The G4ParticleHP package

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ENDF-6 format libraries

There aren't many isotopes with charged particle evaluated libraries. For some of the most common libraries, that information can be found in:

http://www.nndc.bnl.gov/sigma/

A list of some of these libraries, the ones that have been processed at this moment, is presented here, with the incident particle energy range where the reactions are described:

ENDF-6 format libraries

ENDF-VII.0 - proton					
Isotope	Emin (eV)	Emax (eV)	Isotope	Emin(eV)	Emax (eV)
1_2_Hydrogen	3.33712e+06	1.5e+08	28_60_Nickel	1.35493e+06	1.5e+08
1_3_Hydrogen	1.0191e+06	2e+07	28_61_Nickel	1e+06	1.5e+08
2_3_Helium	7.329e+06	2e+07	28_62_Nickel	1.192e+06	1.5e+08
3_6_Lithium	500	2.5e+06	28_64_Nickel	1.36703e+06	1.5e+08
3_7_Lithium	1000	1e+07	29_63_Copper	1e+06	1.5e+08
4_9_Berylium	1e-05	1.13e+08	29_65_Copper	1e+06	1.5e+08
5_10_Boron	9999.99	3e+06	41_93_Niobium	1e+06	1.5e+08
6_12_Carbon	4.81201e+06	1.5e+08	74_182_Tungsten	2e+06	1.5e+08
7_14_Nitrogen	2.4795e+06	1.5e+08	74_183_Tungsten	2e+06	1.5e+08
13_27_Aluminum	888615	1.5e+08	74_184_Tungsten	2e+06	1.5e+08
14_28_Silicon	2e+06	1.5e+08	74_186_Tungsten	2e+06	1.5e+08
14_29_Silicon	1.98201e+06	1.5e+08	80_196_Mercury	4e+06	1.5e+08
14_30_Silicon	2.97886e+06	1.5e+08	80_198_Mercury	4e+06	1.5e+08
15_31_Phosphorous	987998	1.5e+08	80_199_Mercury	4e+06	1.5e+08
20_40_Calcium	3.43e+06	1.5e+08	80_200_Mercury	4e+06	1.5e+08
24_50_Chromium	965087	1.5e+08	80_201_Mercury	4e+06	1.5e+08
24_52_Chromium	1.46205e+06	1.5e+08	80_202_Mercury	4e+06	1.5e+08
24_53_Chromium	948711	1.5e+08	80_204_Mercury	4e+06	1.5e+08
24_54_Chromium	968722	1.5e+08	8_16_Oxygen	6e+06	1.5e+08
26_54_Iron	1.43453e+06	1.5e+08	82_206_Lead	3e+06	1.5e+08
26_56_Iron	1e+06	1.5e+08	82_207_Lead	3e+06	1.5e+08
26_57_Iron	1e+06	1.5e+08	82_208_Lead	3e+06	1.5e+08
28_58_Nickel	1.47982e+06	1.5e+08	83_209_Bismuth	4e+06	1.5e+08

ENDF-6 format libraries

ENDF-VII.0 - deuteron					
Isotope	Emin (eV)	Emax (eV)	Isotope	Emin(eV)	Emax (eV)
1_2_Hydrogen	100	1e+07	3_6_Lithium	2000	5e+06
1_3_Hydrogen	100	3e+07	3_7_Lithium	19998.8	2e+07
2_3_Helium	800	1.4e+06			

ENDF-VII.0 - triton					
Isotope	Emin (eV)	Emax (eV)	Isotope	Emin(eV)	Emax (eV)
1_3_Hydrogen	100	2e+07	3_6_Lithium	19999.9	2e+07
2_3_Helium	1000	2e+07			

ENDF-VII.0 – 3He					
Isotope	Emin (eV)	Emax (eV)	Isotope	Emin(eV)	Emax (eV)
2_3_Helium	4000	2e+07	3_6_Lithium	20000	2e+07

JENDL-3.3 - alpha					
Isotope	Emin (eV)	Emax (eV)	Isotope	Emin(eV)	Emax (eV)
3_6_Lithium	6.31317e+06	1.5e+07	7_14_Nitrogen	6.08805e+06	1.5e+07
3_7_Lithium	4.3809e+06	1.5e+07	7_15_Nitrogen	8.13108e+06	1.5e+07
4_9_Berylium	200000	1.5e+07	8_17_Oxygen	800000	1.5e+07
5_10_Boron	1e+06	1.5e+07	8_18_Oxygen	851698	1.5e+07
5_11_Boron	1e+06	1.5e+07	9_19_Fluorine	2.3629e+06	1.5e+07
6_12_Carbon	1.13376e+07	1.5e+07	11_23_Sodium	3.48187e+06	1.5e+07
6_13_Carbon	780000	1.5e+07			

ENDF-6 format libraries

Other set of libraries are the TENDL libraries, which are libraries in the ENDF-6 format produced by the TALYS code. Information and the libraries can be found in:

ftp://ftp.nrg.eu/pub/www/talys/tendl2010/tendl2010.html

There are TENDL libraries for neutron, proton, deuteron, triton, ^{3}He, alpha and gamma incident particles. There are data for a large amount of nuclei, up to 200MeV incident energy.

The new G4ParticleHP package

The elastic cross section of charged particles includes a Coulombian contribution, a nuclear contribution and an interference between both contributions. Since Coulombian interaction have infinite range, the elastic cross section is infinite. Because of this, some difficulties arise when simulating elastic scattering of charged particles. There are information concerning this reaction in the ENDF-6 format files, but nothing has been done at this moment.

The new G4ParticleHP package

For the non-elastic scattering, the following GEANT4 classes have been modified in order to manage charged particles instead neutrons:

Concerning the cross sections:

G4ParticleHPInteractionData: modification of the G4NeutronHPInelasticData class.

G4ParticleHPElementData: modification of the G4NeutronHPElementData class.

G4ParticleHPIsoData: modification of the G4NeutronHPIsoData class.

Concerning the final states:

G4ParticleHPInteraction: modification of the G4NeutronHPInelastic class.

G4ParticleHPInteractionFS: modification of the G4NeutronHPInelasticBaseFS class.

G4ParticleHPInteractionCompFS: modification of the G4NeutronHPInelasticCompFS class.

G4ParticleHPChannel: modification of the G4NeutronHPChannel class.

G4ParticleHPChannelList: modification of the G4NeutronHPChannelList class.

It is not clear that the latest two classes are necessary.

The ENDF-6 format libraries have been translated into the GEANT4 format in the same way as it is done for neutrons.

The new G4ParticleHP package

```
*****************************************************************************
  G4HadronElasticProcess* theElasticProcess = new G4HadronElasticProcess;
  G4LElastic* theElasticModel = new G4LElastic;
  theElasticProcess->RegisterMe(theElasticModel);
  pmanager->AddDiscreteProcess(theElasticProcess);
#ifndef USEALPHALIB
        //-----------------------------------------------------
        //Old way:
        G4AlphaInelasticProcess* theInelasticProcess =
          new G4AlphaInelasticProcess("inelastic");
        G4LEAlphaInelastic* theLEInelasticModel =
          new G4LEAlphaInelastic;
        theInelasticProcess->RegisterMe(theLEInelasticModel);
        pmanager->AddDiscreteProcess(theInelasticProcess);
        //-----------------------------------------------------
#else
        //-----------------------------------------------------
        //New way:
        G4AlphaInelasticProcess* theInelasticProcess = new G4AlphaInelasticProcess("inelastic");
        G4LEAlphaInelastic* theLEInelasticModel = new G4LEAlphaInelastic;
        theLEInelasticModel->SetMinEnergy(199*MeV);
        theInelasticProcess->RegisterMe(theLEInelasticModel);
        G4ParticleHPInteraction* theAlphaHPInelastic=new G4ParticleHPInteraction("G4ALPHAHP");
        theInelasticProcess->RegisterMe(theAlphaHPInelastic);
        G4ParticleHPInteractionData* theAlphaHPInelasticData=new G4ParticleHPInteractionData(particle,"G4ALPHAHP");
        theInelasticProcess->AddDataSet(theAlphaHPInelasticData);
        pmanager->AddDiscreteProcess(theInelasticProcess);
        //-----------------------------------------------------
#endif
*****************************************************************************
export G4ALPHAHP="/home/u5491/programs/geant4/data/ChargedHP/JENDL330_alpha"
```

The new G4ParticleHP package

The same classes are used for all particles.

There are three folders in the library (located at “G4ALPHAHP” or similar):

- CrossSection: with the total non-elastic cross section.
- Elastic: empty at this moment, for future implementations.
- NonElastic: with the F01, F02, … F36 folders, similar to those in the G4NDL/Inelastic folder, with the information of the final state of the different reactions.

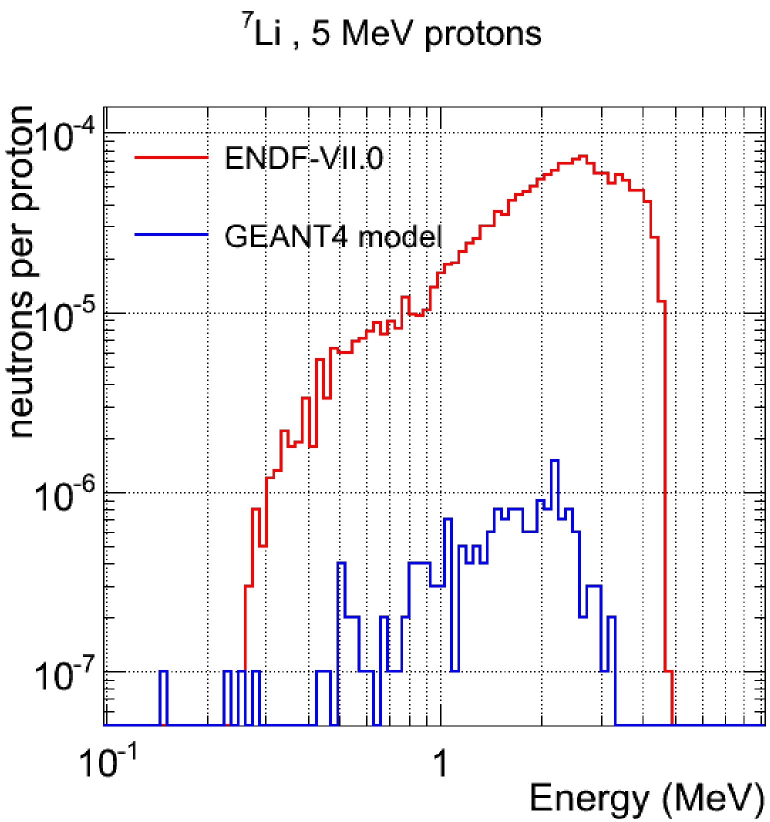
Some results

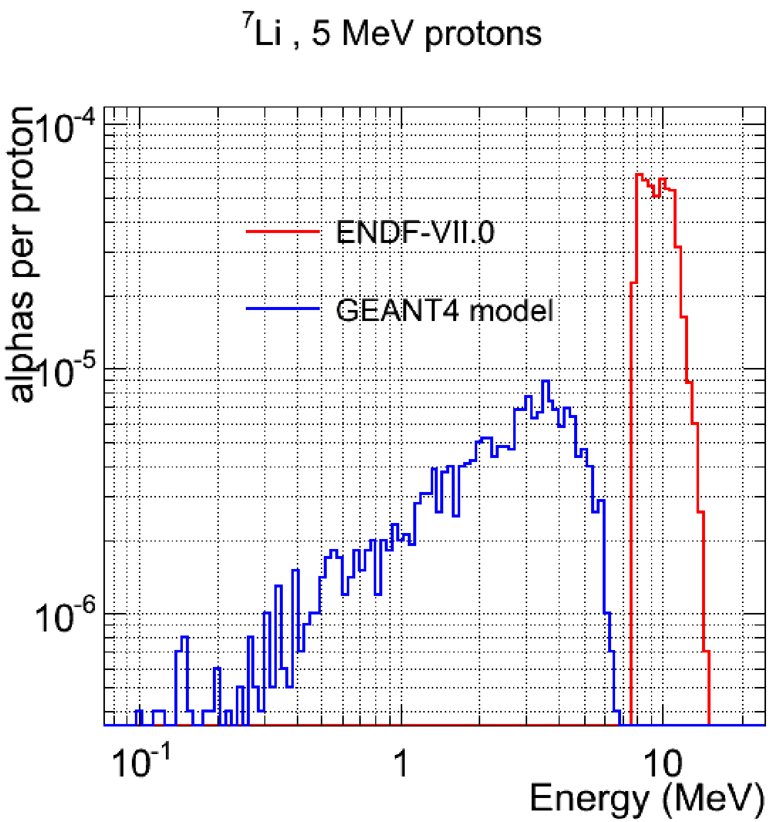
Some MC simulations have been performed, with the standard GEANT4 physics and with the new created libraries.

The geometry is a 0.1mm thick layer, made with different materials, with $1 g/cm^3$ density. Incident monoenergetic particles hit the layer perpendicularly to the surface.

In some simulations the particle production has been stored. In others, the particles exiting the exit surface.

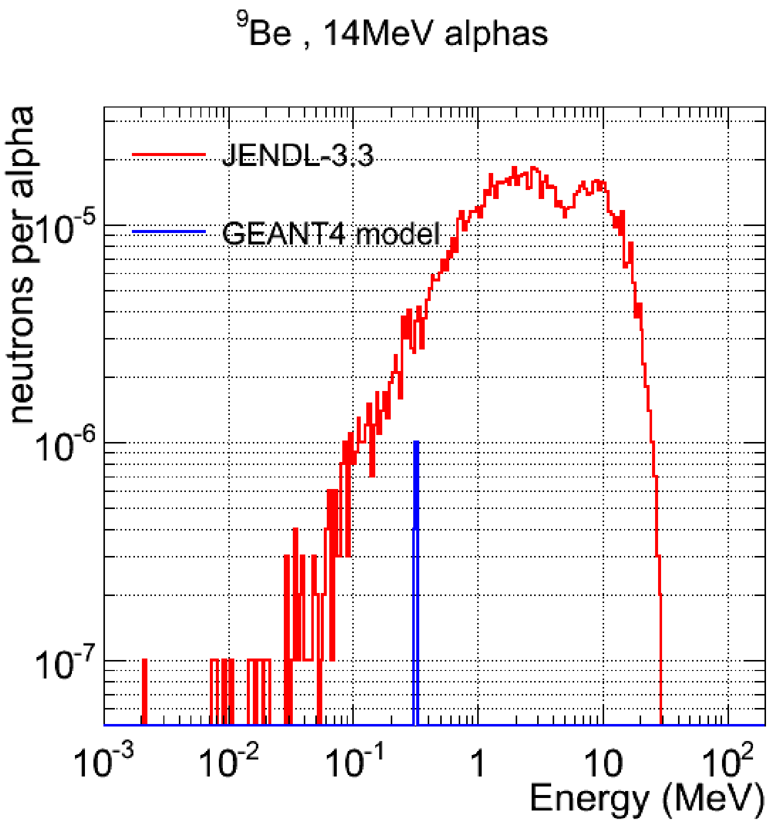
Some results (particle production)

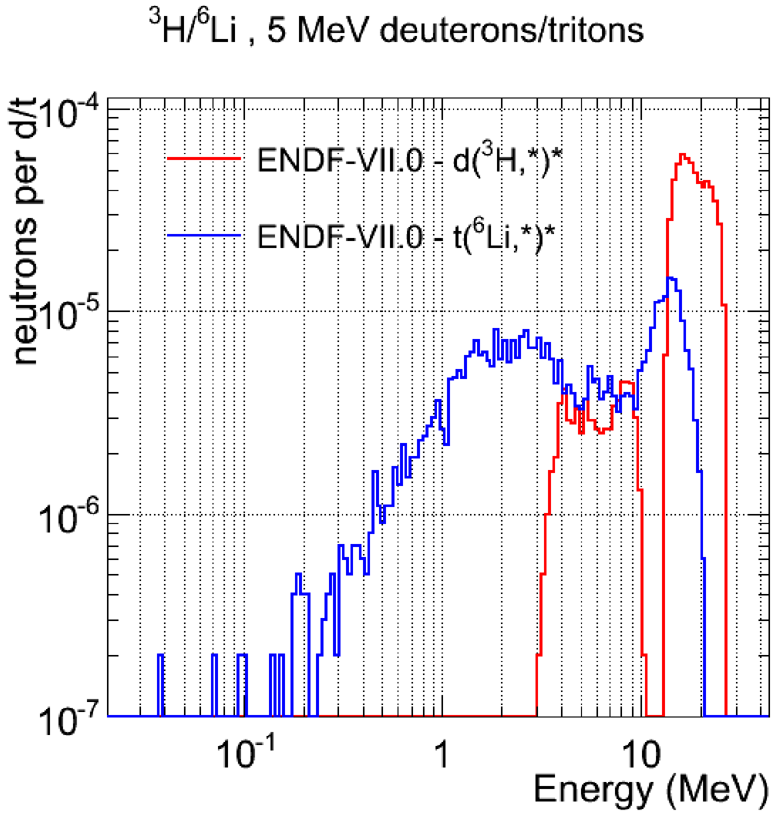




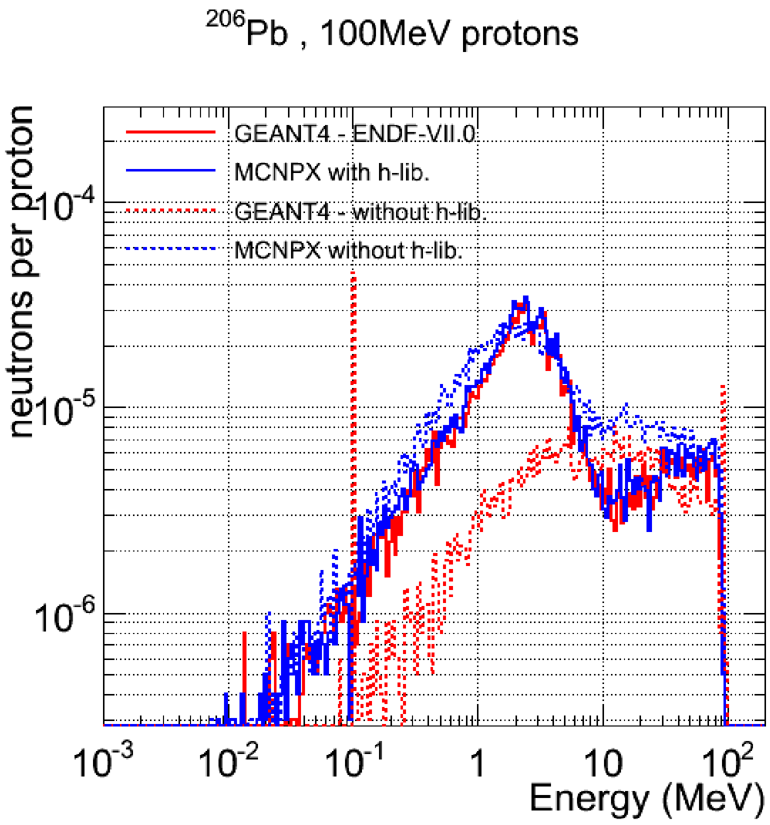
Some results (particle production)

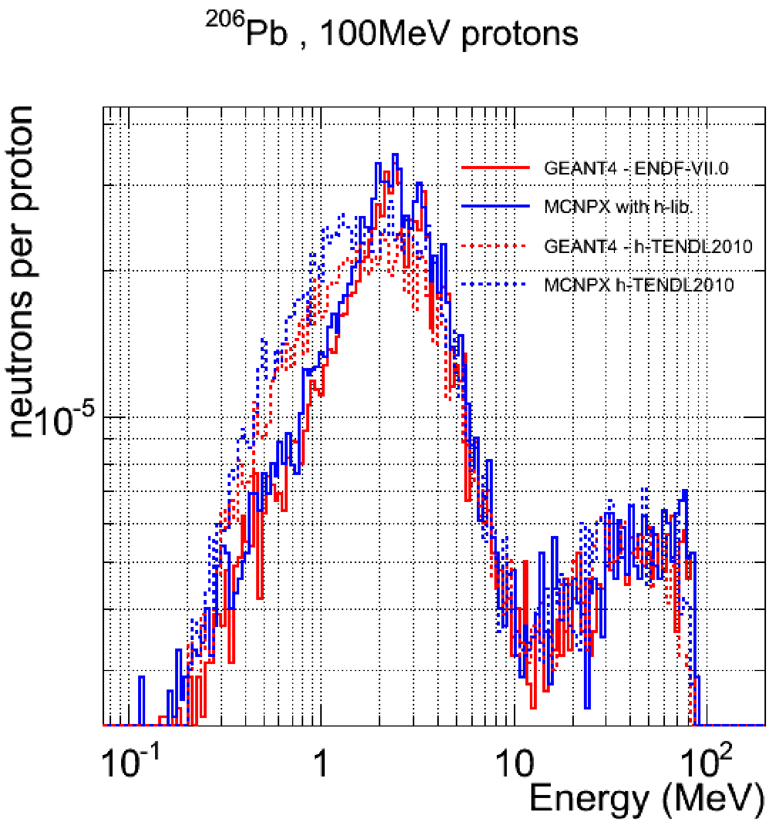
No neutrons are produced with the GEANT4 model



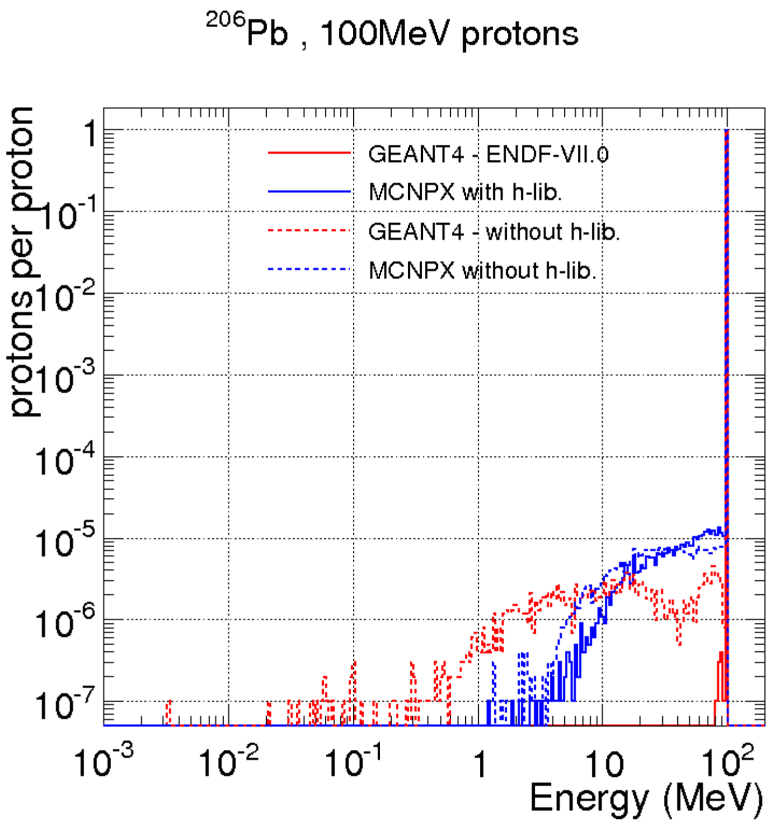


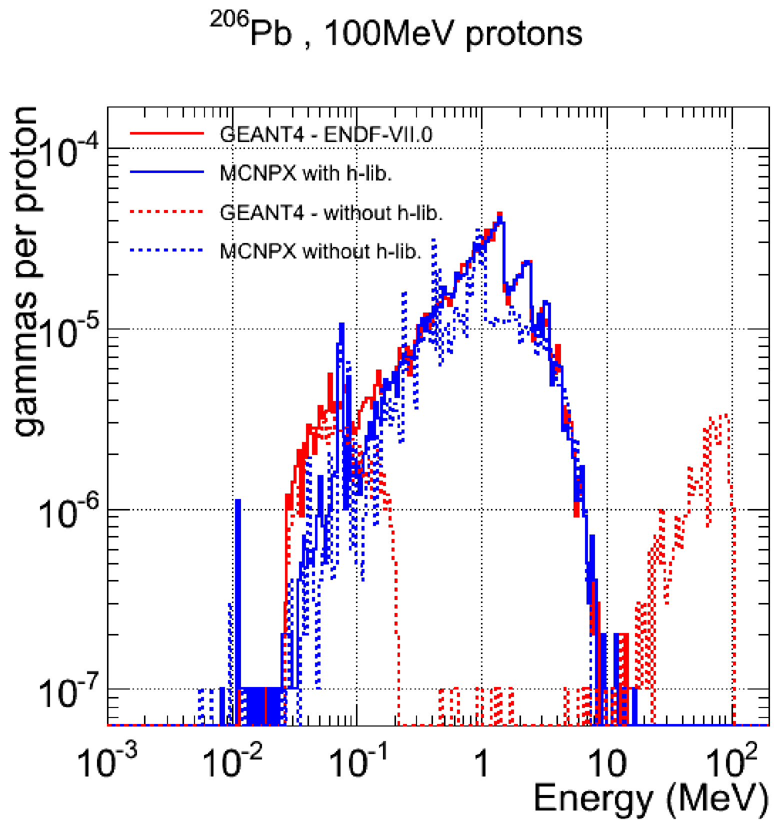
Some results (particles exiting the layer)





Some results (particles exiting the layer)





Comments & conclusions

1- This is a very preliminary development of this package, however, some reasonable results have been obtained. This development should be improved and validated.

2- This package is totally based in the G4NeutronHP package. The charged particles are treated as neutrons, but with their "charged particle" data, instead of neutron data. Probably more parts of the code where it is assumed that it is a neutron what it is being simulated must be changed.

3- Elastic scattering should be included.

4- Residual nuclei & gammas not present in the libraries not yet implemented. This is a non-trivial problem, especially when the reaction is described in MF=5 format.

5- Secondary particles bigger than alphas (residual nuclei) present in the libraries hasn't been translated into the GEANT4 format (same as with neutrons).

6- TENDL libraries could be used to simulate neutrons from 20 to 200 MeV.

Comments & conclusions

7- The evaluated libraries have only a limited number of isotopes (except for neutron incident particles) and the energy range of the libraries is not the same for all the isotopes, as it was shown above. Probably the best way to operate is by using the library information if it is available and the standard G4LE{Proton/Deuteron/…}Inelastic processes (cross sections + final states) if not. However, this is not straightforward, since particles in GEANT4 interact with elements, instead of isotopes, making it more difficult. Another difficulty is that usually the range of validation of the models (G4ParticleInteractio/ G4LE{Proton/Deuteron/…}Inelastic) is set in the physics list, and it is the same for all materials.

One advantage of the TENDL libraries is that they have a large amount of isotopes, all of them with energies up to 200MeV.