Transport of low energy neutrons and charged particles in Geant4

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CIEMAT

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.

In this presentation:

- The ENDF-6 format libraries
- The ENDF-6 format
- Verification tests
- Strengths and limitations
- Future developments

The ENDF-6 format data libraries

- The ENDF-6 format:
  https://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf

- 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

- ENDF-6 format data libraries:
  - https://www-nds.iaea.org/exfor/endf.htm
  - https://www.nndc.bnl.gov/exfor/endf00.jsp

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

- Evaluated libraries:
  - USA: **ENDF/B** → ENDF/B-VIII.0, **ENDF/B-VII.1**,ENDF/B-VII.0 … (ENDF/B-VII.1 → **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 from:

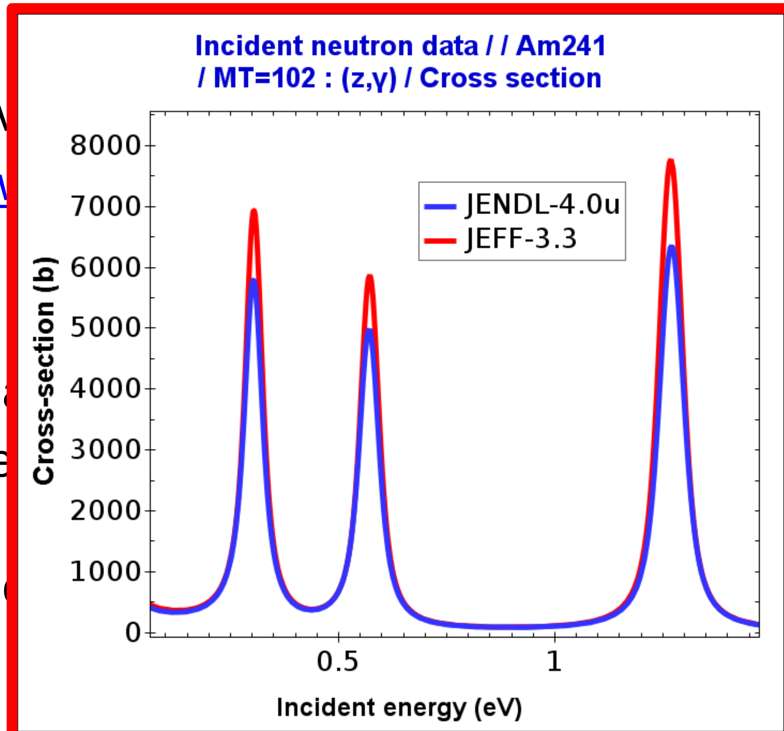
  https://www-nds.iaea.org/geant4/

- Characteristics:
  - Evaluated data
  - Incident energy range covering at least from 10^{-5} eV up to 20 MeV, for all isotopes.
  - Information concerning secondary neutrons are *always* given.

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

G4NDL4.5

- Evaluated libraries:
  - 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 av
  https://www

- Characteristics:
  - Evaluated d
  - Incident ene ⁵ eV up to 20 MeV, for all isotopes.
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ENDF-6 neutron incident data libraries (<20 MeV)

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

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Hot Topics » IAEA-CIELO • TENDL-2017 • JENDL-4.0u2 • ENDF/B-VIII.0 **News** » Damage cross section database extended by SS-316 and Eurofer

Quick Links

- ADS-Lib
- Atomic Mass Data Centre
- CINDA
- Charged particle reference cross section
- DICEBOX
- DROSG-2000
- DXS
- Decay Data Library for Actinides
- EMPIRE-3.2
- ENDF Archive
- ENDF Retrieval
- ENDF-6 Codes
- ENDF-6 Format
- ENDVER
- ENSDF
- ENSDF ASCII Files
- ENSDF programs
- EPICS Electron & photon interaction data
- EXFOR
- FENDL
- Fission Yields

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/

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

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

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```
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.

Example of using different libraries

[J.L. Taín et al, NIMA 774, 17 (2015)]

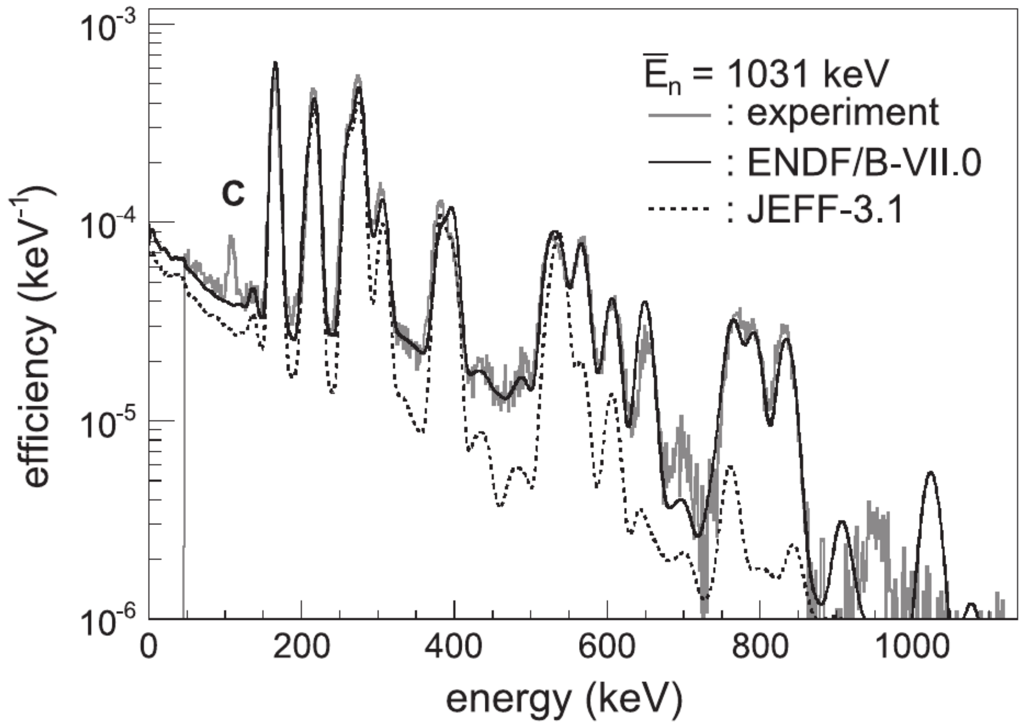


Fig. 6. Comparison of measured and simulated detector response with two different neutron libraries for the distribution with $\overline{E}_n = 1031$ keV. C: contaminant peak.

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

Other ENDF-6 format data libraries

- Incident charged particle (evaluated):
  - **ENDF/B-VIII.0**: proton (48 isotopes), deuteron (5 isotopes), triton (5 isotopes), ^{3}He (3 isotopes), alpha (1 isotope).
  - JENDL/AN-2005: (alpha,n) reaction data file.

G4TENDL1.3.2

- Incident charged particle (computer code):
  - TENDL libraries: TENDL-2017, TENDL-2015, **TENDL-2014** … (~2800 isotopes). Incident n, p, d, t, ^{3}He, α, γ. Up to 200 MeV.
- High energy:
  - ENDF/HE-VI: n,p incident (4 isotopes, up to 1 GeV).
  - JENDL/HE-2007: n,p incident (106 isotopes, up to 3 GeV).
- Thermal data libraries
- …

The ENDF-6 format

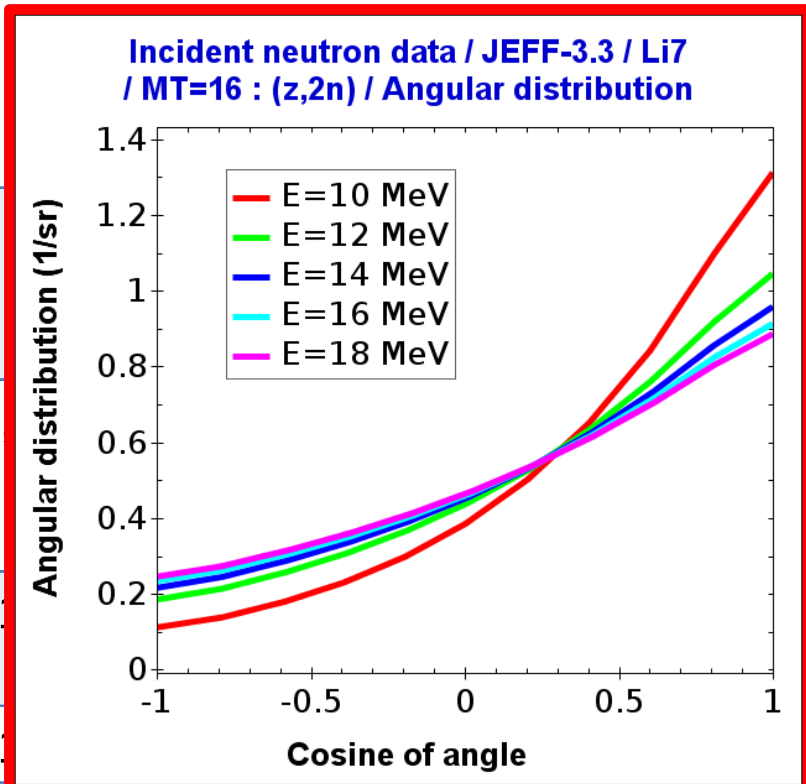
- The understanding of the ENDF-6 format helps to know which results can be expected from a simulation and which ones can not.

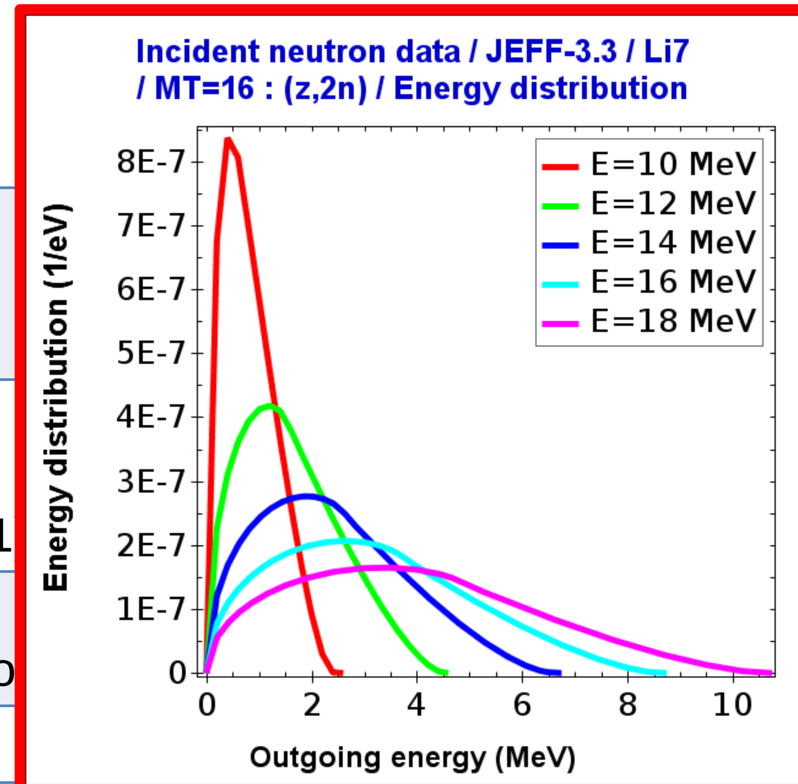
- Information in an ENDF-6 format file:
  - Reaction cross sections
  - Secondary particle yields
  - Energy-angular distributions of secondary particles

- Example 1: n+^{7}Li in JEFF-3.3
- Example 2: p+^{12}C in TENDL-2017

MT	Reaction	n+^{7}Li – JEFF-3.3 Info
2	(n,n)	Cross section (MF=3) neutron angular (MF=4)
4	(n,n’)	Cross section (MF=3)
16	(n,2n)	Cross section (MF=3) neutron angular (MF=4) neutron energy (MF=5)
24	(n,2n+a)	Cross section (MF=3) neutron angular (MF=4) neutron energy (MF=5)
25	(n,3n+a)	Cross section (MF=3) neutron angular (MF=4) neutron energy (MF=5)
51,…,82	(n,n’)	Cross section (MF=3) neutron angular (MF=4) (Only MT=51) Photon production (MF=12+MF=14)
102	(n,γ)	Cross section (MF=3) Photon production (MF=12+MF=14)
104	(n,d)	Cross section (MF=3)

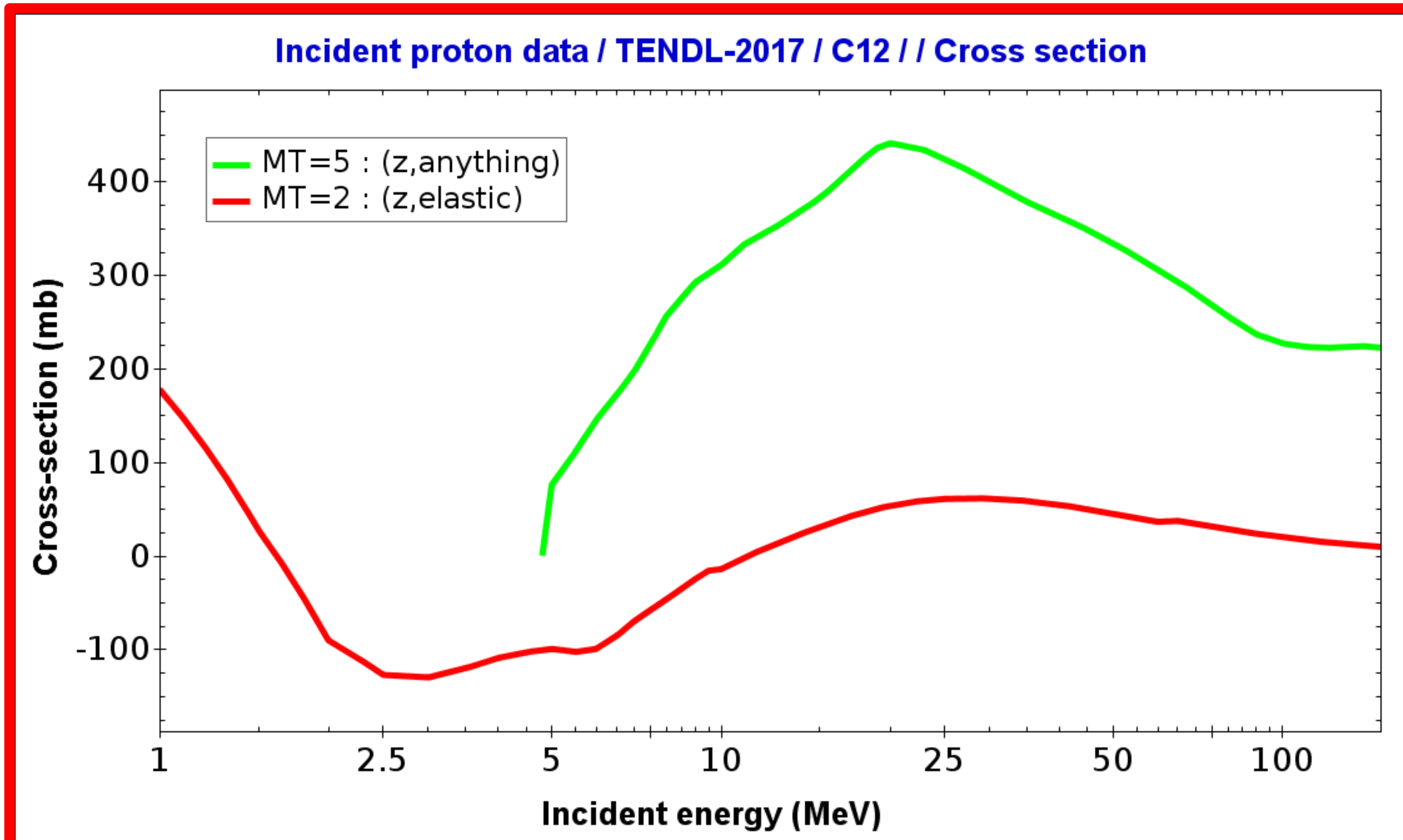
MT	Reaction	n+^{7}Li – JEFF-3.3	Info
2	(n,n)		Cross section (MF=3) neutron angular (MF=4)
4	(n,n’)		Cross section (MF=3)
16	(n,2n)		Cross section (MF=3) neutron angular (MF=4) neutron energy (MF=5)
51			=51
			hoto





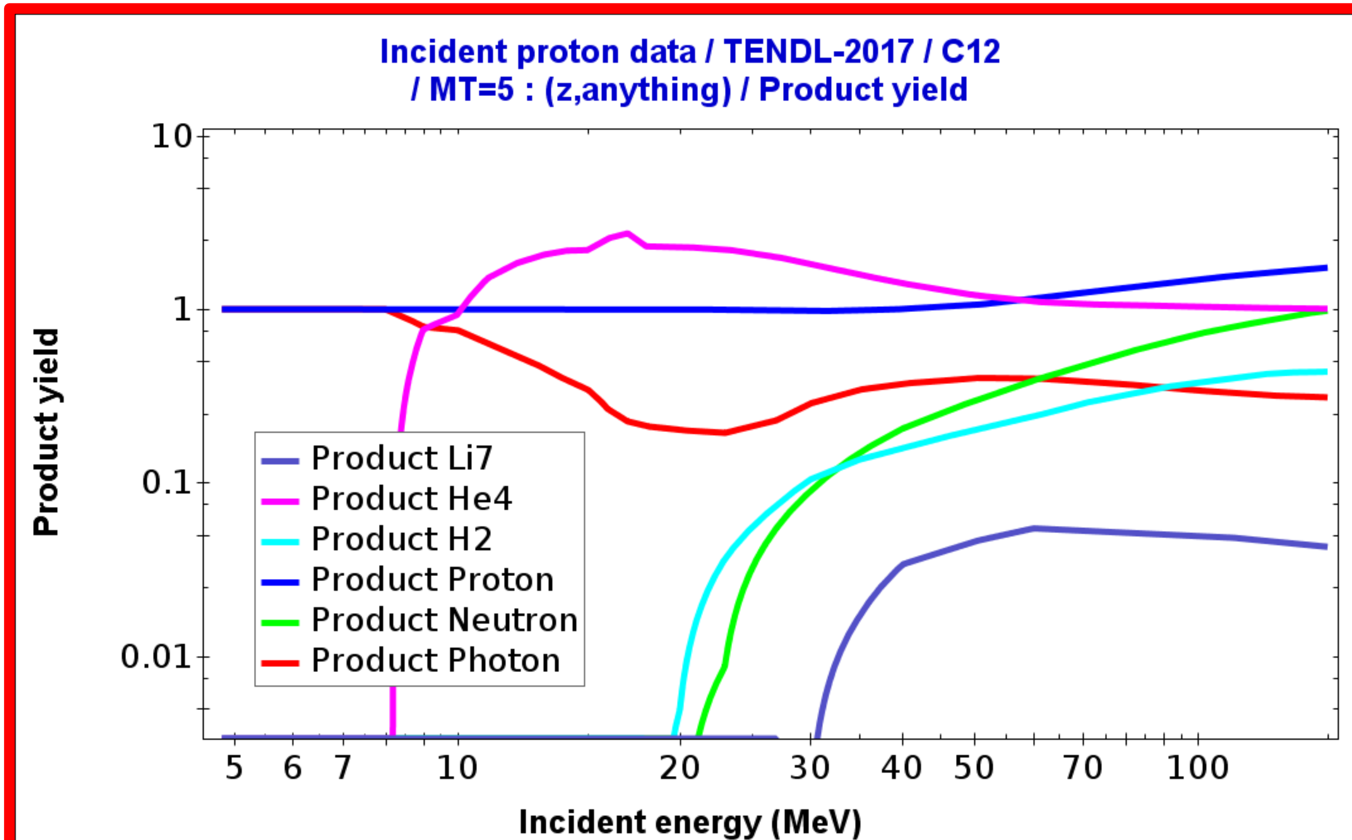
p+^{12}C – TENDL-2017

MT	Reaction	Info
2	(n,n)	Cross section (MF=3) neutron angular (MF=4)
5	(n,x)	Cross section (MF=3) Particle yields (MF=6) Energy-angular distributions (MF=6)



p+^{12}C – TENDL-2017

MT	Reaction	Info
2	(n,n)	Cross section (MF=3) neutron angular (MF=4)
5	(n,x)	Cross section (MF=3) Particle yields (MF=6) Energy-angular distributions (MF=6)

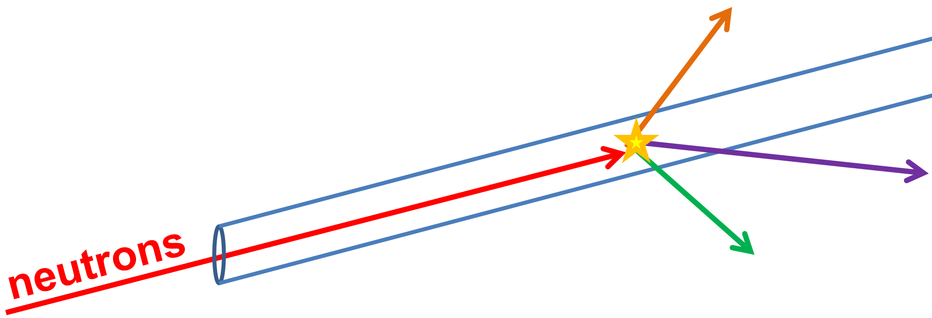


The ENDF-6 format

- In general:
  - Evaluated libraries:
    - Explicit cross sections up to 20 MeV
    - Particle yields + energy-angular distributions above 20 MeV (MT=5)
    - Information concerning energies and angles of secondary neutrons are always given
    - Information concerning energies and angles of other secondary particles are not always given
  - TENDL:
    - Two versions: one with explicit cross sections up to 30 MeV (but errors have been found) and other without explicit cross sections at all.
    - Particle yields + energy-angular distributions above 30 MeV (MT=5)

Verification tests

Verification tests have been performed by comparing Geant4 with MCNP



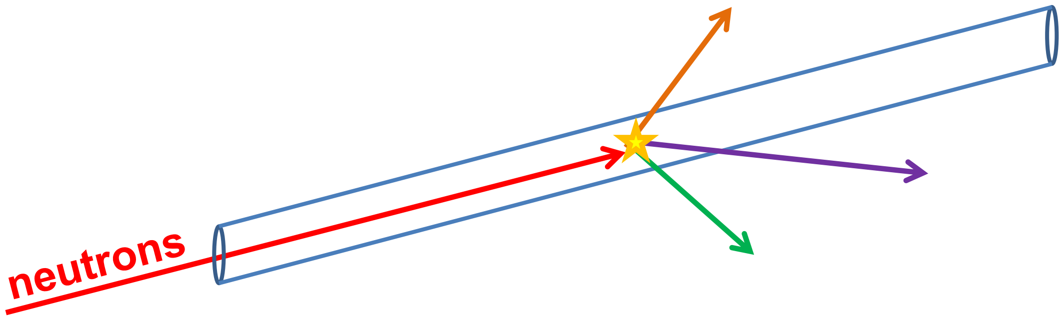
Geometry: 2 m long cylinder with a radius of 1 μm made of an isotopically pure material with density 1 g/cm^3.

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.

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:

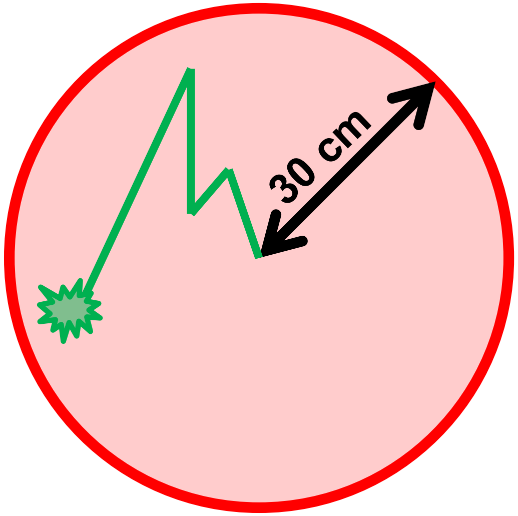
E. Mendoza and D. Cano-Ott, *Update of the Evaluated Neutron Cross Section Libraries for the Geant4 Code*, IAEA technical report [INDC(NDS)-0758](), Vienna, 2018.

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/

Verification tests

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



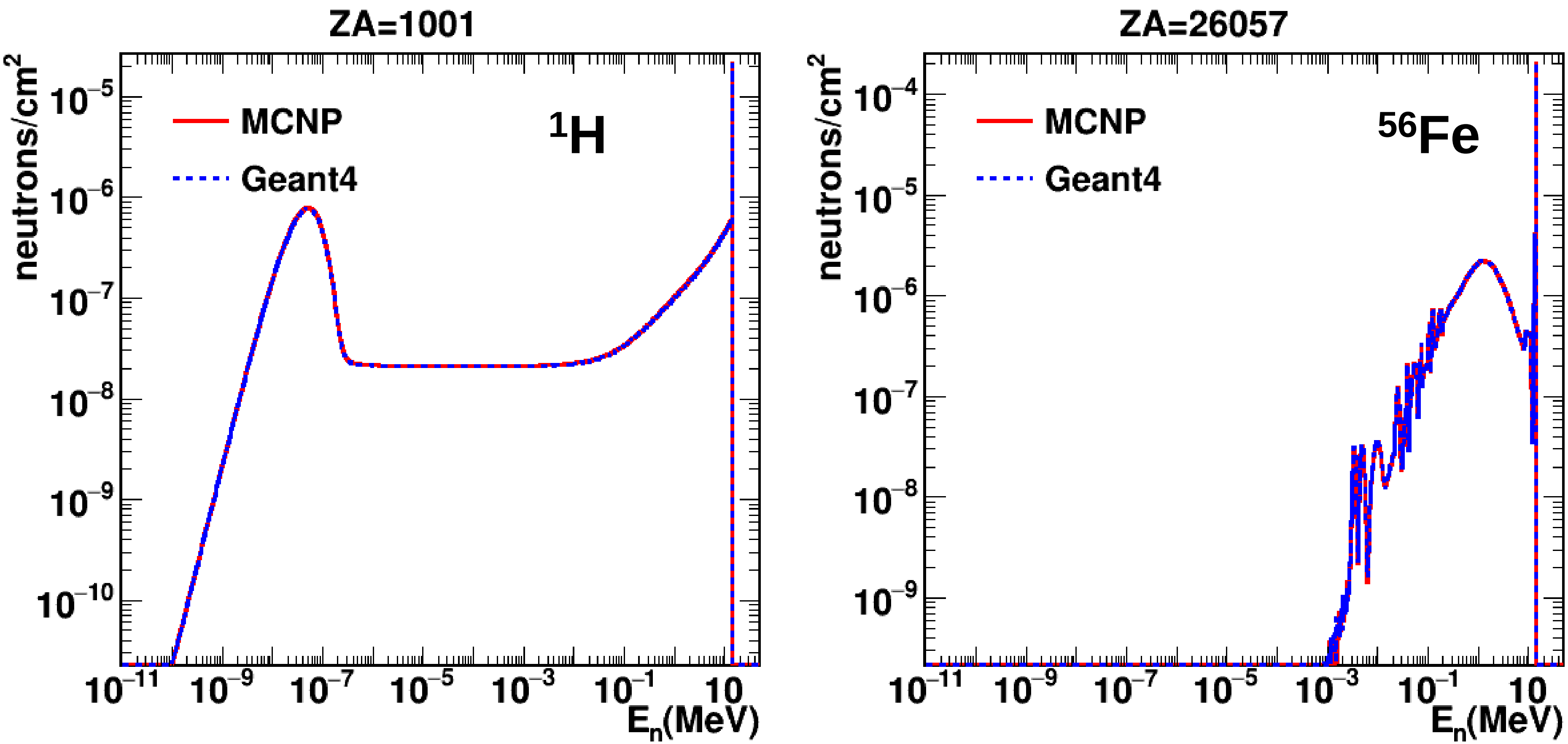
Geometry: 30 cm radius sphere made of an isotopically pure material with density 1 g/cm^3.

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

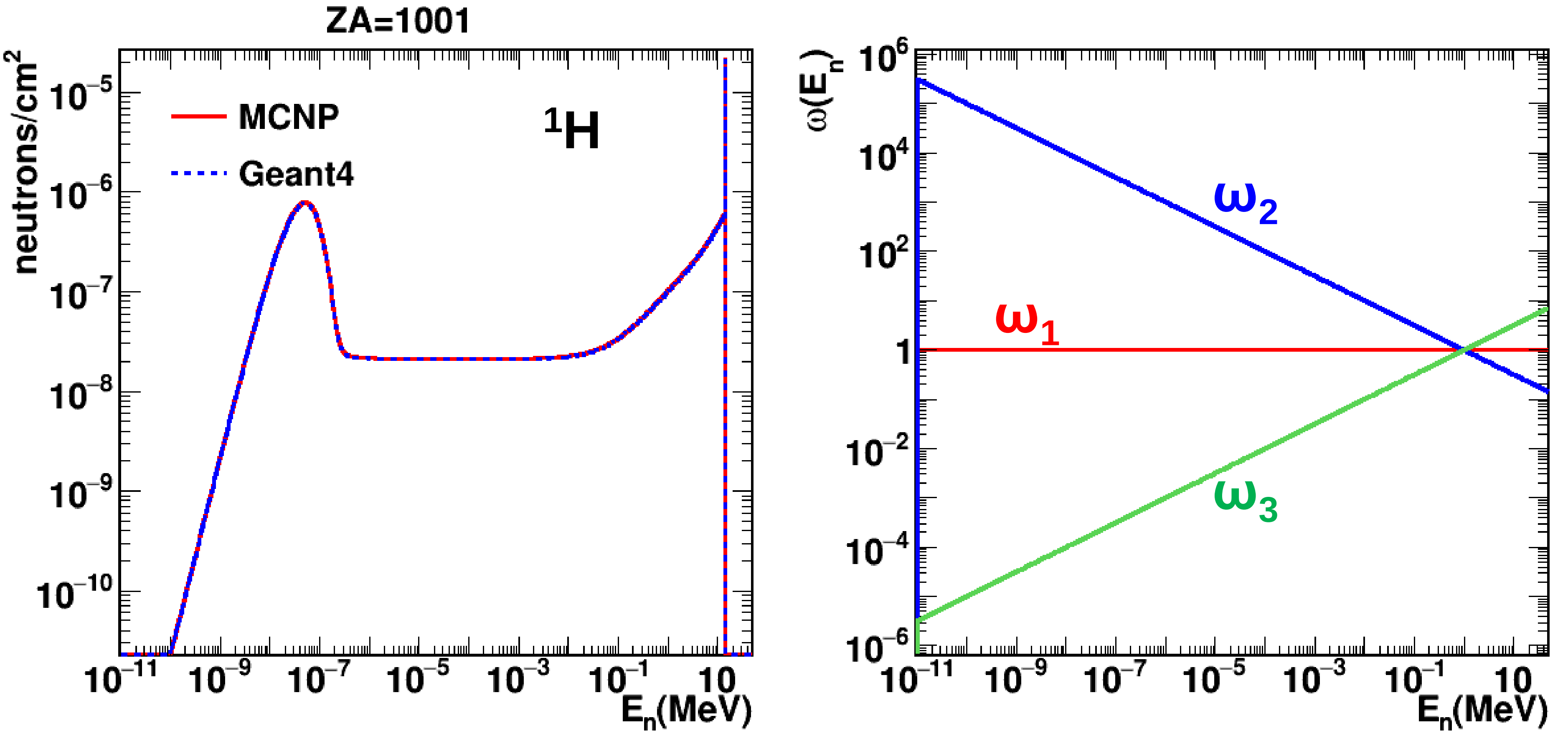
Tallies: neutron flux inside the sphere.

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

Verification tests



Verification tests



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

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

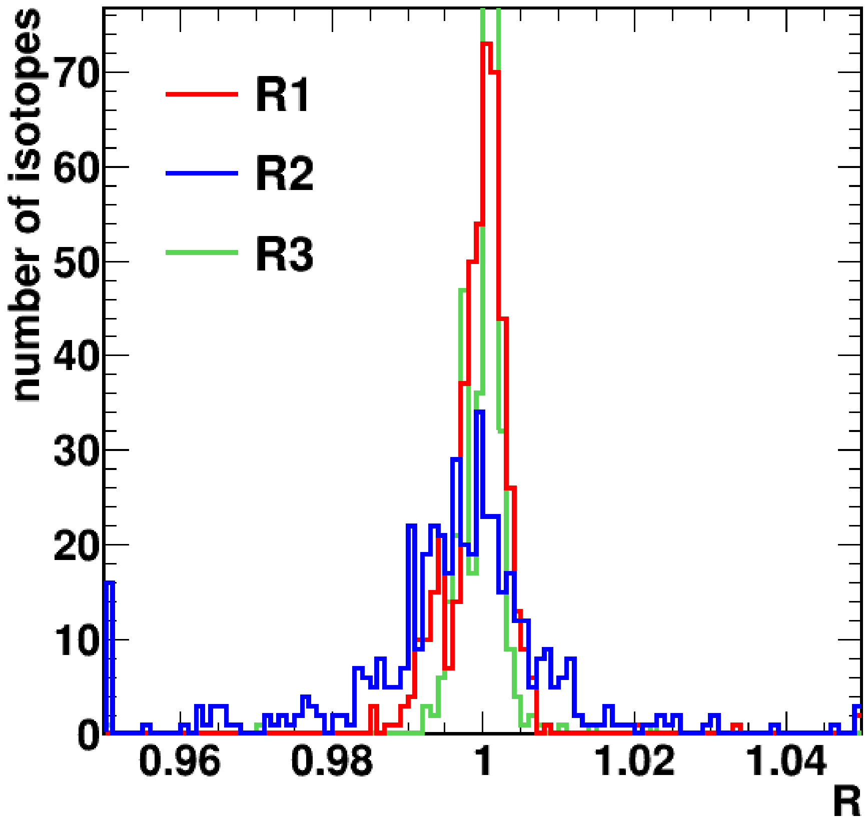
$C_3 = \int \Phi(E) \cdot \sqrt{E}\, dE$

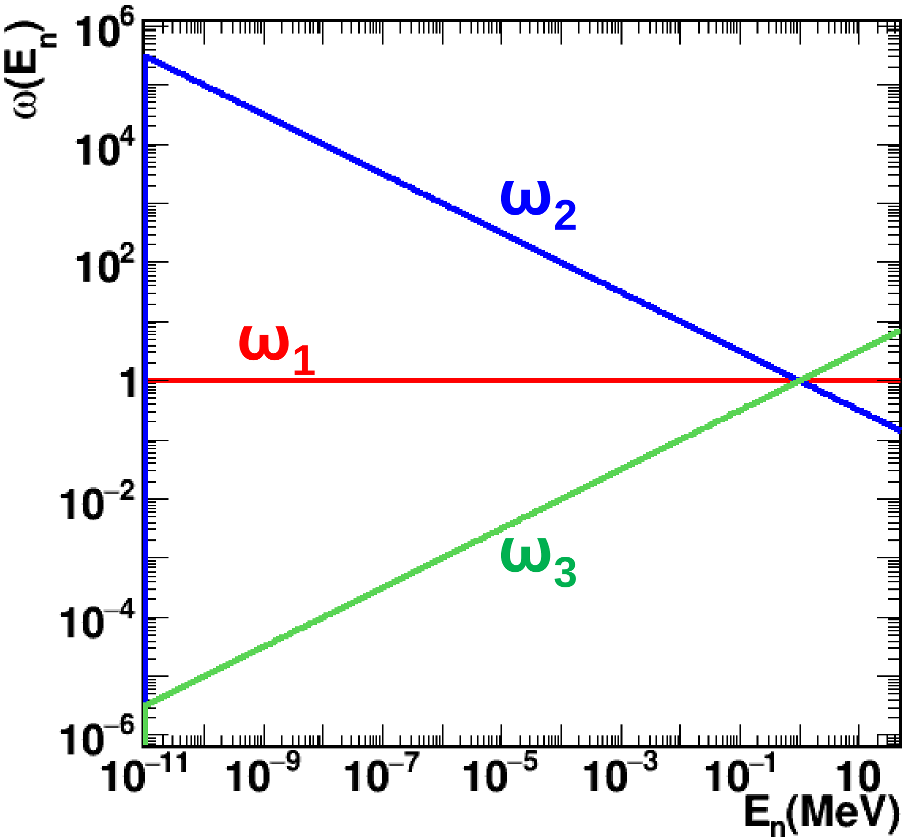
$R_1 = C_1(\text{MCNP})/C_1(\text{Geant4})$

$R_2 = C_2(\text{MCNP})/C_2(\text{Geant4})$

$R_3 = C_3(\text{MCNP})/C_3(\text{Geant4})$

Verification tests





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

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

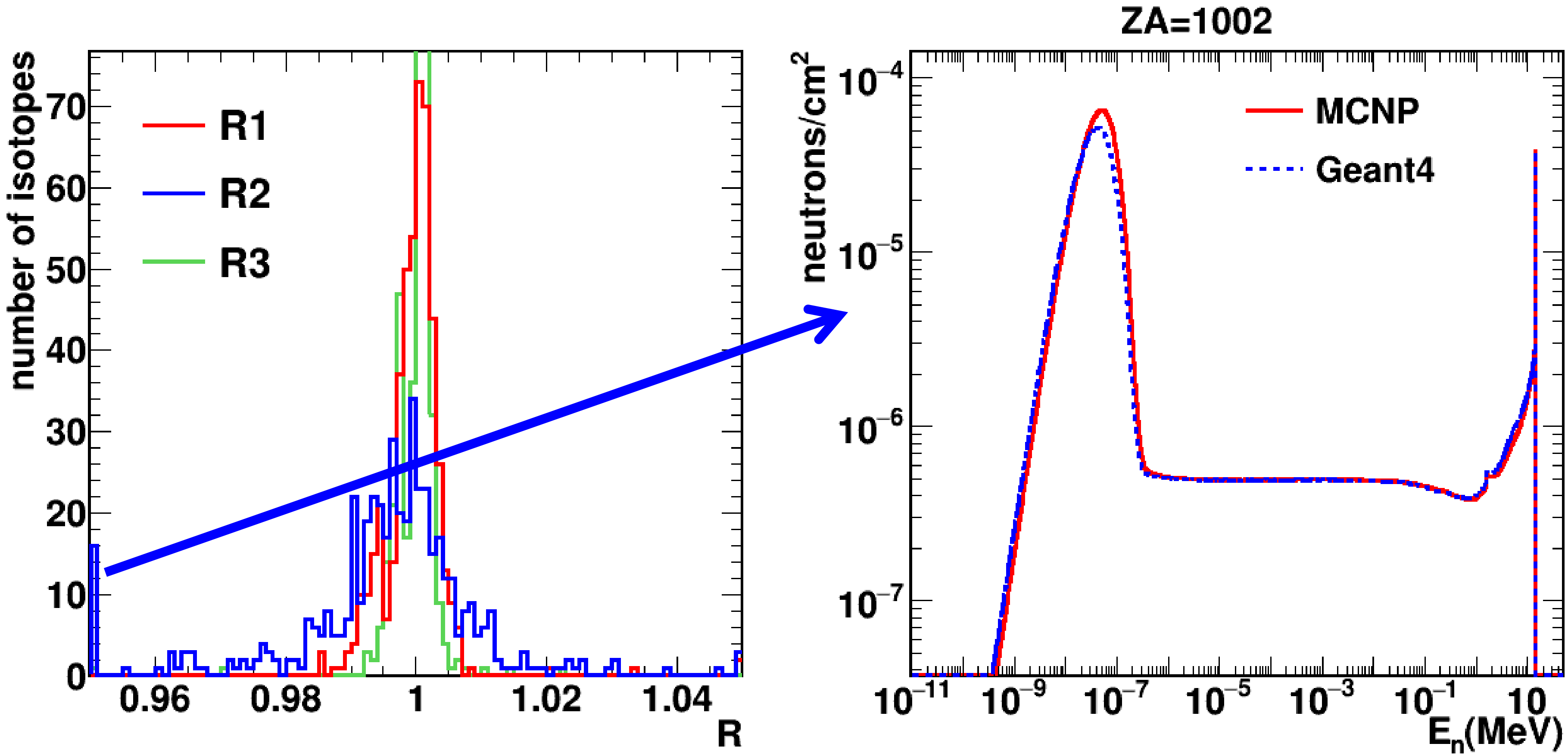
$C_3 = \int \Phi(E) \cdot \sqrt{E}\, dE$

$R_1 = C_1(\text{MCNP})/C_1(\text{Geant4})$

$R_2 = C_2(\text{MCNP})/C_2(\text{Geant4})$

$R_3 = C_3(\text{MCNP})/C_3(\text{Geant4})$

Verification tests



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

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

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

$R_1 = C_1(\mathrm{MCNP})/C_1(\mathrm{Geant4})$

$R_2 = C_2(\mathrm{MCNP})/C_2(\mathrm{Geant4})$

$R_3 = C_3(\mathrm{MCNP})/C_3(\mathrm{Geant4})$

Strengths and limitations

Strengths

- Very nice performance in the neutron transport, according to the verification tests performed (Geant4 VS MCNP).
- Possibility of using different neutron data libraries.

Limitations

- Incident charged particles: has been incorporated more recently → small validation/verification + biasing processes are required in some cases (see talk from D. Cano-Ott 25/04/2019-12:30).
- Energy, momentum, baryonic number … is **in general** not conserved event by event. However, all these quantities are conserved in many practical simulations (case dependent).
- Some complex reactions cannot be described with detail with the ENDF-6 format. Example: $n+^{12}C \rightarrow n+3\alpha$ (organic scintillators – fast neutron detectors) → *A. García et al., NIMA 868, 73 (2017)* :

$$n+^{12}C \rightarrow n'+^{12}C^* \qquad ^{12}C^* \rightarrow \alpha+^{8}Be \qquad ^{8}Be \rightarrow 2\alpha$$

$$n+^{12}C \rightarrow \alpha+^{9}Be^* \qquad ^{9}Be^* \rightarrow n'+^{8}Be \qquad ^{8}Be \rightarrow 2\alpha$$

Future developments

1) Energy-momentum conservation (event by event)

2) Extend the G4ParticleHP 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)

3) Include unresolved resonance range probability table treatment

4) Thermal neutron data libraries: extension + validation (?)

5) Clean-up a bit the code

Energy-momentum conservation

Crucial to calculate response functions

Reaction channels in ENDF-6 databases can be classified as (my classification):

1. **Two body reactions**: (n,n), (n,n'), (n,p), (n,d) …

   → energy-momentum is already conserved in all (*or most of*) the cases

2. **Capture**: (n,γ)

   → energy-momentum is conserved if the G4PhotonEvaporation model is used (can be activated via enviromental variable)

3. **Fission**: (n,f)

   → ?? (Wendt fission model?, GEF?)

4. **Other explicit reactions**: (n,2n), (n,n2a), (n,p2d) …

   → A very simplified model is already inside ParticleHP, used when no data available.

5. **(n,x) reactions**: residual in neutron incident (<20 MeV),dominant in high energy and charged particle incident data libraries.

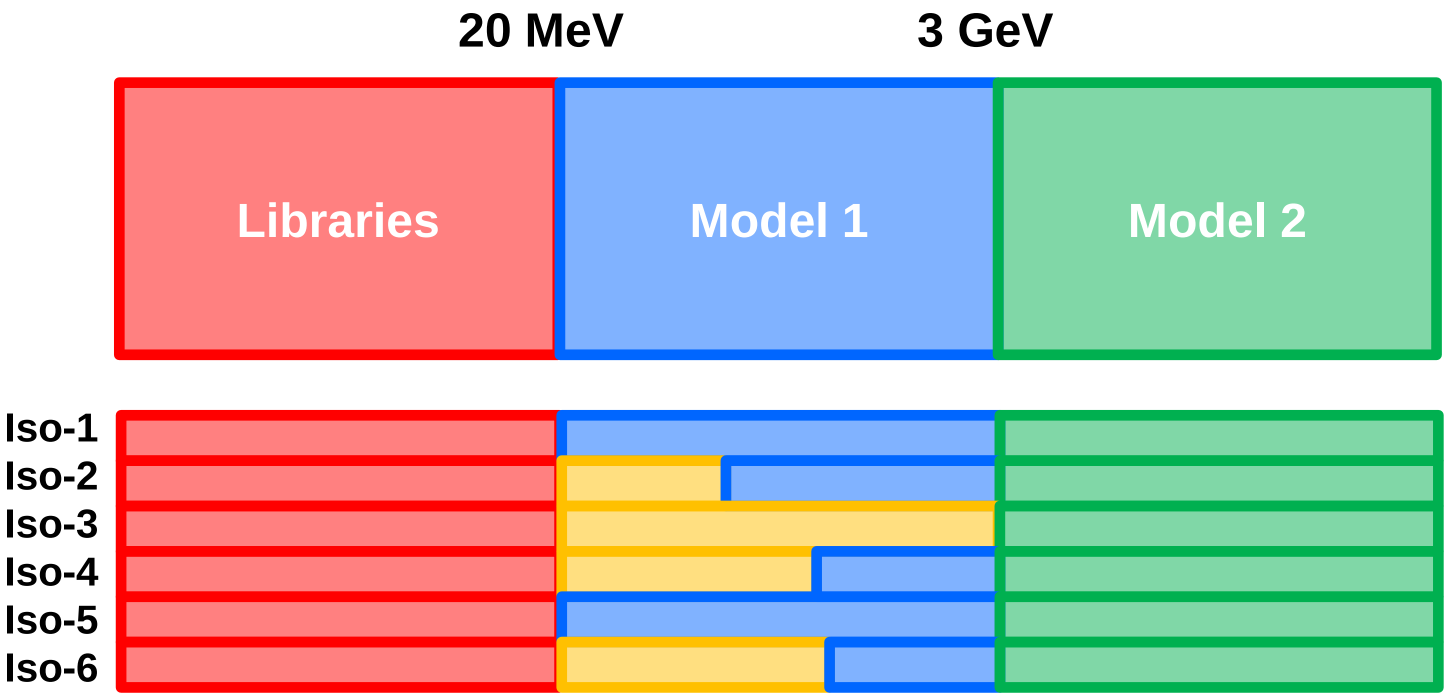
   → ???

Extend the G4ParticleHP model to higher energies

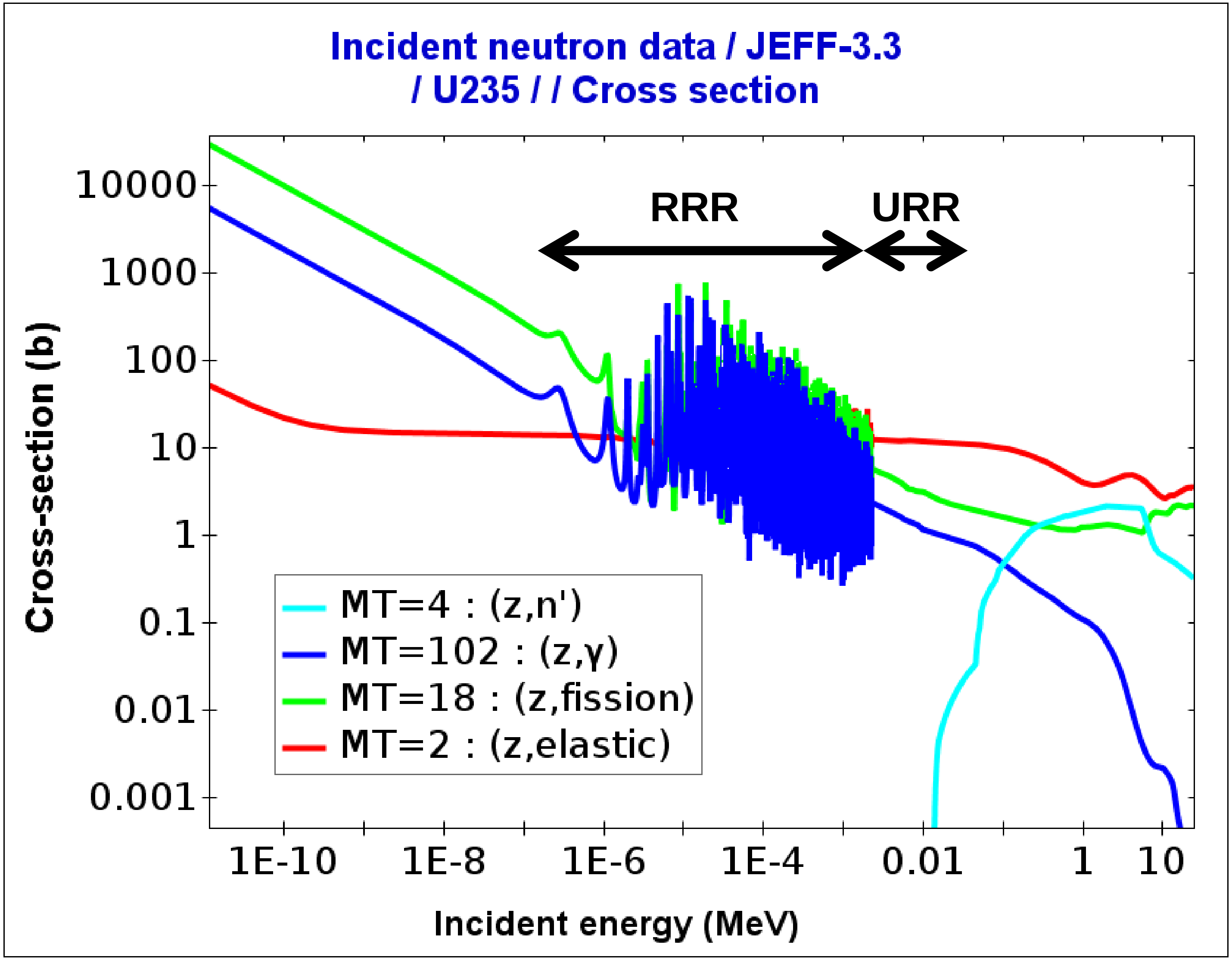
There are some high energy libraries:

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

Difficulty: limited amount of isotopes + not all defined in the same energy range
→ combine data driven models with theoretical models



Include unresolved resonance range probability table treatment



Thermal neutron data libraries

Low energy neutrons (<4 eV) must be transported using the thermal scattering data libraries, which takes into account that the nuclei are in atoms which form part of a certain molecule inside a material.

At present, the isotopes-materials distributed with Geant4 correspond to ENDF/B-VII.0 (20 materials: H in H_2O, C in graphite, O in UO_2 …).

1. Extension of the Geant4 thermal data libraries?
   → ENDF/B-VIII.0 contains 34 materials
   → http://www.cab.cnea.gov.ar/nyr/tsl_eng.html
   → NCrystal code? (https://arxiv.org/abs/1901.08890)

2. Validation/verification of the code?
   → *H.N. Tran, NIMA 893, 84 (2018)*

Summary and conclusions

The G4ParticleHP package is able to use the information available in ENDF-6 format data libraries to transport neutrons (up to 20 MeV) and light charged particles (up to 200 MeV).

The performance of the code has been verified extensively for neutrons. Small verification/validation for incident charged particles.

The result of a simulation performed with G4ParticleHP will depend on the information available in the data library (accuracy + data format). The understanding of the ENDF-6 format helps to know which results can be expected from a simulation and which ones can not.

Future developments have been proposed.