

# MAGE - a GEANT4-based Monte Carlo Application Framework for Low-background Germanium Experiments

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**Abstract**—We describe a physics simulation software framework, MAGE, that is based on the GEANT4 simulation toolkit. MAGE is used to simulate the response of ultra-low radioactive background radiation detectors to ionizing radiation, specifically the MAJORANA and GERDA neutrinoless double-beta decay experiments. MAJORANA and GERDA use high-purity germanium detectors to search for the neutrinoless double-beta decay of  $^{76}\text{Ge}$ , and MAGE is jointly developed between these two collaborations. The MAGE framework contains the geometry models of common objects, prototypes, test stands, and the actual experiments. It also implements customized event generators, GEANT4 physics lists, and output formats. All of these features are available as class libraries that are typically compiled into a single executable. The user selects the particular experimental setup implementation at run-time via macros. The combination of all these common classes into one framework reduces duplication of efforts, eases comparison between simulated data and experiment, and simplifies the addition of new detectors to be simulated. This paper focuses on the software framework, custom event generators, and physics lists.

**Index Terms**—Monte Carlo, neutrinoless double-beta decay, Germanium detectors, Geant4, radiation detection, low background.

## I. INTRODUCTION

MAGE (MAJORANA-GERda) is a GEANT4-based [1], [2] physics simulation software framework jointly developed by the MAJORANA and GERDA collaborations [3], [4]. Both experiments will search for the neutrinoless double-beta decay ( $0\nu\beta\beta$  decay) of the  $^{76}\text{Ge}$  isotope using arrays of isotopically enriched High-Purity Germanium (HPGe) detectors. The discovery of  $0\nu\beta\beta$  decay is the only practical way to determine if the neutrino is a Majorana particle. For further details on the physics motivation, see the review article in [5]. The current lower limit on the  $0\nu\beta\beta$  decay half-life of  $^{76}\text{Ge}$  is  $1.9 \times 10^{25}$  years [6], making this decay extremely rare if it exists. This requires great care to reduce experimental backgrounds from naturally occurring radioactivity and cosmic rays. This is achieved via careful material selection and assay, a deep underground location, passive and active shielding, and analysis cuts. The purpose of MAGE is to simulate the response of the MAJORANA and GERDA experiments to ionizing radiation from backgrounds, calibration sources, and  $0\nu\beta\beta$  decays. MAGE is also used to simulate the response of prototype detectors, test-stands, and low-background assay systems. In the prototyping phase, the simulation is used as a virtual test stand to guide detector design, to estimate the effectiveness of proposed background reduction techniques, and to estimate the experimental sensitivity. During experimental operation, MAGE will be used to simulate and characterize unexpected backgrounds and determine the ultimate sensitivity of the experiments. It will also provide probability distributions for signal extraction analyses. The combination of the two collaboration's simulation package into one framework reduces duplication of efforts, eases comparison between simulated

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data and experiment, and simplifies the addition of new simulated detector geometries. MAJORANA and GERDA are currently constructing detectors with tens of kilograms of enriched isotopes, but it is the goal of parts of the two collaborations to merge and pursue a joint effort towards a tonne-scale germanium experiment. Having a joint simulation package during the very early phases will ease this future integration. This paper focusses on the software framework, custom event generators, and physics lists of MAGE.

The code and physics requirements are given in section II. The code structure of MAGE is discussed in section III. Section IV describes the implemented GEANT4 physics lists that are optimized for low-energy (sub-keV to few MeV), low background applications. Validation of MAGE simulations against experimental data is discussed in Sect. V. Conclusions are provided in the last section.

## II. REQUIREMENTS

The requirements for the MAGE framework can be subdivided into physics requirements and software requirements. The physics requirements define the physical processes that have to be simulated to find the response of the detectors. Software requirements are driven by the use of the GEANT4 toolkit as basis for MAGE and the anticipated end-users.

### A. Physics Requirements

GEANT4 is a simulation toolkit that uses Monte Carlo techniques to simulate the propagation of particles and nuclei through matter. It has extensive capabilities to simulate different experimental geometries, propagating particles, and particle interactions, and has the foundation of the physics requirements for MAGE. The choice of GEANT4 over other packages as the basis for MAGE was motivated by its flexibility and active development within the particle and medical physics communities, as well as its C++ and object-oriented structure. GEANT4 is open-source and allows collaborations with members from multiple countries to use it. It is a standard simulation tool for LHC experiments and will likely be supported for at least another decade.

The most stringent requirements for MAGE are the proper simulation of the relevant background sources for  $0\nu\beta\beta$  decay experiments. GEANT4 fulfills some of these requirements, specifically it simulates:

- 1) Electromagnetic interactions of electrons and  $\gamma$ -rays at MeV and keV energies.
- 2) Radioactive isotope decay chains and nuclear de-excitations.

- 3) Interactions of thermal and fast neutrons.
- 4) Electromagnetic and hadronic showers initiated by cosmic-ray muons.
- 5) Penetration depths and ionization energy loss profiles of  $\alpha$ -particles.

The list of implemented physics models in MAGE was optimized for low-background, underground physics applications [7], with an emphasis on low-energy interactions and hadronic interactions resulting from cosmic-ray spallation. MAGE has implemented different selections of models in its GEANT4 physics list. These are tailored to fit specific physics applications, and the required processes can be selected by the user to optimize computation time and data storage requirements. For example, the simulation of muon propagation through rocks requires different models than that of background from radioactive decays in detector components. Many important tuning parameters, such as the production cuts for  $\delta$ -rays and soft bremsstrahlung photons, may also be set by the user. Specific details of the physics lists implemented in MAGE are discussed in Section IV. The MAGE code is regularly updated and ported in order to make it compatible with the most recent GEANT4 releases.

Other physics processes that are not part of GEANT4 had to be simulated. These include:

- 1) Electric-field solvers are required to simulate the trajectories of charge carriers inside the HPGe crystals under the influence of the biasing field.
- 2) Generators of electronic waveforms by charge carriers in the HPGe detectors as they drift inside the crystal towards the collection electrodes.
- 3) Electronic transfer functions of generated pulses into simulated detector pulses.
- 4) A generic surface sampler that uniformly and randomly samples points on arbitrary surfaces had to be implemented to simulate surface alpha contaminations. The algorithm of this sampler is described in Ref. [8].
- 5) Event generators for physics processes other than normal nuclear decay, such as two neutrino double-beta decay for different models,  $0\nu\beta\beta$  decay, and cosmic-ray muons at depth.

Some of the existing aspects of GEANT4 had to be extended or improved to fulfill the requirements of MAGE. These are described later in this paper.

### B. Software Requirements

The use of GEANT4 as the basis of MAGE made C++ the natural choice for MAGE, and MAGE makes full use

of the object-oriented nature of C++ and GEANT4. The software framework is required to:

- 1) Allow run-time selection of detector configuration, event generators and output format.
- 2) Allow parallel and independent development of different branches of the code. For example, the development of the geometric descriptions of the GERDA and MAJORANA detector geometries should proceed independently and with minimal interference.
- 3) Ease-of-maintenance over the full life time of the experiments.
- 4) Perform simulations with different configurations by physicists that are inexperienced in programming.

The collaboration does not maintain the MAGE source code for public release, since most of components are experiment-specific and not useful beyond the two collaborations. However, some select components, such as physics lists and event generators, are provided to interested parties on a case-by-case basis. The object-oriented nature of the MAGE framework makes the transfer of such code to other users straightforward.

### III. STRUCTURE OF MAGE

To realize the requirements outlined in the previous section we subdivided a simulation task into different components. These components are geometries, generators, output formats, and physics lists. The user instantiates one instance of a class corresponding to each component at run-time, typically via a GEANT4 messenger in a macro file. A component may then also instantiate other components, and have its own macro commands that allow the user to further refine the simulation parameters. This design allows the simulation of many different detectors, prototypes and validations to be performed within the same executable using the same physics processes, geometries and other codes. This greatly eases cross-comparisons and reduces coding and debugging effort. The components are described in this section.

#### A. Geometries

These are the physical geometries of the detectors or experiments that are being simulated. MAGE supports geometric description via the GEANT4 geometry description classes or through an interface with the Geometry Description Mark-up Language [9] (GDML). MAGE currently has about 30 user-selectable geometries. The geometries range from simple cylindrical crystals to a

full detector array with 60 crystals, mounting components, shield and surrounding room. Each geometry is encoded in a class that derives from a geometry base class that contains the following basic components of a geometry:

- A unique identifying serial number string.
- A detector name string.
- A *ConstructDetector()* method that is invoked by GEANT4 to construct the detector geometry during run-time.
- An associated *G4LogicalVolume*.
- A setting of the importance value of the region, used by GEANT4 when performing simulations that require importance sampling of geometries to optimize performance.

This design also allows the reuse of existing geometry classes, since the classes describing a geometry can be instantiated within a class that requires that component. For example, a detailed germanium crystal has been coded that is used many times in other simulated detector geometries. This crystal can be simulated on its own, or be instantiated many times in a complex detector array. Shown in Fig. 1 is an example of how multiple stand-alone geometry classes are combined to create a complex detector. A rendering of the detector is shown in Fig. 2. The GERDA detector array rendering shown in Fig. 3 is constructed in a similar way. A bonus of this approach is that the GERDA and MAJORANA collaborations can share the same basic geometries, such as crystals. This reduces redundant code and increases code scrutiny.

#### B. Event Generators

These classes generate the initial conditions of each event to be simulated. MAGE has several event generators that all inherit from an *MGVGenerator* base class. One such generator is instantiated by the user at run-time via a GEANT4 messenger. The *MGVGenerator* base class contains the following relevant virtual methods that are defined in the daughter class:

- A *BeginOfRunAction()* method that is executed at the beginning of a GEANT4 run. It is primarily used to compute lookup tables from analytic expressions for distributions to be sampled.
- A *EndOfRunAction()* method that is executed at the end of a run. It is primarily used to deallocate memory used by lookup tables.
- A *GeneratePrimaryVertex(G4Event \*event)* method that passes the initial event particle type, position and momentum to the *G4Event* object.
- A *SetParticlePosition(G4ThreeVector vec)* method that can be used by another generator, such as the

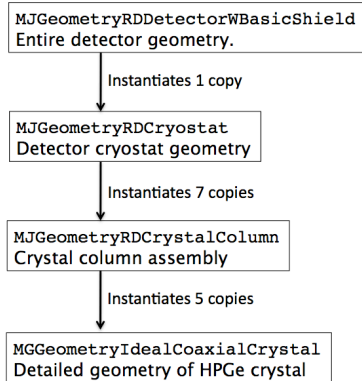


Fig. 1. Classes used to create the geometry of the MAJORANA DEMONSTRATOR. This detector consists of 35 crystals arranged in 7 columns of 5 crystals each. The crystals are placed inside a cryostat that in turn is placed inside a layered shield. This diagram illustrates how this design is realized in the simulation. Each of these classes can be instantiated on its own, or as part of a larger geometry, such as this. A rendering of this geometry is shown in Fig. 2.

position sampler described below, to set the position for the initial vertex.

The generator may also have a GEANT4 messenger associated with it to allow the user to set parameters at run-time. Using this base class, we have created the following specific generators for MAGE:

- A wrapper for the Radioactive Decay Module [10] (RDM) in GEANT4 that generates radioactive decays from unstable nuclei at a point.
- “Hybrid” generators that use the RDM generator to generate the initial decay of a nucleus, but then uses a customized surface or volume sampler to place it at a specific location in our simulated geometry. We developed a volume sampler that can generate points uniformly distributed in any GEANT4 solid. This is required to simulate radioactive contamination embedded in detector components. A surface sampler was also developed that creates points uniformly distributed on the surface of any GEANT4 solid. This surface sampler is complex and is described further in [8]. A surface sampler is required to simulate surface contaminations, in particular  $\alpha$ -emitters and  $\beta$ -emitters on detector

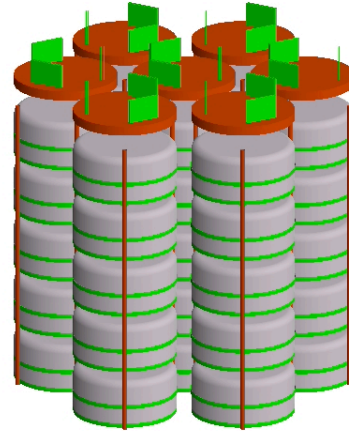


Fig. 2. Rendering of MAJORANA DEMONSTRATOR with cryostat and shields removed that was created using the class structure in Fig. 1. Each of the 7 crystal columns with associated support structures is a stand-alone class, as is each of the 5 crystals in a column.

surfaces inside the cryostat that are within line-of-sight of the HPGe crystals.

- Generators to simulate neutron and muon backgrounds in underground laboratories, using either theoretical models or data-driven approaches. Interfaces are available which read initial conditions for an event from other codes, such as SOURCES4A [11] for neutron flux and MUSUN [12] for muon flux, as well as other selected analytical models, such as that by Wang et al. [13].
- A wrapper for the FORTRAN-based DECAY0 [14] generator. It is primarily used to generate different types of double-beta decays, but can also simulate normal nuclear decays. DECAY0 is able to simulate properly the angular correlation between  $\gamma$ -rays in nuclear de-excitation cascades, that is not accounted for in the GEANT4 Radioactive Decay Module.
- A customized generator to simulate the neutron and gamma flux from an AmBe source used for studying neutron interactions.

### C. Physics Lists

A collection of GEANT4 physics processes is called a physics list. They define the particles that are included in the simulation and the decays and interactions they can undergo. There are several physics lists implemented in MAGE, each optimized for the particular problem being simulated. One list is optimized at higher energies for

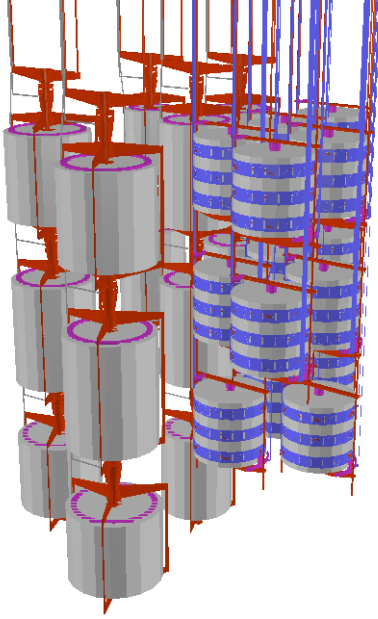


Fig. 3. Rendering of GERDA detector array with cryostat and shields removed. On the right hand side are 18-fold segmented HPGe detectors, while left are unsegmented ones. Detectors of the same type are only modeled once. The codes are reused to construct the whole array.

simulating cosmic-ray muon interactions, while others are optimized for standard electromagnetic interactions at lower energies, i.e. below 10 MeV. These are used to simulate the response of detectors to the decay of radioactive isotopes. Each physics list is contained in its own class that is instantiated at runtime. The physics lists and requirements are discussed in more detail in section IV.

#### D. Output Format

During the simulation GEANT4 generates complete information about the trajectory and interactions of particles as they propagate through the detector. Although all of this information is available to the user, it is typically processed, parsed and saved to an output file for further analysis after the simulation run is complete. Different detector or even different simulations of the same detectors have specific output requirements. MAGE defines a generic base output class and does not have a built-in output format, but we have implemented interfaces to the AIDA-compliant [15] and ROOT [16] analysis tools, as well as simple text-based output. At one extreme MAGE has implemented a class that saves all of the GEANT4 information for each step, at the other end is an output class that only generates a histogram of energy

deposited in a single HPGe crystal. Each output format consists of a class that inherits from a virtual base class (*MGVOutputManager*) that contains the following main methods:

- *BeginOfRunAction()* and *EndOfRunAction()* methods that are executed at the beginning and end of a simulation run respectively. They are used to open and close data files, create file formats, i.e. ROOT trees, create histograms, and allocate and deallocate data structures.
- *BeginOfEventAction()* and *EndOfEventAction()* methods that are executed at the beginning and end of the events. They are used to clear arrays that store stepping information and to perform processing on event data and fill event histograms.
- A *SteppingAction()* method that is executed at the end of each step. It gathers all the information concerning the particle in the given track and adds it to a histogram, or accumulates it in a variable.

These classes, in turn, can be inherited by classes that simulate and store detector responses and save any relevant information.

#### E. Materials

GEANT4 defines materials internally in terms of how they interact with ionizing radiation, but MAGE adds information about radioactive contaminants and other properties of interest to MAJORANA and GERDA. MAGE has the ability to read in all relevant information about materials from a PostgreSQL database. This is currently limited to quantities required by GEANT4 such as density, isotopic abundance, etc. Once the MAJORANA or GERDA detectors are constructed, the materials used will be carefully assayed and characterized. All this information will be saved in a database as well. MAGE can then use this information to include the measured activities in the simulation on a component-by-component and time-dependent level, reducing systematic uncertainties in sensitivity calculations.

#### F. Example

MAGE is typically compiled into a single executable. The user selects the particular instance of the components they require during run-times via macros saved as text files. MAGE macros are based on the GEANT4 *messenger* classes. A simple, self-explanatory example of such a macro is given below. The simulation consists of a simple block that is bombarded with a beam of

neutrons. The scattered neutrons are analyzed by the output class and elastic cross-sections are computed. This example is used to verify the neutron cross-sections implemented by GEANT4.

```
% Select geometry component
% and set parameters describing
% its geometry.
/MG/geometry/detector solidBlock
/MG/geometry/solidblock/material Hydrogen
/MG/geometry/solidblock/edgeLength 1.0 cm

% Select output format component.
/MG/eventaction/rootschema HPNeutronTest

% Select generator component.
/MG/generator/select SPS

% Start run
/run/initialize
/run/beamOn 500000
```

#### IV. PHYSICS

The physics list in MAGE has been optimized for the reliable simulation of the most common background sources in  $0\nu\beta\beta$ -decay experiments. It was designed according to the suggestions of the GEANT4 team [17] and optimized for low-background physics applications [7], [18]. The default MAGE physics list is mainly based on the Underground Physics advanced example which is distributed with GEANT4 [17].

By default, MAGE uses the Low-Energy models based on the Livermore data libraries [19], [20] for the description of the electromagnetic interactions of electrons,  $\gamma$ -rays and ions. These models include atomic effects (e.g. fluorescence and Doppler broadening) and can handle interactions of electrons, positrons and photons with energies down to 250 eV.

For specialized applications, electromagnetic interactions of  $\gamma$ -rays, electrons and ions can be simulated in MAGE by the so-called “standard models” provided by GEANT4 [21]. These models are tuned to high-energy physics applications; they are less precise in the low energy region and do not include atomic effects. However, they are faster in terms of computing time.

MAGE uses the standard GEANT4 models for the electromagnetic interactions of muons and of positrons. Furthermore, synchrotron radiation is included in the physics list for electrons and positrons. The electromagnetic physics processes provided by GEANT4 for  $\gamma$ -rays and  $e^\pm$  (both “standard” and “low-energy”) have been systematically validated by the GEANT4 Collaboration [22] and by other groups [23] at the few-percent level. The precision of the electromagnetic models for muons is discussed in [24].

Interactions of  $e^\pm$  and  $\gamma$ -rays with nuclei are simulated on the basis of the equivalent photon approximation. The reaction cross section is determined according to a parameterization from experimental data for all incident energies from the hadron production thresholds upwards. Different energy regimes are considered separately in the parameterization, as described in Ref. [21]. Hadronic final states are generated using a Chiral Invariant Phase Space (CHIPS) decay model [25].

For energies above 3.5 GeV, the final states of photo-nuclear reactions are generated according to a theory-based parton-string model, called the Quark-Gluon String Precompound model (QGSP). The model is composed of several components: the quark-gluon string (QGS) part handles the formation of the initial strings in the initial collision [26]; string fragmentation into hadrons is handled by the quark-gluon string fragmentation model [27], while the pre-compound model [28] takes care of the de-excitation of the residual nucleus.

Hadronic interaction of muons with nuclei are managed by the `G4MuNuclearInteraction` model. Muons produce virtual photons which are in turn converted to pions which interact with the nucleus using a model derived from the GHEISHA code [29]. The physics list also includes the capture process of  $\mu^-$  by nuclei. The hadronic interactions included in the MAGE physics list handle elastic scattering, inelastic scattering, capture (for neutrons,  $\pi^-$  and  $K^-$ ), fission (neutrons only) and decay.

The elastic scattering of all long-lived hadrons is described by the `G4LElastic` model, which is based on the GHEISHA code [29] and includes a parameterization for cross section and final state. Elastic scattering of neutrons from thermal energies to 20 MeV is simulated according to the data-driven `G4NeutronHPElastic` model, which is based on the tabulated cross section and final state data from the ENDF/B-VI database [30], [31].

Different energy regimes have been considered in the MAGE physics list to simulate the inelastic interactions of long-lived hadrons. Each energy regime has its own specialized model. In particular:

- 1) theory-driven quark-gluon string precompound model (QGSP) for pions, kaons and nucleons in the high-energy region, up to 100 TeV.
- 2) Low-energy parametrized (LEP) model for pions and nucleons with energies between 10 and 12 GeV and for kaons below 25 GeV. Such a model is applicable below about 30 GeV and is derived from the GHEISHA package [29]. The cross section and the final state are determined by parametrized functions which are fitted to experi-

mental data.

- 3) Bertini (BERT) cascade model, based on a re-engineering of the INUCL code [32], to describe nucleon and  $\pi$  interactions below energies of 10 GeV. The model includes the Bertini intra-nuclear cascade model with excitons [33], [34], a pre-equilibrium model [35], [36], a nucleus explosion model [37] and an evaporation model [38].
- 4) data-driven high-precision (HP) model for neutrons from thermal energies up to 20 MeV, based on the ENDF/B-VI database.

Such an ensemble of models for hadronic inelastic interactions is shortly labeled as QGSP\_LEP\_BERT\_HP.

Alternative hadronic physics lists, which differ in the models used to describe the inelastic interactions of nucleons, are available in MAGE and can be instantiated by messenger commands. They are:

- QGSP\_LEP\_BIC\_HP, which employs the Binary cascade [21] model (instead of the Bertini cascade model) for inelastic interactions of nucleons below 10 GeV. The model handles the intra-nuclear cascade as well as the remaining fragment, which is treated by precompound and de-excitation models. Cross sections are parametrized using experimental data. This physics list is similar to the one used in Ref. [39] for the simulation of muon-induced neutrons, the only difference being that the list of Ref. [39] does not include the LEP bridge between the high-energy QGSP regime and the low-energy Binary cascade.
- QGSP\_LEP\_HP, where parametrized LEP models are used for nucleons below 10 GeV, instead of intra-nuclear cascade models. Such a list is much faster than the default one from the point of view of the computation time.
- QGSC\_BERT\_HP, which employs the quark-gluon string CHIPS model (QGSC) instead of the quark-gluon string precompound model (QGSP) to simulate high-energy inelastic interaction of nucleons (from 10 GeV to 100 TeV). The QGSC model differs by the QGSP by the fact that the de-excitation of the residual nucleus is handled by a CHIPS model [25], [40], [41], rather than the precompound model. The physics list does not include the LEP parametrized model. The QGSC model is also used to produce the final state following photo-nuclear interactions above 3.5 GeV.

Multiple alternative lists for hadronic physics based on independent models are used in MAGE mainly for testing purposes, namely to cross-check results and

evaluate systematic uncertainties from the simulations. Crucial background sources for many underground experiments are due to high-energy interactions of cosmic-ray muons. Background estimates (e.g. production of secondary neutrons or long-lived unstable nuclei) often rely on the ability of simulation codes to model high-energy hadronic and electromagnetic showers initiated by muon interactions. Fig. 4 shows the neutron production yield by muons in Germanium vs. the muon energy for the four hadronic physics lists provided by MAGE (one default and three alternative). The simulations are run with GEANT4 9.0. Simulation results are very similar (within 15%) in the full energy range, indicating that details in the physics modeling of high-energy hadronic interactions do not have a large impact on some parameters of interest for underground physics experiments. Neutron yield in Ge obtained with MAGE (about  $1.5 \cdot 10^{-3}$  neutrons per muon per  $\text{g}/\text{cm}^2$  at 280 GeV) is consistent ( $< 10\%$ ) with the results based on the FLUKA-1999 code [42], derived by the power law parameterization of Fig. 5 of Ref. [43].

The GERDA experiment uses a water Cherenkov muon veto and internal shield consisting of liquid Ar. For this reason, MAGE takes advantage of GEANT4 ability to simulate optical photons. While the default MAGE physics list does not include interactions of optical photons these processes can be enabled during runtime. The underlying models encompass scintillation light emission (possibly with different light yields for electrons,  $\alpha$ -particles and nuclei), Cherenkov light emission, absorption, boundary processes, Rayleigh scattering and wavelength shifting. If optical photon treatment is enabled, it is necessary to specify all relevant optical properties of interfaces and bulk materials (refraction index, absorption length, etc.) in the geometry definition.

GEANT4 tracks all simulated particles down to zero range, although various options exist to manually limit step size, track length, time-of-flight, and other parameters. Production cuts for  $\delta$ -rays and for soft bremsstrahlung photons are expressed in spatial ranges and are internally converted into energy thresholds for the production of soft photons and  $\delta$ -rays in the corresponding material. It is necessary to find a trade-off between accuracy and computing time in most applications. Therefore MAGE provides three production cut realms: DarkMatter, DoubleBeta and CosmicRays. The DarkMatter realm is used for high-precision simulations, especially related to background studies for

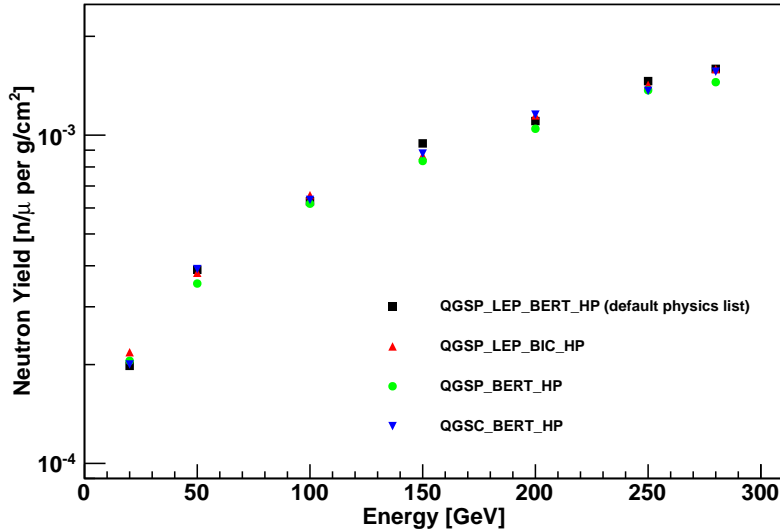


Fig. 4. Neutron yield from muon-induced showers in metallic germanium. MAGE had been run with the version 9.0 of GEANT4.

dark matter applications and surface effects: the cuts for  $\gamma$ -rays and  $e^\pm$  are  $5 \mu\text{m}$  and  $0.5 \mu\text{m}$ , respectively, corresponding to a  $\sim 1 \text{ keV}$  energy threshold in metallic germanium. The DoubleBeta realm (MAGE default) is suitable for signal and background studies related to double-beta decay, i.e. in the MeV energy-region: the range cut for  $\delta$ -ray production is relaxed to  $0.1 \text{ mm}$ , corresponding to a  $100 \text{ keV}$  threshold in metallic germanium. The CosmicRays realm is used for the simulation of extensive electromagnetic showers induced by cosmic-ray muons. The cut-per-region approach is used in this setup. Sensitive regions are defined for which the production cuts are the same as for the DoubleBeta realm. They are more relaxed everywhere else ( $5 \text{ cm}$  for  $\gamma$ -rays and  $1 \text{ cm}$  for  $e^\pm$ ). By avoiding the precise tracking of particles in the inactive detector components, computing time is saved.

MAGE includes some provisions to improve agreement between simulation and experimental results. For instance, simulations do not account for inefficient conversion of germanium nuclei recoil energy to ionization energy, also known as quenching. MAGE contains output classes that simulate this conversion inefficiency using the parameterizations from [56].

GEANT4 performs simulations on an event-by-event basis, where each event begins with the release of a particle from a generator, and ends when the interac-

tions of the primary particle and its secondaries have finished. When long-lived radioactive decays occur, a single GEANT4 event may span many simulated years. Output classes in MAGE divide GEANT4 events into intervals that span user-selectable times. The total energy deposited during specific time intervals can be reported. This information can be used to simulate the effectiveness of timing cuts at removing backgrounds. It can also improve agreement between results of MAGE simulations and experimental data. Simulated energy deposits occurring long after the duration of an experiment can be excluded. Simulated energy deposits in close succession can be summed to approximate the pile-up due to the finite time resolution of data acquisition hardware used in an experiment.

## V. VALIDATION OF THE SIMULATION

The GEANT4 simulation toolkit is used in various applications of modern physics. These range from simulations in high-energy particle physics to astrophysics and medical science. In parallel to the development of new simulation modules the verification of the simulation code is an important task for developers and users. Several modules have been developed to describe the interactions of low energy photons, electrons and hadrons with matter. These are of particular importance for applications such as MAGE and are tested within the two collaborations developing the software. In the following, the current status of



MAGE validation efforts is summarized.

The description of electromagnetic interactions in the energy region up to several MeV was tested with high-purity germanium detector systems. A reverse electrode coaxial germanium detector was operated directly submerged in liquid nitrogen in the so-called cryoliquid-submersion test stand [44]. The crystal was exposed to the radioactive sources  $^{60}\text{Co}$ ,  $^{228}\text{Th}$  and  $^{152}\text{Eu}$ . The comparison between a simple MAGE simulation and recorded data is shown in Fig.5. The biggest deviation was found to be approximately 12%. Most probably the decrease of  $Data/(MC+Bkg)$  with increasing energy is due to the fact that the inactive material between source and detector, e.g. dewar walls, is not precisely known.

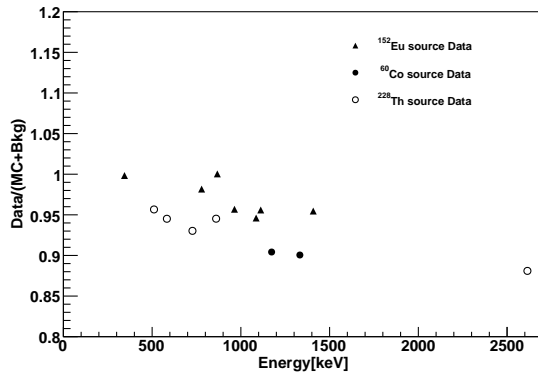


Fig. 5. Difference between number of events in characteristic photon peaks from  $^{60}\text{Co}$ ,  $^{152}\text{Eu}$  and  $^{228}\text{Th}$  sources plus background and a simple MAGE simulation. The maximal deviation was found to be approx. 12%.

The most extensive verification effort was performed with an 18-fold segmented GERDA prototype detector. The segmented germanium crystal was operated in vacuum and exposed to several radioactive sources ( $^{60}\text{Co}$ ,  $^{228}\text{Th}$ ,  $^{152}\text{Eu}$ ) [45], [46]. A large fraction of the emitted  $\gamma$ -rays deposit energy in more than one segment. This feature allows these events to be distinguished from those which deposit energy in relatively small volumes, such as  $0\nu\beta\beta$  decays. Such segmentation-based discrimination between single- and multiple-site interactions was compared between experiment and simulation, with deviations found on the 5% level.

MAGE has been used to simulate the response of a variety of low-background assay detectors in use by the MAJORANA collaboration. In general the

simulation agreed with the data to a few percent and the largest discrepancies were ascribed to uncertainties in the geometry models that have been coded in the simulation. The detailed shape of the Compton continuum for a HPGe detector exposed to variety of sources was also studied in [47]. The simulation and data compared favorably in this study.

The description of neutron interactions with Ge is probed by comparing data from a measurement of an AmBe source with predictions from MAGE. The measurements have been performed with a CLOVER detector and with the 18-fold segmented detector cited previously [48]. At an energy of several MeV, neutrons mostly interact through elastic and inelastic scattering as well as neutron absorption. The measured energy spectra were studied and photon lines from neutron interactions with the germanium detector itself and the surrounding materials were identified [49]. A few discrepancies in the GEANT4 simulation were identified:

- the 2223.0-keV peak from  $\text{H}(n,\gamma)\text{D}$  appears at 2224.6 keV in GEANT4 simulations (bug report # 955) [50];
- meta-stable nuclear states are not produced by GEANT4 as a result of neutron interactions (bug report # 956) [50];
- neutrons do not produce internal conversion electrons in GEANT4 (bug report # 957) [50].

The first and third bugs are related to issues in the G4NDL nuclear data files distributed with GEANT4, and can be solved by editing or augmenting the data library. The third bug also involved several coding errors, corrections for which were provided by the MAGE group. Fixing the second bug requires functionality that the GEANT4 Collaboration does not plan to implement at this time. Nevertheless, a viable solution has been developed by the MAGE group. The work-around for the meta-stable problem consists in identifying at run-time those neutron interactions that might produce a meta-stable nucleus. In this case, the new nucleus track is discarded, since GEANT4 would always generate it in the ground state, but its position and the parent neutron energy are logged in a file. Later on, a new simulation job is launched which uses the position information from the previous one and where the ratio between ground and meta-stable nuclear states is set manually to the proper value.

MAGE was also used to study and verify the simulation of spallation neutron production and propagation. At the CERN NA55 experiment the

neutron production from a 190 GeV muon beam incident on different targets was measured. At the SLAC electron beam dump experiment the neutron propagation through different thicknesses of concrete was measured. Both experiments were simulated within the MAGE framework. The attenuation of the neutron propagation was found to be larger in the simulation than measured in the SLAC experiment [51]. A method to correct the neutron over-attenuation in MAGE-based simulations was implemented in MAGE and is described in [51].

It was also found that MAGE/GEANT4 underestimates the neutron production from muon interactions measured by NA55, especially in high-Z materials, by more than a factor of two [51]. Results obtained in the MAGE simulation of NA55 have been compared with the GEANT4- and FLUKA-based [42] Monte Carlo simulations of the same experiment performed in [43], and found to be consistent. The disagreement between Monte Carlo simulation codes and NA55 data for muon-induced neutron production is discussed in detail in [43] and [52]. The muon-induced neutron yield in lead has been recently re-measured at the Boulby underground laboratory [53]. In this case, in which the neutron energies are much lower, the GEANT4-based simulation is found to over-estimate the experimental neutron yield, which is the opposite behavior with respect to the NA55 data. MAGE results for muon-induced neutron production by muons in liquid scintillator have been compared to the set of experimental data reported in Ref. [43]. Fig. 6 displays the neutron production yield by muons derived by the MAGE simulations (using the alternative hadronic physics lists described in Sect. IV) vs. energy, superimposed with the experimental data [54] reported in [43] and the recent data from the KamLAND experiment [55]. The agreement between MAGE simulations and experimental data is typically better than a factor of two. Results are consistent with those obtained in the recent work Ref. [39].

## VI. CONCLUSIONS

We presented the MAGE framework for simulating interactions in neutrinoless double-beta decay experiments that utilize enriched HPGe detectors. The benefits of MAGE can be summarized as:

- Reliable Monte Carlo framework based on GEANT4 for low-background, low-energy experiments.
- Ongoing tests of the code and validation of the physics processes.

- Flexible geometry and physics code framework that emphasizes code reuse and verification.
- General purpose tools like surface and volume sampling, custom isotope decay generators, etc.

In general there is good agreement between the GEANT4 simulation with the MaGe physics list and the measurements of electromagnetic interactions with average discrepancies of the order of (5-10)%. Several problems have been identified in the simulation of neutron interactions. These problems have been reported to the GEANT4 collaboration and are under investigation by the MAGE developers.

We anticipate that MAGE will form the foundation of the simulation and analysis framework of the GERDA and MAJORANA experiments. This type of framework and its associated event generators and physics lists is also useful for other low-background underground experiments, such as solar, reactor and geological neutrino experiments, direct dark matter searches, and other neutrinoless double-beta decay search. These experiments share many detection techniques and background issues in common with GERDA and MAJORANA.

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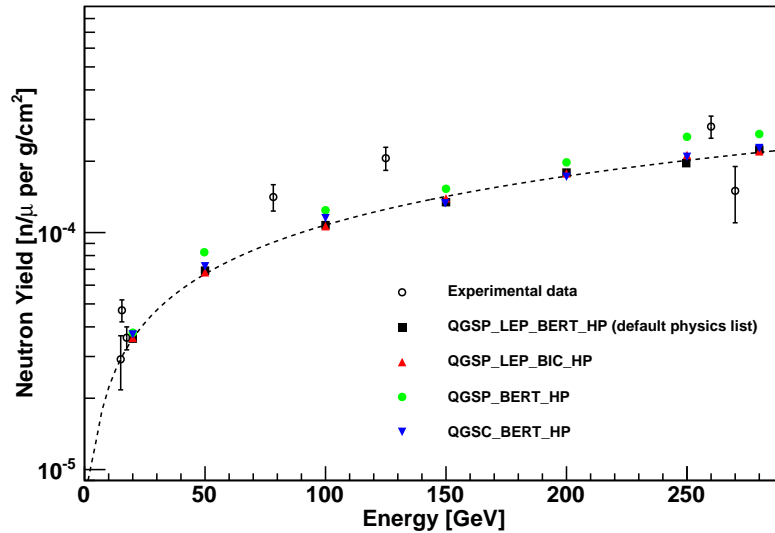


Fig. 6. Neutron yield from muon-induced showers in liquid scintillator ( $C_{10}H_{22}$ ). Experimental data are from the Refs. [54] (reported in [43]) and from Ref. [55]. Monte Carlo results (default physics list) are well parametrized by a scaling law  $E^{0.685}$  (dashed curve). GEANT4 9.0 had been used for this study.

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