SaG4n: Calculation of ($\alpha$,n) yields for low background experiments using Geant4

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Abstract.
SaG4n is a code fully based on Geant4 that we have developed to calculate neutron yields. The code is available in http://win.ciemat.es/SaG4n and works for Geant4.10.6 or superior. The improvements to the ($\alpha$,n) yields introduced by the use of a single Monte Carlo code, fully developed in Geant4, are presented. Neutrons are a potential source of background for all rare-event searches, and is specially relevant for WIMP searches with liquid argon, where they are the only source of irreducible background together with the yet-negligible coherent neutrino scattering. The precision of the neutron yield is critical to evaluate the discovery potential of coming experiments and to reduce systematic effects in current data.

We present the result of evaluating the neutron yield for three different cases and show the sizable effect of interfaces between materials with high ($\alpha$,n) cross section and materials with small mass which contribution to the neutron budget is often considered negligible.

1. Introduction
The field of rare event searches is in constant progress towards the characterization of the backgrounds that are limiting the performance of detectors. Such characterization enables the community to reduce the systematics and finding better solutions in the design of new larger devices to progress in the field. The $\alpha$, $\beta$ and $\gamma$ backgrounds have different effect in different detectors, but their systematics are not always leading the uncertainty on the total background estimates [1, 2, 3]. This is due to the high radiopurity levels achieved in current and new-generation detectors, together with the use of time projection chambers (TPC). Such purity level is being evaluated with more sophisticated and precise techniques and is allowing us to understand the details of naturally occurring decay chains in the materials used for the construction. The TPCs, in particular TPCs filled with liquid argon (LAr) are able to discriminate with an unparalleled efficiency the electronic recoils induced by the $\beta$ and $\gamma$ backgrounds from the WIMP-like nuclear recoils using pulse shape discrimination [3]. In turn, the $\alpha$ background from the bulk of the LAr leave a high energy signal that is not a problem for dark matter searches, and the surface contamination, given the precision in position reconstruction, is efficiently removed with fiducial cuts.
Having these backgrounds under control, neutrons become the dominant source of both background and systematic uncertainty. Radiogenic neutrons are produced by spontaneous fission of $^{238}\text{U}$ and, mainly, by $(\alpha,n)$ induced by the $\alpha$ population produced in the decay chains of $^{238}\text{U}$ and $^{232}\text{Th}$. The large size detectors and the unavoidable level of radioactive impurities, translates into a significant variety of isotopes on which the $(\alpha,n)$ cross sections need to be evaluated.

2. Geant4-based approach: SaG4n

The details of our approach are described in [4], together with its performance with respect to experimental data compared to other codes, like NeuCBOT [5], NEDIS [6], USD [7] and SOURCES-4C [8] widely used in the field of Dark Matter searches [1, 2, 3, 9, 10, 11].

Its main features are that it is flexible in the selection of the data libraries to be used, it exploits the advantages of Geant4 [12], it is transparent for the user to implement modifications as desired and it has is easily executed only by editing an input file (it needs a Geant4 installation).

In particular, the Geant4 capabilities most relevant for this use are three. First, it allows for almost arbitrarily complicated geometries. Second, it benefits from the electromagnetic processes already implemented for $\alpha$ transportation. Third, it allows you to bias a particular process, in this case boosting the $(\alpha,n)$ cross section in to reduce the computation time and make the simulation viable for this kind of studies. The amount of biasing and the step size of the simulation are controlled by the user. For reducing further the computation time, there is an option to kill the process once the neutron is produced.

In order to read the ENDF-6 format tables [13] as input for $(\alpha,n)$ cross section Geant4.10.6 or superior is needed. In the work presented here the JENDL/AN-2005 [14] and TENDL-2017 [15] data libraries were used. It is worth noting that in particular MT5 data was used, so the neutron yields are calculated considering all the channels that produce at least one neutron, regardless the number they produce and if something else is also produced in the process. The code allows for the production of $\gamma$ decays in the same nuclear process, provided that the data libraries used have that information.

The output of the code is editable, but in its native version includes initial position and momentum of the generated $\alpha$, position and momentum of the produced neutron (and $\gamma$ rays) and weight. The weight is given by Geant4 to each generated neutron to compensate the biasing that has been introduced to boost the $(\alpha,n)$ process in first place. The yield of neutrons per alpha can be calculated as

$$Y[n/\alpha] = \frac{1}{N_\alpha} \sum_{i=1}^{N_n} \omega_i,$$

where $N_n$ is the number of neutrons produced in the simulation, $\omega_i$ the weight of each of them, and $N_\alpha$ the number of simulated alphas. It was cross-checked in monoisotopic examples that the yield obtained this way and the one obtained convoluting the simulated $\alpha$ flux and the used data libraries agreed.

3. Results

In this section we show three simple examples that evidence the suitability of SaG4n for a comprehensive study of the neutron yields in low background experiments. The effect of having a copper sheet immersed in a liquid argon bath, of having a fluorine based insulator for copper
Figure 1. Left—Neutron yield along the perpendicular axis of a 0.5 mm thick copper sheet (copper_alone, red). If the sheet is surrounded by liquid argon (copper_lar, black) the neutron yield in the surrounding material is \( \sim 9 \) times larger than in the copper itself. Center—Neutron yield along the radial axis of a 0.5 mm diameter copper cable (copper_cable_alone, red). If the cable is surrounded by FEP the neutron production in the surrounding material is 48 times larger than in the copper itself (copper_fep, black). Right—Neutron yield along the perpendicular axis of a 0.5 mm thick solder paste point with liquid argon in both sides (xsolder_lar, black). The simulation shows that the yield in the interface is boosted by a factor 24 and, in contact with kevlar of a PCB substrate in one side, the neutron production in the surrounding material is \( \sim 4 \) times larger than in the solder paste itself (solder_lar_pcb, red).

cables and of using dirty solder pastes. All the examples were chosen to clarify the importance of the radiopurity of materials, even if the \((\alpha,n)\) cross section of the material itself is low, and how these can end up being sizable contributions in ultrapure detectors.

The variable chosen in order to compare the different scenarios is the yield of neutrons per \( \alpha \) in the last 20 \( \mu \)m of the \( \alpha \)-emitting material with respect to a central slice with the same volume. This comparison is robust with respect to geometry particularities, and evidences at the same time the border effects in the case of surface contamination and in the case of having potentially dirty materials in contact with materials with a high \((\alpha,n)\) cross section. The results presented are obtained using the JENDL/AN-2005 data library where information is available and TENDL-2017 elsewhere.

Case 1: Copper is one of the materials that goes in all detectors in many different formats. The variety of mechanical requirements and the price of electroforming does not make it possible to use it for all the applications, but its \((\alpha,n)\) cross section is low, so neutron yields are expected to be low even when using not-so-radiopure batches. However, a full simulation with SaG4n using a simple geometry of a copper plate surrounded by liquid argon shows an enhancement in the effective neutron production in the surface of a factor 9, see figure 1 a).

Case 2: FEP and other fluorine-based materials are chosen as insulator of cables in low-background cryogenic detectors because of their flexibility at low temperatures and their radiopurity. Notwithstanding, the \((\alpha,n)\) cross section in \(^{19}\text{F}\) is very high. Figure 1 b) shows the result of the simulation with FEP around copper, which multiplies the effective neutron yield by a factor 48 for the \( \alpha \) decays produced in the last 20 \( \mu \)m (in the case of a 0.5 mm diameter copper cable).
Case 3: The electronics associated with the photosensors needs of PCBs with several components that are soldered. The number of solderings is proportional to the number of photosensors and with the development of larger detectors is continuously increasing. Solder pastes with activities below the Bq / kg throughout the $^{238}$U and $^{232}$Th decay chains are hard to find, and the argument of their low $(\alpha,n)$ cross section is used to accept their use. According to our simulation, the contact with a kevlar substrate multiplies the yield by a factor 4 in the surface, and the contact with LAr by a factor 24. This effect can be observed in figure 1 c).

4. Conclusions
This work evidences the enhancement of the effective neutron yield near the interfaces of materials with high $(\alpha,n)$ cross sections in some paradigmatic cases. Calculations, in which only the composition of the material containing the impurities is taken into account, cannot quantify this effect and simulations are fundamental to evaluate the neutron yields and reduce their systematic uncertainty in the new era of ultrapure detectors. Our simulation, using JENDL/AN-2005 data libraries where available and TENDL-2017 else where, show increases in the effective yields near the surfaces above a factor 10 in two cases. This results depends on the cross sections used in first place and must be understood as such.

The code SaG4n, fully based on Geant4, allows the user to define the geometries and quantify this effect by the edition of a single input file, with no hard coding needed. The code allows the selection of ENDF-6 formatted $(\alpha,n)$ data libraries (so far JENDL/AN-2005 and TENDL-2017), and is validated against experimental data and other codes widely used for the estimation of neutron yields.

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