Necessary improvements of G4NeutronHP for the new libraries. Resolved and open questions.

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Necessary implementations

- For the use of the new generated neutron libraries it is necessary to include the possibility of reading capture photon data in MF=6 format. This can be done (and it has been done), by performing a very little modification in the GEANT4 code, since GEANT4 reads and interprets photon data in MF=6 format for other reactions (inelastic = all except elastic, capture and fission).

- Same for neutrons in the fission process, but only for three isotopes: 232Th, 231Pa, 233Pa in ENDF_VII.0. The MF=6 format data has been translated into MF=4,5 (uncorrelated) data, but maybe for a future it would be better to use MF=6 format.

Neutron validation results

In the GEANT4 comparison with MCNPX done up to now, three main differences have been found:

1- Thermal neutrons: include more thermal neutron libraries?. There are only three materials available, whereas there are 20 in ENDF-VII.0, 9 in JEFF-3.1, 15 in JENDL-4.0, …

2- The “inelastic” problem: cross sections should include the QI value for the calculation of the energy secondary particle, instead of using the Inelastic/Gamma folders.

→ include Breakup reactions?

3- Self shielding treatment: some procedure to treat the URR could be implemented. It should be based in cross section evaluated data for the URR: statistical parameters such as the main distance between resonances, size, …

4- Fission???

Non-neutron validation results

- No validation for particle production (different) than neutrons have been performed by CIEMAT.

- Gamma production:

1- Gamma production in ENDF files is usually UNCORRELATED data.

2- Gamma production in ENDF files can be incomplete or missing.

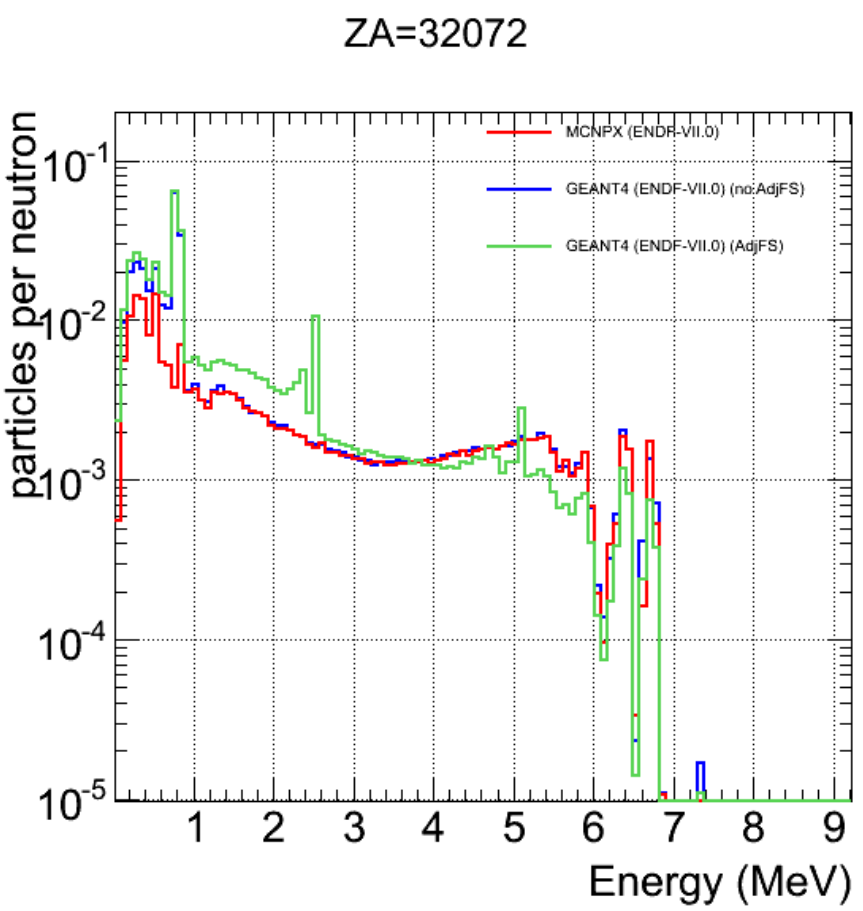
Possibilities to manage the photon production in GEANT4:

1- Use ENDF data (only).

2- Use models.

3- Use both ???

Mixing models with ENDF data has to be done with extremely care.

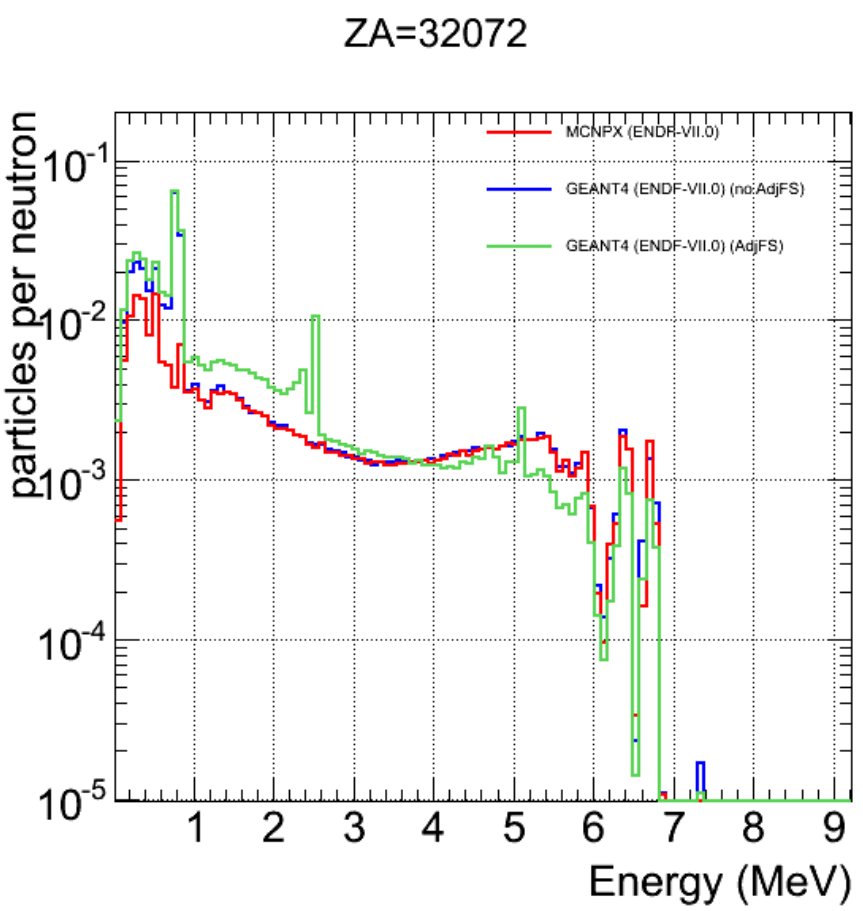


Non-neutron validation results

Possible solution: include a flag which specifies how to manage the photon production data.

- PFlag=0: use ENDF data.
- PFlag=1: use models.
- PFlag=2: use ENDF data, if there is no data, use models.
- PFlag=3: …

→ adjust_final_state method of the G4NeutronHPFinalState class.



General comments

1- Lack of data: ENDF format libraries have some amount of isotopes. However, there are:

A- Some isotopes are missing.

B- The information for each isotope has to be, in principle, complete (exception: ROSFOND library). However, this doesn't mean that all reactions are 100% perfectly described, specially for secondary particles different than neutrons.

What to do?

A- By default, if one isotope is missing, take the natural component (Warning in the output), if there is no natural component, exit.

(export G4NEUTRONHP_SKIP_MISSING_ISOTOPES=1)

B- Several options can be taken:

1- Perform the simulation with the available data (do not generate secondary particles if there is no data).

2- Use models.

3- Distribute only isotopes with some minimal information.

4- Use some flags to determine what to do.

5- …

General comments

- One idea is to implement the possibility of writing into a file information concerning the G4NDL data which has been read, the data which is going to be used in the simulation.

2. Additional ENDF data: There is some information in the ENDF-6 format files which are not used (?) by GEANT4. Some source code can be developed in order to use this information. In particular:

1- File MF=8: Radioactive decay and fission product yield data.

2 – File MF=9: Multiplicities for production of radioactive nuclides.

3 – File MF=10: Cross sections for production of radioactive nuclides.

4- Files MF=30-40: Covariance data.

3. Reaction MT=5: this is an special reaction. It is an undefined reaction, it can be every mix of reactions. The residual nucleus is not well determined.

4. Residual nucleus: sometimes there are residual nuclei information in the ENDF data files, as an outgoing particle. This information is not used by GEANT4.

Additional comments

- Some classes should be revised:

+ G4NeutronHPContAngularPar: there are some ENDF data which is not well interpreted.

+ G4NeutronHPDiscreteTwoBody: some errors in the code.

+G4NeutronGPInelasticComp: the two_body_reaction method should be revised.