Geant4 progress

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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) → **11664 citations** (May-2019)

Geant4 releases

- geant4.10.5 → 2019 (+ patch 01)
- geant4.10.4 → 2018 (+ patches 01,02,03)
- geant4.10.3 → 2017 (+ patches 01,02,03)
- geant4.10.2 → 2016 (+ patches 01,02,03)
- geant4.10.1 → 2015 (+ patches 01,02,03)
- geant4.10.0 → 2014 (+ patches 01,02,03,04) ← Multithreading
- geant4.9.6 → 2013 (+ patches 01,02,03,04)
- …

Geant4 is being continuously improved → Release notes

User forum: http://hypernews.slac.stanford.edu/HyperNews/geant4/cindex

Geant4 examples

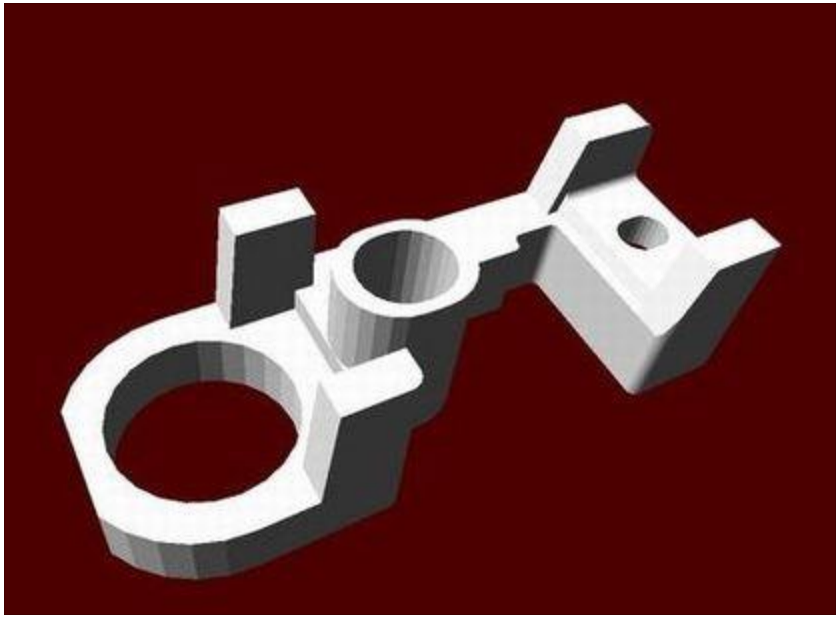
Some characteristics

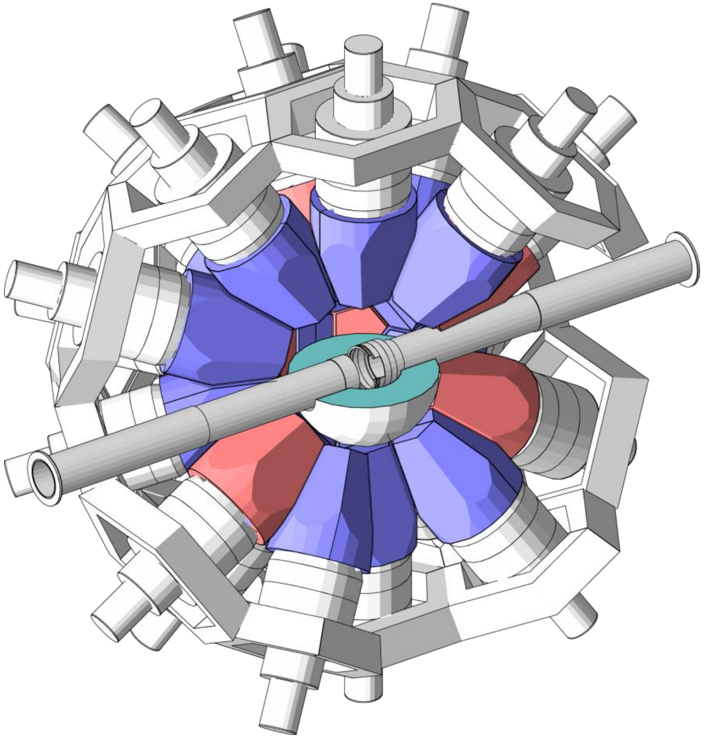
- Written in C++

  Toolkit → C++ code has to be written to build an application

  → Large flexibility (geometry, tallies …)

- Powerful geometry package:





C. Guerrero et al., NIMA 671, 108 (2012)

Outline

In this presentation:

- Radioactive decay
- Biasing
- Low energy neutron transport
- Neutron production in (α,n) reactions

Radioactive decay

The radioactive decay module has been improved considerably in the last releases:

- 10 decay modes implemented:
  - α
  - β^+, β^- → allowed and forbidden transitions
  - electron capture (from K, L, M, N shells)
  - isomeric transition → including EC + atomic relaxation
  - neutron emission
  - proton emission

- Not yet implemented:
  - Spontaneous fission (available soon)
  - Beta-delayed neutrons and protons
  - Double beta decay

Radioactive decay

The radioactive decay module has been improved considerably in the last releases:

- Databases (RadioactiveDecay5.3 + PhotonEvaporation5.3) → ENSDF – ~3000 nuclei included. Both databases consistent.

- *Very good performance* → in most practical cases, more than enough to simulate natural decay chains inside detectors.

Radioactive decay

The radioactive decay module has been improved considerably in the last rel

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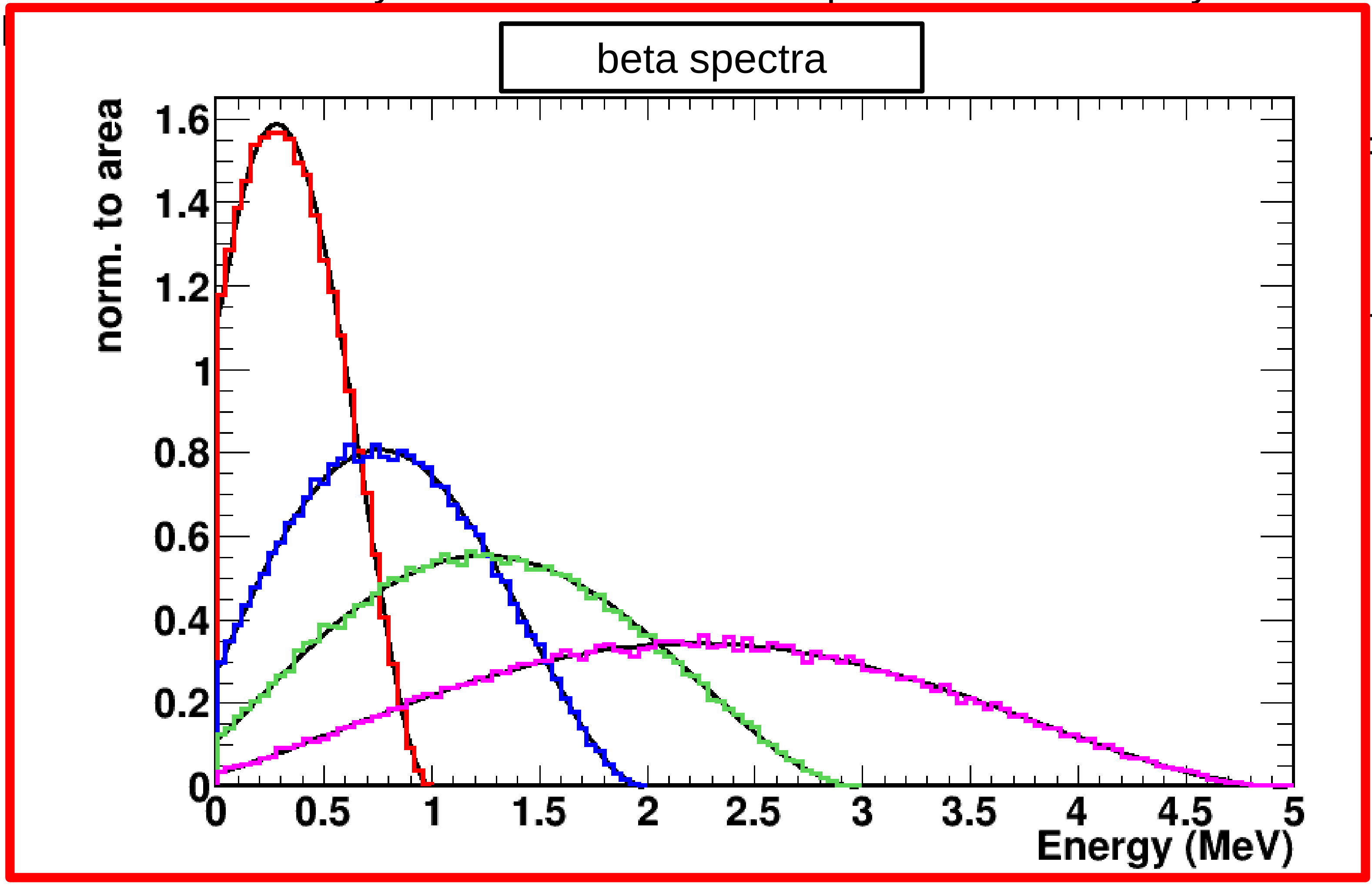


Biasing

Biasing techniques have been included/improved in the last releases. Different biasing options are allowed:

- Physics process biasing:
  - Cross-section biasing, forced interaction, etc.
  - Biasing final products of an interaction, e.g. distribution
- Non-physics biasing :
  - Geometrical importance, splitting / Russian roulette, weight window, etc.
- User defined biasing

→ Check manual + examples

Low energy neutron transport

Low energy neutron transport

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.

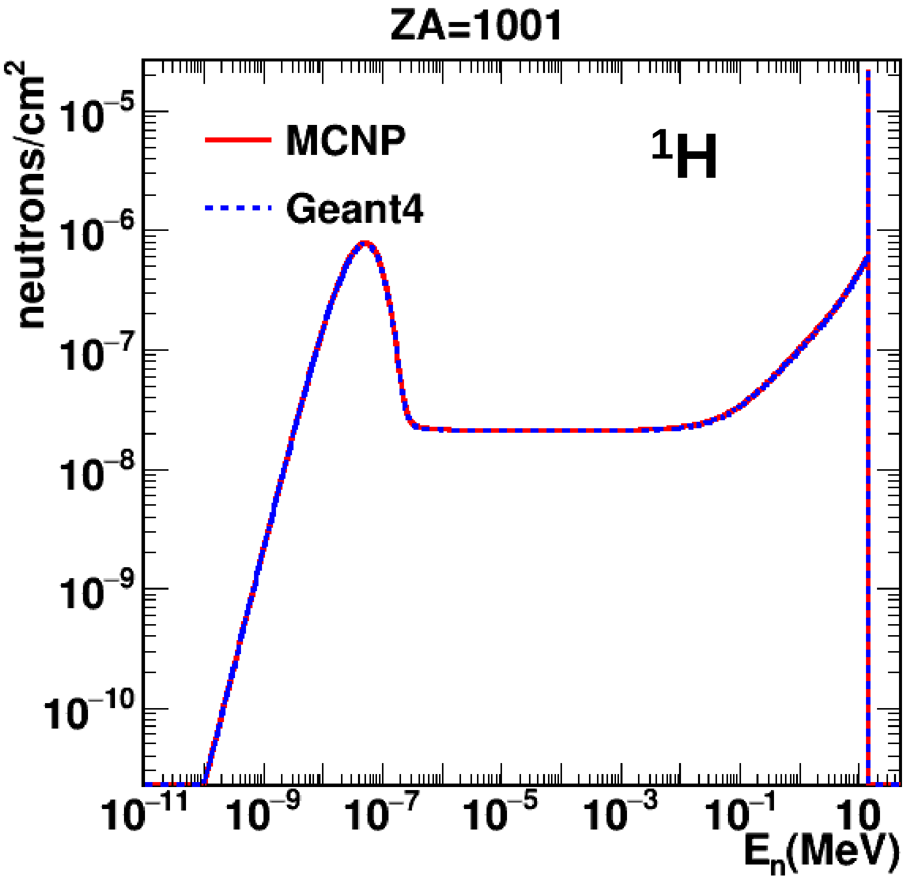
Verification tests have been performed by comparing Geant4 with MCNP. Details of the tests are given in:

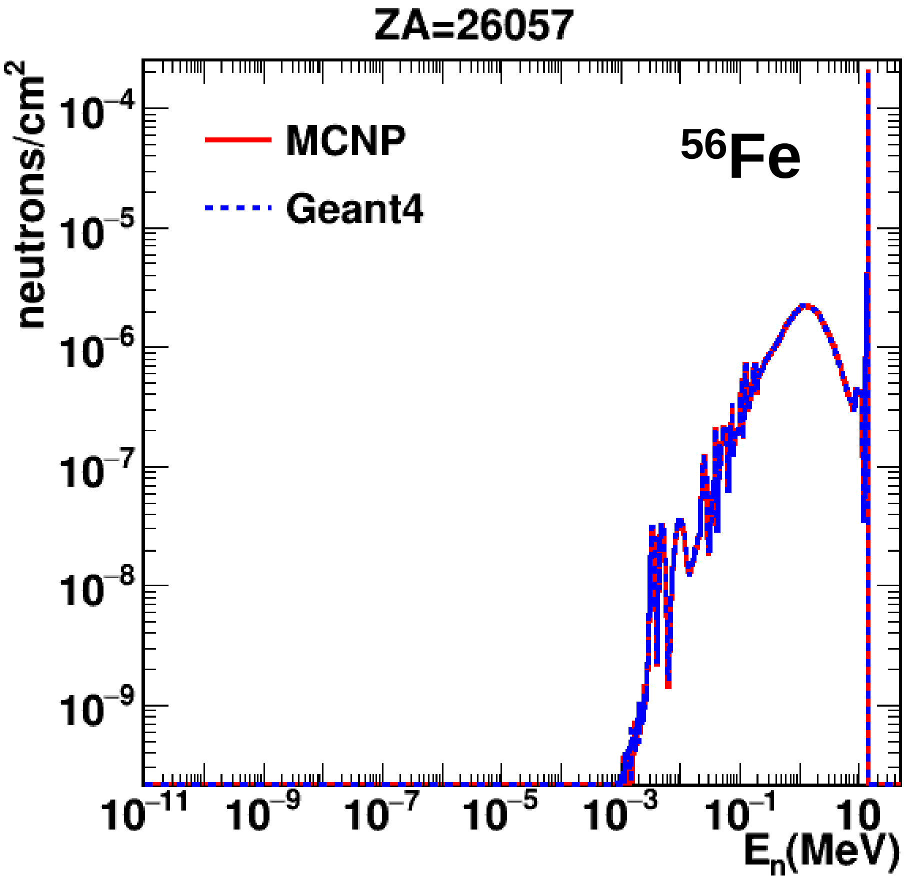
- E. Mendoza, IEEE TNS 61, 2357 (2014)
- E. Mendoza and D. Cano-Ott, *Update of the Evaluated Neutron Cross Section Libraries for the Geant4 Code*, IAEA technical report INDC(NDS)-0758, Vienna, 2018.

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/

Verification tests





ENDF-6 neutron incident data libraries (<20 MeV)

- Evaluated libraries: → **G4NDL4.5**
  - USA: **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

- Many of them available for download from:

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

The ENDF-6 format

- **ENDF-6** format data libraries: originally created to simulate nuclear reactors.

- The understanding of the ENDF-6 format helps to know which results can be expected from a simulation and which ones can not.

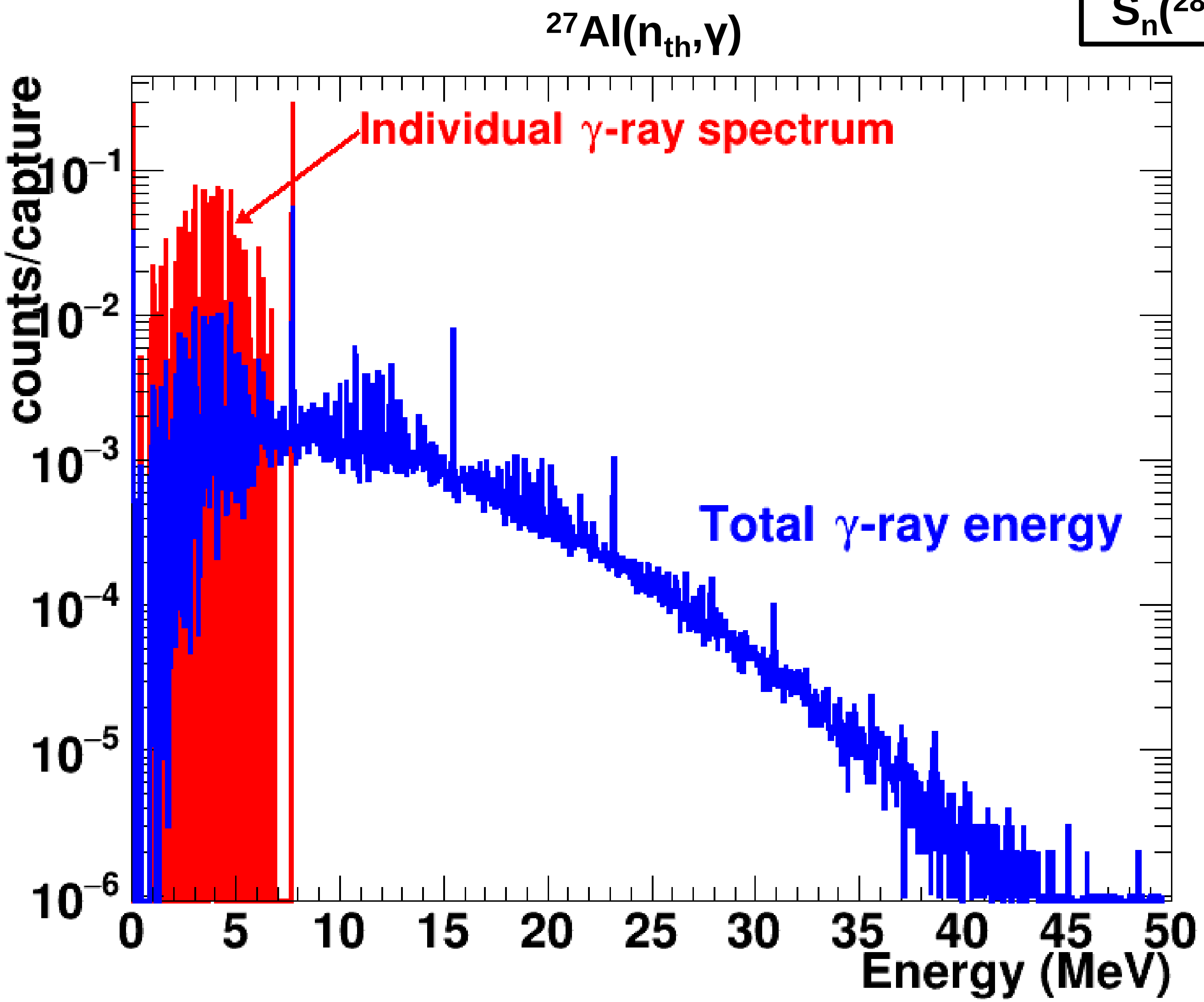
  → https://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf

- Information in an ENDF-6 format file:
  - Reaction cross sections
  - Secondary particle yields
  - Energy-angular distributions of secondary particles

- **In general,** no energy/momentum/baryonic number … conservation event-by-event.
  - Capture, fission, (n,2n), (n,n2a), (n,p2d) …
  - Usually conserved in two body reactions: (n,n), (n,n’), (n,p), (n,d) …

Example: thermal capture on ^{27}Al

$S_n(^{28}Al)$=7.7 MeV



γ-ray production in (n,γ) reactions

Alternative in Geant4 for (n,γ) reactions → G4PhotonEvaporation model, which is used:

1. If no data, i.e. no γ-rays after capture in the ENDF-6 data file.
2. If G4NEUTRONHP_USE_ONLY_PHOTONEVAPORATION environmental flag defined.

The G4PhotonEvaporation model generates the cascade from the capture level using statistical models.

A *new* Photon Evaporation model has been developed, which does the same, but *with more detail*.

New photon evaporation model

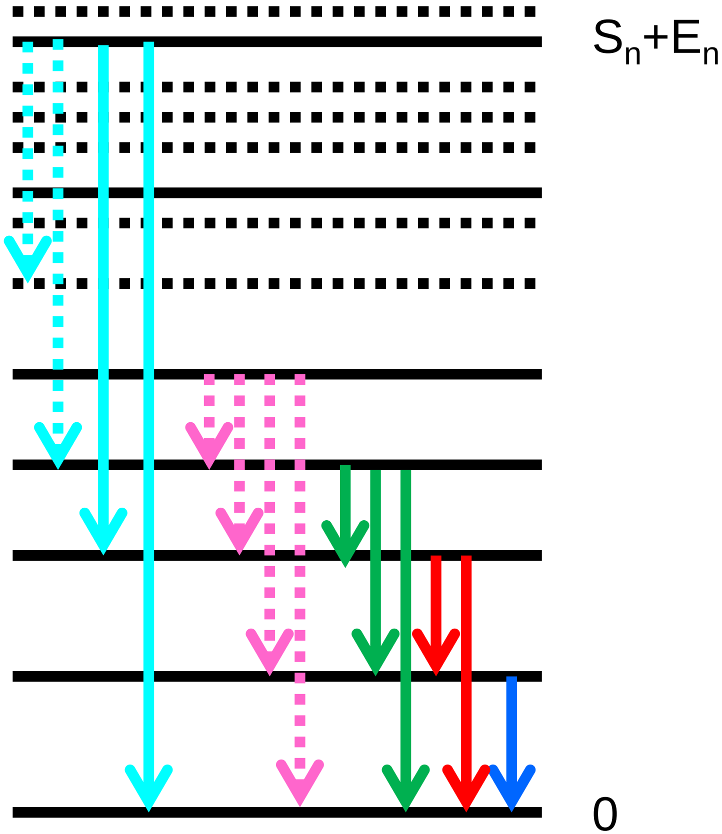
What is needed:
- Levels
- Branching ratios
- Internal conversion coefficients

What the code does is to create the full level scheme + branching ratios + internal conversion coefficients, from:

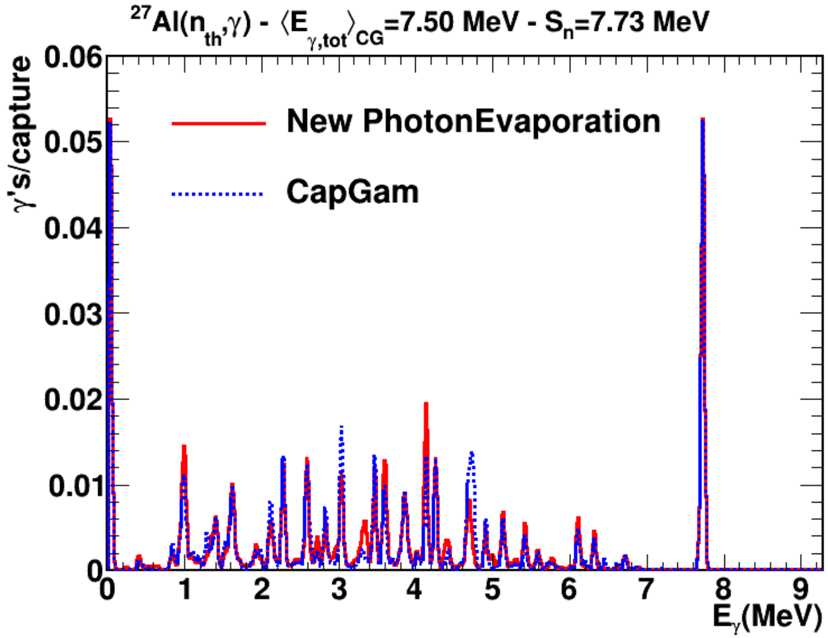
- **Experimental information:** RIPL-3 + ENSDF → G4-PhotonEvaporation library.

- **Missing information:** Statistical models: level density formulas, photon strength functions (parameters from RIPL-3), BrICC …

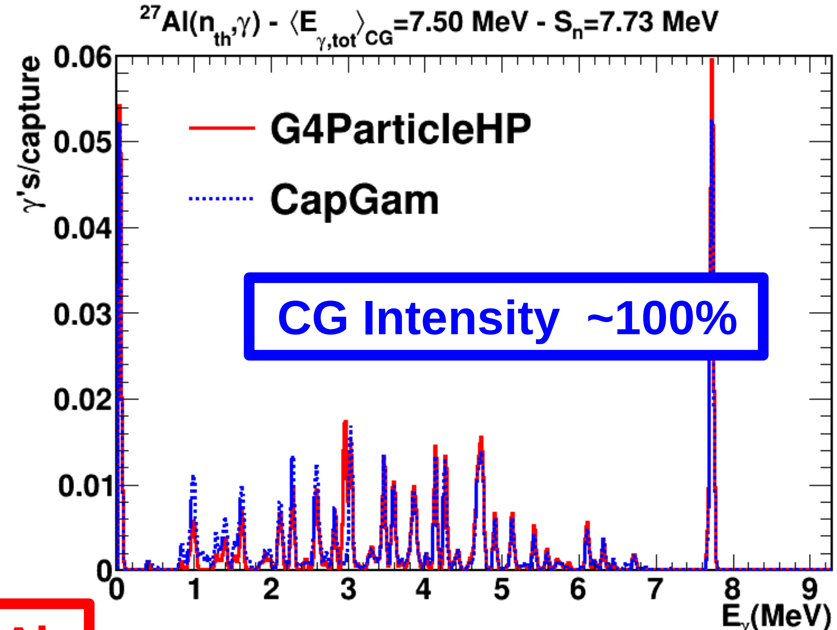
To check γ-ray intensities from (thermal) neutron capture → CapGam: https://www.nndc.bnl.gov/capgam/



$n + {}^{A}X \rightarrow {}^{A+1}X$

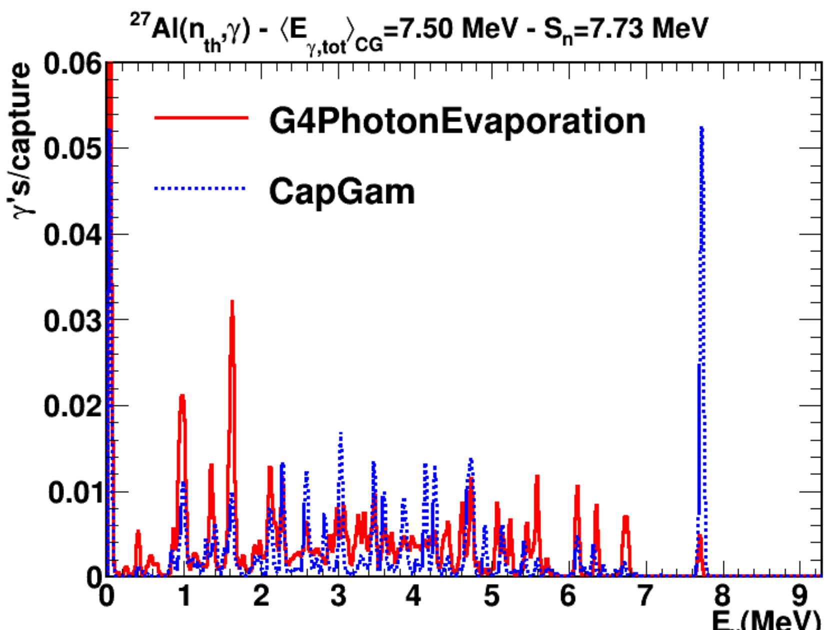


^{27}Al(n_{th},γ) - ⟨$E_{\gamma,tot}$⟩$_{CG}$=7.50 MeV - S_n=7.73 MeV
New PhotonEvaporation
CapGam
γ's/capture
E_γ(MeV)

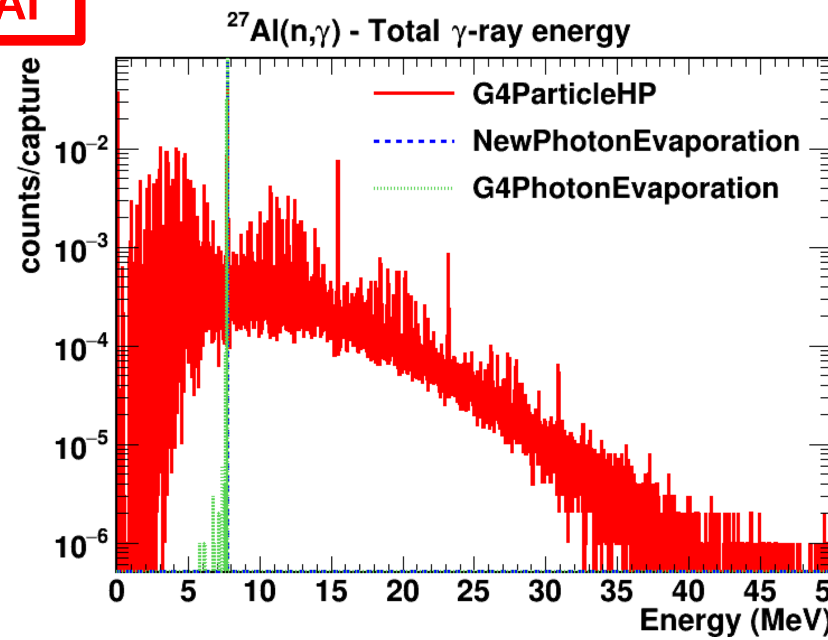


^{27}Al(n_{th},γ) - ⟨$E_{\gamma,tot}$⟩$_{CG}$=7.50 MeV - S_n=7.73 MeV
G4ParticleHP
CapGam
CG Intensity ~100%
γ's/capture
E_γ(MeV)

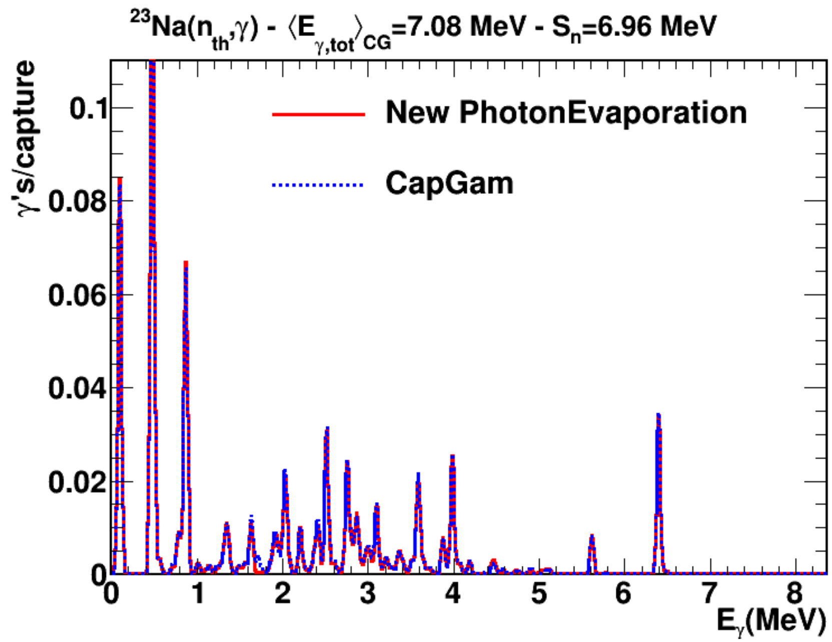
^{27}Al

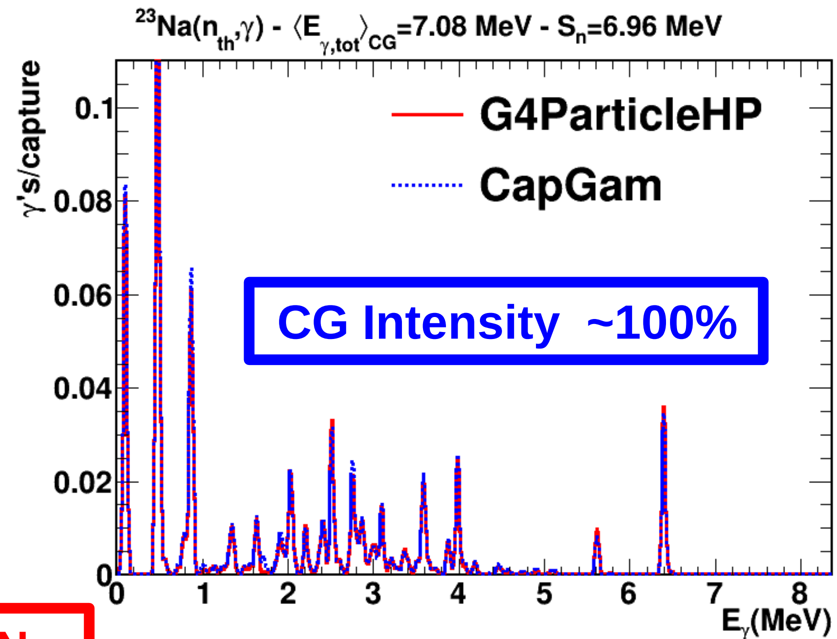


^{27}Al(n_{th},γ) - ⟨$E_{\gamma,tot}$⟩$_{CG}$=7.50 MeV - S_n=7.73 MeV
G4PhotonEvaporation
CapGam
γ's/capture
E_γ(MeV)

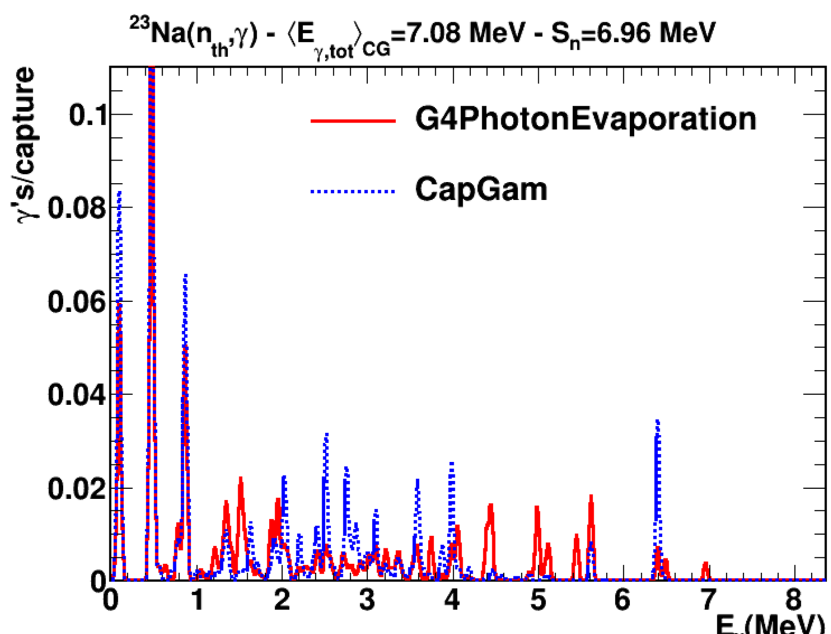


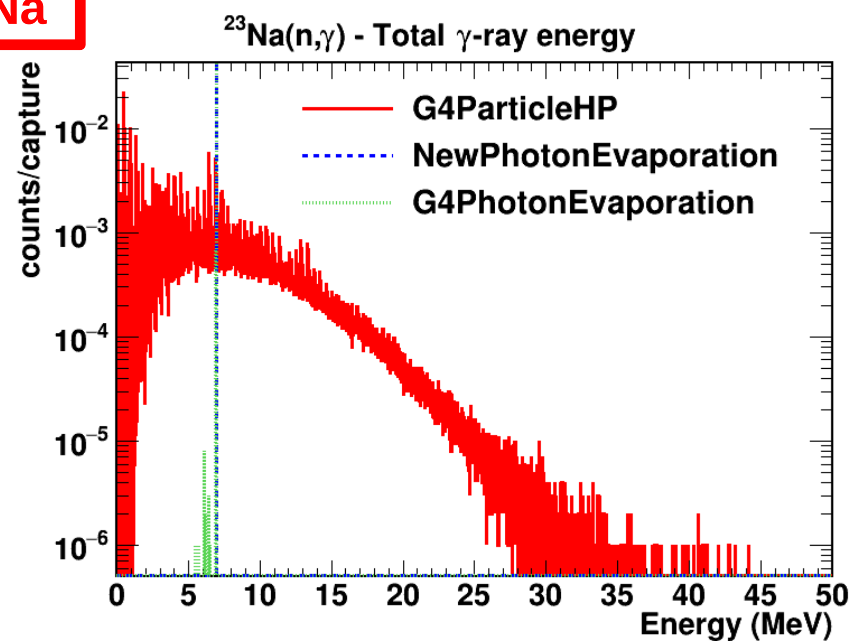
^{27}Al(n,γ) - Total γ-ray energy
G4ParticleHP
NewPhotonEvaporation
G4PhotonEvaporation
counts/capture
Energy (MeV)

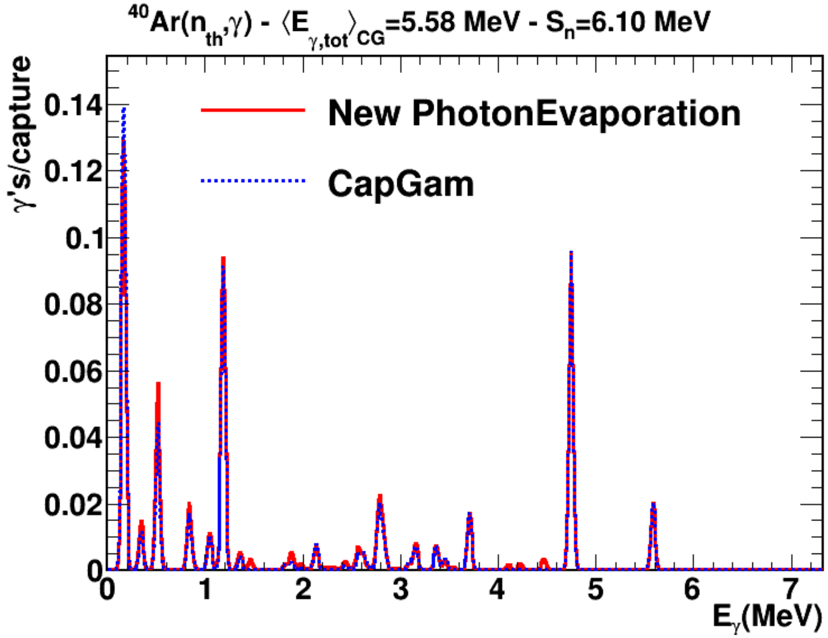

23Na(nth,γ) - ⟨Eγ,tot⟩CG=7.08 MeV - Sn=6.96 MeV
New PhotonEvaporation
CapGam
γ's/capture
Eγ(MeV)


23Na(nth,γ) - ⟨Eγ,tot⟩CG=7.08 MeV - Sn=6.96 MeV
G4ParticleHP
CapGam
CG Intensity ~100%
γ's/capture
Eγ(MeV)

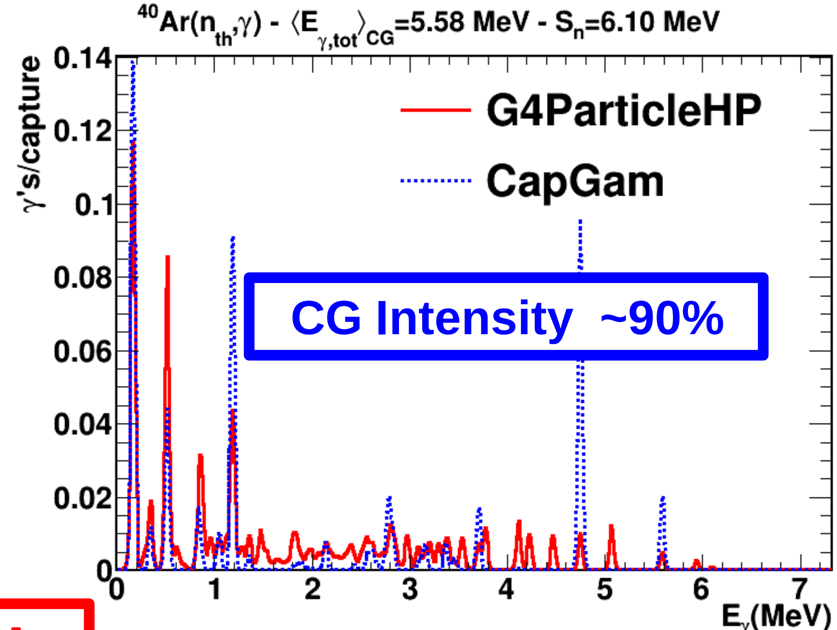
^{23}Na


23Na(nth,γ) - ⟨Eγ,tot⟩CG=7.08 MeV - Sn=6.96 MeV
G4PhotonEvaporation
CapGam
γ's/capture
Eγ(MeV)


23Na(n,γ) - Total γ-ray energy
G4ParticleHP
NewPhotonEvaporation
G4PhotonEvaporation
counts/capture
Energy (MeV)

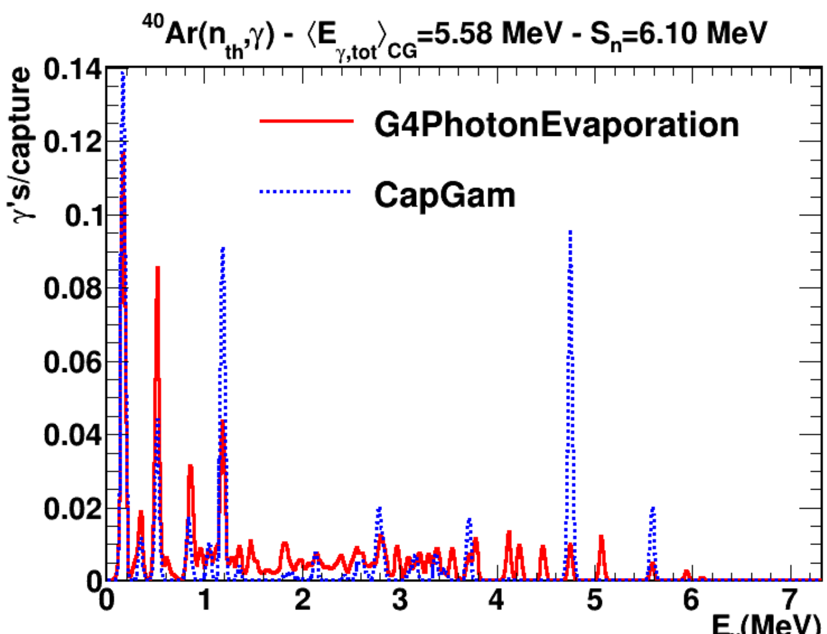


^{40}Ar(n$_{th}$,γ) - ⟨E$_{γ,tot}$⟩$_{CG}$=5.58 MeV - S$_n$=6.10 MeV
New PhotonEvaporation
CapGam
γ's/capture
E$_γ$(MeV)

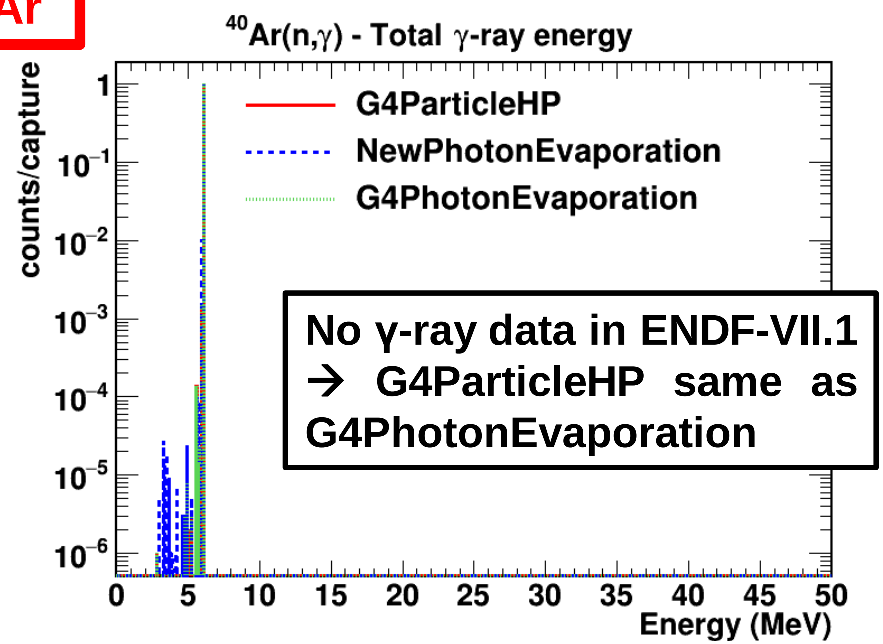


^{40}Ar(n$_{th}$,γ) - ⟨E$_{γ,tot}$⟩$_{CG}$=5.58 MeV - S$_n$=6.10 MeV
G4ParticleHP
CapGam
CG Intensity ~90%
γ's/capture
E$_γ$(MeV)

^{40}Ar



^{40}Ar(n$_{th}$,γ) - ⟨E$_{γ,tot}$⟩$_{CG}$=5.58 MeV - S$_n$=6.10 MeV
G4PhotonEvaporation
CapGam
γ's/capture
E$_γ$(MeV)



^{40}Ar(n,γ) - Total γ-ray energy
G4ParticleHP
NewPhotonEvaporation
G4PhotonEvaporation
No γ-ray data in ENDF-VII.1
→ G4ParticleHP same as
G4PhotonEvaporation
counts/capture
Energy (MeV)

Neutron production in (α,n) reactions

Neutron production in (α,n) reactions

$$Y = V \cdot N \cdot \int \Phi_\alpha(E)\sigma_{(\alpha,Xn)}(E)dE$$

V: material volume N: atom density $\Phi_\alpha(E)$: differential flux

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.
- The energy distributions of the secondary neutrons.

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.

Neutron production in (α,n) reactions

$$Y = V \cdot N \cdot \int \Phi_{\alpha}(E)\sigma_{(\alpha,Xn)}(E)dE$$

Codes:

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)*

Neutron production in (α,n) reactions

Monte Carlo

$$Y = V \cdot N \cdot \int \Phi_\alpha (E) \sigma_{(\alpha,Xn)}(E) dE$$

Codes:

Geant4	**ICRU 49 report**	**+**	**ENDF-6 format library**
NeuCBOT	**SRIM**	**+**	**TALYS**
NEDIS	**SRIM**	**+**	**own library**
SOURCES	**SRIM**	**+**	**own library**
USD	**ICRU 49 report**	**+**	**TALYS**

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

Stopping cross section

Neutron production in (α,n) reactions

Geant4 operates different than the other codes → Monte Carlo

Pros:

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

Cons:

- Slow → large CPU times → biasing techniques are needed

Modifications to the Geant4 source code are needed → next Geant4 release

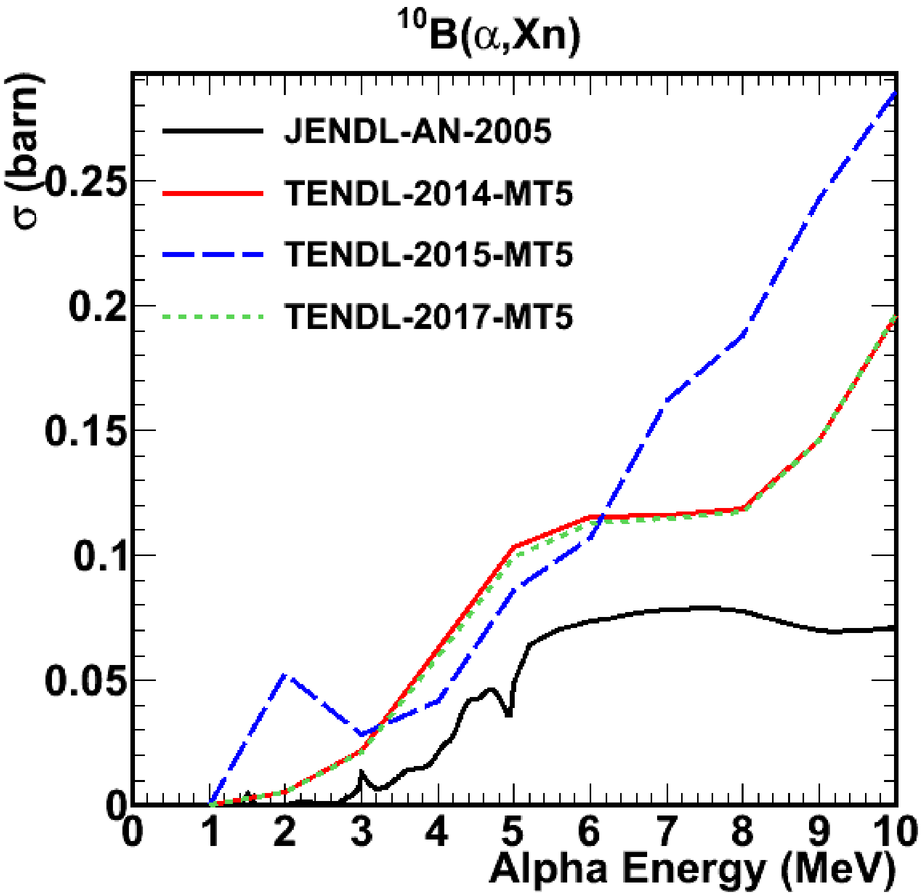
ENDF-6 α-incident libraries

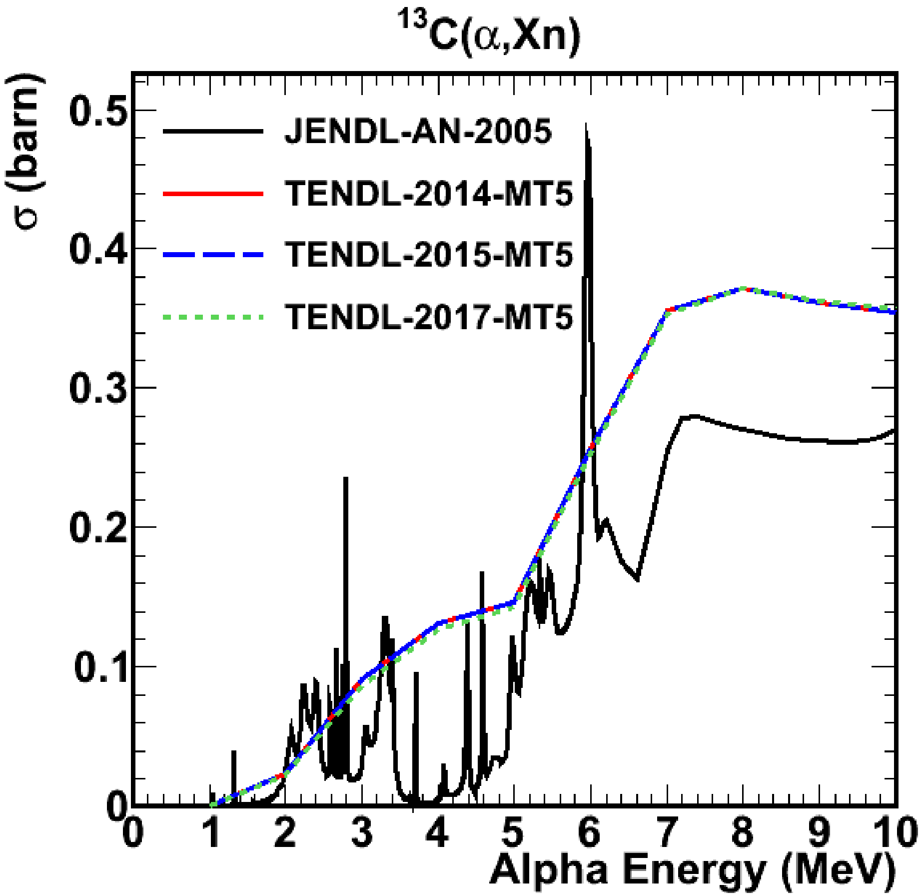
The ENDF-6 α-incident data libraries available are:

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.

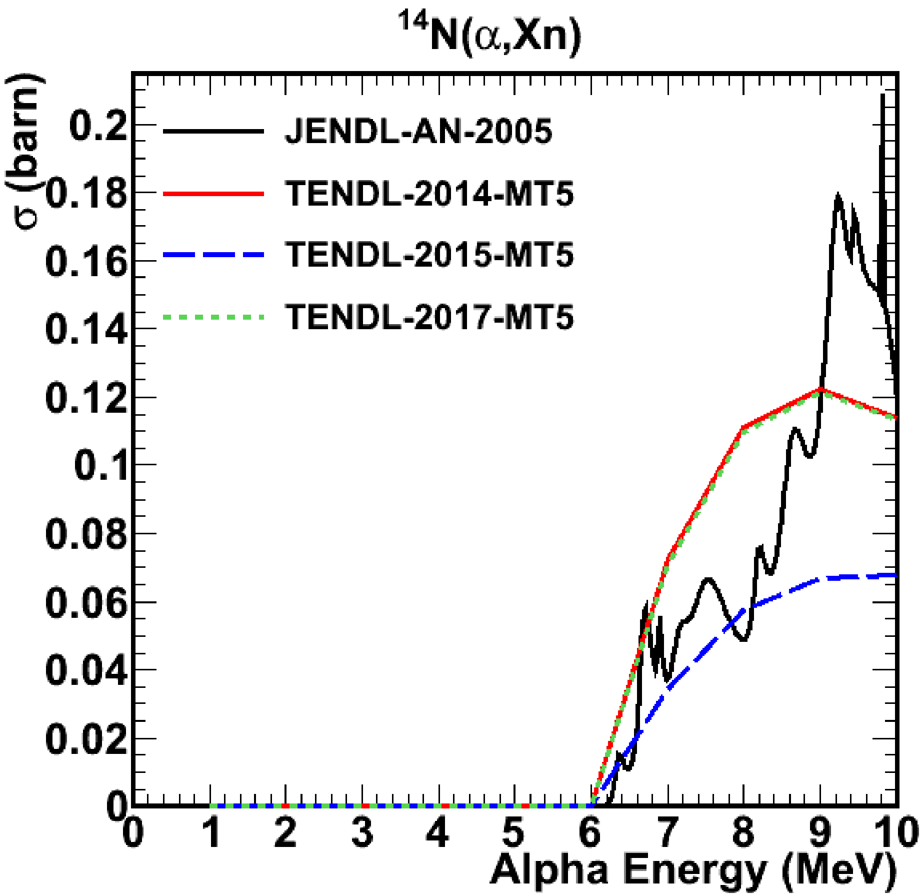
TENDL libraries: they have been made with the results of the **TALYS** code. There are several versions: TENDL-2017, TENDL-2015, TENDL-2014 ... They contain a large amount of isotopes.

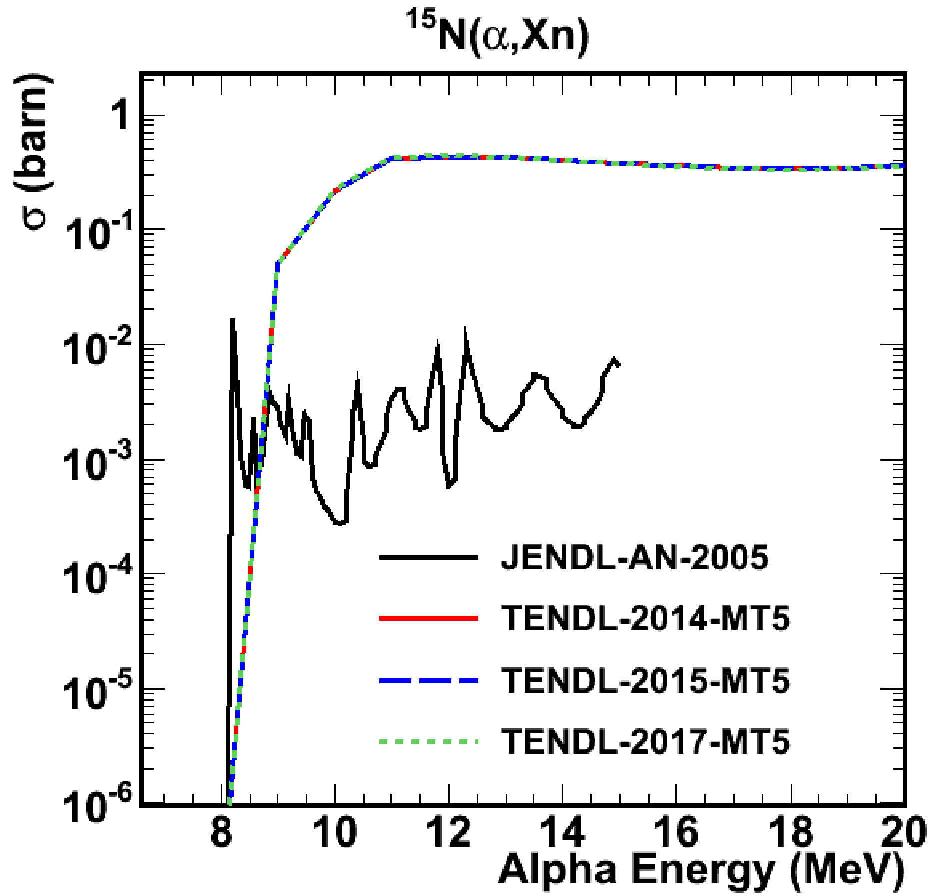
ENDF-6 α-incident libraries



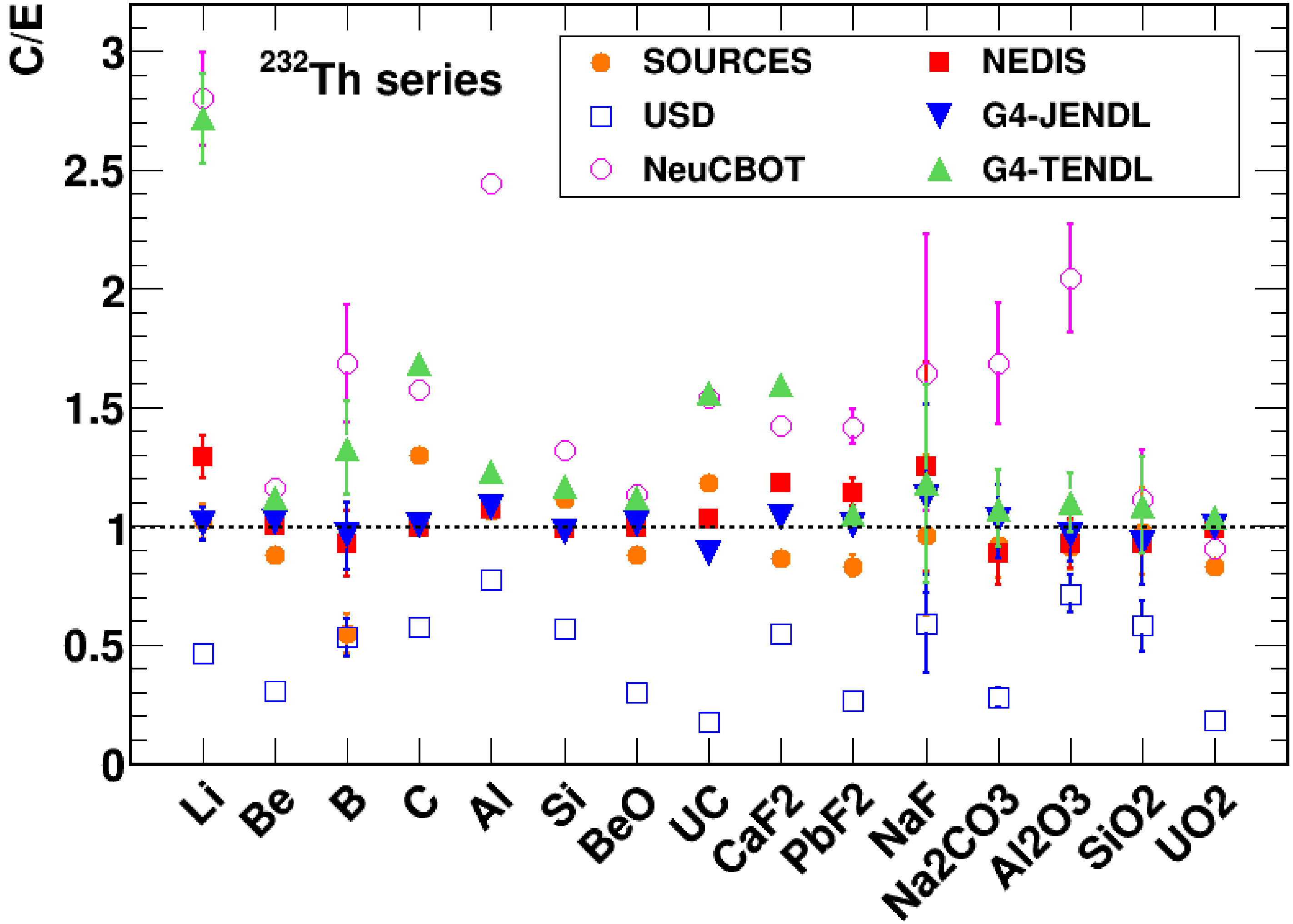


ENDF-6 α-incident libraries





Comparison: neutron yields



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

Summary & conclusions

- **Geant4** is a general purpose Monte Carlo simulation tool for elementary particles passing through and interacting with matter.
- Geant4 is being continuously improved → update
- C++ knowledge is needed

- The **radioactive decay** module has been improved in the last releases.
- **Biasing** techniques have been included/improved in the last releases.
- **Low energy neutron transport:**
  - Verification tests with MCNP
  - Based on ENDF-6 format data libraries, originally created to simulate nuclear reactors → **In general,** no energy/momentum/baryonic number … conservation event-by-event.
  - Improvements in future releases
- **Neutron production in (α,n) reactions:**
  - A verification & validation study has been performed.
  - Advantages: complex geometries + γ-rays in coincidence with neutrons + same code for generating and for transporting the neutrons.