Developments for G4NeutronHP

E. Mendoza, D.Cano-Ott
Nuclear Innovation Unit (CIEMAT)

Presented by P. Arce
Medical Physics group (CIEMAT)

Introduction

The **G4NeutronHP** is the GEANT4 package for simulating the **detailed interaction of neutrons with energies <20 MeV**. The physics relies on the cross section G4NDL libraries, which have been obtained from evaluated neutron data libraries in the ENDF-6 format.

The performance of G4NeutronHP relies on the accuracy of the underlying nuclear experimental and evaluated data. Different evaluated files are available and users should have access to all of them, since there is NO BEST evaluated file.

Work done so far:

•**Eight different libraries** corresponding to the state of art of the evaluated nuclear data. The major libraries have been translated into the G4NDL format.

•**Several bugs** have been found in the GEANT4 code and **corrected/reported**. **New GEANT4 code** has been written for **extending the package capabilities** (i.e. new photon tables). **The work has been reported to T. Koi** and **included in the new Geant4 release**.

•A validation method “isotope by isotope” has been made. The GEANT4 results have been compared systematically with MCNPX for the ENDF-B.VII.0 library. Furthermore, a less exhaustive comparison has been made for other libraries.

Creation of G4NeutronHP data libraries

The following libraries have been translated into the G4NDL format:

ENDF-VII.0 (USA) – 385 isotopes, ENDF-VI.8 (USA) – 317 isotopes, JEFF-3.0 (EU) – 373 isotopes, JEFF-3.1 (EU) – 334 isotopes, **JENDL-4.0 (Japan) – 400 isotopes**, JENDL-3.3 (Japan) – 332 isotopes, BROND-2.2 (Russia) – 120 isotopes, CENDL-3.1 (China) – 239 isotopes.

The latest GEANT4 version tested was: **G4NDL-3.14 (GEANT4) – 181 isotopes**.

Any future release of evaluated libraries will be translated into the G4NDL format and validated before being released.

The files will be distributed by the IAEA nuclear data service (under the agreement CIEMAT – IAEA) and will be kept compatible with the future Geant4 releases (see T. Koi).

Improvements of the Geant4 source code

Description of our contribution to the G4NeutronHP code:

1. Some **bugs have been found and corrected** in the following classes: G4NeutronHPDiscreteTwoBody and G4NeutronHPPartial (see T. Koi talk).
2. Some new upgrades in the ENDF-6 neutron data format were not yet implemented in the GEANT4 code (gamma emission after neutron capture in a specific format). Some new GEANT4 code has been developed in order to be able to read neutron data in this new format.
3. The class G4NeutronHPInelasticCompFS has been modified in order to obtain the energy of the outgoing particles in the (n,{n',p,d,t,^{3}He,α}) reactions from the neutron data libraries information, instead of the excitation energy of the residual nucleus. With the unmodified GEANT4 version, wrong results were obtained for several nuclei.
4. Some additional "problems" are under investigation.

Validation strategy

CIEMAT has defined a validation strategy for the G4NeutronHP code and the new libraries. The same strategy has been adopted for validating the LENDL development (see T. Koi's presentation) and the G4ProtonHP development (see P. Arce's presentation).

Three different validation methods have been applied to the old and new G4NDL neutron data libraries. These methods can be automatically run for an entire library (typically ~300-400 isotopes each library), so a check "isotope-by-isotope" can be easily performed.

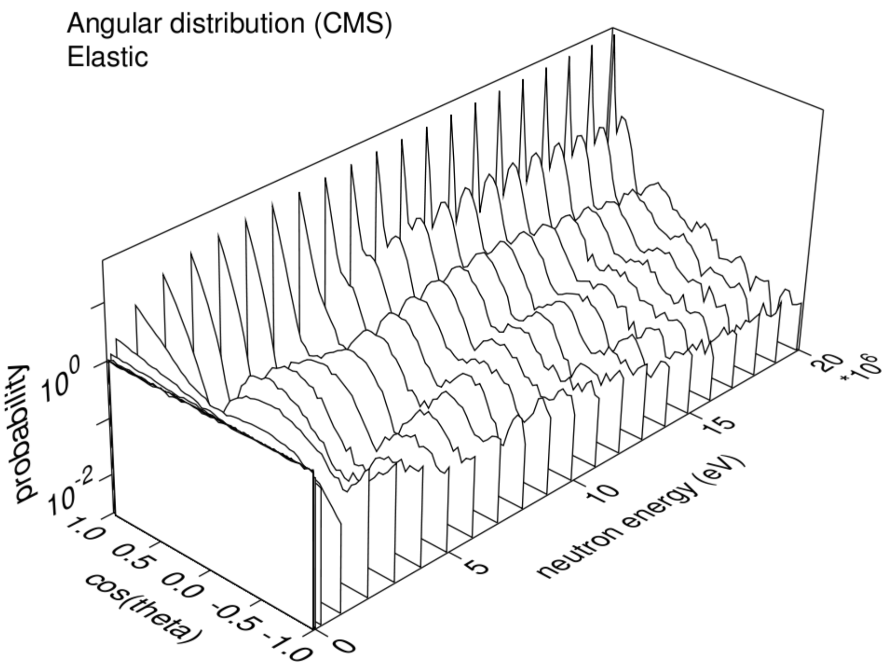
1. The GEANT4 classes are used for sampling all the secondary particle distributions and documented. The users can compare them to the evaluated files, looking for possible discrepancies.

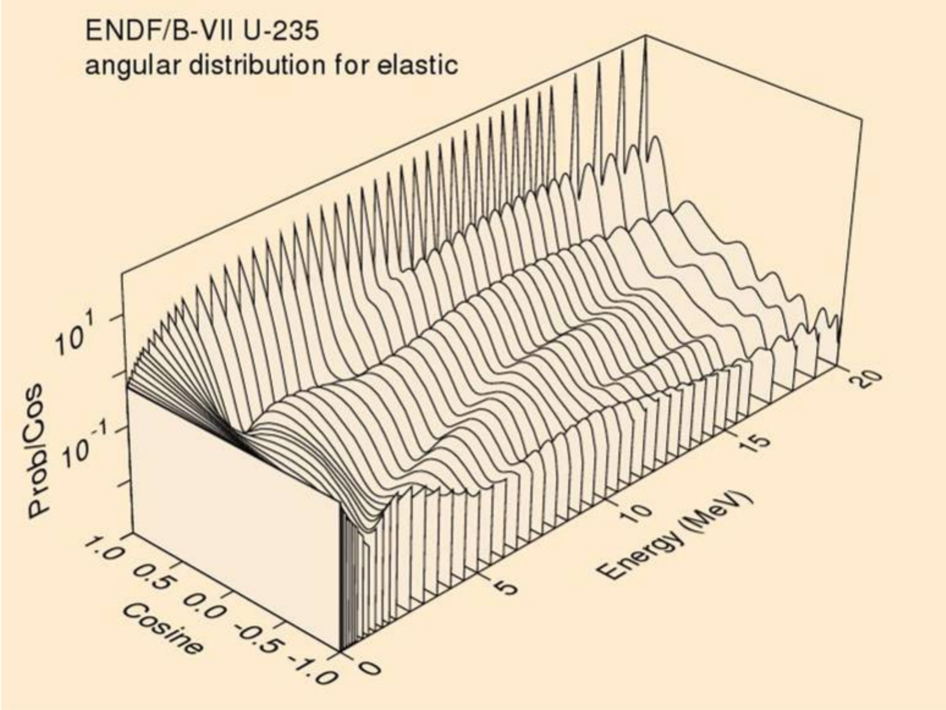
2. + 3. Identical Monte Carlo simulations **for each isotope** are performed with GEANT4 and MCNPX and compared. Again, the same simulation is automatically done for all the isotopes of a certain library.

Validation I (example – elastic scattering on ^{235}U)

Plot obtained by sampling with the GEANT4 classes

Plot obtained with NJOY

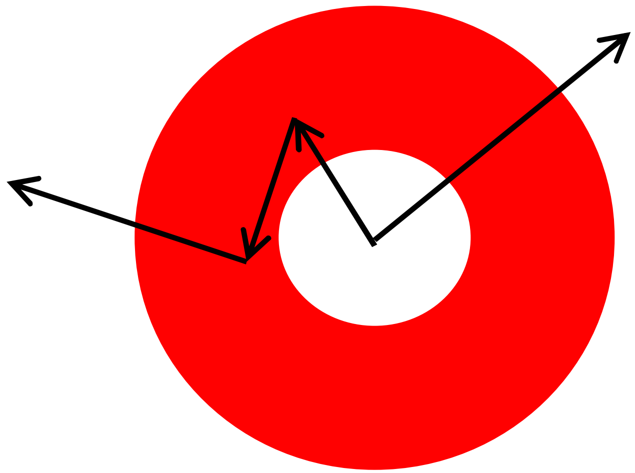




Every quantity has been sampled 50000 times at each energy. Similar plots can be obtained with NJOY. At the moment, the comparison can only be done "by eye". In a future, mathematical quality tests will be applied.

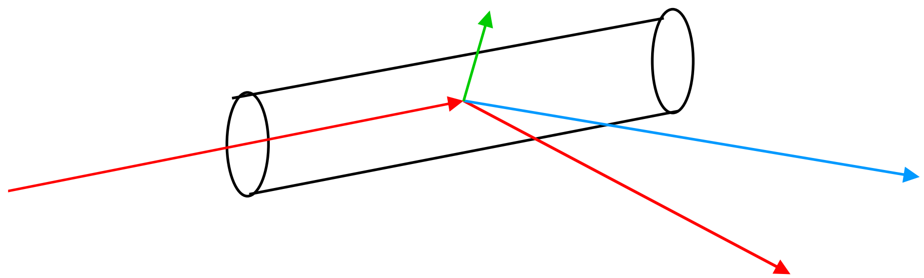
Validation II (MC simulations - sphere)

The transmission through a sphere of 5 cm inner radius and 15 cm outer radius, made of different materials, has been simulated with both Geant4 and MCNPX. 10^6 neutrons have been emitted from the center of the sphere, with energies distributed isolethargicaly between 1.e-10 MeV and 19MeV. Neutrons and gammas crossing the outer surface of the sphere have been histogrammed.



Validation III (MC simulations - cylinder)

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. 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}He,α).

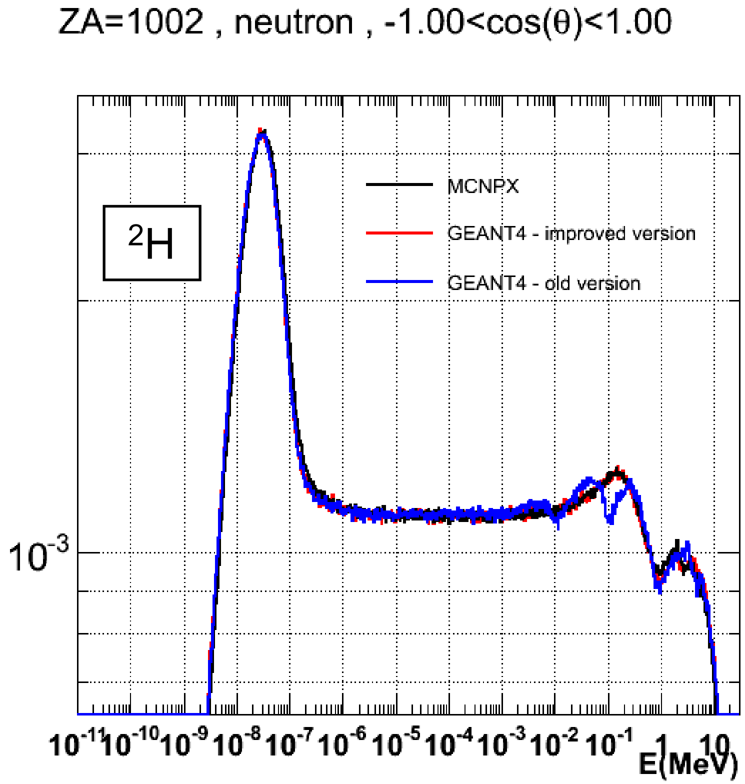


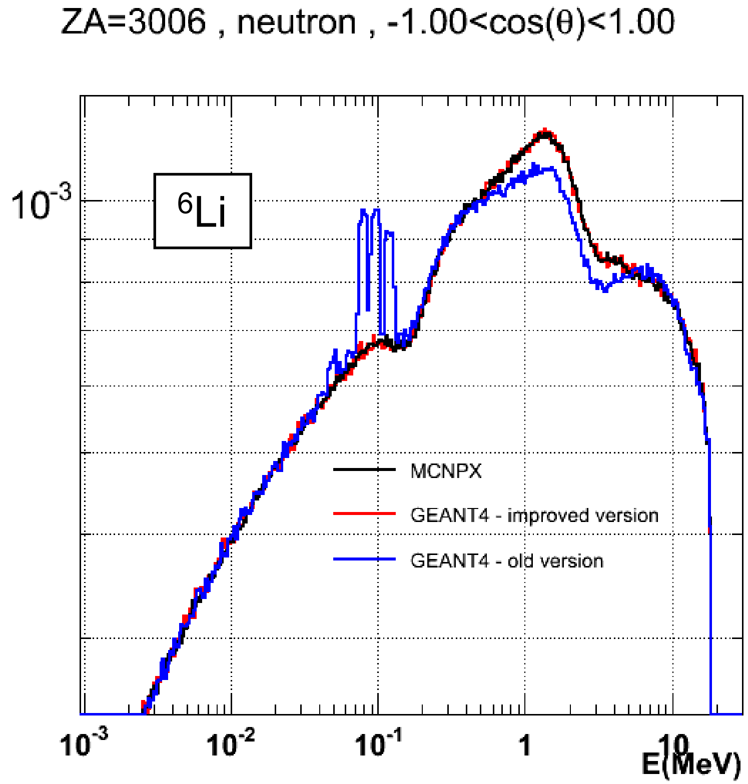
With these simple MC results it is easy to:

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

Validation III - examples

One simulation for each isotope (385) present in the ENDF-VII.0 library has been performed with the cylinder configuration, using MCNPX and different GEANT4 versions. The energy of the outgoing neutrons, for all directions, are presented below, for some example isotopes.





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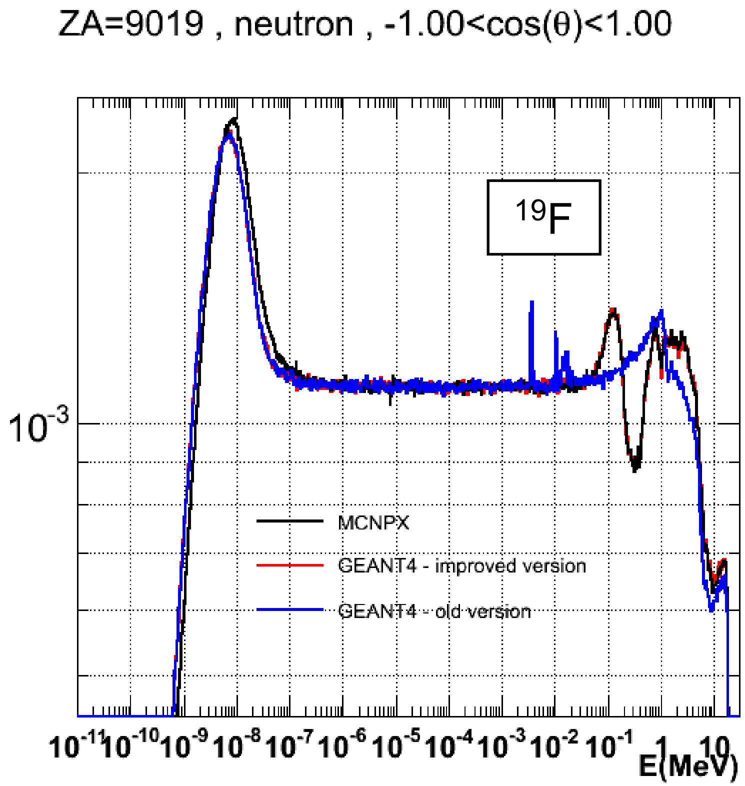
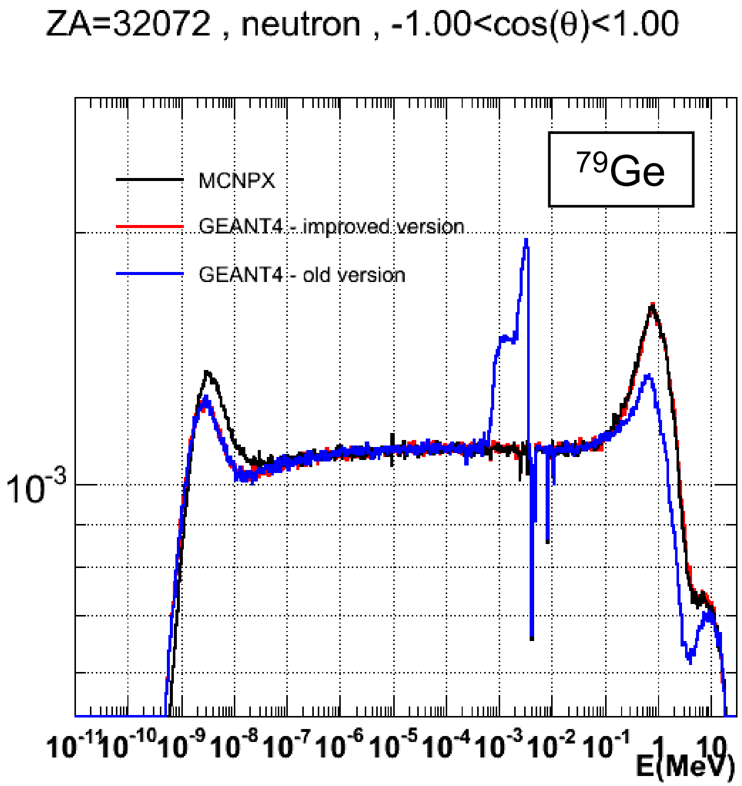
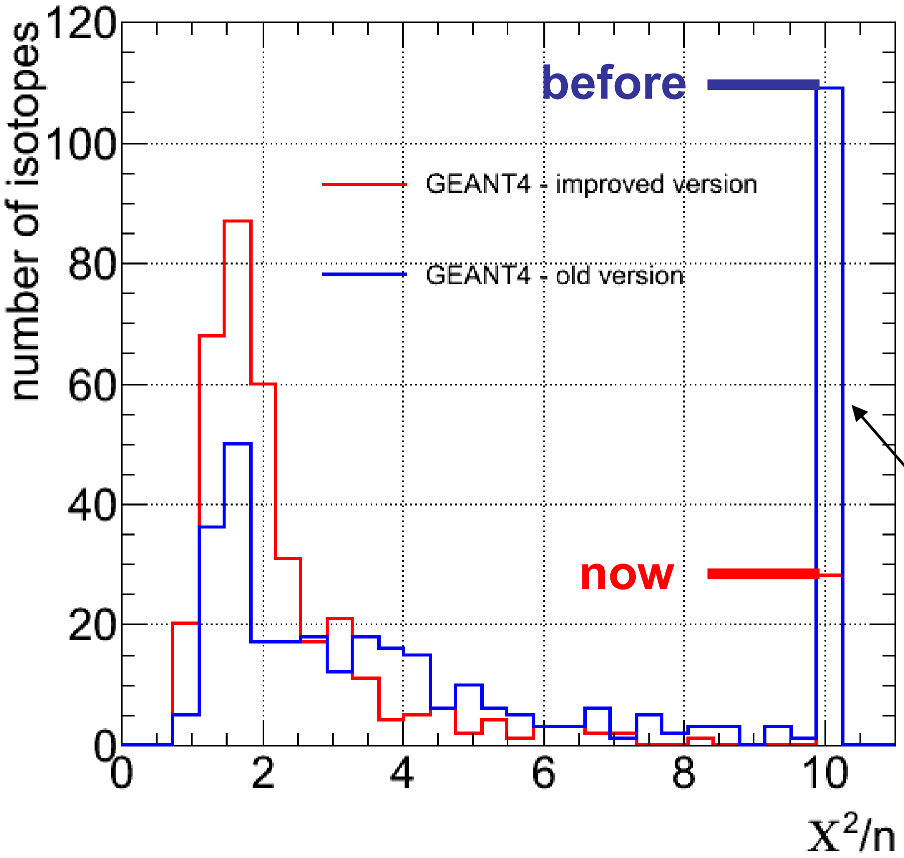




Validation III - results



The $\chi^2/2$ value between the MCNP and GEANT4 results have been computed systematically for all the ENDF-VII.0 isotopes.

$X^2/2$ values greater than 10 have been included in this bin

Conclusions

- A program which “translates” the ENDF-6 neutron data libraries into the G4NDL data format libraries has been developed. Eight different libraries have been translated and they will be distributed from the IAEA web page. This will allow to the users to have a better quality control on their simulations.
- Some validation tools have been developed, capable of making a systematic comparison between codes and libraries for all the isotopes of a certain neutron data library. This tools are useful to detect bugs in the Geant4 code.
- The results of the validations will be make public, to allow the users to compare results between different codes and libraries, isotope by isotope.
- All the developments have been included in the new Geant4 release.

Conclusions

- Some desirable future capabilities of the code have also been identified (breakup reactions, thermal treatment, URR statistical treatment, …).

- As a final conclusion, it can be stated that with additional effort, the G4NeutronHP package can be improved to reach a reliability close to MCNPX in neutron transport problems. MCNPX is however significantly faster and a large programming effort should be made for changing this feature.