Recent developments and prospects of ParticleHP

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Recent developments of ParticleHP

- New neutron library G4NDL4.6 : validation and CPU implications.

  More info in the had-meeting presentation (Feb. 2020) → here

- New UI commands to replace environmental variables.

  More info in the had-meeting presentation (Jun. 2020) → here

- SaG4n (G4 tool developed to calculate neutron production due to (α,xn) reactions).

  More info in the had-meeting presentation (Apr. 2020) → here

New neutron library G4NDL4.6

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 …
- OECD-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

New neutron library G4NDL4.6

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.

Main changes:

ENDF/B → JEFF

Isotopes with Z>92 now available

The main advantage of G4NDL4.6 over G4NDL4.5 is that 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

New neutron library G4NDL4.6

CPU performance: 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.

The results of the study were presented in the G4 Hadronic meeting February 2020 → link

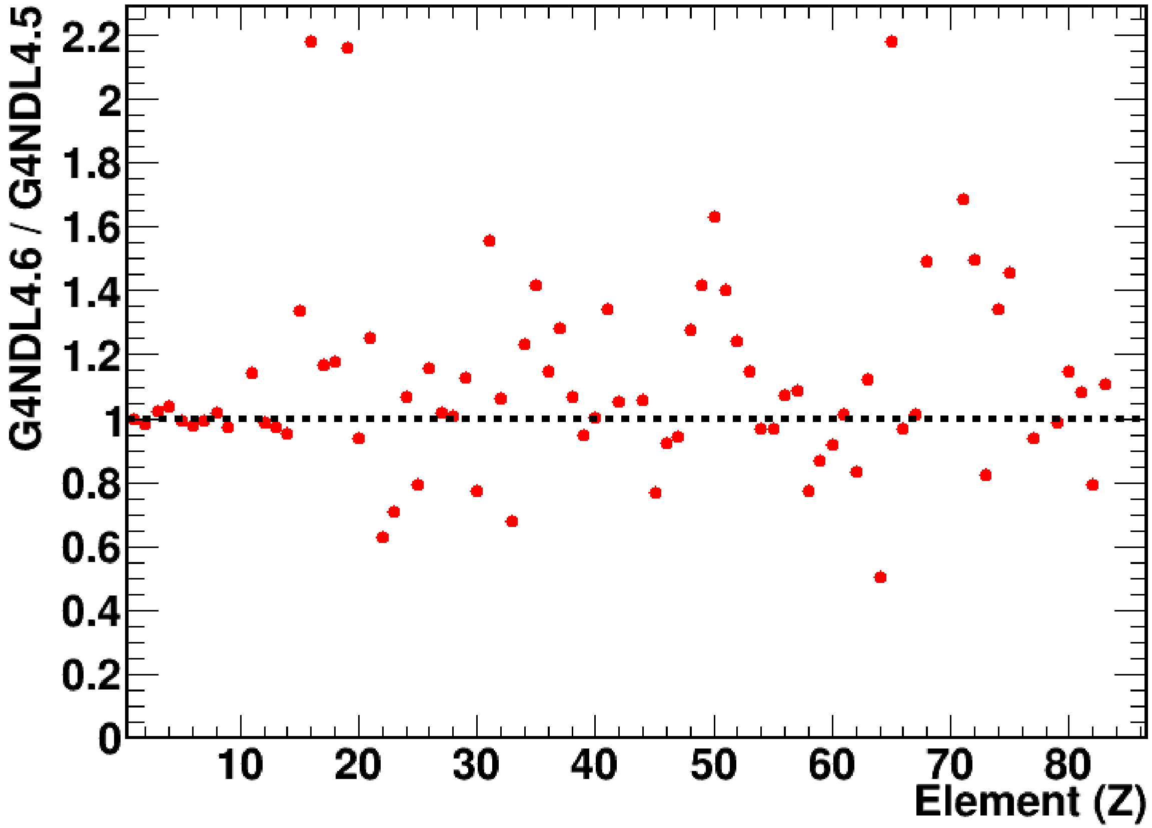
Conclusions of the study:

1- CPU time difference depends on the simulation: not always G4NDL4.6 (JEFF-3.3) is slower than G4NDL4.5 (ENDF/B-VII.1). However, in the tested cases, there were more simulations where G4NDL4.6 was slower than G4NDL4.5 → G4NDL4.6 is *usually* slower 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.

New neutron library G4NDL4.6



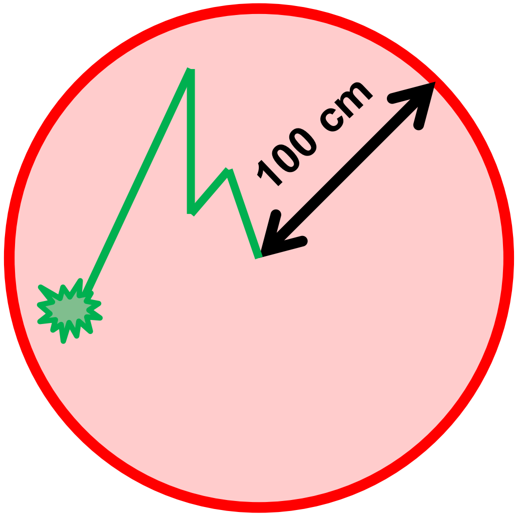


Figure 1a: ratio between CPU times when performing simulations using 14.1 MeV neutrons transported in a 10 g/cm^3 sphere made of different elements, using G4NDL4.6 and G4NDL4.5. R = 7.3%.

New neutron library G4NDL4.6

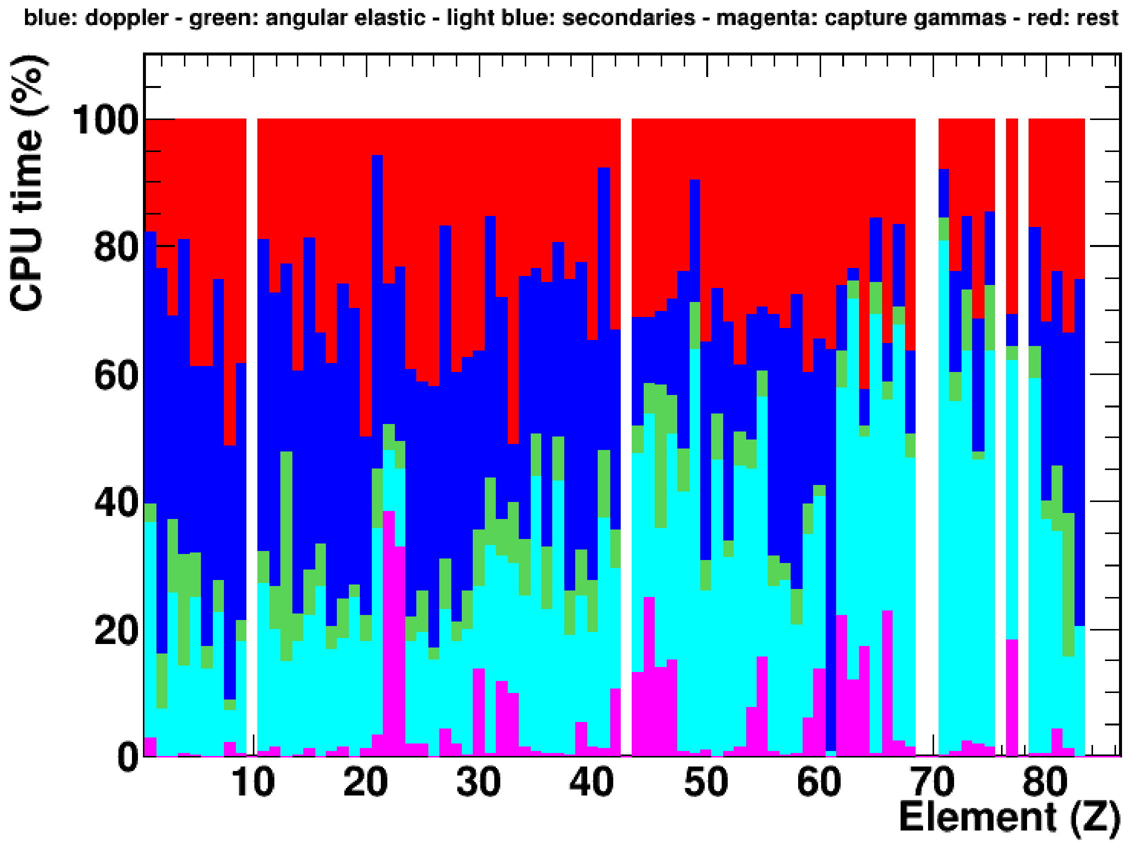


Figure 2a: estimated fraction of the CPU time dedicated to perform the Doppler broadening (blue), the sampling of the angle of the elastic scattered neutron (green), the transport of no-neutrons secondary particles (light blue) and the generation of the capture gamma rays (magenta) in simulations performed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

New UI commands to replace environmental variables

There are several options in ParticleHP which are controlled via environmental variables:

G4NEUTRONHP_USE_ONLY_PHOTONEVAPORATION
G4NEUTRONHP_NEGLECT_DOPPLER
G4PHP_NEGLECT_DOPPLER
G4NEUTRONHP_SKIP_MISSING_ISOTOPES
G4NEUTRONHP_PRODUCE_FISSION_FRAGMENTS
G4PHP_USE_NRESP71_MODEL
G4PHP_DO_NOT_ADJUST_FINAL_STATE
G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE
G4NEUTRON_HP_USE_WENDT_FISSION_MODEL

New UI commands to replace environmental variables

Alternatively, the options can be controlled via UI commands:

/process/had/particle_hp/use_photo_evaporation
/process/had/particle_hp/skip_missing_isotopes
/process/had/particle_hp/neglect_Doppler_broadening
/process/had/particle_hp/do_not_adjust_final_state
/process/had/particle_hp/produce_fission_fragment
/process/had/particle_hp/use_NRESP71_model
/process/had/particle_hp/verbose
/process/had/particle_hp/use_Wendt_fission_model

(Work done by A. Ribon)
This will be the situation for Geant4.10.7, but if the env. variables are used then you get a warning that it is deprecated → **environmental variables will be removed for G4.11**

There is also another env. variable: PHP_AS_HP, which is used at build-time of Geant4. It still works but it is depreacted and will be removed in G4.11 → now there is a new CMake building option: GEANT4_BUILD_PHP_AS_HP which is OFF by default (work done by Ben Morgan).

Env. Variables related to data libraries → a common solution for all, not only ParticleHP, will be implemented in a future, for G4.11 (Ben Morgan).

SaG4n: Simulation of (α,xn) reactions with Geant4

We have been investigating the performance of Geant4 in the simulation of **neutrons generated by α-decay**, via (α,xn) reactions.

Motivation:

- Low background experiments. (e.g. dark matter detection).
- Nuclear technology.
- …

We have published a paper → E. Mendoza et al., *Neutron production induced by α-decay with Geant4*, NIMA 960, 163659 (2020)

Other codes:

NeuCBOT	*S. Westerdale et al., NIMA 875, 57 (2017)*
NEDIS	*G. N. Vlaskin et al., Atomic Energy 117, 357 (2015)*
SOURCES	*W. Wilson et al., Progress in Nuclear Energy 51, 608 (2009)*
USD	*D.M. Mei, NIMA 606, 651 (2009)*

SaG4n: Simulation of (α,xn) reactions with Geant4

We have created a Geant4 application → **SaG4n**, which is a tool to to calculate neutron production due to (α,n) reactions in different materials. This tool is available at:

http://win.ciemat.es/SaG4n/

It **works with an input**, i.e. once compiled, SaG4n takes from an input file written by the user all the information necessary to define the geometry of the problem, the source, parameters of the physics, the type of output, etc...

It needs an **α–incident data library** to work: there are four available for download in the same web as the source code.

There you will find:

- The source code
- Data libraries (x4), needed to run Geant4, with XS and FS data from ENDF-6 format data libraries.
- The manual

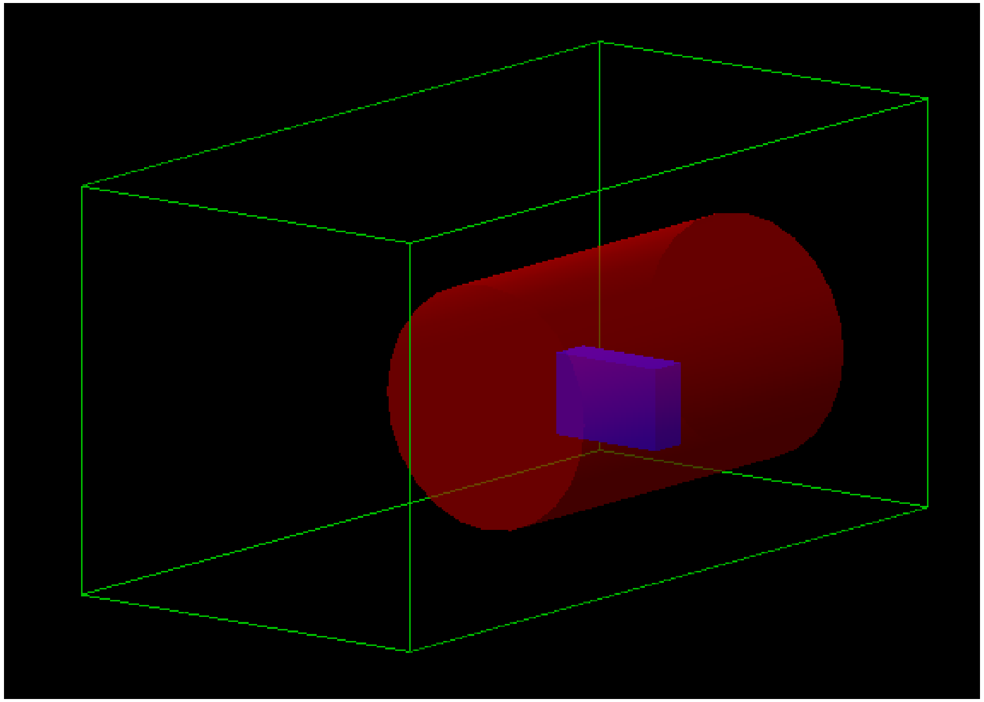
SaG4n: Simulation of (α,xn) reactions with Geant4

Input:

```
# VOLUMES:
VOLUME 12 Box01    7 2 0 - 10 10 20 0 0 0
VOLUME 14 Cylinder01    8 3 12 -  3 10 1 -1 -3
VOLUME 25 Box02    9 2 14 - 3 2 1 0.5 -0.5 0.5
```

```
MATERIAL 9 H2O 1.00 2
1 2
8 1
ENDMATERIAL
```

```
SOURCE 0 27
1.00 3
Chain_Th232  0 30.00
Chain_U235    0 50.00
Chain_U238    0 20.00
ENDSOURCE
```



Future developments

1- Implement an option to force ParticleHP to respect event-by-event conservations (energy-momentum, baryonic number, etc.) → to be done

2- Extend ParticleHP model to higher energies → in progress

3- Introduction of NuDEX, to generate EM de-excitation cascades. NuDEX is a code written in C++ which generates EM de-excitation cascades by creating full level schemes + BR of a large variety of nuclei. Similar to PhotonEvaporation but with more detail → in progress (almost done).

4- Create a tool to automatically change charged particle cross-sections adding user experimental data → to be done (P. Arce)

More info concerning these developments can be found → here