Neutron library G4NDL4.6 : validation and computing performance

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Introduction

G4NDL are the nuclear data libraries used for the neutron transport below 20 MeV by the G4ParticleHP module of Geant4. They come from libraries written originally in ENDF-6 format.

The information in the G4NDL libraries are pointwise cross sections of the different reaction channels and different probability distributions for the production yields and energy-angular distributions of the emitted particles in the FS.

Evaluated data libraries (neutron incident):

- USA+Canada: **ENDF/B** → ENDF/B-VIII.0, **ENDF/B-VII.1**,ENDF/B-VII.0 …
- NEA (Europe): **JEFF** → **JEFF-3.3**, JEFF-3.2, JEFF-3.1.2, JEFF-3.1.1 …
- Japan: **JENDL** → JENDL-4.0, JENDL-3.3
- Russia: **BROND**, **ROSFOND** → BROND-3.1, ROSFOND-2010 …
- China: **CENDL** → CENDL-3.1, CENDL-2

Most of these releases are available in Gean4 format in https://www-nds.iaea.org/geant4/

Official libraries:

G4NDL4.0 → ENDF/B-VII.0
G4NDL4.1-G4NDL4.5 → ENDF/B-VII.1
G4NDL4.6 → JEFF-3.3

Introduction & validation

G4NDL4.5 → incident neutron data library used up to Geant4.10.5. It comes mainly from ENDF/B-VII.1.

G4NDL4.6 → incident neutron data library used in Geant4.10.6. It is JEFF-3.3.

Advantages of G4NDL4.6 over G4NDL4.5 :

1- Geant4 results are closer to MCNP when using JEFF-3.3 than when using any other library, i.e. the performance of Geant4 seem to be the best when using JEFF-3.3. A verification study has been performed and is available in:

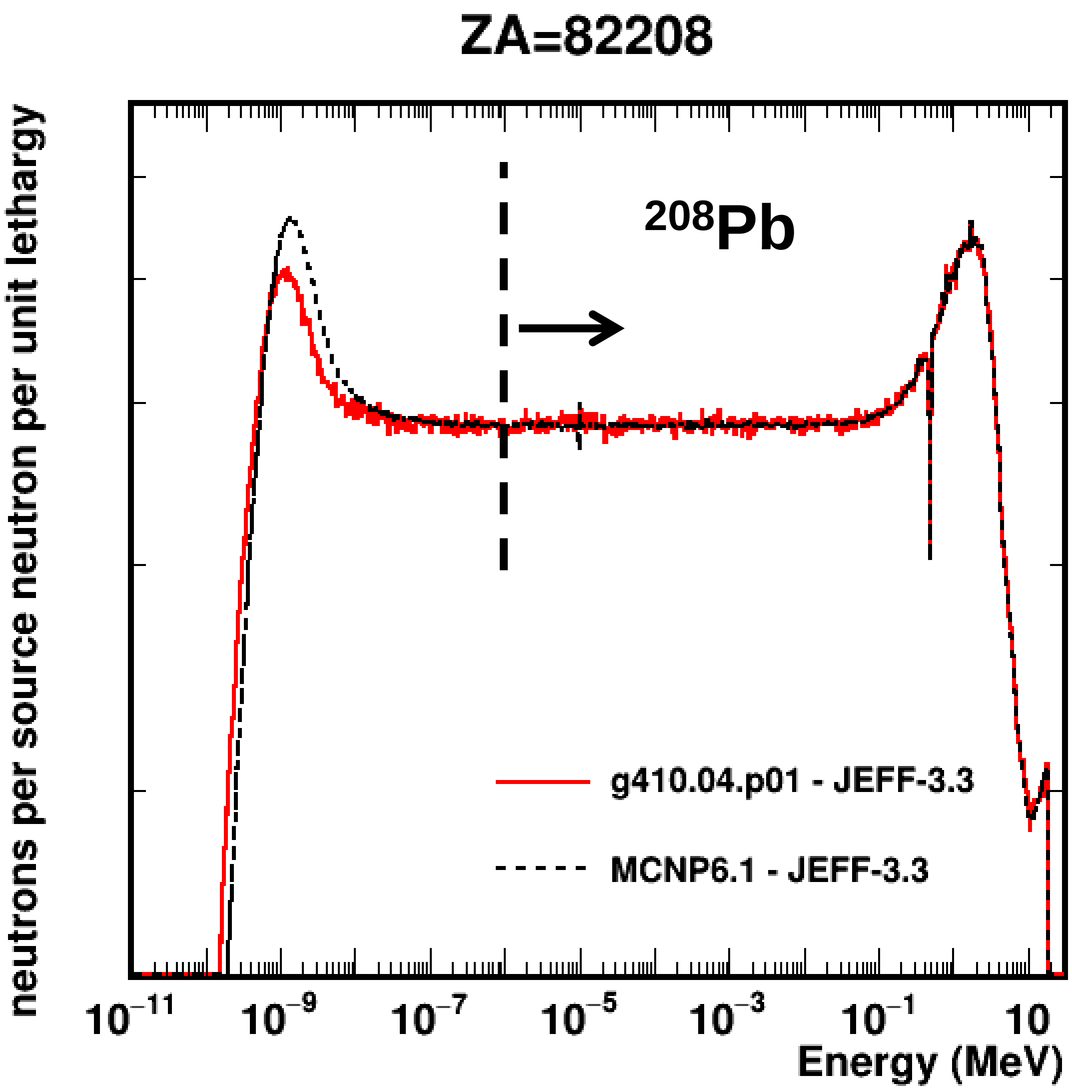
IAEA report → https://www-nds.iaea.org/publications/indc/indc-nds-0758/

G4 Hadronic meeting June 2018 → link

2- More isotopes than G4NDL4.5: 562 VS 363 isotopes, i.e. 199 more. 45 of them correspond to transuranium (Z>92) elements, not present in G4NDL4.5 (ENDF/B-VII.1 has 423 isotopes).

The next 3-4 slides are from the talk of the G4 Hadronic meeting June 2018

Validation

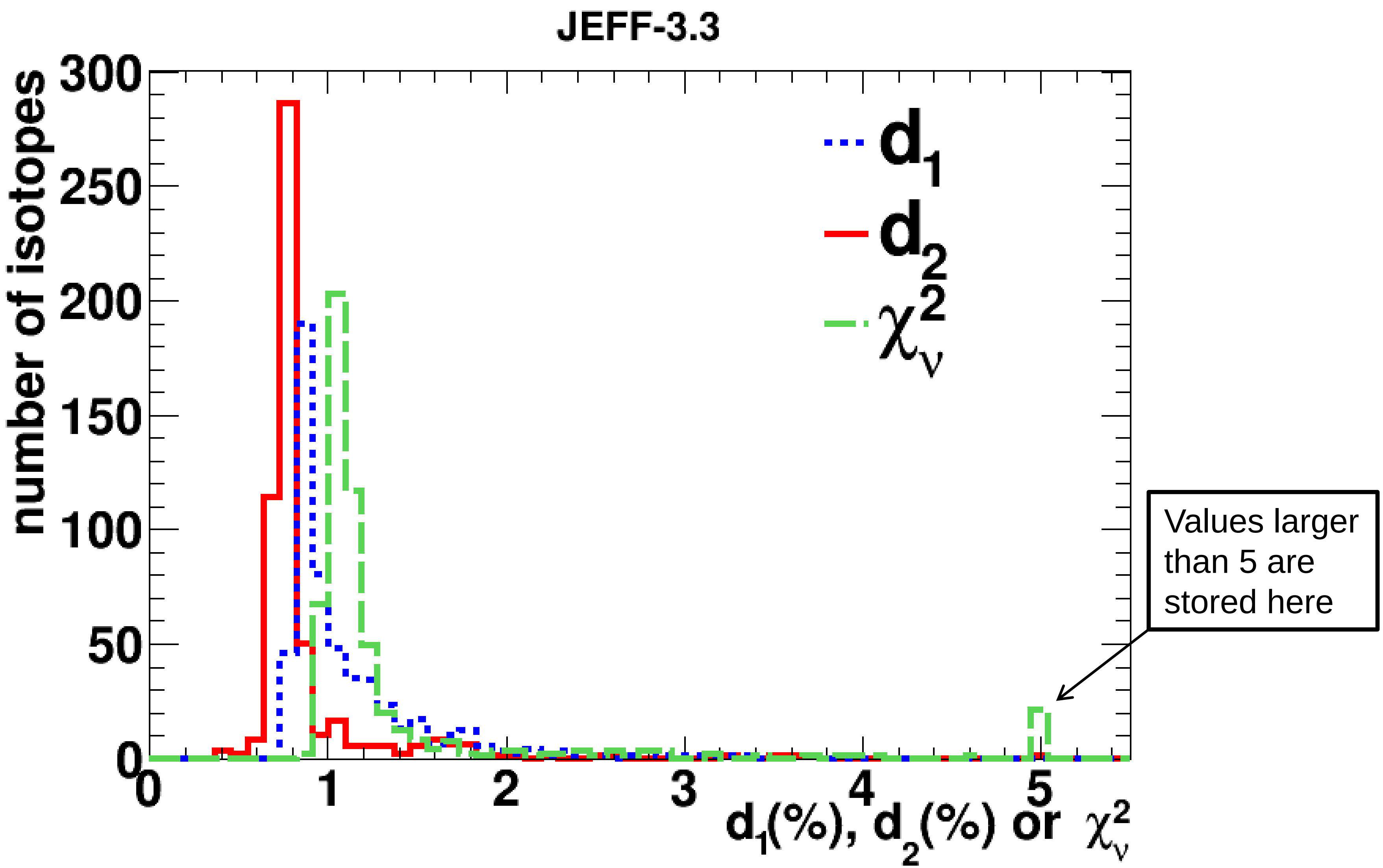


$$d_1 = \frac{1}{N} \sum_{E_i > 1\ eV} \frac{|x_i^G - x_i^M|}{\frac{1}{2}(x_i^G + x_i^M)}$$

$$d_2 = \frac{1}{N} \sum_{E_i > 1\ eV, \sigma_i < 1\%} \frac{|x_i^G - x_i^M|}{\frac{1}{2}(x_i^G + x_i^M)}$$

$$\chi_\upsilon^2 = \frac{1}{N} \sum_{E_i > 1\ eV} \left(\frac{x_i^G - x_i^M}{\sigma_i} \right)^2$$

Validation



JEFF-3.3
number of isotopes
300
250
200
150
100
50
0
0
1
2
3
4
5
$d_1(\%)$, $d_2(\%)$ or χ^2_ν
d_1
d_2
χ^2_ν
Values larger than 5 are stored here

Validation

Library	Total number of isotopes	Number of isotopes tested	Number of isotopes with $\chi_\upsilon^2 > 2$ and $d_2 > 1.5\%$	Fraction of isotopes with $\chi_\upsilon^2 > 2$ and $d_2 > 1.5\%$	Number of isotopes with $\chi_\upsilon^2 > 2$	Fraction of isotopes with $\chi_\upsilon^2 > 2$
JEFF-3.3	**562**	**546**	**34**	**6%**	**51**	**9%**
JEFF-3.2	472	460	52	11%	78	17%
ENDF/B-VIII.0	556	533	84	16%	114	21%
ENDF/B-VII.1	423	411	90	22%	120	29%
BROND-3.1	372	361	64	18%	78	22%
JENDL-4.0u	406	398	58	15%	87	22%

Energies of the secondary neutrons

Validation

Summary and conclusions (G4 Hadronic meeting June 2018):

[…]

A comparison between Geant4 and MCNP6 when using these six evaluated libraries has been performed concerning the neutron transport. Some of the differences have been quantified. According to our comparison, JEFF-3.3 is the library that yields more similar results between both codes. A detailed report has been written and will be available from https://www-nds.iaea.org/publications/indc/indc-nds-0758/

[…]

Geant4.10.6: G4NDL4.5 → G4NDL4.6 i.e. ENDF/B-VII.1 → JEFF-3.3 (+ including Z>92 isotopes).

In any case, many other libraries are available in https://www-nds.iaea.org/geant4/

Some people reported that Geant4 is slower (10%-40%) when running with G4NDL4.6 with respect to G4NDL4.5. They used calorimeters to detect protons of a few GeV.

We have investigated the computing performance of G4NDL4.6 and G4NDL4.5.

Computing performance

Simulation

For this study, we have performed a set of simulations with the following characteristics:

Geometry: 100 cm radius sphere made of a certain material, with a density which can vary from one simulation to other (default 10 g/cm^3).

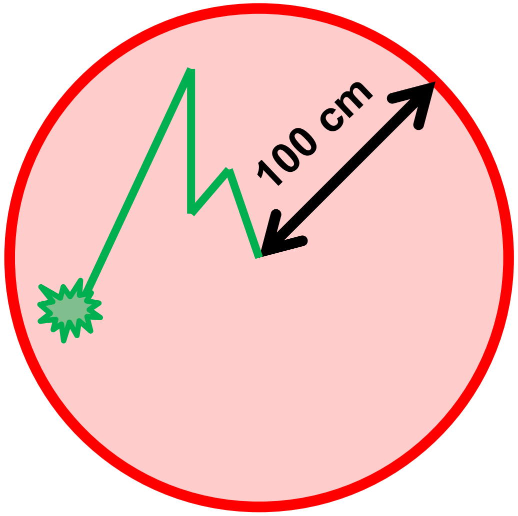
Source: neutrons emitted from the center of the sphere (default 14.1 MeV)

Physics List: Shielding physics list.

Tallies: neutron flux inside the sphere + **CPU time** (obtained using the C++ *clock()* function).

The following flags were used in the simulations:

export G4NEUTRONHP_SKIP_MISSING_ISOTOPES=1
export G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE=1
export G4PHP_DO_NOT_ADJUST_FINAL_STATE=1



Simulation

We have performed different simulations varying:

- The material of the sphere: in particular we performed simulations with each of the elements from Z=1 up to Z=86. The isotopic composition of the elements have been obtained from the NIST database inside Geant4. We didn't simulate Z>86 elements to avoid fission reactions. When using G4NDL4.5 we could not simulate the following elements, due to lack of data: Z= 10, 43, 69, 70, 76, 78, 84, 85, 86 (Ne, Tc, Tm, Yb, Os, Pt, Po, At and Rn).
- The data library used.
- The energy of the source neutron.
- The density of the sphere, which is equivalent to vary the radius.
- Some physics options, in order to estimate the CPU time dedicated to different processes: Doppler, generation of secondary particles, transport of secondary particles …

When comparing the simulations performed with all the elements with Z=1-86, we evaluate the **average difference if CPU time between using G4NDL4.5 and G4NDL4.6** with ($t_{1,z}$ and $t_{2,z}$ are the CPU times of the simulations for material with Z=z when using G4NDL4.5 and G4NDL4.6, respectively):

$$\boldsymbol{R = \sum_{z=1}^{z=86} \frac{t_{2,z} - t_{1,z}}{(t_{2,z}+t_{1,z})/2}}$$

Results01

We have performed a first set of simulations with different densities and neutron energies. In particular:

- E=14.1 MeV and ρ=10 g/cm^3 → Figure 1a – R = 7.3%.
- E=14.1 MeV and ρ= 1 g/cm^3 → Figure 1b – R = 12.6%.
- E=14.1 MeV and ρ= 0.1 g/cm^3 → Figure 1c – R = 11.0%.
- E=1 keV and ρ= 10 g/cm^3 → Figure 1d – R = 15.2%.

We can observe from these results that, according to these simulations, **G4NDL4.6 seem to be *on average* slower than G4NDL4.5, but not for all the cases** (materials), i.e. there are materials where G4NDL4.6 is faster than G4NDL4.5.

We have investigated if the differences come from the processing of the data library, instead of the data library itself. This is, G4NDL4.5 was generated by T. Koi using NJOY and G4NDL4.6 by E. Mendoza using PREPRO. The answer is **no**: we have run simulations using ENDF/B-VII.1 generated by E. Mendoza using PREPRO and the results were the same as those using G4NDL4.5.

→ **differences do not come from the processing of the data library**

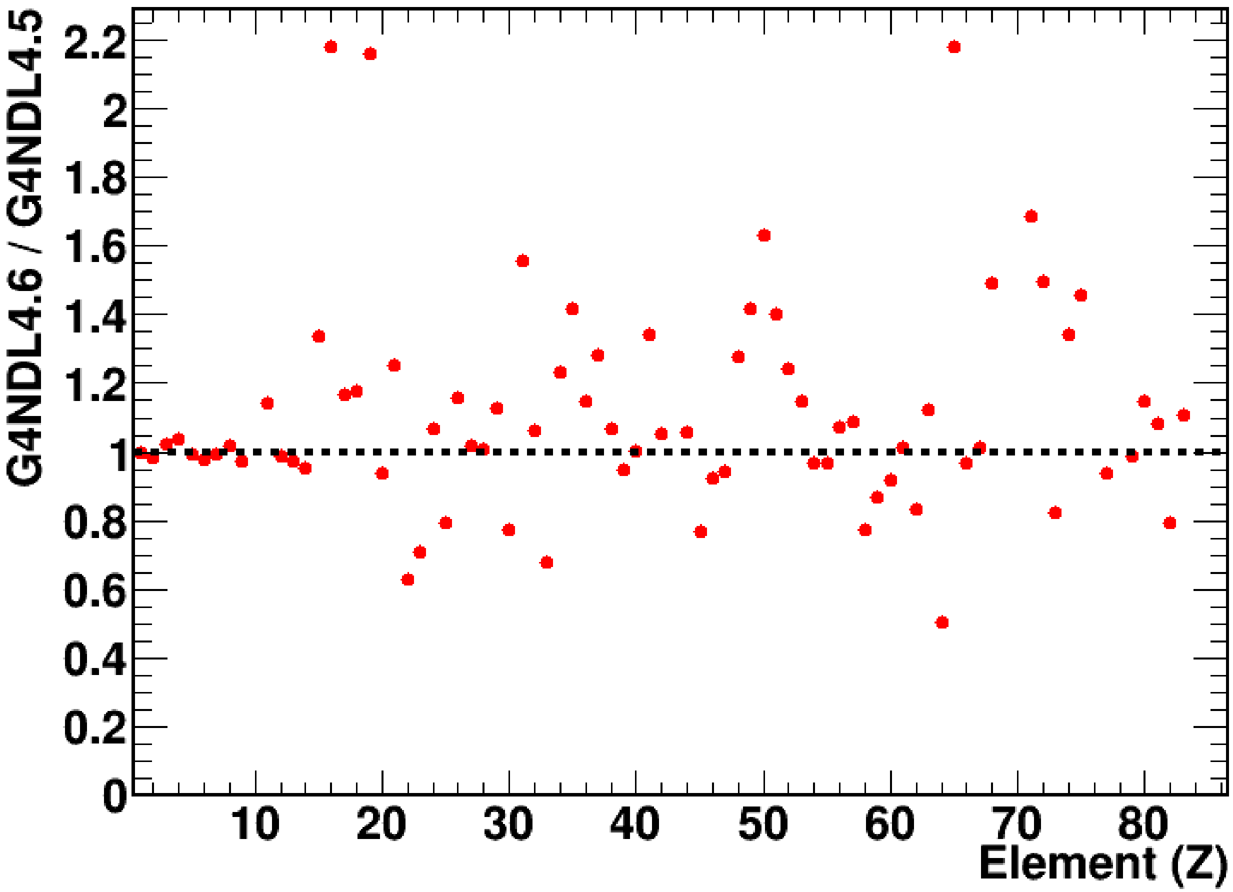


Figure 1a: ratio between CPU times when performing simulations using 14.1 MeV neutrons transported in a 10 g/cm^3 sphere made of different elements, using G4NDL4.6 and G4NDL4.5. R = 7.3%.

Results02

We have quantified, for some specific simulations, what is the difference in CPU time between G4NDL4.5 and G4NDL4.6. The next step has been to study in which processes Geant4 dedicate the CPU time.

For this, we run the same simulations using different physics options:

- Sim01: standard simulation.
- Sim02: without Doppler.
- Sim03: isotropic sampling of the angle of the emitted neutron after elastic scattering.
- Sim04: secondary particles different than neutrons are not transported.
- Sim05: Sim04 + gamma rays from capture reactions are not generated.

From the results of this simulations we estimated the CPU time used in different processes by subtracting the CPU time used in the different simulations according to:

- The **Doppler broadening**: Sim01-Sim02.
- The **sampling of the angle of the elastic scattered neutron**: Sim01-Sim03.
- The **transport of no-neutrons secondary particles**: Sim01-Sim04.
- The **generation of the capture gamma rays**: Sim04-Sim05.

Results02

The results of these simulations, for some of the previous cases are:

- Figure 2a: E=14.1 MeV and ρ=10 g/cm^3 using G4NDL4.5
- Figure 2b: E=14.1 MeV and ρ=10 g/cm^3 using G4NDL4.6
- Figure 3a: E=14.1 MeV and ρ=1 g/cm^3 using G4NDL4.5
- Figure 3b: E=14.1 MeV and ρ=1 g/cm^3 using G4NDL4.6
- Figure 4a: E=14.1 MeV and ρ=0.1 g/cm^3 using G4NDL4.5
- Figure 4b: E=14.1 MeV and ρ=0.1 g/cm^3 using G4NDL4.6
- Figure 5a: E=1 keV and ρ=10 g/cm^3 using G4NDL4.5
- Figure 5b: E=1 keV and ρ=10 g/cm^3 using G4NDL4.6

Note that the CPU time fractions shown are estimations. In some cases the sum of them exceeds 100%. Note also that when simulating 1 keV neutrons, only elastic and capture channels are open in most of the cases. On the contrary, at 14.1 MeV there are usually many *inlelastic* channels opened.

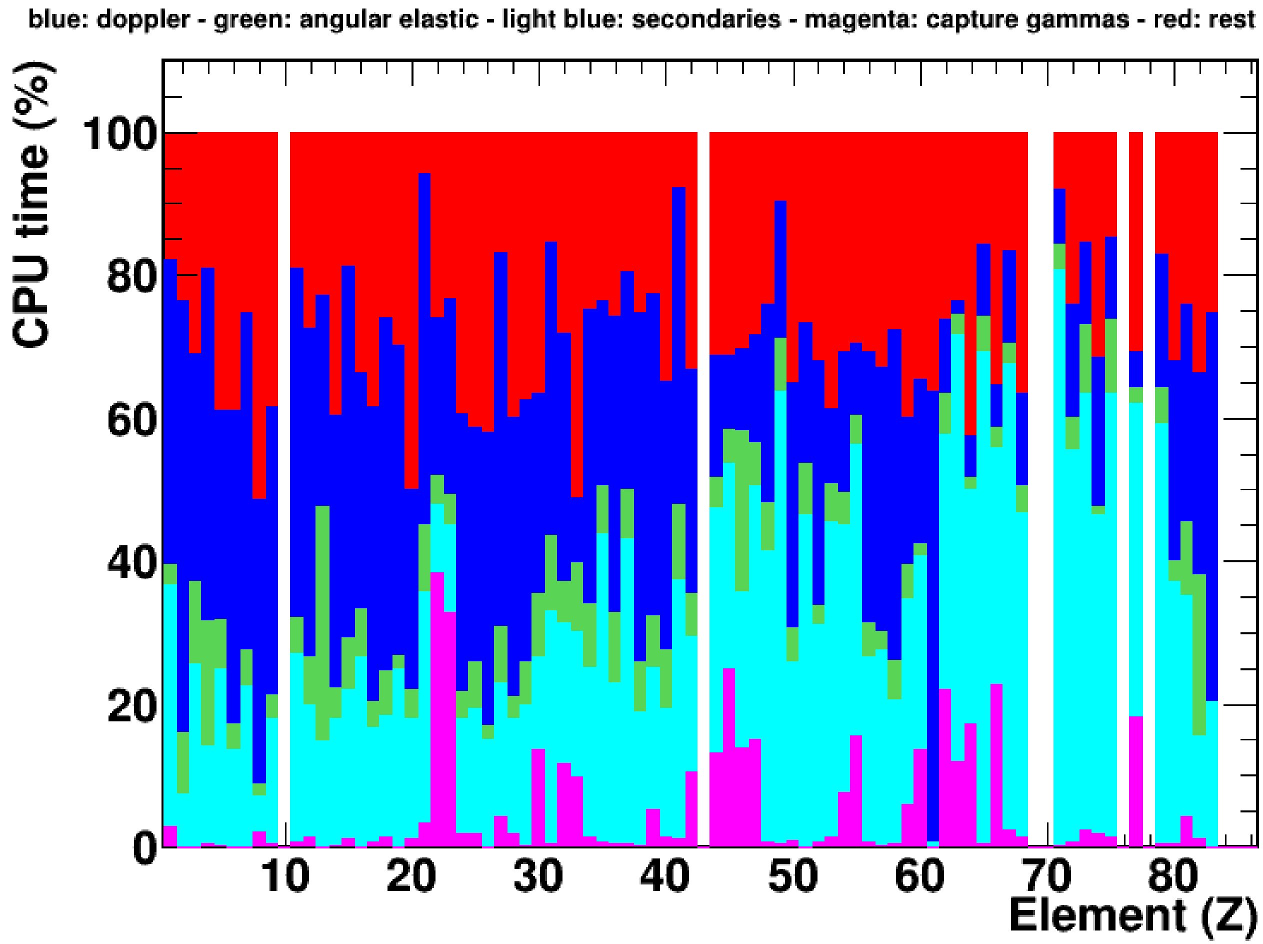


Figure 2a: estimated fraction of the CPU time dedicated to perform the Doppler broadening (blue), the sampling of the angle of the elastic scattered neutron (green), the transport of no-neutrons secondary particles (light blue) and the generation of the capture gamma rays (magenta) in simulations performed with 14.1 MeV neutrons in a sphere of 10 g/cm^3 and using G4NDL4.5.

Results03

We have also make an estimation of the CPU time used by Geant4 for the following processes: Transport of neutrons in elastic collisions, transport of secondaries (including non-elastic neutrons), generation of secondaries (inelastic and capture). Again, we run the same simulations using different physics options:

- Sim01: standard simulation.
- Sim02: secondary particles are not transported.
- Sim03: Sim02 + inelastic secondaries are not generated.
- Sim04: Sim03 + gamma rays from capture reactions are not generated.

From the results of this simulations we estimated the CPU time used in different processes by subtracting the CPU time used in the different simulations according to:

- The **transport of secondary particles**: Sim01-Sim02.
- The **generation of (the first) inelastic secondaries** (just after the elastic transport, inelastic reactions induced by secondary particles are not considered here): Sim02-Sim03.
- The **generation of capture secondaries** : Sim03-Sim04.
- The ***elastic transport***: rest of the CPU time.

Results03

The results of these simulations, for some of the previous cases are:

- Figure 6a: E=14.1 MeV and ρ=10 g/cm^3 using G4NDL4.5
- Figure 6b: E=14.1 MeV and ρ=10 g/cm^3 using G4NDL4.6
- Figure 7a: E=14.1 MeV and ρ=1 g/cm^3 using G4NDL4.5
- Figure 7b: E=14.1 MeV and ρ=1 g/cm^3 using G4NDL4.6
- Figure 8a: E=14.1 MeV and ρ=0.1 g/cm^3 using G4NDL4.5
- Figure 8b: E=14.1 MeV and ρ=0.1 g/cm^3 using G4NDL4.6
- Figure 9a: E=1 keV and ρ=10 g/cm^3 using G4NDL4.5
- Figure 9b: E=1 keV and ρ=10 g/cm^3 using G4NDL4.6

Note that the CPU time fractions shown are estimations.

Results02 + Results03 summary

So now we have quantified the CPU time difference between G4NDL45 and G4NDL46. We have also estimated the CPU time dedicated to different processes. The next step is to see which processes are slower in G4NDL46 respect to G4NDL45. In the following table, we show the R-factor defined above, but considering the CPU time dedicated to the processes described in Results02 and Results03

	14.1 MeV 10 g/cm^3	**14.1 MeV 1 g/cm^3**	**14.1 MeV 0.1 g/cm^3**	**1 keV 10 g/cm^3**
Total	7%	13%	11%	15%
Doppler	5%	3%	1.5%	14%
Transport of no neutrons sec.	4%	5%	3.5%	15%
Capture gammas generation	55%	75%	-36%	60%
Inelastic sec. generation	33%	36%	40%	-5%
Elastic transport	3%	3%	0.3%	9%

Conclusion: most of the time difference seem to come from the generation (not the transport) of secondaries.

Results04

What about other data libraries?

In the following table we show the R-values obtained when performing the same comparison as before but with ENDF/B-VIII.0 and JEND-4.0u. The first two lines are the same just to remain that G4NDL4.6 is JEFF-3.3 and G4NDL4.5 is ENDF/B-VII.1.

	14.1 MeV 10 g/cm^3	**14.1 MeV 1 g/cm^3**	**14.1 MeV 0.1 g/cm^3**	**1 keV 10 g/cm^3**
G4NDL4.6 VS G4NDL4.5	7%	13%	11%	15%
JEFF-3.3 VS ENDF/B-VII.1	7%	13%	11%	15%
ENDF/B-VIII.0 VS ENDF/B-VII.1	3.3%	1.1%	0%	14%
JENDL-4.0u VS ENDF/B-VII.1	0.9%	-5%	-4%	8%

Example: $PbWO_4$

We show in Table 1, as an example, the ratio between the CPU times obtained when using G4NDL4.6 and G4NDL4.5 in the simulations of the sphere, using $PbWO_4$, Pb, W, O and their isotopes present in their natural compositions.

Isotopes ^{18}O and ^{180}W have no data in G4NDL4.5.

In Table 2, the same ratios as before, but using $PbWO_4$ only, and different physics options, which are:

- Elastic transport: simulations are killed before the generation of non-elastic secondaries.
- No sec. transport: simulations are killed after the generation of non-elastic secondaries, i.e. secondaries are not transported.

Example: $PbWO_4$

	14.1 MeV 10 g/cm^3	14.1 MeV 1 g/cm^3	14.1 MeV 0.1 g/cm^3	1 keV 10 g/cm^3
$PbWO_4$	1.42	1.13	1.09	1.59
O	0.98	1.04	1.00	0.98
W	1.30	1.31	1.20	3.33
Pb	0.94	1.04	1.09	1.03
8016	1.00	1.03	0.97	0.98
8017	1.97	3.02	2.37	1.65
8018	-	-	-	-
74180	-	-	-	-
74182	1.31	1.22	1.11	2.30
74183	1.22	1.33	1.28	4.77
74184	1.20	1.37	1.26	1.47
74186	1.83	1.39	1.27	2.06
82204	0.98	0.84	0.82	1.18
82206	1.35	1.03	1.12	1.06
82207	1.10	1.13	1.29	1.28
82208	0.73	0.98	1.00	0.93

Table 1: CPU time (G4NDL4.6) / CPU time (G4NDL4.5)

Example: $PbWO_4$

	14.1 MeV 10 g/cm^3	14.1 MeV 1 g/cm^3	14.1 MeV 0.1 g/cm^3	1 keV 10 g/cm^3
Standard	**1.42**	**1.13**	**1.09**	**1.59**
Elastic transport	**0.94**	**0.97**	**0.98**	**1.60**
No sec. transport	**1.14**	**1.12**	**1.06**	**1.68**

Table 2: CPU time (G4NDL4.6) / CPU time (G4NDL4.5) when simulating $PbWO_4$ with different physics options

Conclusions

We have run large amount of simulations, using different materials and neutron energies, and we have defined a quantity to evaluate the CPU time difference between two sets of simulations $\boldsymbol{R} = \sum_{z=1}^{z=86} \frac{t_{2,z} - t_{1,z}}{(t_{2,z} + t_{1,z})/2}$. From the study presented here we can conclude that:

1- G4NDL4.6 (JEFF-3.3) is *on average* slower than G4NDL4.5 (ENDF/B-VII.1), according to these simulations, but not for all the cases (materials), i.e. there are materials where G4NDL4.6 is faster than G4NDL4.5.

2- We have tried to estimate which are the time dedicated by Geant4 to simulate different processes. The larger difference in CPU time between G4NDL4.5 and G4NDL4.6 seem to be in the generation of the (non-elastic) secondary particles.

Why is slower the generation of secondaries in G4NDL4.6 (JEFF-3.3) than in G4NDL4.5 (ENDF/B-VII.1)? → There are several format in the ENDF-6 files to store the probability distributions for the production yields and energy-angular distributions of the emitted particles in the FS. *Probably* JEFF-3.3 uses more often some formats which are slower in Geant4.

Rest of the figures

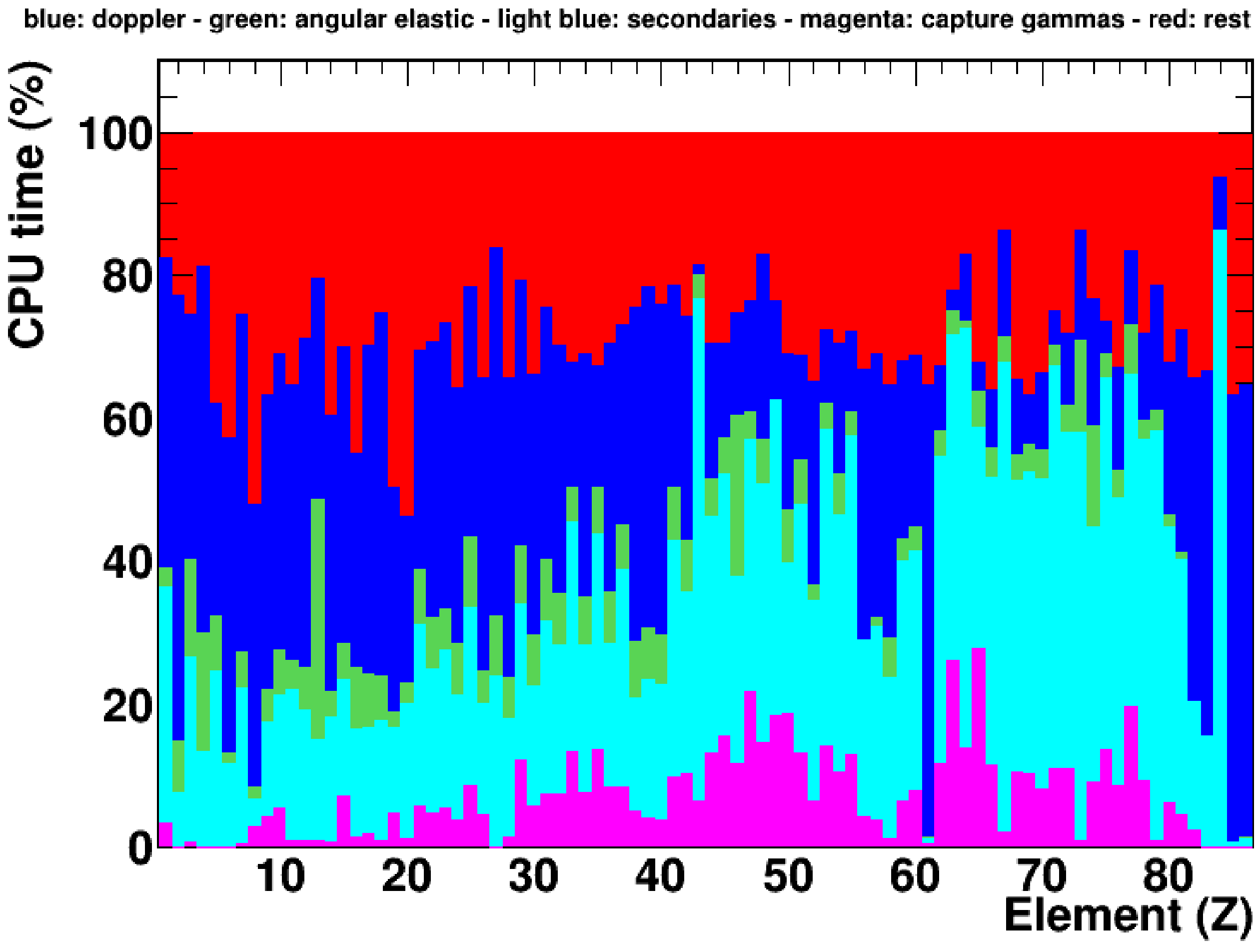


Figure 2b: estimated fraction of the CPU time dedicated to perform the Doppler broadening (blue), the sampling of the angle of the elastic scattered neutron (green), the transport of no-neutrons secondary particles (light blue) and the generation of the capture gamma rays (magenta) in simulations performed with 14.1 MeV neutrons in a sphere of 10 g/cm^3 and using G4NDL4.6.

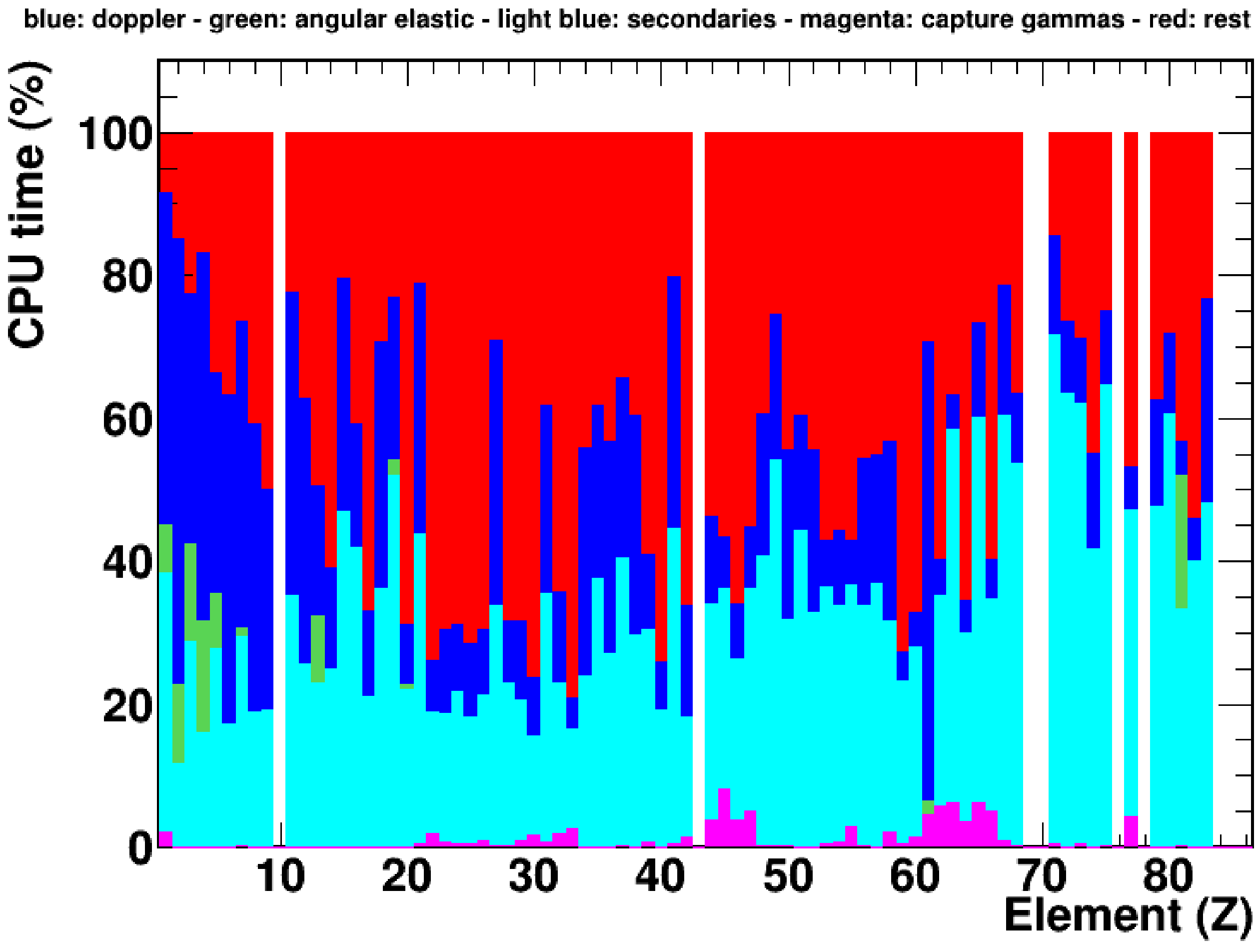
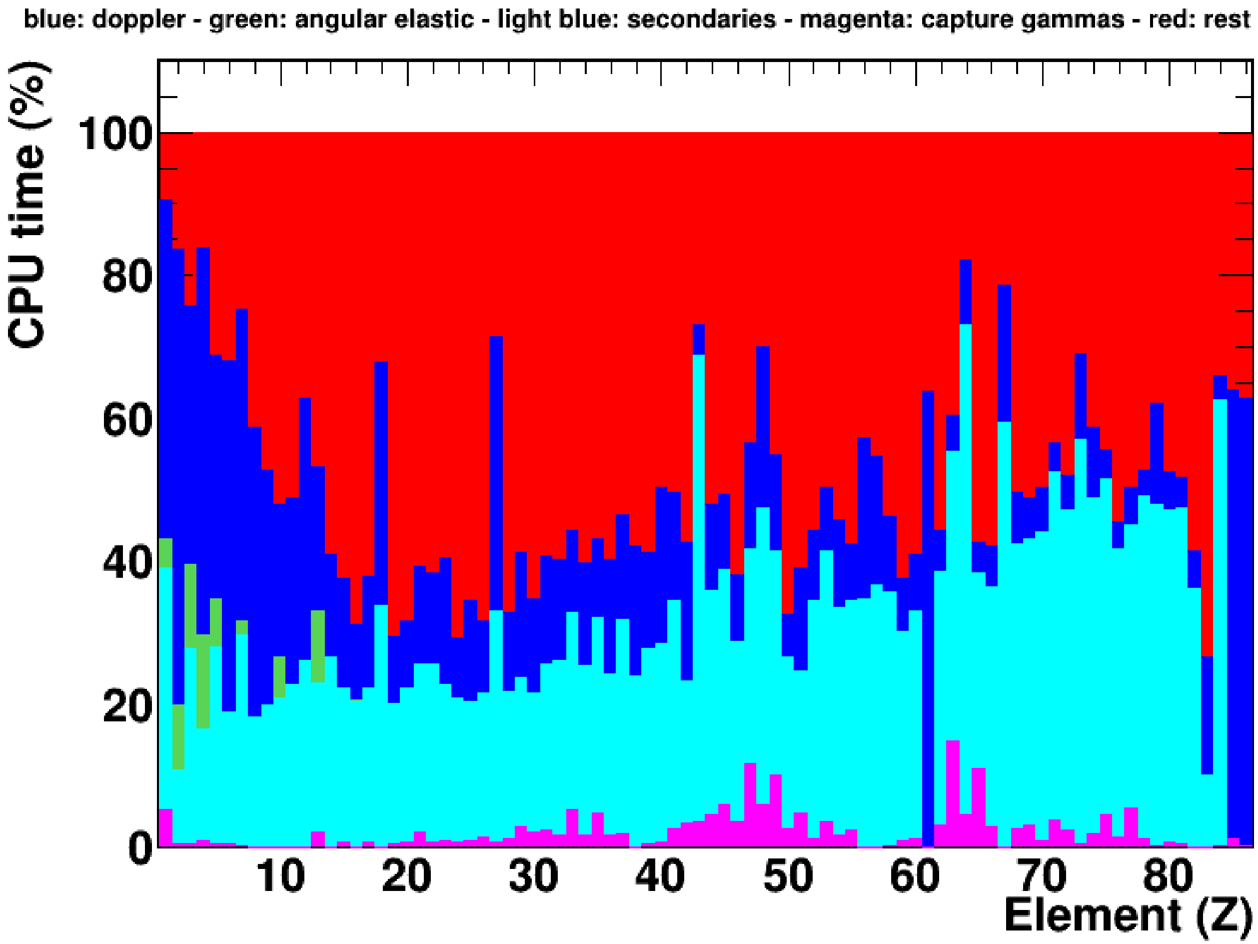


Figure 3a: estimated fraction of the CPU time dedicated to perform the Doppler broadening (blue), the sampling of the angle of the elastic scattered neutron (green), the transport of no-neutrons secondary particles (light blue) and the generation of the capture gamma rays (magenta) in simulations performed with 14.1 MeV neutrons in a sphere of 1 g/cm^3 and using G4NDL4.5.



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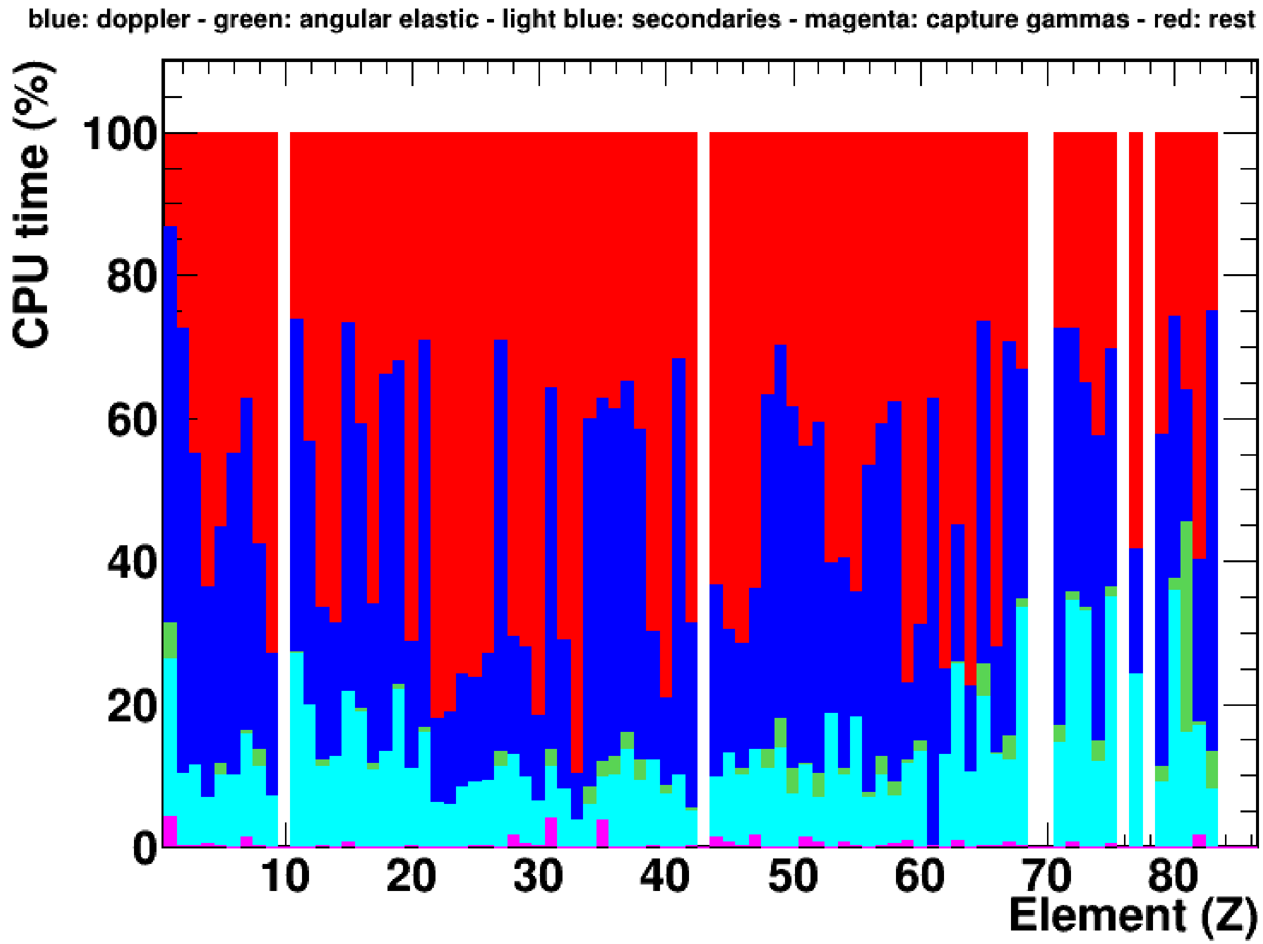
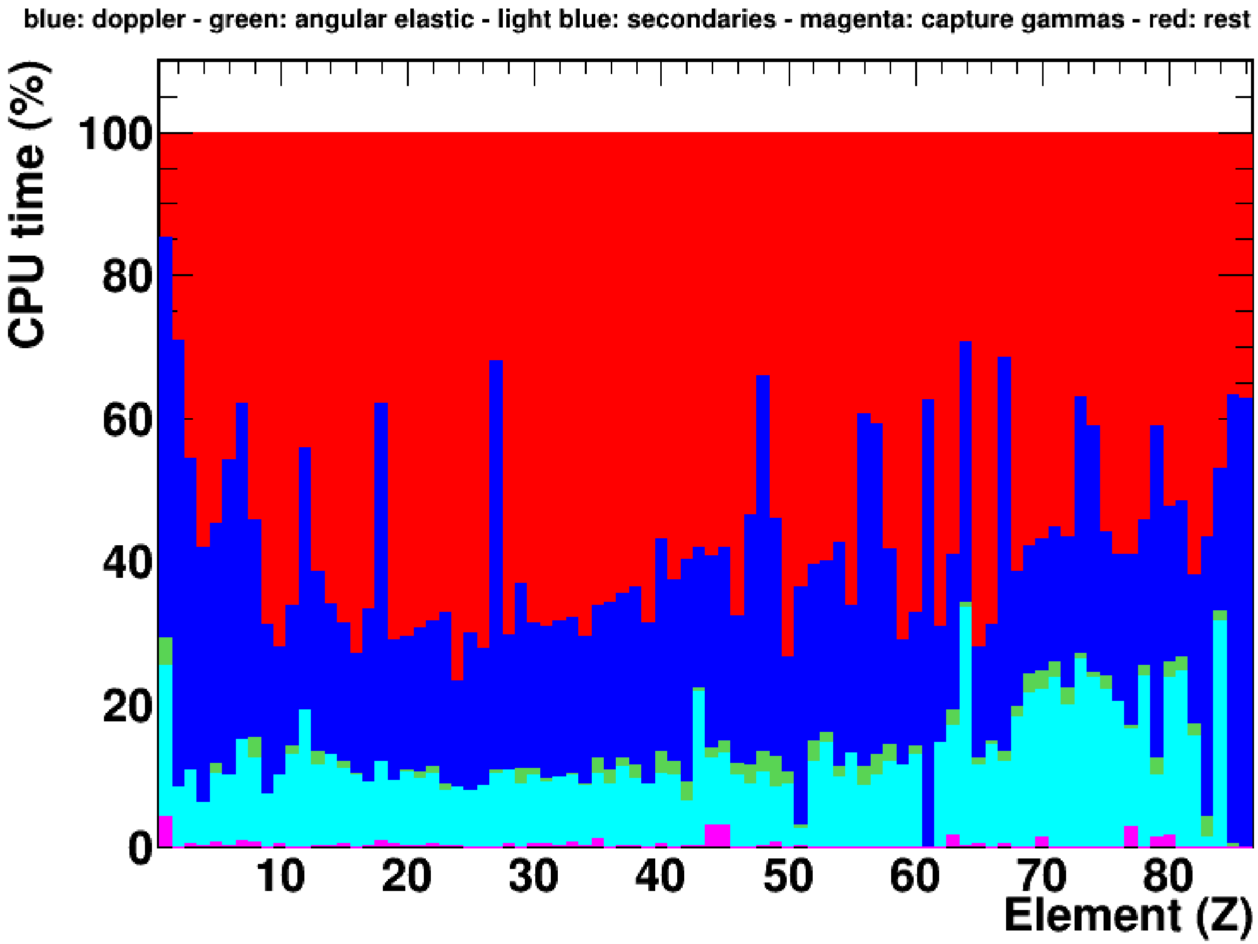


Figure 4a: estimated fraction of the CPU time dedicated to perform the Doppler broadening (blue), the sampling of the angle of the elastic scattered neutron (green), the transport of no-neutrons secondary particles (light blue) and the generation of the capture gamma rays (magenta) in simulations performed with 14.1 MeV neutrons in a sphere of 0.1 g/cm^3 and using G4NDL4.5.



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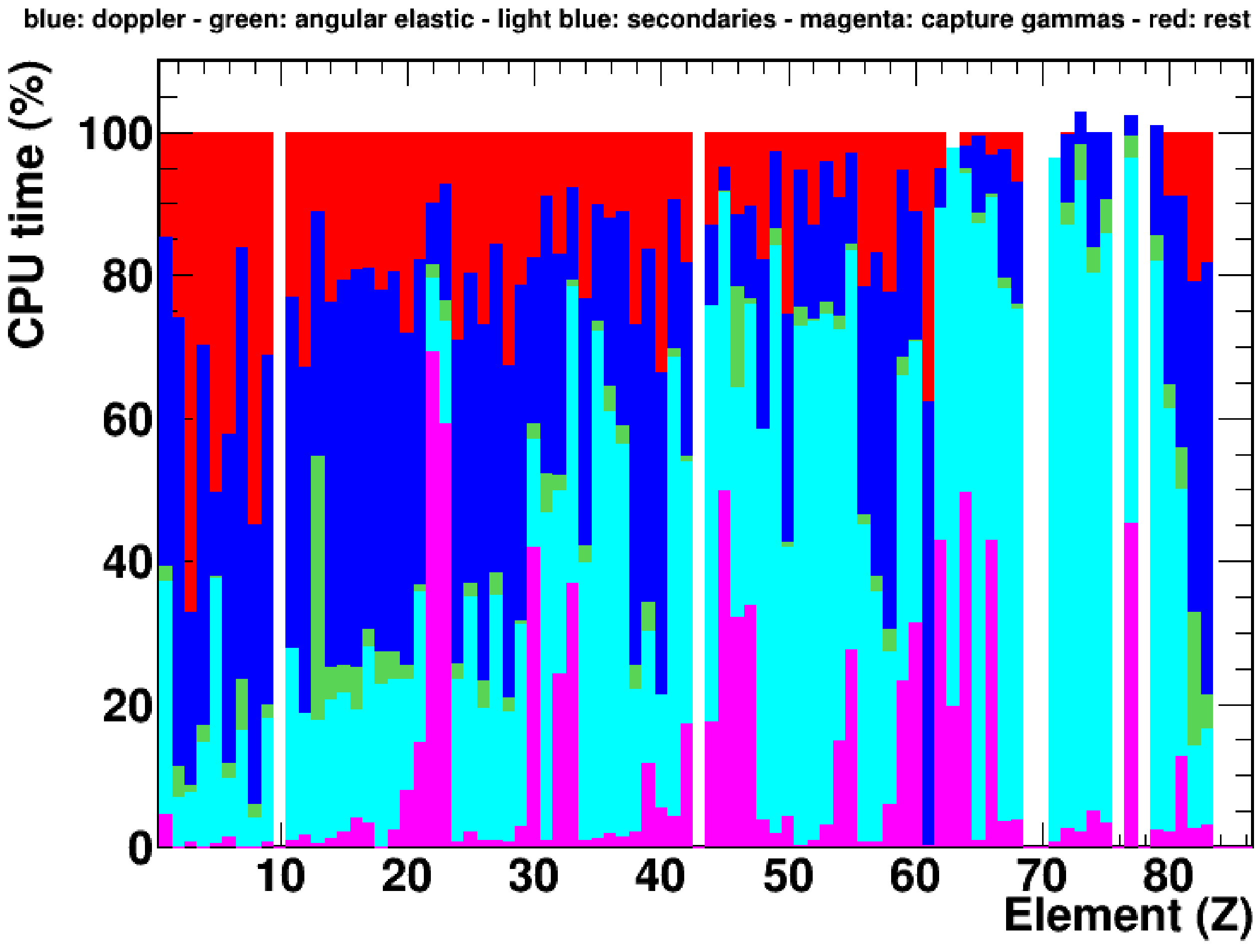


Figure 5a: estimated fraction of the CPU time dedicated to perform the Doppler broadening (blue), the sampling of the angle of the elastic scattered neutron (green), the transport of no-neutrons secondary particles (light blue) and the generation of the capture gamma rays (magenta) in simulations performed with 1 keV neutrons in a sphere of 10 g/cm^3 and using G4NDL4.5.

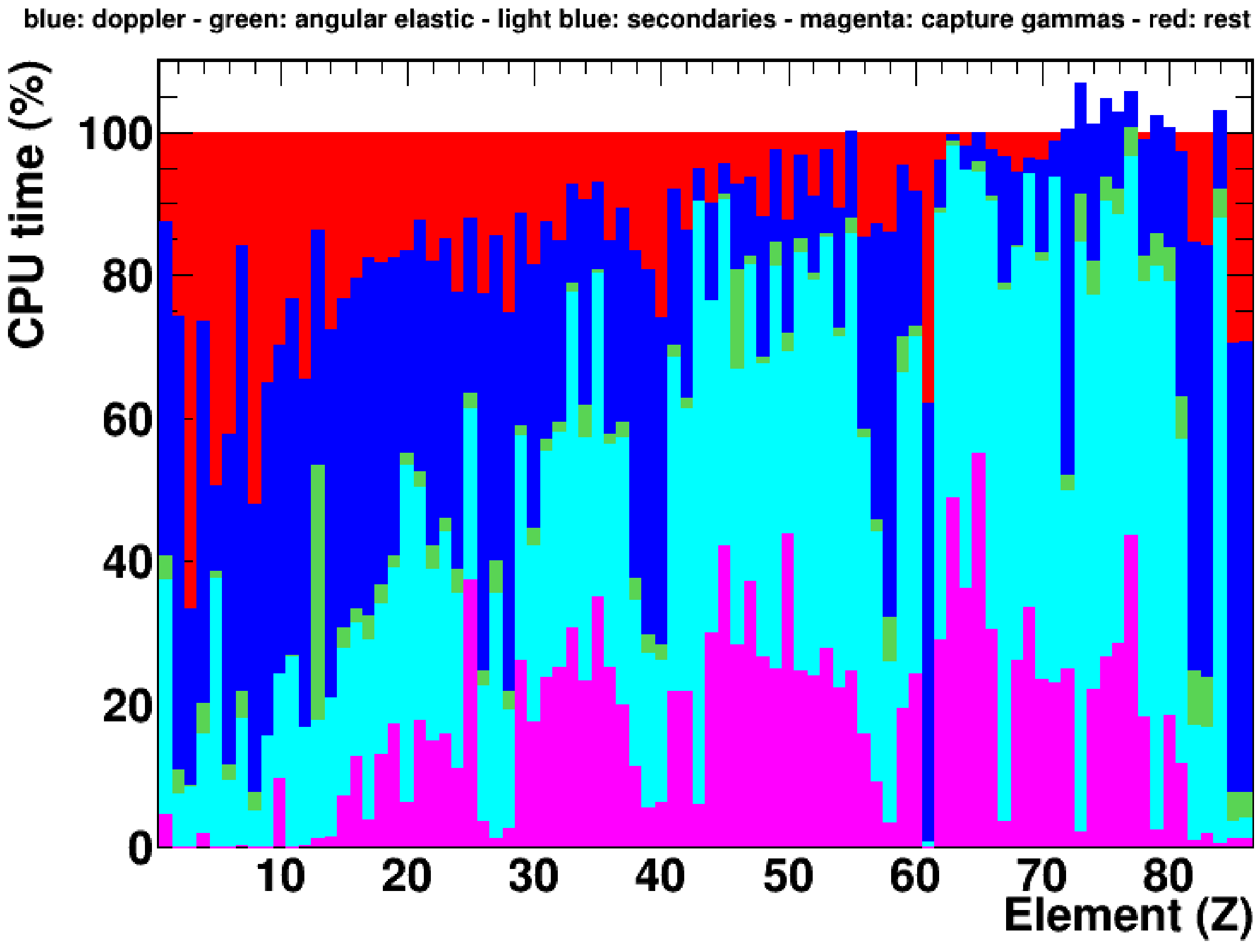


Figure 5b: estimated fraction of the CPU time dedicated to perform the Doppler broadening (blue), the sampling of the angle of the elastic scattered neutron (green), the transport of no-neutrons secondary particles (light blue) and the generation of the capture gamma rays (magenta) in simulations performed with 1 keV neutrons in a sphere of 10 g/cm^3 and using G4NDL4.6.

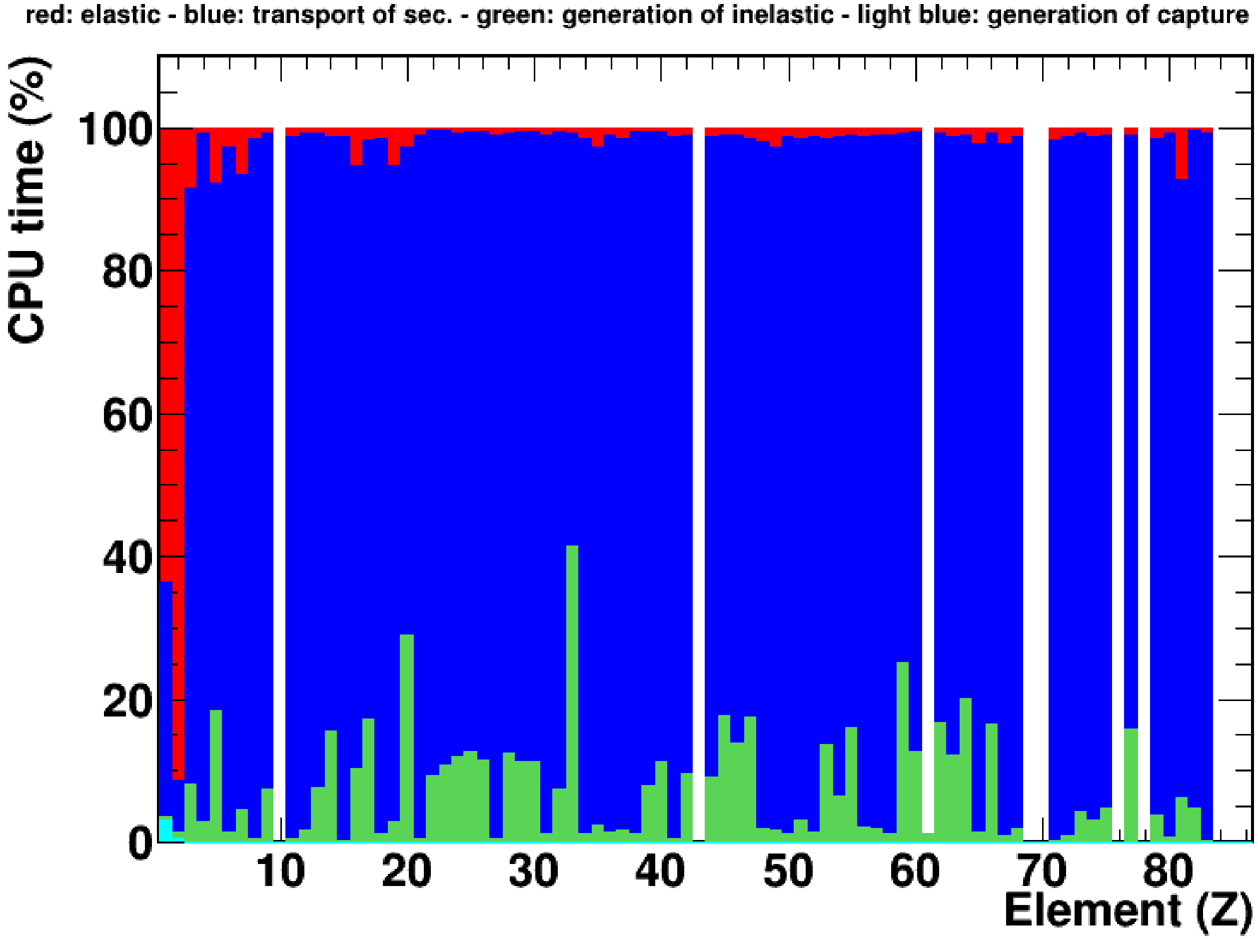
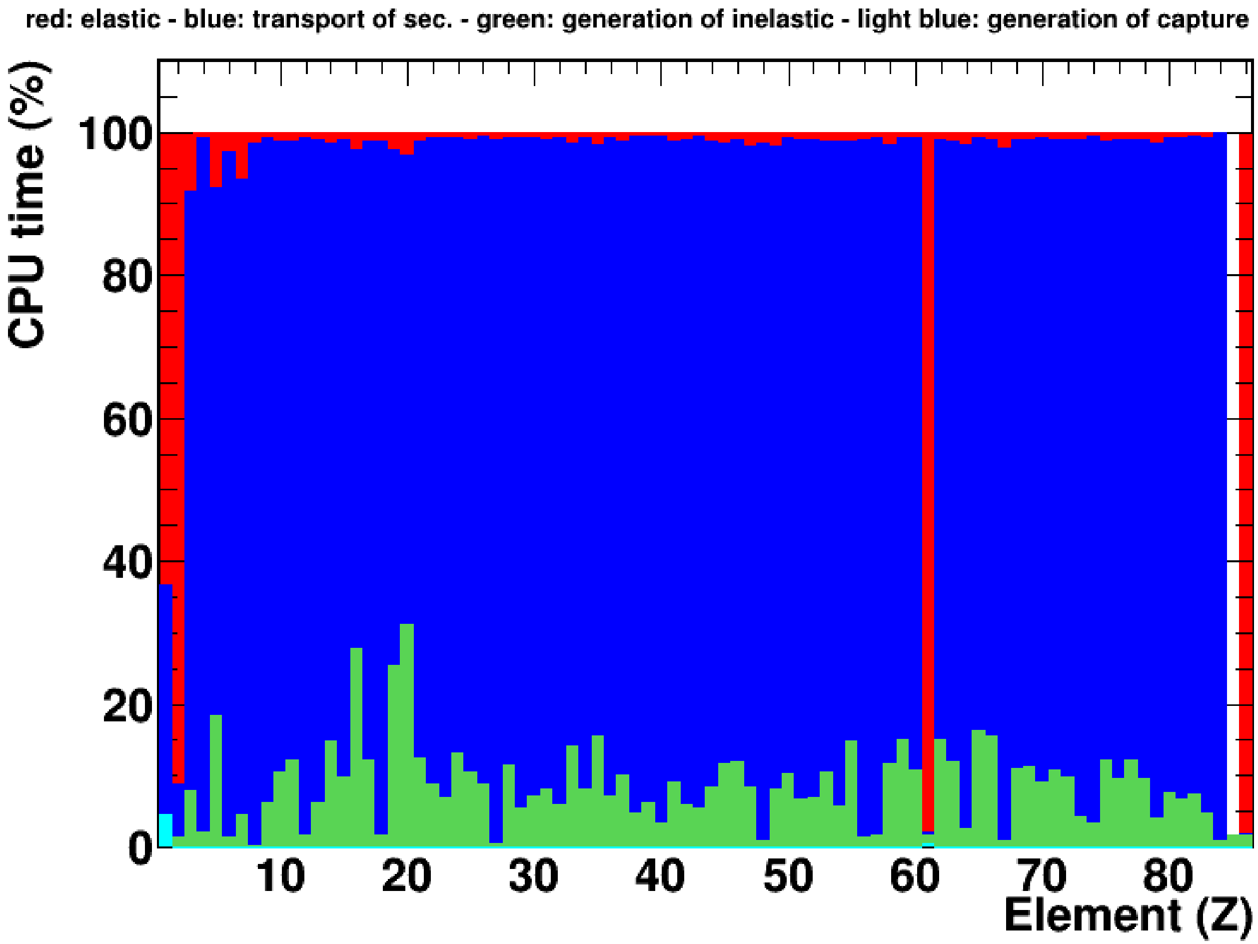


Figure 6a: estimated fraction of the CPU time dedicated to perform the elastic transport (red), the transport of secondary particles (blue), the generation of the first inelastic particles (green) and the generation of the capture secondaries (light blue) in simulations performed with 14.1 MeV neutrons in a sphere of 10 g/cm^3 and using G4NDL4.5.



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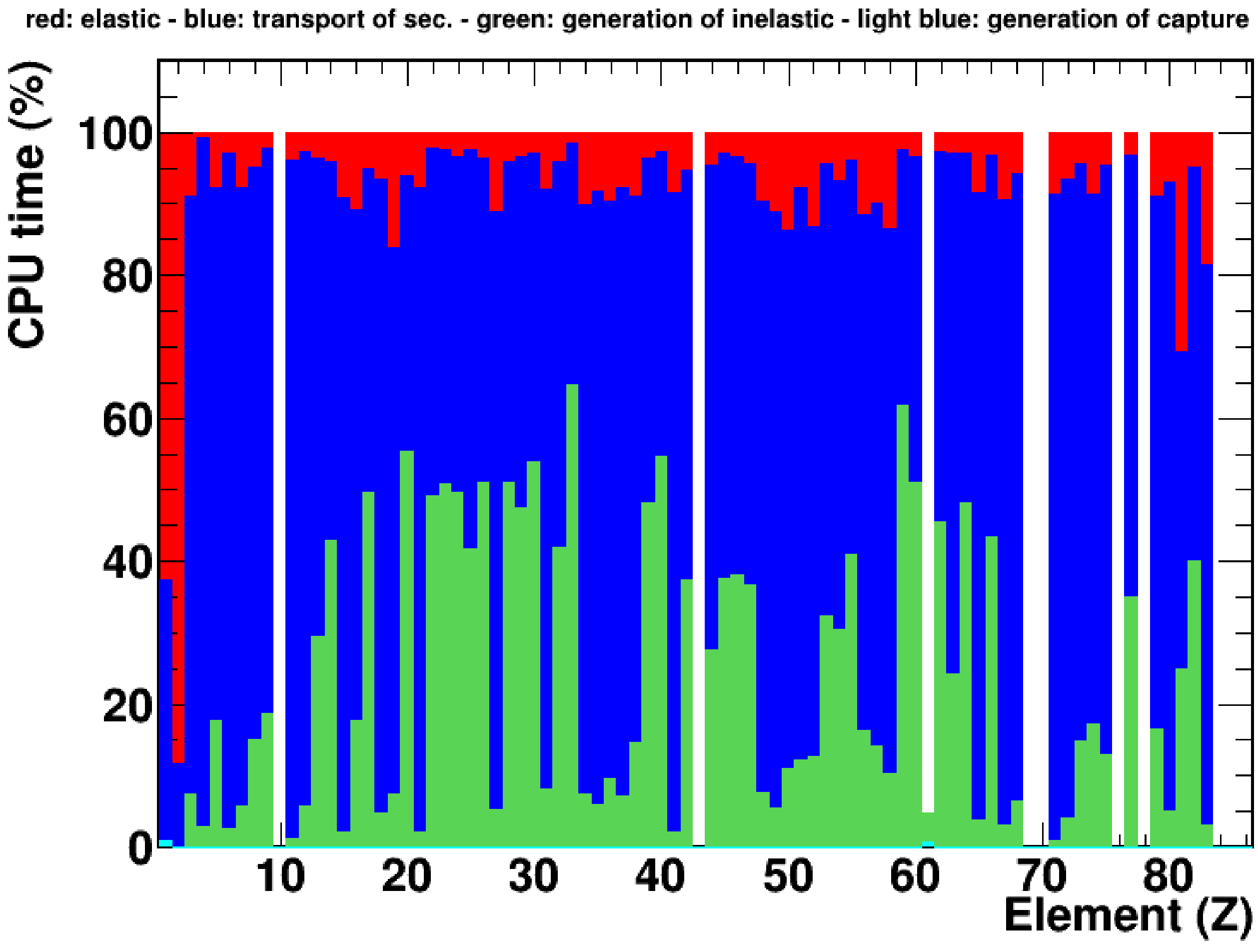

Figure 7a: estimated fraction of the CPU time dedicated to perform the elastic transport (red), the transport of secondary particles (blue), the generation of the first inelastic particles (green) and the generation of the capture secondaries (light blue) in simulations performed with 14.1 MeV neutrons in a sphere of 1 g/cm^3 and using G4NDL4.5.

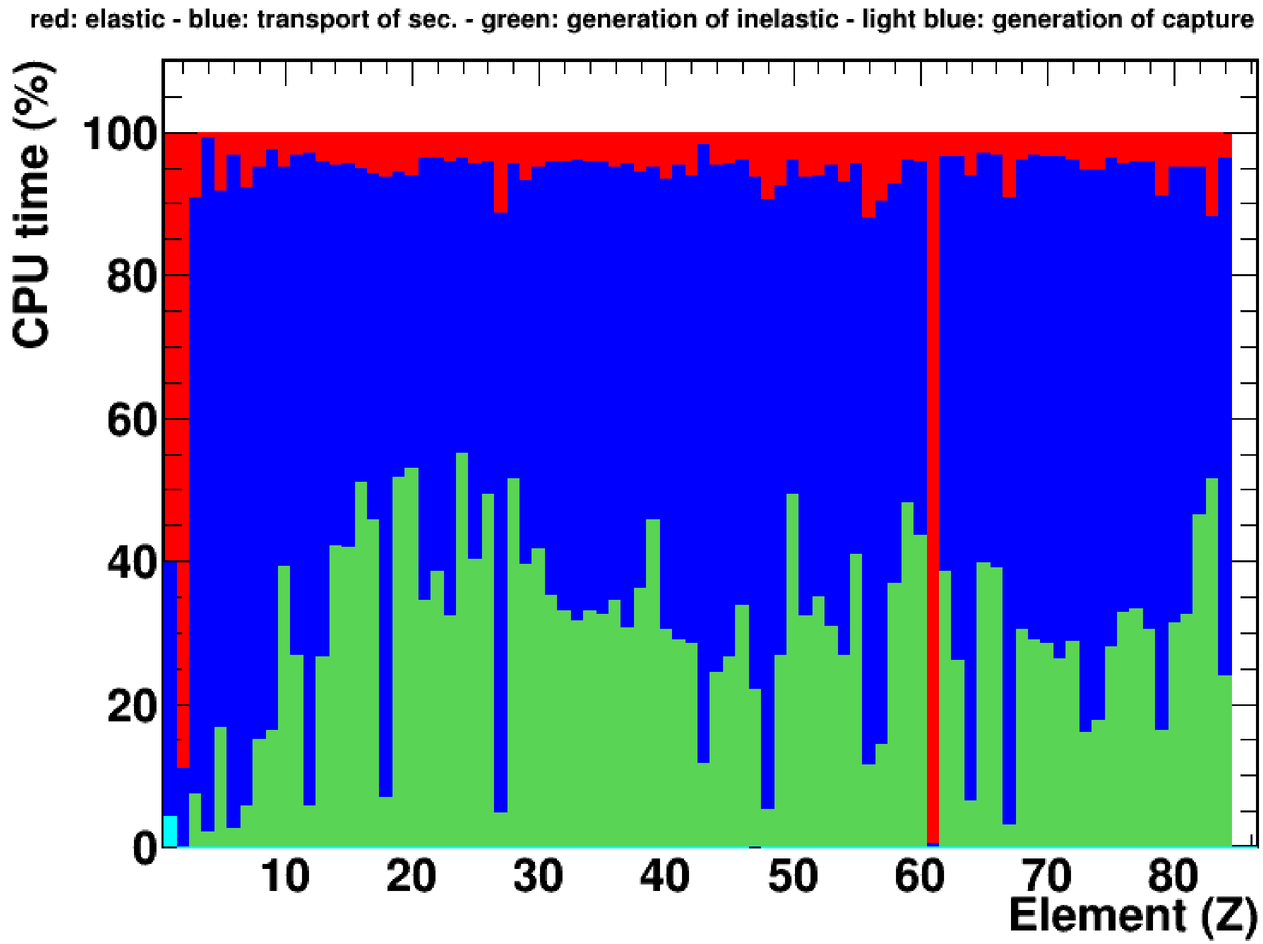

Figure 7b: estimated fraction of the CPU time dedicated to perform the elastic transport (red), the transport of secondary particles (blue), the generation of the first inelastic particles (green) and the generation of the capture secondaries (light blue) in simulations performed with 14.1 MeV neutrons in a sphere of 1 g/cm^3 and using G4NDL4.6.

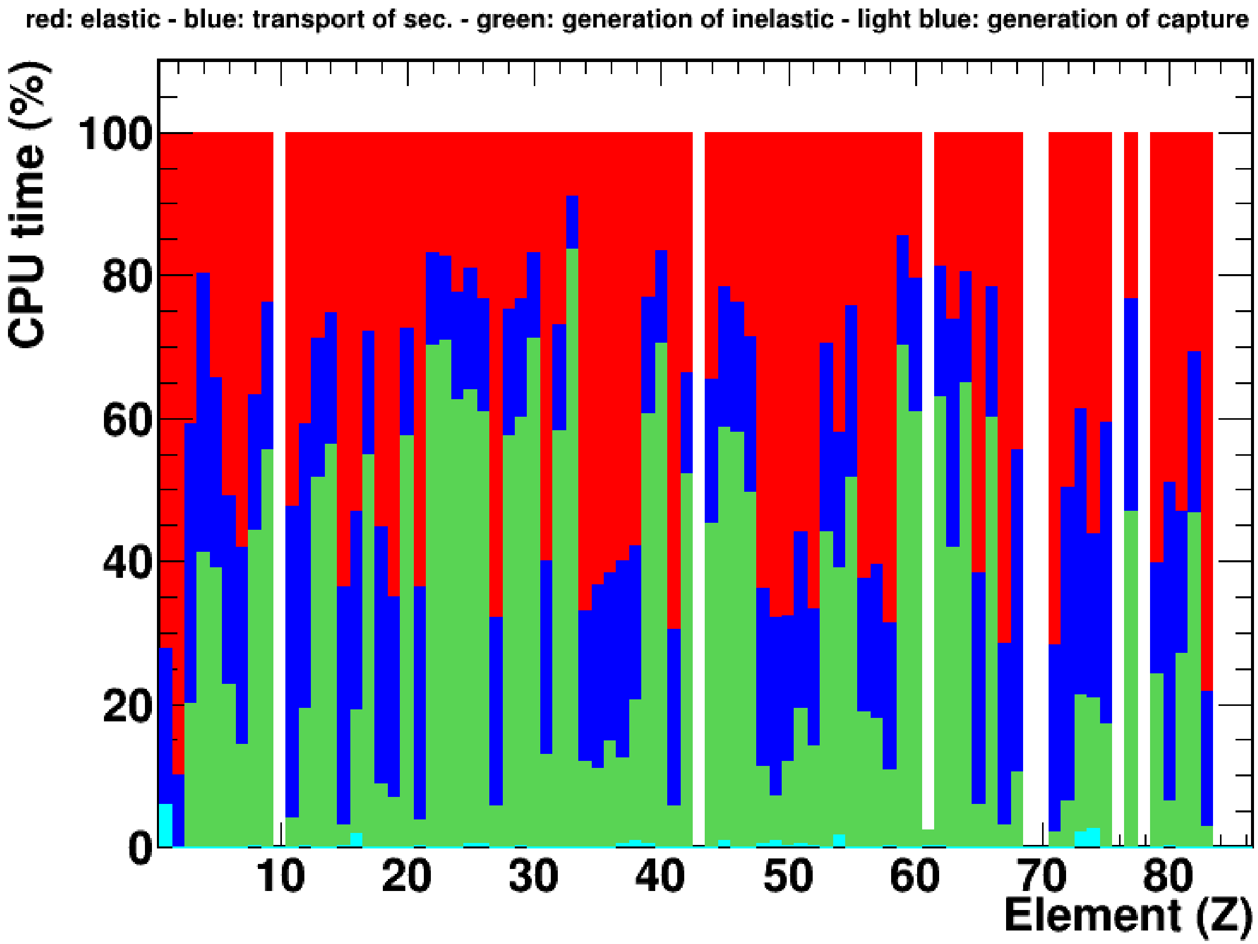

Figure 8a: estimated fraction of the CPU time dedicated to perform the elastic transport (red), the transport of secondary particles (blue), the generation of the first inelastic particles (green) and the generation of the capture secondaries (light blue) in simulations performed with 14.1 MeV neutrons in a sphere of 0.1 g/cm^3 and using G4NDL4.5.

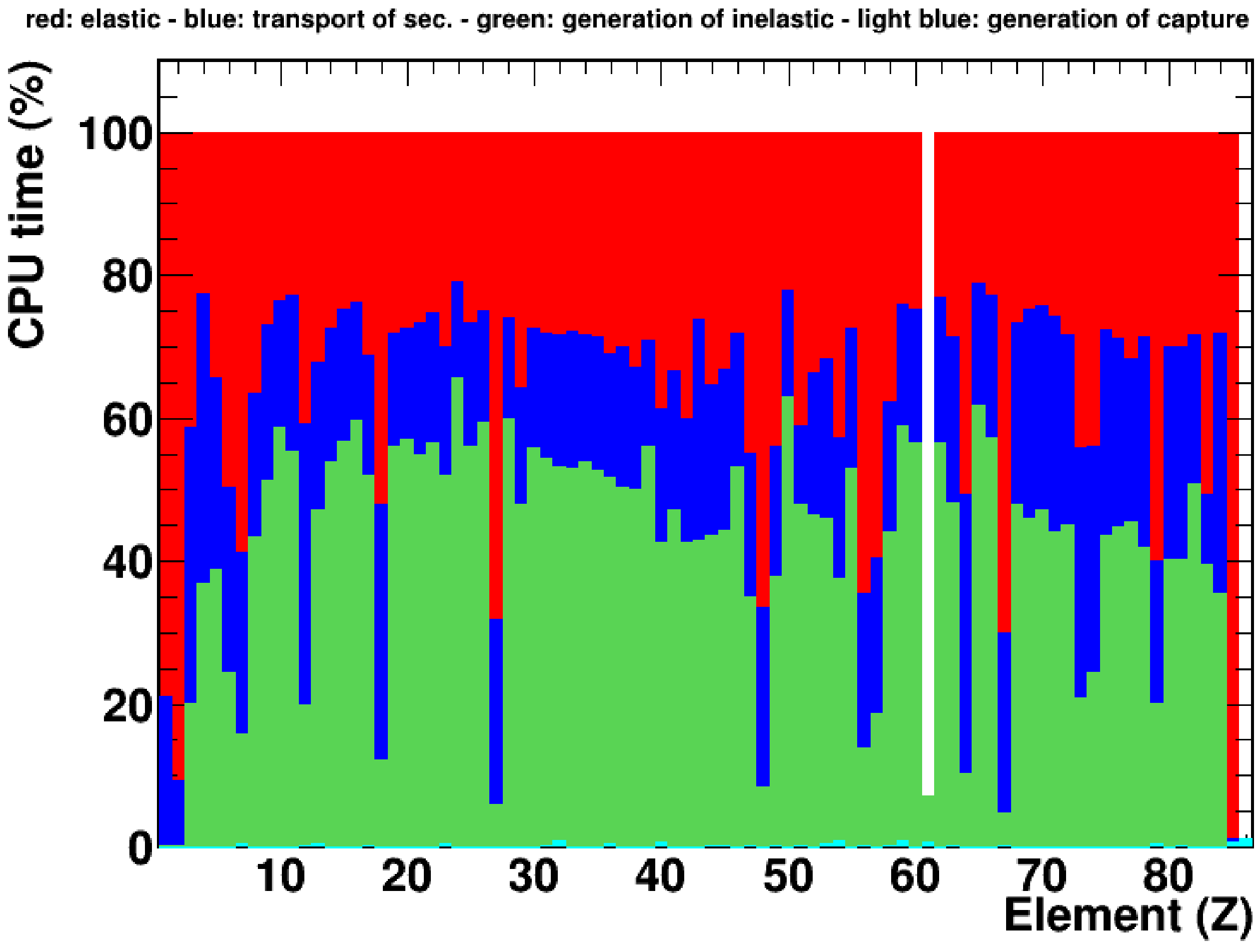

Figure 8b: estimated fraction of the CPU time dedicated to perform the elastic transport (red), the transport of secondary particles (blue), the generation of the first inelastic particles (green) and the generation of the capture secondaries (light blue) in simulations performed with 14.1 MeV neutrons in a sphere of 0.1 g/cm^3 and using G4NDL4.6.

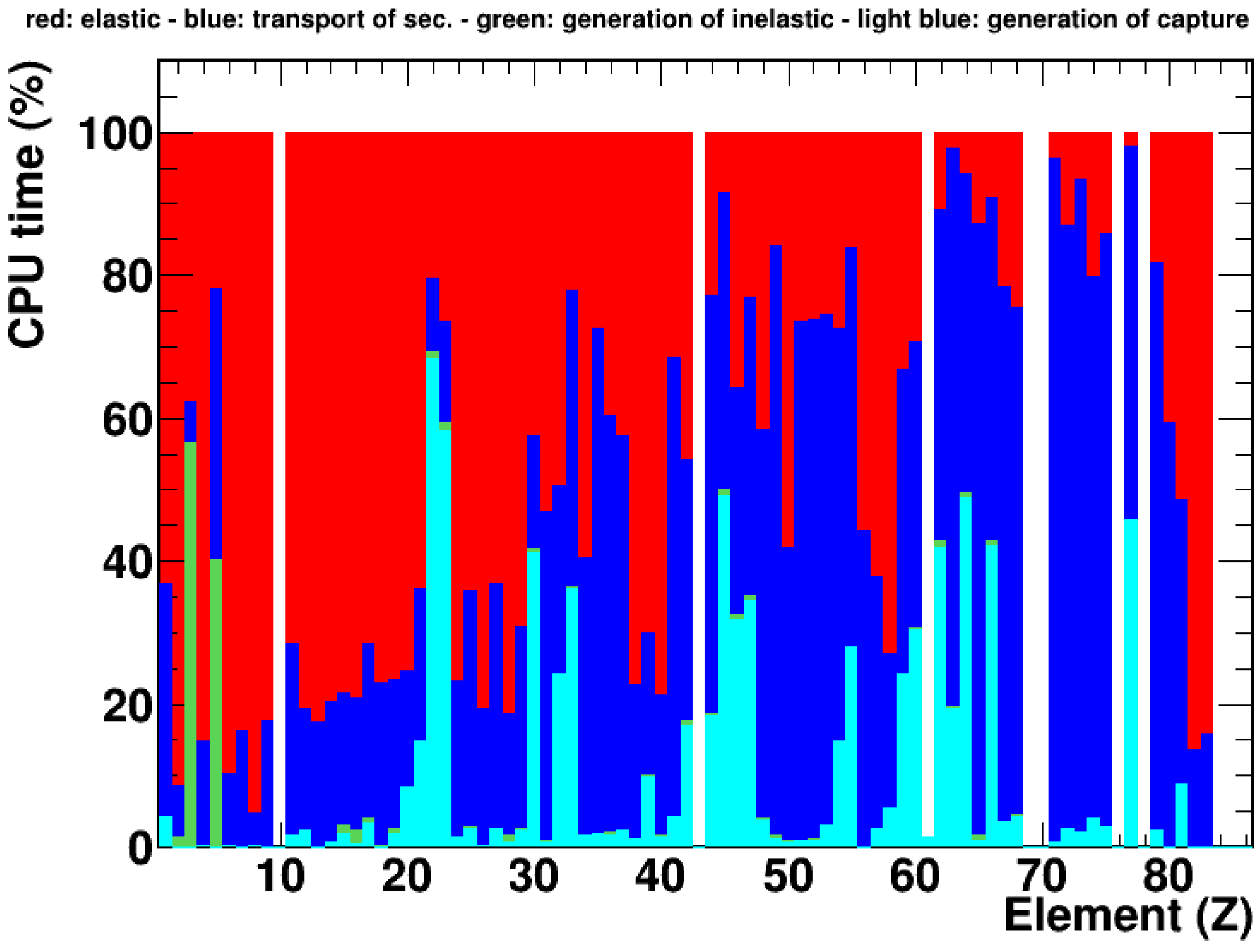

Figure 9a: estimated fraction of the CPU time dedicated to perform the elastic transport (red), the transport of secondary particles (blue), the generation of the first inelastic particles (green) and the generation of the capture secondaries (light blue) in simulations performed with 1 keV neutrons in a sphere of 10 g/cm^3 and using G4NDL4.5.

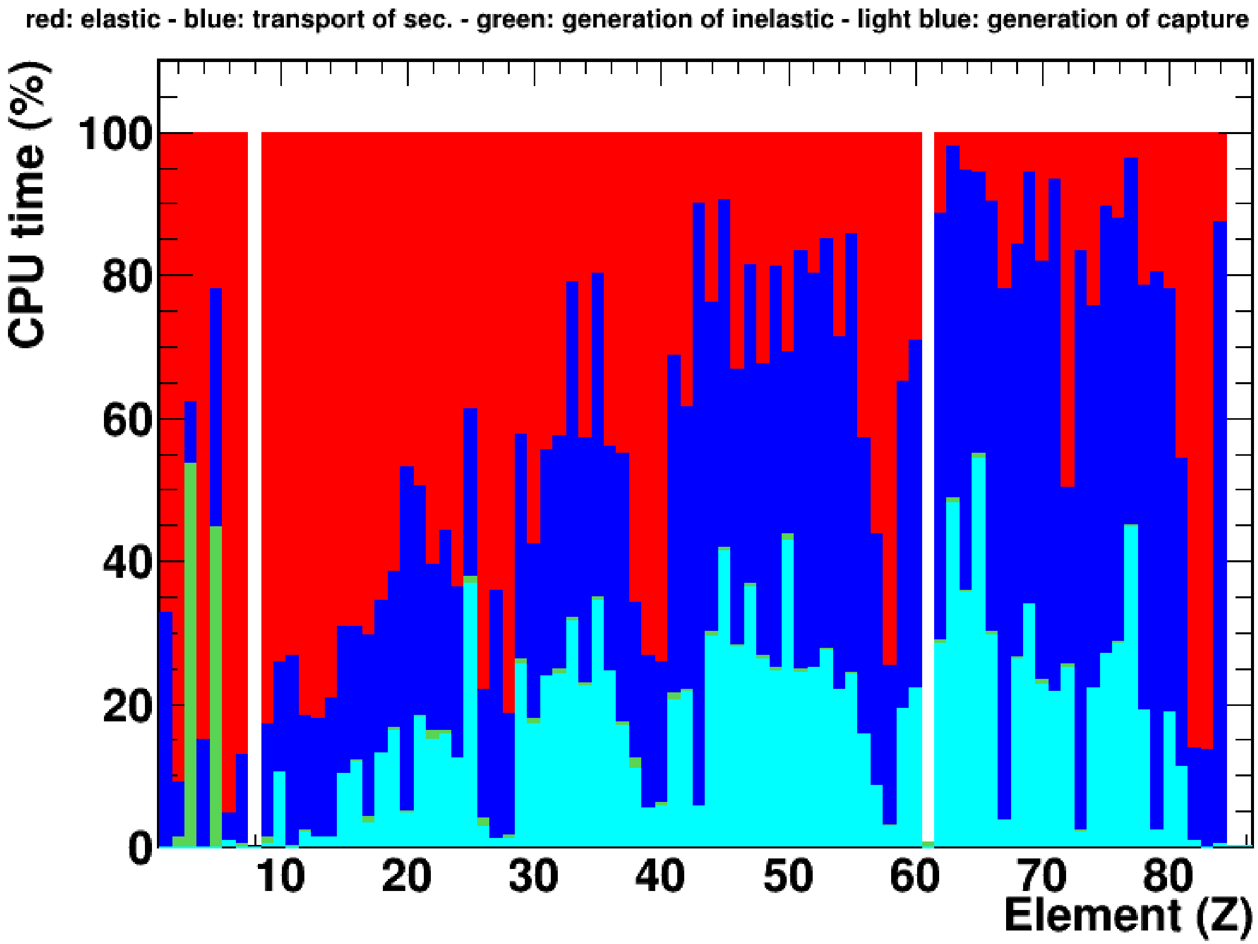

Figure 9b: estimated fraction of the CPU time dedicated to perform the elastic transport (red), the transport of secondary particles (blue), the generation of the first inelastic particles (green) and the generation of the capture secondaries (light blue) in simulations performed with 1 keV neutrons in a sphere of 10 g/cm^3 and using G4NDL4.6.

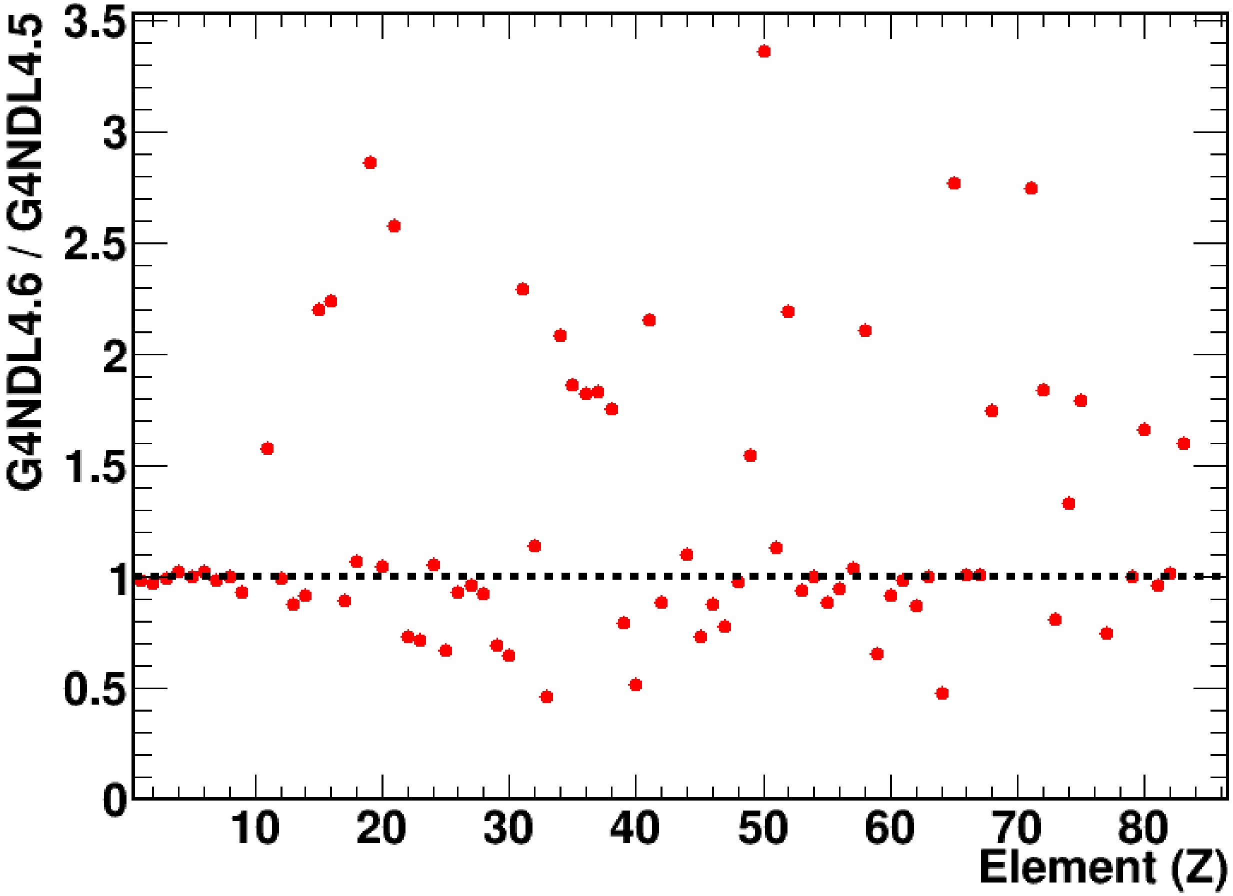

Figure 1b: ratio between CPU times when performing simulations using 14.1 MeV neutrons transported in a 1 g/cm^3 sphere made of different elements, using G4NDL4.6 and G4NDL4.5. R = 12.6%.

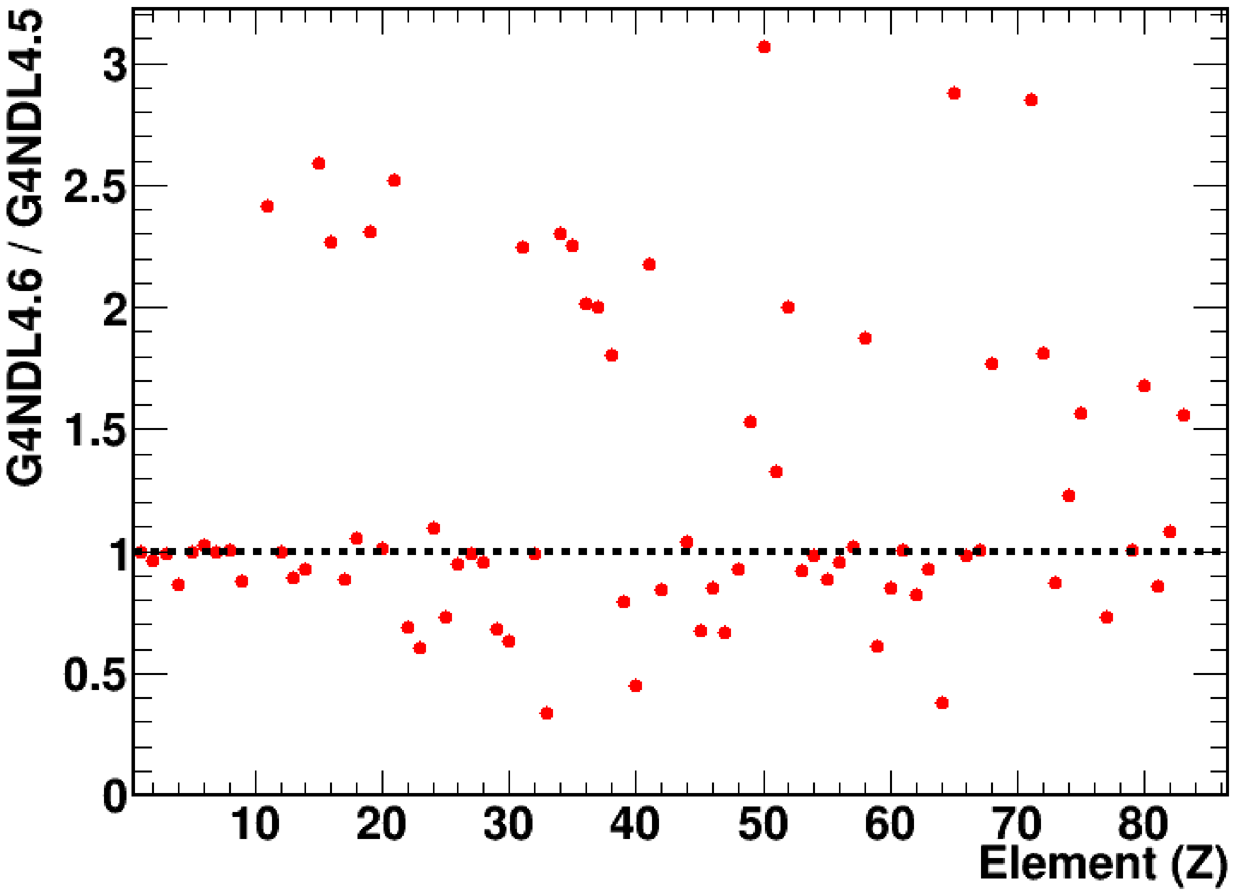

Figure 1c: ratio between CPU times when performing simulations using 14.1 MeV neutrons transported in a 0.1 g/cm^3 sphere made of different elements, using G4NDL4.6 and G4NDL4.5. R = 11.0%.

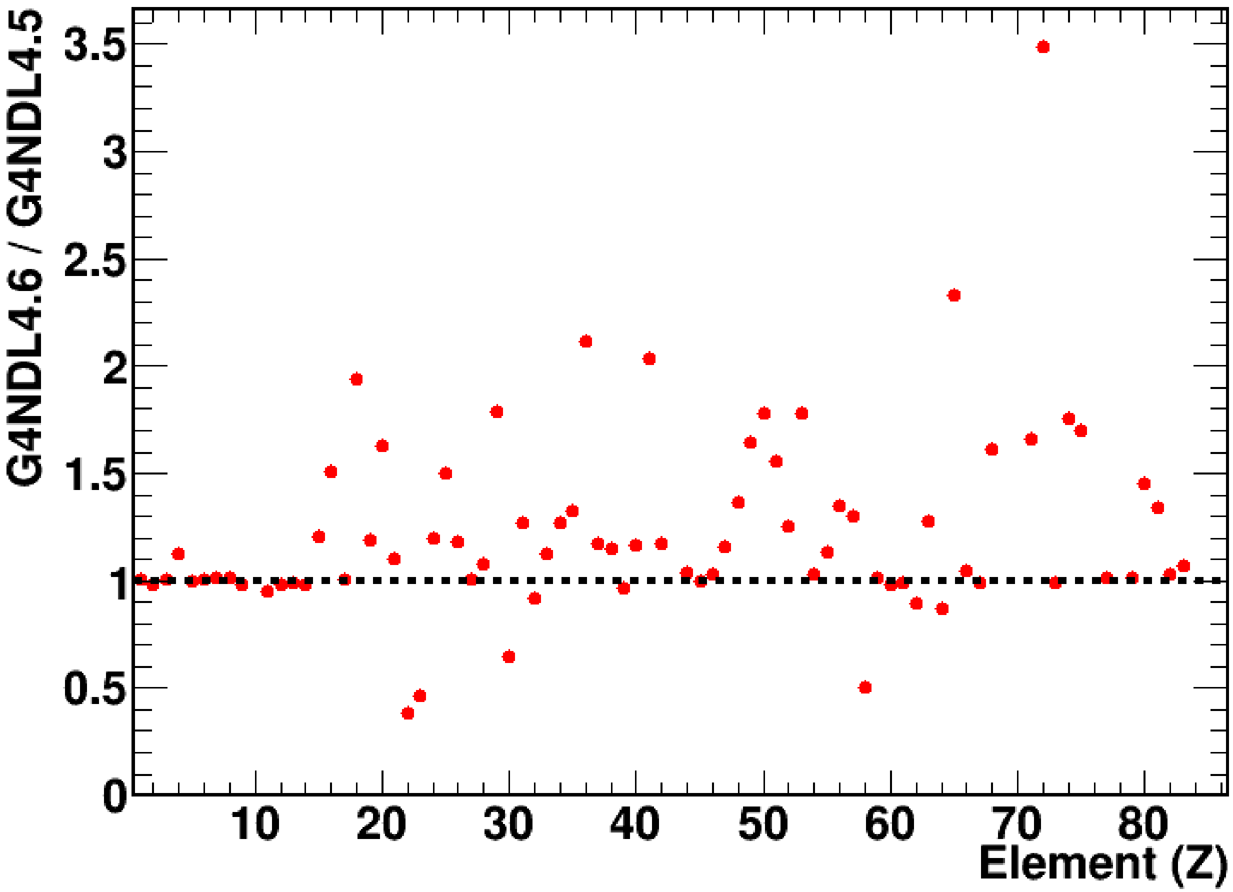

Figure 1d: ratio between CPU times when performing simulations using 1 keV neutrons transported in a 10 g/cm^3 sphere made of different elements, using G4NDL4.6 and G4NDL4.5. R = 15.2%.