Validation of the new neutron data libraries

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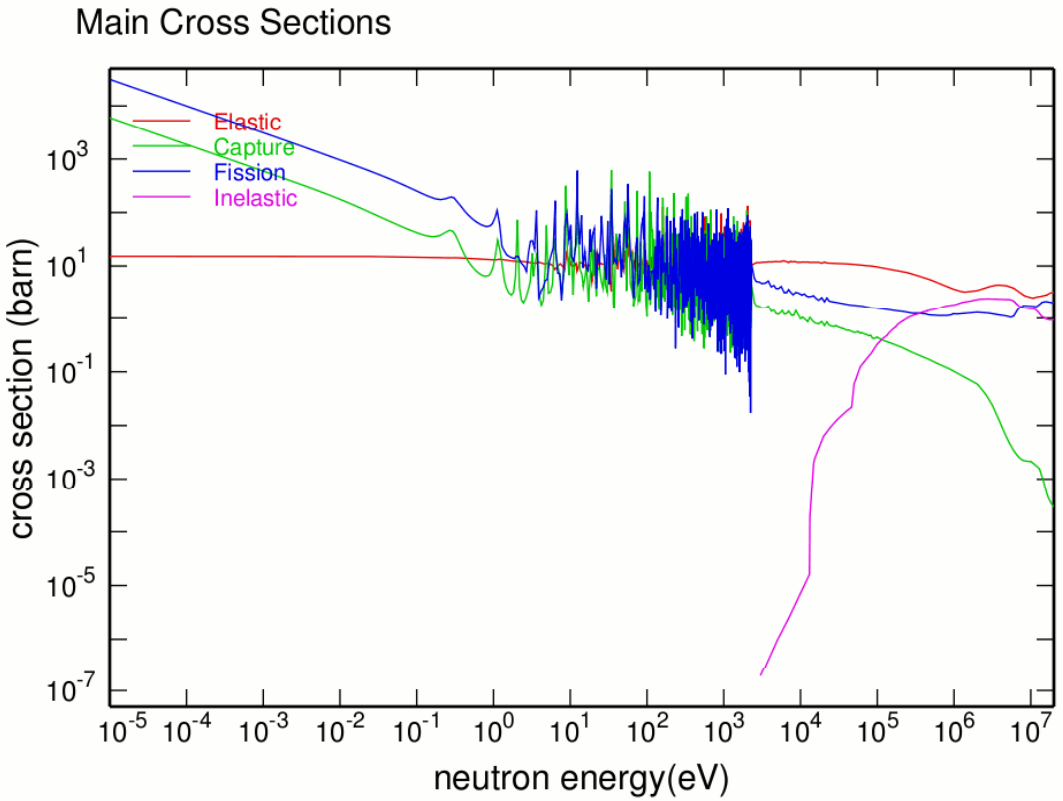
Validation method I

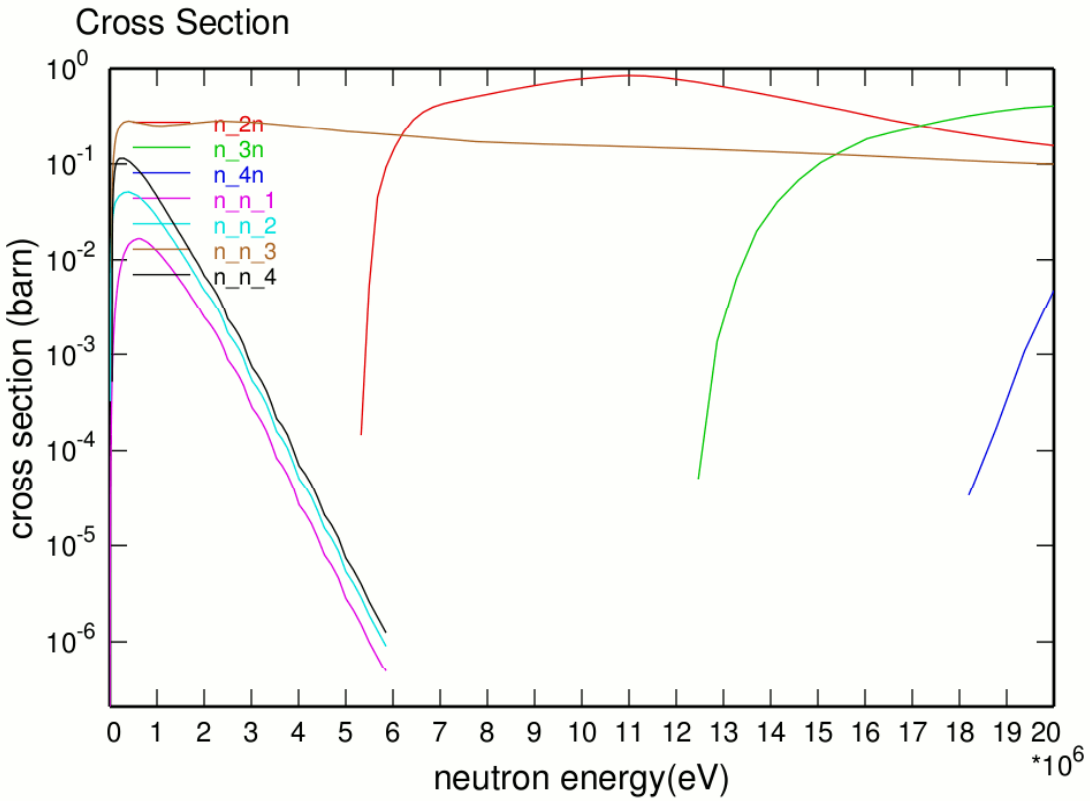
A computer program based in the GEANT4 classes has been developed for sampling a given number of times every probability distribution present in the G4NDL: angular and energy distribution of outgoing particles for every reaction, gamma multiplicities and number of neutrons emitted in fission reactions, prompt and delayed.

The sampling has been done for every reaction of every isotope of every library. It has been done for 40 incident neutron energies: 20 values distributed isolethargicaly from 1e-11MeV to 1MeV and 20 distributed uniformly from 1 to 20MeV. Every quantity has been sampled 50000 times at each energy.

Validation method I (^{235}U)



Validation method I (^{235}U)



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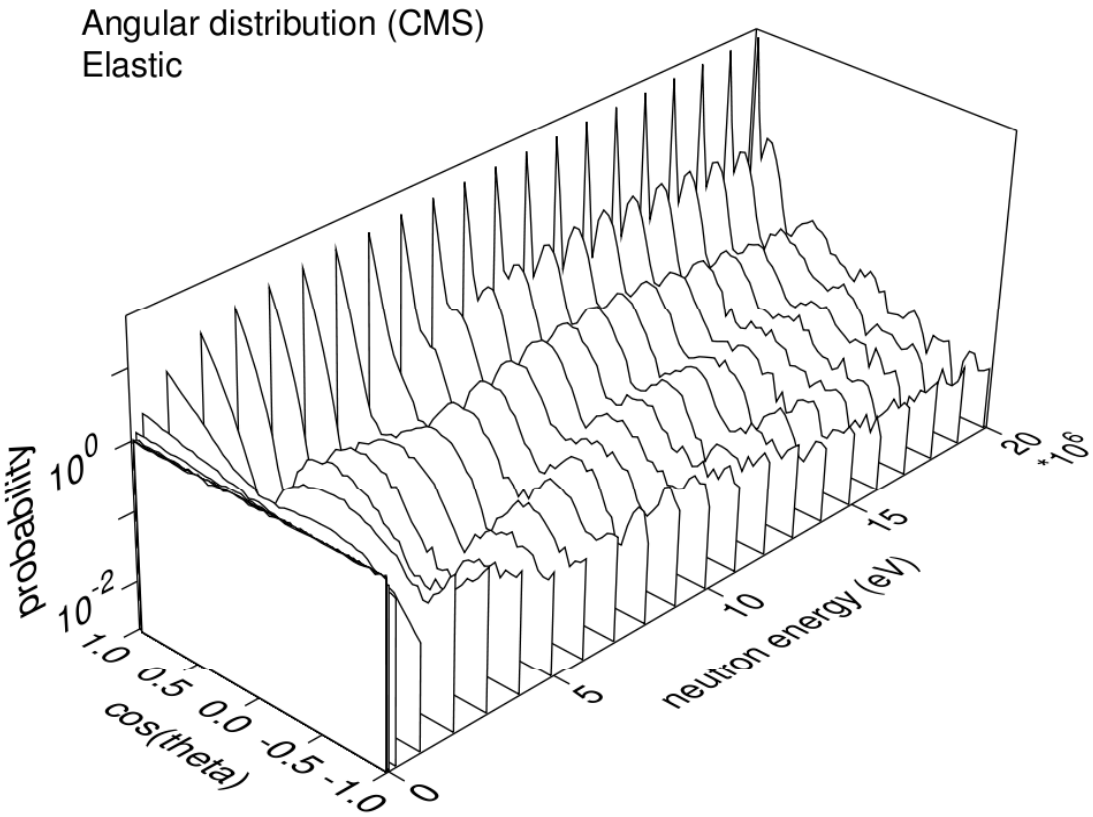

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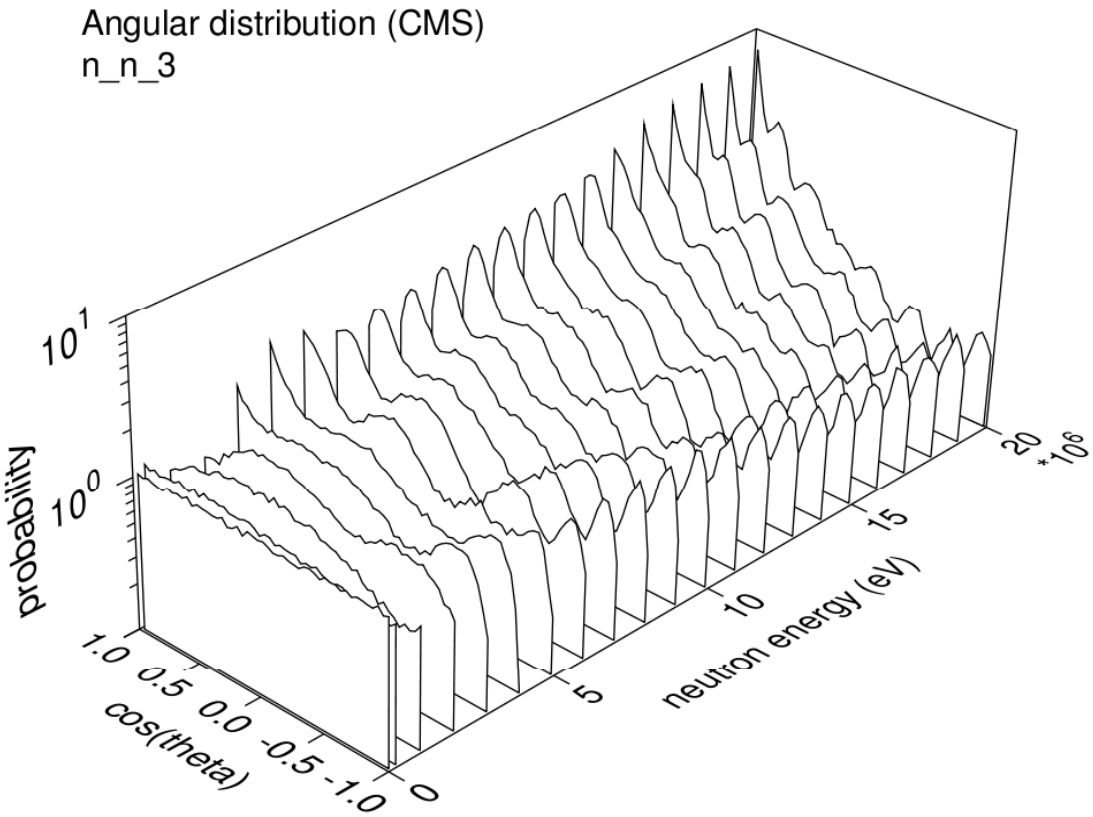

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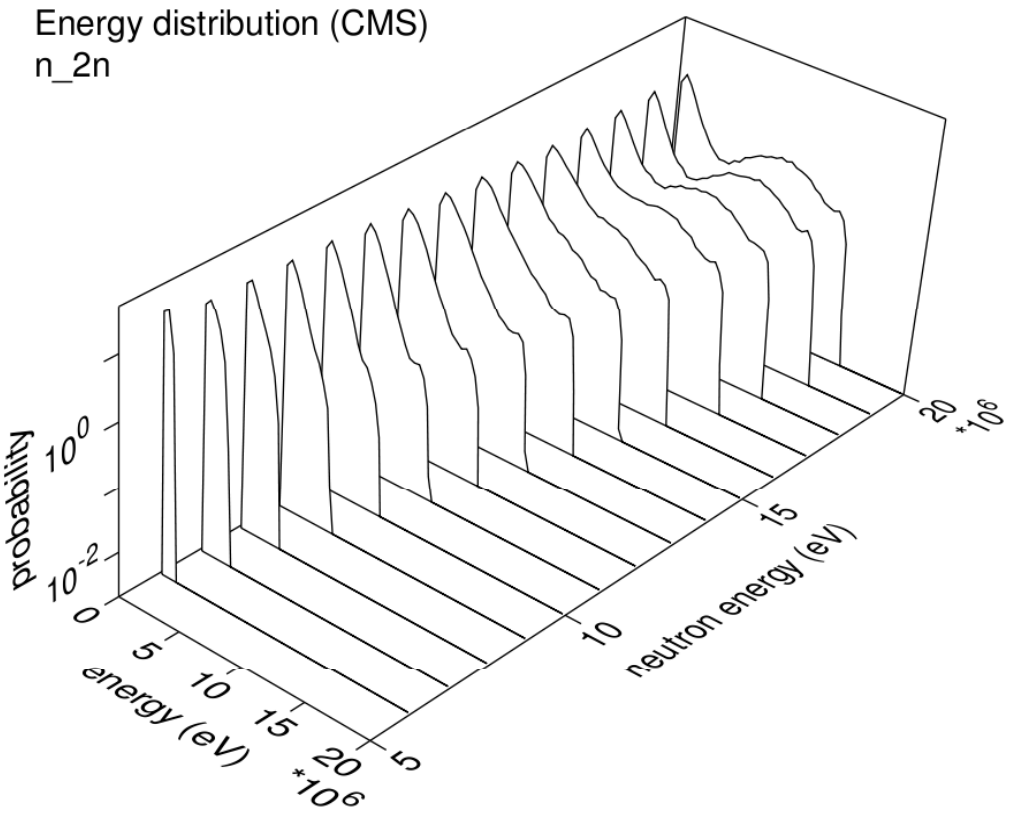

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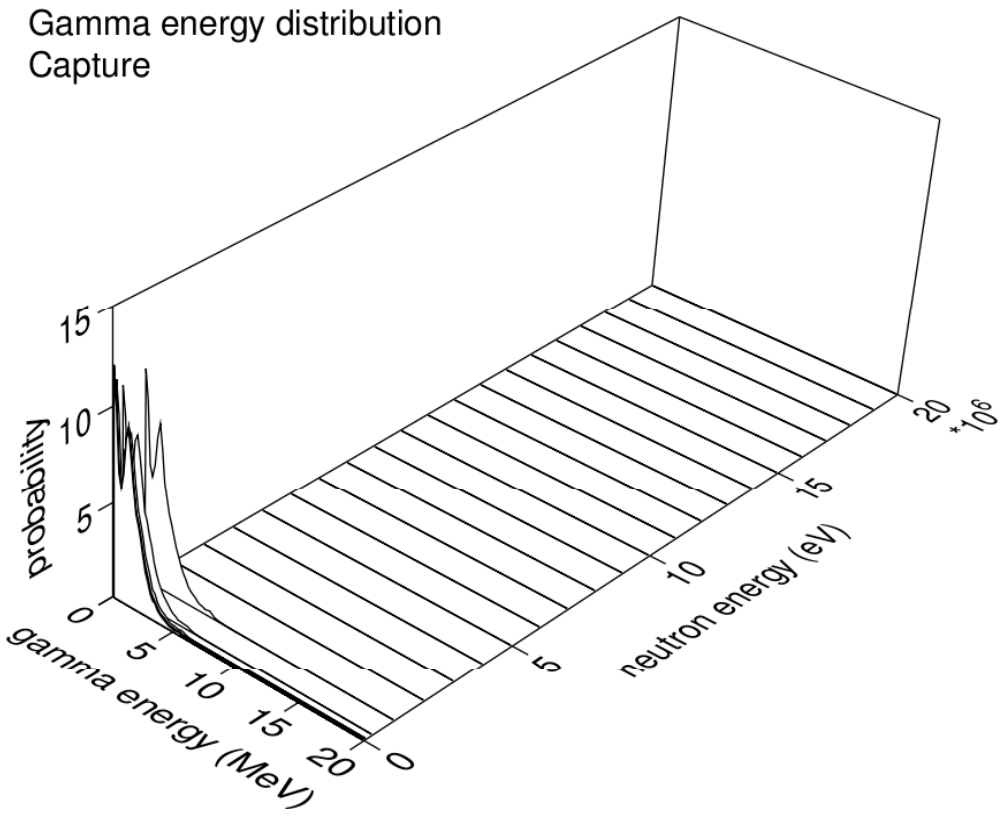

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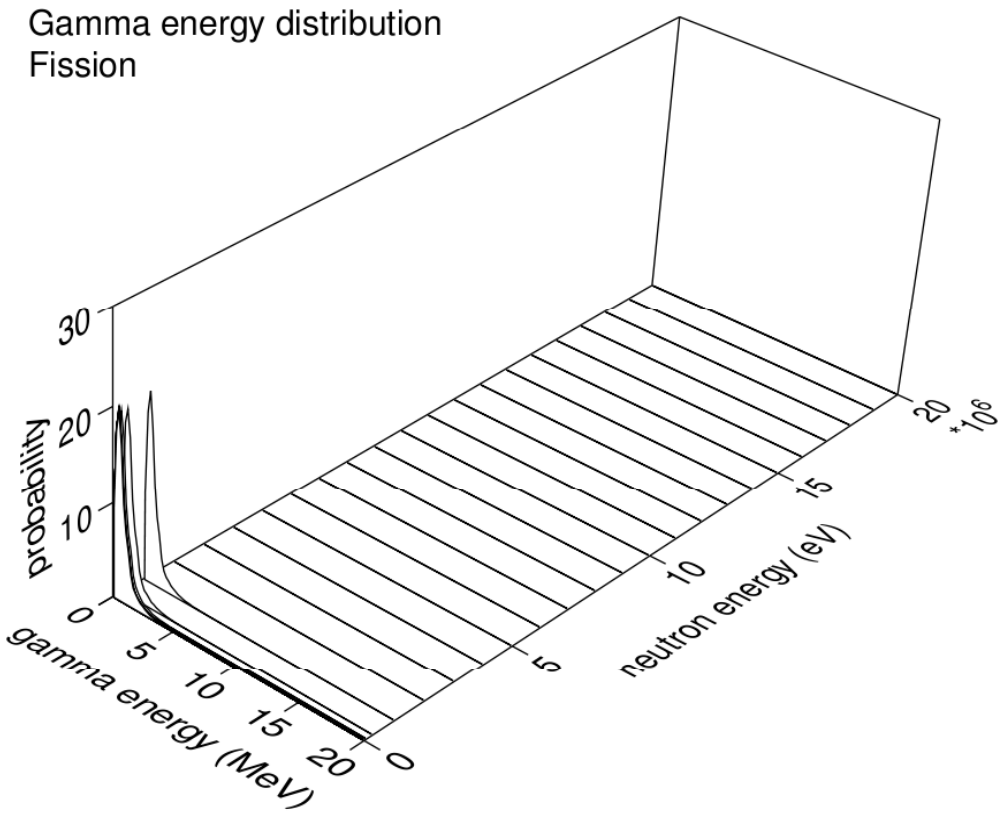
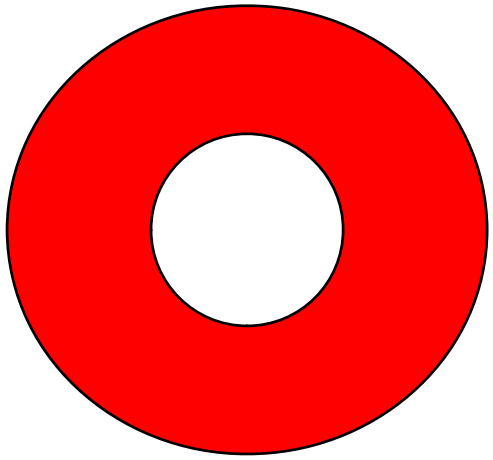


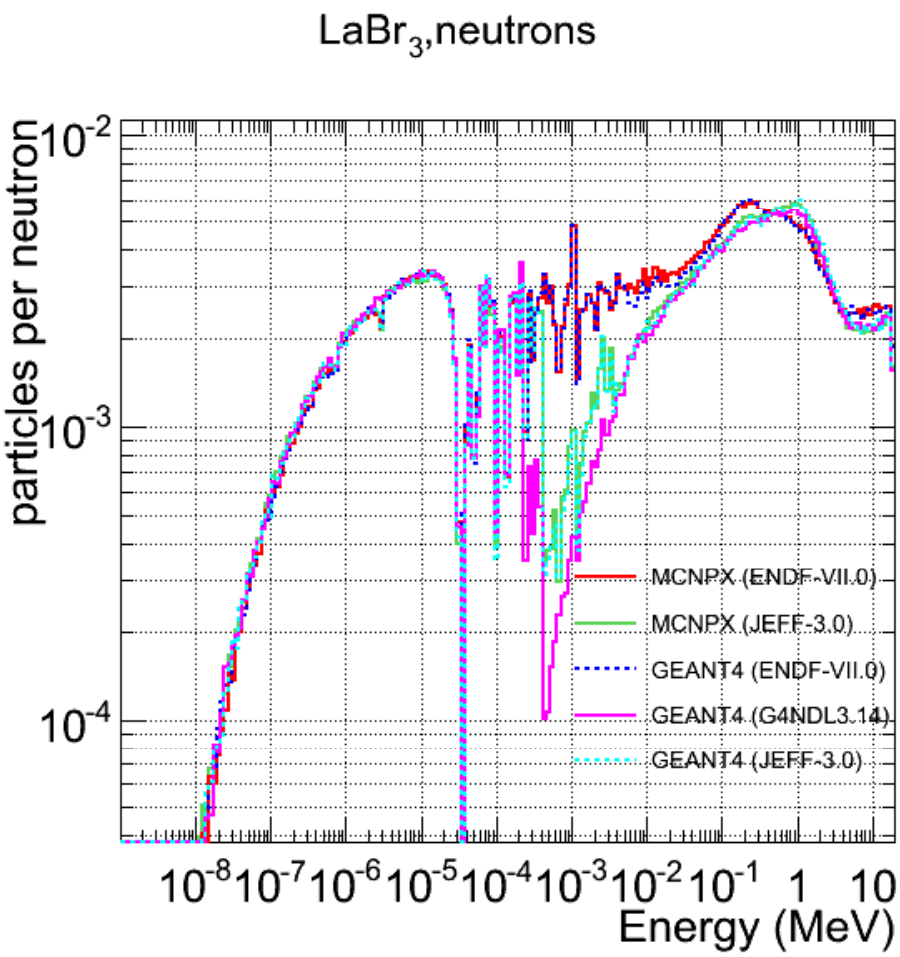
Validation method II

Several MC simulations have been performed using a sphere of 5cm inner radius and 15cm outer radius, made with different materials. Neutrons have been thrown from the center of the sphere. 1e6 neutrons each simulation, with energies isolethargicaly distributed between 1.e-10 MeV and 19MeV. Neutrons and gammas crossing the outer surface of the sphere have been counted. The simulations have been made with GEANT4 and MCNPX, using different libraries.

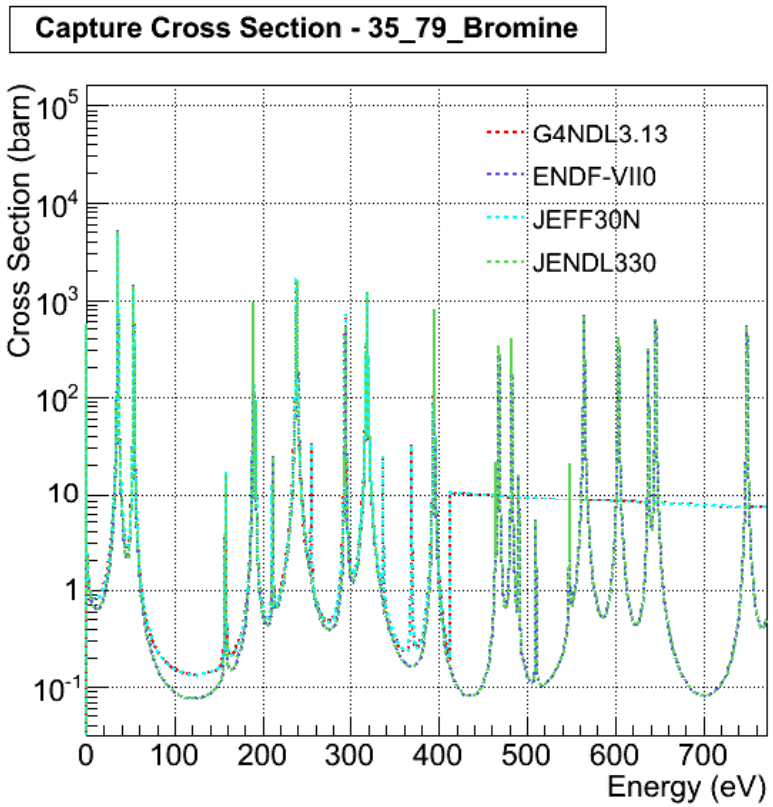


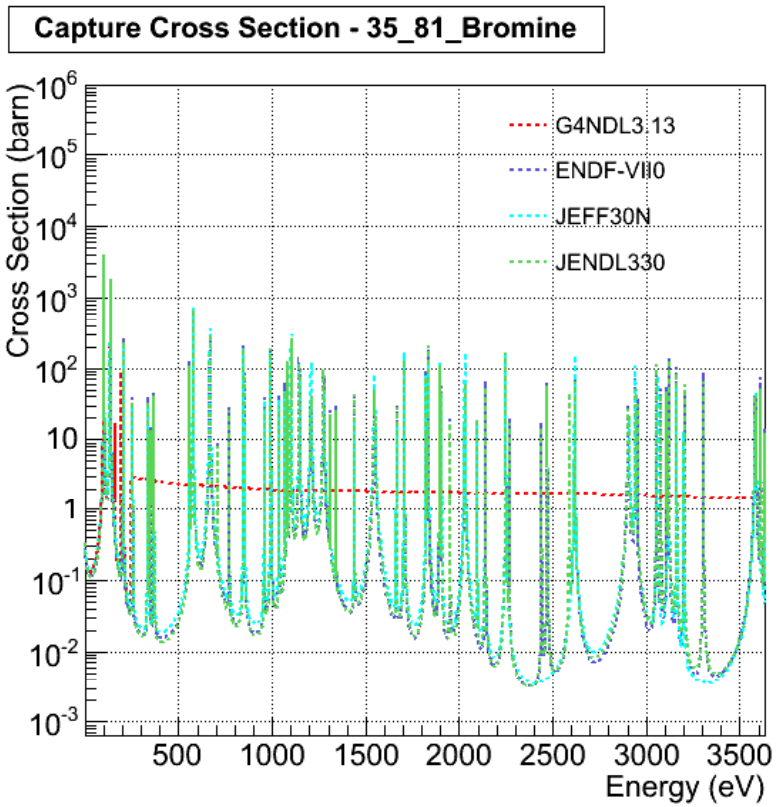
Validation method II

This is just to show differences in the libraries

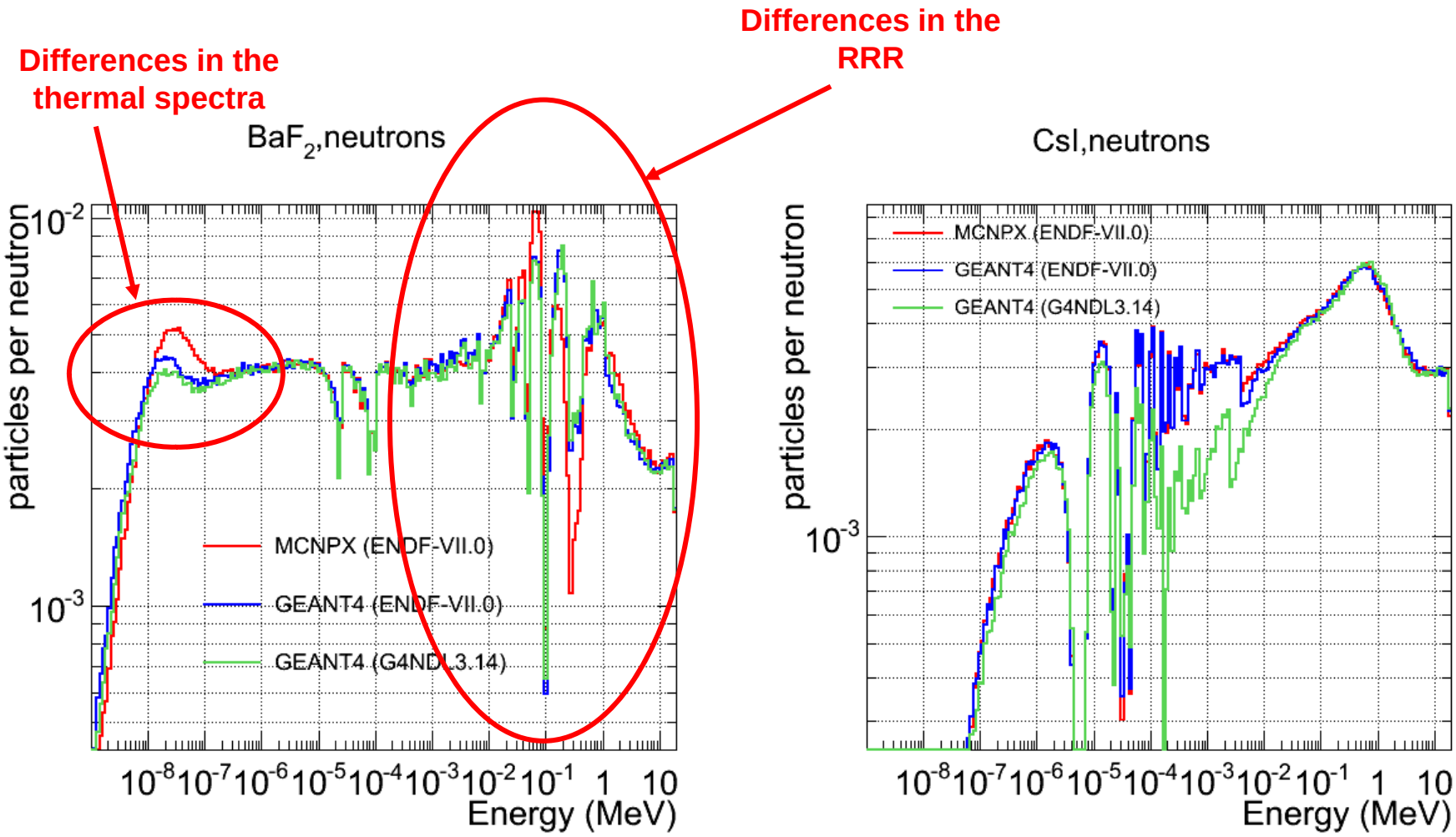


Validation method II

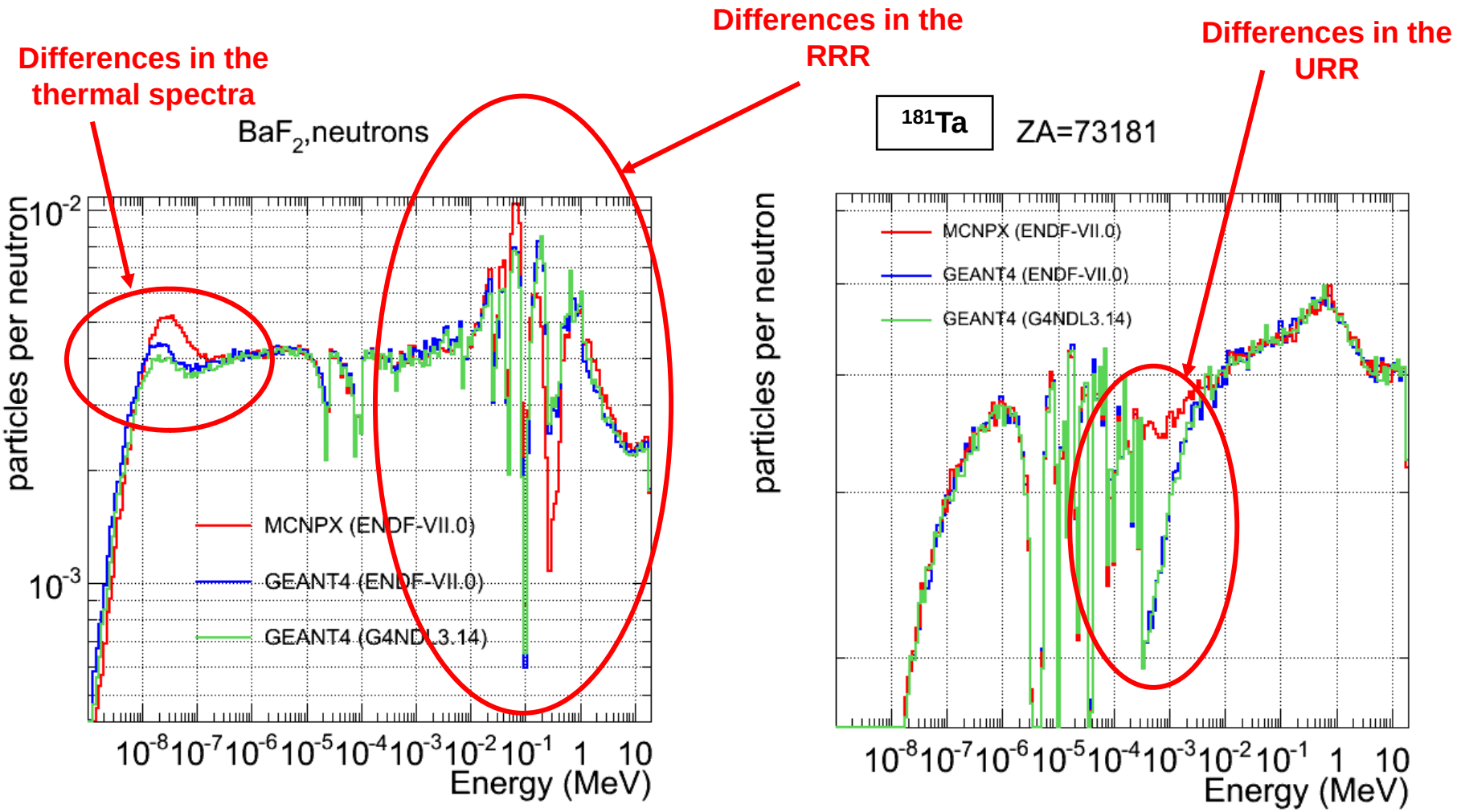




Validation method II



Validation method II



Validation method II

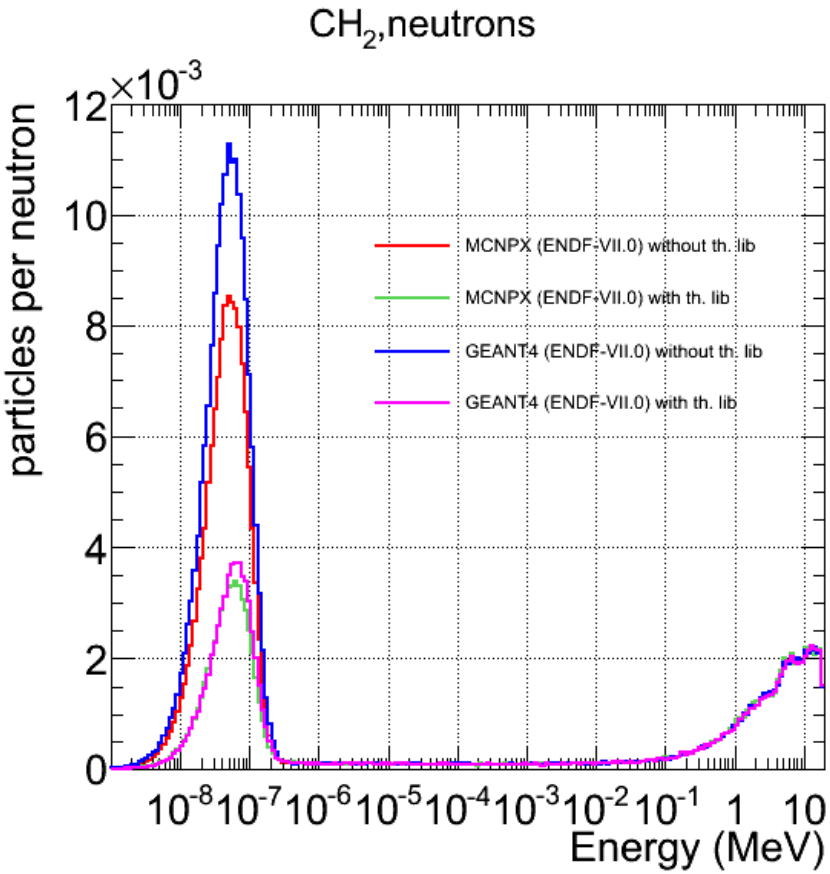
An iterative method has been developed in order to make the “sphere simulation” for a large amount of isotopes. All ENDF-VII.0 isotopes have been simulated with GEANT4 and MCNPX, using the 5-15 cm sphere, with 1g/cm^3 density. At the view of the results, three main differences have been observed and identified:

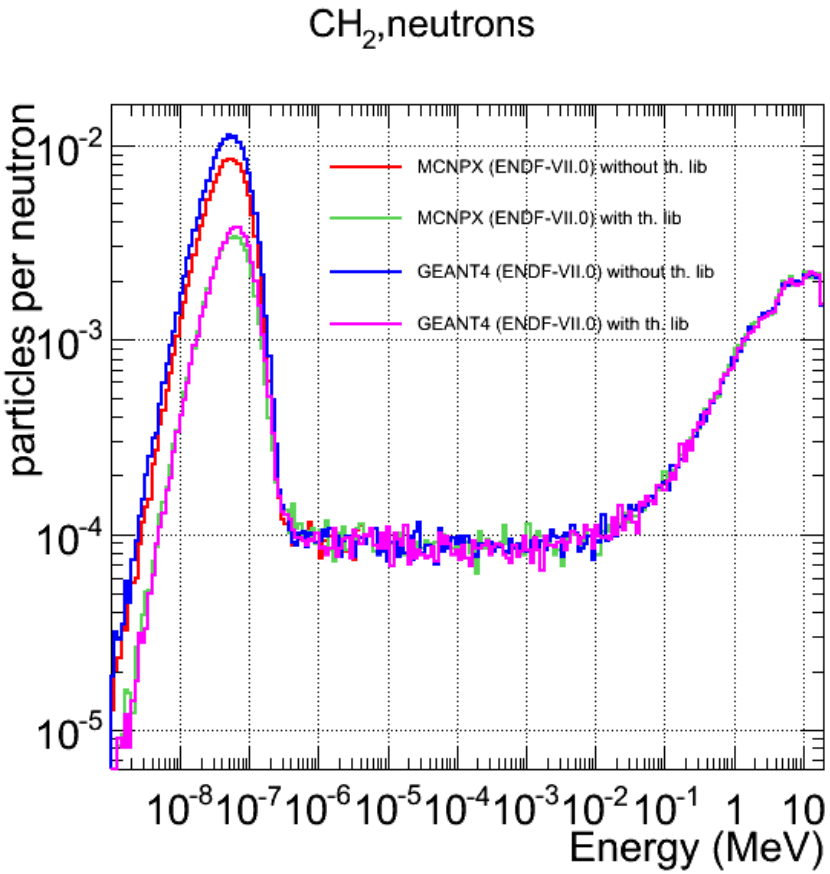
1- If there is thermal spectrum, the results obtained with both codes is always different. However, if thermal libraries are used, the results are the same. So thermal neutrons are treated differently in both codes when there are not thermal libraries. However, there is no way to simulate thermal neutrons without thermal libraries.

2- There are some differences which come from some error in the code: for (n,n’), (n,p), (n,d), (n,t), (n,3He) and (n,a) reactions, the energy of the outgoing particle is calculated by looking at the Inelastic/Gammas folder (*Example: the energy of a (n,n_3) neutron is calculated by looking the energy of the 3th excited level of the nucleus, not from “G4NDL file” information*). Some of these files are wrong, and some others do not correspond exactly with the level to which the XS refers (breakup reactions). A correction has been made in the GEANT4 code.

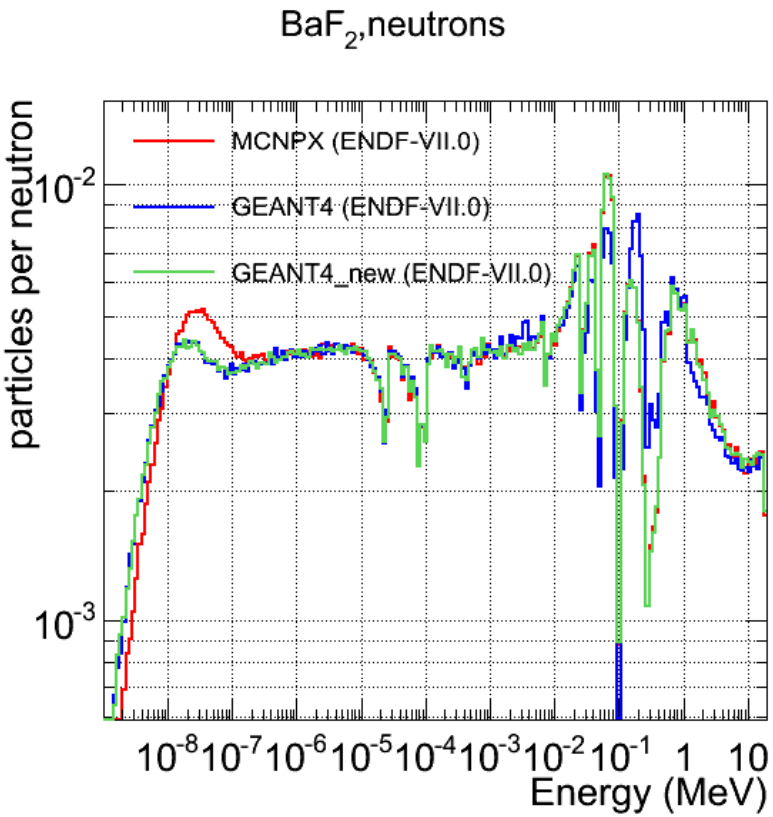
3- MCNPX uses by default an statistical treatment for the URR. If it is deactivated the MCNPX result matches the GEANT4 result.

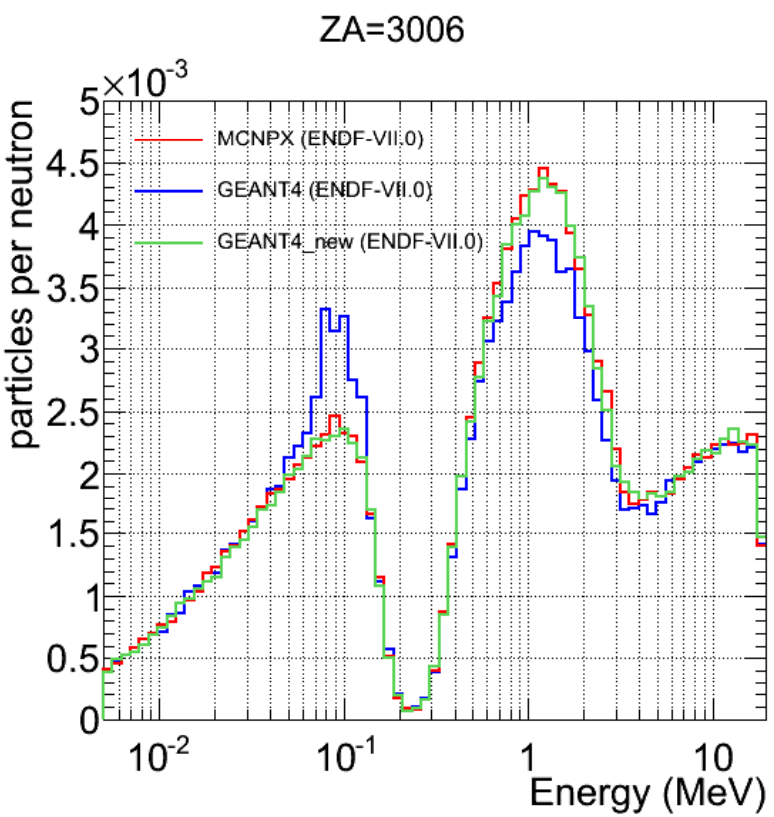
Thermal spectra (1)





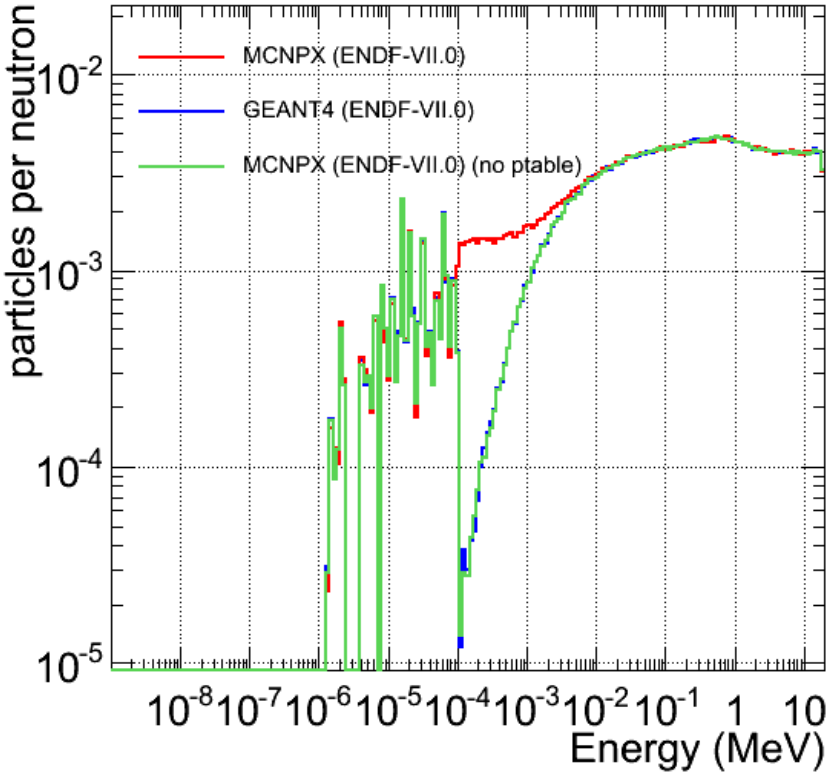
Inelastic scattering (2)



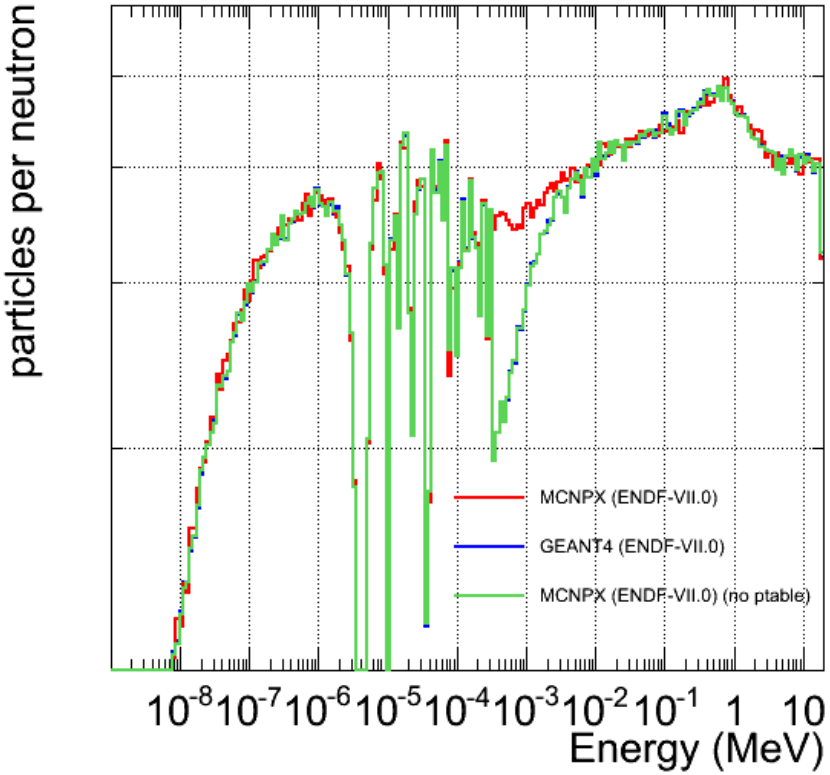


Shelf shielding (3)

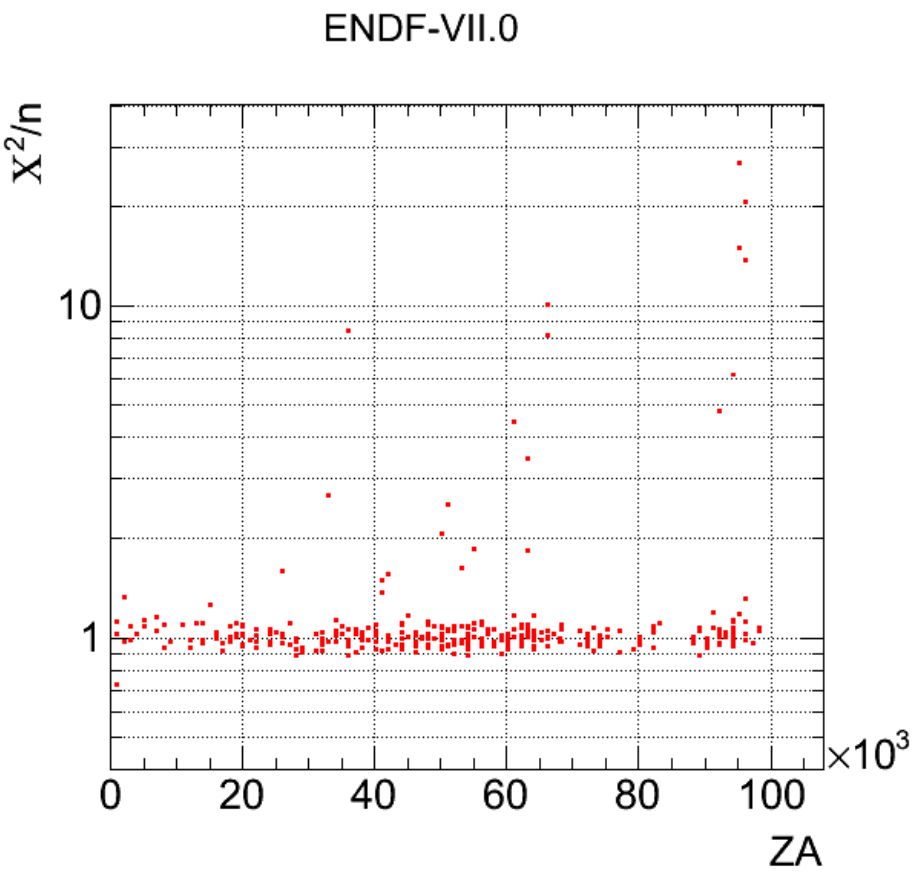
^{151}Eu ZA=63151



^{181}Ta ZA=73181



Validation method II

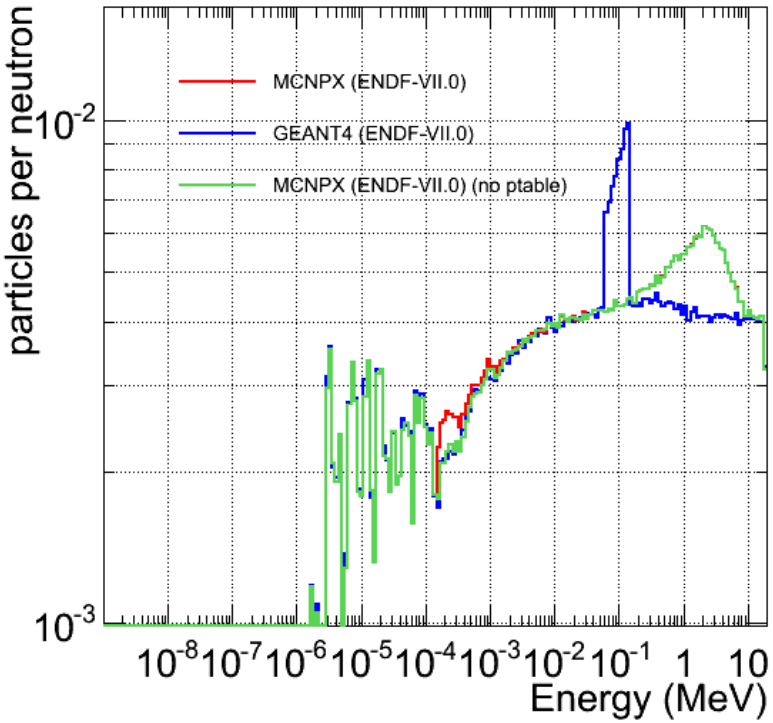


- 351(/385) ENDF-VII.0 isotopes have been compared up to now.
- GEANT4 simulations with the “inelastic correction”.
- MCNPX without the statistical treatment for the URR.
- The Chi2/n value between both results has been calculated, for the part of the spectrum over 1eV, to avoid the thermal problem.
- 25/351 isotopes with Chi2/n values grater than 1.2.
- 19/351 isotopes with Chi2/n values grater than 1.5.
- 14/351 isotopes with Chi2/n values grater than 2.

Validation method II

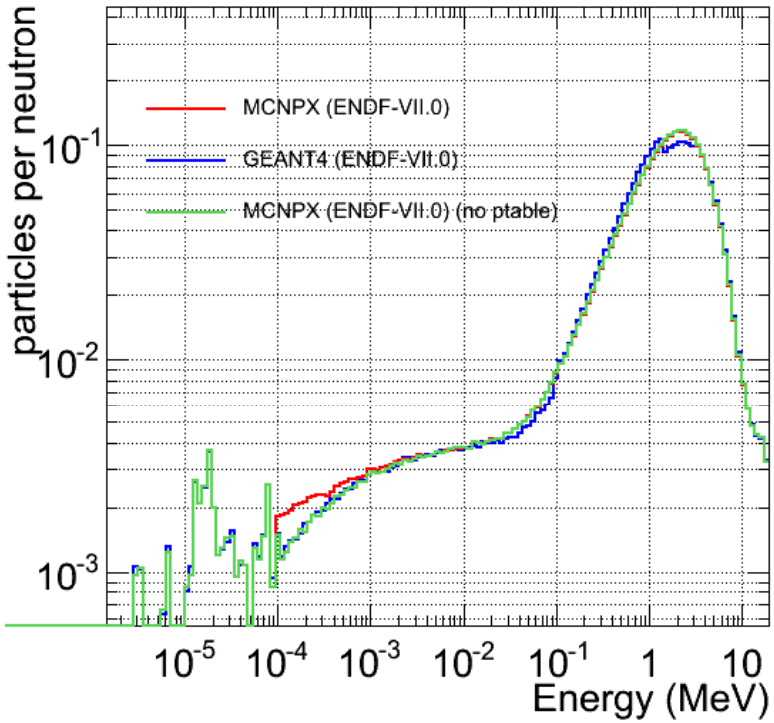
Chi2/n=27

ZA=95241



Chi2/n=20

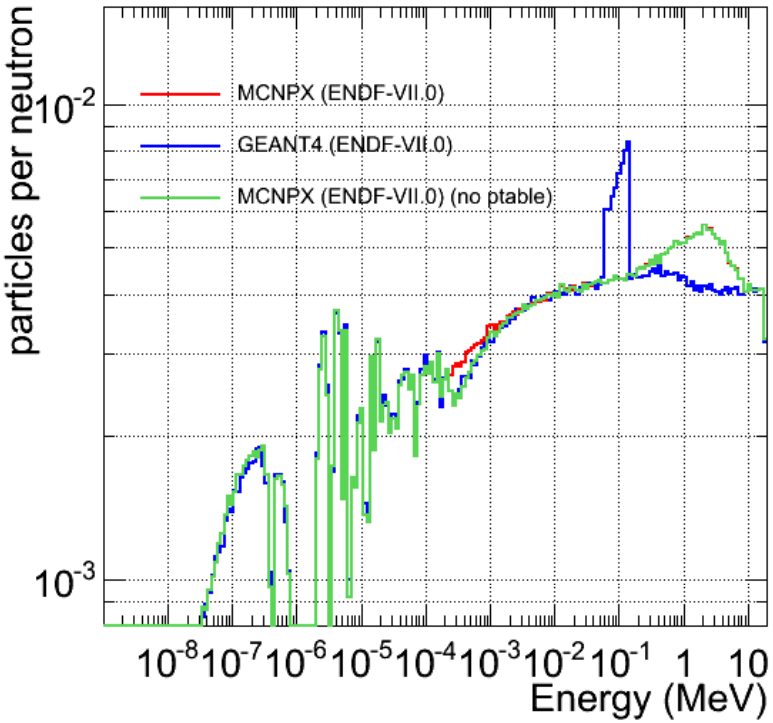
ZA=96245



Validation method II

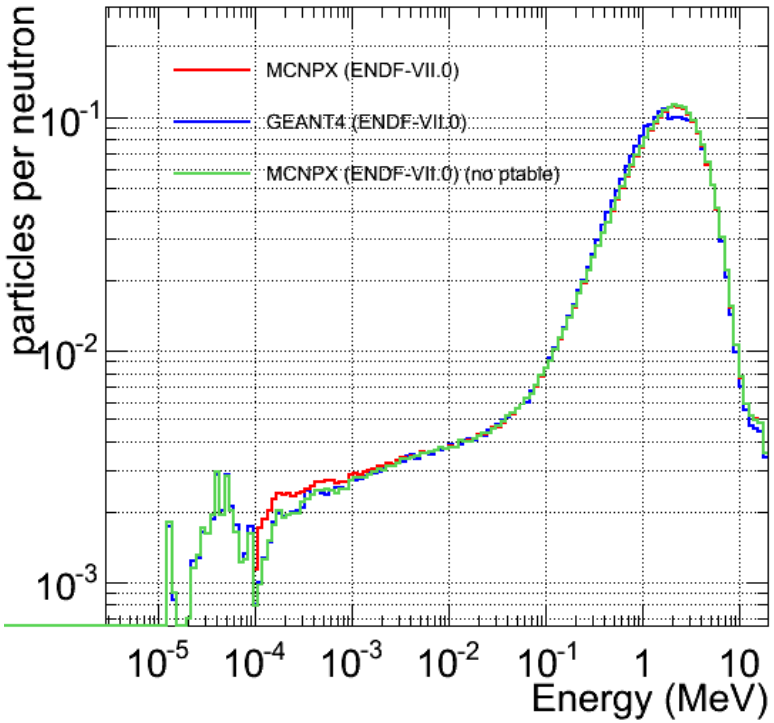
Chi2/n=15

ZA=95243



Chi2/n=13.7

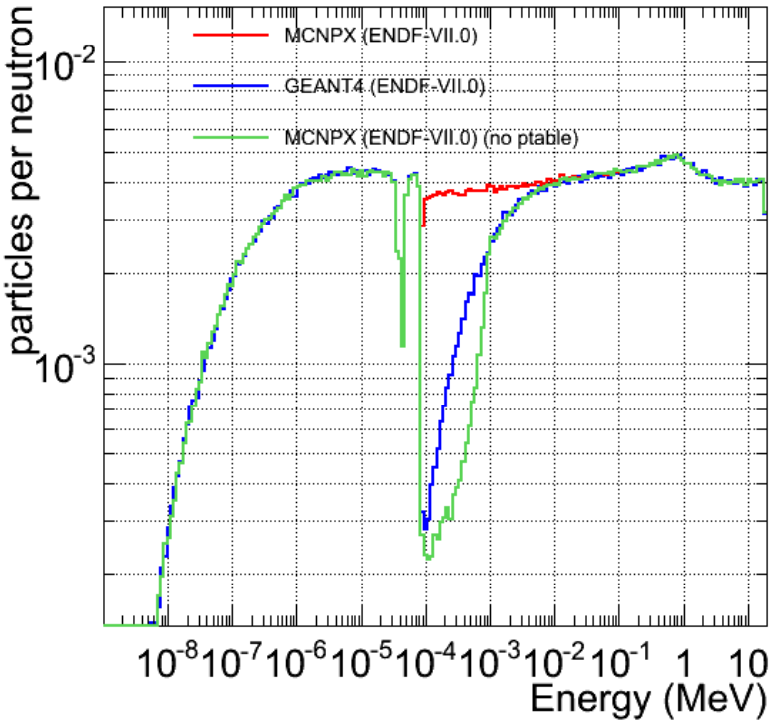
ZA=96243



Validation method II

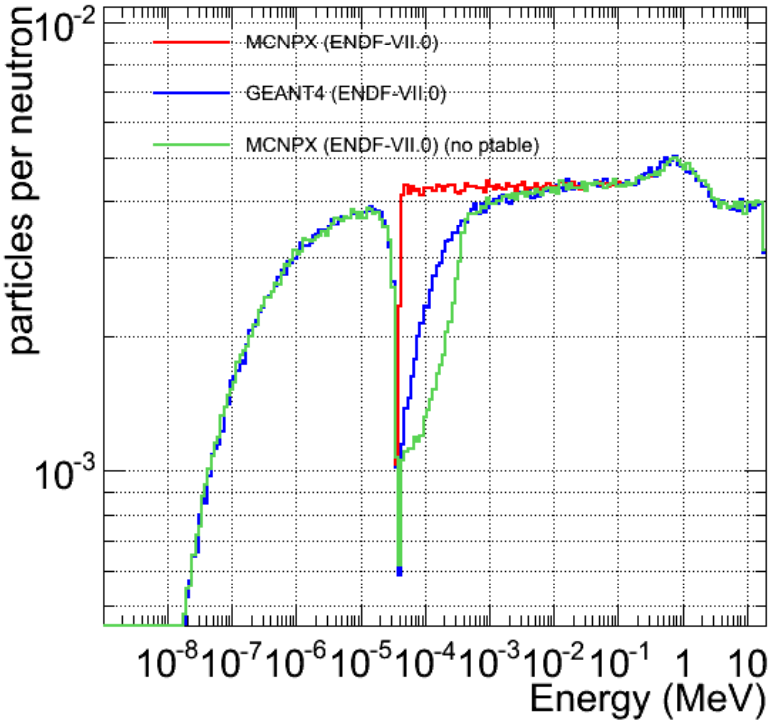
Chi2/n=10

ZA=66158



Chi2/n=8.4

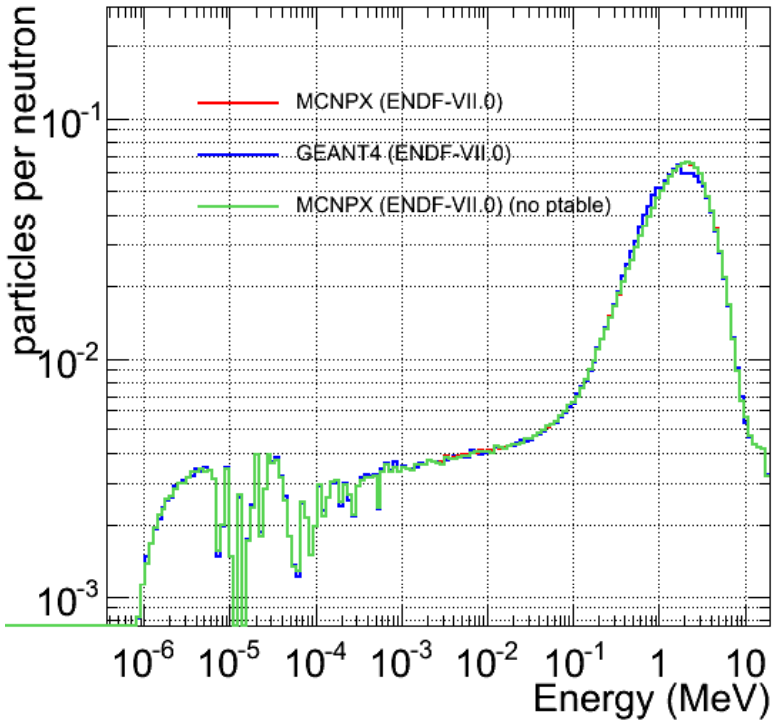
ZA=36082



Validation method II

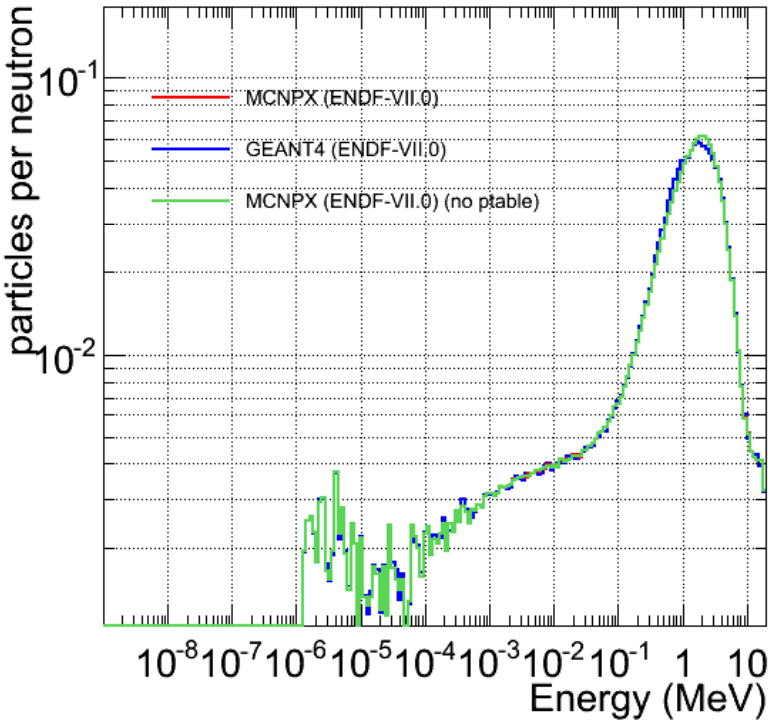
Chi2/n=6.2

ZA=94239

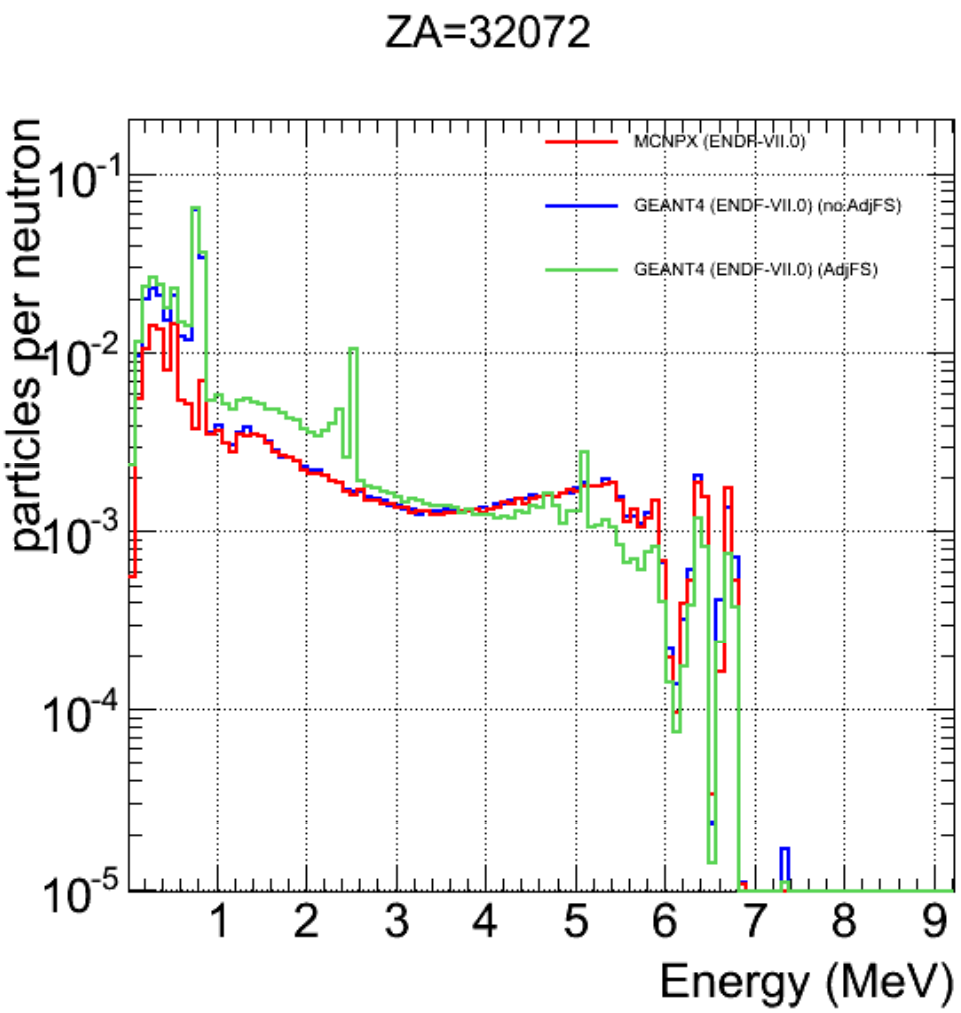


Chi2/n=4.8

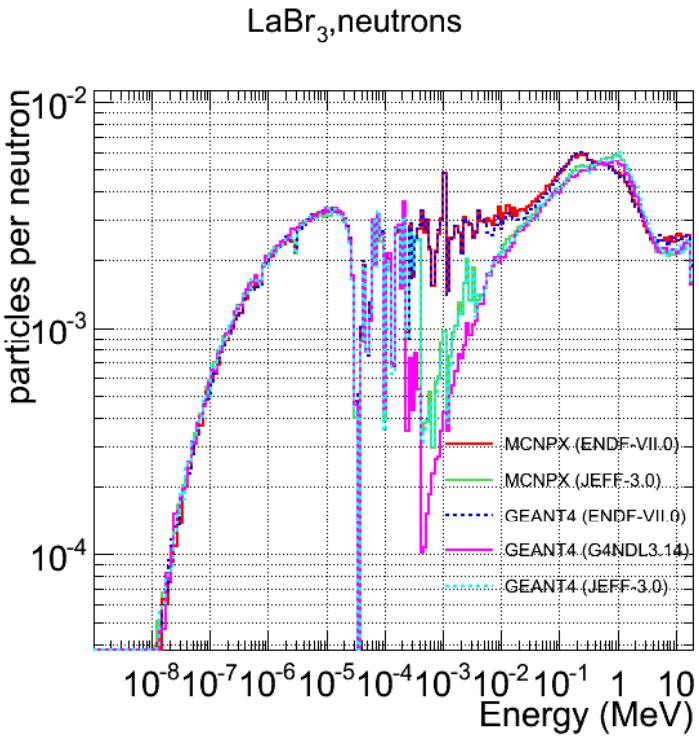
ZA=92235



Gammas


ZA=32072
MCNPX (ENDF-VII.0)
GEANT4 (ENDF-VII.0) (no AdjFS)
GEANT4 (ENDF-VII.0) (AdjFS)
particles per neutron
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
1 2 3 4 5 6 7 8 9
Energy (MeV)

GEANT4 sólo distribuye su propia librería: G4NDL3.14 (181 isótopos). Se han generado 8 nuevas librerías: ENDF-(VI.8/VII.0)-(317/385), JEFF-(3.0/3.1)-(373/334) JENDL-(3.3/4.0)-(332/400), BROND-2.2 (120), y CENDL-3.1 (239).



Las nuevas librerías se han validado haciendo simulaciones con una geometría que consiste en una esfera de 5-15cm, en la que se tiran neutrones isoletárgicos en el centro, en todo el rango de energías, contando los neutrones que salen, y comparando GEANT4 con MCNPX.

Se han encontrado y corregido algunos errores en el código.