

## GEANT4 Simulation of the GTAF

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### Abstract

To meet the demands for neutron capture reaction cross-section measurements in the keV energy regime for nuclear astrophysics and advanced nuclear energy system development, the  $4\pi$  BaF2 Gamma-ray Total Absorption Facility (GTAf), developed by the Key Laboratory of Nuclear Data at the China Institute of Atomic Energy (CIAE), was relocated and installed at the Backstreaming White Neutron Source (Back-n) of the China Spallation Neutron Source (CSNS) in 2019. Since then, a series of results have been achieved and published based on the GTAf, which has rendered the need for background reduction increasingly urgent. To understand the origins of backgrounds and to optimize the facility, a detailed simulation program based on the GEANT4 toolkit was established and is presented in this paper. To demonstrate the validity of the developed code, several practical examples that assist in experimental data processing and verify optimization proposals are also presented in this paper.

### Full Text

### Preamble

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To meet the demands of neutron capture reaction cross-section measurements in the keV energy range for nuclear astrophysics and advanced nuclear energy system development, the  $4\pi$  BaF<sub>2</sub> Gamma-ray Total Absorption Facility (GTAF) developed by the Key Laboratory of Nuclear Data at the China Institute of Atomic Energy (CIAE) was relocated and installed at the Back-streaming White Neutron Source (Back-n) of the China Spallation Neutron Source (CSNS) in 2019. Since then, a series of results have been achieved and published, making background reduction increasingly urgent. To understand the origins of backgrounds and optimize the facility, a detailed simulation program using GEANT4 toolkits was established and is presented in this paper. To demonstrate the utility of the validated codes, several practical examples illustrating their role in assisting experimental data processing and verifying optimization proposals are also shown.

**Keywords:** Gamma-ray Total Absorption Facility, White Neutron Source, Neutron Capture Cross Section, Monte Carlo simulation, GEANT4, Geometry optimization.

## Introduction

The  $4\pi$  BaF<sub>2</sub> Gamma-ray Total Absorption Facility (GTAF), shown in Fig. 1 [Figure 1: see original paper], is designed for neutron capture cross-section measurements under keV-scale neutron beams for applications in nuclear astrophysics and advanced reactor design, leveraging its large angular coverage and high detection efficiency [1-7]. It was installed at Back-n of CSNS in 2019 [7, 8].

To support experimental data analysis, a set of detailed and reliable Monte Carlo simulation codes was developed using GEANT4 toolkits [9], as described in Sections II and III. Validation against standard library and experimental data is presented in Sections IV and V, and based on this validation, several practical examples are provided in Section VI. These examples demonstrate the codes' capabilities in assisting experimental data processing and verifying geometric optimization variants to address background problems.

## II. Basis of Facility

### A. Time-of-Flight Method

The Time-of-Flight (ToF) method is a widely used technique for particle measurement [10, 11]. It relies on the principle that the time required for a neutron to travel a known distance is inversely proportional to its energy, which can be calculated theoretically using Equation (1) [10, 11]:

$$t = 72.3 \times \frac{L}{\sqrt{E_n}}$$

where  $t$  is the flight time,  $L$  is the flight distance, and  $E_n$  is the primary neutron energy. Neutron flight time measurement is designed with high accuracy [12] using specialized timing hardware and software systems [13], as it is crucial for determining neutron energy and reconstructing spectra at the GTAF [14-16].

## B. Multiplicities of $(n,\gamma)$ Reactions

Multiplicity is defined as the number of detector volumes that particles traverse through inelastic reactions before being fully absorbed or escaping the sensitive crystal array, as illustrated in Fig. 2 [Figure 2: see original paper]. It provides key benchmark information about reaction channels and underlying physical processes [17, 18], such as elastic scattering, inelastic scattering, and radiative capture, since each event exhibits a distinctive multiplicity signature. Ideally, all data can be restored as shown in Equation (2).

## C. Pilled-up Energy of Event Cascades

The de-excitation principle of isotopes in GTAF is shown in Fig. 3 [Figure 3: see original paper]. In GTAF, identifying neutron capture reactions is of paramount importance as they represent key data of interest [2, 19]. A practical method to distinguish neutron capture reactions is to examine the piled-up released gamma-ray energy  $E_{ex}$ , which remains constant regardless of the number of reaction channels experienced, provided that  $E_{ex} = E_n + Q$ , where  $E_n$  is the neutron energy and  $Q$  is the reaction Q-value.

# III. Monte Carlo Simulation

## A. General Idea

As discussed in Section I, a reliable Monte Carlo simulation is needed to facilitate facility improvements and assist in experimental data analysis. The reliability of Monte Carlo simulations depends on detailed reconstruction of various components: (1) detailed geometry reconstruction; (2) accurate physics configurations; (3) reasonable calibration and neutron beam sources; (4) capable event reconstruction algorithms; and (5) logical data restoration design. The GEANT4 simulation toolkit [9] was selected due to its widespread use and verification in nuclear and high-energy physics, offering extensive physics configurations and flexible geometric reconstruction methods. The GEANT4 kernel version used in this simulation is 11.1.2. The general workflow is shown in Fig. 4 [Figure 4: see original paper].

## B. Geometry Reconstruction

To accommodate different geometry simulation needs under specific experimental conditions, Boolean variables are provided to users as switches for geometry construction, as listed in Table 1. The geometry is reconstructed with the most reasonable detail possible. Apart from mechanical fabrication errors, geometric parameters and related materials are set to match those measured directly from the actual arrangement at Back-n of CSNS [20]. In addition to using Constructed Solid Geometry (CSG) methods or CSG-like methods embedded in GEANT4, facility subassemblies are also reconstructed using the CADMesh method [21] as a backup and agile development option.

CADMesh is a valuable tool for reconstructing detector geometries in GEANT4 simulations, allowing complex geometries created in Computer-Aided Design (CAD) software to be imported directly into GEANT4 simulation programs with support for various common ASCII format files. While both CSG and CADMesh methods are based on computer graphics geometric logic, commercial CAD software provides more preset basic graphics and logical operations, enabling CADMesh to rapidly build highly accurate geometric volumes. This ensures that simulations of detector physical characteristics meet the critical needs for particle tracking results. The CADMesh method is particularly advantageous for handling complex 3D shapes and curved surfaces when simulating detectors like the GTAF series, which contain numerous intricate or irregular geometric elements.

Based on the topological definition of different fields in ASCII format CAD files created by FreeCAD [22]—such as vertex positions, normals, mappings, etc., as shown in Table 2—an interface program reads and translates parameters to enable the GEANT4 core program to complete the corresponding geometric construction. Materials are subsequently defined in the same manner as the CSG method in GEANT4. The two methods can be switched via a Boolean variable as shown in Table 1. For certain elements where local geometric effects need not be considered in detail, related parameters are calculated and set using an equal-volume factor. For instance, a bellows type BP300 can be considered as a tube with a volume equivalent coefficient of 1.2, while quick-release flanges type KF100 have a coefficient of 1.47. The geometric simulation and typical subassemblies are shown in Fig. 5 [Figure 5: see original paper].

## C. Physics Models

Constructing a reasonable physical model is crucial for detector simulation. For both calibration mode and neutron beam mode simulations, interest focuses on the low-energy response. The QGSP\_{{BIC}}\_{{HP}} preset physics package [23] is used as the basic physics model, containing a series of physics references including low-energy reactions, decay, elastic scattering, and inelastic processes that meet preliminary simulation needs, with results shown in Section V. The “HP” type physical process package is used because “HP” refers

to High Precision physics models [23] in GEANT4, which provide more accurate and detailed simulations of particle interactions across a broader energy range, enabling more comprehensive simulations of various physics processes. The preliminary applied physics processes and models are listed in Table 3 and will continue to be refined in subsequent work according to different simulation needs.

#### D. Primary Sources

Two types of sources are reconstructed using specific macro files containing matrices of spectral and spatial parameters with related normalized weighting coefficients: (1) calibration sources recommended by the standard Evaluated Nuclear Data File (ENDF) library [24, 25]:  $^{60}\text{Co}$ ,  $^{137}\text{Cs}$ , and  $^{22}\text{Na}$ ; and (2) neutron beams including (a) neutron beams from Back-n and (b) 4.9 eV mono-energetic neutron beams.

**1. Calibration Sources** Three calibration sources recommended by the ENDF library— $^{60}\text{Co}$ ,  $^{137}\text{Cs}$ , and  $^{22}\text{Na}$ —are reconstructed in the simulation with the same geometric parameters used in real experiments [26]. The dimensions are set as  $32\text{\$}\times 4\text{mm}$ ,  $\phi 32\times 4\text{mm}$ , and  $25\times 25\text{ mm}$ , respectively.

**2. Neutron Sources** Two neutron beam sources are simulated: mono-energetic and spectral neutron beams. Due to hardware time-resolution limits in real experiments, Time-of-Flight (ToF) spectra of beams with initial energies above 1 MeV cannot be well resolved. Therefore, an upper energy limit of 1 MeV has been set for both options in the first simulation stage [26]. The neutron energy spectrum matrix and initial momentum spectrum are written in a macro file.

- **Mono-energetic neutron beams** are simulated with parameters of 4.9 eV mono-energy and a spatial beam spot obtained from CMOS experiment data at Back-n of CSNS. This is used to obtain a clear image of the largest resonant cross-section of the standard  $^{197}\text{Au}$  sample, which helps verify code reliability and calculate theoretical efficiency or other required information.
- **Spectral neutron beams** are simulated with the same spectral [27, 28] and spatial [29, 30] characteristics as those from Back-n. They are used for background analysis and theoretical neutron capture cross-section calculations of samples. The simulated beam spot is shown in Fig. 6 [Figure 6: see original paper].

**3. Pseudo-random Number Generator** The statistical properties of the Pseudo-Random Number Generator (PRNG) significantly impact Monte Carlo simulation reliability. Several popular PRNG candidates exist for nuclear physics, including James Random, Mersenne Twister, and Ranlux64. The

MTWistEngine pseudo-random number generator [31] is selected for two main reasons: (1) it can generate a sufficiently large pool of valid pseudo-random numbers ( $2^{19937} - 1$ ) in a single operation, supporting the need for approximately  $2 \times 10^9$  events per run in GEANT4 and fulfilling potential needs for further studies using accumulated simulation data; and (2) it has high reliability, having passed almost all rigorous random number tests referenced in [32-34].

To obtain system time via an I/O data channel as initial seeds for the pseudo-random generator, a time seed interface program is designed, programmed, and linked to the EventAction class of the simulation program.

### E. Simulation Run and Action Classes

In both Calibration mode and Neutron Beam mode, the simulation begins by emitting primary particles through the General Particle Sources (GPS) function embedded in GEANT4, calling detailed parameters of initial particles from the macro file (including initial energy, momentum, and position) and the specific operation mode defined in the RunMessenger interface. After emission, particle behavior depends on the physical models and process definitions from Section III.C while traveling through various spatial volumes in the geometry described in Section III.B, with information cutoff or truncation according to demands in various action classes.

According to the design logic of built-in GEANT4 action classes, each Run consists of the number of Events defined in the macro file. In each Event, according to particle step length and physical process settings, the corresponding Step is included, and required information can be filtered through Stack and Track action classes. At the end of each Run (after the last Event), corresponding data and information are saved and output according to the preset format in RunMessenger.

## IV. Primary Data Analysis Program

To meet basic pre-processing requirements for simulation data, a general data processing program with a Qt-based GUI interface was designed and tested.

### A. GUI Interface

To facilitate implementation of commonly used data pre-processing functions, a visual human-machine GUI interface was designed using Qt version 5.9.7, as shown in Fig. 7 [Figure 7: see original paper]. With PythonQt and PyRoot, commonly used functions are implemented by transporting data flow through various interfaces, including import and export of files in various basic formats, switching between neutron beam mode and calibration mode, and display and fitting functions for energy spectra and ToF spectra. The visualization program

uses Qt controls to implement the data interface required to call these functions, enabling basic data pre-processing.

## B. Reconstruction Algorithm of Event Cascades

Simulations can be performed per event or per run as required. Consistent with experimental data processing, two general and basic event reconstruction algorithm subprograms are designed in the data processing program: energy reconstruction and position reconstruction. Reconstruction is relatively simpler in simulation since target data can be retrieved directly from GEANT4 built-in functions. Particles are transported and tracked via Action Class functions in the GEANT4 framework until absorbed in certain volumes or escaping preset cutoff areas. Essential values such as deposition energy, time-of-flight, multiplicities, geometric volumes, materials, reaction channels, and other relevant information can be extracted and recorded after each step or event. Meanwhile, data for each reaction channel can be distinguished by calling the physics model or physics process of each track.

For situations requiring further energy deposition processing, a TrackingAction class retaining interface functions is designed to filter specific required deposition energy according to user simulation needs. According to user requirements, data can be transferred to the Analyzer after preliminary processing in the TrackingAction class, where more preprogrammed reorganization tools are set as described in Section IV.C.

Original simulation data output from the above dataflow are saved by separate detector crystals. The reconstructed energy spectrum can be output directly in divided crystal form, or according to user needs, a deposited energy spectrum reconstruction output in total detector units can be achieved by summing total deposition data of each crystal in the same Event. These functions can be implemented in RunMessenger by adjusting Boolean variables or through GUI tabs. Thus, after each Run, the energy spectrum of particles can be reconstructed.

**1. Energy Reconstruction** Deposited energy can be traced in each particle transportation step using GEANT4's built-in algorithms. One privilege of processing simulation data compared to experimental data is that piled-up energy peaks and event cascade reconstructions are much easier to perform. Particles are transported via action class functions in each Step until absorbed in certain volumes or escaping preset cutoff areas. During simulation, each particle is labeled by generation, and associated particle information is transferred via a user-set personalized function to the TrackingAction class for further processing. Since simulation results of interest are those with responses in the detector array, geometric volume information is crucial; therefore, volume numbers (CopyID) are recorded simultaneously.

For situations not requiring further energy deposition processing, extracted data can be transferred directly from the SteppingAction class to the EventAction

class for accumulation and storage, then passed to the Analyzer for saving in a specific format according to the dataflow shown in Fig. 4 [Figure 4: see original paper].

**2. Time-of-Flight Spectrum Simulation** To verify results with experimental data, particle flight time is recorded in the simulation. The start time point  $T_0$  is preset in the EventAction class at the beginning of each Event when primary particles are emitted. When triggered in each Step (under SteppingAction mode) or in each Sensitive Detector zone (under SensitiveDetector mode), the corresponding time is recorded and saved in a tuple or histogram predeclared in the RunAction class. The recorded time is Global Time in the entire Event since  $T_0$  marks each Event' s beginning. At each Event' s end, corresponding time data are recorded in different tuples or trees in ROOT files through pre-selection conditions in Step, Track, Stack, or Event action classes. Therefore, a ToF Spectrum can be generated at the end of the whole Run.

Additionally, similar to experimental data processing, the corresponding simulated energy spectrum (E-ToF) can be calculated using particle flight length and simulated ToF spectrum through Equation (1). Flight length is obtained by adding the flight distance in each Step, calculated in the geometric simulation program and transferred to analysis functions via two switchable methods: (1) extracting geometric length of corresponding passing elements in the Detector Construction source file, with parameters transferred to the Analyzer source file; or (2) calculating directly in the Step action class through GEANT4' s built-in variable function, then passing step length to the Event action class function to store and generate the E-ToF spectrum directly.

**3. Position Reconstruction** Similar to ToF spectrum reconstruction, position information (3D vector tuple) of each step can be traced and recorded while deposited energy (difference between pre-step and post-step energy) in dedicated geometric volumes is non-zero in the SteppingAction class.

## C. Reorganization Tools

**1. Multiplicities** During experimental installation setup, as discussed in Section II.B, proper design should consider electronic circuitry based on NOT gate circuits of nuclear electronics technology with well-preset key parameters including energy and timing thresholds to identify particle interactions [14]. In the simulation program, a similar but more precise and practical method is applied. Technically, multiplicities of each Event are counted by the number of different CopyIDs of geometric volumes where deposited energy is non-zero before particles are fully absorbed or escape sensible arrays, since each geometric volume reconstructed in the simulation codes has a unique CopyID.

**2. Reaction Channels** Distinguishing data from different reaction channels is the core algorithm in experimental data processing, realized through different

gates to help understand experimental data and phenomena. In simulation, the physical process occurring at each step can be traced before or after each step. To avoid null pointer errors in the C++ coding environment, apart from usual protection by a judgment function, the post-step physics model filter is used. A string value preset in GEANT4 or user-set to the dedicated physics model or process is returned due to Boolean switch values chosen in the RunManager. After transfer to Stack and Track classes, string values of relevant physics processes or models are passed to the Analyzer and stored in corresponding tuples or other formats in ROOT files. After simulation completion, physics process or model values can be called in the Primary Data Analysis Program, and ToF or energy spectra for different reaction channels can be classified and plotted.

## D. Spectrum Broadening and Semi-automatic Peak Finding

**1. Broadening of the Energy Spectrum** Since GEANT4 cannot simulate nuclear electronic effects in preset physical processes, the electronic response ratio is obviously 100%. Thus, simulated data need broadening before supporting experimental data analysis. In the preliminary analysis program, Gaussian functions are used as the broadening algorithm. The specific process is as follows: (1) determine the total normalized bin number and corresponding coordinate values of the spectrum; (2) determine an energy resolution set according to experiment or user specification; (3) determine Gaussian broadening constants by ensuring the integral of Gaussian broadening with the above parameters matches the original count value.

**2. Semi-automatic Fitting and Peak Finding** Spectrum fitting and peak finding are generally performed in ranges of interest during data processing. Semi-automatic spectrum fitting and peak finding can be implemented in the primary data analysis program. The algorithm is similar to energy spectrum broadening, achieved by fitting with Gaussian functions using basic initial parameters including approximate peak position regions and fitting adjustment parameters that can be modified directly in the GUI interface mentioned in Section IV.A. Peak positions and final fitting iteration coefficients are displayed in the GUI interface or printed in the Terminal for storage and subsequent data analysis.

## V. Validation of Reliability

### A. Responses to Calibration Source

Three simulated calibration sources mentioned in Section III.D are designed to validate geometric simulation reliability and reconstruction algorithms. Results are shown in Fig. 8 [Figure 8: see original paper], where piled-up deposition energy peaks are in good agreement with ENDF library data, demonstrating geometry and physics configuration reliability. Preliminary processing of multiplicities and reunited BaF<sub>2</sub> crystal event reconstruction is performed on simula-

tion data. Taking  $^{60}\text{Co}$  source calibration as an example, two gamma rays with energies of 1.17 MeV and 1.33 MeV emit spontaneously. The piled-up energy of 2.5 MeV serves as a benchmark to evaluate detector array efficiency as discussed in Section III.E, as shown in Fig. 9 [Figure 9: see original paper]. This preliminarily proves that geometric reconstruction of the simulation program is effective and the basic reconstruction algorithm is functional. Experimental data processing of GTAF is ongoing, and control results from experiments will be published subsequently.

## B. Response to Neutron Capture Reactions

Considering that isotope  $^{197}\text{Au}$  has a very large resonant neutron capture cross-section at 4.9 eV—several orders of magnitude larger than other cross-sections such as elastic scattering—monoenergetic neutron beams are commonly used to verify simulation physics configurations. To this end, a 4.9 eV monoenergetic neutron beam with the same geometric spatial distribution as Back-n neutrons starts from the vacuum tube 72.7 m upstream of the sample tray, and a standard thin cylindrical  $^{197}\text{Au}$  sample with the same geometric dimensions as the experiment (0.2 mm thickness and 40 mm diameter) is simulated. A lower energy threshold of  $10^{-2}$  eV is preset for each simulated crystal unit to facilitate preliminary data processing. Particle response information on  $\text{BaF}_2$  crystals is recorded as described in Section IV.B, and energy and ToF spectra are output through event reconstruction. As shown in Fig. 10 [Figure 10: see original paper], a deposited energy peak around 6.51 MeV and a typical time peak of  $2.478 \times 10^6$  ns are clearly visible in the Energy Spectrum and ToF Spectrum respectively, consistent with standard values and demonstrating simulation code validation.

## VI. Practical Examples

### A. Assistant Processing and Understanding Experimental Impact

**1. Impact of Different Neutron Beam Energy** To accelerate simulation and considering characteristics of electronic devices in real experiments, the Back-n neutron beam energy segment below 1 MeV is often used as the input neutron beam source. However, neutron beams in different energy bands may have different effects on backgrounds [35]. To confirm high-energy band influence on the effect of interest, four different initial input neutron beam sources are simulated, with effect-background ratio results shown in Table 4. Although the high-energy segment has some influence on spectral structure, it has little effect on key data such as the background-effect ratio. Therefore, when using simulation calculations for rough analysis, a simplified neutron source term filtered under 1 MeV can be used to improve computational efficiency.

**2. Discrimination of Different Reaction Channels** Discriminating different reaction channels is a major advantage of using simulation codes since

they provide an ideal panorama of all reactions occurring. A demonstration is shown in Fig. 11 [Figure 11: see original paper]. By implementing these functions, theoretical neutron capture reaction detection efficiency can be calculated. This serves as an important analysis tool to help better understand experimental data phenomena and optimize structure by reducing background impact.

## B. Assistant in Evaluation of Preliminary Geometric Optimization

**1. Theoretical Analysis of Background** To support upcoming facility upgrades, theoretical backgrounds can be analyzed using simulation codes while comparing with experimental results [36]. With all experimental facilities in Hall 2 simulated, since part of the background could be produced by scattering neutron interactions with surroundings [37], a series of abnormal resonant peaks appear in the ToF spectrum ranging from  $8 \times 10^5$  ns to  $1.1 \times 10^6$  ns according to Fig. 11 [Figure 11: see original paper]. Preceding geometric volumes and related materials of abnormal data are traced by simulation codes, as shown in Fig. 12 [Figure 12: see original paper]. Since most background precursor origins are concrete-made volumes (walls, ceilings, or floors), a preliminary geometric optimization proposition can be made: one possible approach to reduce abnormal background impact is to isolate sub-particles caused by scattering from walls, ceilings, or floors, especially those affecting responses in the central area where the crystal array is located.

**2. Evaluation of Geometric Optimization Proposition** One possible structural optimization option is adding a vacuum tube in the central area (the area through the center of the detector array) with a ball-shaped neutron absorber outside the sample tray/support, as shown in Fig. 13 [Figure 13: see original paper]. Simulation results for different preliminary geometric propositions are summarized in Table 5, showing that adding the central vacuum pipe and absorber outside the sample tray can significantly help reduce anomalous background influence. Obviously, the final geometric optimization plan will be decided after considering more details, including effects of in-beam  $\gamma$  rays at Back-n sources [38]. Several validation experiments are prepared, after which all simulated and experimental data will be verified and analyzed in the near future.

## VII. Summary

A Monte Carlo simulation program for GTAF based on GEANT4 toolkits has been established and verified in this paper. The geometry of the entire facility is reconstructed in great detail according to as-built drawings and actual layout conditions on site. Together with reasonable physics configurations and event reconstruction algorithms, the codes have been tested and validated by comparing simulated data with experimental data from three calibration sources

and two neutron beam sources. All comparison results show positive agreement, demonstrating code reliability.

Two typical application examples are presented to show common scenarios where these codes can be applied. More work will be done to enhance code performance, and more applicable scenarios will be developed to assist data analysis and other needs using the validated simulation codes.

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