Neutron Interactions

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1. Introduction:

Geant4 is a toolkit for the simulation of the passage of energetic particles through matter. Its areas of application include production by numerous HEP experiments. Nuclear & Accelerator physics, as well as studies in space and medical science.
Also in the past, validation for many application areas has been made. This work undertakes a new validation of neutron interactions in gases relevant for gaseous detectors. Various improvements to Geant4 code are being introduced quasi continuously by people working in this field. Contrary to the theoretically predictable electromagnetic interaction of particles like γ, $e^{\pm}$, etc., the interaction of neutrons with matter, i.e. the atomic nuclei, relies rather on measurements up to about 10 MeV neutron kinetic energy. This is also the range of interest in LHC detectors. Geant4 created its own library of cross sections for neutrons, derived from evaluations current in the late 1990s, with some updates undertaken also during the last ~5 years. One aim is to find the origin of neutron cross sections used in Geant4 (for elements where this information is not directly available), and identify ones for which the use of newer evaluations will be necessary.
In this work, we make a comparison between cross sections from the neutron libraries and those used by Geant4, aiming to improve the performance of Geant4 and its reliability too. We validate the Geant4 Cross Sections for key chamber gases against benchmark data from several Neutron Libraries, including recent and also older evaluations. For this we used JANIS 3.0 (Java-based Nuclear Information Software) including all libraries which had data available for each element.
The simulation of the interaction of a low energy neutron field (below 10-20 MeV) with matter is still not so easy, or, to put it differently, it cannot be as precise as one would wish to have. This is shown by the fact that several neutron data libraries have been created being continuously updated/improved, while they are used by Monte Carlo codes like the Geant4 and others.
The inaccuracy of the neutron propagation in and interaction with matter has to do with the fact that not all neutron cross sections with the various stable isotopes are precisely known. These nuclear reactions include for example a plethora of final nuclear levels, which participate in the neutron nucleus interaction mode, and they are often not known at all. In addition, in nuclear physics one cannot predict completely, or, at least not satisfactorily, the neutron cross sections with all elements and their isotopes based on first principles. For comparison, this is actually the case with the electromagnetic interactions of photons and electrons/positrons with the constituent atoms of matter, whose quantized states are actually well known experimentally, and, most of them can be predicted quite reliably. After all, QED, the theory that describes this kind of interactions is the most precise theory available so far. Therefore, even now one measures at CERN the neutron cross sections with various elements in the nTOF experiment.
Furthermore, at a more fundamental level, the nuclear potential itself of the various nuclei is not precisely known, and it cannot be compared with the one single law of the nuclear Coulomb potential, which describes the involved atomic states. Thus, it is this at the origin of the not well known interaction of neutrons with matter (i.e., its constituent nuclei) and therefore one depends actually on the measurements.

All this, is also the reason why one encounters so diverse discrepancies between the various input data used in related hadronic Monte Carlo simulation of low energy neutrons as it happens with the Geant4 code. To converge all these occasionally divergent neutron cross sections to a final set of values/curves, it is a necessary, though also not an easy task.

In fact, Geant4 code is already widely used to reproduce or predict the interaction of all kind of energetic particles with matter, and this in particular in HEP experiments, where it was also born in 1994. Thus, in HEP experiments a variety of particles appear, like photons, electron/positrons, pions (π^+, π^-, π^0), Kaons (K^+, K^-, K^0) etc., which do interact with the surrounding detector material. Some of the reaction products do not actually interact with the detector material like the neutrinos and other as yet unidentified exotica like dark matter particle candidates, e.g., the expected Weakly Interacting Massive Particles (WIMPs) with a rest mass of ~1GeV/c^2 to eventually several TeV/c^2. Nevertheless, about their production in HEP reactions it can be concluded indirectly measuring all other particles in the primary reaction including their decay products. In such situations only the performance of a complete Monte Carlo simulation of the whole chain of reactions can help to conclude about the appearance of such quasi invisible (i.e., very feebly interacting) particles.

Of the interacting particles, the photons and the electrons/positrons obey the electromagnetic interactions, which Geant4 code follows with high precision from very high to very low energies down to the keV range. The reason is, as it said before, the underlying and well established theory of QED. In fact, below the limit at ~1 keV, Geant4 description becomes less and less precise or reliable. This has to do rather with the not so well known atomic cross sections at this level where also other effects in the actual material play a role, be solid state physics phenomena, be gas dynamics, etc. As a relevant example we mention the propagation and energy loss or ionization of a recoiling heavy nucleus struck by a neutron. The underlying processes are still theoretically and experimentally not well known, and they certainly deserve further investigations. However simulations at high energies, like in LHC or sLHC experiments, are not affected by this range of inaccuracy, since any simulation program like Geant4 assumes that particles which arrive at ? low energies deposit their entire energy locally.

However, the low energy limitations of the Monte Carlo codes are indeed a serious constraint for the simulation of processes at low energy experiments as those encountered, e.g., in space science, biomedical studies, nuclear physics or elsewhere.

Moreover, particles like charged pions, charged Kaons, etc interact not only electromagnetically but also hadronically, since they are mesons. The appearance of hadrons, like protons, neutrons and their antiparticles, can take place directly in HEP collisions like those expected to occur at high rate and with high multiplicity in LHC, and even more so in sLHC collisions. Furthermore, neutrons and protons, even though we focus here exclusively on neutrons, appear predominantly as secondary by-products during the interaction of all various high energy particles involved. We refer to the interaction of energetic particles with the detector active material or also the inactive material surrounding the detector itself.

Thus one has in HEP experiments a neutron background field, which in case of LHC and sLHC is expected to have up to 10-20 MeV kinetic energy (still open). Some detector components have real difficulties to live with this neutron background field. Since they have to localize it fast and if possible, to suppress it also fast from further consideration, provided they get not switched off by the recoiling and highly ionising active detector

material nuclei (e.g. Argon in chambers). Note, neutrons can appear also in the interaction of the accelerator beams with the beam pipes or even with more outwards located accelerator elements like the bending magnets, the focusing quadrupoles, etc.
Thus, detectors in LHC and sLHC will be exposed to an unprecedented neutron flux of ~1-20 MeV energy, and they will suffer also damages, in particular if they are solid state detectors like the Silicon trackers or the crystalline calorimeters. The neutron damages can affect the performance of the detectors, due to the defects in their crystalline structure, and this in turn will change also their performance as detectors.
The interaction of neutrons with the detectors has unavoidable impact also on the actual data evaluation, since those events must be recognized first by the data analysis algorithm and be rejected at the earliest possible level of the analysis program, if it is possible at all, i.e. if their impact does not switch-off the detector performance.

2. Workshops – Training Events

The last ~11 months I have visited the laboratory in Frascati and attended some courses / workshops:

1) 25 - 28 November: Geant4 courses in Annecy.
   (http://indico.in2p3.fr/conferenceDisplay.py?confId=443)

2) 30 March - 3 April: 8th Fluka Course, Demokritos, Athens, Greece.
   (http://www.fluka.org/fluka.php?id=course⊂=intro&which=demokritos2009)

3) 27 April - 26 June: General and Professional French Courses (Level 2).

4) 3 - 8 May: Visit Frascati (Italy) and KLOE experiment in order to get informed about simulations that have been already done and discuss about the possibility of getting involved in the Geant4 simulation for KLOE.

5) 11-15 May: Attendance to the 1st EIROforum School on Instrumentation at CERN.

6) 19 - 22 May: Participation to the 6th Geant4 Space User's Workshop in Madrid (Spain).

7) 16-19 September 2009: Attendance to the 1st MC-PAD Network Training on Readout Electronics in Krakow, Poland - Contributed with a poster -This poster contains actually most of my work done in the period Dec. 2008 - Sept. 2009.
8) 12 October - 16 December: General and Professional French Courses (Level 3).

9) October - November: Self study of SRIM (Stopping and Range of Ions in Matter). SRIM is a group of computer programs which calculate interaction of ions with matter. More specifically, work on how Argon ions behave inside noble gases i.e. Argon gas. Search for ALICE and ATLAS documents related to their gaseous detectors.

10) 26-28 October: C++ Part 1 at CERN: Hands-On Introduction.

11) 3 - 6 November: C++ Part 2 at CERN: Object-Oriented and Generic Programming.

3. Motivation of the work

In November 2008, I have started working at CERN as MC-PAD researcher.
A detailed simulation of gaseous detectors and lead/scintillating fibres (Scifi) calorimeters of different structures using Monte Carlo tools (Fluka, Geant4) is relevant to evaluate and improve their energy response and sensitivity to neutrons. The first part is to concentrate on the impact of the expected strong neutron background on the energy deposition measured in chambers, which might be a significant limitation of the performance of gaseous detectors in HEP experiments. The accuracy of the modelling of neutron interactions in the physics models used by Geant4 is being validated using published benchmark and test beam data. These studies will be completed with simulation of resulting secondary photons and the ionization in Geant4 and the transport of low energy electrons/gammas using Garfield with the aim to create an integrated tool for assessing the influence of neutrons in gaseous detectors.
What has been done so far is the validation of the existing Geant4 cross-sections and physics models for key gases against benchmark data from neutron data libraries, in order to update anyone for which a significant deviation has been identified. For the next two years I will create an application interfacing Garfield with GEANT4; this will allow to model the effect of neutrons on the energy deposition in gas chambers and will elaborate on the Geant4 description of the neutron interaction in calorimeters.
More specifically, as part of my work as fellow at CERN, I have performed a new validation on the Geant4 code of the neutron interactions (=cross sections) with typical gaseous constituents like Helium, Argon, Krypton, Xenon, and elements used as quenchers as Hydrogen, Oxygen and Carbon, which are widely used in HEP gaseous detectors.
It is worth repeating here that, in general, the interaction of neutrons with the detector atomic nuclei, relies on measurements which limit the simulation accuracy.
One task in this work was to trace back the origin of the used neutron cross sections by Geant4, and eventually update them with more recently derived values. This is appropriate, in order to make Geant4 performance better and therefore accordingly even more reliable. In this work, the Geant4 neutron cross sections have been validated for key chamber gases against benchmark data from various Neutron Libraries, using recent as well as older evaluations.

4. Setup

- Geant4:

In order to obtain the neutron cross sections we use the extended hadronic example Hadr00. We used two different physics lists.

1. QGSP_BERT (=QGSP BERTINI) and
2. QGSP_BERT_HP (=QGSP BERTINI HIGH PRESICION).

QGSP is the basic physics list applying the quark gluon string model for high energy interactions of protons, neutrons, pions and Kaons and nuclei.
Like QGSP, but using Geant4 Bertini cascade for primary protons, neutrons, pions and Kaons below ~10 GeV, is QGSP_BERT.
QGSP_BERT_HP list is similar to QGSP_BERT and in addition uses the data driven high precision neutron package (NeutronHP) to transport neutrons below 20 MeV down to thermal energies.

- Data Libraries:

The libraries used in this work are:

ENDF/B-VII.0 & ENDF/B-VI.8: Evaluated Nuclear Data File (December 2006 and 2001, respectively)
JEF-2.2 : Joint Evaluated File (January 1997)
JEFF-3.0 : Joint Evaluated Fission and Fusion,
"...this library superseded JEF-2.2..." (April 2002)
JEFF-3.1 : "...this library superseded JEFF-3.0..." (May 2005)
JEFF-3.0/A : Neutron Activation File
JENDL-3.3 : Japanese Evaluated Nuclear Data Library (2002)

5. Validation and Results

The following figures show the comparison of Geant4 performance with various libraries for Argon, Helium, Oxygen, Xenon, Krypton, Hydrogen and Carbon.

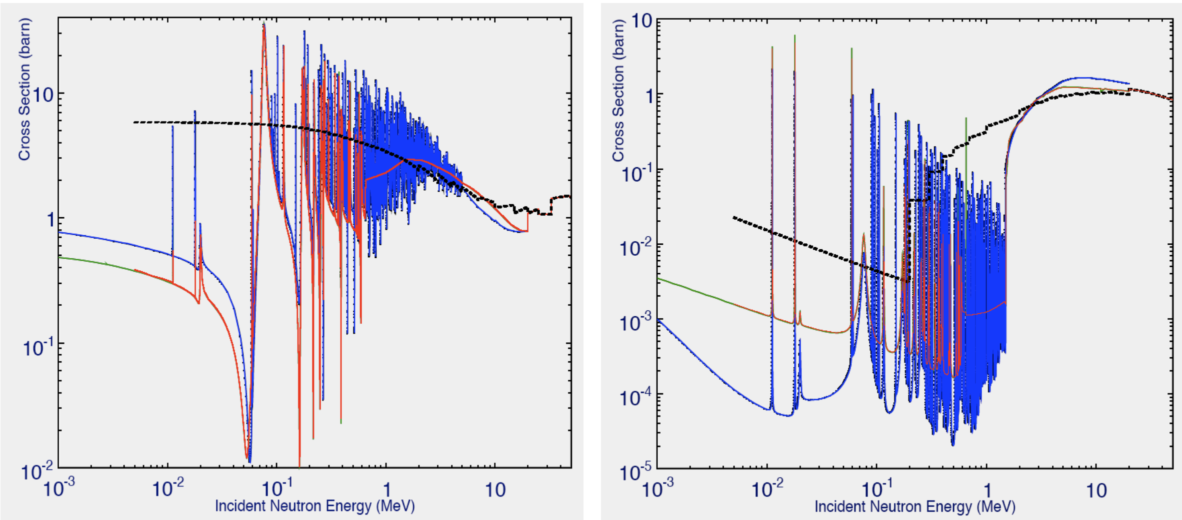

Figure 1. There is agreement between Geant4 and the “old” libraries at all energy regions. Large discrepancies appear with the “new” libraries. For the case of Argon, G4NDL uses JEF 2.2 / JEFF 3.0.

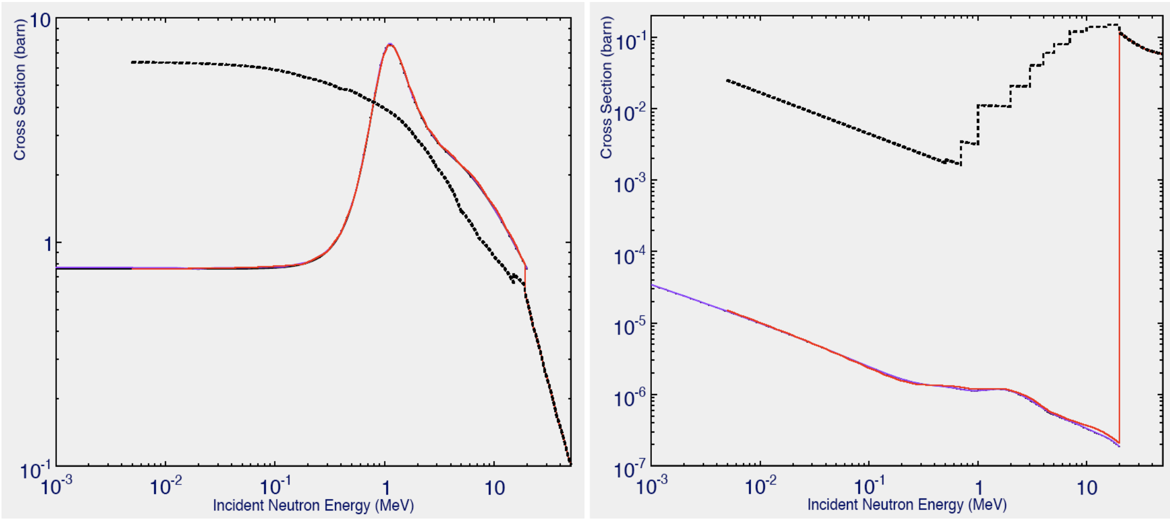

Figure 2. No differences between “old” and “new” libraries. There is agreement between Geant4 and all the available libraries, almost in the entire energy region below 20 MeV. For the case of Helium, G4NDL follows ENDF and JEFF

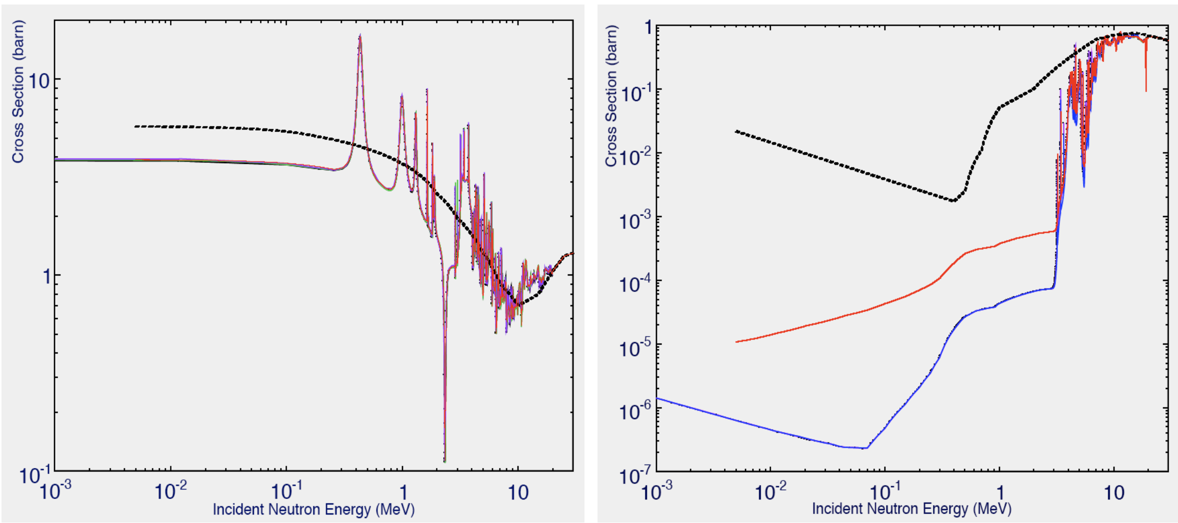

Figure 3. Small differences exist between “old” and “new” libraries. Elastic interactions: Geant4 is in quite good agreement with all the libraries. Non-Elastic: Geant4 follows the libraries for energies higher than 3 MeV. Large differences appear below 3 MeV. JEFF-3.0 has few data for non-elastic xs (10 – 20 MeV). For the case of Oxygen, G4NDL uses ENDF and JEFF.

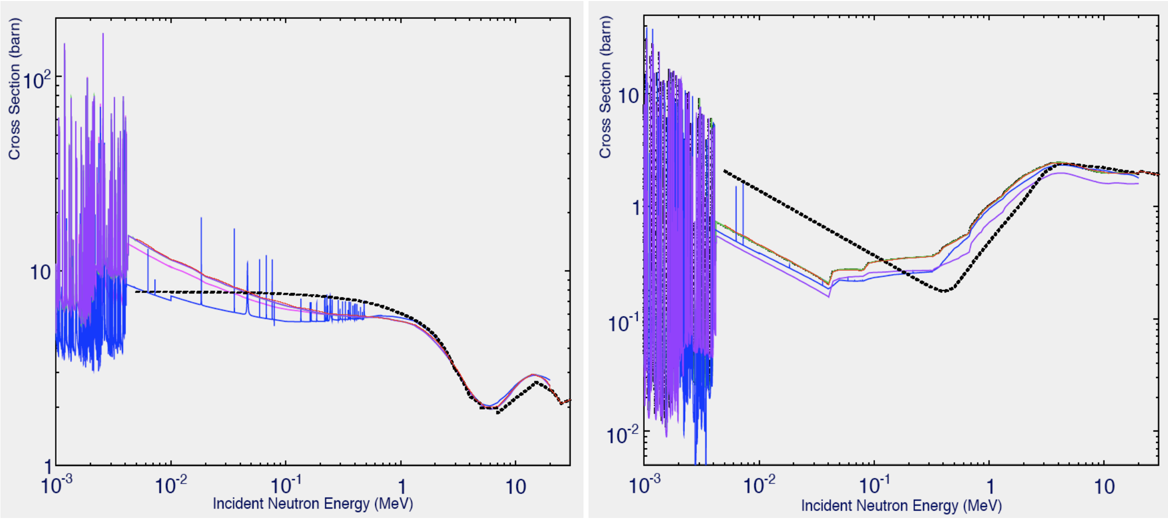

Figure 4. Elastic interactions: Geant4 agrees with the most recent JEFF. Large discrepancies exist even between recent libraries for energies below 1 MeV. Non-Elastic: Geant4 follows the "old" libraries. For the case of Xenon, G4NDL uses the latest version of JEFF for elastic xs and ENDF / JEFF for the non-elastic xs.

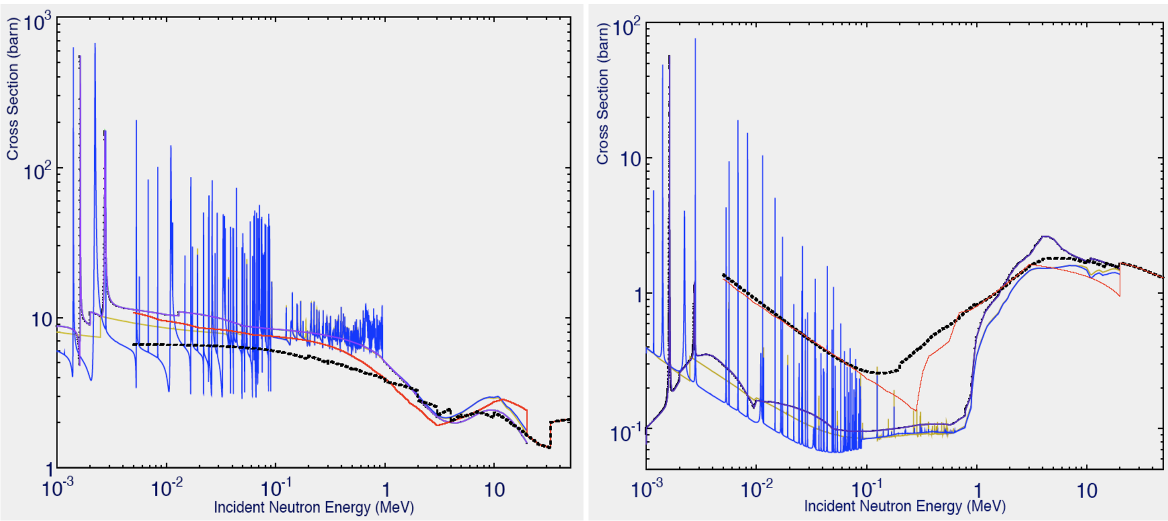

Figure 5. G4NDL is missing xs for Krypton (Z=36). Instead, is using Bromine's (Z=35) xs. Geant4 does not follow any of the libraries. Large differences appear in the case of non-elastic interactions. For the case of Krypton, G4NDL needs Krypton's data for a more reliable comparison.

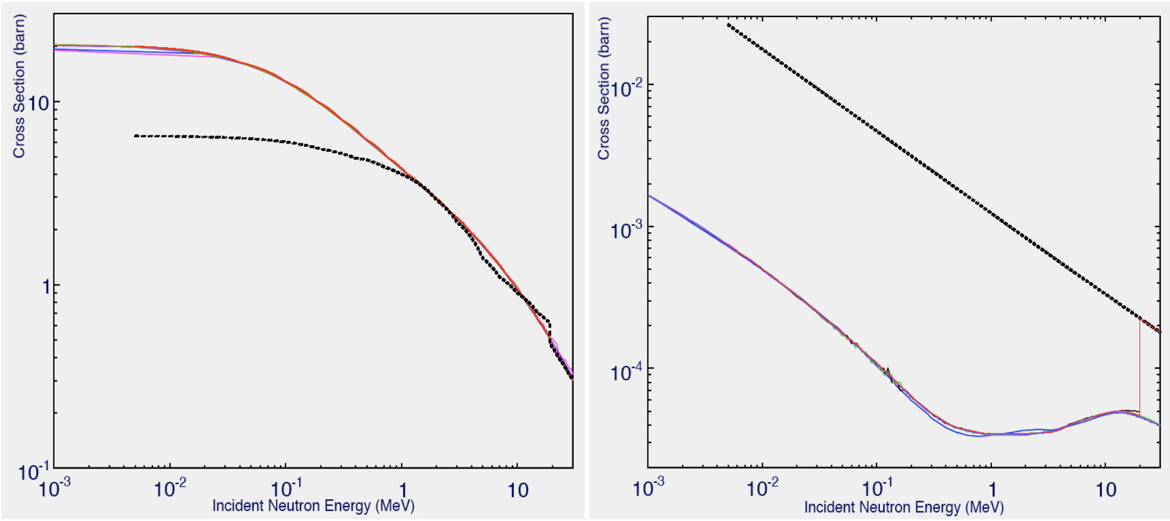

Figure 6. Small differences exist between "old" and "new" libraries. The appearing peak of Geant4 above 20MeV for elastic xs is not yet identified. Geant4 agrees with all the available libraries. For the case of Hydrogen, G4NDL follows ENDF / JEFF and JENDL.

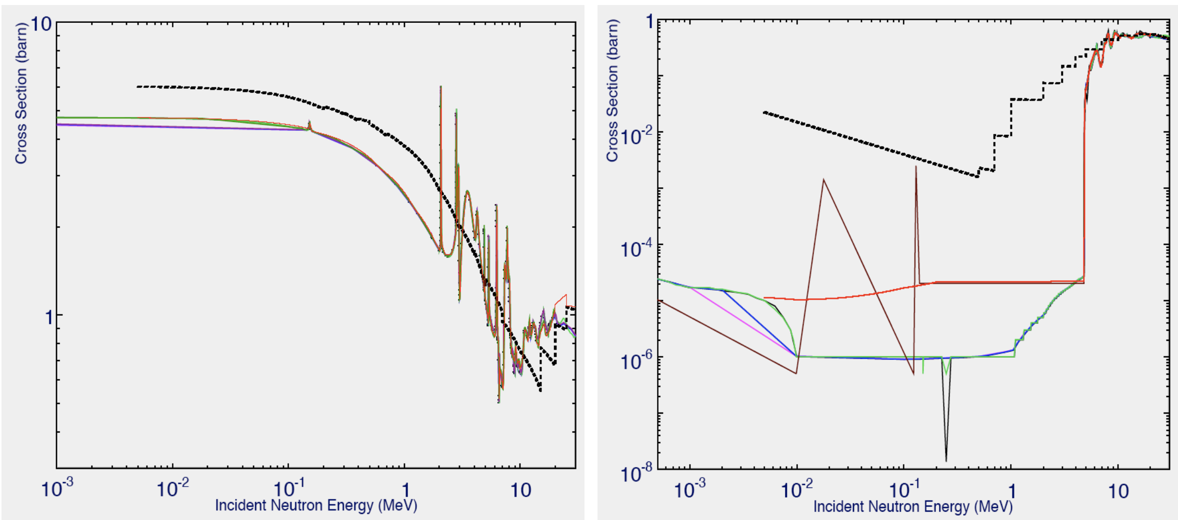

Figure 7. Elastic interactions: Geant4 follows the "old" libraries. Non-Elastic: Geant4 follows JENDL above ~100 keV. For high energies, it agrees with many of the libraries while having always small differences. For the case of Carbon, G4NDL uses the "old" ENDF / JEFF and JENDL. Non-elastic xs: JENDL-3.3 is used for energies below ~5 MeV.

6. Simulation with Quencher Gases

The high reaction multiplicity and the high rate in LHC collisions result to a high neutron background in the detectors mostly up to ~10 MeV. The eventual goal of this work is to simulate first monochromatic neutrons of energies equal to 1 and 10 MeV. Elastic recoils of heavy nuclei like Argon deposit energy below ~10-100 keV, which increases however with decreasing atomic number A due to the two body kinematics involved, for example, the maximum energy loss, i.e. the minimum energy (E') of an elastically scattered neutron, occurs for a head-on collision ($\theta=180^{\circ}$), $(E'/E)_{min}=[(A-1)/(A+1)]^2$. Notice that for A=1 (neutron scattering with Hydrogen), the neutron can give all its energy to the struck proton.

Therefore, the case of Hydrogen constituents is the most extreme one. Even though Hydrogen is not used as principle active gas in chambers, it is part of the chemical composition of various quenchers, making ~5-10% of the total gas composition. Thus, the impact of the quencher is eventually not at all negligible, since an elastically recoiling proton can take a large fraction (maximum up to 100%) of the energy of the interacting neutron. In fact, such recoiling protons will deposit their energy as relatively long tracks and they cannot be suppressed easily, i.e. fast, from further consideration. This work allows to quantify the implications of hydrogen compositions like the occasionally used quencher gas CH_4.

7. Conclusions

Once this work is completed, it might make future Geant4 updates easier to implement. This is an ambitious but necessary first step, keeping in mind the wide applications Geant4 has found in various disciplines. Throughout this work we have focused on typical gaseous compositions used in chambers in HEP experiments, and in particular in LHC experiments. We have identified that for Ar, Xe, Kr, H, C and O (not shown here) Geant4 follows rather well JEF 2.2. This justifies that an update of the input used by the Geant4 code is in place. Moreover, neutron cross sections from recent libraries are now available. The structure of these data files allows an easy access by Geant4 itself without the need of further treatment. As a first by-product, we applied the same reasoning also for the quenchers, which are inherent to the working principle of any gaseous detector. After all, their part makes about 5-10% of the total detector gas, which is certainly not negligible. More specifically, we conclude in this work, as expected, that a quencher with Hydrogen composition seems to be sensitive to the neutron background in experiments in LHC and even more so in sLHC with the expected much higher neutron fluxes.

8. Neutrons Simulation

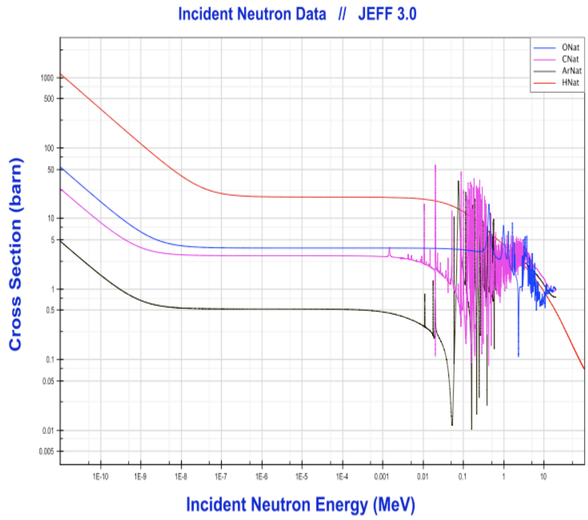

Figure 8. Neutron Cross Section in natural composition of oxygen (blue line), carbon (pink line), argon (black line) and hydrogen (red line).

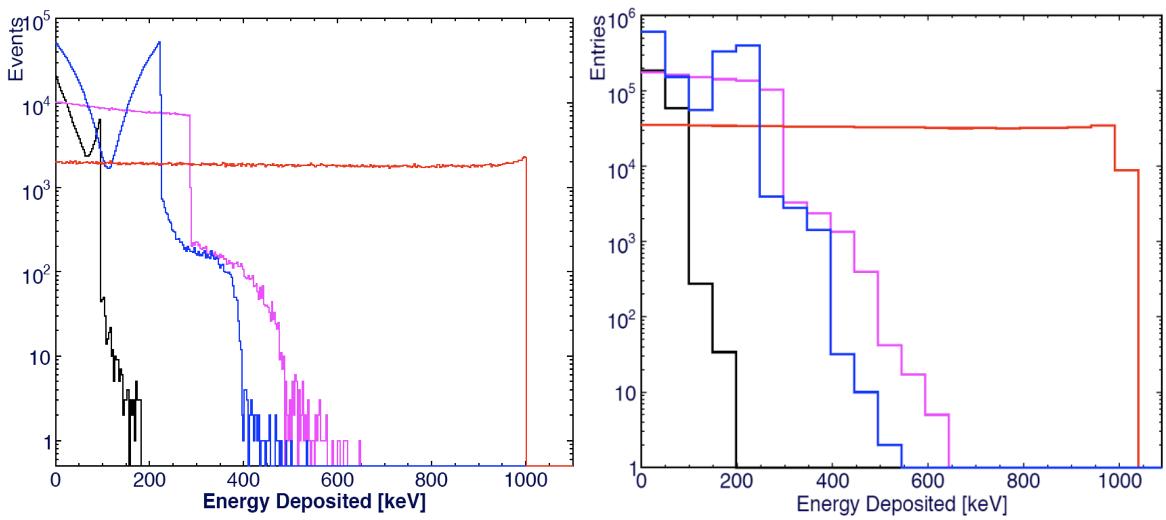

Figure 9. Energy deposition for 1 MeV neutrons in oxygen (blue line), carbon (pink line), argon (black line) and hydrogen (red line) gaseous chambers (1mx1mx1m).

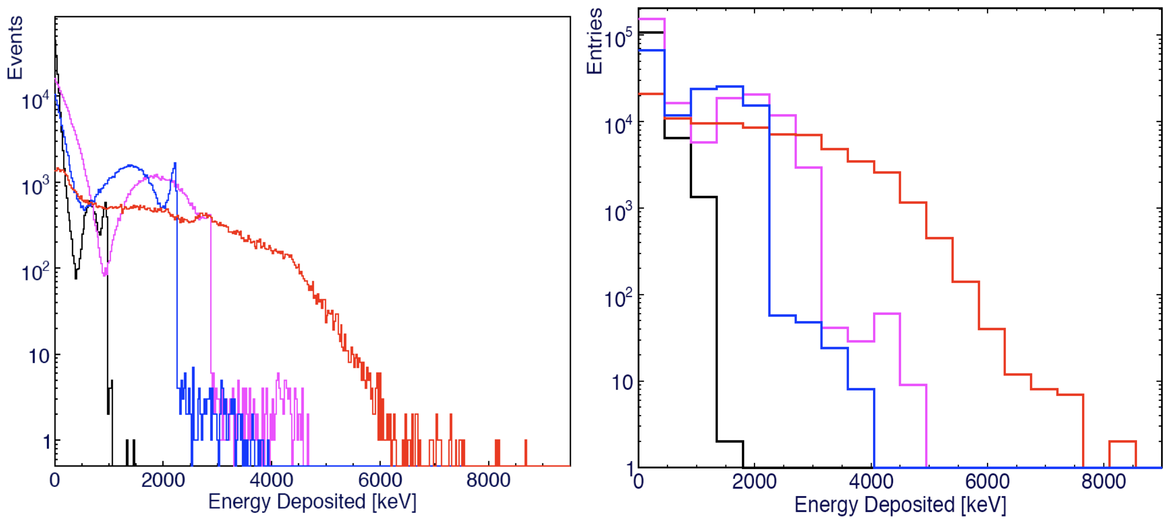

Figure 10. Energy deposition for 10 MeV neutrons in oxygen (blue line), carbon (pink line), argon (black line) and hydrogen (red line) gaseous chambers (1mx1mx1m).

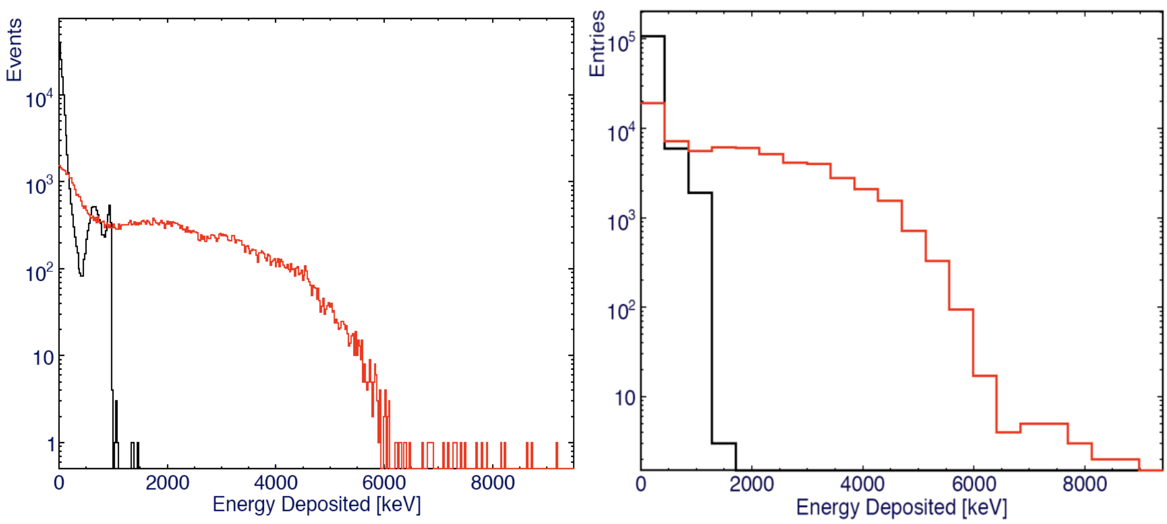

Figure 11. Energy Deposition in 90% argon (black line) (1.782mg/cm3) and 10% CH_4 (red line) (0.1782mg/cm3) gaseous chambers, for 10 MeV neutrons.

9. Dynamics of neutron recoil energy deposition (Ongoing work)

The process of the energy deposition of the recoiling neutrons off detector nuclei like Argon etc implies a series of atomic reactions, which take place. For example, a struck nucleus like Ar will get first highly ionized, i.e. loosing some (if not all) of its atomic electrons to the chamber enviroment. Then, this slow and highly charged Argon projectile has high ionisation power: it looses all its kinetic energy rapidly, while at the end of its penetration length, before it comes to rest, the ionization is the highest. The dynamics of this process much be understood, in order to explain experimental observations (like the response of chambers to neutrons) and eventually allow to choose appropriate detector conditions to improve its performance. Fig. 12 shows the ionization of recoiling Ar nuclei due to elastic neutron scattering. For comparison, if a minimum ionising particles deposits ~2[MeV]/[g/cm^2], the corresponding value derived from Fig. 12 is ~300 times higher. Such a high degree of ionization might explain why some chambers cannot stand out such local events.