Validation of the thermal neutron physics in GEANT4

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Why using thermal neutron physics?

If not absorbed, neutrons loose energy with the medium in inelastic and elastic collisions. Therefore, in every simulation it is necessary to consider a wide energy range, form several tens of MeV (or larger) down to thermal energies ($E_{thermal}$=0.025 eV).

At energies close to thermal, the collisions of the neutron with atoms or molecules can result in a gain or loss of energy, by reducing or increasing the velocity of the molecule (translational modes), and they can interact to make the molecule slow down or speed up its rotations (rotational modes) or vibrations (vibrational modes).

A thermal neutron treatment is therefore necessary, in order to account accurately for the low energy neutron interactions with matter, and such a treatment depends on the structure of the material/molecules (crystaline, liquid...)

The thermal “scattering law” provides this treatment: cross sections written in terms of the scattering matrix S(α,β).

$$\sigma(E \rightarrow E', \mu) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}S(\alpha,\beta) \qquad \alpha = \frac{E' + E - 2\mu\sqrt{E'E}}{AkT} \qquad \beta = \frac{E' - E}{kT}$$

Why using thermal neutron physics?

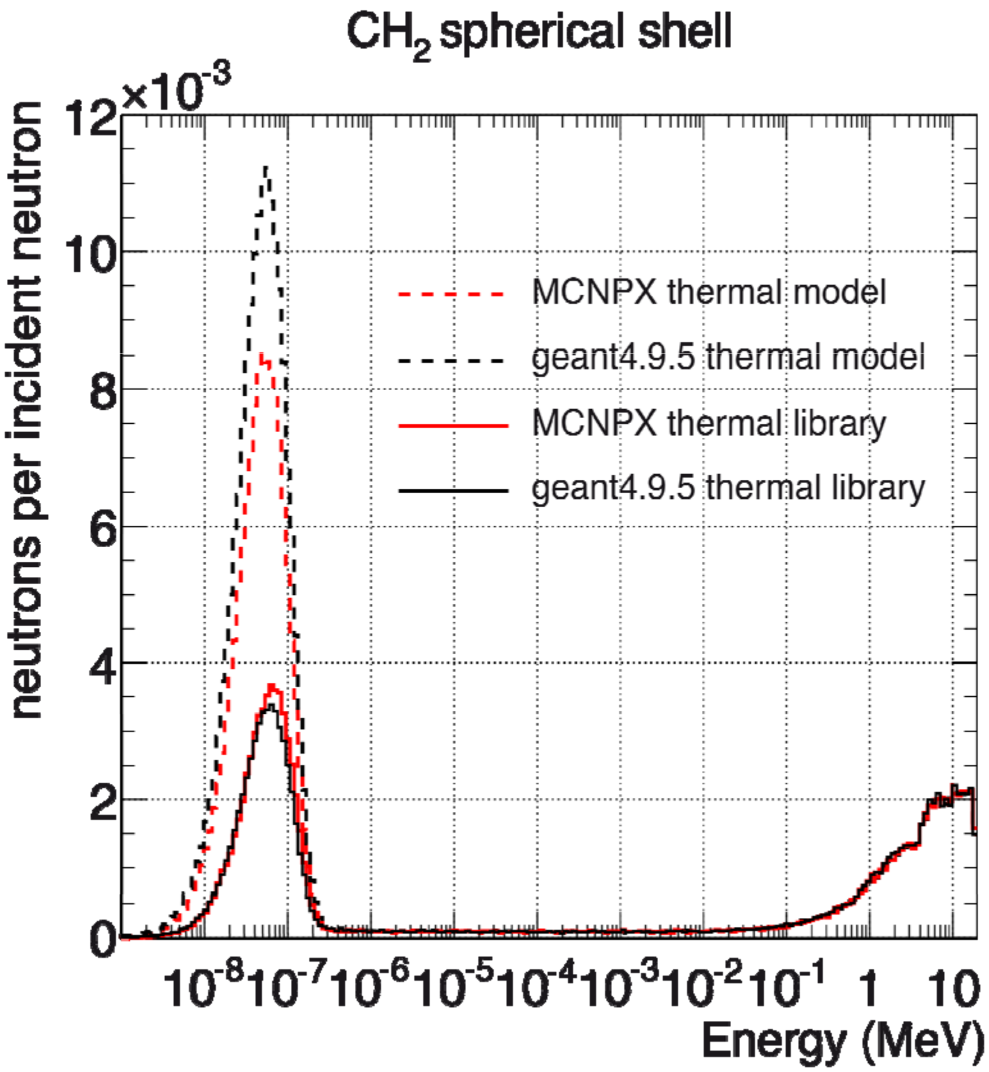
The scattering matrix needs to be determined for specific elements present in the moderator material, e. g., hydrogen in water, hydrogen in polyethylene, carbon in graphite...

Such data comes from dedicated experiments or from solid state physics models. They are delivered together with the standard evaluated neutron data libraries (ENDF/B, JEFF, JENDL...)

Scattering matrices are not ready to be used directly in practical calculations. They have to be converted into energy dependent cross sections and scattering distributions in appropriate formats by a nuclear data processing code such as NJOY.

Geant4.9.3 had thermal data for only 3 materials. The current release 4.9.6 does have thermal data for ~20 materials.

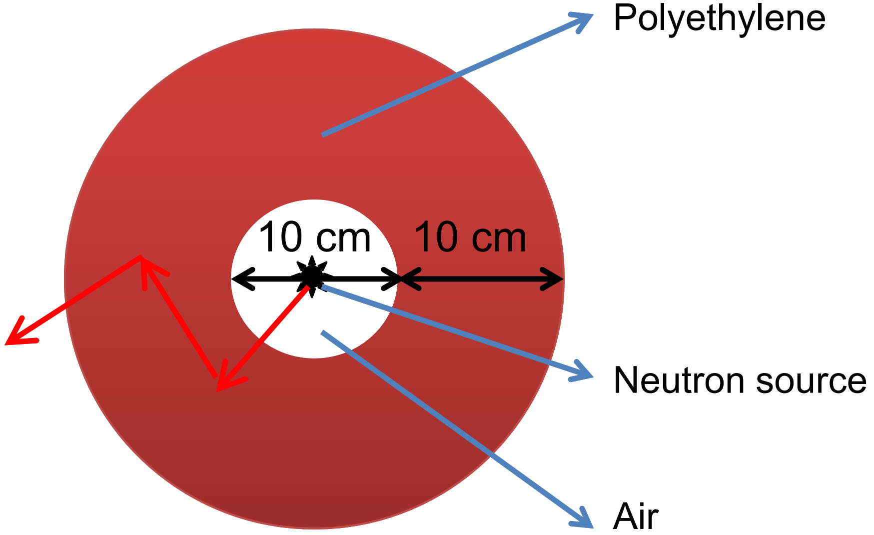
Thermal neutron treatment in MCNPX and GEANT4



The thermal neutron physics in MCNPX and GEANT4 is not the same.

Both codes show a better agreement this physics is used with the same thermal scattering data, although differences remain at the level of 10% - 20%.

Still important for several applications (reactors, moderated neutron detectors…)



Activation of the thermal neutron physics in GEANT4

DETECTOR CONSTRUCTION

```
…
G4Element *C  = new G4Element("C", "C", 2);
…
G4Element *H = new G4Element("TS_H_of_Polyethylene", ”H", 1., 1.0079*g/mole);

G4Material *POLYMAT = new G4Material("POLYMAT ", 0.94*g/cm3, 2, kStateSolid, 293.15*kelvin);
POLYMAT->AddElement(H, 0.143711);
POLYMAT->AddElement(C, 0.856289);
…
```

1. The elements in the moderator material which are relevant for the thermal processes must be defined with their corresponding specific names defined in the class *G4NeutronHPThermalScatteringNames*.

2. The real temperature of the moderator material must be specified since, by default, materials are defined in GEANT4 at a temperature *STP_temperature* which is a CLHEP constant equal to 273.15ºK.

Activation of the thermal neutron physics in GEANT4

PHYSICS LIST

```
…
else if ( particleName == "neutron" )
            {
            …
            G4HadronElasticProcess *elasticnp = new G4HadronElasticProcess;
            G4NeutronHPElastic *elasticn = new G4NeutronHPElastic;
            …
            elasticn->SetMinEnergy(4.*eV);
```

3. Set the minimum energy limit of the elastic scattering model to 4 eV (the limit imposed by ENDF/B is 5 eV but GEANT4 has only data up to 4 eV)

Activation of the thermal neutron physics in GEANT4

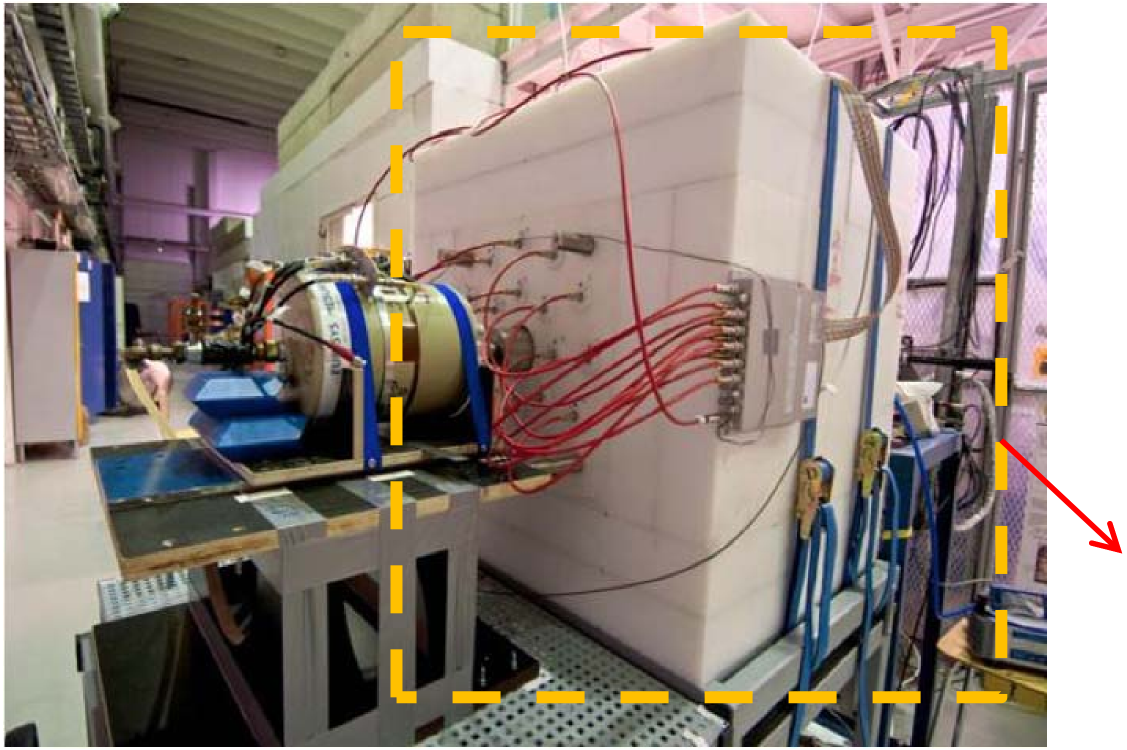
PHYSICS LIST

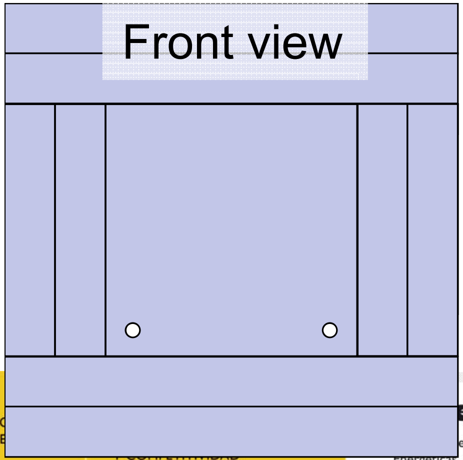
```
G4NeutronHPThermalScattering *thermaln = new G4NeutronHPThermalScattering;
thermaln->SetMaxEnergy(4.*eV);
elasticn->RegisterMe(thermaln);

G4NeutronHPThermalScatteringData *hpthermaldata
                                   = new G4NeutronHPThermalScatteringData;
hadelasticp->AddDataSet(hpthermaldata);
…
}
…
```

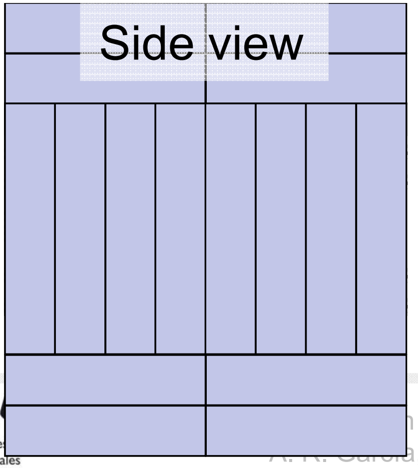
4. Create and register the thermal neutron scattering model and set its maximum energy limit to 4 eV.

5. Add the thermal neutron data set G4HadronElasticProcess.

The BEta deLayEd Neutron detector (BELEN)







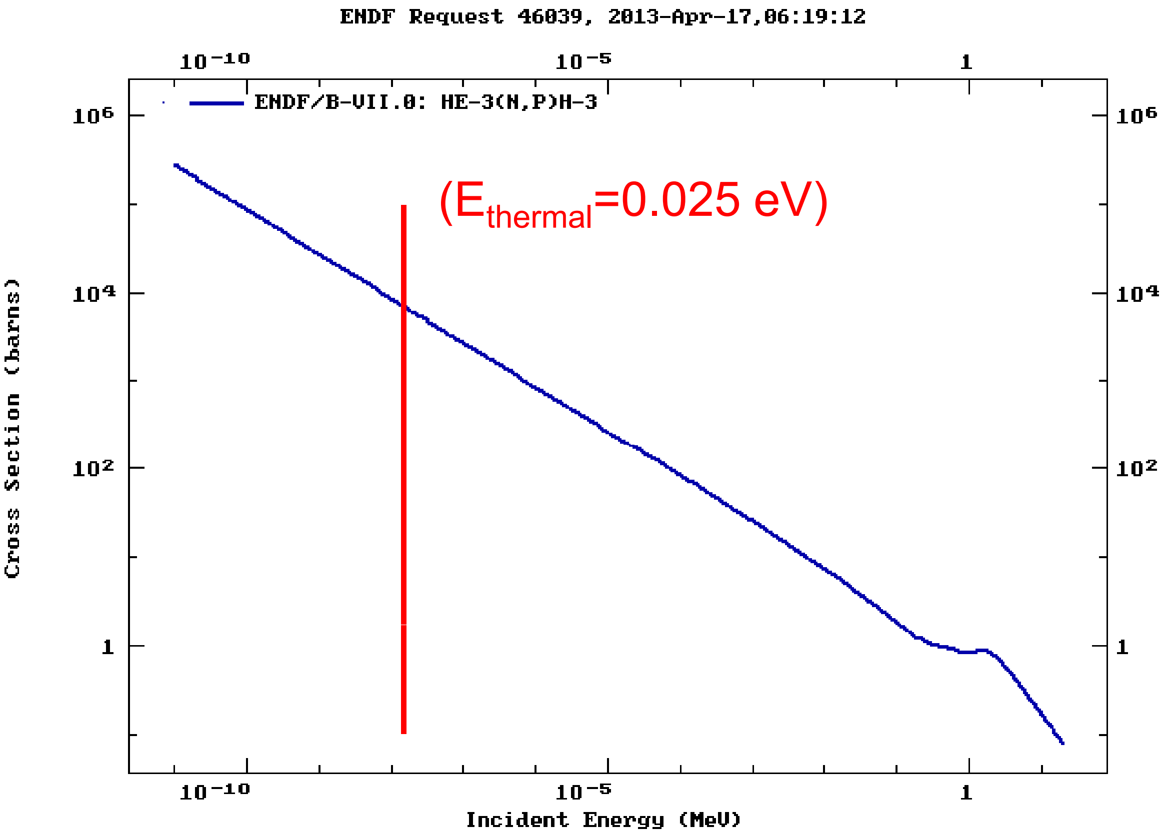
Polyethylene matrix ~1 m^3 with 20 ^{3}He neutron counter tubes (20 atm) embedded in two concentric crowns:

- 8 cm inner radius
- 12 cm outer radius

Such detectors are used because of their large intrinsic efficiency (30% - 80%) and because the efficiency is nearly constant with the incident neutron energy (E_n<2 MeV).

The BEta deLayEd Neutron detector (BELEN)

The neutrons emitted in a radioactive decay at the centre of the detector are moderated inside the polyethylene matrix and absorbed (with a large probability) in one of the ^{3}He tubes. The ^{3}He(n,p) cross section is very large at thermal energies.



$n+^{3}He \longrightarrow p+t$

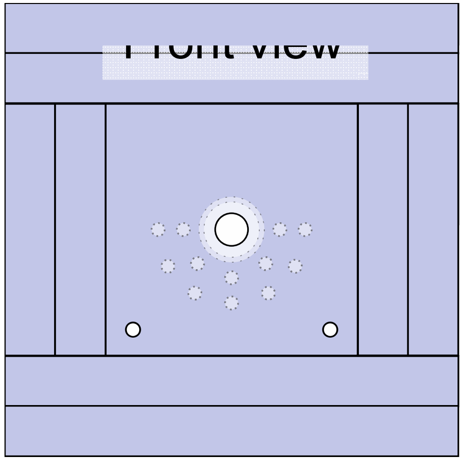
E_p = 573 keV,
E_t = 191 keV,
Q = 764 keV

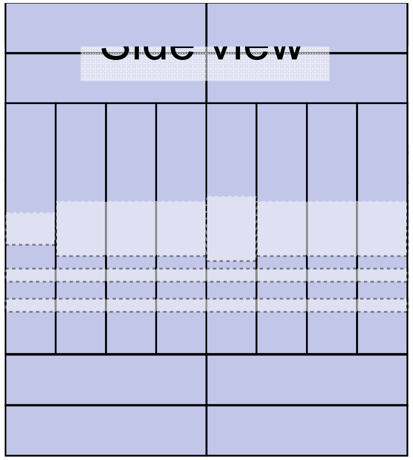
Simulation of BELEN with MCNPX and GEANT4

The BELEN detector was simulated in detail with MCNPX 2.7a with ENDF/B-VII.0 and GEANT4.9.3 with ENDF/B-VII.0 (same CIEMAT neutron libraries >4 eV + “presumably” the same thermal neutron data).

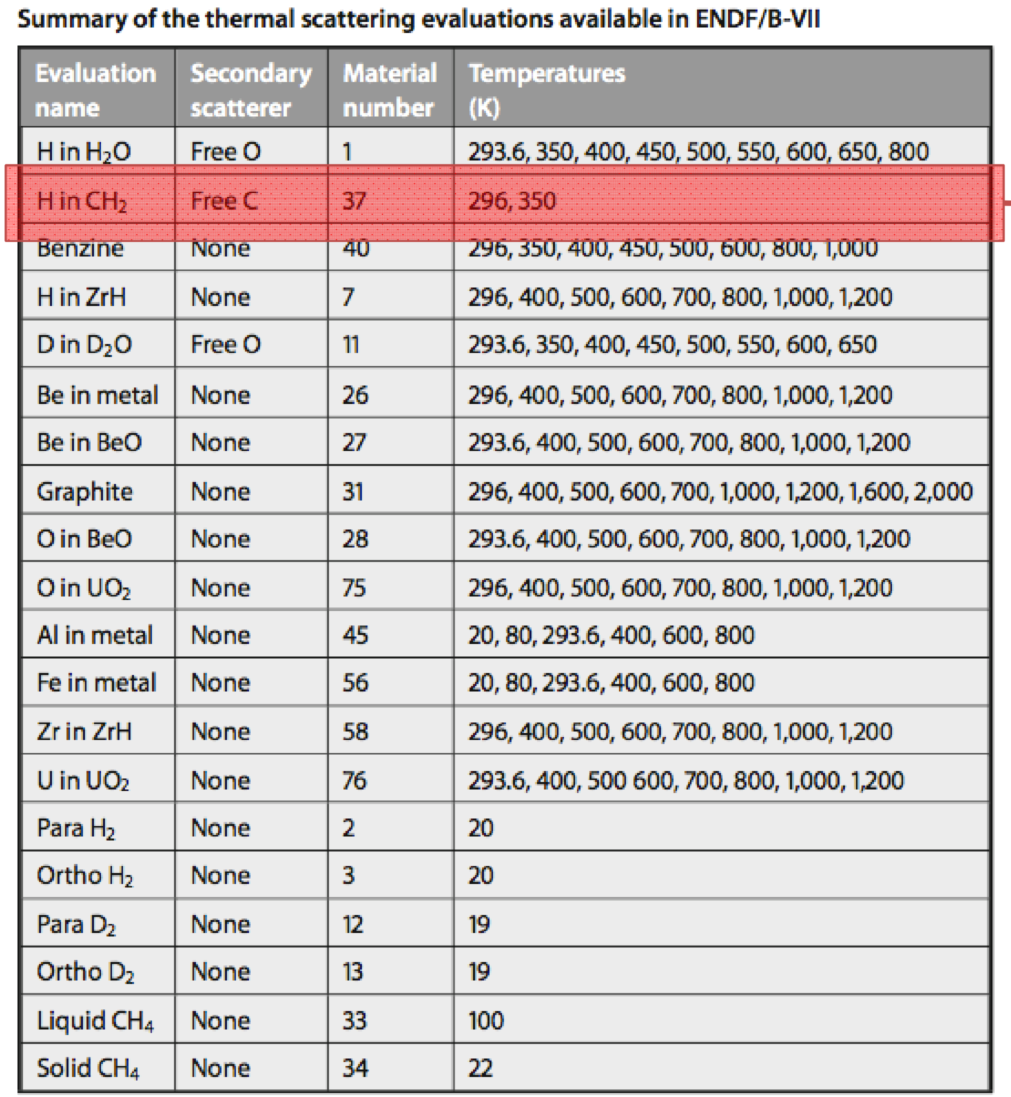
10^6 monoenergetic neutrons (0.01, 0.05, 0.1, 0.25, 0.7, 1, 1.5, 2.5 and 5 MeV) were generated isotropically from the center of the detector.

In the n+^{3}He, reaction products are emitted in opposite directions. The minimum detected energy is therefore that of the tritium (191 keV) when the proton escapes out of the detector. The detection efficiency was then calculated by integrating the energy deposition distribution from 191 keV up to the Q value at 764 keV for all the ^{3}He tubes.





Polyethylene thermal neutron data in ENDF/B-VII.0



Summary of the thermal scattering evaluations available in ENDF/B-VII

Evaluation name	Secondary scatterer	Material number	Temperatures (K)
H in H_2O	Free O	1	293.6, 350, 400, 450, 500, 550, 600, 650, 800
H in CH_2	Free C	37	296, 350
Benzine	None	40	296, 350, 400, 450, 500, 600, 800, 1,000
H in ZrH	None	7	296, 400, 500, 600, 700, 800, 1,000, 1,200
D in D_2O	Free O	11	293.6, 350, 400, 450, 500, 550, 600, 650
Be in metal	None	26	296, 400, 500, 600, 700, 800, 1,000, 1,200
Be in BeO	None	27	293.6, 400, 500, 600, 700, 800, 1,000, 1,200
Graphite	None	31	296, 400, 500, 600, 700, 1,000, 1,200, 1,600, 2,000
O in BeO	None	28	293.6, 400, 500, 600, 700, 800, 1,000, 1,200
O in UO_2	None	75	296, 400, 500, 600, 700, 800, 1,000, 1,200
Al in metal	None	45	20, 80, 293.6, 400, 600, 800
Fe in metal	None	56	20, 80, 293.6, 400, 600, 800
Zr in ZrH	None	58	296, 400, 500, 600, 700, 800, 1,000, 1,200
U in UO_2	None	76	293.6, 400, 500 600, 700, 800, 1,000, 1,200
Para H_2	None	2	20
Ortho H_2	None	3	20
Para D_2	None	12	19
Ortho D_2	None	13	19
Liquid CH_4	None	33	100
Solid CH_4	None	34	22

H in Polyethylene (MT 37)

These evaluations contain the scattering matrix S(α,β) from 0 to 5 eV.

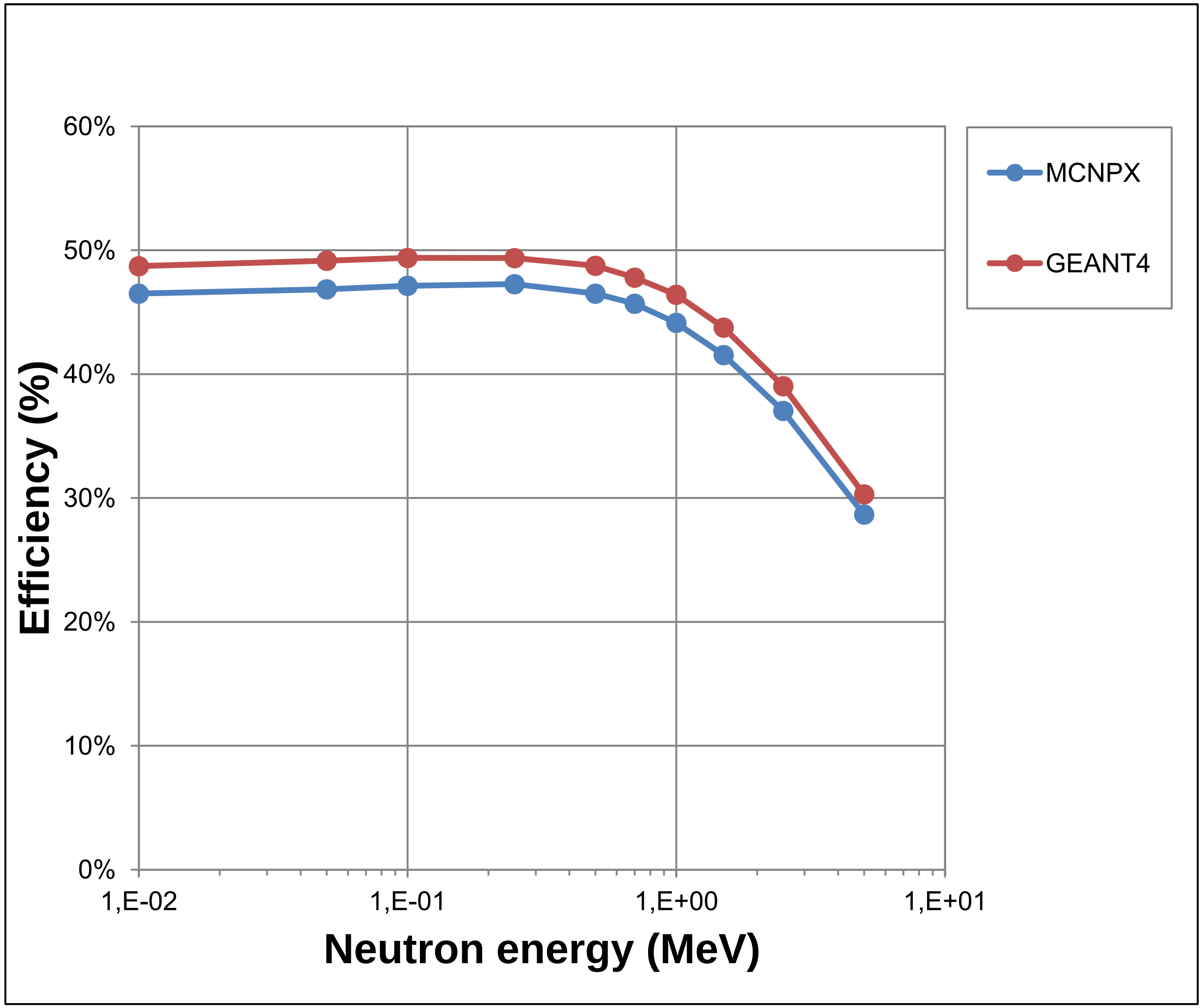
Polyethylene thermal neutron data in MCNPX and GEANT4

MCNPX uses its own ACE format. The thermal neutron data for Polyethylene was processed with NJOY 99.0 for 293.6 ºK. Cross sections and scattering distributions were calculated from the scattering matrix and applied the corresponding Doppler broadening. Calculations for other temperatures requires the creation of new libraries.

GEANT4 uses its own G4NDL format. The thermal neutron data for Polyethylene was processed with its own processing tools for 296 and 350 ºK. Doppler broadening is applied in run time. Calculations for other temperatures are also possible with linear interpolation/extrapolation of cross sections and scattering distributions.

In order to compare both codes, simulations were performed at 293.6 ºK since that is the only temperature for which MCNPX has thermal data.

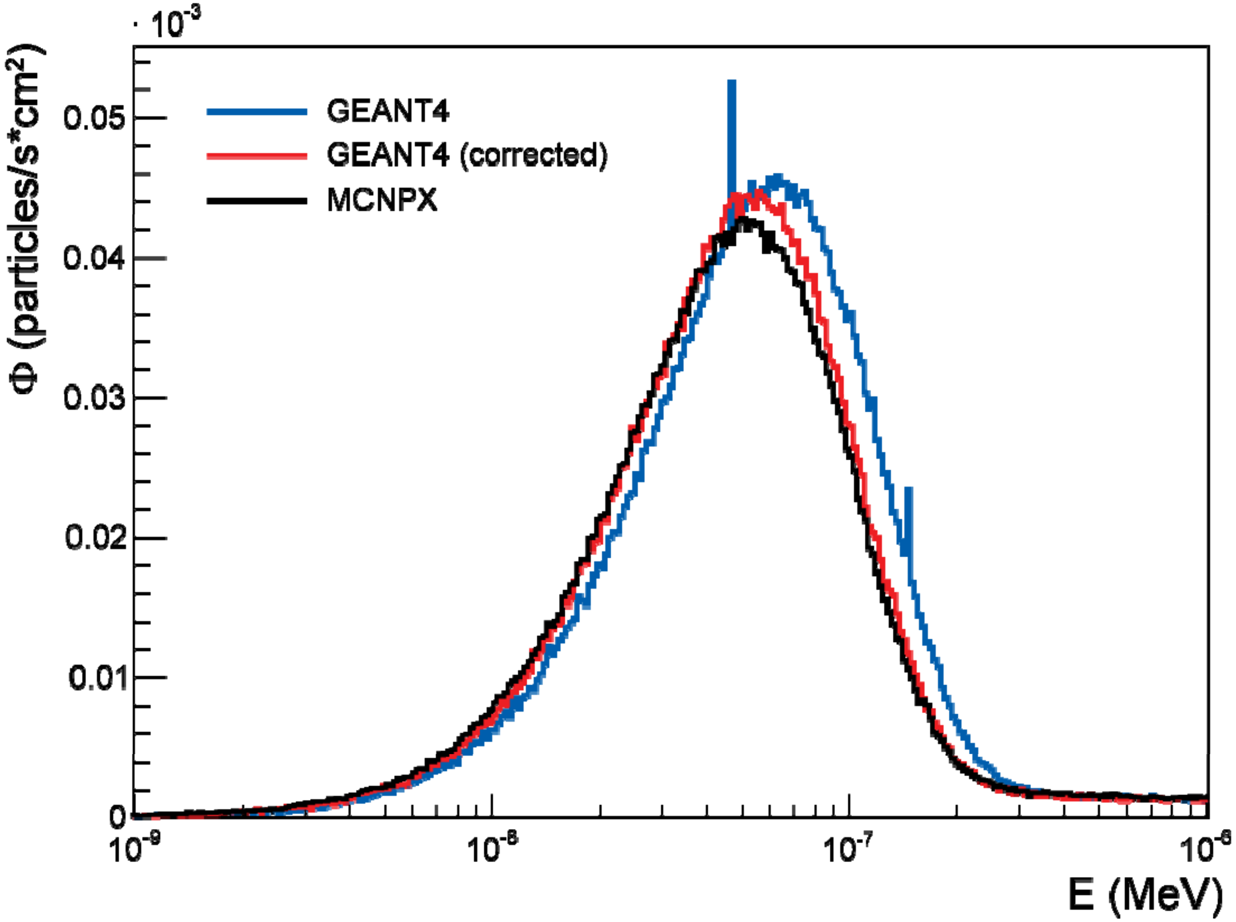
Simulation results without corrections



Conclusion: GEANT4 overestimates systematically the detection efficiency up to a 7% compared to MCNPX when the thermal neutron physics is activated in both codes.

Thermal neutron energy distribution in GEANT4 and MCNPX

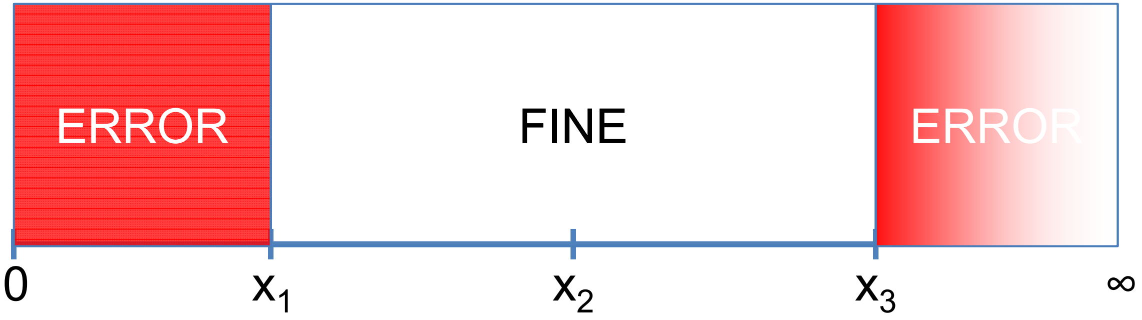
It has been found that the differences in the simulated efficiencies are related to differences in the thermal neutron spectra calculated by GEANT4 and MCNPX.



1. The temperature of the Maxwellian spectra is not the same (and they should) since the same temperature was defined in the two simulations.
2. The temperature reconstructed from the MCNPX distribution is the correct one. The GEANT4 is 60 K larger.
3. There are strange spikes in the Maxwellian distribution calculated by GEANT4.

Corrections made to *G4NeutronHPThermalScattering*

All errors found concerned the extrapolation of data when the extrapolation point was below the lower or above the upper data values. The interpolation/extrapolation routine itself was not wrong (simple linear algorithms), but in most extrapolation cases the routine was not provided with the correct data points.

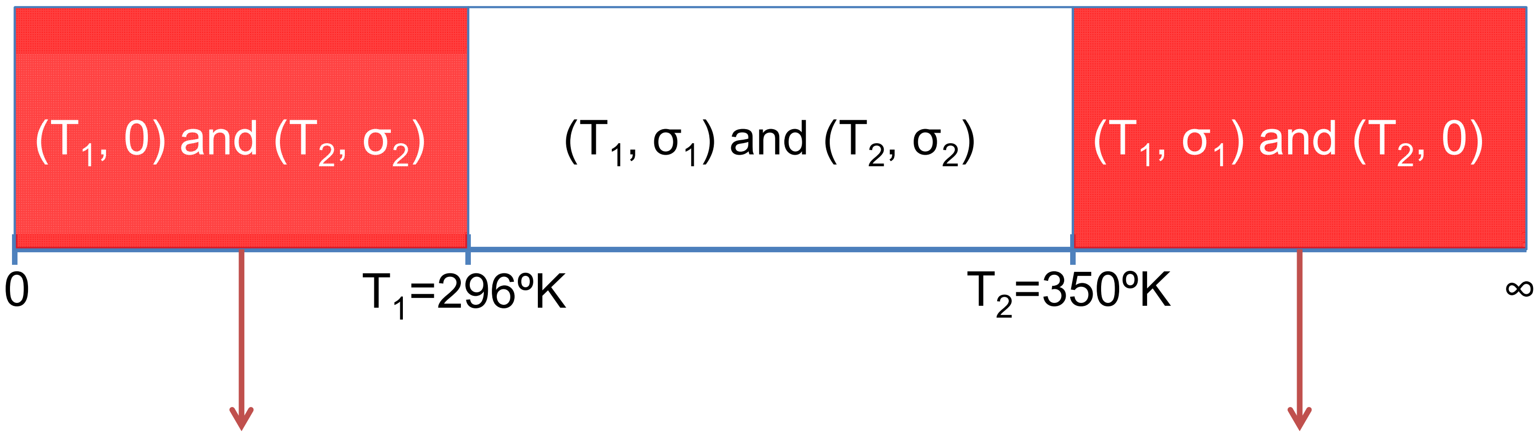


Specifically, errors were found in the extrapolation of the:

1. temperature of the moderator material,
2. angular distributions of outgoing neutrons,
3. energy distribution of outgoing neutrons,

Corrections made to *G4NeutronHPThermalScattering*

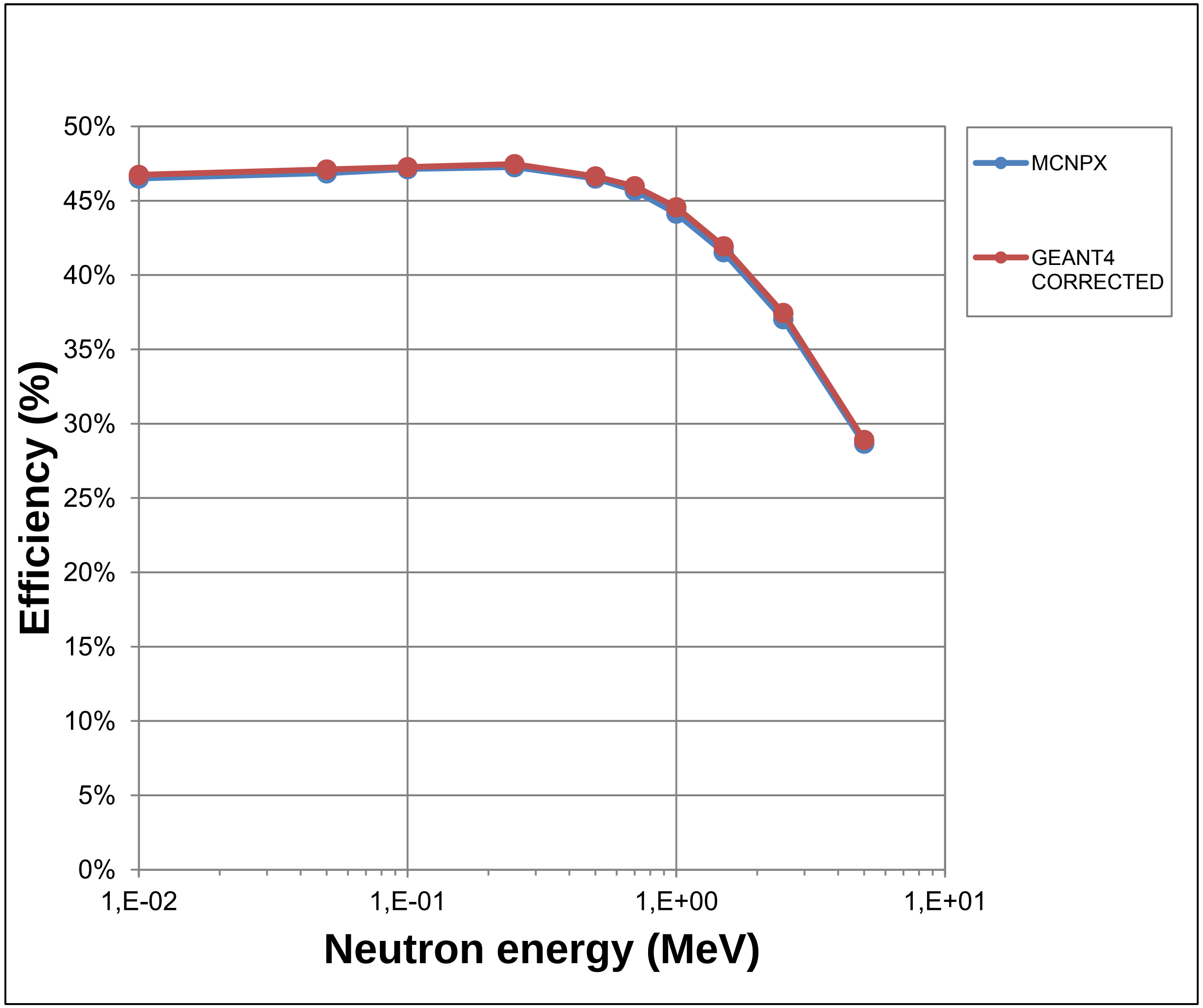
For instance, the interpolation/extrapolation of the cross section given only two datasets for temperatures T_1=296ºK and T_2=350ºK was performed by providing the points:



It should have been given instead:
(T_1, σ_1) and (T_2, σ_2)

It should have been given instead:
(T_1, σ_1) and (T_2, σ_2)

Simulation results with corrections to GEANT4



After having corrected the G4NeutronHP-ThermalScattering class, the detection efficiency calculated with GEANT4 and MCNPX using the thermal neutron physics differ in less than 1%.

Thermal neutron treatment

The interaction of thermal neutrons (E_n = 0.025 eV) with matter needs to be treated in detail as a function of the temperature of the material for obtaining accurate results from Monte Carlo simulations. Such a treatment is important for a wide range of applications: neutron shielding problemes –polyethylene or water–, neutron detectors, dosimetry, reactors, ultra cold neutron applications – liquid methane or helium moderators – ….

If no data are available, both MCNPX and GEANT4 (E_n < 4 eV) use models for the treatment of thermal neutrons. The models in GEANT4 and MCNPX are different, and so tare the results. The differences can be as large as 100% or even worse.

The most accurate/reliable results are obtained by using the thermal neutron data libraries for materials delivered together with the evaluated data libraries. They do exist only for a reduced set of materials (i.e. Moderators). Using the same data, MCNPX and GEANT4 are “comparable”, but not identical.

We have validated the performance of GEANT4 in simulations with thermal neutrons with experimental data from a state of art ^{3}He-based neutron detector and simulations with MCNPX. The efficiency of the detector calculated with GEANT4 shows a systematic deviation ~10% with respect to the experimental values and simulations with MCNPX.

Thermal neutron treatment

We have investigated the nature of the differences and found:

1. One important bug in the calls to the temperature interpolation routine.
2. Differences in the interpolation schemes of the thermal libraries.

We have corrected the bugs and now found a much better agreement between GEANT4 and MCNPX.

Small differences do still remain, attributed mostly to the different sampling methods applied in GEANT4 and MCNPX. The revision of the code and models is in progress.