SaG4n

Simulation of (α,n) reactions with Geant4

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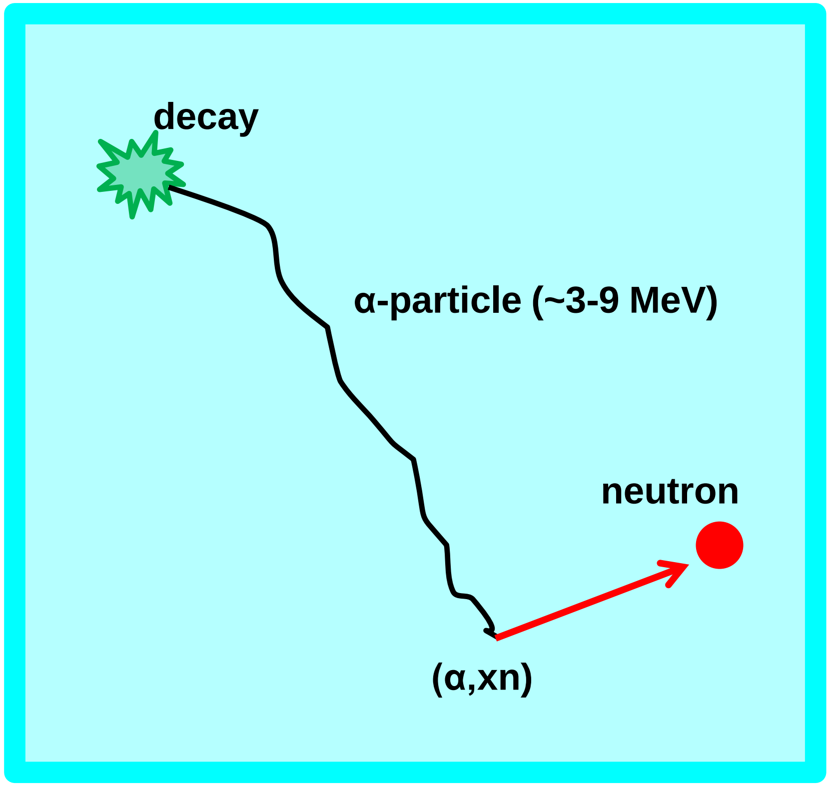
Introduction

Goal: calculate the neutron production due to (α,xn) reactions.



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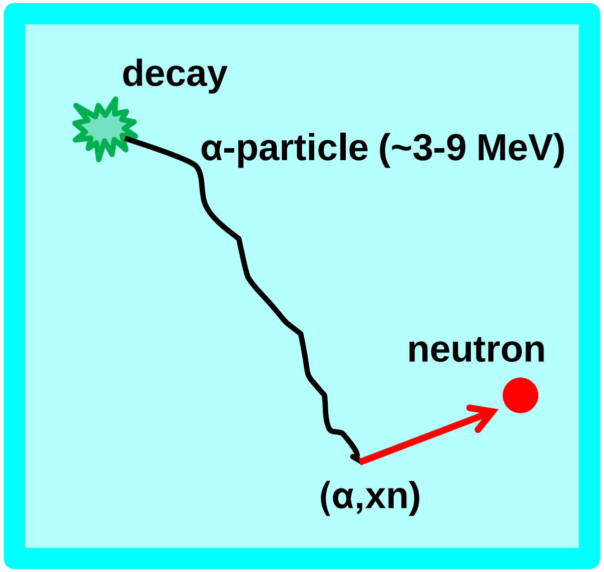

What do we need:

- Material composition
- Activity
- Calculation of the α-tracks → stopping powers.
- (α,xn) cross sections
- Energy distributions of the outgoing neutrons.

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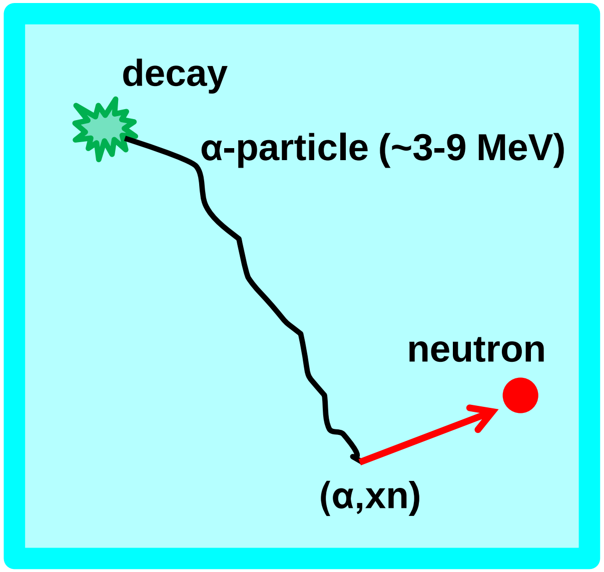

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Simulation code

(other) Simulation codes

The calculation of the neutrons produced in (α,xn) reactions in a certain material require:

- The calculation of the α-tracks → **stopping powers**.
- The **cross sections** of the neutron production reactions involved.
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NeuCBOT	*S. Westerdale et al., NIMA 875, 57 (2017)*
NEDIS	*G. N. Vlaskin et al., Atomic Energy 117, 357 (2015)*
SOURCES	*W. Wilson et al., Progress in Nuclear Energy 51, 608 (2009)*
USD	*D.M. Mei, NIMA 606, 651 (2009)*

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$$Y(E_\alpha) = \int_0^{E_\alpha} \frac{\sigma_{(\alpha,Xn)}(E)}{\varepsilon(E)} dE$$

Stopping cross section

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All these ingredients are present in **Geant4**:

- Slowing down of the alpha particles → EM processes.
- Neutron production cross sections + energy distributions → ParticleHP module, based on ENDF-6 formatted data libraries.
- Particle and process biasing techniques.

(other) Simulation codes

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→ Stopping cross section

What is Geant4?

Geant4 is a general purpose Monte Carlo simulation tool for elementary particles passing through and interacting with matter.

Web: http://geant4.web.cern.ch/ (code, user guides, publications …)

User domains:

- High energy physics
- Nuclear physics
- Space engineering
- Medical applications
- Material science
- Radiation protection
- Security
- …

S. Agostinelli et al., NIMA 506, 250 (2003) → **16840 citations** (Oct-2022)

Why Geant4?

Geant4 operates different than the other codes → Monte Carlo

Pros:

- Complex geometries
- Event generator: γ-rays in coincidence with neutrons (in some cases)
- Same code for generating and for transporting the neutrons

Cons:

- Slow → large CPU times → biasing techniques are needed

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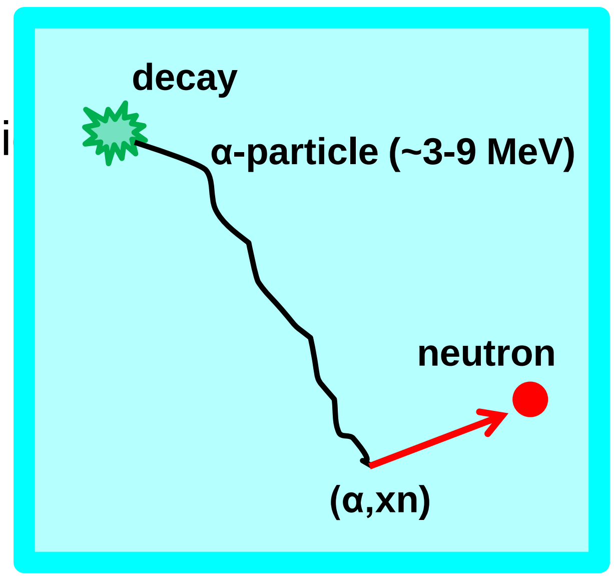

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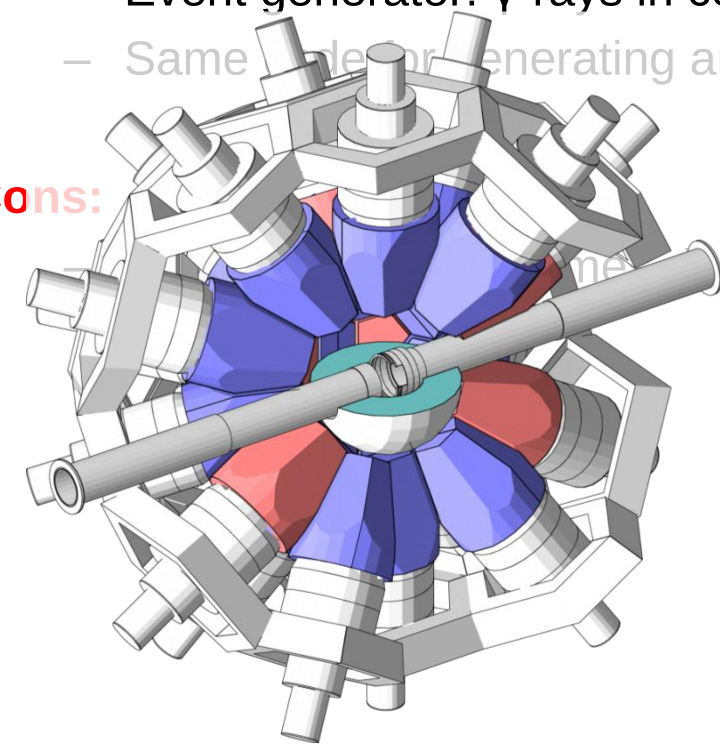
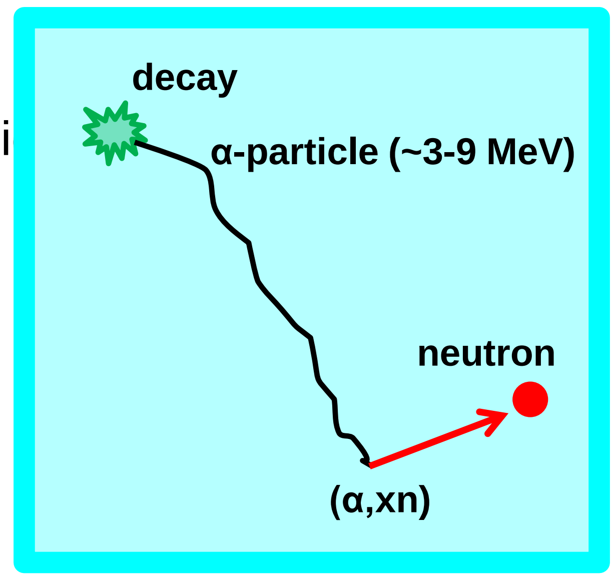




SaG4n

We have created a **Geant4 application** → **SaG4n**, which is a tool to to calculate neutron production due to (α,xn) reactions in different materials. This tool is available at:

http://win.ciemat.es/SaG4n/

There you will find:

- The source code
- Data libraries (x4), needed to run geant4, with XS and FS data from ENDF-6 format data libraries.
- The manual

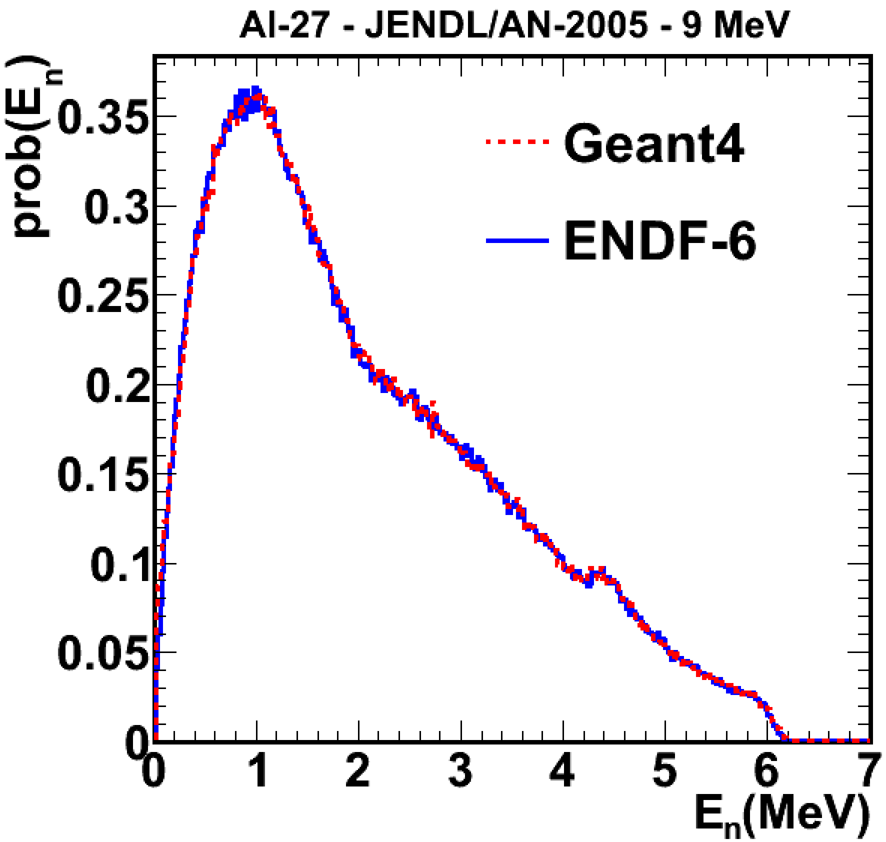
→ **SaG4n** works with an input, i.e. once compiled, SaG4n takes from an input file written by the user all the information necessary to define the geometry of the problem, the source, parameters of the physics, the type of output, etc... → **no Geant4 knowledge is needed**.

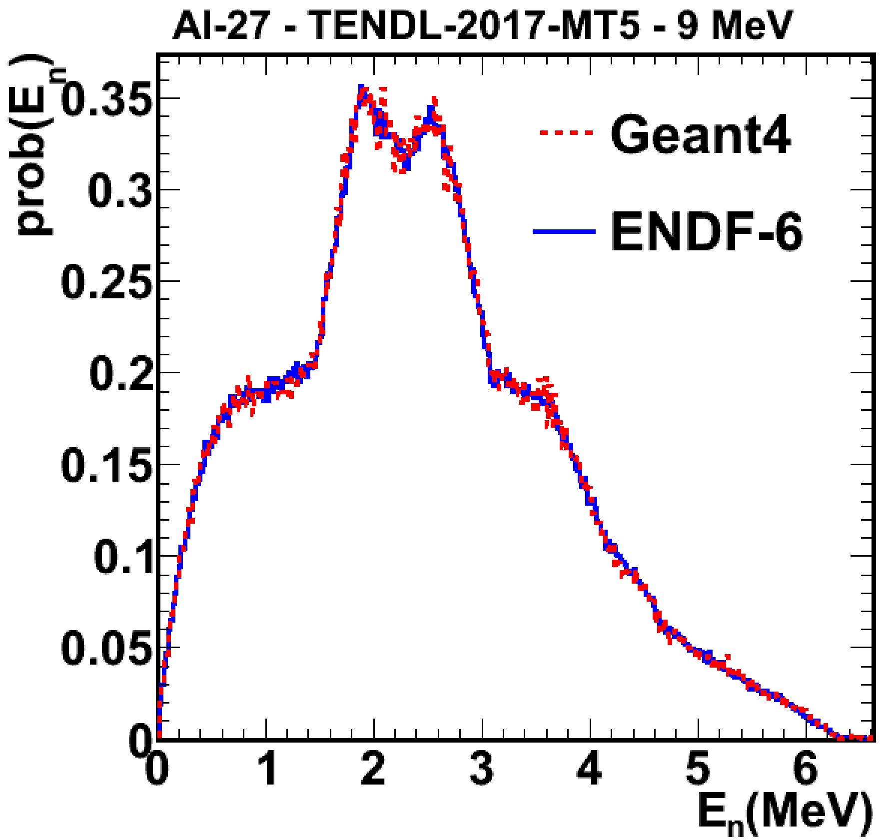
Paper → E. Mendoza et al., *Neutron production induced by α-decay with Geant4*, NIMA 960, 163659 (2020)

- Verification: ParticleHP + biasing
- Studied the existing input data libraries
- Validation and comparison with other codes.

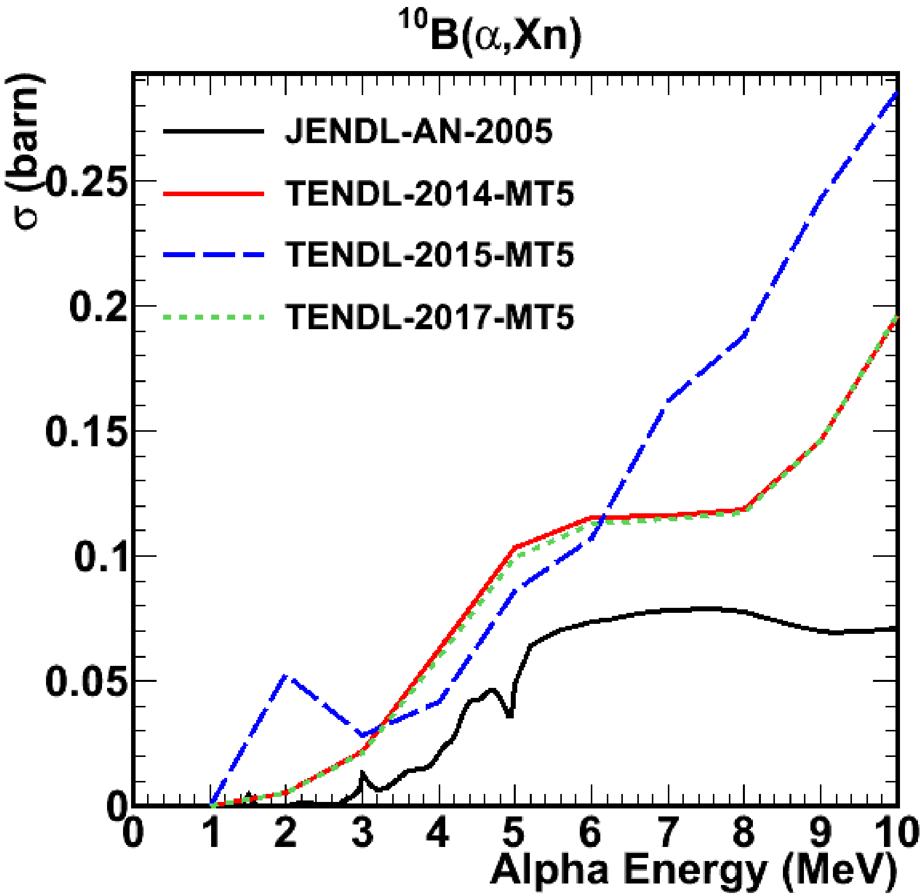
Verification of the neutron energy spectra

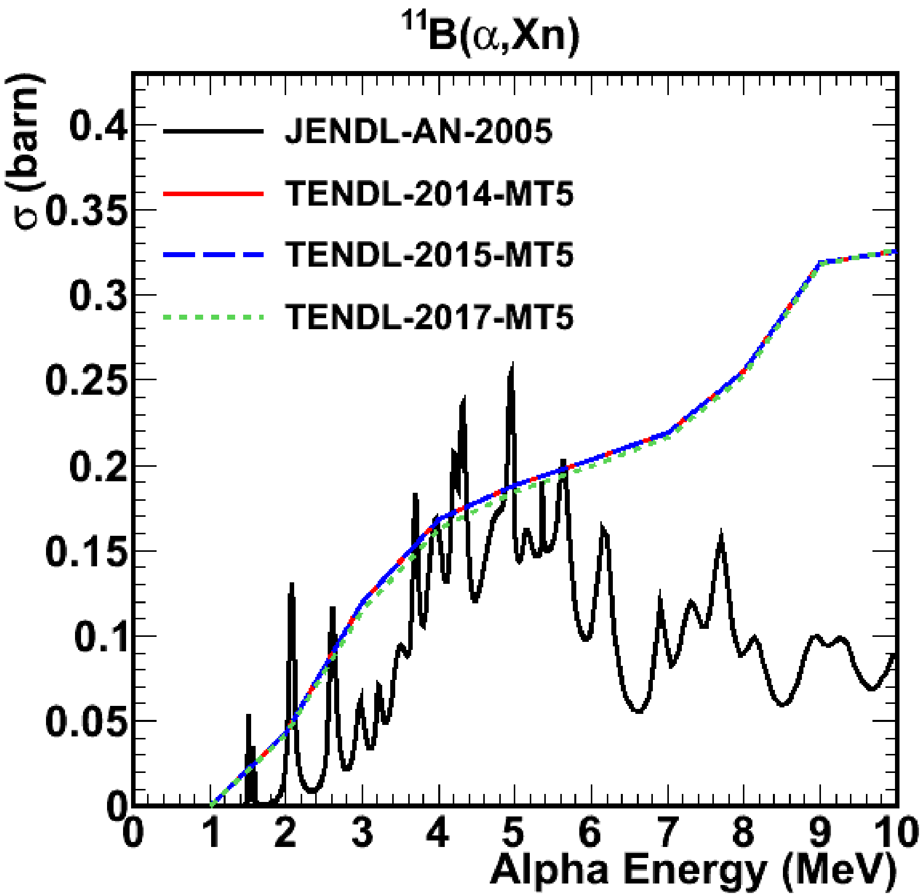
We have compared neutron energy spectra obtained with Geant4 with the data tables inside the ENDF-6 format data libraries.



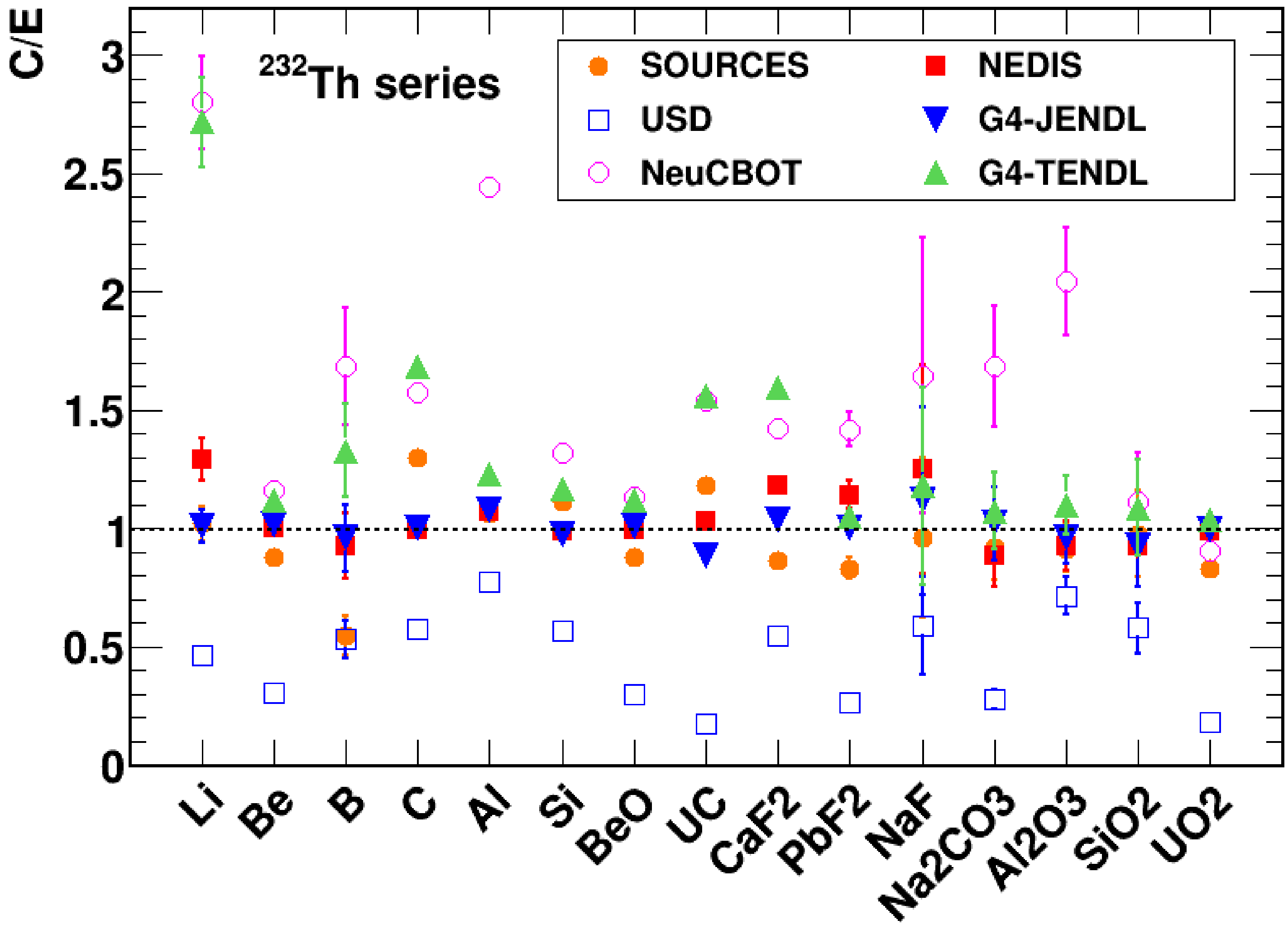


Comparison between data libraries





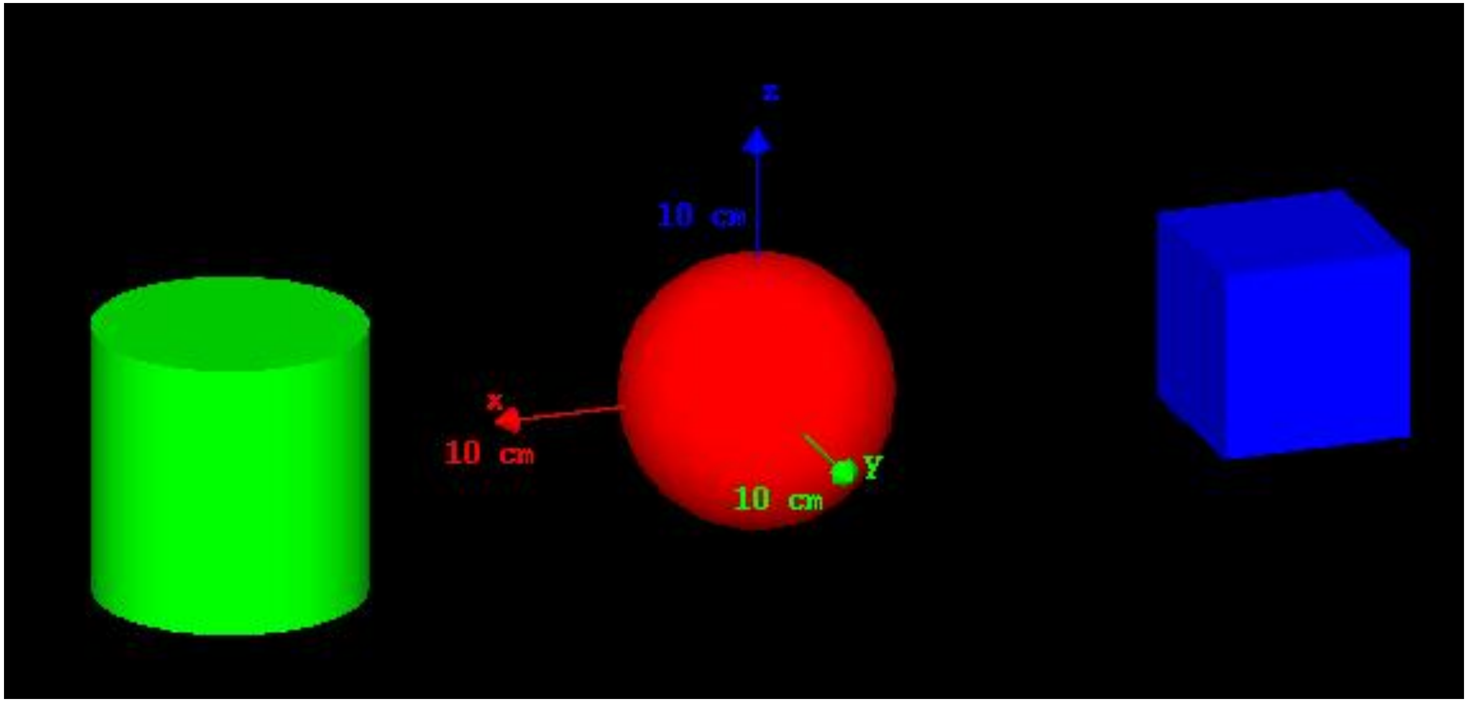
Comparison: neutron yields



Source: [A. C. Fernandes et. al, EPJ Web Conf. 153, 07021 (2017)]

SaG4n input - geometry

```
# VOLUMES:
VOLUME 77 Sphere01      7  1 0 - 5 0 0 0
VOLUME 49 Box01           8  2 0 - 7 7 7  -20 0 0
VOLUME 54 Cylinder01  9  3 0 - 5 10  +20 0 0
```



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```

VolID

VolName

MatID

MotherID

λ_1 λ_2 … $\lambda_{N\lambda}$

VolType

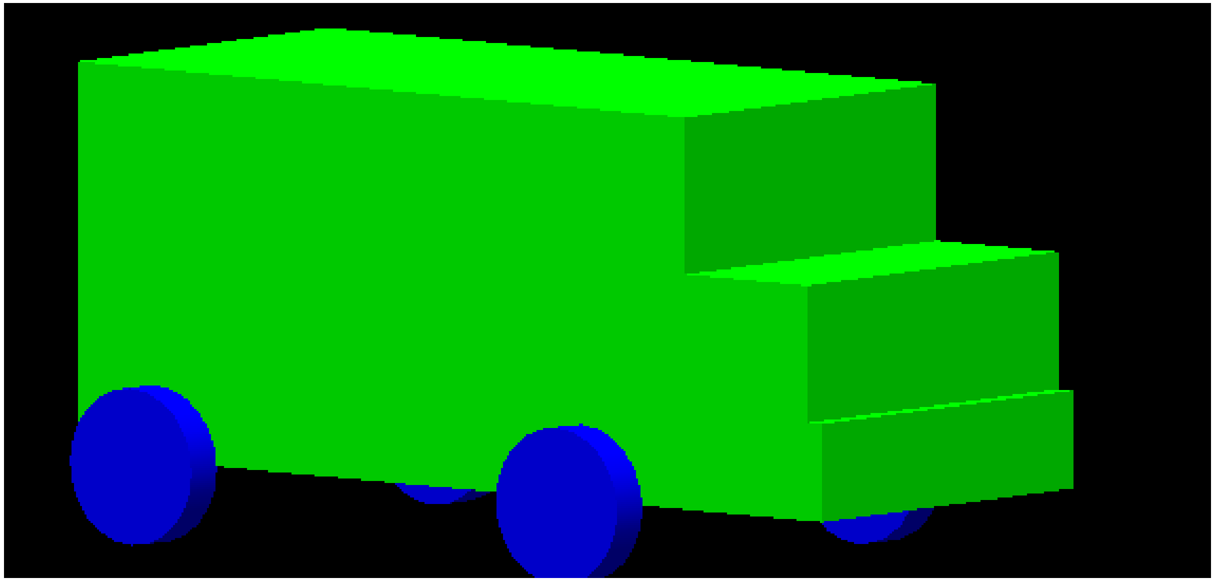
1 – sphere

2 – parallelepiped parallel to the XYZ axis

3 – cylinder parallel to the Z axis

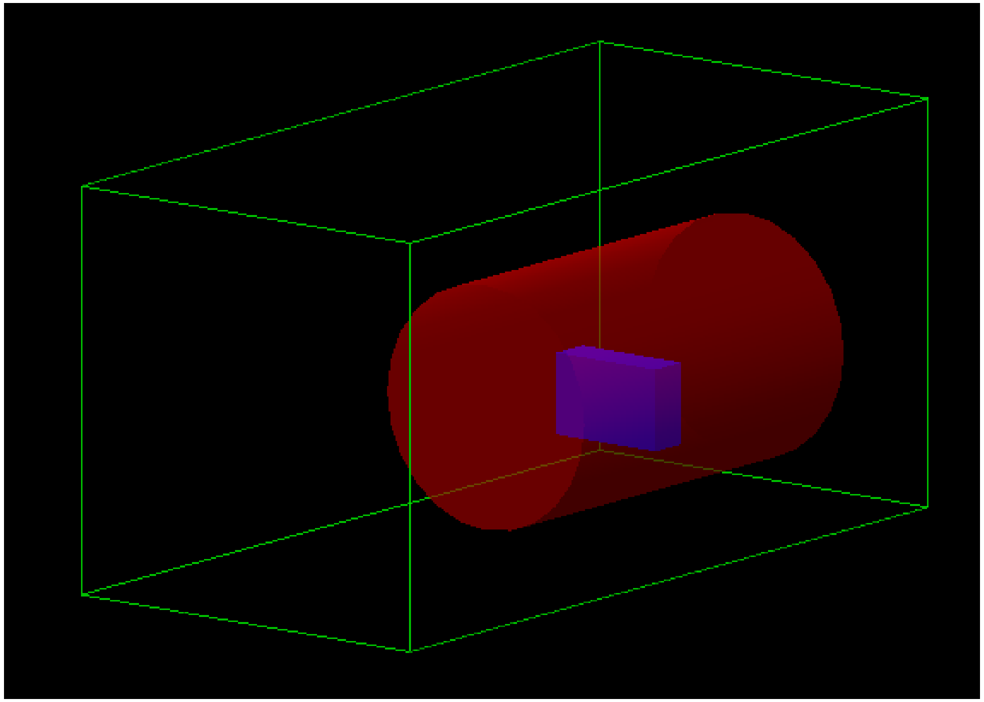
SaG4n input - geometry

```
# VOLUMES:
VOLUME 1 BigBox    7 2 0 - 20 10 10 0 0 0
VOLUME 2 MedBox01 7 2 0 - 4 6 10 12 -2 0
VOLUME 3 MedBox02 7 2 0 - 0.5  2.5 10 14.25  -
3.75 0
VOLUME 4 Wheels01 8 3 0 - 2 1 -7 -5 6
VOLUME 4 Wheels02 8 3 0 - 2 1 +7 -5 6
VOLUME 4 Wheels03 8 3 0 - 2 1 -7 -5 -6
VOLUME 4 Wheels04 8 3 0 - 2 1 +7 -5 -6
```



SaG4n input - geometry

```
# VOLUMES:
VOLUME 12 Box01    7 2 0 - 10 10 20 0 0 0
VOLUME 14 Cylinder01    8 3 12 -  3 10 1 -1 -3
VOLUME 25 Box02    9 2 14 - 3 2 1 0.5 -0.5 0.5
```



SaG4n input - geometry

```
MATERIAL 9 H2O 1.00 5
1001 1.99977
1002 0.00023
8016 0.99757
8017 0.00038
8018 0.00205
ENDMATERIAL

MATERIAL 9 H2O 1.00 2
1 2
8 1
ENDMATERIAL

MATERIAL 9 H2O 1.00 2
1 -11.19
8 -88.81
ENDMATERIAL

MATERIAL 9 G4_WATER 0 -1
```

4 different ways of defining water material

SaG4n input - source

Monoenergetic alphas in some region:

```
SOURCE 3 10 20 +15 0 0
1.00 3
ThreeMeVAlpha 3.00 1.00
FiveMeVAlpha  5.00 1.00
EightMeVAlpha 8.00 1.00
ENDSOURCE
```

Particle beam:

```
SOURCE -1 3 2 1 0 0 1 2 -1
1.00 2
ThreeMeVAlpha 3.00 1.00 0.2
FiveMeVAlpha  5.00 1.00 0.2
ENDSOURCE
```

Decay series in some volume:

```
VOLUME 15 Cylinder01 9 3 0 - 10
20 +15 0 0
SOURCE 0 15
1.00 3
Chain_Th232 0 30.00
Chain_U235  0 50.00
Chain_U238  0 20.00
ENDSOURCE
```

SaG4n input – rest of the input

```
MAXSTEPSIZE 0.00001     # OPTIONAL
BIASFACTOR 100000   # OPTIONAL

NEVENTS 10000000       # OPTIONAL
OUTPUTFILE ./outputs/yields/yield01 # without the extension
OUTPUTTYPE 1 0 #OPTIONAL

# if defined, interactive running mode:
# INTERACTIVE

# if defined, secondary particles are not killed when
created:
# DONOTKILLSECONDARIES

# New seed for the MC (default is 1234567):
SEED 1234567 #OPTIONAL
```

SaG4n - output

Two types of output files:

1 – A **rootfile**, with two histograms per volume:

- One with the energy spectrum of the neutrons generated in the volume.
- Other with the fluence of the source alpha particles in the volume.

2 – A **text file**, with a list of the neutrons and the gamma rays generated in the simulation, together with their position, energy momentum, weight …

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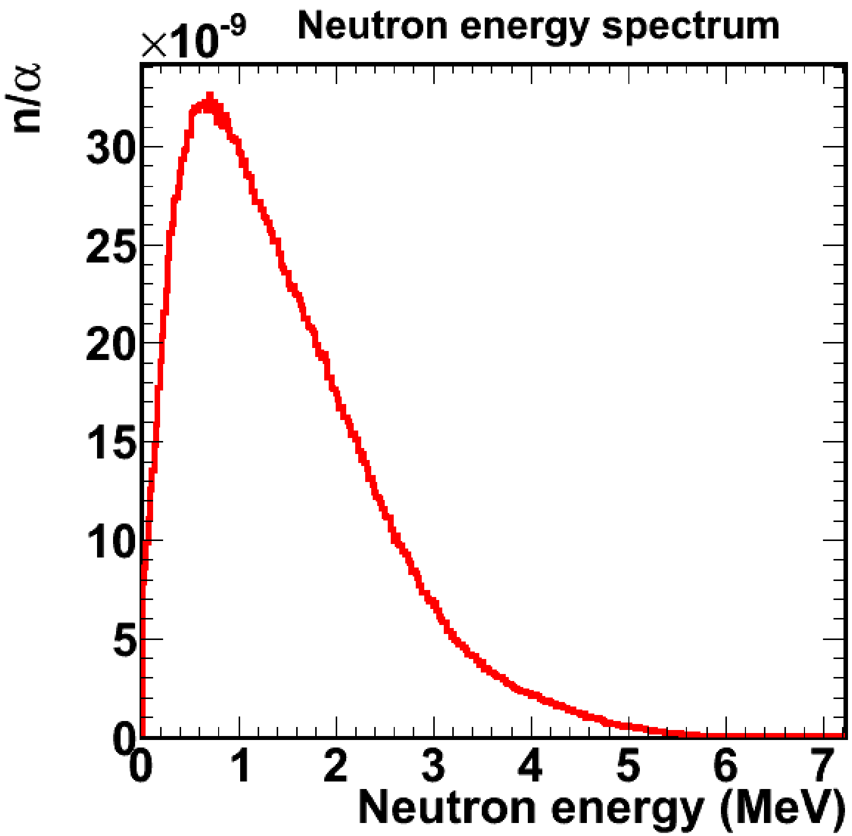

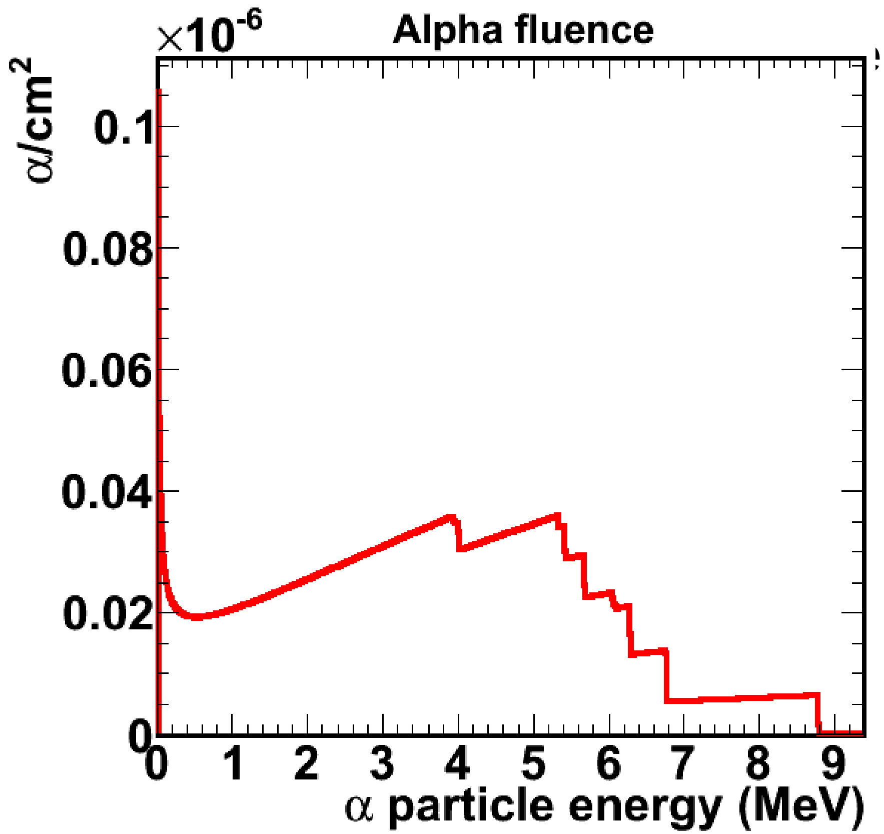

How reliable are the obtained results?

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A few percent differences are expected from here

Main source of uncertainty comes from here

$$Y(E_\alpha) = \int_0^{E_\alpha} \frac{\sigma_{(\alpha,Xn)}(E)}{\varepsilon(E)}\, dE$$

Stopping cross section

ENDF-6 format libraries

The ENDF-6 α-incident data libraries available are:

JENDL-AN-2005: this is an *evaluated* library (experimental data + theoretical calculations). There are only a few isotopes: ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{12,13}C, ^{14,15}N, ^{17,18}O, ^{19}F, ^{23}Na, ^{27}Al, ^{28,29,30}Si.

TENDL libraries: they have been made with the results of the TALYS code. We have performed calculations with TENDL-2014, TENDL-2015 and TENDL-2017 (there is no TENDL-2016). They contain a large amount of isotopes.

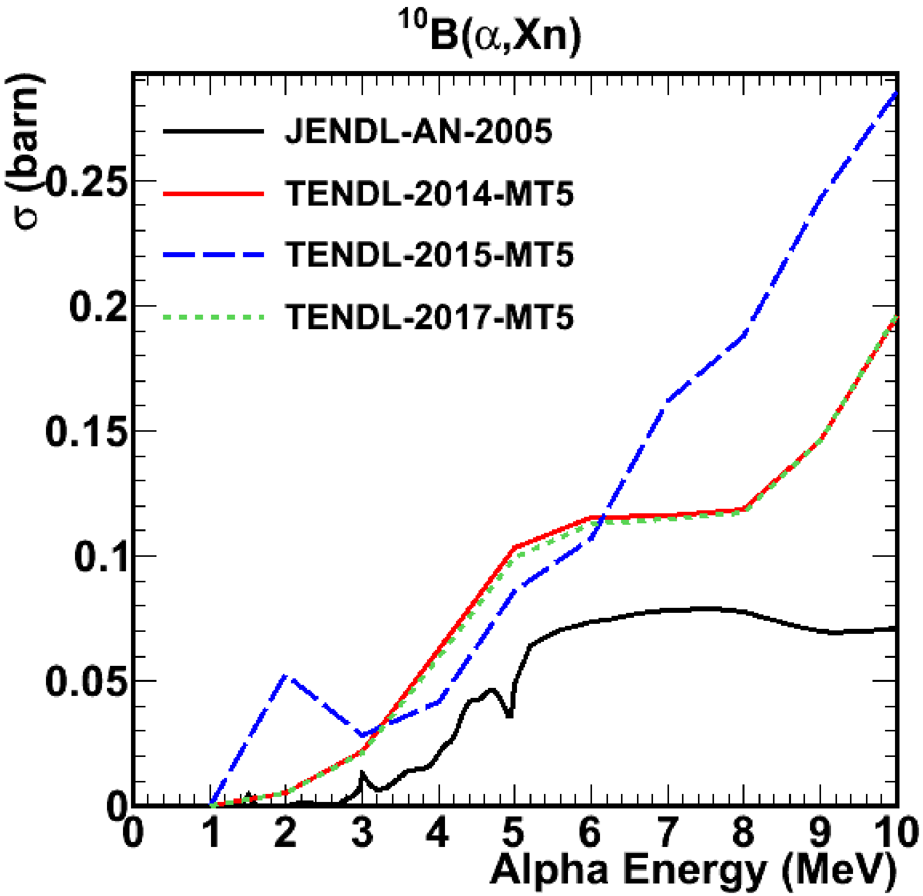
Conclusions from the comparison study:

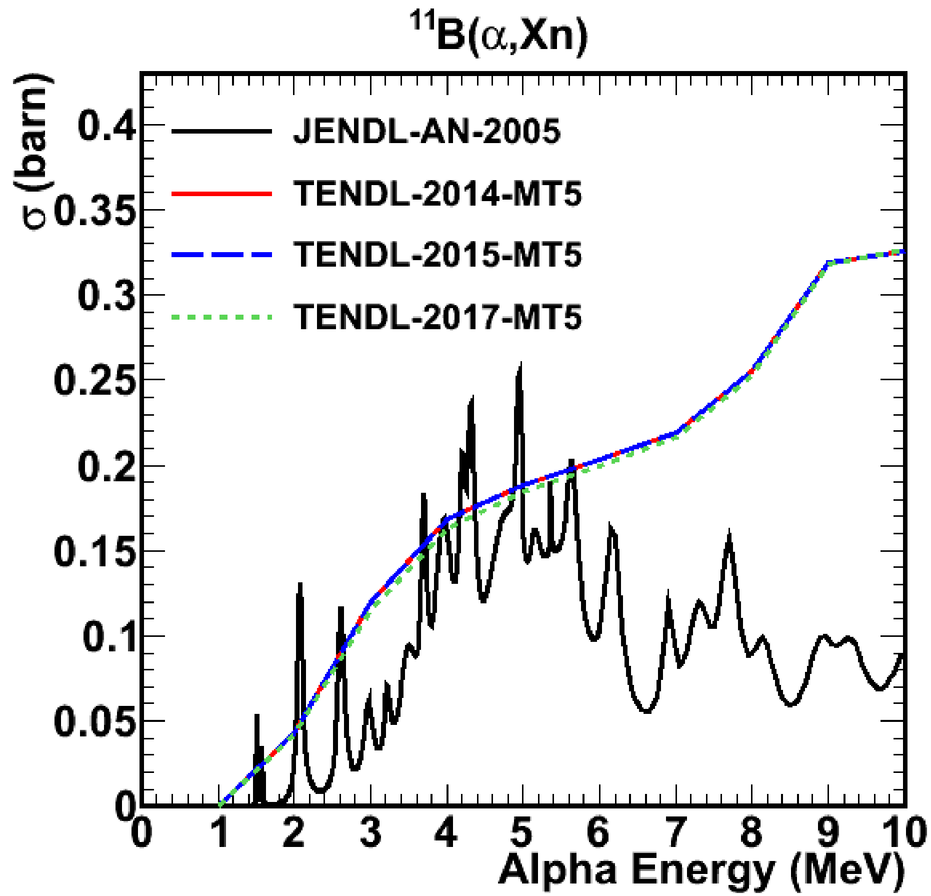
1- The different versions of the TENDL libraries do not differ so much.

2- The neutron production in TENDL is higher than in JENDL in most of the cases.

3- The neutron energy spectra from JENDL seem to underestimate the energy of the produced neutrons.

Comparison between JENDL-AN-2005 and TENDL-MT5





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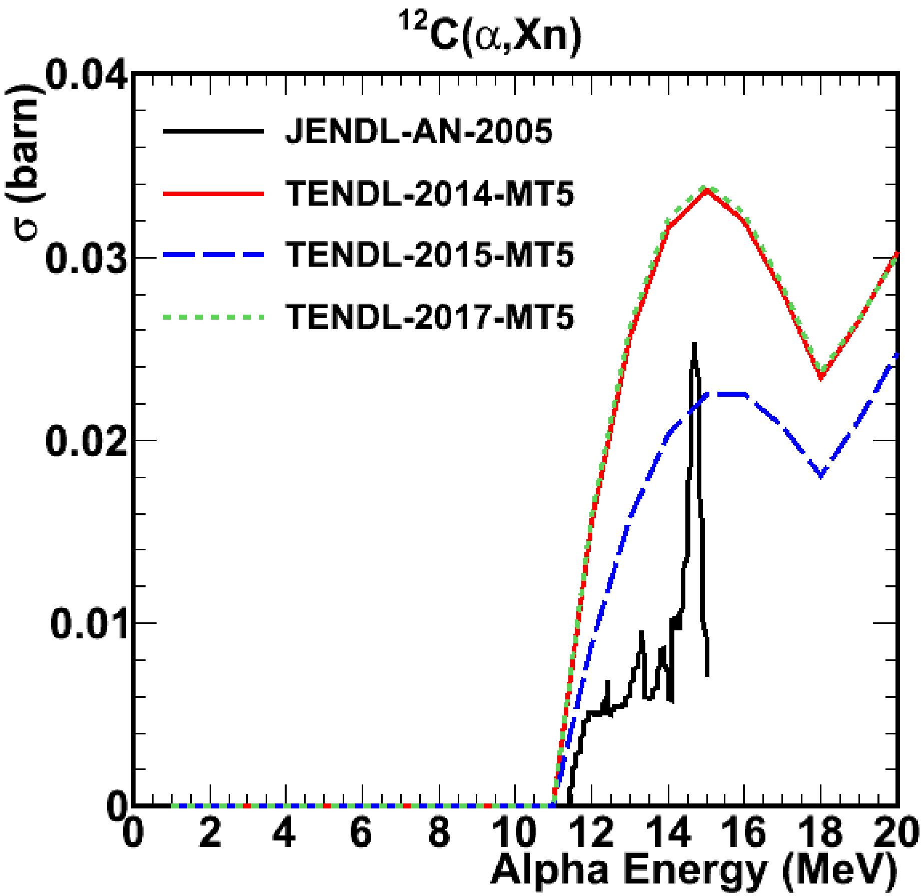

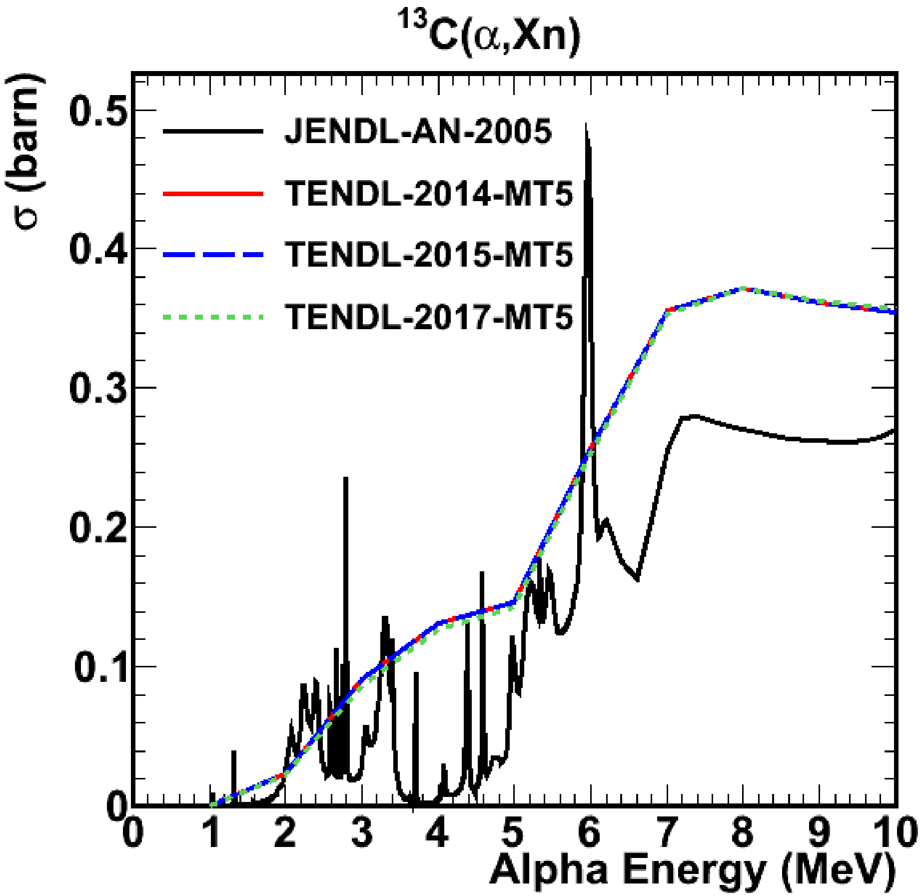

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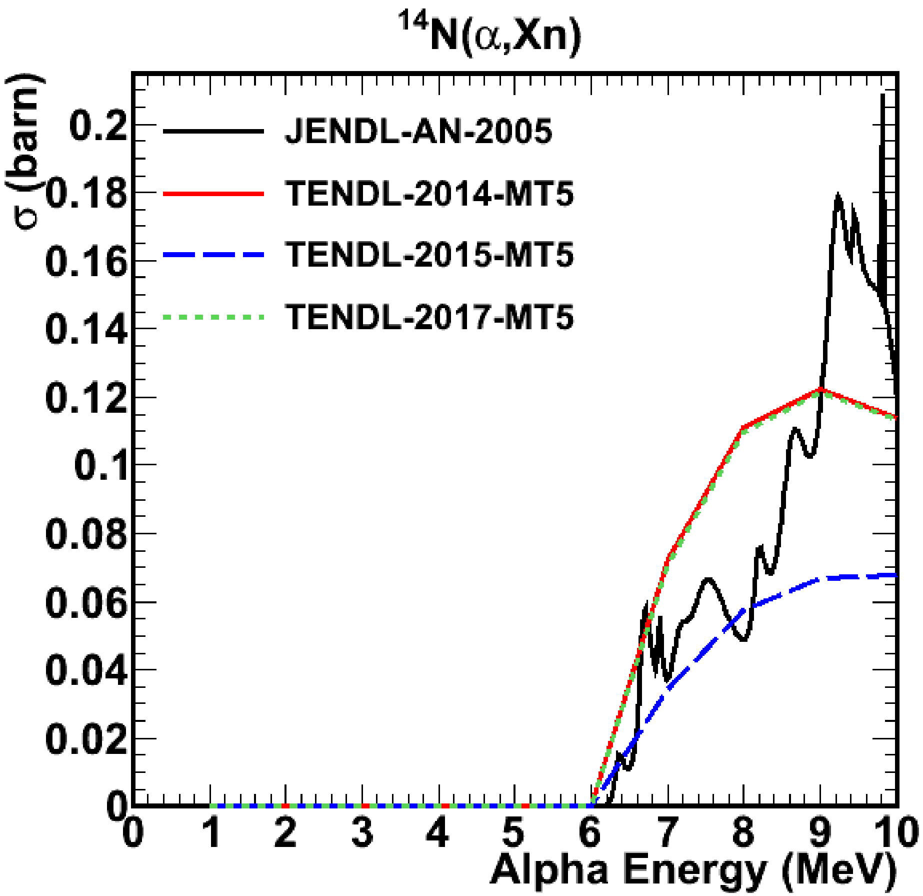

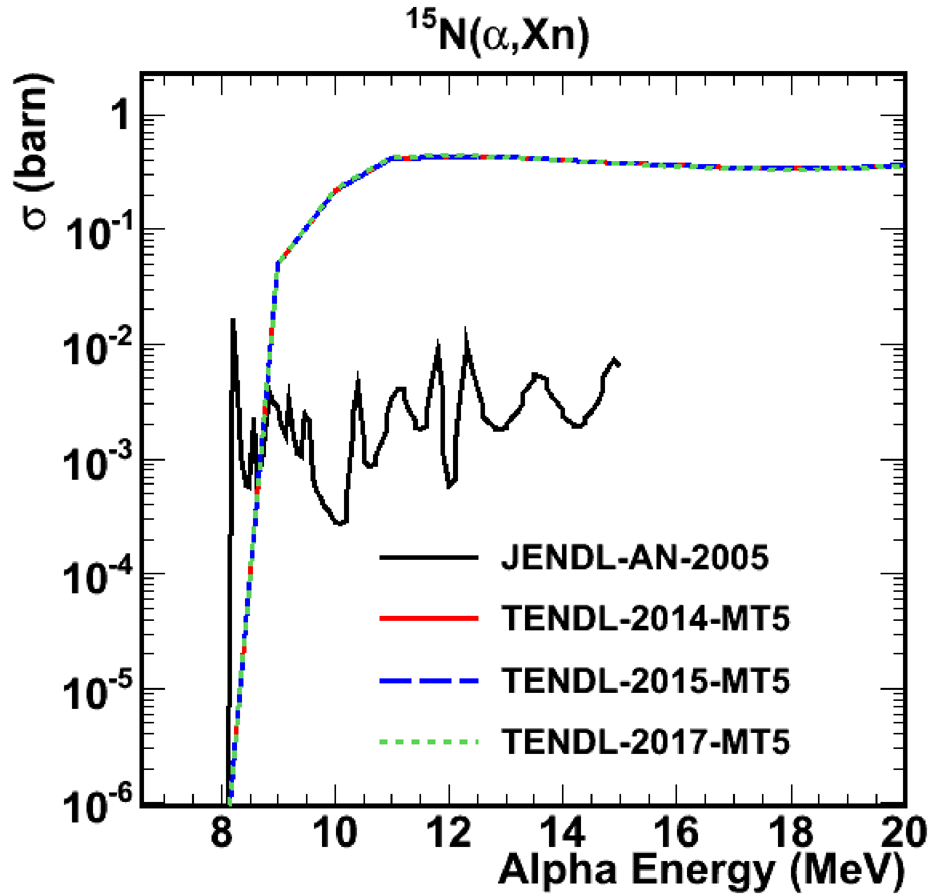

ENDF-6 format libraries available for SaG4n

In the SaG4n web (http://win.ciemat.es/SaG4n/) we can find:

Data libraries

SaG4n uses libraries originally written in ENDF-6 data format to model the (α,xn) reactions. The following libraries are available for download:

JENDL/AN-2005. It contains only (α,n) cross sections and secondary neutron energy-angular distribution data tables for the following isotopes: ^{6,7}Li, ^{9}Be, ^{10,11}B, ^{12,13}C, ^{14,15}N, ^{17,18}O, ^{19}F, ^{23}Na, ^{27}Al and ^{28,29,30}Si. This library relies on experimental data and theoretical calculations.

TENDL-2017. It contains cross sections and secondary neutron energy-angular distribution data tables for a large variety of isotopes. This library relies on theoretical calculations performed with the TALYS code. This is the version of the TENDL-2017 library where all the non-elastic reactions are grouped together into a single channel.

JENDL/AN-2005_noSec01. This is the same as JENDL/AN-2005, but the data tables concerning the energy-angular distributions of the neutrons from (α,n) reactions (MT=4) on ^{6,7}Li, ^{10,11}B, ^{13}C, ^{14,15}N and ^{17,18}O have been removed. These energy-angular distributions are then computed by Geant4 from the information of the excited state of the residual nucleus (information provided by the library). An isotropic neutron angular distribution in the center-of-mass system is assumed, and the energy of the emitted neutrons is obtained from two-body kinematics.

JENDLTENDL01 **(recommended)**. This is the TENDL-2017 library, in which the 17 isotopes of JENDL/AN-2005 have been replaced with those of the JENDL/AN-2005_noSec01 library.

Conclusions

SaG4n is a Geant4 tool to to calculate neutron production due to (α,xn) reactions in different materials. The source code + manual + data libraries are available at:

http://win.ciemat.es/SaG4n/

SaG4n works with an input (simple geometries, sources … but enough for many practical cases) → once compiled, no geant4 knowledge is needed.

SaG4n can be also used as a basis to develop more complex applications.

Advantages of Geant4 over other codes:

- Complex geometries
- Event generator: gamma rays in coincidence with neutrons (in some cases)
- Same code for generating and for transporting the neutrons

Disadvantages:

- Slow