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# Integration and Validation of Nuclear Fission Physics in the SWORD Simulation Suite

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# INTEGRATION AND VALIDATION OF NUCLEAR FISSION PHYSICS IN THE SWORD SIMULATION SUITE

## 1. SOFTWARE FOR OPTIMIZATION OF RADIATION DETECTORS

### 1.1 Abstract

SoftWare for Optimization of Radiation Detectors (SWORD) is a vertically integrated software package developed at the Naval Research Laboratory that offers a CAD-like interface to several cutting-edge radiation transport codes. SWORD allows users to design and optimize radiation detectors for maximum-likelihood detections of nuclear materials. Despite using cutting edge radiation transport codes, SWORD lacked the ability to simulate nuclear fission accurately. This limited the types of scenarios and detectors that could be modeled. Through the work I have accomplished under the Jerome and Isabella Karles Distinguished Scholar Fellowship Program, SWORD now has the ability to accurately and efficiently model nuclear fission physics. With this new capability, SWORD provides Navy and other DoD users with a powerful and flexible tool to model quickly and accurately a wide range of new and highly complex scenarios involving active interrogation, space-based and ship-based nuclear reactors and shielding, transportation and handling of nuclear materials, novel methods and materials for detection of special nuclear materials, and more.

### 1.2 Introduction to radiation transport

The physics of particle interactions is well understood, but one cannot derive analytical solutions to radiation transport problems except in the most trivial cases. However, an effective way to evaluate complex particle interactions is through Monte Carlo simulation, and a number of simulation libraries exist. These libraries require significant expertise to run and have a wide variety of adjustable parameters. These difficulties motivated the construction of a tool that could be used by a person without specialized radiation transport experience to create and evaluate a range of defense and homeland security scenarios.

### 1.3 SWORD, a CAD-like environment for radiation transport modeling

SWORD is a vertically integrated development tool and front end for nuclear radiation transport modeling developed at the US Naval Research Laboratory (NRL). SWORD provides a library of prebuilt objects, including various detectors, vehicles, border portals, and buildings as well as a library of common spectra. SWORD was designed to allow for easy use of these radiation transport codes without the need for radiation transport subject matter experts and to quickly make changes to the scenario being modeled. SWORD also allows scenarios where objects move to be easily simulated. SWORD is funded jointly by the Department of Defense/Defense Threat Reduction Agency (DTRA) and the Department of Homeland Security/Countering Weapons of Mass Destruction (CWMD). The primary use of SWORD is to study and optimize detector responses in a variety of scenarios. SWORD is the primary tool for simulating radiation/nuclear environments for DHS/CWMD and DTRA/RD-NTI, and it has over 300 government and commercial registered

users across the United States. Potential licensees are screened by the Radiation Safety Information Computational Center for security concerns related to certain organization affiliations and country of origin. In particular, applicants from Department of Energy 810.8a list countries are not allowed to receive SWORD.

SWORD can use three different radiation transport codes: Geant4 [1], MCNP [2], and Omnibus/Denovo [3]. An advantage of SWORD is that it gives the user an easy way to compare a model very closely between all of these radiation transport codes. All three codes have different limitations, and one of the major limitations of the Geant4 engine is that, since it has its roots in high energy experimental physics, it has a very poor model for nuclear fission interactions. This is the limitation we sought to address with this work.

Geant4 and its predecessors were initially developed by the European Organization for Nuclear Research (Conseil européen pour la recherche nucléaire, CERN) as a way to help design detectors and shielding for big experimental nuclear and elementary particle physics programs at the Large Hadron Collider (LHC) such as the Compact Muon Solenoid. While it has been designed to work at a variety of energy scales, the physics interaction models have been built with the primary purpose of studying how radiation will affect a detector at the extremely high energy scales of a modern accelerator facility, a factor of  $\sim 10^6$  above those relevant for nuclear fission in DoD and security-related applications. While a simple fission physics model is adequate for the former, it cannot meet the requirements of the latter. As such, only a simple physics model of fission was developed.

Monte Carlo N-Particle Transport (MCNP) was developed at Los Alamos National Laboratory and has its roots in code developed during the Manhattan project. Classified radiation transportation codes used to develop nuclear weapons had key components removed, and a declassified radiation transportation code was released to authorized persons. MCNP inputs were designed from a punch card system whose use requires significant expertise which makes SWORD support for MCNP very valuable.

Denovo is a radiation transport code developed by Oak Ridge National Lab. Unlike Geant4 and MCNP, which use Monte Carlo methods for radiation transport, Denovo is a 3-dimensional discrete ordinate radiation transport code. Denovo is significantly faster than Geant4 and MCNP, however, without adequate computing resources, it can produce misleading results in some circumstances. It is commonly used for reactor designs, where evaluation of large-scale radiation environments is important.

## 1.4 Fission introduction

Nuclear fission is the process by which a nucleus splits into two (or more) lighter nuclei. Aside from defense applications, nuclear fission has applications in power generation, industry, space propulsion, radiation detection, materials science, and nuclear medicine. While SWORD is used in defense radiation detection applications, it is not directly applicable to nuclear weapons development. It is, however, well-suited to developing reactor shielding for space reactors (which require lightweight shielding) and developing novel detectors to study or exploit fission reactions (some examples of which will be given below) once nuclear fission is properly modeled.

The default Geant4 nuclear fission library has a number of glaring discrepancies that make it unsuitable to Navy, DoD, and DHS usage. First, however, it is important to understand how current and future SWORD users will make use of nuclear fission; here we will highlight two prominent (unclassified), examples.

### 1.4.1 Active interrogation

Active interrogation is a technique that enables direct detection of nuclear materials in a container without needing to open the container to inspect it. The container and contents to be tested are first bombarded with a beam of high energy photons or neutrons. If nuclear material is present, it will be fissioned by the beam; in the case of high energy photon beam, this is done via photofission (when a nucleus absorbs a high energy photon and subsequently splits into two smaller nuclei) and in the case of a neutron beam, this is done via neutron-induced fission.

A suite of detectors can then be used to look for the specific gamma ray emission that is associated with nuclear fission. Other techniques look for a specific neutron signature from the fission. If no nuclear materials are inside the container, only backscattering of the source particles is detected. The key to the detection method is to differentiate between the fission spectrum and normal backscatter spectrum using both energy and time profiles of the resulting particles.

Active interrogation has been studied and evaluated by Navy, DoD, DHS, and other government agencies that are SWORD users. DHS/CWMD is interested in using this technology to secure border portals. This technology is much more sensitive to weapons-grade nuclear material than other methods used today. DTRA is also researching ways to use active interrogation for force protection overseas, for example, to inspect a vehicle or crate without opening it and risking triggering an improvised explosive device or nuclear weapon. The reliability of these studies is, however, strongly limited by the fidelity of the physics model.

### 1.4.2 Space-based nuclear reactors

Space-based nuclear reactors are again becoming a focus of research. NASA is actively pursuing a nuclear thermal propulsion system for launch as soon as 2024 [4] and several near-peer adversaries have publicly announced various forms of space-based nuclear reactors.

An accurate model of nuclear fission would be useful in a number of different space-based scenarios. Nuclear fission reactors are a strong candidate for power systems for human space travel, and it is crucial for the safety of the crew to evaluate the performance of shielding designs. In ground based shielding applications, it's easy to overbuild shielding, but in spaceflight, weight will be very important and shielding simulations will be critical. Accurate fission simulation will also be instrumental in developing detection of adversarial spacecraft.

## 2. GEANT4 FISSION LIMITATIONS AND THE LLNL FISSION LIBRARY FOR GEANT4

### 2.1 Geant4 limitations

Currently, the version of Geant4 that SWORD uses has serious weaknesses for studying fission applications because it has been designed for high-energy, particle physics accelerator use, where fission processes are utterly negligible at the relevant energy scales. The energy spectrum of the fission, the number of neutrons and gamma rays produced, and the atomic number of the fission product nuclei are all incorrect. All of these issues make the current nuclear physics fission model unsuitable for simulating many state-of-the-art instruments and evaluating many security-related scenarios. In addition, the Geant4 fission model only supports neutron-induced fission, not photofission, which dramatically reduces the types of active interrogation scenarios that could be studied.

## 2.2 LLNL fission library

LLNL sought to address many of these issues by producing its own nuclear fission physics library. In the LLNL library, photofission was enabled with the simplifying assumption that nuclear fission proceeds independently of the type of particle inducing the fission. This implies that the nucleus will fission based entirely upon its excitation level, but also means that the neutron separation energies and Watt spectra must be known in order for the model to work. Data is included only for thorium, uranium, neptunium, plutonium, americium and californium. The fission fragments now produce the correct number of fragments with the proper atomic number.

## 2.3 Rapiscan Laboratories improvements

For elements with atomic numbers higher than Uranium, no data was provided by LLNL. Rapiscan, a commercial laboratory which produces active interrogation equipment, used cross section data produced by Stanford Linear Accelerator Center (SLAC) to fill this gap. Rapiscan also modified the Geant4 Cascade and NeutronHP models to correct the multiplicity of neutrons and photons generated by fission and atomic number of the fission fragments by integrating, and, where required, modifying the LLNL fission library. In addition, the Rapiscan program performed significant validation and testing of the resulting library. This work was done under contract to CWMD.

## 3. SUMMARY OF WORK DONE

### 3.1 Integration overview

In FY19-20, we undertook a substantial revision to the SWORD simulation engine, a significant portion of this work was supported by this Karles. In order to utilize this new physics library, SWORD had to be modified, and the LLNL/Rapiscan physics library had to be integrated and the implementation validated.

### 3.2 Integrating LLNL fission into SWORD

First, we redesigned the Geant4 interface to accommodate the new physics library. We decided to rewrite the existing Geant4 implementation for a number of reasons, including features important for the fission work. Previous versions of SWORD could not handle the amounts of data produced by Geant4's built in version of fission, so it was important for us to increase the efficiency of SWORD. We also implemented the ability to select different physics lists at runtime, which is a critical feature for fission.

We also made changes to SWORD7 to allow long fission runs that were not possible with the previous SWORD engine. SWORD's geometry backend was initially designed to index volumes on the name of volume string. Since NRL developed SWORD to handle relatively simple geometries and interactions, using string-identified volumes was an acceptable solution. However, this resulted in string compares in critical parts of the code. String compares are highly inefficient. Every time a particle entered or exited a volume, multiple string compares were run to determine if the volume was a detector. Now SWORD7 leverages existing Geant4 sensitive detectors to tell when a particle enters a detector. Additionally, previous versions of SWORD would cache all data in memory and write it all out at the end of a simulation. Now, we have changed SWORD7 to use cached writes after each event. This allows the SWORD data to become arbitrarily large (limited only by hard disk drive space) and writes to data files are more efficient since the buffer flush is governed by the operating system.

Geant4 allows the user to select among a range of physics lists, which are libraries of physics models of the fundamental interactions of particles. SWORD has a physics list which has been vetted and validated carefully over many years, so extra care had to be taken when integrating the LLNL physics library. Separate physics interactions can have an effect on each other. For example, when a fission occurs, it creates secondary neutrons, gammas, and unstable fission product isotopes. Even if the fission is correctly modeled, the transport of the secondary products via electromagnetic interactions, neutron transport, and radioactive decay is important to properly modeling the full fission process.

Since Rapiscan created its own physics list which incorporates all its changes and improvements, and SWORD had an existing physics list, when making the union of the two, it was important to fully understand the effects of all choices. There were several differences between the SWORD physics list and the Rapiscan provided physics list. These differences were studied to ensure accuracy of the Rapiscan configuration when used by SWORD.

### 3.3 Validation

We chose to validate the changes to SWORD fission using the same figures of merit that Rapiscan used when validating its improvements to the nuclear fission library. This usually involved comparing to the MCNP radiation transportation code, which has had its fission physics validated for years, or comparing to NIST nuclear databases. All of the following validation was done under the Karles fellowship.

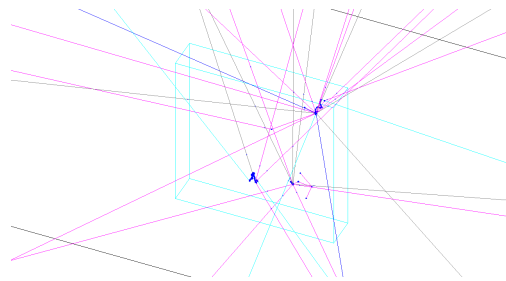


Fig. 1: Box (cyan) is the  $^{235}_{92}\text{U}$  foil used in all simulations. Neutrons (pink) and  $\gamma$  (blue) were generated at the surface of the foil. Lines represent secondary particles generated by the fission. Blue “points” are actually many different lines representing small ionizations as the energy is deposited in the foil.

#### 3.3.1 Simulation setup

Both prompt and delayed fission products were studied for thermal neutron-induced fission and photofission. Prompt fission products are those fission fragments generated by the fission. Delayed fission products are those products made by the radioactive decay of the prompt fission products.

To test thermal neutron fission, 0.025 eV thermal neutrons were generated at the face of a fissile material foil. Both  $^{235}_{92}\text{U}$  and  $^{238}_{92}\text{U}$  were tested, but only  $^{235}_{92}\text{U}$  results are presented as they are representative of the accuracy of the model. To test photofission, 12 MeV photons were generated at the face of the same target geometry. The  $^{235}_{92}\text{U}$  foil, shown in Figure 1, was  $5 \times 5 \times 1$  mm, surrounded by vacuum.

1000 thermal neutrons and 500000  $\gamma$  were generated to produce the following results. All events were written using the standard SWORD output. The output files were used for all of the studies in this section.

### 3.3.2 Fission cross section

Cross section is the absolute probability of an interaction occurring: in this case, the probability that a particle will fission a nucleus. This, above all else, is the most important thing to get right. If the absolute cross section is wrong, every important figure of merit will also be incorrect. After checking the absolute cross section, other variables derived from the absolute cross section will be tested for this validation.

The absolute cross section is given as

$$I = I_0 e^{-n\sigma z}, \quad (1)$$

where  $n$  is the number density of particles,  $\sigma$  is the cross section, and  $z$  is the thickness of the material. This can be rewritten in terms of the molar mass  $m_a$  and density  $\rho$  as

$$\frac{I}{I_0} = e^{\frac{N_A}{m_a} \sigma \rho z}, \quad (2)$$

where  $N_A$  is Avogadro's number. Solving for  $\sigma$  gives

$$\sigma = \left[ \frac{\ln\left(\frac{I}{I_0}\right) m_a}{N_A \rho z} \right]. \quad (3)$$

Since simulation provides the number of fissions  $n_{\text{fission}}$  and the total number of events generated  $n$ , the intensity ratio can be calculated as

$$\frac{I}{I_0} = 1 - \frac{n_{\text{fission}}}{n}. \quad (4)$$

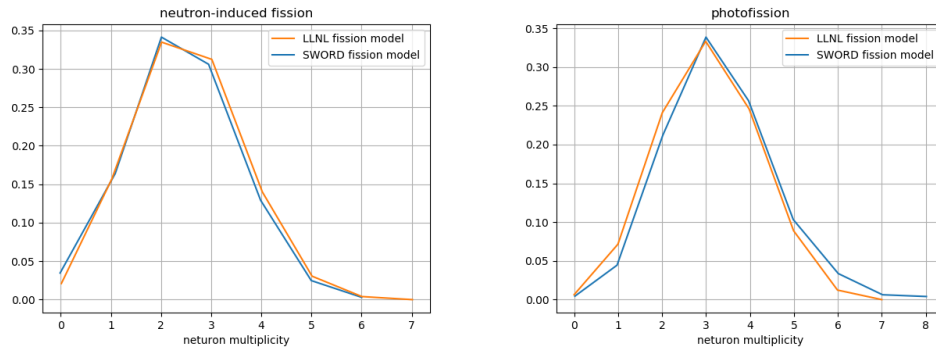
Using this method, the fission cross sections for thermal neutron fission ( $E_{\text{neutron}} = 0.025$  eV) and photofission ( $E_\gamma = 12$  MeV) of  $^{235}_{92}\text{U}$  were calculated to be<sup>1</sup>

$$\sigma_{\text{neutron}} = 354 \text{ b}, \quad (5)$$

$$\sigma_{\text{photofission}} = 0.223 \text{ b}. \quad (6)$$

The cross section for neutron-induced fission  $^{235}_{92}\text{U}$  is measured to be 588 b [5]. While the cross section of 354 b we derive from the LLNL fission library is 40% too low, it is dramatically closer than the native cross sections in Geant4, which were incorrect by orders of magnitude. In the following section, we will show good agreement between SWORD and the Rapiscan implementation for many variables sensitive to cross section. This indicates the problem is not with the SWORD implementation, but in the LLNL model. Additionally, since the model produces results that are in good agreement with data (shown below), this discrepancy does not adversely affect the usefulness of the model. For photofission of  $^{235}_{92}\text{U}$ , the cross section is measured to be 0.224 b, which is in very good agreement with the data [5].

<sup>1</sup>b = barn =  $1 \times 10^{-24}$  cm<sup>2</sup> (approximately the cross sectional area of one uranium nucleus).



(a) Neutron multiplicity with thermal neutron fission.

(b) Neutron multiplicity with photofission.

Fig. 2: Neutron multiplicity comparison with thermal neutron fission and photofission of  $^{235}_{92}\text{U}$ . The SWORD implementation and LLNL fission model agree closely, thus validating the implementation of the LLNL model within SWORD. SWORD data in blue, LLNL [6] in orange.

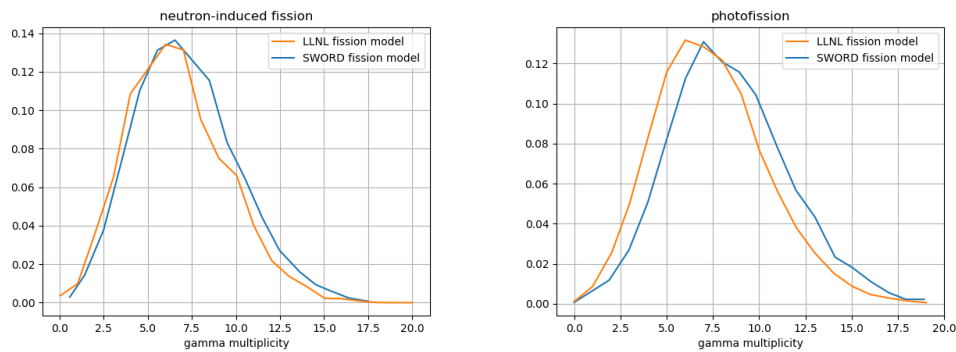
(a)  $\gamma$  multiplicity with thermal neutron fission.(b)  $\gamma$  multiplicity with photofission.

Fig. 3:  $\gamma$  multiplicity comparison with thermal neutron fission and photofission of  $^{235}_{92}\text{U}$ . The SWORD implementation and LLNL fission model agree closely, thus validating the implementation of the LLNL model within SWORD. SWORD data in blue, LLNL [6] in orange.

### 3.3.3 Prompt photon and neutron multiplicity

The next improvement tested was the neutron and  $\gamma$  prompt multiplicity, i.e. the number of particles created directly by the fission. Prompt fission multiplicity refers to the number of particles that are created directly by the fission and not by decay of the fission products.

Figures 2 and 3 show the neutron and  $\gamma$  multiplicities for thermal neutron and photon induced fission. Table 1 shows the mean multiplicities for both fission type and prompt particle type. For neutron-induced fission, very good agreement is apparent. For photofission, SWORD shows a slight excess of 0.26 neutrons and 0.80  $\gamma$  relative to the LLNL fission model, an excesses of about 10%. For comparison, the default

Table 1—Multiplicities of  $\gamma$  and neutrons from neutron and photon induced fission. Reference data sourced from [6].

Prompt particle	Fission type	Sim mean multiplicity	Ref mean multiplicity
neutron	thermal neutron	2.50	2.41
neutron	photofission	3.32	3.06
$\gamma$	thermal neutron	6.72	6.74
$\gamma$	photofission	8.21	7.41

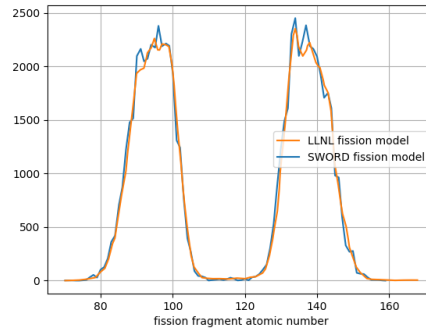


Fig. 4: Fission fragment atomic mass distribution with thermal neutron and photofission of  $^{235}_{92}\text{U}$ . SWORD data in blue, LLNL [6] in orange.

Table 2—Fission fragment mean and standard deviation for both peaks. LLNL data sourced from report [6].

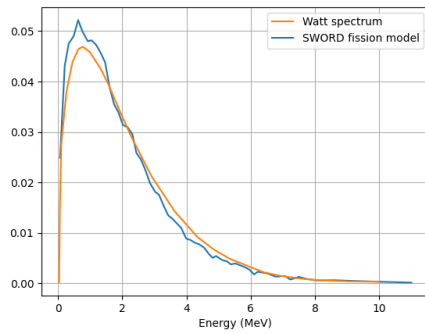
Peak	Simulation source	Mean (atomic number)	Standard deviation (atomic number)
First peak	SWORD	94.2	5.4
First peak	LLNL	94.7	5.3
Second peak	SWORD	137.5	5.5
Second peak	LLNL	137.3	5.4

Geant4 fission library gives mean neutron and  $\gamma$  multiplicities for thermal neutron and photofission of less than 2, smaller than the values reported in [6] by  $\sim 150\%$  and  $\sim 300\%$ . The SWORD implementation is therefore a significant improvement over the base Geant4 fission library.

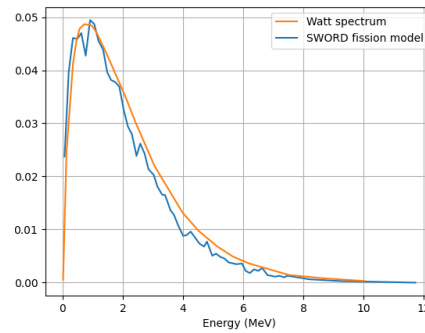
### 3.3.4 Fission fragment distribution

We also studied the prompt fission fragments. The mass distribution of prompt fission fragments is important since the radioactive decay chains of the fragments will determine the spectrum of delayed fission products; if the mass distribution of the fission fragments is incorrect, then the radioactive decay products will also be incorrect, leading to large, compounding errors in delayed  $\gamma$  and neutron spectra.

The shape of the bimodal fission fragment distribution matches qualitatively with what is shown by Rapiscan [6] in Figure 4, with small variations attributed to differences in statistics. The means and standard deviations of each peak in the bimodal distribution are shown in Table 2. The means agree extremely well (within about 0.4 atomic number), validating this portion of the SWORD implementation.



(a) Prompt neutron spectrum with thermal neutron fission.

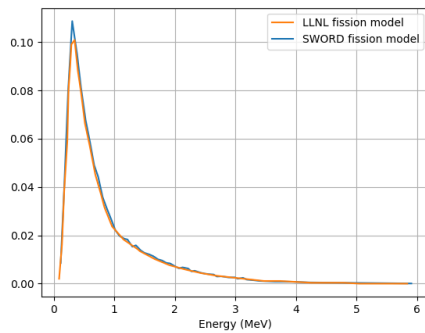


(b) Prompt neutron spectrum with photofission.

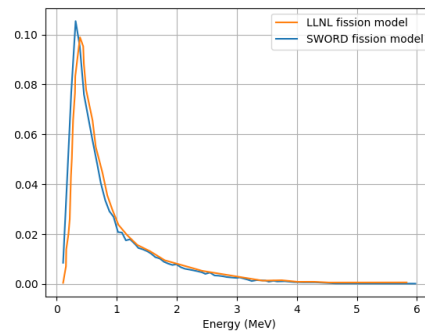
Fig. 5: Prompt neutron spectrum with thermal neutron fission of  $^{235}_{92}\text{U}$ . SWORD data in blue, Watt spectrum [6] in orange.

### 3.3.5 Prompt $\gamma$ and neutron energy spectra

The energy spectra of prompt fission  $\gamma$  and neutrons are important for several reasons. Simulation of active interrogation detectors and other instruments that use fission spectra to identify materials rely on these spectra. For prompt neutrons, the energy should be close to a Watt spectrum; the LLNL fission library uses a modified Watt spectrum to set the energy of the neutrons. We studied both the neutron and gamma prompt spectra.



(a) Prompt  $\gamma$  spectrum with thermal fission.



(b) Prompt  $\gamma$  spectrum with photofission.

Fig. 6: Prompt  $\gamma$  spectrum with thermal neutron fission of  $^{235}_{92}\text{U}$ . SWORD data in blue, LLNL [6] in orange.

Comparison between SWORD’s fission implementation and the LLNL fission library are shown in Figure 5 for neutron spectra and Figure 6 for  $\gamma$  spectra. For neutron induced fission, the SWORD library has its neutron spectral peak at 0.91 MeV, whereas the LLNL library has its neutron spectral peak at 0.80 MeV [6]. This 10% difference is likely due to differences in binning, since this difference is less than one bin width (SWORD uses bin widths of 0.15 MeV). For neutron induced fission, the SWORD library has its  $\gamma$  spectral peak at 0.31 MeV, and the LLNL library has its  $\gamma$  spectral peak at 0.34 MeV.

### 3.3.6 Time spectra of delayed products

One of the important Rapiscan fixes to the LLNL fission model was the addition of delayed neutrons through a virtual daughter particle. This particle does nothing except decay into a neutron at some time; it exists solely to implement delayed neutron decays which are not included in the Geant4 radioactive decay model.

The delayed gamma spectrum is a dependent on the fission fragments, which have already been validated (see section 3.3.4). This is because the time history is determined by the superposition of the decay lives of the radioactive fission products. Here, time delay refers to the time at which the particle is produced after the initial fission. For competence, we studied the time spectra, and good qualitative agreement is shown in Figure 7 of the normalized time spectra. Table 3 shows very good agreement in particle populations between reference data and SWORD at 1, 10 and 100 seconds after the fission.

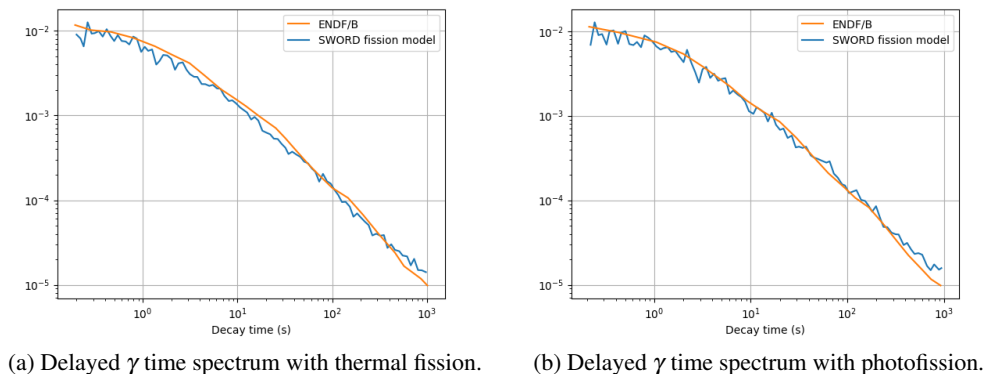


Fig. 7: Delayed  $\gamma$  time spectrum with thermal neutron fission of  $^{235}_{92}\text{U}$ . The histograms show normalized counts versus time in seconds. SWORD data in blue, ENDF/B [5] in orange.

## 4. CONCLUSIONS

The primary achievement of this work done under the Jerome and Isabella Karles Distinguished Scholar Fellowship was the successful implementation of accurate fission physics into the SWORD software package. The SWORD implementation was a threefold effort. First, the SWORD simulation engine was updated to accommodate a new physics library and increase performance. Next, the new fission physics library was carefully integrated into SWORD using modern software engineering methods. Finally, the newly integrated library was validated to ensure that it had been properly integrated and that fission physics was accurately modeled. This work will be included in the upcoming release of SWORD 7. SWORD can now model nuclear reactors and other fissions sources, as well as the next-generation of fission based detectors.

Table 3—Comparison of normalized time-delayed counts from SWORD simulation and reference. Reference data sourced from [6].

time delay (s)	Fission type	Sim normalized counts	Ref normalized counts
1	thermal neutron	0.0060	0.0074
1	photofission	0.0068	0.0074
10	thermal neutron	0.0013	0.0014
10	photofission	0.0011	0.0014
100	thermal neutron	0.00014	0.00013
100	photofission	0.00012	0.00013

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