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INDC(NDS)-0612
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New evaluated neutron cross section libraries for the GEANT4 code

Prepared by

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April 2012

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Printed by the IAEA in Austria

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Abstract

The so-called High Precision neutron physics model implemented in the GEANT4 simulation package allows simulating the transport of neutrons with energies up to 20 MeV. It relies on the G4NDL cross section libraries, prepared by the GEANT4 collaboration from evaluated cross section files and distributed freely together with the code.

Even though the performance of the G4NDL library has been improved over the time, users running complex simulations which involve the transport of neutrons do need more flexibility, in particular when assessing the uncertainties in the simulation results due to the neutron (and hence the nuclear) data library used. For this reason, a software tool has been developed for transforming any evaluated neutron cross section library in the ENDF-6 format into the G4NDL format. Furthermore, eight different releases of ENDF-B, JEFF, JENDL, CENDL and BROND national libraries have been translated into the G4NDL format and are distributed by the IAEA nuclear data service at www-nds.iaea.org/geant4. In this way, GEANT4 users have access to the complete list of standard evaluated neutron data libraries when performing Monte Carlo simulations with GEANT4. Consistency checks and a first validation of the libraries have been made following the methods described in this report.

April 2012

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1. INTRODUCTION

The G4NeutronHP (High Precision) model implemented in the GEANT4 Monte Carlo 0,[1] code is used to simulate the neutron transport at low energies (below 20 MeV). It relies on G4NDL neutron data files which contain the same type of information that can be found in the standard ENDF-6 formatted data files (cross sections, energy-angular distributions of secondary particles, ...), but the data is written in a different format. A description of the ENDF-6 data format can be found in [3].

A tool which converts the ENDF-6 data files into the GEANT4 ones has been developed for having more flexibility and control of the nuclear data used in GEANT4 simulations. The tool has been used for creating G4NDL like neutron data libraries from any standard evaluated cross section library (ENDF, JEFF, JENDL, CENDL, BROND, ...). In addition, files for some isotopes which are not included in the original G4NDL3.14 library have been created as well: typically G4NDL has information for 180 isotopes, whereas the recent evaluated libraries have about 300 – 400 isotopes.

The GEANT4 data format had been deduced from the GEANT4 source code, since no documentation was available. A computer program was then developed for translating the ENDF-6 formatted evaluated nuclear data libraries into the G4NDL format. This procedure is described in Section 2.

Some new GEANT4 source code had to be written as well, in order to accommodate the most recent upgrades present in the standard libraries. It affects in particular the photon production data associated to the neutron capture process. The standard GEANT4 source code (up to version 9.4) does only allow to deal with data from ENDF-6 files 12,13,14 and 15, while the more recent evaluations like ENDF/B-VII.0 provide information in file 6 for some isotopes. The software developments are described in Section 3 together with some difficulties and limitations associated to the creation of the libraries.

A first validation of the libraries has been made by performing extensive consistency and integrity tests. In addition, Monte Carlo simulations have been performed with GEANT4 for specific cases and compared to the results obtained with MCNPX [4]. Section 4 shows a few examples of the validations and the performance of the new libraries. The conclusions of this work can be found in Section 5.

2. THE PRODUCTION OF THE LIBRARIES

The cross sections used in GEANT4 files have to appear in a linear interpolable form. For this reason, it was necessary to pre-process the ENDF-6 libraries, since the cross section data are given in files MF=2 (resonance parameters) and MF=3 (data points). It was necessary to transform the MF=3 file (which can be expressed also in log-log or linear-log interpolation laws) into a linear-linear interpolable form, and then add the contribution of file MF=2 to file MF=3.

The procedure was performed with the PREPRO software package [5], a collection of public and standard computing codes distributed by the IAEA which allow converting the ENDF-6 libraries into a form required by many applications. The production scheme used is as follows:

1. First, the LINEAR program was applied, for changing the cross section data points in file MF=3 into linear-linear interpolation form. The allowable error was set to 0.1%.
2. Then, the RECENT program was applied, in order to convert the resonance contribution into cross section data points. The allowable error was set to 0.1%.
3. Then, the LINEAR program was applied again, in order to reduce the number of cross section points in file MF=3. The allowable error was set to 1%, since an error smaller than 1% leads to an excessively large number of points (>500.000) for some cross sections.
4. Then, the FIXUP program was applied. It reads the ENDF-6 file and performs some format corrections, if needed.

Once the ENDF-6 data file is processed with PREPRO, the result (still in ENDF-6 format) is translated with a specific program developed by the authors into the G4NDL data format.

3. THE NEUTRON CROSS SECTION LIBRARIES

Eight different libraries have been translated into the G4NDL format: ENDF/B-VI.8 [6], ENDF/B-VII.0 [7], JEFF-3.0 [8], JEFF-3.1 [9], JENDL-3.3 [11], JENDL-4.0 [10], CENDL-3.1 [12] and BROND-2.2. [13]. The corresponding ENDF-6 formatted libraries can be downloaded without restriction from the NEA [14], IAEA [15] or BNL [16] web pages, among other nuclear data services.

Complete G4NDL libraries have been produced for the isotopes listed in there. The files are downloadable from the IAEA nuclear data service website [17].

There were a reduced number of cases for which it was not possible to generate the libraries or the information in the evaluated data library was not complete and additional actions had to be taken. Such exceptions are listed below, together with some additional comments:

1. It has not been possible to generate the G4NDL neutron libraries for three isotopes due to format errors in the evaluated files:
   - ^{nat}Zn (30_nat_Zinc) in the BROND-2.2 library. For the reaction MT=102 (capture) in file MF=12, the value of the flag LO is set to 3, while according to the ENDF-6 manual LO can only take the values 1 or 2.

- ^{nat}S (16_nat_Sulfur) in the ENDF/B-VI.8 library and ^{nat}Fe (26_nat_Iron) in the BROND-2.2 library. PREPRO interprets that some resonance parameters correspond to fission widths and assigns to the isotopes an unphysical fission cross section.
- ^{95}Mo (42_95_Molybdenum) in the JEFF-3.1 library. There is an inconsistency for the reaction MT=849 in file MF=6. The assignments NEP=8, NA=0, NW=24, are wrong, since according the ENDF-6 manual the variables must follow the relation NW=NEP*(NA+2).

2. GEANT4 requires data on the fission (MT=18) cross section and the secondary neutron energy and angular distributions for simulating the fission process. This information does not always appear in the ENDF-6 libraries. Some isotopes do have cross section data but no information is available on the energy of the secondary neutrons or on their angular distributions. If no information on the neutron energy is found, GEANT4 does not crash but no secondary neutron is generated. In order to bypass this problem, if both cross section data and secondary neutron energy distributions are available, the G4NDL libraries have been created by completing the ENDF-6 information with an isotropic angular distribution of the secondary neutrons in the center of mass (CM) system. The correction was made for:

- ^{242}Am (95_242_Americium) in the ENDF/B-VII.0 library.
- ^{241}Am (95_241_Americium) in the JENDL-3.3 library.

The same applies for the reactions MT=19, 20, 21, 38 (first, second, third and fourth chance fission). For some isotopes listed in the ENDF-6 files, the neutron energy distribution is given but their angular distribution is missing. The corresponding G4NDL libraries have been created assuming an isotropic angular distribution in the CM system of the secondary neutrons.

There are three cases for which the energy and angular distributions of the secondary neutrons and gamma rays for MT=18 (fission) reactions are described in MF=6 files:

- ^{232}Th (90_232_Thorium) in the ENDF/B-VII.0 library.
- ^{231}Pa (91_231_Protactinium) in the ENDF/B-VII.0 library.
- ^{233}Pa (91_233_ Protactinium) in the ENDF/B-VII.0 library.

GEANT4 is not able to read such data in MF=6 format. For this reason, the SIXPAK program distributed as part of PREPRO has been used for transforming the MF=6 files into MF=4,5,12,14,15 files, before the translation into the G4NDL format.

3. For some specific reactions and isotopes, the ENDF-6 libraries provide information in the MF=6 file on the angular and energy distributions of the recoil nucleus as an outgoing particle. This information can't be handled by GEANT4 and correspondingly, does not exist in the G4NDL libraries. The information on recoil nuclei in the ENDF-6 files has been omitted during the translation into the G4NDL format.

4. In the ENDF-6 format, the information on the photon production associated neutron capture is usually given in files MF=12, 14 and 15. Some recent evaluations, however, provide the information in MF=6 files (i.e. production yield plus correlated energy and angular distributions) for some isotopes. These isotopes are the ones present in the Capture/FSMF6/ folder. Such a feature was not foreseen in the original GEANT4 source code and thus the class which manages the photon production after capture

(G4NeutronHPCaptureFS) has been modified for supporting the information in MF=6 format. The MF=6 capture data have been translated into G4NDL format in the same way as for other reactions.

5. There are some specific reactions: (n,n'), (n,d), (n,t), (n,^{3}He) and (n,α), i.e., with only one outgoing particle plus the residual nuclei, where the energy of the outgoing particle can be deduced from the emission angle and the energy of the excited state of the residual nucleus. Up to the geant4.9.4 version, this excitation energy was obtained from some specific (non-ENDF) files located in the $G4NEUTRONHPDATA/(library name, i.e. G4NDL3.14)/Inelastic/Gamma folder. It has been observed that in several cases this energy does not correspond to the excitation energy present in the ENDF file and/or the energy of the outgoing particle was calculated wrongly. In order to solve this problem the excitation energy values present in the ENDF files have been included in the new G4NDL files and the class which manages this process (G4NeutronHPInelasticCompFS) has been changed. Such a solution has forced to modify slightly the G4NDL format. The change will be included in the geant4.9.5 release and future versions.

6. The elastic cross sections in ENDF/B-VI.8 of

- ^{40}Ar (18_40_Argon)
- ^{92}Mo (42_92_Molybdenum)
- ^{98}Mo (42_98_Molybdenum)
- ^{100}Mo (42_100_Molybdenum)
- ^{115}In (49_115_Indium)

do not contain the data on the angular distribution of the scattered neutrons, which are necessary for running a GEANT4 application. The G4NDL libraries have been created assuming an isotropic angular distribution for the neutrons in the CM system.

7. In the ENDF-6 libraries, some probability distributions are expressed in terms of Legendre polynomials. The maximum allowed number for the coefficients is 64, whereas G4NDL3.14 (and earlier versions) does only accept up to 30. For the cases where the number of coefficients exceeded the maximum allowed value, the coefficients of order greater than 30 have been omitted.

8. A warning message can appear when using the new G4NDL libraries: "*Warning Transition Energy of repFlag3 is not consistent.*" The warning message can be ignored, since it results from the condition on the equality of two real numbers which are the same within the precision, but not strictly identical. The message "*080808 Something unexpected is happen in G4NeutronHPLabAngularEnergy*" can also appear with some libraries when using the ^{9}Be isotope. The cause of this warning has not been yet identified.

9. The following UNIX environment variables should be set when running a GEANT4 program:

- G4NEUTRONHP_SKIP_MISSING_ISOTOPES=1. It sets to zero the cross section of the isotopes which are not present in the neutron library. If GEANT4 doesn't find an isotope, then it looks for the natural composition data of that element. Only if the element is not found then the cross section is set to zero. On the contrary, if this variable is not defined, GEANT4 looks then for the neutron data of another isotope close in Z and A, which will have completely different nuclear properties.

- G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE=1. If this variable is not defined, a GEANT4 model that attempts to add energy and momentum conservation to some nuclear reactions, by generating artificially some unphysical gamma rays, is activated. The definition of this variable avoids the correction and leads to the result obtained with the ENDF-6 libraries, which intrinsically violate energy and momentum conservation for several processes.
- AllowForHeavyElements=1. Activates the physics for isotopes with Z>92.

10. Evaluated data of isomeric nuclei have also been translated into the G4NDL format. The name of the files of the isomeric nucleus is the same as the ground state ones, but adding "_1" at the end of the name. For example, for the ^{242}Am isomeric nucleus the information is given in the "95_242_Americium_1" files, whereas the ground state one is in the "95_242_Americium" files. It is not possible to define isomeric nucleus in the GEANT4 code, and these new files ending in "_1" are not read by the code. For using them it is necessary to remove the "_1" placed at the end of the file name. It is not possible to use both, the isomeric and the ground state nucleus, at the same time.

4. VALIDATION OF THE LIBRARIES

The validation of the integrity of new G4NDL libraries has been performed by two methods. First, a large collection figures with the graphical representation of cross section data and associated probability distributions has been generated for each isotope and library. The figures are delivered together with the libraries (also from [17]) and will allow the users to verify the correctness of the input data. Second, identical Monte Carlo simulations with the same data library have been performed with GEANT4 and MCNPX, and compatible results were found. More systematic validations are in progress and will be published in a future. However, it should be said that neither the standard G4NDL neutron libraries, nor the codes used for processing them or the GEANT4 simulation package can be declared as bug free. For this reason, users are encouraged to verify always the correctness and coherence of the results obtained.

Validation of the probability distribution sampling

The sampling of the probability distributions contained in the G4NDL data files is carried out by different methods (functions) which are defined in several GEANT4 classes. A computer program based on the GEANT4 classes has been developed for sampling a given number of times every probability distribution present in the G4NDL libraries: the angular and energy distribution of outgoing particles (neutrons, gammas and charged particles) for every reaction (except the energy distribution in elastic scattering, which is calculated from the angular distribution), gamma ray multiplicities for any reaction which emits gammas, and number of neutrons emitted in the fission reaction (prompt and delayed). The GEANT4 version used is 4.9.4.

The sampling has been made for every reaction and every isotope present in all the data libraries at 40 incident neutron energies: 20 discrete energy values distributed isolethargicaly from 10^{-11} MeV to 1 MeV and 20 distributed uniformly from 1 to 20 MeV. Every quantity has been sampled 50000 times for each neutron energy.

Figures for every distribution have been generated with the "*viewr*" program of NJOY [18] and compiled in postscript files together with the cross sections, one for each isotope in each library processed. An example of the plots generated is shown in Figure 1. The sampling of the data with the GEANT4 classes facilitates the detection of possible errors in both the data and the source code.

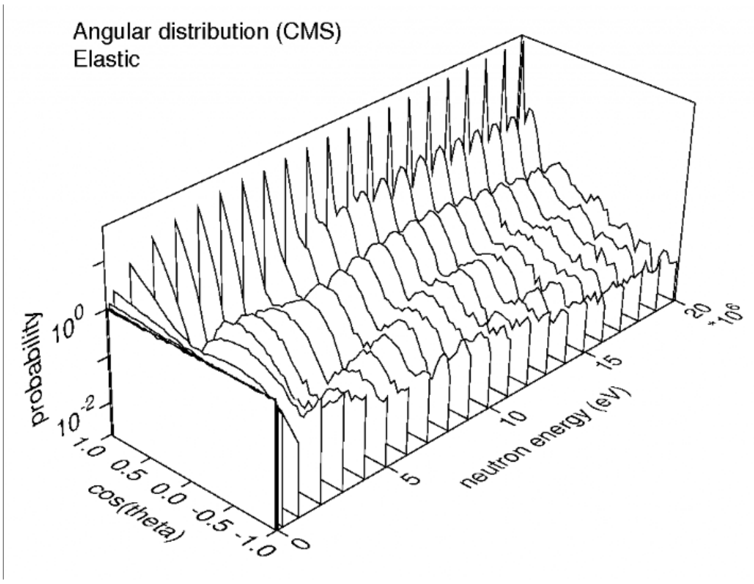

Figure 1 Angular distribution of outgoing neutrons in elastic scattering on $^{235}_{92}U$ *(ENDF/B-VII.0).*

Test Monte Carlo simulations

The performance of the new libraries has been investigated with specific Monte Carlo simulations of simple geometries done with GEANT4 (version 4.9.4). The validation did not pretend to be exhaustive but to reveal differences for materials of common use in experimental nuclear physics and verify the proper functioning of the code with real simulations. The simulations were performed with different libraries and compared to identical calculations performed with the MCNPX Monte Carlo code (version 2.7). The geometry defined consists in a 10 cm thick spherical shell, with an inner radius of 5 cm and an outer radius of 15 cm. An isotropic point like neutron source is located at the geometric centre of the shell and for each case, 10^6 neutrons have been generated with an isolethargic energy distribution ranging from 10^{-10} MeV to 19 MeV. The neutrons and gammas leaving the spherical shell were histogrammed as a function of energy. Despite its simplicity, such geometry is representative of a large variety of problems like a neutron/gamma shielding or a 4π detector.

The materials used in the simulations are: Ge (ρ=5.32g/cm^3), Pb (ρ=11.34g/cm^3), BaF_2 (ρ=4.89g/cm^3), CsI (ρ=4.51g/cm^3), $LaBr_3$ (ρ=5.3g/cm^3), $LaCl_3$ (ρ=3.64g/cm^3), CH_2 (ρ=1g/cm^3) and C_6D_6 (ρ=1g/cm^3), which are detector, shielding and moderator materials commonly used in nuclear physics experiments. Vacuum was used for the void parts of the geometry.

As expected, the results of the simulations depend on the neutron library used, and in several cases the standard neutron library G4NDL3.14 did not show the best performance. For example, the left panel of Figure 2 shows the transmission of the neutrons through a $LaBr_3$ shell, obtained with both codes GEANT4 and MCNPX. As it can be seen, the results obtained when using the same ENDF/B-VII.0 library with both codes are in agreement. The Figure shows as well that the quality of the results depends largely on the nuclear database used. For example, the results for ENDF/B-VII.0 deviate strongly from the calculation obtained with the G4NDL3.14 in the neutron energy region over 400 eV. Even more, the results obtained with JEFF-3.1, which seem to be closer to G4NDL3.14, deviate also from ENDF/B-VII.0. Indeed, this is one illustrative example of why users need access to various nuclear databases, for being able to verify the dependence of their simulations on the nuclear library use.

The reason of the discrepancies observed in Figure 2 originates in the different ^{79}Br neutron capture cross sections in the libraries, as it is shown in the right panel of Figure 2: the description of the ^{79}Br(n,γ) cross section in terms of resolved resonances ends at 400 eV for both the JEFF-3.1 and G4NDL3.14 libraries, whereas it extends up to 5.5 keV in the ENDF/B-VII.0 library. This causes the large differences observed in the transmission spectra above 400 eV. The smaller differences between JEFF-3.1 and G4NDL3.14 result from the resonant description of the ^{81}Br(n,γ) cross section. For G4NDL3.14 the resolved resonance region ends at 400 eV, while in JEFF-3.1 it extends up to 3.63 keV. Thus, it can be concluded that the use of the ENDF/B-VII.0 library leads to more accurate results for this particular case. It should be noticed, however, that this does not allow concluding at all that the ENDF/B-VII.0 library will have a better performance than other evaluated libraries.

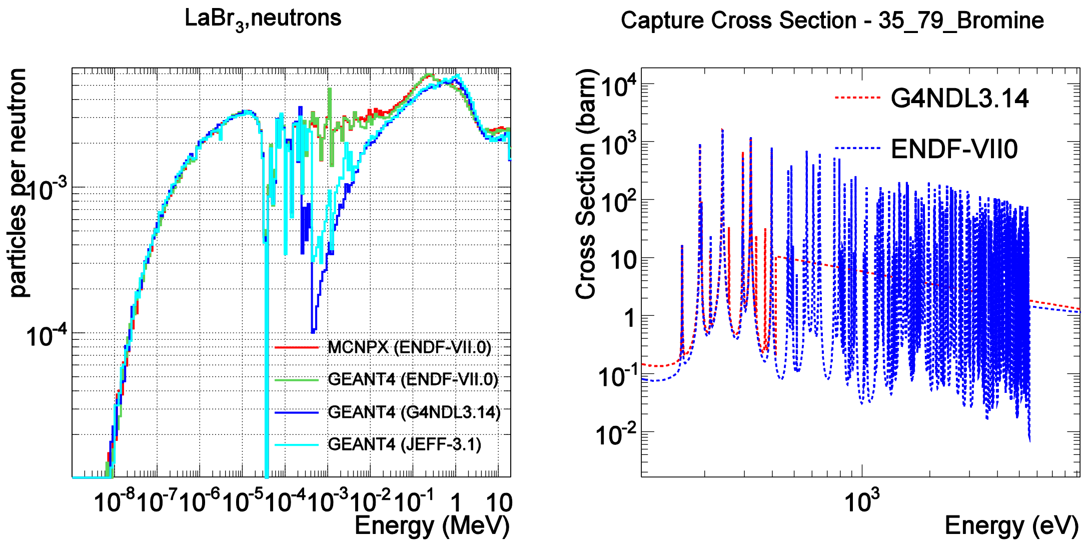

Figure 2 In the left panel, neutrons crossing a $LaBr_3$ sphere for MCNPX and GEANT4 simulations, using different neutron libraries. In the right panel, capture cross section of ^{79}Br in the standard distributed GEANT4 library (G4NDL3.14) and in the ENDF/B-VII.0 library.

A similar behavior has been found in the simulation of a CsI shell, where the energy threshold of resonant description of ^{133}Cs(n,γ) and ^{127}I(n,γ) cross sections did show a significant effect on the results in the range between 100 eV and 10 keV, as it can be seen in the left panel of Figure 3. Such a behavior can however not be made extensive to all the list of materials. As it can be seen in the right panel of the same Figure, the results obtained for a $LaCl_3$ shell with all libraries and codes are compatible.

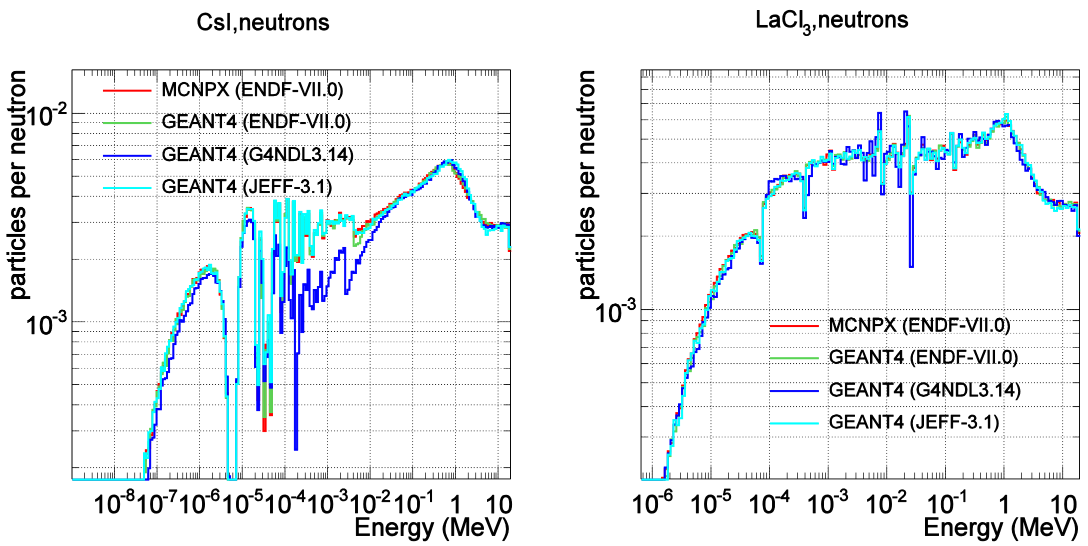

Figure 3 Neutrons crossing a CsI (left) and a $LaCl_3$ (right) sphere for MCNPX and GEANT4 simulations, using different neutron libraries.

The production of secondary particles does also depend on the library used. In particular, the implementation of the treatment of capture data in MF=6 format in GEANT4 has allowed to use evaluated capture data instead of model based parameterisations. Due to its wide use in gamma ray detection, the ^{70}Ge, ^{72}Ge, ^{73}Ge, ^{74}Ge and ^{76}Ge isotopes are a striking example. Only the ENDF/B-VII.0, JEFF-3.1 and JENDL-4.0 libraries do have gamma ray capture data (in file MF=6) and no information is present in the rest of the libraries, including G4NDL3.14. Such a situation is extremely unpleasant due to the many applications that Germanium has in nuclear physics, since it can limit severely the accuracy of Monte Carlo simulations when calculating the interactions of neutrons with Ge, and it has been improved significantly with the new libraries discussed in this work.

Figure 4 shows the photon spectra leaving a spherical shell made of ^{nat}Ge after neutron bombardment. The results obtained with MCNPX and GEANT4 with ENDF/B-VII.0 are identical, thus showing the correctness of the implementation of the new source code for the MF=6 file treatment. The results are also identical to the simulation performed with JENDL-4.0, and are remarkably different from the JEFF-3.1 case, which does also provide capture gamma ray data. This is another example of how the use of different data libraries can lead to incompatible results. Last, the use of the G4NDL3.14 library, which triggers a gamma production model, is not compatible with any of the previous libraries mentioned.

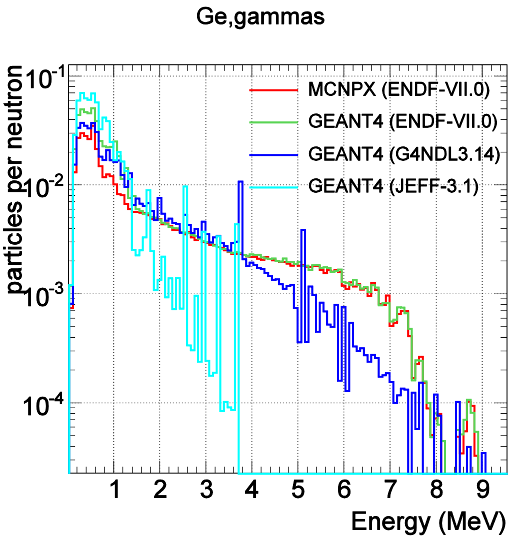

Figure 4 Gammas crossing a Ge sphere for MCNPX and GEANT4 simulations, using different libraries. Results obtained with JENDL-4.0 are the same as those obtained with ENDF/B-VII.0.

For the comparison of the results between MCNPX and GEANT4, it is necessary to consider also the physics models or thermal neutron libraries which describe the neutron interactions of neutrons at thermal energies. Most of the evaluated neutron data libraries do have a reduced set of specific thermal neutron data libraries for the most relevant materials used as moderators. Such libraries have not been processed and the standard thermal libraries distributed with GEANT4 have been used when possible. For the large majority of isotopes, the thermalisation process is described by models.

The simulations have evidenced differences due the neutron energy physics models implemented in both MCNPX and GEANT for the description of the thermalisation process. Such differences become particularly large when dealing with low mass number materials, which act as neutron moderators. The right panel of Figure 5 shows the energy distribution of the neutrons transmitted through a spherical shell made of polyethylene (CH_2). The four calculations visible have been performed with both GEANT4 and MCNPX and the ENDF/B-VII.0, with and without thermal libraries for ^{1}H in polyethylene. It can be appreciated that all four curves do agree for neutron energies above 1 eV. It can be also observed that the magnitude of thermalisation peaks obtained with GEANT4 and MCNPX differ largely when physics models are used (solid and dashed lines). However, when a detailed thermal treatment is made in both codes (represented by the grey and dotted lines) by using the thermal scattering data for polyethylene, the results do agree. The conclusion is that users interested in problems where moderation is relevant will have to pay special attention in using the adequate thermal data and, if they are not available, will very likely obtain different (and presumably inaccurate) results with both GEANT4 and MCNPX.

Even though the effect is enhanced for light materials, it can be still sizeable for heavier materials and should be therefore taken into account. The right panel of Figure 5 shows the energy distribution of the neutrons transmitted through a spherical shell made of BaF_2, calculated with different libraries. Since no thermal data are available for BaF_2, a model based thermalisation is applied in both codes. As it can be seen, the three results obtained with GEANT4 are similar at neutron energies below 1 eV, but deviate substantially from the calculation made with MCNPX. Again, this is explained due to the differences in the thermalisation models used by MCNPX and GEANT4.

The source of the differences is still under investigation and will be subject of a future work. At present, it has been attributed to the different treatment of the Doppler Effect in the two codes.

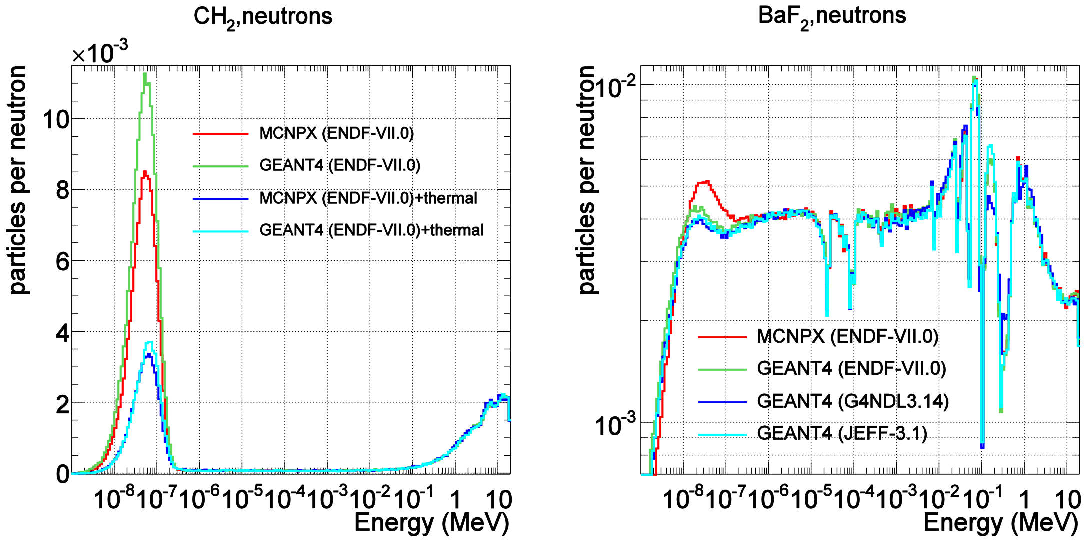

Figure 5 Neutrons crossing a CH_2 (polyethylene) sphere for MCNPX and GEANT4 simulations, using the ENDF/B-VII.0 library in both cases, and performing the simulations with and without neutron thermal libraries (left). Neutrons crossing a BaF_2 sphere for MCNPX and GEANT4 simulations, using different libraries. Results obtained with JEFF-3.0 and JENDL-3.3 are similar to those obtained with G4NDL3.14 (right).

5. CONCLUSIONS

A tool which converts ENDF-6 formatted neutron data files into the G4NDL format used by the GEANT4 simulation package has been developed. A new set of G4NDL neutron data libraries has been created from the following evaluated neutron data libraries: ENDF/B-VI.8, ENDF/B-VII.0, JEFF-3.0, JEFF-3.1, JENDL-3.3, JENDL-4.0, CENDL-3.1 and BROND-2.2. Any future release of the ENDF-6 formatted data libraries will be created as well.

New GEANT4 source code has been written for reading capture data in the MF=6 files, for which GEANT4 was not prepared. This has allowed replacing the model driven gamma ray production by experimental data for elements as important as Ge.

The libraries produced have been tested by sampling all the probability distributions for all the isotopes with the same C++ classes used in the standard GEANT4 code.

Specific Monte Carlo simulations of simple geometries have been performed with GEANT4 and MCNPX for validating the new libraries. It has been concluded that both GEANT4 and MCNPX do obtain compatible results when the same libraries are used. Furthermore, both GEANT4 and MCNPX agree when thermal data are used, but such data are available only for a reduced set of materials. Discrepancies have been found however in simulations where the thermalisation of the neutron becomes important.

6. ACKNOWLEDGMENTS

This work was supported in part by the Spanish national company for radioactive waste ENRESA, through the CIEMAT-ENRESA agreements on “Transmutación de residuos radiactivos de alta actividad", the Spanish “Plan Nacional de I+D+i de Física de Partículas (project FPA2008-04972-C03-01)”, the Spanish Ministerio de Ciencia e Innovación through the “CONSOLIDER CSD 2007-00042” project and the European Commission 7th Framework Program project ENSAR.

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