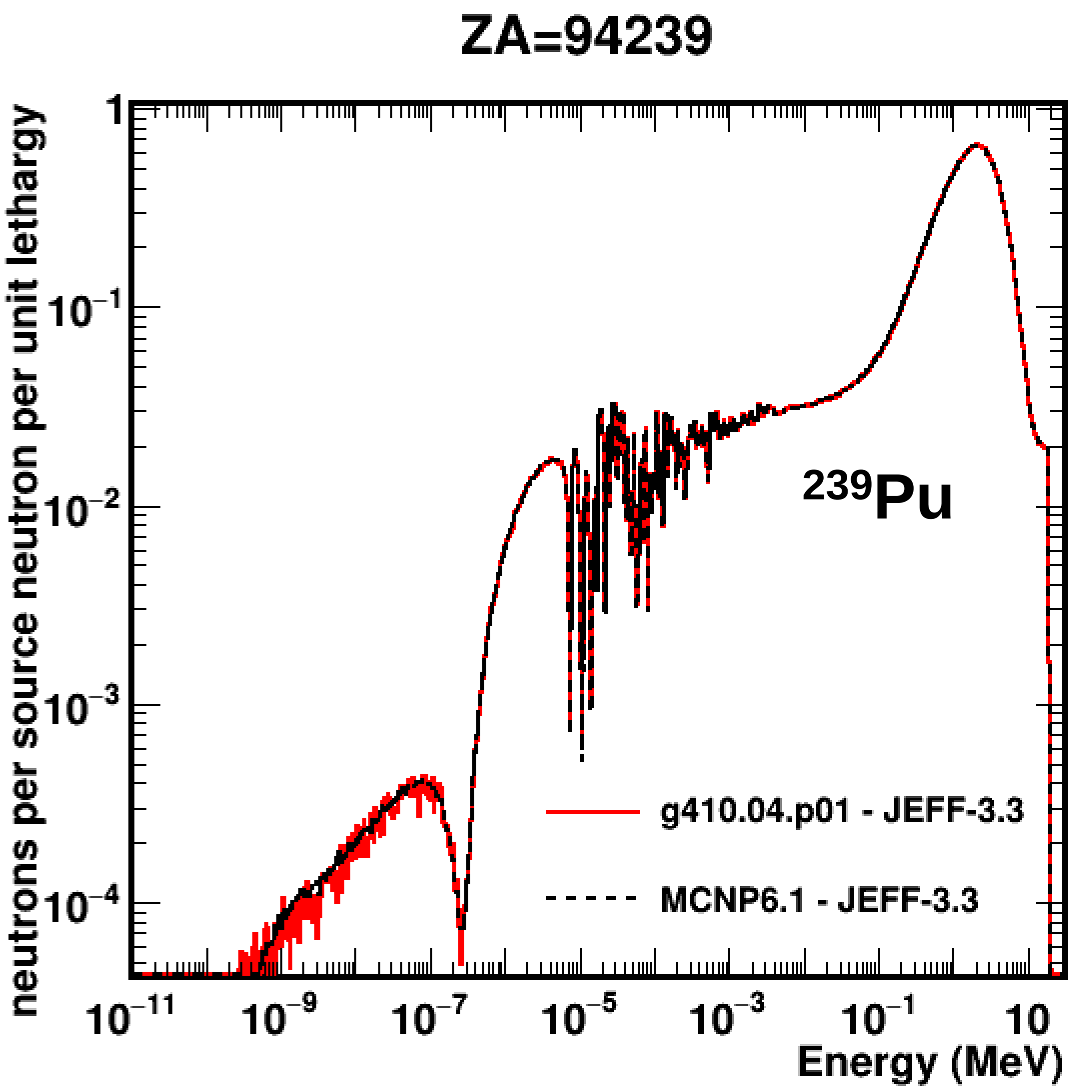

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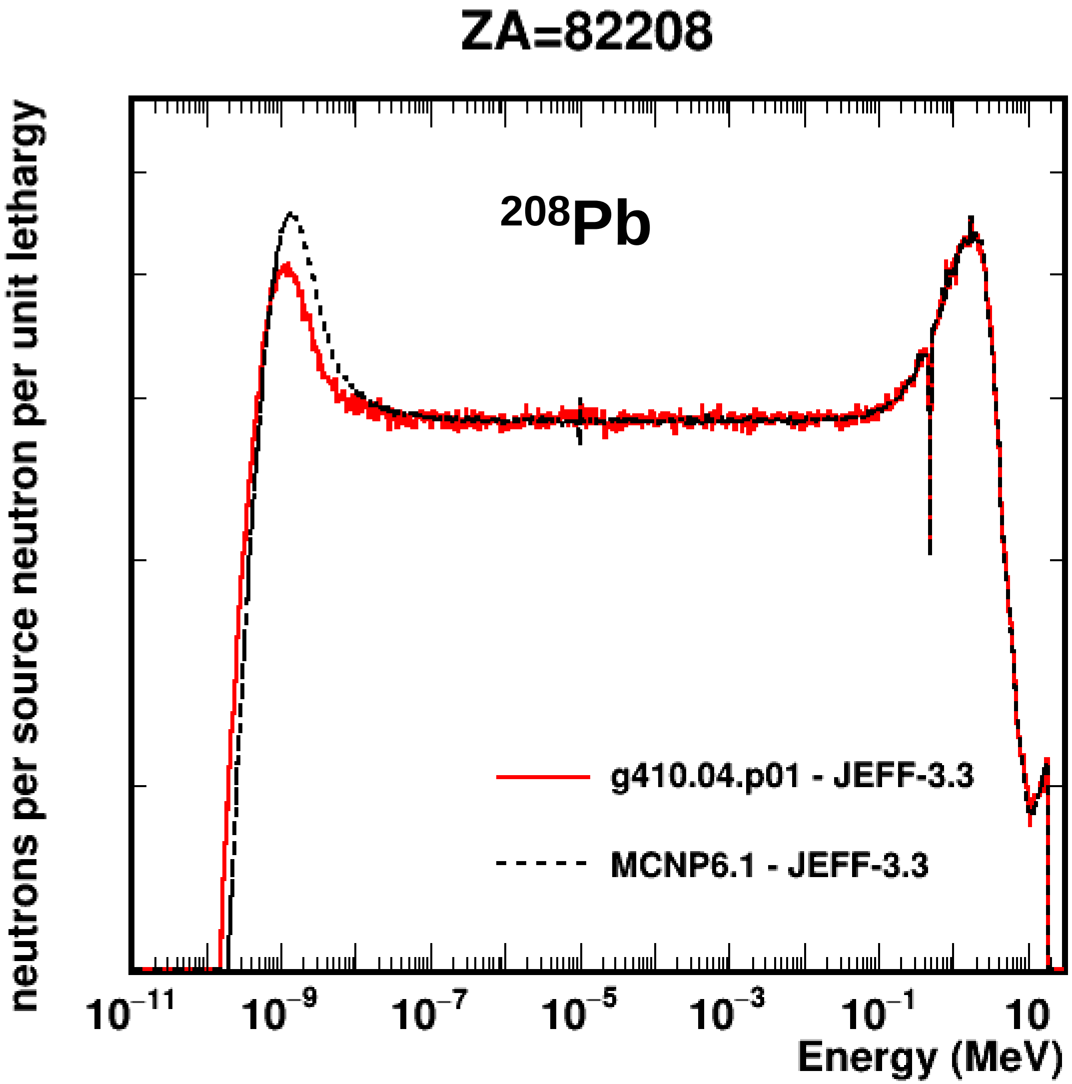

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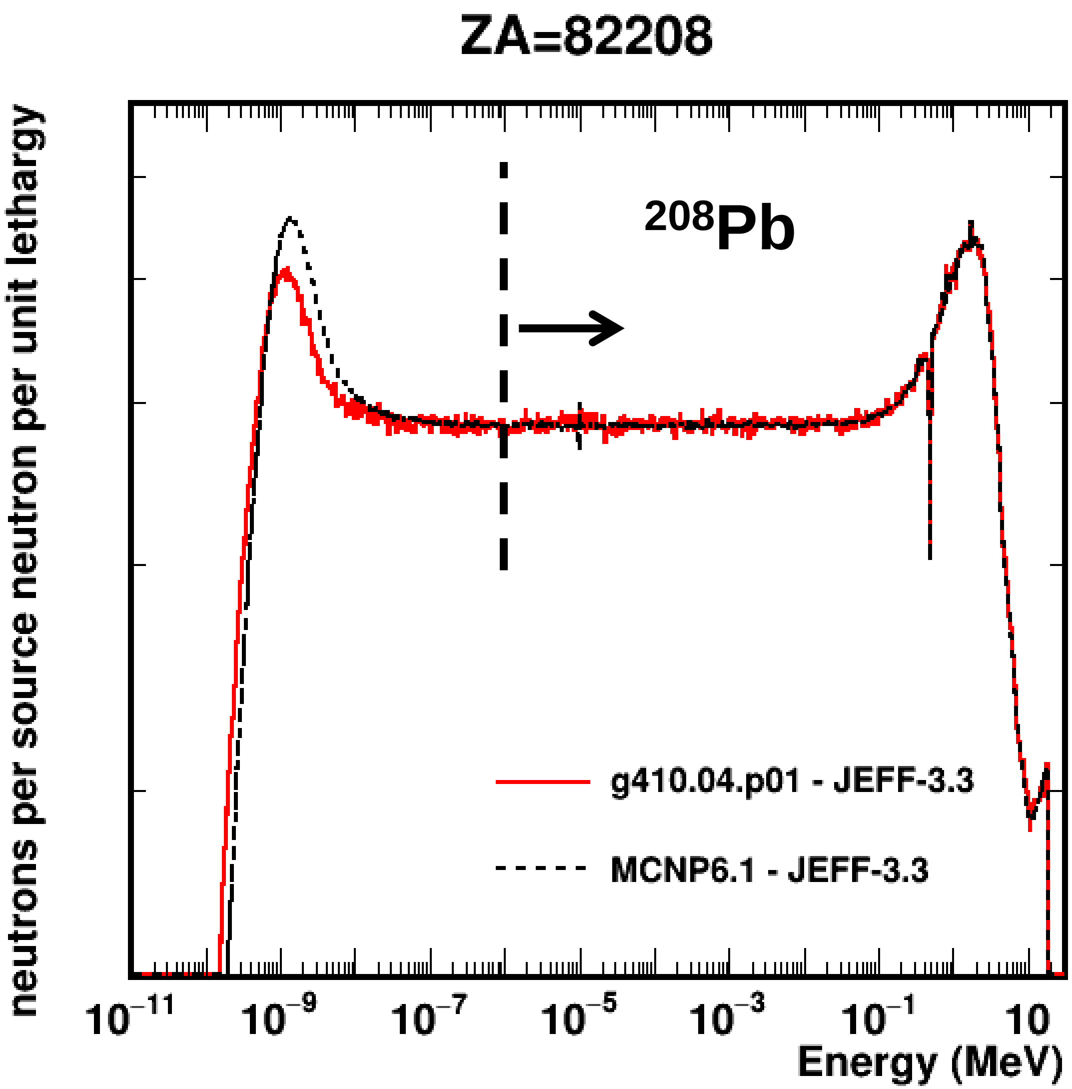
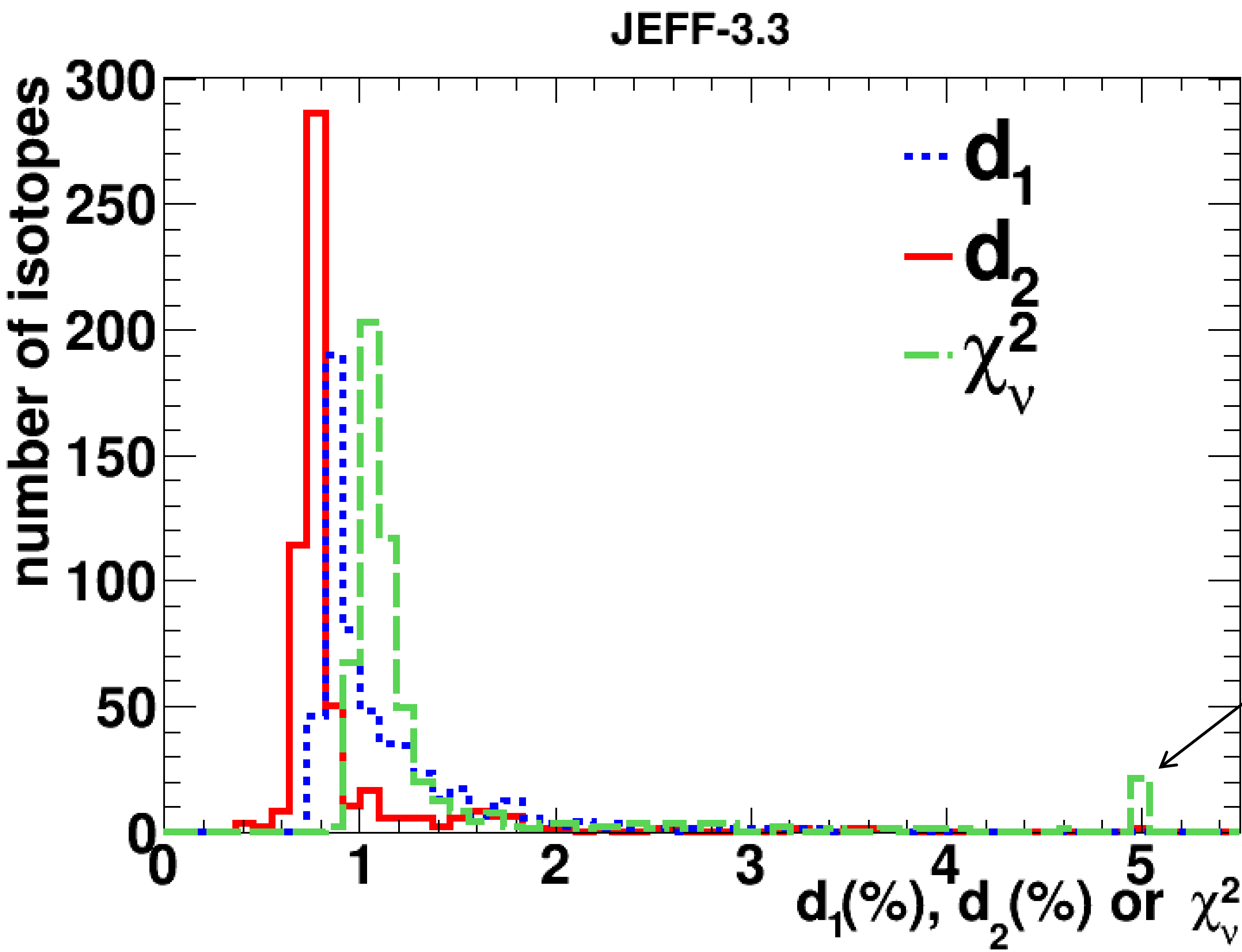


$$d_1 = \frac{1}{N} \sum_{E_i > 1\,eV} \frac{\left| x_i^G - x_i^M \right|}{\frac{1}{2}\left(x_i^G + x_i^M\right)}$$

$$d_2 = \frac{1}{N} \sum_{E_i > 1\,eV, \sigma_i < 1\%} \frac{\left| x_i^G - x_i^M \right|}{\frac{1}{2}\left(x_i^G + x_i^M\right)}$$

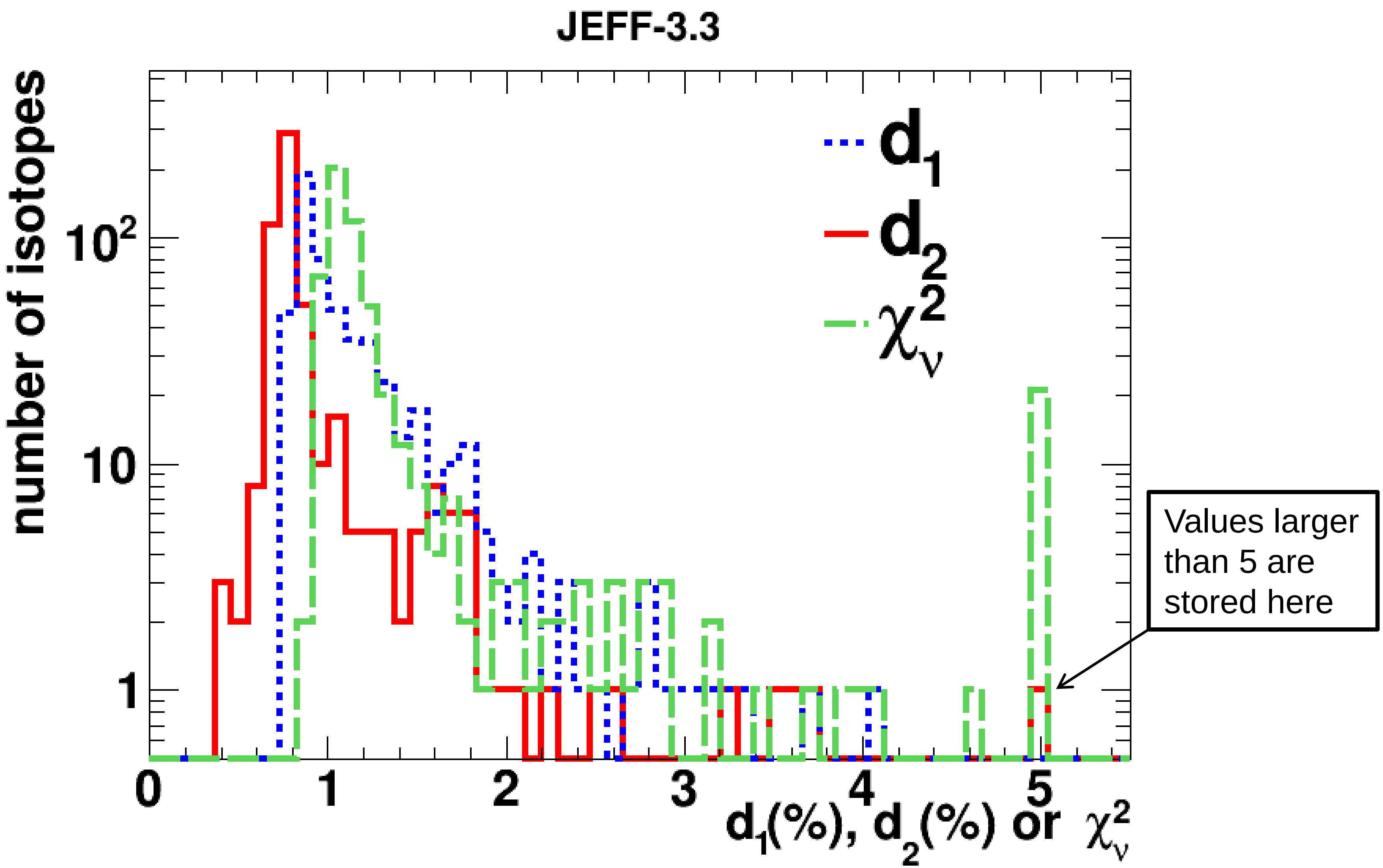
$$\chi_\upsilon^2 = \frac{1}{N} \sum_{E_i > 1\,eV} \left(\frac{x_i^G - x_i^M}{\sigma_i} \right)^2$$

Energies of the secondary neutrons



Values larger than 5 are stored here

Energies of the secondary neutrons



Energies of the secondary neutrons

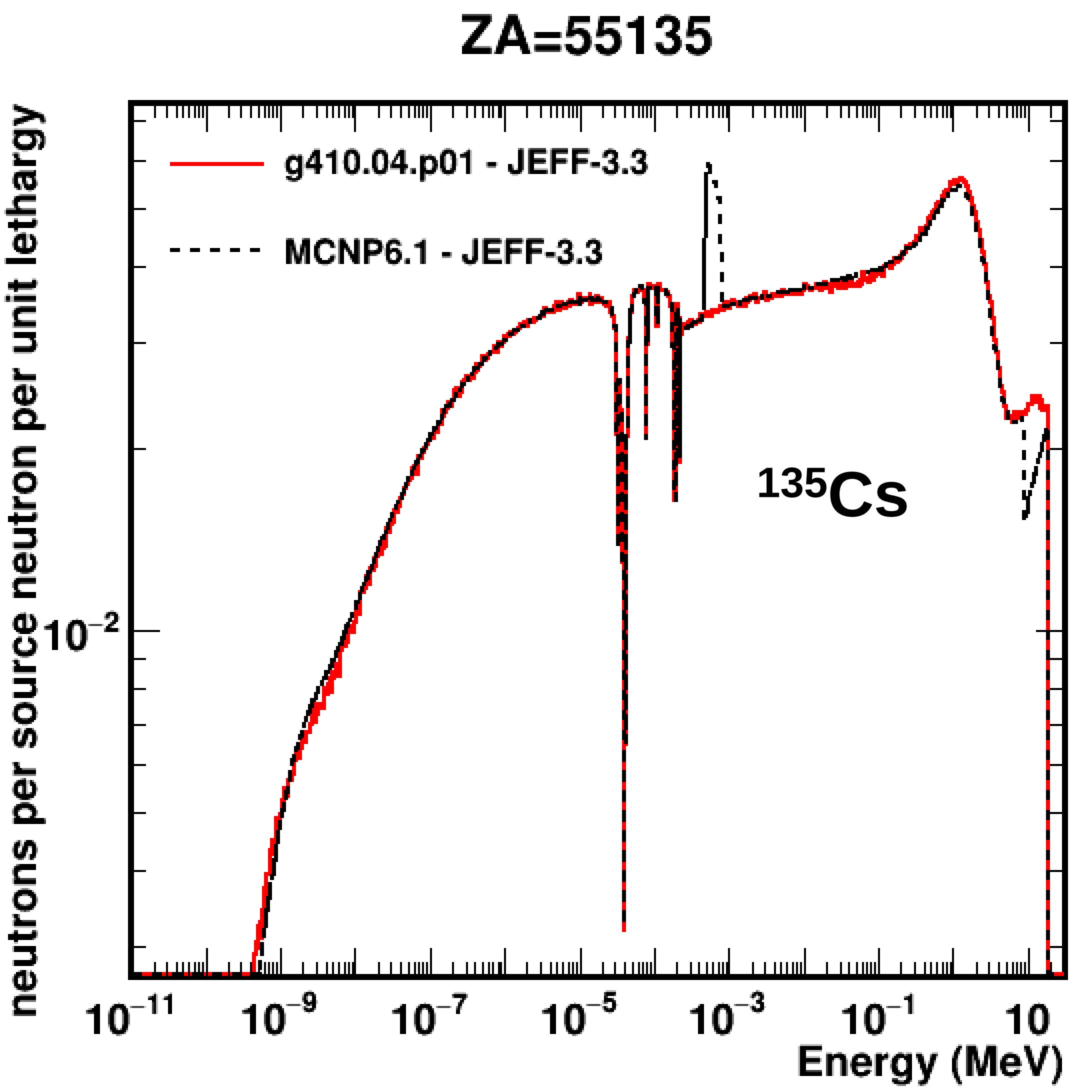
Library	Total number of isotopes	Number of isotopes tested	Number of isotopes with $\chi_v^2 > 2$ and $d_2 > 1.5\%$	Fraction of isotopes with $\chi_v^2 > 2$ and $d_2 > 1.5\%$	Number of isotopes with $\chi_v^2 > 2$	Fraction of isotopes with $\chi_v^2 > 2$
JEFF-3.3	**562**	**546**	**34**	**6%**	**51**	**9%**
JEFF-3.2	472	460	52	11%	78	17%
ENDF/B-VIII.0	556	533	84	16%	114	21%
ENDF/B-VII.1	423	411	90	22%	120	29%
BROND-3.1	372	361	64	18%	78	22%
JENDL-4.0u	406	398	58	15%	87	22%

JEFF-3.3 isotopes with $\chi^2_v > 2$ and $d_2 > 1.5\%$

ZA	$d_1(\%)$	$d_2(\%)$	χ^2_v
46107	1.22	1.64	2.41
53131	1.30	1.81	2.80
55135	4.04	6.98	122
56130	1.16	1.80	2.05
56132	1.18	1.89	2.39
56134	1.14	1.70	2.23
56135	1.24	1.95	2.62
56136	1.14	1.69	2.60
56137	1.10	1.75	2.34
56138	1.13	1.64	2.88
59143	1.26	1.61	3.13
61147	1.55	2.48	3.94
61148	2.36	3.22	6.18
63151	2.18	2.63	3.68
63154	1.97	1.58	2.19
91231	2.00	2.26	4.11
91232	1.76	1.56	5.94

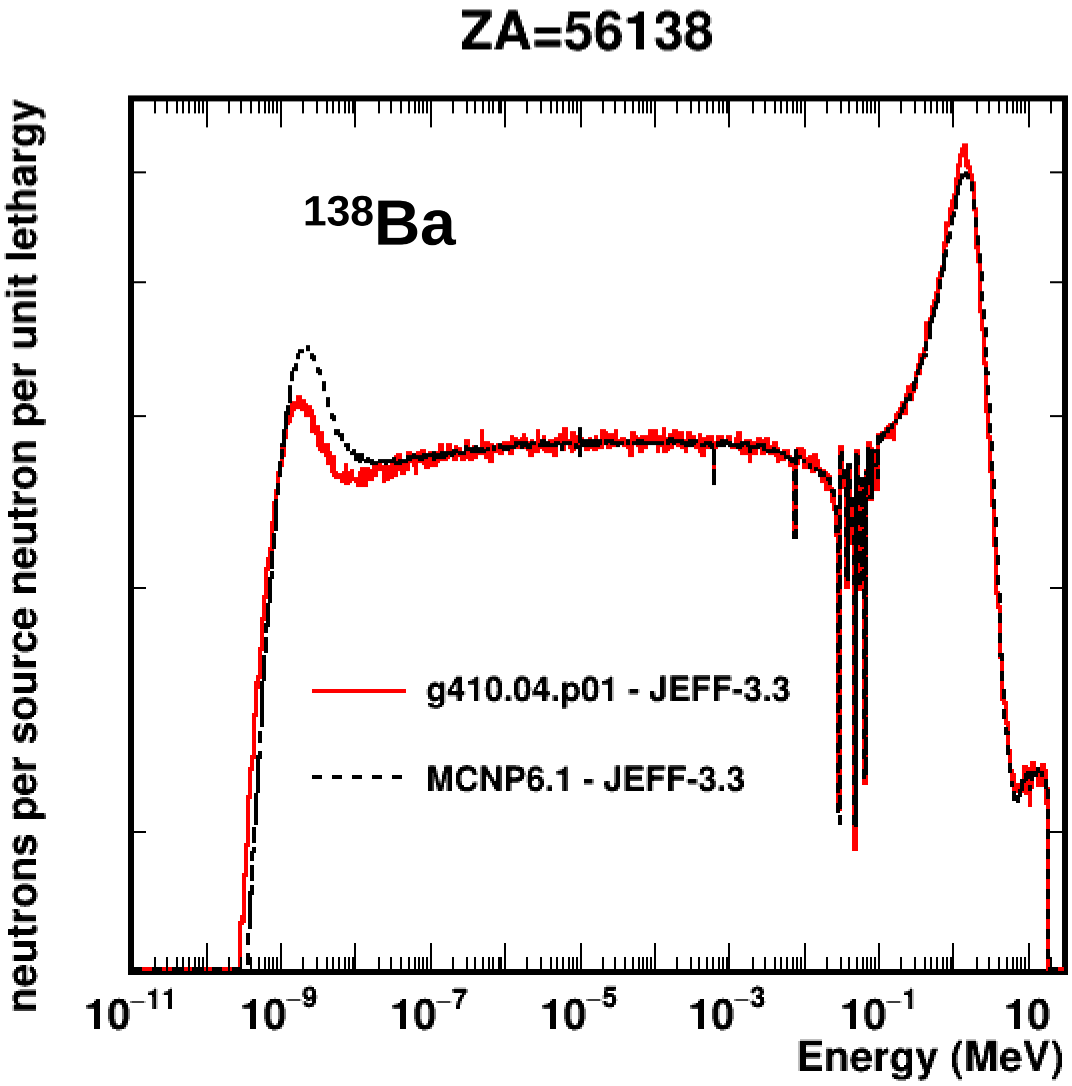
ZA	$d_1(\%)$	$d_2(\%)$	χ^2_v
92232	1.49	1.51	5.28
92233	2.77	3.56	51.7
93236	1.95	1.56	7.32
94236	1.90	1.76	9.18
94241	1.73	1.55	7.29
95242	2.18	1.79	18.3
95244	1.73	1.58	6.72
96241	1.83	1.73	10.3
96242	1.62	2.07	7.55
96243	3.29	3.67	64.5
96245	2.81	3.74	72.4
96247	1.87	1.62	8.85
96249	1.72	1.68	8.92
98249	1.74	1.67	9.87
98253	1.87	1.59	9.27
99254	2.29	1.73	12.1
100255	2.17	1.76	12.8

Energies of the secondary neutrons



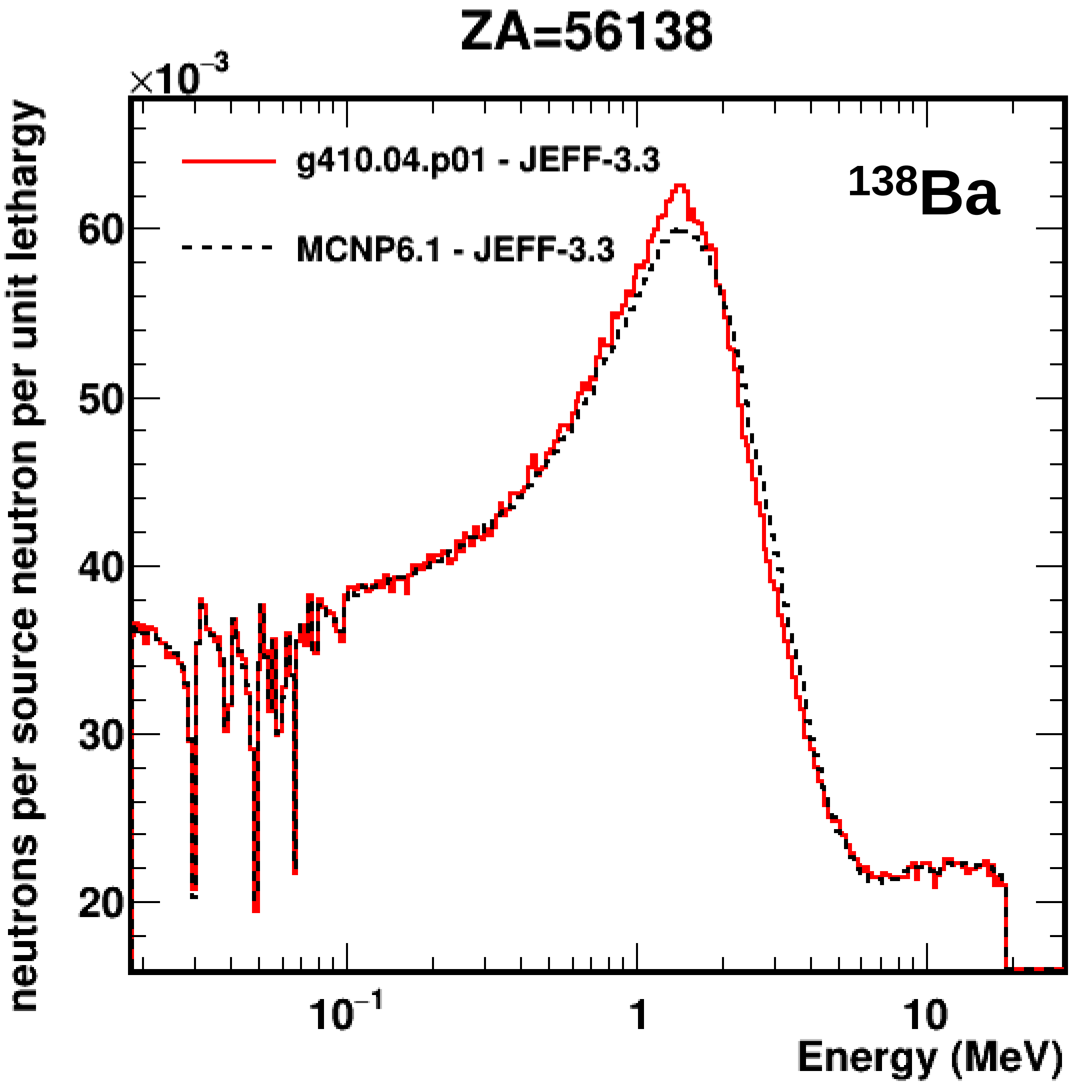
$d_1 = 4.0\%$
$d_2 = 7.0\%$
$\chi^2_v = 122$

Energies of the secondary neutrons



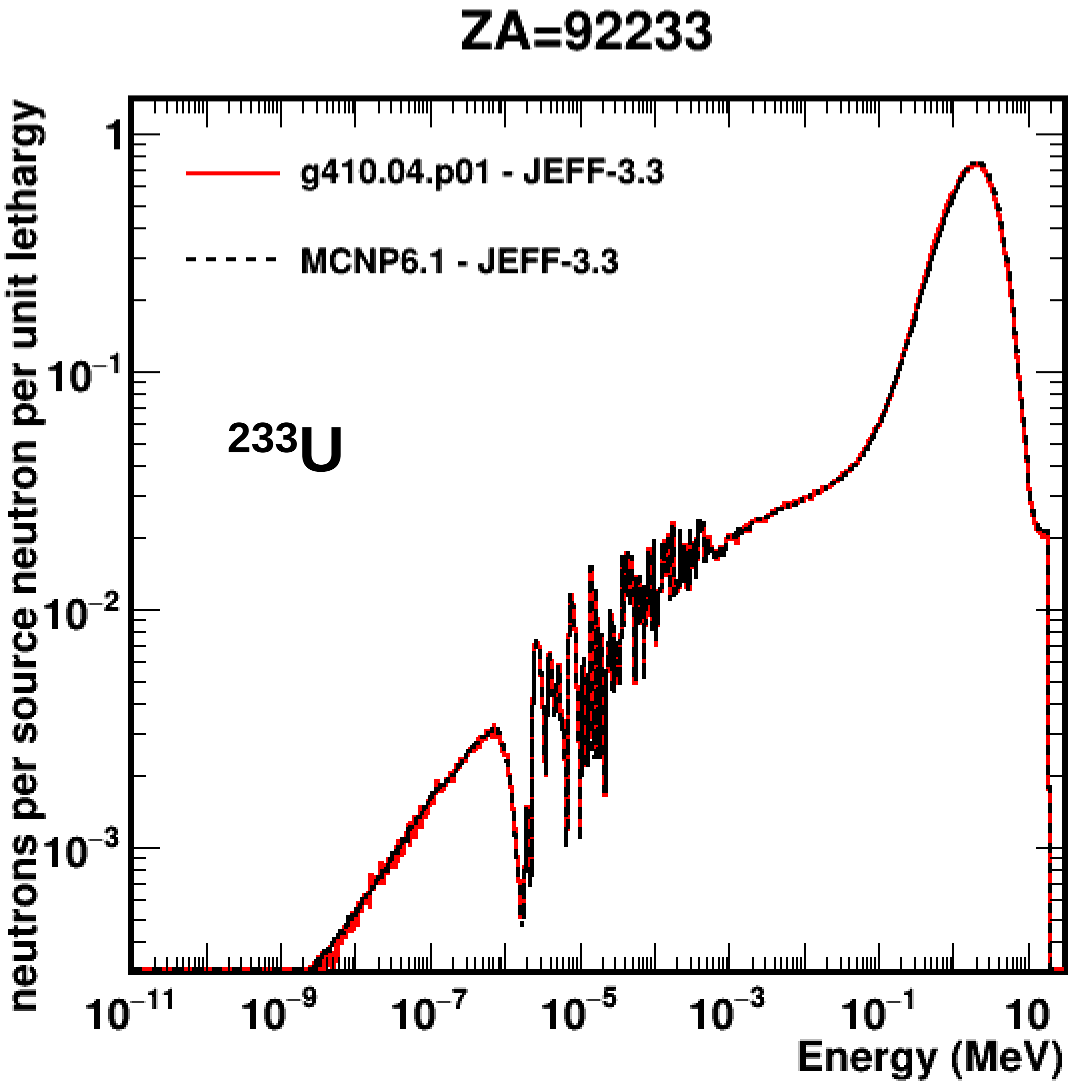
$$d_1 = 1.1\%$$
$$d_2 = 1.6\%$$
$$\chi_v^2 = 2.9$$

Energies of the secondary neutrons



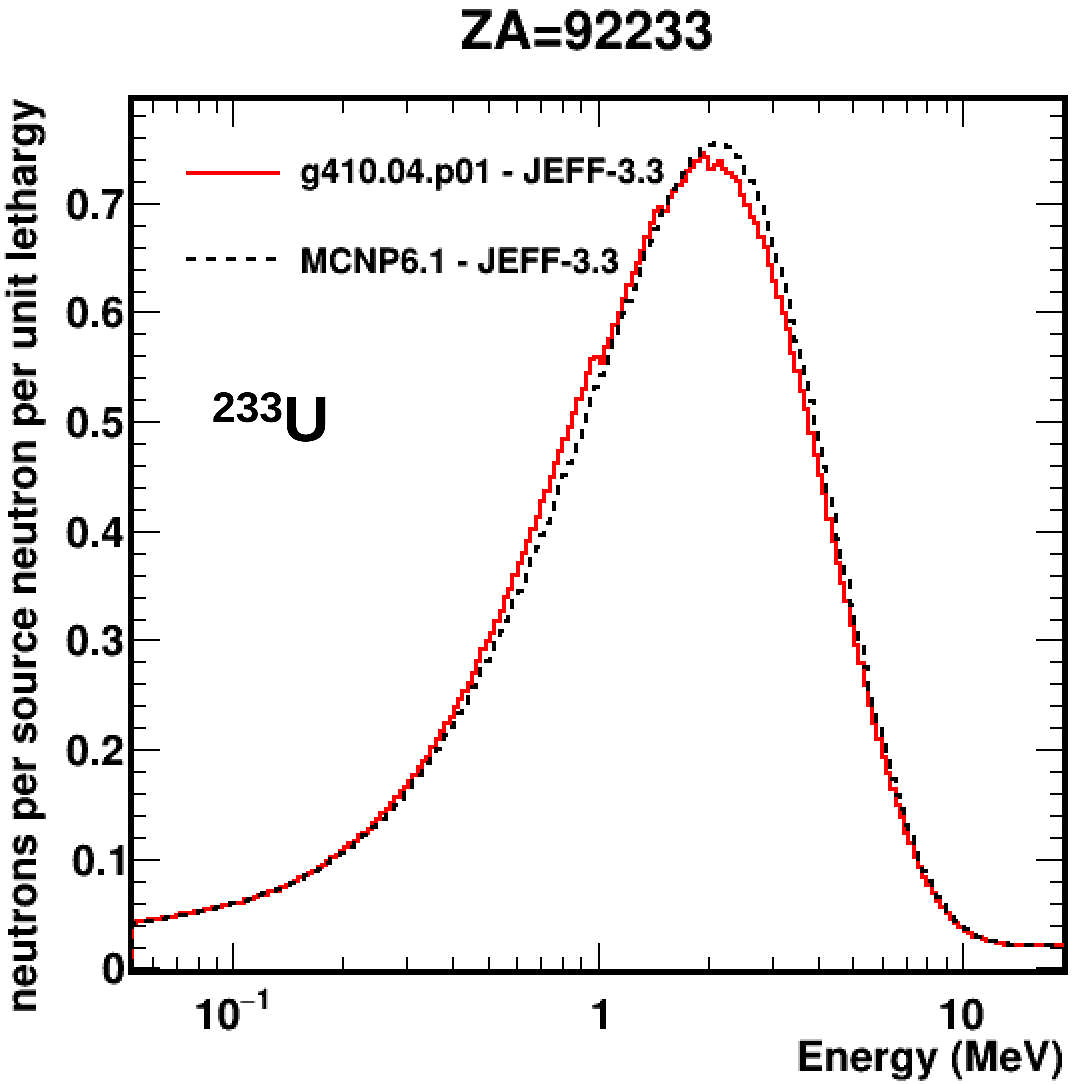
$d_1 = 1.1\%$
$d_2 = 1.6\%$
$\chi_v^2 = 2.9$

Energies of the secondary neutrons



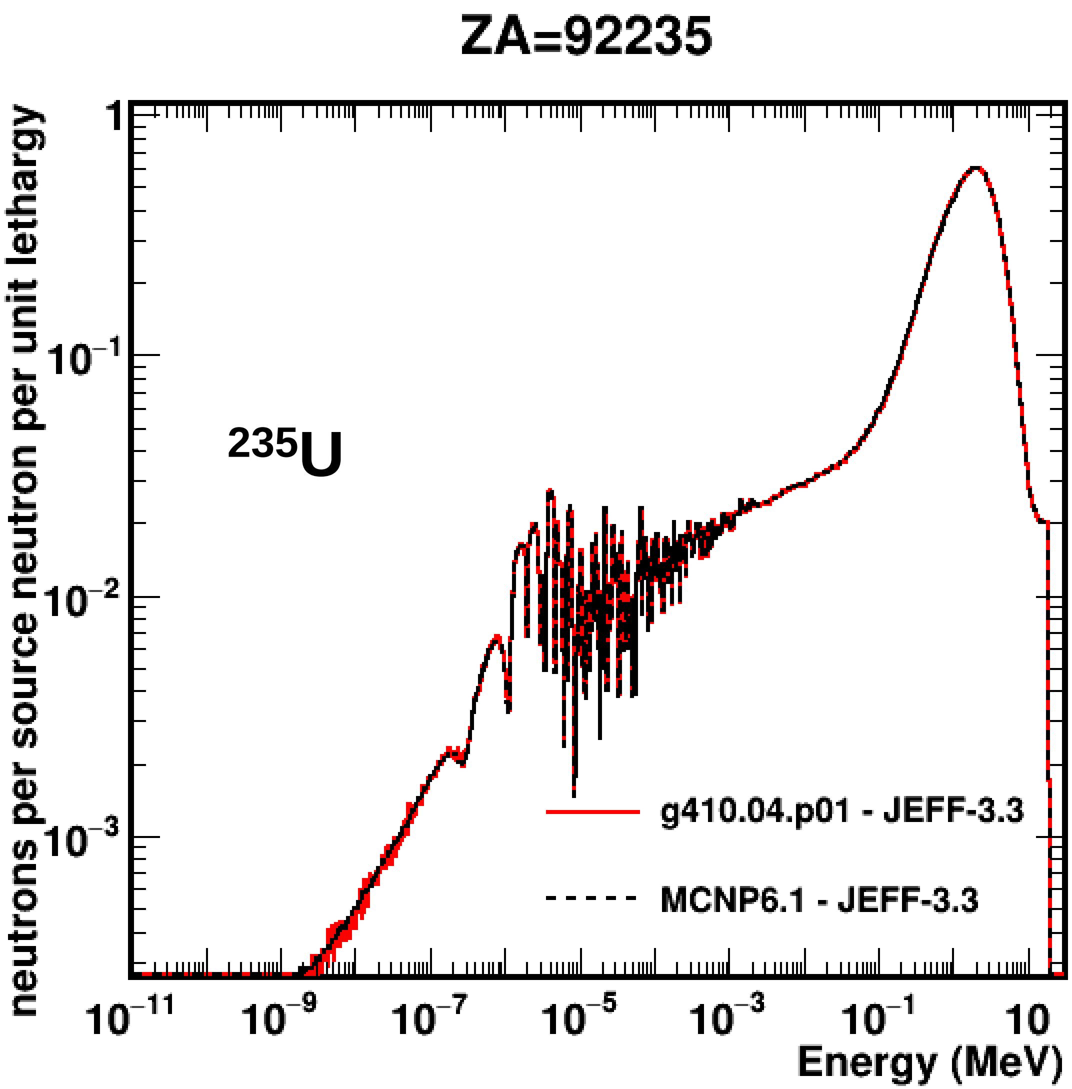
$d_1 = 2.8\%$
$d_2 = 3.6\%$
$\chi_v^2 = 52$

Energies of the secondary neutrons



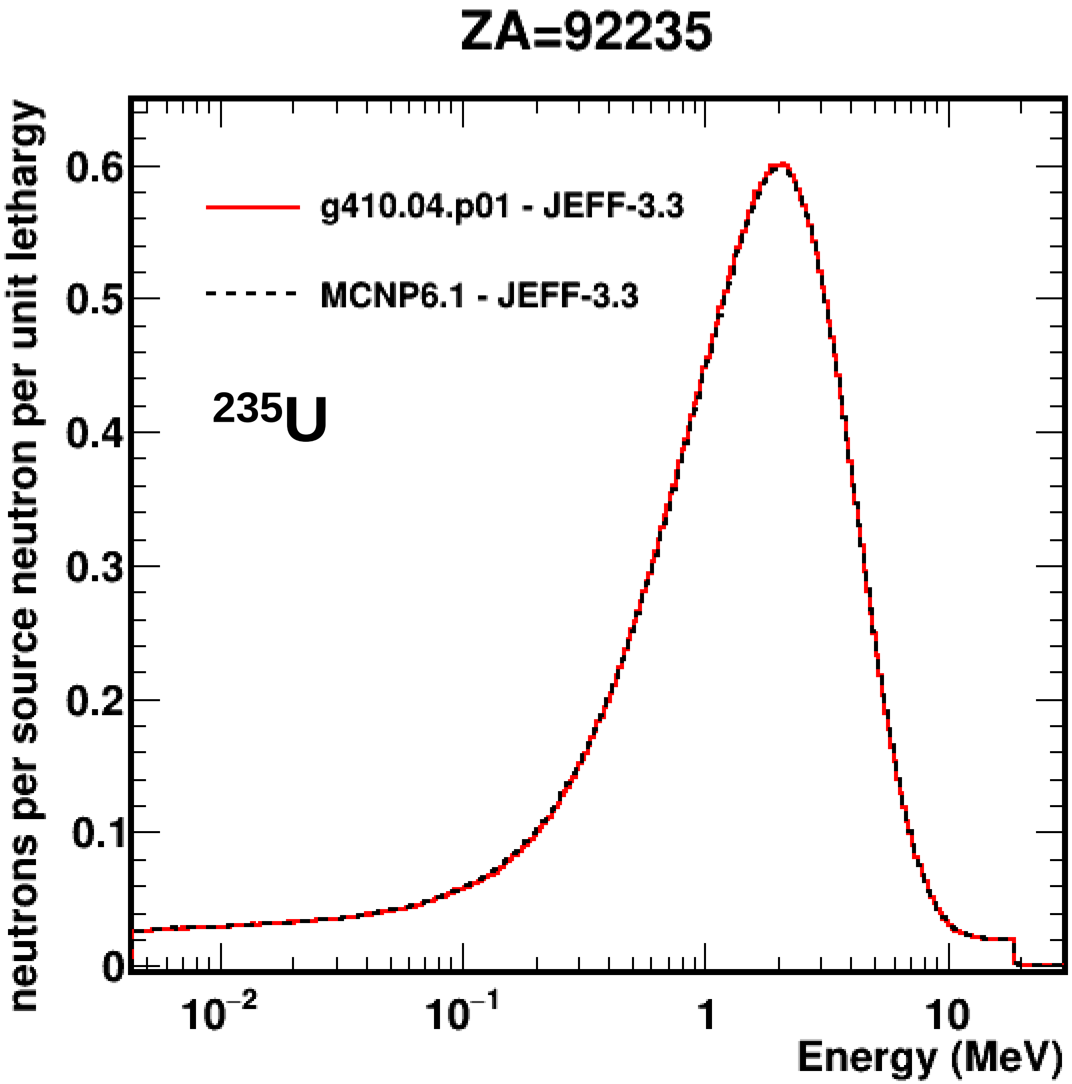
$d_1 = 2.8\%$
$d_2 = 3.6\%$
$\chi^2_\upsilon = 52$

Energies of the secondary neutrons



$d_1 = 1.8\%$
$d_2 = 1.1\%$
$\chi^2_v = 3.2$

Energies of the secondary neutrons



$d_1 = 1.8\%$
$d_2 = 1.1\%$
$\chi^2_v = 3.2$

Energies of the secondary γ-rays, p, d, t, ^{3}He and α

In this case a systematic comparison between Geant4 and MCNP6 d_1, d_2 and χ_v^2 similar to the one performed to neutrons has not been performed.

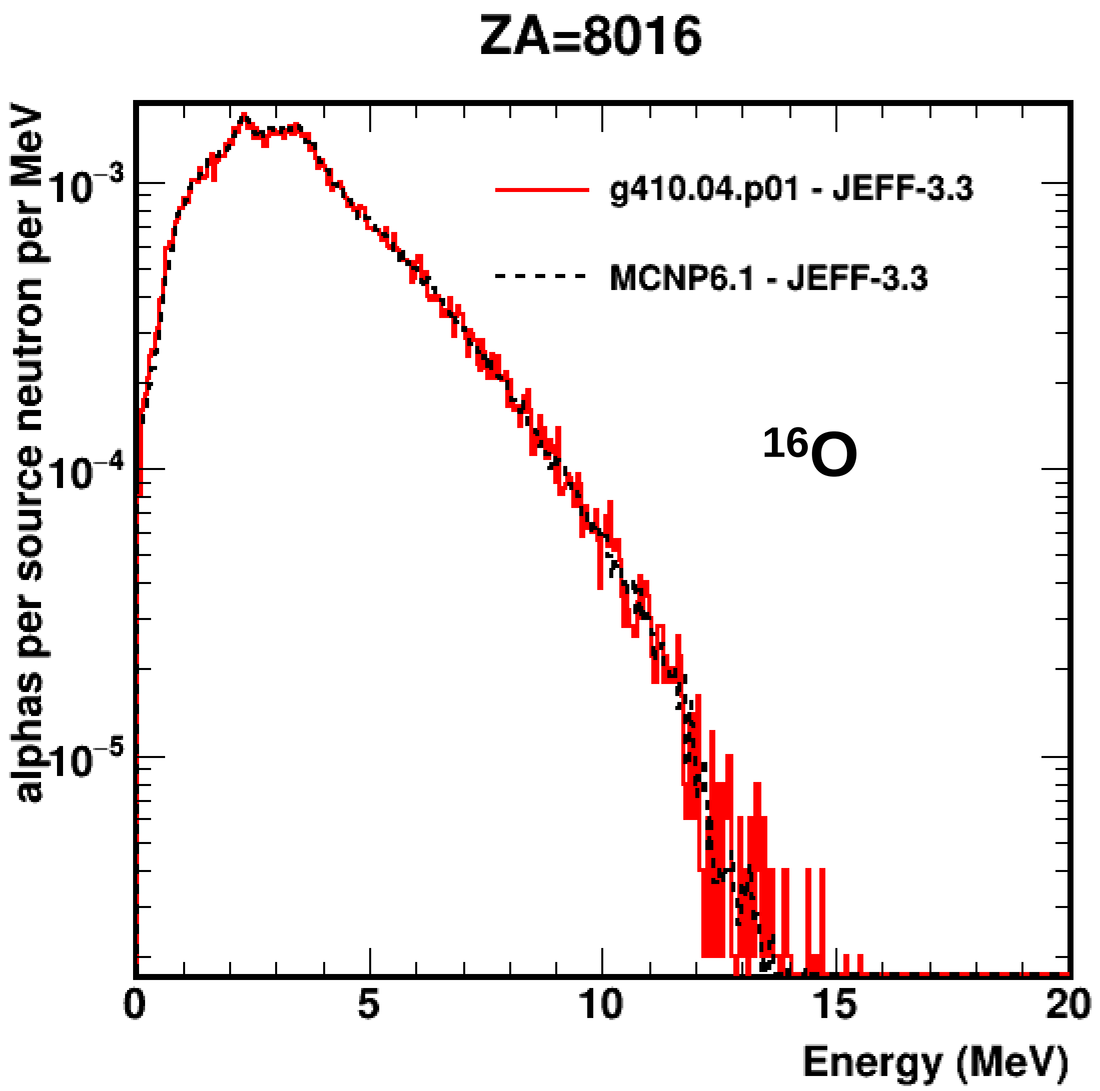
In the ENDF-6 format libraries the energy and angles of the secondary neutrons are always provided, but for the rest of the secondary particles these distributions are sometimes omitted.

If they are omitted then Geant4 will use a model to generate them whereas MCNP6 will not produce them. Thus, results obtained with both codes are more difficult to compare.

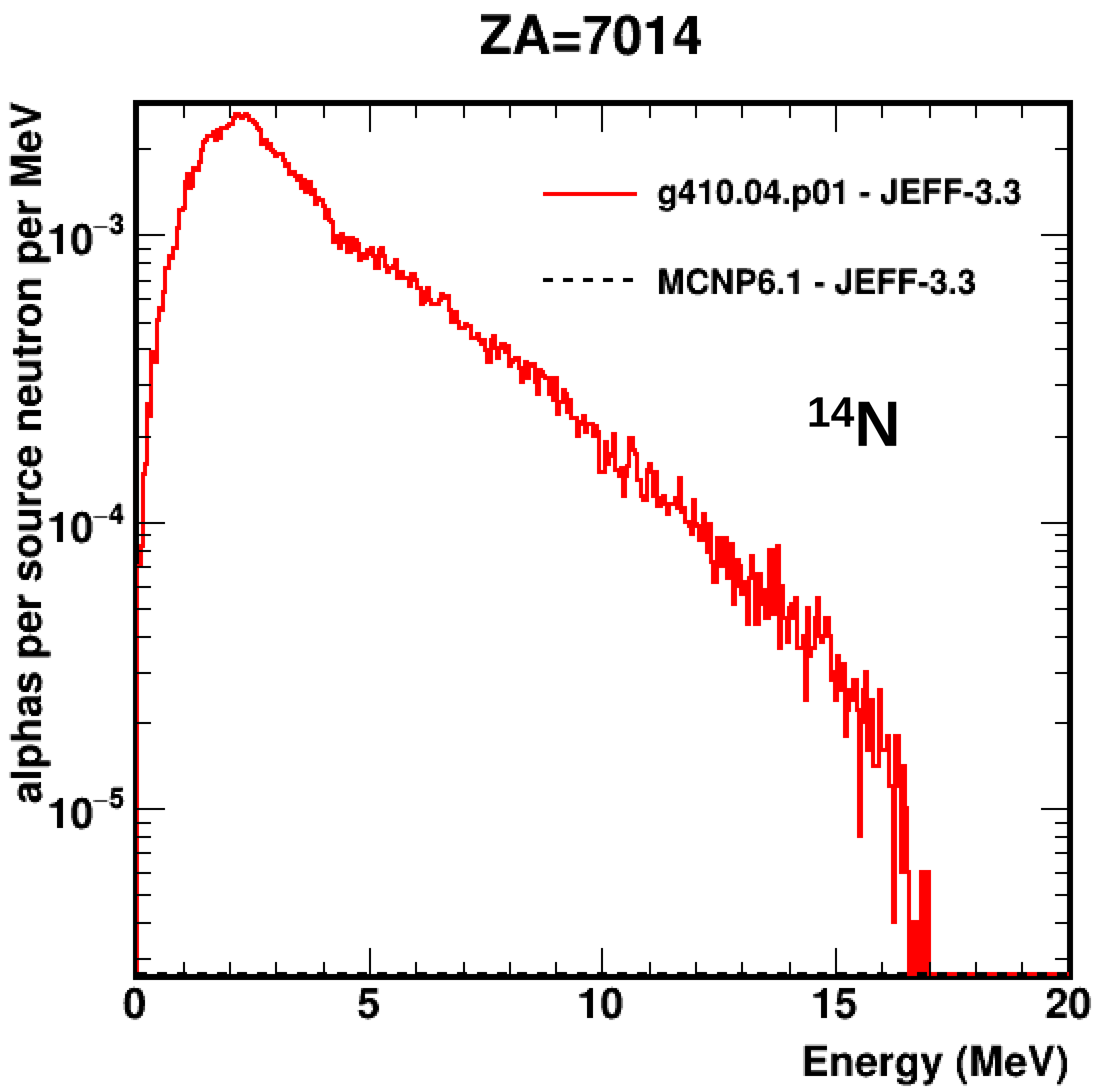
The full set of plots (for all nuclei in all of the six libraries) of the energy distributions integrated over all angles of the secondary neutrons, γ-rays, p, d, t, ^{3}He and α are available from the IAEA nuclear data service together with the libraries.

https://www-nds.iaea.org/geant4/figures/G4_10.04.p01_VS_MCNP6_JEFF33.pdf
https://www-nds.iaea.org/geant4/figures/G4_10.04.p01_VS_MCNP6_ENDF80.pdf
…

Energies of the secondary alphas

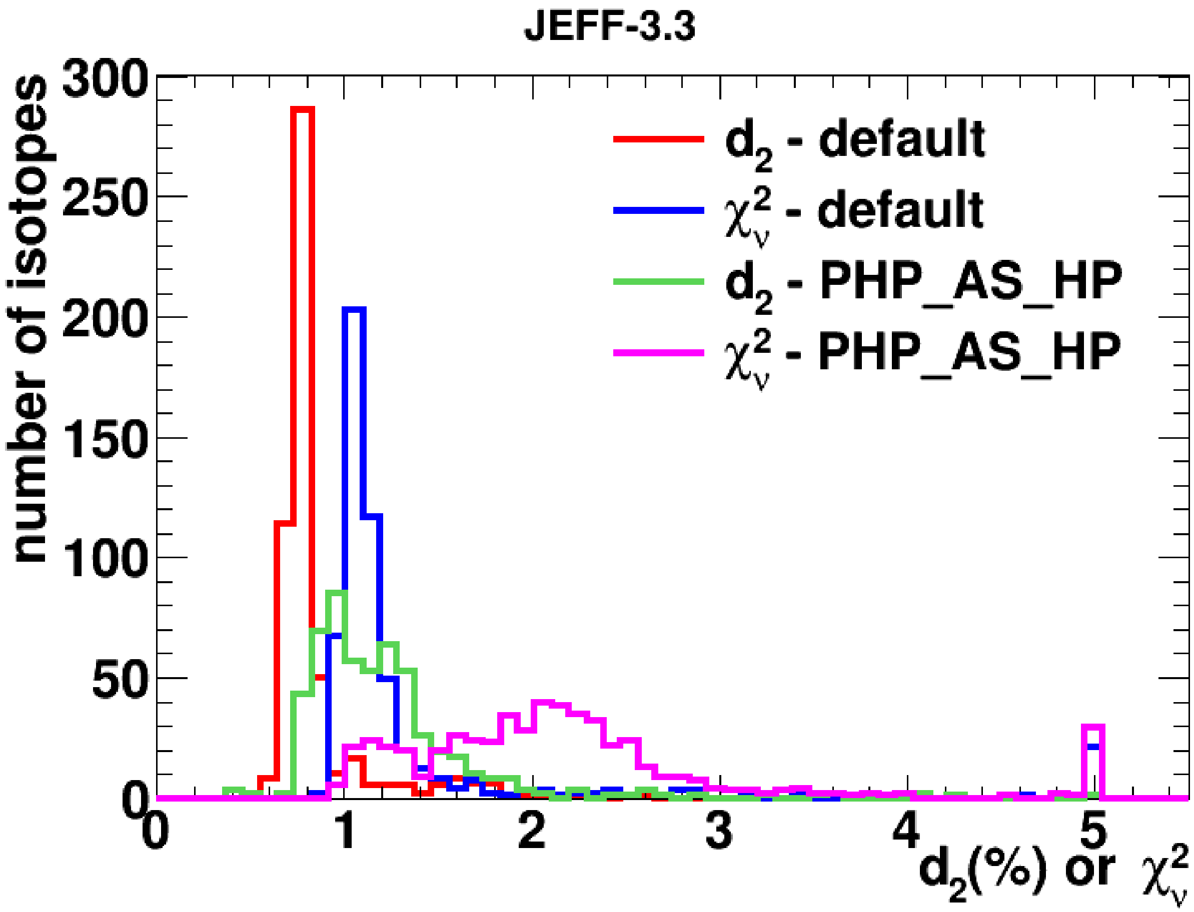


Energies of the secondary alphas



The PHP_AS_HP flag

At compilation time it is possible to define the following flag in Geant4: PHP_AS_HP. If this flag is defined then the sampling procedure to generate secondary particles will be slightly different.



Summary and conclusions

Six new ENDF-6 neutron library releases in G4NDL format are available for download from the IAEA nuclear data service: https://www-nds.iaea.org/geant4/: JEFF-3.3, JEFF-3.2, ENDF/B-VIII.0, ENDF/B-VII.1, BROND-3.1 and JENDL-4.0u (version 2016/1/6).

A comparison between Geant4 and MCNP6 when using these six evaluated libraries has been performed concerning the neutron transport. Some of the differences have been quantified. According to our comparison, JEFF-3.3 is the library that yields more similar results between both codes. A detailed report has been written and will be available from https://www-nds.iaea.org/publications/indc/indc-nds-0758/

A large set of plots containing energy distributions from Geant4 and MCNP6 simulations of the secondary neutrons, γ-rays, p, d, t, ^{3}He and α are available from the IAEA nuclear data service together with the libraries.

Concerning the neutron transport, the default compilation of Geant4 seems to be, in general, better than when compiling with the PHP_AS_HP flag.