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ADVANCING NEUTRON SAFETY AND DOSIMETRY IN NUCLEAR FACILITIES: APPLICATIONS AND CURRENT STATUS OF THE DEVELOPMENT OF NEREIDA

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ABSTRACT

The development of nuclear facilities necessitates reliable tools for design, licensing, and safety assessments. NEREIDA (the Spanish acronym for fast neutrons for the exploitation of facilities with atomic devices) is being developed for providing a robust solution. Utilizing Geant4-based Monte Carlo methods, NEREIDA characterizes neutron flux spectra and calculates dosimetric quantities such as environmental and personal dose equivalents in any neutron-production facility. This innovative tool integrates state-of-the-art codes for neutron transport, interaction, moderation, and material activation. Our preliminary results, obtained after the first year of a three-year development period, demonstrate computational scalability across various high-performance computing clusters and clouds. NEREIDA will generate the Geant4 facility's models from CAD files, structural materials, and neutron source characteristics without requiring programming expertise. Additionally, NEREIDA models the impact of the cosmic ray background and includes anthropomorphic phantoms for comprehensive safety assessments. This work discusses NEREIDA's current status and future directions, emphasizing its critical role in enhancing nuclear facility safety.

1 INTRODUCTION

For the licensing of complex fast-neutron generating facilities, such as the upcoming IFMIF-DONES or the CLPU (*Centro de Láseres PUlsados*) in Spain, it is essential to rely on tools capable of characterizing both the architectural features and the evolution of neutron phenomena within such facilities. Codes such as MCNP (Monte Carlo N-Particle transport code) (Werner et al. 2018), PHITS (Sato et al. 2013), and Geant4 (Agostinelli et al. 2003) play a vital role in neutron transport and interaction Monte Carlo calculations. Geant4, in particular, not only offers an open license, but also stands out for its versatility in simulating neutron interactions in complex geometries (Thulliez et al. 2022).

Currently, Geant4 simulations occupy a central role in the development of various applications related to the calculation of fast neutron transport and interaction. It has been utilized in studies of beams produced in spallation sources, in the characterization of Bonner sphere-based detectors (Hu et al. 2020), in the development of new detection techniques (Tripathi et al. 2018; Sidelnik et al. 2020), and even in studies of concrete activation including an exhaustive performance comparison between PHITS, MCNP, and Geant4 (Tesse et al. 2018). While MCNP faces certain usage restrictions globally, Geant4 benefits from its open-source status (Ge et al. 2022). Recent studies further highlight Geant4's advantages in predicting microscopic observables more realistically compared to MCNP6 (Lee and Kang 2023; Ge et al. 2022).

However, it is known that Geant4 can present challenges in implementation for different geometries and materials in a modular and adaptable way. The new tool Meiga facilitates the integration of Geant4 simulations, sophisticated geometry descriptions, advanced 3D visualization tools, and validated physical models. It simplifies the development of any Geant4 application by integrating middle-ware layers between Geant4 libraries and non-specialized users (Taboada et al. 2022). Structurally, Meiga is composed of various C++ classes, each dedicated to a specific functionality. It integrates Geant4 simulations for particle transport and detector response calculations, providing interfaces for users to manage detector descriptions and simulation executions. Moreover, Meiga is compatible with data output from ARTI (Sarmiento-Cano et al. 2022), a computational framework that combines CORSIKA (Heck et al. 1998) with Geant4 for accurate atmospheric radiation flux calculations and the corresponding signals in typical astroparticle detectors installed anywhere around the World. Given the computational demands associated with these tools, our team has developed OnedataSim (Rubio-Montero et al. 2021), to facilitate the execution of such tools at high-performance computing and cloud environments, ensuring portability across computational environments through the use of virtualized containers. It also adapts data and metadata to comply with the FAIR principles (Wilkinson et al. 2016), ensuring data findability, accessibility, interoperability, and reusability (Rubio-Montero et al. 2021).

Our current objective is to integrate these tools for developing NEREIDA (*NEutrones Rápidos para la Explotación de Instalaciones con Dispositivos Atómicos* for fast neutrons for the exploitation of facilities with atomic devices), an autonomous solution based on Geant4 Monte Carlo methods. NEREIDA is designed to produce a digital representation of the facility to be licensed, incorporating its main geometry, construction materials, location, and characteristics of the neutron sources. It also aims to obtain the discretized three-dimensional distribution of the expected neutron spectrum and doses both inside and outside the irradiation rooms. Additionally, the values of the environmental (H^*) and personal (H_p) dose equivalents at the points of interest will be determined. This application incorporates the most up-to-date algorithms and libraries available for neutron transport, interaction, and moderation, as well as for neutron activation of the materials present (Thulliez et al. 2022). It will be able to run in local computing environments and/or in the cloud, and the data produced will adhere to the FAIR principles (Wilkinson et al. 2016).

In summary, NEREIDA is designed to meticulously characterize any relevant nuclear facility, given a CAD file, regardless of the complexity of its geometry and the type of source used. It is particularly useful where understanding the neutron flux and spectrum is important, with an emphasis on dosimetric quantities.

The future validation of NEREIDA will be performed by comparing the results of our simulations with existent and to-be-performed MCNP simulations and measurements at the *Laboratorio de Patrones Neutrónicos* (LPN) at CIEMAT, Madrid, Spain, and in some facilities at *Centro Atómico Bariloche* (CAB), depending of the *Comisión Nacional de Energía Atómica*, Argentina. In this paper, the design and the first preliminary results of NEREIDA after the first year of its 3-year development plan are presented, along with the planned upcoming developments and future perspectives.

2 MATERIAL AND METHODS

2.1 NEREIDA Simulation Development

Geant4 is a widely used and standard code for Monte Carlo simulation of radiation-matter interaction. NEREIDA relies on Geant4 tools and libraries for its core computational engine, using the NEUTRON-HP package for neutrons with energy $E_n < 20\,\text{MeV}$. This includes interaction libraries for low-energy neutrons, such as ENDF/B-VIII.0 and JEFF-3.3, and a transport algorithm implementing the Sampling of the Velocity of the Target nucleus (SVT) method for the epithermal range. For higher energy neutrons and other interactions, the general-purpose physics list library QGSP_BERT_HP was implemented to simulate various physical processes depending on the energy of the incident particles. Additionally, the G4_INCL libraries are used for neutron activation of elements, tracking all possible radioactive interactions with neutrons, including gamma emissions from neutron activation of facility materials. These compounds can be defined using the internal Geant4 database based on NIST standards or as new materials, utilizing their composition and the natural isotopic composition of each element. All particle interaction processes are primarily described by the included physics lists, selected to best represent current validations available in the literature (Thulliez et al. 2022). Besides neutron interaction, other standard model interactions, such as electromagnetic or nuclear interactions, are also computed using the standard physics lists included in Geant4.

The second layer of the application serves as the interface between the physics core and the user and is built as a Meiga application (Taboada et al. 2022). This layer supports the construction of the NEREIDA application and the development of its user interfaces. Meiga's design enables the creation of JSON input files using a controlled vocabulary, eliminating the need for programming knowledge. Additionally, when complete, NEREIDA will include a user web interface deployed in a software-as-a-service model. Users will upload a CAD-compatible file containing the architectural details of the facility. Using the McCAD library (Große et al. 2013), NEREIDA will convert the structural models of the installations into the semi-algebraic models used to define the geometry of installations and detectors in Geant4 Monte Carlo simulation codes (Lu et al. 2017). This library is currently being integrated into the NEREIDA application.

For the calculation of dose distribution within the facility, a voxelization sub-module was developed to generate a three-dimensional cubic mesh of the installation, accurately replicating its geometry. This spatial discretization is adaptable, allowing for mesh refinement and improving dose calculation precision in areas of interest by preventing the inclusion of multiple materials within a single voxel. Our algorithm checks for volumetric consistency and makes the necessary adjustments to meet this constraint. Additional checks are performed to avoid excessive detail in the Geant4 model geometry description, such as, e.g., bolts or knots present in the original CAD files. Sensitive volumes are placed within these voxelized regions to obtain information about various quantities of interest, such as deposited energy or the neutron spectrum within each voxel volume.

NEREIDA incorporates standard neutron sources such as the ^{252}Cf fission source and the ^{241}AmBe standard source. For these cases, the simulation only requires the source type and the measured activity at the calibration date. NEREIDA performs all the calculations needed to determine the source's current activity and the total number of particles to be injected based on the irradiation time defined at the beginning of the simulation. It is also possible to simulate non-standard neutron sources by providing a text file containing the measured spectrum of the source. Basic computational statistical techniques like rejection sampling and the inverse transformation method are used to accurately mimic the emission energy of any generic neutron source. The input data, simulation setup, and outputs, such as spectra or doses, are defined through its own semantic analyzer. For this purpose, text files in JSON are used, providing a lightweight standard for data exchange based on associative arrays of name/value pairs.

2.2 Simulated Radiation Detectors

To validate the simulation accuracy, NEREIDA outputs will be compared with measurements from various neutron detectors installed in the facility. Additionally, water Cherenkov detectors (WCDs) installed near the testing facility will be used to validate the atmospheric radiation neutron background simulation (Sidelnik et al. 2020; Sidelnik et al. 2020). Reliable simulation models of the detectors' responses to the present radiation fields are essential. Meiga's modular and adaptable framework provides significant advantages, as it includes a set of pre-configured detector models, such as WCDs, and Geant4 physics lists that can be extended or modified to develop customized detectors and processes. Furthermore, the framework supports the development of new action classes to introduce specific operations during the simulation process.

2.2.1 Bonner Spheres Spectrometers and Neutron Long Counters

Meiga's detector libraries are extended in the NEREIDA application to include Bonner Sphere Spectrometers (BSS) (Bramblett et al. 1960; Garny et al. 2009) and neutron long-counters (Lacoste 2010; Park et al. 2013). These devices are essential in neutron metrology laboratories and facilities where precise spectral information is crucial, allowing the comparison of digital dose estimations with actual measurements. BSS are particularly useful for measuring neutron spectra over a broad range of energies. Our BSS model, based on the physics libraries and implementations detailed in prior studies (Cao et al. 2015; Garny et al. 2009), employs a series of polyethylene or composite material spheres as neutron moderators. The thickness of each sphere is carefully selected to fine-tune the energy sensitivity of the detectors, enabling the detection of neutrons across a wide energy spectrum. For development and testing, our initial setup includes five polyethylene spheres, ranging from 4 to 15 inches in diameter, each with a density of 0.946 g/cm^3. A centrally placed ^{3}He gas-filled sphere at 2 atmospheres acts as a proportional counter.

While BSS is appropriate for determining neutron spectra across a wide range of energies, neutron long counters are noted for their low sensitivity to gamma rays and their flat response over a vast neutron energy spectrum. In our model of the neutron long counter, based on standard designs, we aim to flatten the response function down to neutron energies of a few eV. This model includes a ^{3}He tube, type 25He/76/38E, from Centronic Ltd., designed with a nominal active length of 25 cm and operating at 10 atm.

Geometric details and the simulation results of these detectors can be seen in Section 3

2.2.2 Water Cherenkov Detector

Meiga was initially developed for muography, a technique that uses atmospheric muon flux to image the density distribution of large objects, such as volcanoes (Vesga-Ramírez et al. 2021), and for the development of new astroparticle detectors and techniques (Rubio-Montero et al. 2021). Consequently, Meiga includes a configurable Water Cherenkov Detector (WCD), commonly used in many astroparticle observatories. WCDs typically consist of a cylindrical water container (1-10 m^3), an 8-9" photomultiplier tube (PMT), and an internal coating that diffuses Cherenkov radiation produced by relativistic charged particles moving through the water. The WCD model included in NEREIDA accounts for variables such as water quality, the PMT model and its position, the type and quality of the internal coating, and the detector's electronic response. Due to their large detection volume, WCDs can also detect neutral particles like neutrons and photons through secondary processes such as neutron capture followed by prompt gamma emission, Compton scattering, or pair creation within the water (Sidelnik et al. 2020). The detector's electronic response is simulated to generate the final signal, and the pulse is analyzed in both real and simulated detectors. Pulse characteristics and information about secondary particles are logged for further analysis.

2.3 Additional Modules

2.3.1 Atmospheric Background Radiation

The interaction of cosmic rays (CR) with Earth's atmosphere results in the phenomenon of extensive air showers (EAS). These showers generate secondary particles through radiation and decay processes that are initiated by the incident cosmic ray energy (E_p) and continue until reaching the ground. Modeling this complex secondary spectrum requires significant computational resources due to the need to simulate numerous physical interactions and track a vast number of particles produced by many cosmic rays simultaneously impacting the Earth's atmosphere. Among the available tools, CORSIKA is highly preferred for its extensive use and continuous enhancements in simulating EAS (Heck et al. 1998). To augment these capabilities, NEREIDA is designed to be compatible with onedataSim-ARTI (Sarmiento-Cano et al. 2022; Rubio-Montero et al. 2021), a simulation toolkit developed by the LAGO collaboration for predicting the expected flux of atmospheric radiation backgrounds under varying atmospheric and geomagnetic conditions. This toolkit integrates seamlessly with CORSIKA, Magnetocosmics, and Geant4 (Sarmiento-Cano et al. 2022). It has been applied in diverse scenarios, ranging from studying space weather impacts on neutron detection to developing neutron detectors for security purposes, and even calculating radiation exposure during commercial flights (Asorey et al. 2023).

ARTI operates efficiently on high-performance computing clusters and is optimized for virtualized platforms like the European Open Science Cloud (EOSC), handling vast data across multiple storage solutions (Rubio-Montero et al. 2021). By leveraging this tool, NEREIDA is also able to determine the impact of atmospheric background radiation on the global dose received in the installation.

2.3.2 Anthropomorphic Voxelized Phantom Models

As part of the auxiliary tools included in NEREIDA, the RadPhantom application (Núñez-Chongo et al. 2023) has been adapted and incorporated as an optional module. Initially developed for radiation therapy dose calculations, this application simulates the interaction between various radiation fields, including neutrons, and different tissues in the human body. RadPhantom can generate models of a voxelized anthropomorphic phantom using two approaches: (a) by voxelizing real patients' body geometries from Digital Imaging and Communications in Medicine (DICOM) images (Bidgood Jr et al. 1997), or (b) by creating a 3D mesh based on the Adult Male or Female reference computational models defined in the ICRP110 publication (Large et al. 2020). Customized methods import information from specific files containing the 53 compound tissue materials and the geometries and compositions of 142 organs within the modeled human body (Núñez-Chongo et al. 2023).

For NEREIDA, the geometry constructor of RadPhantom allows for the adaptation of variable voxel sizes once the voxelization of the facility is completed. This strategy optimizes memory access and consumption, enabling faster navigation through the large number of voxels in both models. The dose information recorded in each phantom voxel is exported to a JSON file for external analysis using dedicated Python scripts. This module within NEREIDA provides the capability to obtain the discretized distribution of absorbed dose over the entire volume of the human phantom and the dose in depth along the trajectory of the incident particle beam. This allows for a detailed analysis of the radiation received in different parts of the body and the calculation of effective dose values in various scenarios.

2.4 HPC and Cloud Implementation

Several approaches were developed for meet the computational demands of NEREIDA. Container virtualization ensures that NEREIDA runs efficiently on High Performance Computing (HPC) clusters equipped with Singularity or uDocker, as well as on federated cloud-based infrastructures such as the European Open Science Cloud (EOSC) or public clouds like Amazon Web Services (AWS) (Calatrava et al. 2023). The flux of any radiation field follows a Poisson distribution, making parallelization straightforward, as the initial neutron and/or gamma flux, calculated from the source activity in each of these fields and the requiered total simulation time, is divided into $n \times c$ sub-executions, where n is an adjustable integer depending on the initial flux, installation size, and the total number of voxels, and c is the number of available cores. These values are selected automatically by the NEREIDA's launcher at the beginning of the run. Consequently, $n \times c$ virtualized instances are deployed after each of the corresponding JSON input files is automatically adjusted. During execution, only information related to the run's progress is shared from the different instances to a central daemon where the parallelization is orchestrated. For large fluxes, scalability tests and performance benchmarking are planned for the third year of NEREIDA's development, once all the modules have been integrated and tested. However, preliminary tests after the first year of development indicate that scalability has been achieved with the expected performance and are shown in the next section. Additionally, the development plan includes adapting OnedataSim (Rubio-Montero et al. 2021) to NEREIDA's output data. OnedataSim is a virtualizable application that enables atmospheric radiation simulations in HPC and cloud-based environments, autonomously producing FAIR (Findability, Accessibility, Interoperability, and Reusability) (Wilkinson et al. 2016) data.

To meet the computational demands of NEREIDA, the application and its required dependencies, including, e.g., ARTI, Geant4, and Meiga, are deployed using container virtualization. This approach ensures operation on High Performance Computing (HPC) clusters with Singularity or uDocker, as well as on federated cloud infrastructures like the European Open Science Cloud (EOSC) and public clouds such as Amazon Web Services (AWS) (Calatrava et al. 2023). Parallelization is straightforward, given that the flux of any radiation field follows a Poisson distribution. The initial neutron and/or gamma flux, determined from the source activity and the required total simulation time, is divided into $n \times c$ sub-executions, where n is an adjustable integer based on the initial flux, installation size, and total number of voxels, and c is the number of available cores. NEREIDA's launcher automatically selects these values at the start of the run. Consequently, $n \times c$ virtualized instances are deployed, with each JSON input file automatically adjusted. During execution, only progress-related information is shared from the instances to a central daemon that orchestrates the parallelization. Scalability tests and performance benchmarking for large fluxes are planned for the third year of NEREIDA's development, once all modules have been integrated and tested. Preliminary tests after the first year indicate that scalability has been achieved with the expected performance, as demonstrated in the following section. Additionally, the development plan includes adapting OnedataSim (Rubio-Montero et al. 2021) to NEREIDA's output data.

This implementation enables NEREIDA to be deployed and executed locally, in High Performance Computing (HPC) environments, and in cloud infrastructures while generating standardized data catalogs. These catalogs utilize a linked open data schema (Bauer and Kaltenböck 2011) and adhere to FAIR principles, as mandated by the European Commission. The development of FAIR-compliant modules for NEREIDA, in accordance with the project management and Data Management Plan (DMP), is scheduled for the third year of the project. This phase will include the selection of standard ontologies and controlled vocabularies to further enhance data interoperability and reusability.

2.5 Validation Plans

The validation of NEREIDA involves MCNP simulations and measurements at two facilities. Initially, comparisons are made using two Water Cherenkov Detectors (WCDs) at the Neutron Physics Department of the Bariloche Atomic Center (DFN/CAB), in Argentina. Each detector is equipped with electronics for slow control, pulse setting, digitization, pulse labeling, preliminary data analysis, and data transmission to a central repository. The use of two identical detectors enables differential response studies. For instance, one detector can be used to evaluate the effectiveness of water additives in improving neutron detection. Measurements involve ^{252}Cf and ^{241}Am-Be sources (Sidelnik et al. 2020), which are used for NEREIDA validation experiments. These experiments employ various shielding configurations for neutrons and photons, including cadmium for thermal neutron absorption, paraffin for fast neutron moderation, and lead for gamma radiation shielding.

The second validation stage is based on performing NEREIDA simulations of the *Laboratorio de Patrones Neutrónicos* at CIEMAT (LPN/CIEMAT, Spain). LPN is a facility within the Ionizing Radiation Metrology Laboratory (LMRI) at CIEMAT, which is responsible for establishing, maintaining, and disseminating the SI National Standards for ionizing radiation in Spain. The LPN specializes in neutron dosimetry, spectrometry, and calibration, offering a controlled environment for high-precision measurements. The LPN hosts two calibrated neutron sources: ^{252}Cf and ^{241}Am-Be. These sources are stored in water within the Irradiation Room (IR-LPN), a bunker measuring approximately 8 m x 8 m x 8 m, with 1.25 m thick concrete walls. The facility provides remote manipulation capabilities for the sources, ensuring safety and precision during experiments. The IR-LPN is equipped with state-of-the-art instruments for neutron detection and measurement. The LPN has extensive experience in neutron spectrometry using BSS (Méndez-Villafañe et al. 2019; Méndez-Villafañe et al. 2018). For this validation, the CIEMAT-BSS spectrometer will be used. It consists of 12 polyethylene spheres that house proportional counters, ^{3}He-type SP9. The CIEMAT-BSS has already determined the neutron spectrum at various points inside and outside the IR-LPN, providing a solid baseline for NEREIDA's validation. Spectrometry measurements using BSS spheres are complex and have been limited to a few points. However, LPN is now exploring multi-point creep rate measurements using a long counter detector developed specifically for this work. These experimental results have been previously compared with MCNP simulations, and the outcomes of those comparisons will be utilized to validate NEREIDA's accuracy as it's showed in Figure 3.

3 FIRST RESULTS AND DISCUSSION

The first case study involved creating a reliable digital model of the LPN-IR facility's interior and its neutron sources. At this stage of NEREIDA's development, the LPN-IR model is based on a simplified geometry representing three significant volumes: an internal cubic volume of $(8 \times 8 \times 8 = 512)\,\mathrm{m}^3$ filled with dry air, surrounded by 1.25 m thick concrete walls, and situated on a Geant4 model of Madrid's soil. The implementation of these volumes utilized Geant4's semi-geometric models, based on dimensions provided in user input data.

After defining the volumes, voxelization is performed for each structure by dividing the geometry into cubic voxels of configurable size. Materials are assigned to each voxel based on their spatial location within the LPN-IR. NEREIDA's capability to generate a mesh with varying voxel sizes is illustrated in Figure 1. This feature allows NEREIDA to obtain precise and detailed information on physical quantities resulting from simulations in specific areas of interest. Voxel sizes are dynamically adapted based on the criticality of a specific area, generating a voxel size that is inversely proportional to the deposited energy in that area. This adaptive voxelization is shown in panels 1 and 2 of Figure 1. Panel 3 of Figure 1 shows the result of injecting 10^5 neutrons from the simulated ^{252}Cf source located at the geometric center of the installation, reflecting one of the potential real-world source locations. In addition to the primary neutrons, beams of secondary particles resulting from interactions with the air, concrete, and soil are observed. The model accurately mimics the expected shielding behavior of the concrete walls, where only ν (neutrinos) and $\bar{\nu}$ (antineutrinos) escape from the LPN irradiation room. This figures were obtained by using the Geant4 visualization capabilities based on the OpenGL library.

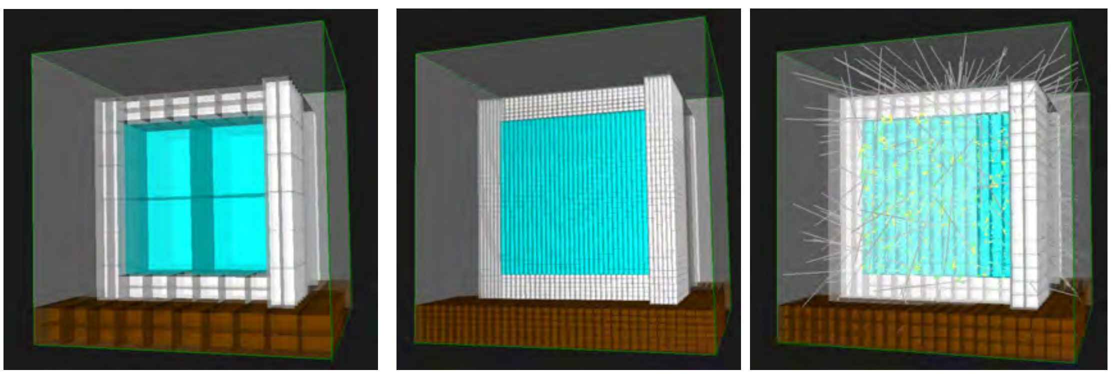

Figure 1: Spatial discretization of the voxelized model for the LPN facility at the initial stage of NEREIDA, depicting different materials: air (blue voxels), concrete (gray voxels), and Madrid's soil (brown voxels). Left: robust geometric voxelization model for a fast simulation. Center: refined voxelization, where different voxel sizes can be implemented for the different areas. Right: visualization of the nuclear and radiative interactions produced by the injection of 10^5 neutrons emitted by the simulated ^{252}Cf source. As expected, only neutrinos escape from the LPN facility.

The energy spectrum of the ^{252}Cf and ^{241}AmBe LPN's sources were modeled and incorporated into NEREIDA as configurable sources for future use. The energy distribution of the primary neutrons is randomly generated according to the methods described in the previous section. The energy spectrum of ^{252}Cf and other fission neutron sources can be described by Watt's distribution, $N(E_n) = \exp\left(-E_n/a\right)\sinh\left(\sqrt{bE_n}\right)$, where E_n represents the neutron energy in MeV, while $a = 1.18\,\mathrm{MeV}$ and $b = 1.03419\,\mathrm{MeV}^{-1}$ are the corresponding Watt's parameters for the ^{252}Cf source. A comparison between the source spectrum generated by NEREIDA and the expected distribution for this source is presented in Figure 2-left. The ^{241}Am-Be source, based on the $^9\mathrm{Be}(\alpha,n)^{12}\mathrm{C}$ reaction, where ^{241}Am serves as the alpha emitter and Be as the target nuclei, is simulated in NEREIDA using the discrete probability function obtained from the source spectrum data (ISO8529-1 2021).

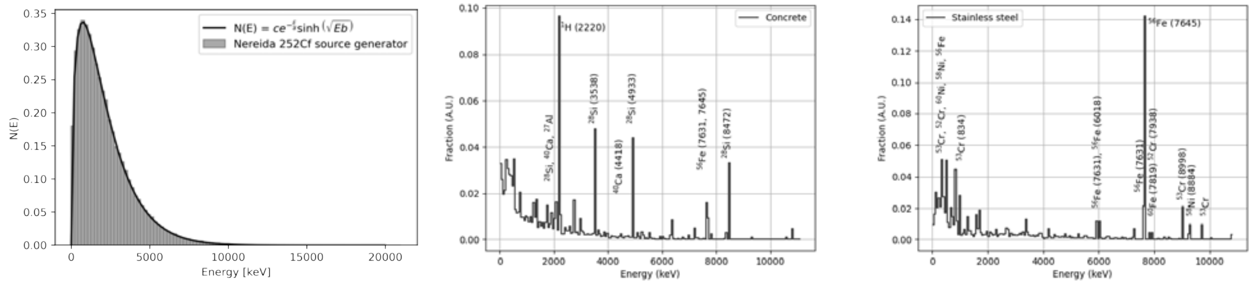

Figure 2: Left: Neutron emission spectra generated by NEREIDA (bars) compared with the corresponding Watt's distribution for ^{252}Cf (solid line). Center and Right: Neutron activation of common building materials: concrete (center) and stainless steel (right), as obtained in NEREIDA simulations. These panels illustrate the γ emission photon lines identified for key elements such as iron, silicon, cobalt, hydrogen, an oxygen.

As detailed in the previous section, NEREIDA is capable of accounting for neutron activation of building materials, a crucial consideration for facilities where high neutron fluxes may occur. The central and right panels of Figure 2 illustrate the γ emission spectra resulting from neutron activation of concrete (center) and stainless steel (right). The observed gamma emission lines are compared with γ prompt emission tables, enabling the identification of activated elements in the tested building materials, such as iron, silicon, cobalt, hydrogen, and oxygen. These significant results demonstrate NEREIDA's proficiency in simulating neutron interactions with facility materials and accurately accounting for their responses.

We estimated the response functions for both the CIEMAT-BSS and the long-counter detectors by exposing them to mono-energetic neutron beams ranging from 10^{-9} MeV to 20 MeV and calculating the count rate per incident neutron fluence (Mares et al. 1991). The results are presented in the Figure 3, where the second panel displays the responses for each BSS sphere, illustrating the efficiency of various sphere radii in detecting specific neutron energies, and the fourth panel shows the preliminary results from the long counter model, evidencing the expected flat response across the full energy range. These results, which aligns well with results reported in the literature (Lacoste and Gressier 2010), show NEREIDA's capability to accurately model complex neutron detection systems and their energy-dependent responses.

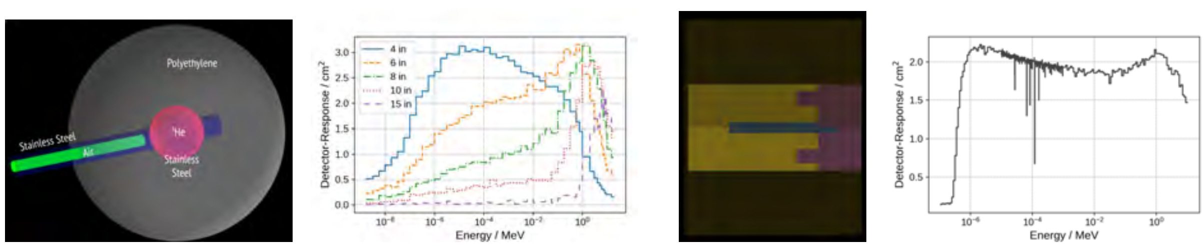

Figure 3: First: Snapshot of the CIEMAT-BSS with a ^{3}He proportional counter (red), an air cavity (green), a stainless steel shell (0.5 mm thick), and a variable-radius polyethylene sphere (gray). Second: Neutron detection efficiency as a function of neutron energy. Third: Neutron long-counter model with high-density polyethylene layers (yellow), borated polyethylene, and a cylindrical section between the thermal neutron counter and the cadmium front window (green). The ^{3}He tube (blue) serves as the proportional counter. Fourth: Preliminary response of the neutron long-counter model, showing a flat response across the energy spectrum.

The energy spectrum of the primary neutrons and the three-dimensional distribution of the deposited dose were recorded using sensitive volume detectors to create a voxelized map of dose distribution within the facility, as illustrated in the left panel of Figure 4. A color scale provides visual information about the spatial dose distribution. These simulations enable the estimation of dose values and the identification of high-exposure areas, both inside and outside the irradiation room. Furthermore, this mapping serves as a visual design tool, facilitating simple modifications to geometry or shielding materials to optimize dose reduction in critical zones.

The spatial representation of deposited dose assists in identifying potential safety concerns within the installation, allowing for targeted interventions. This visualization was performed offline, the final version of NEREIDA foresees to incorporate a web-based visualization tool.

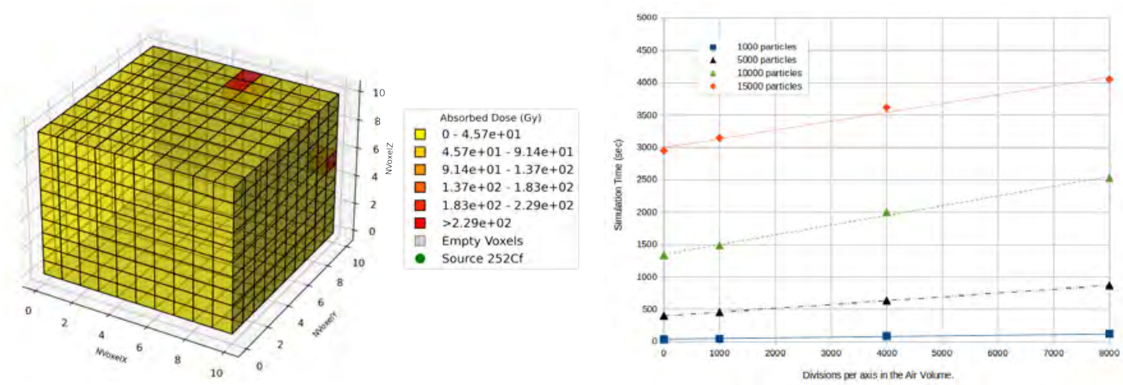

Figure 4: Left: Voxelized map showing dose distribution in grays (1 Gy=1 J kg^{-1}) within the facility, with a color scale highlighting significant dose areas. Right: Computing scalability of the NEREIDA code, displaying simulation time as a function of the number of voxels and injected neutrons (symbols).

Scalability tests were conducted by deploying the NEREIDA docker in a virtual cluster (v-cluster) configured on EOSC. The v-cluster comprised a master and four virtual nodes, each equipped with 8 Intel Xeon E7 Haswell @ 2.3GHz cores, 16 GB of RAM, and 200 GB of disk space. We explored two key simulation parameters: the total number of injected neutrons from a ^{252}Cf source (ranging from 1,000 to 15,000) and the total number of voxels (ranging from 1 to 8000 divisions per axis, equivalent to 1 to $8000^3 = 5.12 \times 10^{11}$ voxels, corresponding to 1 mm^3 voxels in a 512 m^3 facility). Each simulation was configured to use a single core of the v-node. The right panel of Figure 4 presents the results, showing the evolution of total run time as a function of axis divisions for 1k, 5k, 10k, and 15k injected neutrons. Even with this modest cluster configuration, the scalability results are impressive. It's possible to increase the spatial resolution of the dose distribution by several orders of magnitude while only doubling the total time in the worst-case scenario. Regarding scalability in terms of injected neutrons, parallelization is straightforward. The simulation can be divided into smaller runs, with the total dose per voxel summed upon completion of all runs.

4 CONCLUSIONS AND FUTURE WORK

After its first year of development, NEREIDA is demonstrating significant advances in enhancing neutron safety and dosimetry within nuclear facilities. By integrating and combining Geant4-based Monte Carlo methods with other tools, such as Meiga, NEREIDA accurately characterizes neutron flux spectra and provides precise dosimetric calculations.

Preliminary validation activities conducted at LPN/CIEMAT and CAB have highlighted NEREIDA's capability to simulate neutron interactions with various materials and produce reliable measurements. Initial results show excellent agreement with MCNP simulations, underscoring the tool's accuracy and reliability.

The project's next phase will focus on completing the validation of simulations, developing a user-friendly web-based interface, optimizing performance on high-performance computing and cloud infrastructures, and implementing FAIR modules. These advancements will enhance accessibility, efficiency, and data interoperability, aligning with the project's data management plan and facilitating broader scientific collaboration.

NEREIDA's development represents a significant advancement in neutron safety and dosimetry. The tool's ability to generate detailed voxelized maps of dose distribution within a neutron production facility, and its capacity to model complex neutron detection systems demonstrate its potential for improving nuclear facility safety protocols. Furthermore, its scalability and performance in handling large-scale simulations position it as a valuable asset for future research and applications in nuclear engineering.

As NEREIDA continues to evolve, it is well-positioned to address emerging challenges in the field. Its proactive approach to development, coupled with its focus on user accessibility and data interoperability, ensures that NEREIDA will contribute significantly to advancements in nuclear engineering and related disciplines. The project's commitment to producing FAIR data also aligns with broader trends in scientific research, potentially accelerating progress through enhanced collaboration and data sharing.

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