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Development of Experimental and Computational Non-Destructive Assay Techniques for the Safe- guards of Lead-Cooled Reactor fuel

TESI DI LAUREA MAGISTRALE IN
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Abstract

Computational methods for particle transport play an important role in developing Non-Destructive Assay (NDA) techniques for Nuclear Safeguards. Simulations support the design and optimization of NDA instruments, the interpretation of measurements, and the study of scenarios not easily accessible experimentally. Validation against experimental data is essential to ensure predictive reliability and confidence in numerical models for safeguards applications.

This work, conducted during the Scientific Traineeship program at the Joint Research Centre (JRC) of the European Commission in Ispra, combines Monte Carlo and deterministic approaches to address challenges in safeguards verification for advanced nuclear reactor systems.

The main contribution is the design and assessment of a Passive Neutron Coincidence Collar (PNCC) for the safeguards verification of fresh fuel assemblies in the ALFRED (Advanced Lead Fast Reactor European Demonstrator) concept. The use of highly plutonium-enriched Mixed Oxide (MOX) fuel results in significant spontaneous neutron emission, making passive coincidence measurements a suitable NDA approach. A Monte Carlo model was developed using MCNP-PTA, an extension of MCNP for neutron coincidence counting applications developed at JRC Ispra, and experimentally validated using ^{252}Cf and plutonium oxide (PuO_2) samples. The validated model was then applied to ALFRED fuel assemblies, demonstrating the capability to quantify plutonium content and assess sensitivity to diversion scenarios.

In parallel, advanced deterministic methods based on low-rank Tensor Train representations were investigated for solving high-dimensional particle transport problems with improved computational efficiency.

The results demonstrate how experimentally validated particle transport modeling and efficient numerical methods can expand the capabilities of NDA methodologies for safeguards applications in next-generation nuclear systems.

Keywords: Nuclear Safeguards, Non-Destructive Assay, Neutron Coincidence Collar,

Lead-Cooled Reactor, Tensor Train

Abstract in lingua italiana

I metodi computazionali per il trasporto di particelle svolgono un ruolo importante nello sviluppo di tecniche di Analisi Non Distruttiva (NDA) per le salvaguardie nucleari. Le simulazioni supportano la progettazione e l'ottimizzazione degli strumenti NDA, l'interpretazione delle misure e lo studio di scenari non facilmente accessibili sperimentalmente. La validazione rispetto ai dati sperimentali è essenziale per garantire l'affidabilità predittiva e la fiducia nei modelli numerici per applicazioni di salvaguardia.

Questo lavoro, svolto durante il programma di tirocinio scientifico presso il Centro Comune di Ricerca (JRC) della Commissione Europea a Ispra, combina approcci Monte Carlo e deterministici per affrontare le sfide legate alla verifica di salvaguardia.

Il contributo principale consiste nella progettazione e nella valutazione di un Collare Passivo a Coincidenza Neutronica (PNCC) per la verifica di salvaguardia degli assemblaggi di combustibile freschi del concetto di reattore ALFRED (Advanced Lead Fast Reactor European Demonstrator). L'impiego di combustibile a ossidi misti (MOX) ad alto arricchimento in plutonio comporta una significativa emissione neutronica spontanea, rendendo le misure passive di coincidenza una metodologia NDA particolarmente adatta. È stato sviluppato un modello Monte Carlo mediante MCNP-PTA, un'estensione di MCNP per applicazioni di conteggio in coincidenza dei neutroni sviluppata presso il JRC di Ispra, e validato sperimentalmente utilizzando campioni di ^{252}Cf e ossido di plutonio (PuO_2). Il modello validato è stato successivamente applicato ad assemblaggi di combustibile ALFRED, dimostrando la capacità di quantificare il contenuto di plutonio e di valutare la sensibilità a possibili scenari di diversione.

Parallelamente, sono stati investigati metodi deterministici avanzati basati su rappresentazioni a basso rango nel formato Treno di Tensori per la risoluzione efficiente di problemi di trasporto delle particelle ad alta dimensionalità.

I risultati dimostrano come la modellazione del trasporto neutronico validata sperimentalmente e l'impiego di metodi numerici efficienti possano ampliare le capacità delle metodologie NDA per applicazioni di salvaguardia nei sistemi nucleari di nuova generazione.

Parole chiave: Salvaguardie Nucleari, Analisi Non Distruttiva, Collare a Coincidenza
Neutronica, Reattore al Piombo, Treno di Tensori

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1 | Introduction

1.1. Nuclear safeguards

Since the dawn of the atomic age, it has been understood that nuclear materials can offer significant benefits to society while also introducing unprecedented risks. The development and expansion of nuclear energy after the Second World War created an urgent need for international mechanisms capable of preventing the proliferation of fissile materials and nuclear components for military purposes.[1]

In the United States, the Atomic Energy Act [2] marked a turning point by permitting the civilian use of nuclear technology in private industry. Nuclear materials began to be employed for power generation, medical diagnosis and therapy, scientific research, space applications, and industrial processes. However, the growth of peaceful nuclear programs raised concerns about the potential diversion of nuclear materials for the production of nuclear weapons or radiological dispersal devices.

In response, the international community moved toward institutional safeguards. In 1957, the Euratom Treaty [3] established a regional safeguards system within Europe, granting inspectors authority to verify nuclear activities in member states. In the same year, the International Atomic Energy Agency (IAEA) was founded as an autonomous organization within the United Nations. The IAEA has the mandate to both promote the peaceful use of nuclear energy and to ensure that such activities would not contribute to military purposes.

Safeguards in principle differentiate between nuclear materials such as uranium, plutonium and thorium, and non-nuclear materials such as heavy water, graphite or Zircaloy tubes. For the former a significant quantity (SQ) is defined as the amount of material that could be used to manufacture a nuclear explosive device. Timely detection criteria and verification methods are then established for various possible diversion scenarios and material types.

During the 1960s, the rapid expansion of nuclear technology intensified global proliferation

concerns. Although safeguards already existed in the form of facility-specific agreements, the entry into force of the Treaty on the Non-Proliferation of Nuclear Weapons (NPT, [4]) in 1970 marked a fundamental shift toward comprehensive safeguards. Under Article III of the NPT, non-nuclear-weapon states committed to accepting safeguards inspections on all of their nuclear facilities.

The technical and legal framework for these comprehensive safeguards was formalized in 1972 through INFCIRC/153 [5]. This framework, often referred to as “traditional safeguards,” was primarily based on nuclear material accountancy, supported by containment and surveillance measures, and focused on verifying the non-diversion of declared nuclear material.

The discovery in the early 1990s of undeclared nuclear activities in Iraq revealed limitations in the traditional safeguards system, which had been designed mainly to verify declared material and facilities. In response, the IAEA developed a strengthened safeguards system through the Model Additional Protocol, INFCIRC/540 (1997) [6]. The Additional Protocol expanded the Agency’s access to information and sites, enabling it not only to verify the non-diversion of declared nuclear material but also to provide credible assurance of the absence of undeclared nuclear activities. This evolution laid the foundation for what is now referred to as integrated safeguards.

The most straightforward ways to account for nuclear material are weighing, item counting, volume determination. A complete assay of nuclear materials needs also more advanced measuring methods that are able, within their sensitivity, to verify the composition of the examined sample. These are generally subdivided in Destructive Assay (DA) and Non-Destructive Assay (NDA) techniques.

1.2. Non-Destructive Assay (NDA)

In order to determine nuclear material properties such as mass and composition, both for accounting and verification purposes, a series of measurement methods can be employed. These are divided in Destructive Assay and Non-Destructive Assay. [7, 8]

NDA methods mainly rely on the detection of radiation emitted from the sample, either by spontaneous decay (passive methods) or by reactions induced by an external interrogation source (active methods). In this way, the sample is not altered or destroyed during the measurement process, allowing the preservation of the integrity of the material. In contrast, Destructive Assay requires taking samples which have to be processed chemically to be studied and therefore cannot be returned to the original batch. While NDA is

generally less precise and accurate, it allows for faster and repeated measurements of the item as a whole.

NDA techniques are mainly classified in gamma spectrometry, neutron assay and calorimetry. Gamma-ray spectrometry is the most commonly used technique for isotopic composition verification. Each radionuclide emits photons at various energies, which make up its signature. The intensity of each peak is also recorded, hence making this both a qualitative and quantitative measurement.

Unlike gamma-rays, which are emitted by several isotopes, neutron emission is characteristic of only a few nuclear reactions, many involving special nuclear materials (SNM, enriched uranium and plutonium). This is why the detection of neutrons is widely employed in nuclear safeguards and security to verify the presence and quantify the mass of these type of materials.

Spontaneous fission can be an important source of neutrons, especially when even isotopes of plutonium are present. Fissions in the sample can also be induced by external neutron sources, most commonly (α, n) sources like AmBe or AmLi. Since most uranium and plutonium isotopes are α emitters, (α, n) reactions can also happen in the sample, for example on oxygen in oxide fuels. Both induced and spontaneous fission emit a variable number of neutrons with a certain probability distribution, known as multiplicity distribution, typical of each isotope. This is exploited by techniques like coincidence counting or multiplicity counting to assay the fissile material in the sample.

Calorimetry is based on the measurement of the decay heat in the sample. It can be quite accurate to quantify Pu content but because of the time needed to reach thermal equilibrium it does not find extensive application in safeguards.

1.3. Computational methods for particle transport

Computational methods are widely employed in the field of NDA in order to predict the response of NDA instruments and to analyze and support the results of measurements. With growing computational power and the development of more sophisticated algorithms, numerical simulations have become an indispensable tool for the design, optimization, and interpretation of NDA techniques. They bypass the need for extensive experimental campaigns, which can be costly and time-consuming, and to explore a wide range of scenarios and configurations that may not be easily accessible in the laboratory.

Neutrons and high-energy photons are the most common particles of interest for NDA applications. They are electrically neutral and can penetrate deeply into materials, mak-

ing them ideal for probing the internal structure of objects. Also their emission, either induced or spontaneous, is a signature that helps characterize nuclear materials. Their motion is governed by first-order kinetic (integro-differential) equations that describe the behavior as they move through a medium through distribution functions. [9]

When the full transport equation is needed, numerical solutions are required. Deterministic methods solve for the expected phase-space density directly, so the stochastic nature of individual histories is averaged into the distribution function and the cross sections. In these approaches, the phase space is approximated by a tensor-product discretization in space, angle, and energy, leading to a coupled system of algebraic equations whose size scales multiplicatively with the resolution in each variable. In realistic calculations, this results in extremely large linear systems.

Because of these computational challenges, the Monte Carlo method has historically been the dominant approach for simulating particle transport with detailed physics [10, 11]. Monte Carlo methods rely on random sampling to simulate the trajectories of individual particles, without solving the transport equation. In this way the stochastic nature of each interaction is captured at each simulation step, in which cross section data is used as the probability density from which to sample. During the simulation of the particle lifetimes, some aspects of their average behaviour (tallies) can be recorded and used to derive physical quantities of interest such as fluxes and reaction rates. Because of the central limit theorem, Monte Carlo tallies converge to the expected value for the model with statistical error decreasing with $(NPS)^{-1/2}$, where NPS is the number of particles simulated. Provided that N is sufficiently large, and that the cross section data are precise, the tallies will converge to real physical quantities with high accuracy. However, this can be computationally expensive, for example in problems with deep penetration or rare events, where they may require variance reduction techniques to obtain results in a reasonable time frame.

1.4. Aim of the thesis

This thesis is based on the work performed as part of the Scientific Traineeship program at the Joint Research Centre (JRC) of the European Commission in Ispra, Italy.

The main effort was devoted to the development of a NDA method for the fresh fuel verification of the ALFRED (Advanced Lead Fast Reactor European Demonstrator) fuel assembly. The fuel is a Mixed Oxides fuel (MOX) with high plutonium enrichment. For this scope a solution based on a Passive Neutron Coincidence Collar (PNCC) was proposed, and a Monte Carlo model was developed with the MCNP-PTA [12] software,

which is an extension of the widely used MCNP code for particle transport developed and benchmarked at JRC Ispra. The model was validated with experiments at the laboratories in Ispra, with ^{252}Cf and plutonium oxide (PuO_2) samples. The validated model was then used to run simulations with the ALFRED fuel assembly in porder to create calibration curves for the quantification of the plutonium content. Also diversion scenarios were simulated, like pin removal and replacement.

The objective of this research was to begin the development of NDA methodologies for advanced and small modular reactors (AMR/SMR), which are expected to play an increasingly important role in future low-carbon energy systems. As these reactor concepts often employ innovative fuel cycles and operating conditions, dedicated safeguards techniques will be required to verify nuclear material inventories and mitigate proliferation risks with good operational efficiency.

Contributions have also been made to another recently established research activity of the NDA team: the development of numerical methods to directly solve partial differential equations (PDEs) such as the ones governing neutron and photon transport physics. These methods are based on the Tensor Train format, which is a way to decompose high dimensional arrays which arise in the PDE discretization in a series of low dimensional ones. This can reduce memory and computational cost by orders of magnitude, enabling simulations before considered intractable. Support was given to the NDA team to implement a finite element solver for the neutron transport equation in TT format. Preliminary results for a simplified model are presented in the last chapter of this thesis, together with a discussion on future developments.

2 | The ALFRED project

This chapter introduces the ALFRED (Advanced Lead Fast Reactor European Demonstrator) project, which serves as the primary case study of this thesis. ALFRED is a lead-cooled fast reactor demonstrator and represents an important step toward the deployment of Generation IV nuclear technologies.

A brief history of Lead Fast Reactor development in Europe is provided, highlighting the key milestones and design efforts that have led to the current ALFRED concept.

Focus is then placed to the design of the fuel assembly and the characteristics of the fuel, which are relevant for the development of the NDA method presented in this thesis.

2.1. Lead fast reactor technology development in Europe

The next generation of nuclear energy systems, commonly referred to as Generation IV reactors, is being developed to achieve substantial improvements in safety, sustainability, reliability, and proliferation resistance, while remaining economically competitive with currently deployed nuclear power plants. These advanced systems aim to address the long-term challenges of nuclear energy, including more efficient fuel utilization, the reduction of long-lived radioactive waste, and enhanced intrinsic safety features [13].

A significant share of these advanced concepts is oriented toward Small Modular Reactors (SMRs), which are designed for factory fabrication and modular installation. Numerous private companies are actively involved in the research and development of SMRs technologies, supported by governments and international initiatives, such as the European Industrial Alliance on SMRs. This initiative seeks to facilitate and accelerate the development, demonstration, and deployment of the first SMR projects in Europe in the early 2030s [14].

Among the technologies selected by the Generation IV International Forum and European Industrial Alliance on SMRs, the Lead-cooled Fast Reactor (LFR) has emerged as a

promising candidate. The LFR concept is based on a fast neutron spectrum and employs liquid lead or lead-bismuth eutectic as primary coolant. The thermo-physical properties of lead provide several advantages: its very high boiling point allows reactor operation at near-atmospheric pressure, eliminating the risk of coolant boiling and its high density and thermal conductivity of lead enable efficient heat removal from the reactor core. The fast neutron spectrum also allows for the transmutation of minor actinides and efficient breeding or burning of plutonium, supporting the implementation of a closed nuclear fuel cycle and contributing to the reduction of long-lived radioactive waste.

The first major coordinated European design effort on LFR technology was the ELSY project (European Lead-cooled System), carried out between 2006 and 2010 and funded by the EURATOM Sixth Framework Programme (FP6) [15]. The objective of ELSY was to develop a conceptual design for a large-scale LFR suitable for commercial electricity production. The reference design consisted of a pool-type reactor with a thermal power of approximately 600 MW, using MOX fuel and liquid lead as coolant. The project successfully demonstrated the technical feasibility of a large lead-cooled fast reactor and provided a reference design for subsequent European research activities [16].

Building upon the results of ELSY, research continued through the LEADER project (Lead-cooled European Advanced Demonstration Reactor) between 2010 and 2014, funded under the EURATOM Seventh Framework Programme (FP7) [17, 18]. The primary goal of LEADER was to further develop the LFR concept and to design a demonstration reactor capable of validating the key technologies required for future commercial systems. This work led to the development of the ALFRED (Advanced Lead Fast Reactor European Demonstrator) project.

ALFRED [19] is conceived as a pool-type lead-cooled fast reactor demonstrator with a thermal power of approximately 300 MW, corresponding to an electrical output of roughly 100–125 MWe. The reactor is designed to use mixed oxide (MOX) fuel and operate with pure liquid lead coolant in the primary system. The pool-type configuration was selected in order to enhance passive safety and reduce the complexity of the primary circuit. The design incorporates several passive safety features, including natural circulation capability for decay heat removal and large thermal inertia provided by the lead coolant.

The main objective of ALFRED is to demonstrate the technological maturity of LFR systems, including materials compatibility with liquid lead, fuel performance in fast spectra, and the reliability of passive safety systems. In addition, the demonstrator aims to validate industrial construction techniques and operational procedures necessary for the deployment of commercial LFR plants. The project is being developed through a Euro-

pean collaboration involving industrial and research partners, including Ansaldo Nucleare, ENEA, and RATEN-ICN, and is currently planned to be constructed at the Mioveni nuclear research site in Romania.

Recent developments in European lead-cooled fast reactor programs include the collaboration agreement between the EAGLES consortium and Newcleo for the development of LEANDREA, a technology demonstrator and experimental facility intended to support the validation of materials and fuels for future Lead-cooled Fast Reactor (LFR) systems and enable subsequent demonstrators such as ALFRED. [20]

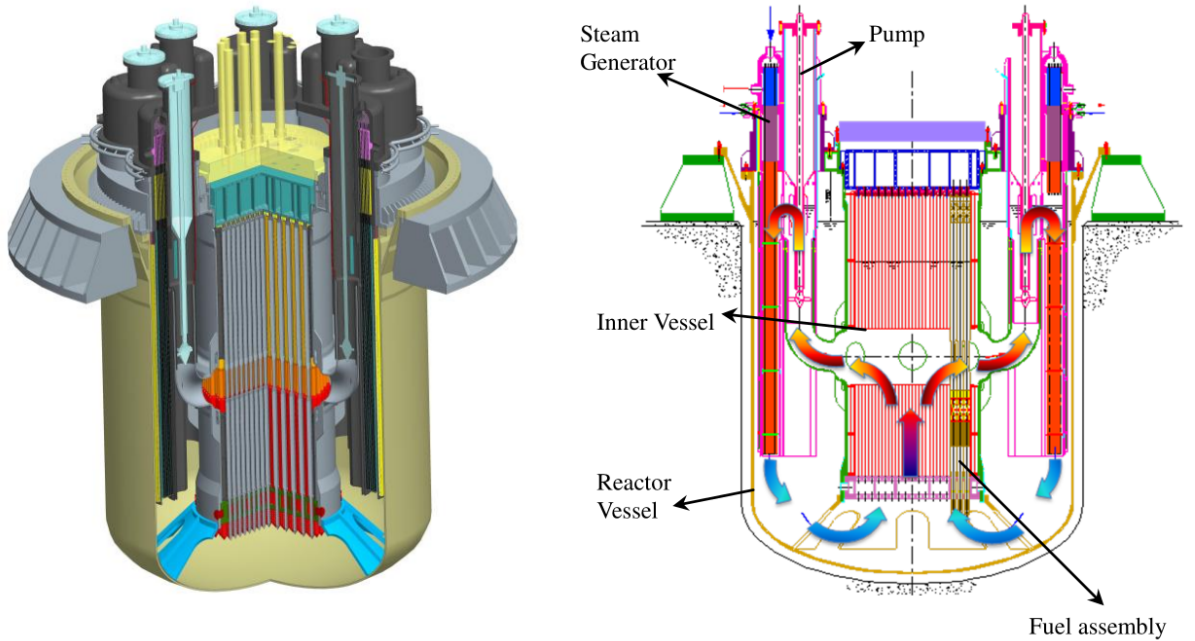


Figure 2.1: ALFRED 3D sketch and reactor block vertical section [18].

2.2. ALFRED fuel assembly design

The most recent core design of ALFRED [21] presents a hexagonal fuel assembly dimensioned as shown in figure 2.2

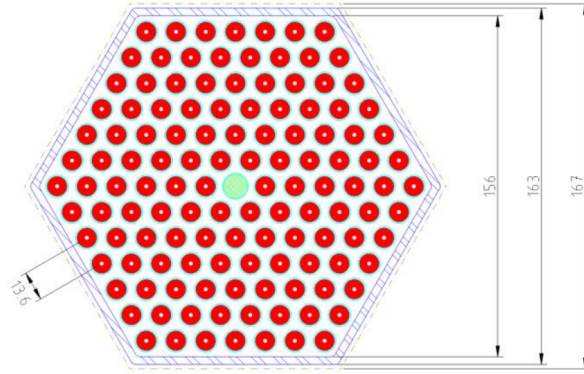


Figure 2.2: ALFRED fuel assembly cross section, dimensions in mm [21].

The core contains 134 fuel assemblies, each containing 126 fuel pins. Figure 2.3 shows a cross section of the core, which is divided in inner (lower enrichment) and outer (higher enrichment) zones. In the outermost part of the core, a layer of reflector assemblies is present, surrounded by another layer of absorbing assemblies. The core contains a total of 16 control and safety rods, and also a test assembly at its center.

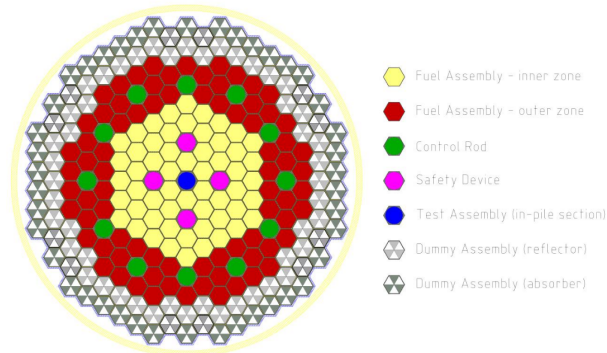


Figure 2.3: ALFRED core cross section [21].

The fuel pin geometry is described in detail in an older core design work [22]. Since then the fuel pin design has not appeared to have changed; we refer to that work for more details. The geometry is shown in figure 2.4.

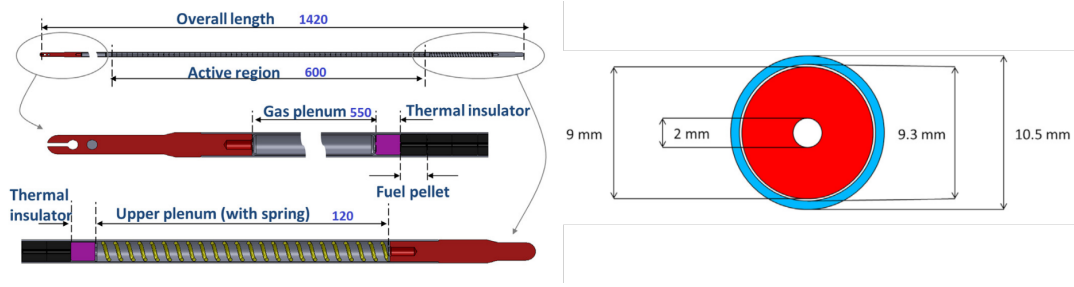


Figure 2.4: ALFRED fuel pin geometry. Dimensions in mm [22].

The fuel used in a 2014 optimization study [23] was a highly enriched in plutonium MOX fuel. The plutonium content expressed as fraction of total heavy metal was 21.7 wt% for the inner zone and 27.8 wt% for the outer zone. The fuel isotopic composition dated back to a 2009 study for the ELSY project [24] which described an oxide with reactor grade plutonium (^{240}Pu 26.9% of total plutonium). Tables 2.2 and 2.3 show the weight percentages for each isotope relative to the total oxide mass. The same optimization study considers a cladding made of AIM1 stainless steel with composition shown in table 2.1.

Element	Cr	Ni	Mo	Mn	Si	Ti	C	B	Fe
[wt%]	15.0	15.0	1.50	1.50	0.90	0.40	0.09	0.006	65.604

Table 2.1: Nominal chemical composition of AIM1 steel used as cladding material in the ALFRED fuel assembly [23].

Plutonium		Uranium		Oxygen (natural)	
A	wt%	A	wt%	A	wt%
238	0.447	234	0.002	16	11.651
239	10.900	235	0.279	17	0.004
240	5.174	236	0.007	18	0.024
241	1.170	238	68.864		
242	1.474				
Total	19.165		69.152		11.679

Table 2.2: Isotopic composition by weight percent (Inner zone) [24].

Each fuel pin contains 362 g of oxide, leading to a total fuel mass of 45.6 kg per assembly. The plutonium masses are 9.9 kg and 12.7 kg for the inner and outer zone respectively, which are both above the IAEA defined significant quantity for plutonium of 8 Kg. [25].

The high presence of even plutonium isotopes, especially ^{240}Pu , makes the fuel a strong neutron emitter via spontaneous fission processes. Using dedicated nuclear data [8] one

Plutonium		Uranium		Oxygen (natural)	
A	wt%	A	wt%	A	wt%
238	0.573	234	0.002	16	11.651
239	13.964	235	0.258	17	0.004
240	6.629	236	0.006	18	0.024
241	1.499	238	63.502		
242	1.889				
Total	24.553		63.768		11.679

Table 2.3: Isotopic composition by weight percent (Outer zone) [24].

can estimate the spontaneous fission yield of a single assembly to be 4.15×10^6 and 5.31×10^6 neutrons per second for the inner and outer zone respectively.

Since most of the heavy metal isotopes are α emitters, (α, n) reactions on oxygen are also a very important source of neutrons. In order to have a first order of magnitude estimate of the neutron yield from (α, n) reactions, one can use experimental coefficients for pure Pu oxide [26]. For a single assembly it is found to be 3.4×10^6 and 4.4×10^6 neutrons per second for the inner and outer zone respectively.

The very high emission of neutrons suggests that passive neutron assay techniques would be definitely sufficient to verify the presence of the fuel and to quantify its plutonium content. This is the main reason why a Passive Neutron Coincidence Collar will be proposed in this work as a NDA technique for the verification of ALFRED fuel assemblies.

3 | Design of a Passive Neutron Coincidence Collar (PNCC)

This chapter introduces the theoretical background of neutron coincidence counting and the main characteristics of neutron coincidence collars, which constitute the selected non-destructive assay (NDA) technique for ALFRED fuel assemblies.

The Monte Carlo modeling approach adopted for the analysis is then presented, with particular focus on the MCNP-PTA software developed at the JRC.

Finally, the chapter describes both the experimental setup and the computational design methodology used for the development and assessment of the neutron collar.

3.1. Coincidence counting

Neutrons emitted by a nuclear item can originate from several physical processes, principally spontaneous fission, induced fission and (α, n) reactions. These mechanisms differ not only in their neutron energy spectra but also in the temporal correlations of the emitted neutrons [8].

Each fission event produces a multiplicity of prompt (and delayed) neutrons. As a consequence, neutrons originating from the same fission event are said to be correlated in time. In contrast, neutrons generated by (α, n) reactions are emitted individually, producing an essentially random time sequence of detections.

In a typical coincidence counter used in safeguards applications, after their emission neutrons undergo transport and moderation and are captured in the detector system. During these processes the time correlations remain observable over a characteristic response time of the order of tens of μs .

Neutron coincidence counting exploits these temporal signatures to distinguish correlated fission neutrons from random neutron backgrounds. Rather than attempting to identify individual fission events, the method analyzes the statistical properties of the detector

pulse train and quantifies the probability of observing detections within predefined time windows.

In neutron coincidence measurements, detected events are classified according to their temporal correlation. The simplest observable is the singles rate S , defined as the total count rate of detected neutrons, regardless of their origin or correlation.

More informative is the doubles rate D , which represents the rate of correlated neutron pairs detected within a short time interval. These pairs predominantly arise from fission events, where multiple neutrons are emitted nearly simultaneously. In contrast, neutrons from (α, n) reactions contribute mainly to the singles rate and only weakly to the doubles rate due to their random emission.

Higher-order correlations, such as the triples rate T , can also be measured, corresponding to the detection of three correlated neutrons. However, for many practical applications, the singles and doubles rates provide sufficient information for material characterization. This also happens because the detection of triples is statistically less probable and requires longer measurement times to achieve acceptable precision.

The knowledge of both singles and doubles count rates allows discrimination between different neutron sources and enables quantitative assay of nuclear material. Operationally, the doubles rate is considered proportional to the fission rate in the sample and therefore to the fissile content. A calibration curve can be established for a specific fuel assembly, either experimentally or computationally, allowing the determination of unknown samples based on their measured singles and doubles rates.

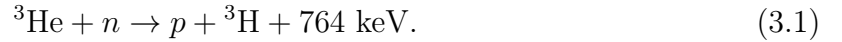
In the 1980's a mathematical model was developed at the JRC by Hage and Cifarelli [27–30] for the probability distribution of neutron signal multiplets from a detector in a time interval. It is called the point model, and it is based on assumptions that may not always be verified in real measurements (such as constant uniform efficiency in the detector geometry), but that allow to derive analytical equations for the singles, doubles and triples rates as a function of the sample properties and the detector characteristics. The expressions are not reported here because, as it will be shown in the experimental validation campaign (chapter 4.2), the detection efficiency varies significantly in the neutron collar cavity, hence the point model is not applicable to the ALFRED fuel assembly. However, it is still a very useful tool to understand the physics of neutron coincidence counting and to derive first order estimates of the expected count rates.

3.2. Neutron coincidence collars

A neutron coincidence collar is a NDA instrument designed to measure correlated neutron emissions from nuclear fuel assemblies. It is routinely employed by international safeguards authorities to verify the fissile content of fresh nuclear fuel, particularly for light water reactor fuel assemblies [31–33]. By exploiting neutron multiplicity and time-correlation measurements, coincidence collars provide sensitivity to the amount of fissile material while remaining non-invasive.

The detector typically consists of an array of cylindrical ^3He proportional counters embedded in a moderating material, usually high-density polyethylene (HDPE), and arranged around the inspected item. The role of the moderator is to thermalize fast neutrons emitted by the sample. Since the neutron capture cross section of ^3He strongly increases at low energies, moderation substantially improves the detection efficiency.

Neutron detection occurs through the reaction [34]



After entering the proportional counter, a thermal neutron is captured by a ^3He nucleus, producing a proton (p) and a triton (^3H). These charged particles deposit their kinetic energy through ionization of the detector gas. Under the electric field applied between the detector wall and the central anode wire, the ionization electrons (ions) drift toward the wire (tube wall) and initiate gas multiplication near the anode, generating a measurable current pulse.

Since the (n, p) cross section increases at low neutron energies, the presence of a moderator is essential to thermalize fast neutrons and enhance the detection efficiency.

Coincidence collars, designed to identify fission events, exploit not only the total neutron count rate but also the temporal correlations between detections. By counting correlated detections (doubles count rate), the system becomes sensitive to spontaneous or induced fission processes and therefore to the quantity of fissile material present.

Two operational modes are commonly employed. In active assay mode, an external neutron source, typically AmLi (of about 300 keV) is used to induce fission in the sample, increasing the correlated neutron signal and enabling measurements of low spontaneous-emission materials such as ^{235}U enriched fuel. In passive mode, the instrument relies exclusively on spontaneous neutron emission from the item.

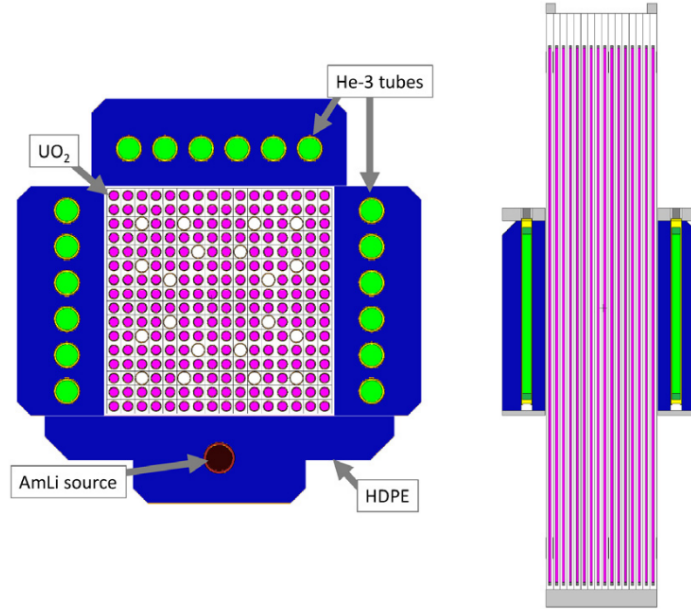


Figure 3.1: Example of a neutron coincidence collar in active configuration, with the fuel assembly in the central cavity and the ^3He detectors arranged around it [33].

The electronic processing chain is designed to preserve the timing information of detector pulses required for coincidence analysis. Signals generated in the ^3He counters are amplified and shaped by the front-end electronics, which also apply discrimination via single channel analyzer (SCA) to reject noise and spurious events. Digital logic pulses are generated and the resulting pulse train is analyzed by coincidence counting electronics, typically implemented using shift-register logic.

3.3. Shift register counting logic

Coincidence information in neutron detection systems is commonly extracted using shift register electronics. In this approach, each detected neutron triggers a pre-delay (P) designed to mitigate issues due to double-pulse pile-up and electronic transients. After this delay, the event opens a temporal coincidence gate of fixed width (G), during which subsequent detections are recorded as either true or accidental coincidences. The measured rate within this gate is therefore the sum $D+A$, where D is the true doubles rate and A represents accidental coincidences.

The Rossi- α distribution characterizes the time-correlation of neutrons. It is the conditional probability of detecting a correlated neutron at the time interval $[t, t + \Delta t]$ after the detection of a trigger neutron at $t = 0$.

The Rossi- α distribution can usually be well described by a single exponential with time constant τ , which is called the die-away time of the detector system. The value of τ mainly depends on the geometry, materials and their moderating and capture properties.

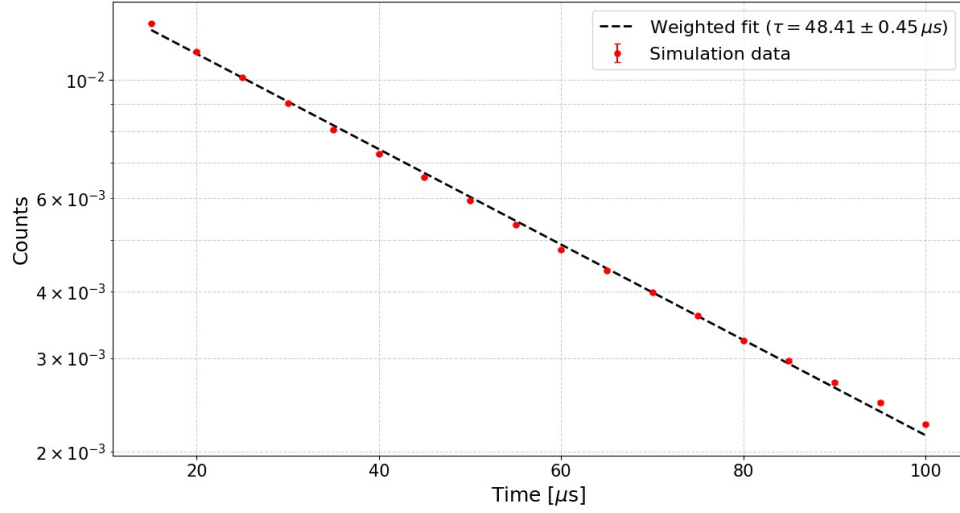


Figure 3.2: Die-away time ($\tau = 48.41 \pm 0.45 \mu s$) of the Passive Neutron Coincidence Collar designed in this work. Counts were computed via Monte Carlo simulations with time bin tallies and a ^{252}Cf point source, and a linear fit weighted with the simulation uncertainties was applied to their logarithm.

The die-away time plays a central role in determining the optimal coincidence gate width. The gate must be sufficiently long to capture correlated neutrons originating from the same fission event, while remaining short enough to minimize contributions from uncorrelated (accidental) coincidences.[35]

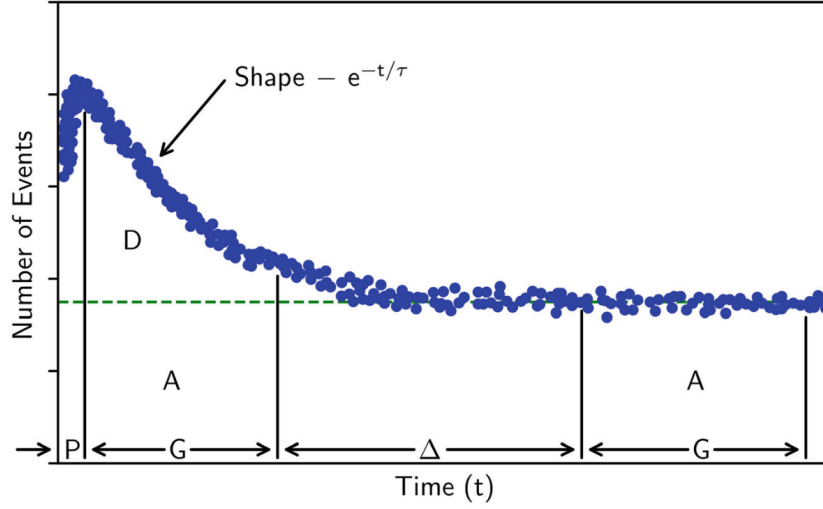


Figure 3.3: Rossi- α distribution illustrating the different time gating logic following a trigger neutron detection: pre-delay (P), gate width (G) and long delay (Δ) [8].

To estimate and correct for the accidental contribution, a second delayed gate of identical width G is introduced. This gate is shifted in time by an interval Δ relative to the prompt gate, ensuring that it samples only uncorrelated events. The accidental rate A is then estimated from this delayed gate, allowing the true doubles rate to be obtained as:

$$D_{\text{true}} = \underbrace{(D + A)}_{\text{prompt}} - \underbrace{A}_{\text{delayed}} \quad (3.2)$$

Modern systems often also support list-mode acquisition, in which each detected neutron is recorded with a timestamp and detector identifier. This approach enables offline reconstruction of coincidence gates, flexible adjustment of timing parameters, and improved dead-time correction. It also allows more advanced correlation analyses without requiring repeated measurements. [8]

3.4. Monte Carlo modeling with MCNP-PTA

For neutron detection systems such as neutron coincidence collars, the assumptions underlying point models are generally not valid. In these systems, the detector geometry, material heterogeneities, neutron moderation, absorption, and spatial correlations strongly influence the measured response. As a consequence, simplified analytical models cannot accurately predict the multiplicity response of the system.

Computer simulations therefore play a fundamental role in the design and calibration of

neutron coincidence counting systems. Their main advantage lies in the ability of supporting and reducing experimental effort and associated costs. To achieve reliable predictions, a numerical tool must be capable of accurately modeling the detector geometry, material compositions, nuclear cross sections, and, most importantly, solving the neutron transport equation within complex computational domains. To ensure this, an experimental validation of the simulation model can be performed using well-characterized neutron sources and reference materials, allowing for the comparison of simulated and measured count rates. This validation step is crucial to establish confidence in the predictive capabilities of the simulation tool. Once validated, the model can then be used to explore a wide range of scenarios, including materials and configurations that may not be easily accessible in the laboratory.

Because of the geometrical and physical complexity of these systems, deterministic transport methods often become impractical due to their high memory and computational requirements. For this reason, Monte Carlo methods progressively emerged during the 1990s as the preferred approach for non-destructive assay (NDA) applications in nuclear safeguards [12]. By statistically simulating individual particle histories, Monte Carlo techniques can naturally handle arbitrary geometries and detailed interaction physics with high accuracy. Among the available Monte Carlo particle transport codes, MCNP (Monte Carlo N-Particle), developed at Los Alamos National Laboratory, is one of the most widely used and validated tools [36]. Over the years, it has been extensively applied to nuclear safeguards problems and, in particular, to the simulation of neutron coincidence collars [33, 37, 38]. MCNP enables detailed modeling of detector systems, including complex geometries, material compositions, and neutron interaction physics based on evaluated nuclear data libraries.

MCNP-PTA (Pulse Train Analysis) is an extension of MCNP developed at the JRC Ispra specifically for coincidence and multiplicity counting applications [12]. In addition to particle transport, MCNP-PTA includes the capability to simulate the time-dependent response of neutron detectors and to reconstruct detector pulse trains, allowing a realistic analysis of coincidence counting observables.

MCNP-PTA is based on the 4c2 version of standard MCNP, to which various modifications have been made. Firstly, spontaneous fission and (α, n) sources were added with respective yields and spectra. A user has to define the isotopic composition of the source material, and the code will automatically calculate the neutron emission rate and energy distribution based on the nuclear data made available to the software. The user can choose to simulate spontaneous fission only, (α, n) only or both sources, hence being able to study their contribution separately. The standard MCNP source definition (SDEF) is

also available to be used.

In order to simulate spontaneous fission events, which emit multiple neutrons, the code was modified to generate a number of particles sampled from the appropriate multiplicity distribution for each source event. This allows for a more accurate representation of the correlated neutron emissions that are critical for coincidence counting analysis. Fission neutron multiplicity sampling can be selected to be based on J. Frehaut's method [39] which approximates the distribution as a Gaussian with mean and variance depending on the isotope, or on a polynomial fit to experimental data. (α, n) yields and spectra are calculated with the code SOURCES-4C [40, 41].

Another key feature of MCNP-PTA is its ability to model the detector electronics. User-defined parameters include detector dead time, pulse shaping time, and counterbank configuration (i.e., the number of detectors connected to a single amplifier channel).

During the particle transport simulation, MCNP-PTA records neutron detection events in list mode, storing the detection time and associated counterbank identifier for each event. After the transport simulation is completed, the PTA module processes this event list to generate the corresponding electronic pulse train and account for count losses due to pulse-shaping amplifier updating dead time. Additional losses introduced by logical-OR summation are also included unless digital mixing is selected.

The simulated pulse train is then analyzed using a shift-register algorithm with user-defined pre-delay and gate width, reproducing the processing performed in experimental measurements and yielding the singles and doubles count rates.

It must be noted that MCNP-PTA was developed in the early 2000s, with the last updates dating back to 2009. Since then, the code has been used for various applications in the field of nuclear safeguards, but it has not been actively maintained or updated. For this reason, some memory constrained were encountered while trying to use newer cross section libraries (ENDFB-VII.1, available with MCNP6), which have a much higher resolution than the ones available at the time of the code development. For each simulation presented in this thesis will therefore indicate which cross section library was used. Also the number of particles simulated (NPS) was reported for each simulation, since it is a key parameter to estimate the statistical uncertainty of the results.

The statistical uncertainty of the simulated count rates was estimated by repeating the Pulse Train Analysis (PTA) procedure 20 times using independent realizations of the source event sequence and time sampling. The resulting variation among the repeated analyses provides a practical estimate of the statistical uncertainty associated with the

simulated count rates.

In order to have comparison with experiments, nuclear data relative to some isotopes of californium (^{250}Cf) and curium (^{246}Cm , ^{248}Cm) were added [42], containing spontaneous fission decay constants and multiplicity distribution, which previously were present only for ^{252}Cf .

3.5. Proposed design of the PNCC for the ALFRED fuel assembly verification

As already mentioned, the high spontaneous neutron emission of the ALFRED fuel assembly suggests that passive neutron assay techniques, without an interrogation source, would be sufficient to verify the presence of the fuel and to quantify its plutonium content. This has been historically done to verify Pu content in fast-breeder reactors, MOX fuels for light water reactors and spent fuel assemblies [43].

A JCC-71 collar by Canberra Industries Inc. was used, which is a standard and well characterized detector of this type [44], routinely employed by nuclear safeguards inspectorates (IAEA and Euratom) for spent fuel verification measurements. As shown in 4.2, the system was operated in passive neutron coincidence configuration. In contrast with the active configuration, the bank containing the neutron source is replaced with a fourth ^3He bank, in order to maximize the detection efficiency and therefore the sensitivity to the spontaneous neutron emission of the fuel assembly. Each bank contains six ^3He proportional counters, for a total of 24 detectors.

The ^3He tubes used were Reuter-Stokes model RS-P4-0813-101 [45]. The proportional fill gas mixture at 5.35 atm pressure shown in table 3.1. The tubes have an outer diameter of 2.54 cm and an active length of 33.02 cm. The detector wall is made of Aluminium Alloy 1100-F with a thickness of 0.8 ± 0.06 mm, which was computed experimentally via gamma ray attenuation at the JRC-Ispra laboratories.

Species	Mass %
^3He	20.935
Ar	69.323
CH_4	9.742

Table 3.1: Gas mixture composition in the ^3He proportional counters.

The moderator geometry was reproduced as a polyethylene matrix with density to be $\rho = 0.965\text{g/cm}^3$, which is a measured value for the HDPE available at the JRC-Ispra

laboratories used for coincidence counting systems. Each bank has a height of 39 cm, while the central cavity is 23.5×17 cm to comfortably accommodate the ALFRED fuel assembly. The polyethylene blocks included an aluminium support plate at the bottom of each bank of 1 cm in thickness.

The full detector geometry and materials composition was implemented in MCNP-PTA, reproducing the exact spatial arrangement of the four banks, the positioning and detailed geometry of the ^3He tubes, and the central measurement cavity.

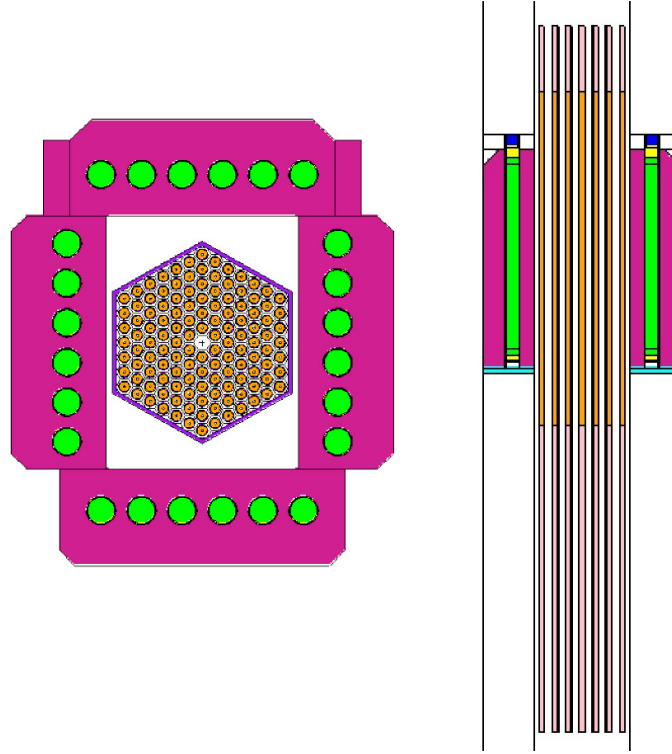


Figure 3.4: MCNP-PTA geometry of the Passive Neutron Coincidence Collar with the ALFRED fuel assembly in the central cavity. (The views are not to scale for better visualization)

The electronics acquisition chain, as well modeled in MCNP-PTA, consists of a single amplifier connected to each bank of six ^3He tubes. For all experiments and simulations, the shift register module was configured with a $4.5 \mu\text{s}$ pre-delay and a $64 \mu\text{s}$ coincidence gate width, which are typical values for neutron coincidence counting systems. Also the detector dead-time was set to $1 \mu\text{s}$ and the pulse shaping time to 50 ns .

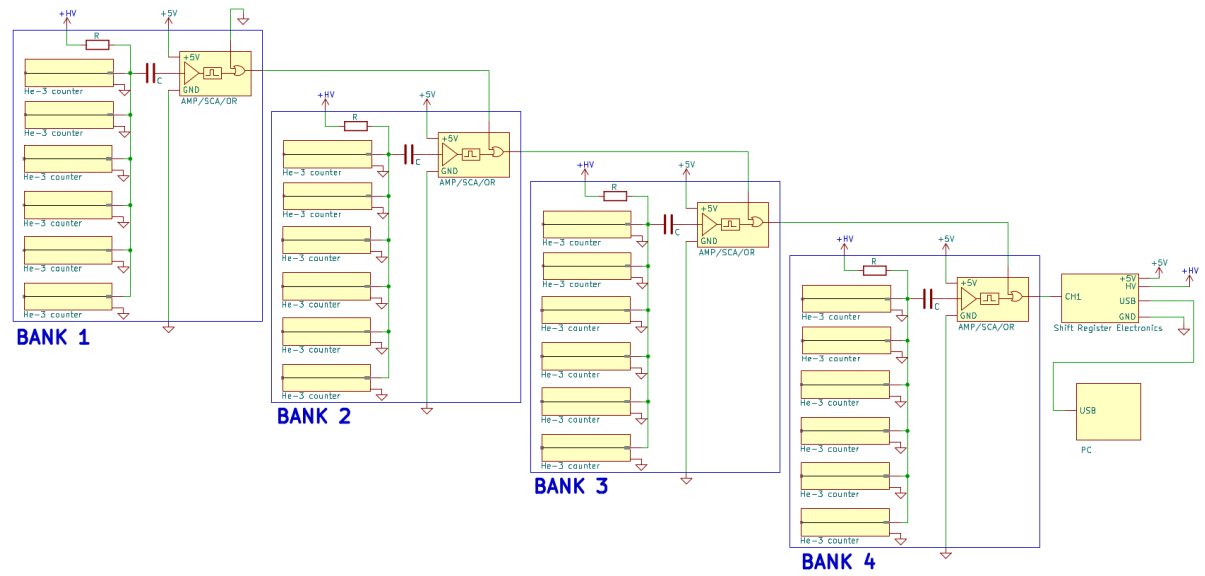


Figure 3.5: Schematic of the electronics acquisition chain of the Passive Neutron Coincidence Collar. Each bank of six ^3He tubes is connected to a single amplifier, and the outputs are processed by a shift register module for coincidence analysis.

4 | Experimental validation of the Monte Carlo model

Before the Monte Carlo model can be used to predict the response of the Passive Neutron Coincidence Collar for the ALFRED fuel assembly, its ability to reproduce measured detector signals must be demonstrated. This chapter therefore (i) describes the experimental arrangements used at the JRC-Ispira laboratories, (ii) presents the validation against a calibrated ^{252}Cf spontaneous-fission neutron source, and (iii) reports the comparison with reference measurements obtained using plutonium-oxide reference materials. The validated model in MCNP-PTA will subsequently provide the calibration curve employed in Chapter 5, allowing the detector performance to be extrapolated to the full fuel assembly.

4.1. Experimental setup

Experimental sessions were performed at the JRC laboratories in Ispira, Italy.

A first experimental setup in Ispira's Physics Lab, shown in Figure 4.2, was used for the first measurements with ^{252}Cf . The collar was placed on a table at a height of 70 cm from the floor, and the sources were placed in various positions within the central cavity. The floor was made of standard concrete, which was included in the simulation geometry to account for neutron back-scattering effects.

The electronic acquisition chain of the collar consists of a standard neutron coincidence counting system, in which a single amplifier was connected to each ^3He tube bank, hence having six tubes per amplifier. A detector bank is shown in Figure 4.1.

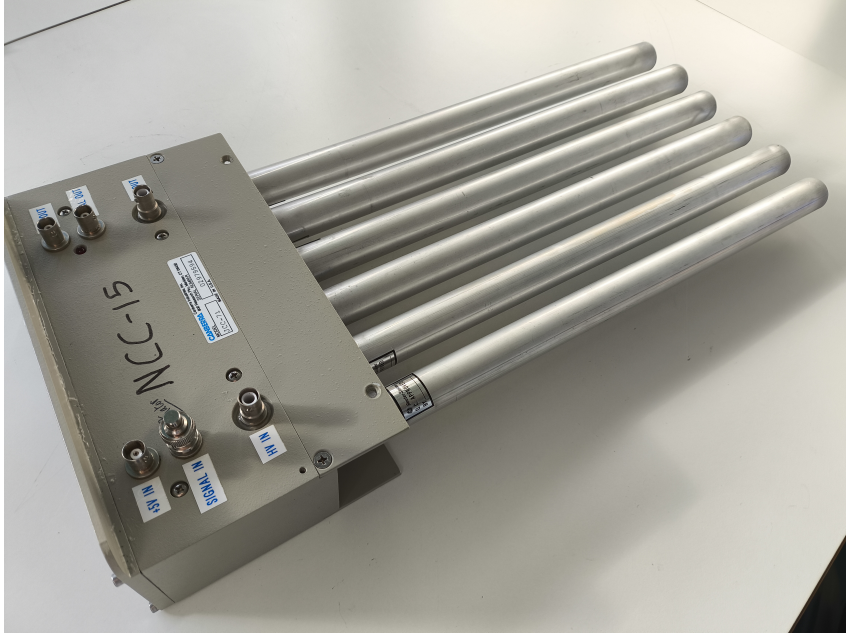


Figure 4.1: He-3 tube bank to be inserted in the HDPE matrix. The six tubes, signal ports, 5V, and HV in/out ports can be seen.

The detector banks were powered using a daisy-chain configuration for both the high-voltage (HV) supply and signal distribution. In this arrangement, only one of the four banks was directly connected to the main electronics and power supply unit. This primary connection provided the operating high voltage for the ^3He proportional counters, set to 1680 V, together with the 5 V supply required for the associated signal processing electronics.

The remaining detector banks were connected sequentially through dedicated input/output (in/out) connectors located on each bank. In this way, the HV and low-voltage signals were distributed from one bank to the next without requiring independent cabling from the main acquisition system to each individual module. The signal output port in each bank was then connected independently to the shift register module.

A N2000 shift register module by ANTECH [46] was used for real-time multiplicity analysis, applying $4.5 \mu\text{s}$ pre-delay and a $64 \mu\text{s}$ coincidence gate width.

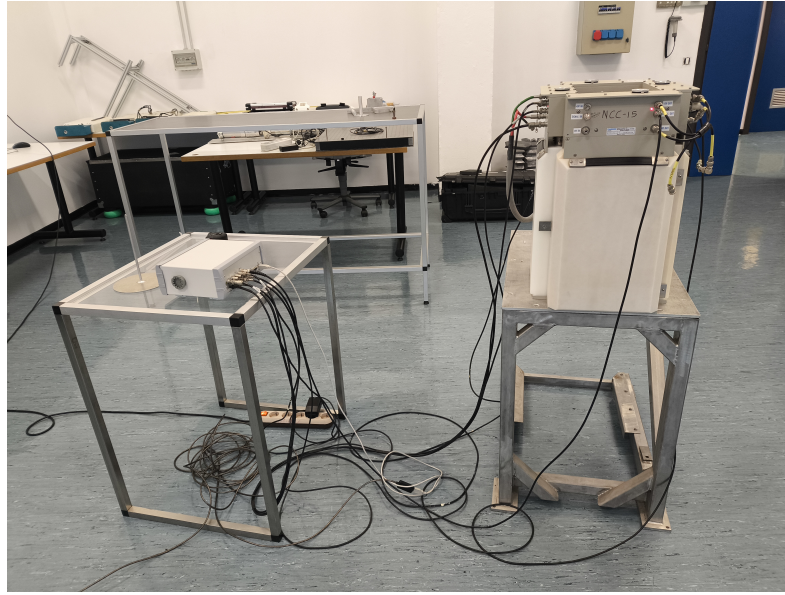


Figure 4.2: Experimental setup in Physics Laboratory

In order to remove the uncertainty related to neutron backscattering from the floor, a second setup was built in the laboratory, 4.3 which allowed to place the collar at a height of 150 cm from the floor. This setup was used for a second measurement with a different ^{252}Cf source.

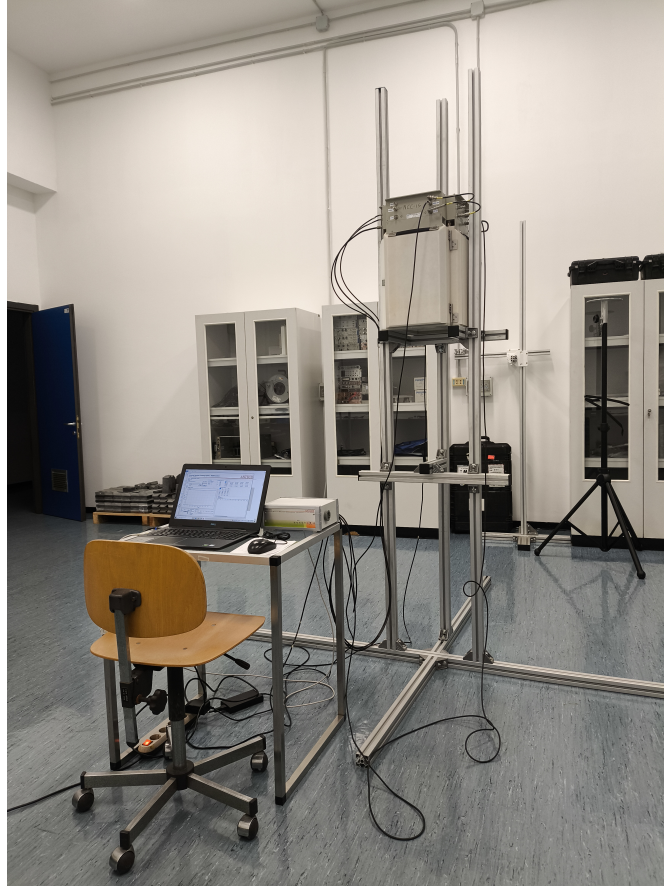


Figure 4.3: Low backscattering structure built to place the collar at 150 cm from the floor.

Experimental sessions with plutonium oxide samples were performed in PERLA (PERformance LABoratory) in a similar setup as the first measurement with ^{252}Cf , with the collar placed on a table at 80 cm from the floor.

Before going through the validation results, it is important to note that all simulations presented in this chapter were performed using the ENDFB-VII.1 nuclear data library. The only unresolved compatibility issue was with the thermal scattering data $S(\alpha, \beta)$ for polyethylene, which was taken from the ENDFB-V library.

4.2. Validation with ^{252}Cf spontaneous-fission neutron sources

A series of measurements was performed using ^{252}Cf spontaneous-fission neutron sources. Such sources are widely employed for the calibration and characterization of neutron

coincidence counters because they provide a well-known neutron yield and can be handled safely as sealed sources under laboratory conditions.

The relevant nuclear data for ^{252}Cf are an average number of neutrons emitted per fission of $\bar{\nu} = 3.7573 \pm 0.0056$ and a half-life of 2.650 ± 0.003 years [47, 48]. The isotopic composition of the sources were updated to the measurement date using the source certification data and decay corrections. The mass of each active isotope and the equivalent spontaneous fission neutron yield computed by MCNP-PTA are reported in table 4.1

Isotope	Q2-988		Q2-987	
	Mass [μg]	SF yield [n/s]	Mass [μg]	SF yield [n/s]
^{246}Cm	4.117×10^{-2}	3.582×10^{-1}	7.477×10^{-3}	7.0×10^{-2}
^{248}Cm	6.717×10^{-1}	2.703×10^1	1.178×10^{-1}	4.76×10^0
^{250}Cf	7.705×10^{-2}	8.414×10^2	1.287×10^{-2}	1.4062×10^2
^{252}Cf	9.361×10^{-2}	2.156×10^5	1.387×10^{-2}	3.2025×10^4
Total	8.780×10^{-1}	2.160×10^5	1.600×10^{-1}	3.217×10^4

Table 4.1: Masses of active isotopes and spontaneous fission (SF) neutron yields computed by MCNP-PTA for the Q2-987 and Q2-988 sources.

The first measurement campaign was performed with source Q2-988. The objective was to investigate the spatial dependence of the collar detection efficiency within the cavity. For this study, only the singles count rate was considered. The efficiency is defined as $\varepsilon = S/Y$ where S are the singles count rates and Y the neutron yield of the source

The source was initially positioned at the center of the collar cavity and subsequently moved to several locations along the horizontal axes while remaining at the vertical mid-plane. To achieve realistic simulations, the source encapsulation was explicitly modeled in MCNP-PTA using the geometry and material specifications provided in the manufacturer's technical drawings.

To compare experimental C_e and Monte Carlo simulations C_m count rates, a percent relative deviation of a value was defined as

$$\text{Dev.}(\%) = 100 \cdot \left| 1 - \frac{C_m}{C_e} \right| \quad (4.1)$$

The uncertainties σ_{ref} and σ were propagated to the deviation as

$$\sigma_{\text{Dev.}}(\%) = 100 \frac{C_m}{C_e} \sqrt{\left(\frac{\sigma_e}{C_e} \right)^2 + \left(\frac{\sigma_m}{C_m} \right)^2} \quad (4.2)$$

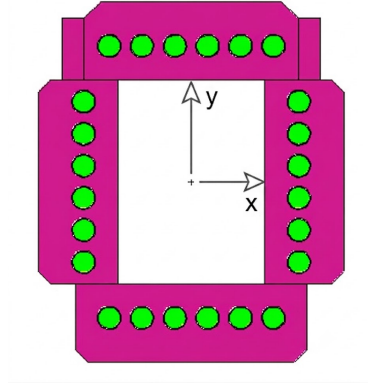


Figure 4.4: x and y horizontal axes at the collar vertical midplane.

While comparing measurements and simulations, the reference value was always considered to be the experimental one. The measured and simulated singles count rates for the different source positions are presented in Fig. 4.5.

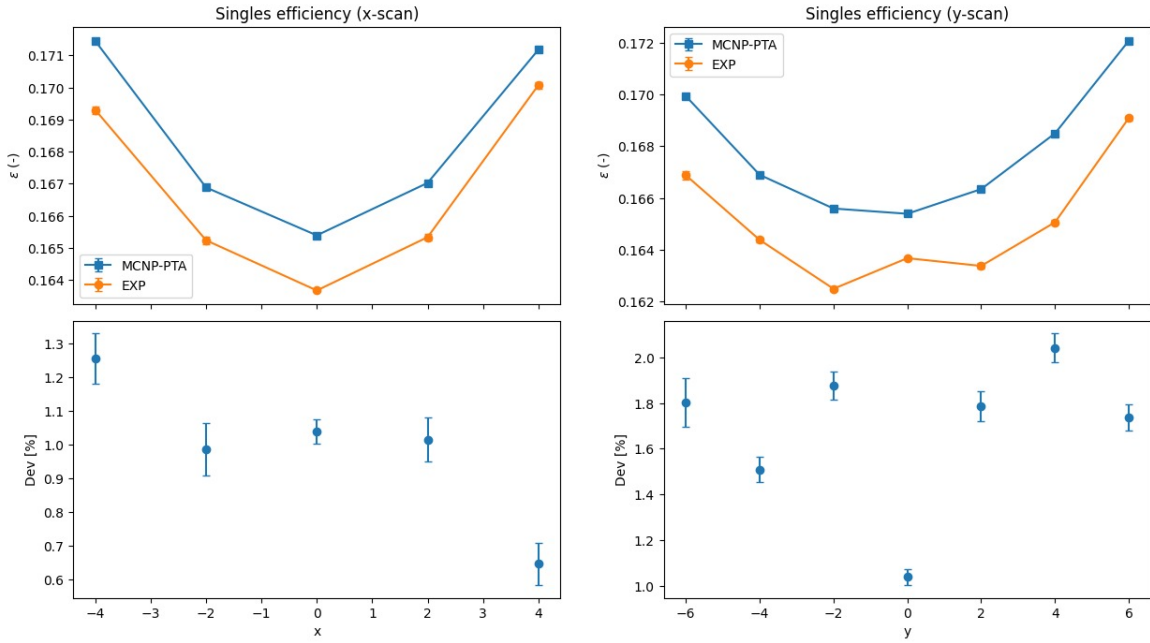


Figure 4.5: Singles efficiency comparison along the x and y axis. Time of measurement was 2 hours and 40 minutes for the central point ($x = 0, y = 0$) and an average of 9 minutes for the rest. NPS $1e7$ for all simulations

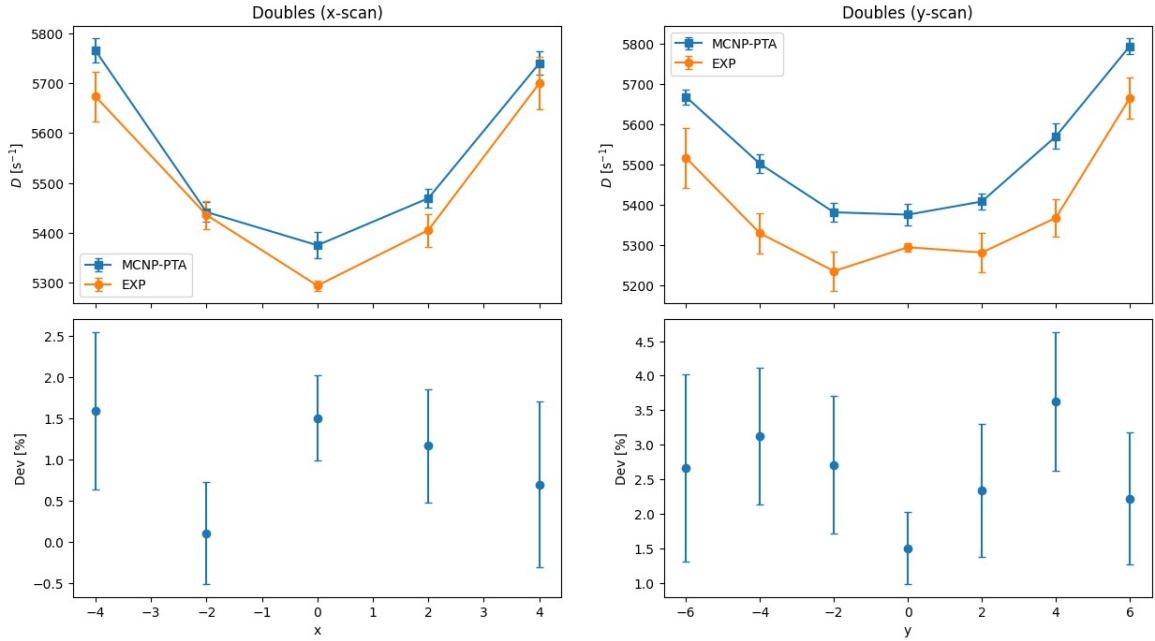


Figure 4.6: Doubles comparison along the x and y axis. Time of measurement was 2 hours and 40 minutes for the central point ($x = 0, y = 0$) and an average of 9 minutes for the rest. NPS $1e7$ for all simulations

The results show that the detection efficiency increases when the source is positioned closer to one of the collar walls rather than at the center of the cavity. This behavior is expected because a larger fraction of the emitted neutrons enters the moderator of the nearest detector bank, increasing its response. This observation provides useful insight into the collar sensitivity to localized changes in neutron production within a fuel assembly, such as those caused by missing fuel pins.

The deviations with the experimental points were within 2% for the singles and 4.5% for the doubles. This may be due to unaccounted model and experimental uncertainties such as misalignment of the source within the cavity, which is more likely to occur when the source is moved to different positions. The asymmetry of the x-axis scan in figure 4.5 suggests this, as well as the central data point which seems to deviate from the physical trend. These results should therefore be considered preliminary, and the measurements should be repeated to validate the model's predictive capabilities in this scenario.

The laboratory floor was modeled as standard concrete to account for neutron backscattering. Additional simulations showed that floor-scattered neutrons have a negligible effect on the detector response when the collar is positioned more than 120 cm above the floor. Consequently, the second experimental setup was performed with the collar elevated to a height of 150 cm.

The second measurement campaign used source Q2-987 positioned at the center of the collar cavity. In contrast to the first study, the objective was not to investigate spatial effects but rather to obtain a high-precision reference measurement of the collar detection efficiency and to validate the capability of MCNP-PTA to accurately predict doubles count rates.

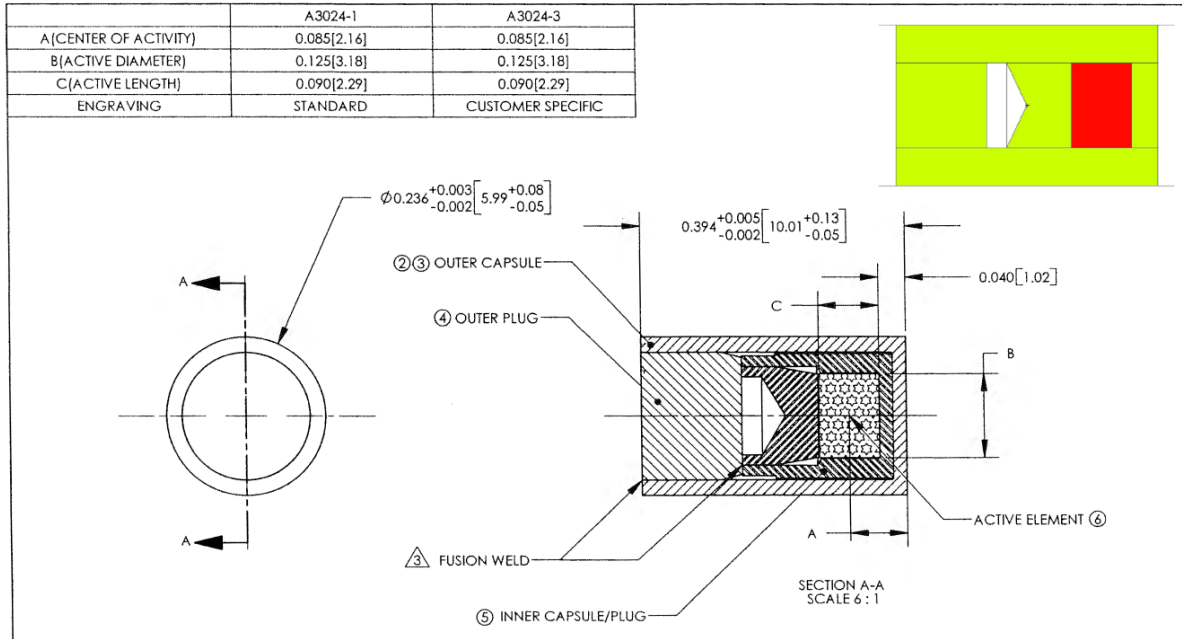


Figure 4.7: Technical drawing of the Q2-988 source encapsulation with its MCNP-PTA geometry (upper right corner). Dimensions are in inches [mm]

	Experimental	MCNP-PTA	Dev. (%)
Singles	5410.80 ± 1.12	5419.50 ± 0.91	0.161 ± 0.027
Doubles	837.66 ± 1.22	844.25 ± 0.88	0.781 ± 0.178

Table 4.2: Comparison between experimental and Monte Carlo results for the measurement with the Q2-987 source. NPS $1e7$ and measurement time 3h.

The results, shown in table 4.2, present a minuscule deviation compared with the previous measurements obtained using the Q2-988 source, this measurement, performed with the source precisely placed at the center of the cavity, is therefore considered more reliable and is used as a reference for validation.

The very successful result with the Q2-987 source shows that MCNP-PTA is capable of accurately predicting the response of the Passive Neutron Coincidence Collar for a well-characterized ^{252}Cf source, including both singles and doubles count rates. The agreement between simulation and measurement indicates that the model correctly captures the

relevant physics of neutron transport, moderation, and detection, as well as the effects of the electronics acquisition chain.

4.3. Validation with plutonium oxide samples

A second set of measurements was performed with plutonium oxide samples. These samples were the ones available that most accurately reproduced a MOX fuel composition and its neutron emission via both spontaneous fission and (α, n) reactions. This campaign had the scope to verify the capability of the model to correctly compute the neutron yields of the sources and the detector response for a more complex scenario, which is crucial for the subsequent simulations of the ALFRED fuel assembly.

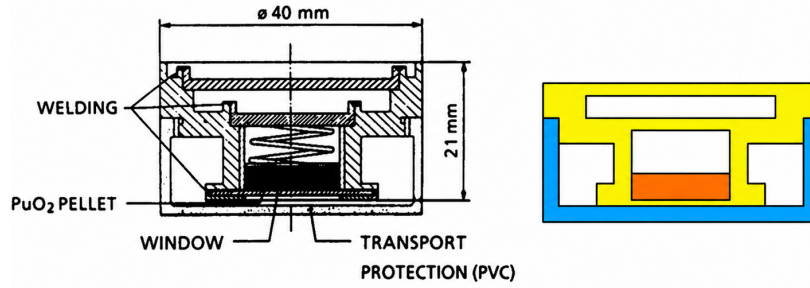


Figure 4.8: Technical drawing of the CBNM source capsule and its MCNP-PTA model geometry.

The samples used were the Nuclear Reference Material 271 of the Central Bureau for Nuclear Measurements (CBNM NRM 271), which were assembled in 1986 at The Joint Research Centre in Geel, Belgium [49]. This set consists of 4 samples of PuO₂ with different isotopic compositions and plutonium content, which was for decay to the date of measurement.

The weight fractions relative to the total oxide mass were computed considering an oxygen to metal ratio of 1.97, since in the source certificate the deviation from stoichiometry is reported to be less than 0.05. Given the isotopic composition of the samples, the neutron emission rates computed by MCNP-PTA are reported in table 4.4.

ID	Mass (g)	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{241}Am
Pu93	6.625	0.0076	82.4279	5.5539	0.0294	0.0349	0.2482
Pu84	6.690	0.0455	74.3945	12.4940	0.1349	0.3158	0.9217
Pu70	6.665	0.5442	64.3389	16.0052	0.7138	1.8247	4.8876
Pu61	6.626	0.7694	54.8143	22.2052	0.8718	3.6793	5.9812

Table 4.3: Isotopic composition (wt%) and sample masses used for the simulations. Values were updated for decay to the measurement date using data from the source certificate.

ID	SF yield [n/s]	(α, n) yield [n/s]	Total yield [n/s]
Pu61	953.1	2126.0	3079.1
Pu70	656.6	1728.4	2385.0
Pu84	424.6	530.2	954.8
Pu93	180.5	321.2	501.7
Total	2214.8	4705.8	6920.6

Table 4.4: Neutron emission rates computed by MCNP-PTA for the CBNM plutonium oxide reference samples.

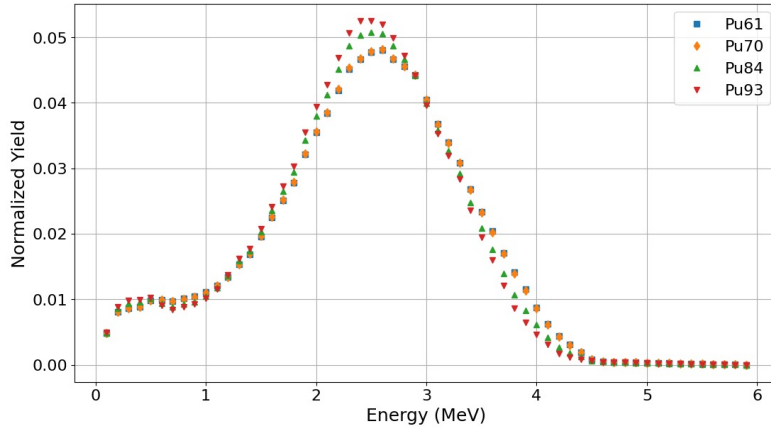


Figure 4.9: (α, n) spectra for the CBNM samples computed by SOURCES-4C. The spectra are normalized to the total (α, n) yield of each sample.

The relatively low neutron yield of these sources makes dead time effects negligible in these measurements, of which two were carried out. The first run used the Pu61 sample alone, positioned in the middle of the collar cavity, and a second one with all 4 samples disposed in the cavity as in figure 4.10. The source capsule geometry was reproduced in MCNP-PTA accordingly to the technical drawing in figure 4.8, and the isotopic composition of each sample was included in the model. The results of the measurements were compared with the Monte Carlo simulations, which are shown in table 4.5.

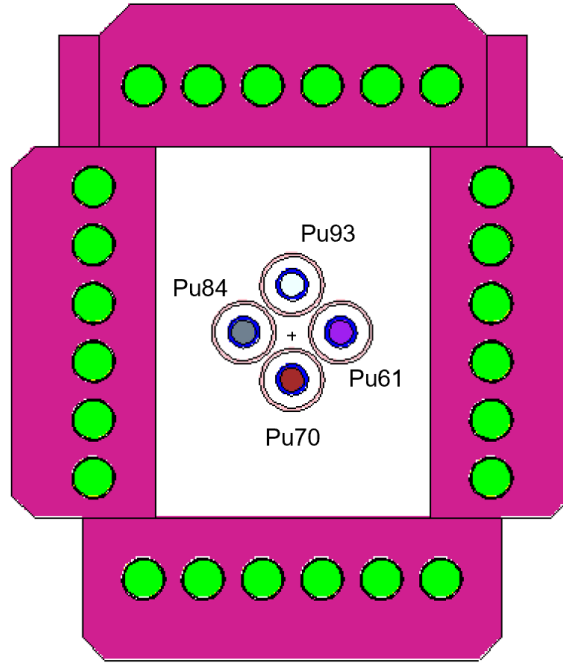


Figure 4.10: MCNP-PTA model of the CBNM source with all 4 samples placed together in the collar cavity. The centre of each sample was shifted by 3 cm along the respective horizontal axis.

	Experimental	MCNP-PTA	Dev. (%)
Pu61			
Singles	681.9 ± 0.4	676.7 ± 0.2	0.762 ± 0.063
Doubles	34.51 ± 0.15	35.13 ± 0.05	1.789 ± 0.466
Full set			
Singles	1545.8 ± 0.66	1535.5 ± 0.3	0.671 ± 0.046
Doubles	81.51 ± 0.34	82.69 ± 0.16	1.369 ± 0.467

Table 4.5: Comparison between experimental and Monte Carlo results for CBNM. NPS 5e6 for Pu61 and 1e7 for the full set, while measurement times were 1h 10m and 4h 56m respectively.

The simulations were run with a NPS of 5×10^6 and 1×10^7 for the Pu61 and the full set respectively, which is much lower than the ones emitted during the measurement time (around 63×10^6 and 122×10^6).

The statistical uncertainties reported by MCNP-PTA reflect only the convergence of the Monte Carlo estimators and are therefore fundamentally different from the total experimental uncertainty. In particular, the simulations model an idealized detector system with fixed geometry and deterministic electronic response, whereas the measurements are affected by additional sources of variability, including electronic noise, material composition deviation and small geometric misalignments of the source capsules. Also the backscattering from the floor and surrounding structures could not be perfectly reproduced in the simulations, which can introduce additional discrepancies.

Since MCNP-PTA explicitly models the multiplicity logic and coincidence processing, each history can contribute multiple correlated events, leading to efficient statistical convergence of singles and doubles estimators.

4.4. Discussion

The results of the experimental validation campaign presented in this chapter demonstrate that the Monte Carlo model is capable of reproducing the response of the Passive Neutron Coincidence Collar with good agreement across a range of neutron source configurations. Measurements with ^{252}Cf spontaneous-fission sources indicate that MCNP-PTA is able to capture the spatial dependence of detector efficiency within the collar cavity, reproduce the behaviour of the front end electronics, and predict singles and doubles count rates with good overall accuracy.

The subsequent validation with plutonium oxide samples showed fine results for a (α, n) and spontaneous fission emitter, which is crucial for the subsequent simulations of the ALFRED fuel assembly. MCNP-PTA proved to be able to compute the correct yields given the isotopic composition of the samples, and to predict the detector response with discrepancies within 1% and 2% for the singles and doubles count rates respectively. Since these measurements and simulations were the most relevant ones for benchmarking, a validation-derived uncertainty estimate for the doubles count rate could be set at a conservative 2%. This should be considered when using the MCNP-PTA model to predict the response of the collar for the ALFRED fuel assembly, as it provides a conservative estimate of the expected accuracy of the simulations compared to real measurements.

In Appendix B, the results of the experimental validation was presented in the form of

an extended abstract submitted and accepted for the 2026 INMM (Institute of Nuclear Materials Management) Annual Meeting, which will be held 2-6 August 2026 in Austin, Texas. The abstract was compiled right before the simulations of the ALFRED fuel assembly, and it summarizes the experimental validation campaign described in this chapter, including the measurements with ^{252}Cf sources and plutonium oxide samples, as well as the comparison with MCNP-PTA simulations.

5 | Simulations of ALFRED fuel assembly verification

Having validated the MCNP-PTA neutron collar model against ^{252}Cf spontaneous-fission neutron sources and plutonium-oxide measurements (Chapter 4), the present chapter employs the validated model to (i) generate a calibration curve relating the doubles count rate of the Passive Neutron Coincidence Collar (PNCC) to the plutonium content of the ALFRED fuel assembly, and (ii) assess the sensitivity of the system to realistic diversion scenarios.

The doubles count rates constitute the primary observable used for plutonium quantification. Since this was the most representative measurement conducted, and being a measurement with a mock-up fuel assembly not possible, the discrepancy identified during validation against plutonium oxide (PuO_2) measurements was incorporated as an additional source of model uncertainty in all subsequent simulations. Based on the level of agreement obtained between MCNP-PTA predictions and experimental doubles count rates, a conservative relative systematic uncertainty of $f = 0.02$ (2%) was assigned to account for model bias and limitations in reproducing experimental observations.

This systematic component was combined in quadrature with the statistical uncertainty of the Monte Carlo simulation to obtain the total uncertainty associated with the simulated doubles count rate:

$$\sigma = \sqrt{\sigma_D^2 + (fD)^2} \quad (5.1)$$

where D is the simulated doubles count rate and σ_D is the statistical uncertainty returned by the Monte Carlo calculation.

The resulting combined uncertainty is intended to account for both stochastic fluctuations inherent to Monte Carlo transport calculations and the estimated predictive accuracy of the validated model relative to experimental measurements.

Throughout this section, reported numerical values are presented together with both uncertainty components in the form

$$x \pm \sigma_x (\pm \sigma) \quad (5.2)$$

where σ_x denotes the Monte Carlo statistical uncertainty and σ denotes the total uncertainty after inclusion of the validation-derived systematic component.

In this set of simulations, being the investigated item more complex than the ones used for the validation, some memory constraints were encountered within MCNP-PTA, which prevented the usage of the ENDFB-VII.1 nuclear data library for all isotopes. For this reason, the fuel assembly wrapper was not modeled, and the cladding composition was simplified to a mixture of 70% Fe, 15% Cr and 15% Ni, which is a reasonable approximation of the actual cladding material. Furthermore, for a couple of nuclear material isotopes (the less relevant to our study ^{234}U and ^{236}U) cross section data was taken from the ENDFB-V library, which has a lower resolution than the ENDFB-VII.1 library. The impact of these approximations on the simulation results is expected to be negligible, since the main source of neutrons is the plutonium content of the fuel assembly, and the cladding and wrapper materials have a minor effect on neutron transport and detection. For the polyethylene moderator, the thermal scattering data ($S(\alpha, \beta)$) was again taken from the ENDFB-V library.

5.1. Calibration curve for plutonium content quantification

In order to provide a reference for determining the plutonium content of the ALFRED fuel assembly, several calibration curves were obtained by performing Monte Carlo simulations for different plutonium enrichments. The curves relate the doubles count rate measured by the collar to the linear plutonium density of the fuel assembly. Since plutonium can be present in different isotopic compositions, the plutonium mass was expressed in terms of the ^{240}Pu effective linear density [g/cm], defined as [8]:

$$m_{240}^{eff} = 2.52 m_{238} + m_{240} + 1.68 m_{242} \quad (5.3)$$

This definition accounts for the different neutron emission rates of the plutonium isotopes by weighting their masses with coefficients proportional to their spontaneous fission yield

and second factorial moments of their multiplicity distribution.

Five enrichments were simulated, ranging linearly from 21.7% to 27.8% Pu/(Pu+U), which corresponds to a linear ^{240}Pu effective density range of 66.19 g/cm to 84.86 g/cm. The isotopic composition of the plutonium vector was maintained constant across the different enrichments.

As discussed previously, the large plutonium inventory results in a very high spontaneous neutron emission rate, ranging from 7.56×10^6 n/s to 9.68×10^6 n/s. Such intense emission is advantageous for safeguards measurements because it enables short acquisition times and high statistical precision. However, it also introduces significant detector dead-time effects that can compromise the measurement reliability.

To mitigate this effect, all simulations were performed with the collar operating in fast mode by introducing a 1 mm thick cadmium liner around the cavity. The cadmium absorbs thermal neutrons returning to the cavity after moderation in the polyethylene, thereby reducing induced fission multiplication inside the fuel assembly. This configuration serves two purposes: reducing the overall count rate and associated dead-time losses, and increasing sensitivity to spontaneous fission neutrons, which constitute the signal of interest for plutonium quantification.

Nevertheless, the reduction obtained with the cadmium liner alone was insufficient. Although the doubles count rate decreased by a factor of approximately 1.7, simulations performed using the same acquisition configuration adopted during the experimental validation (four amplifiers, one per detector bank) still resulted in saturation of the doubles response. Under these conditions, all simulated enrichments produced nearly identical count rates because the acquisition electronics could not process all events due to updating dead-time.

To overcome this limitation, a dedicated study was conducted to evaluate alternative amplifier configurations. Increasing the number of amplifiers reduces the number of ^3He tubes connected to each channel and therefore limits dead-time losses caused by signal pileup and OR-gate processing. The configuration employing one amplifier per detector tube provided the best performance and was adopted for subsequent analyses, as shown in Figure 5.1. In the MCNP-PTA input file, detector dead-time and pulse time were still set to 1 μs and 50 ns respectively.

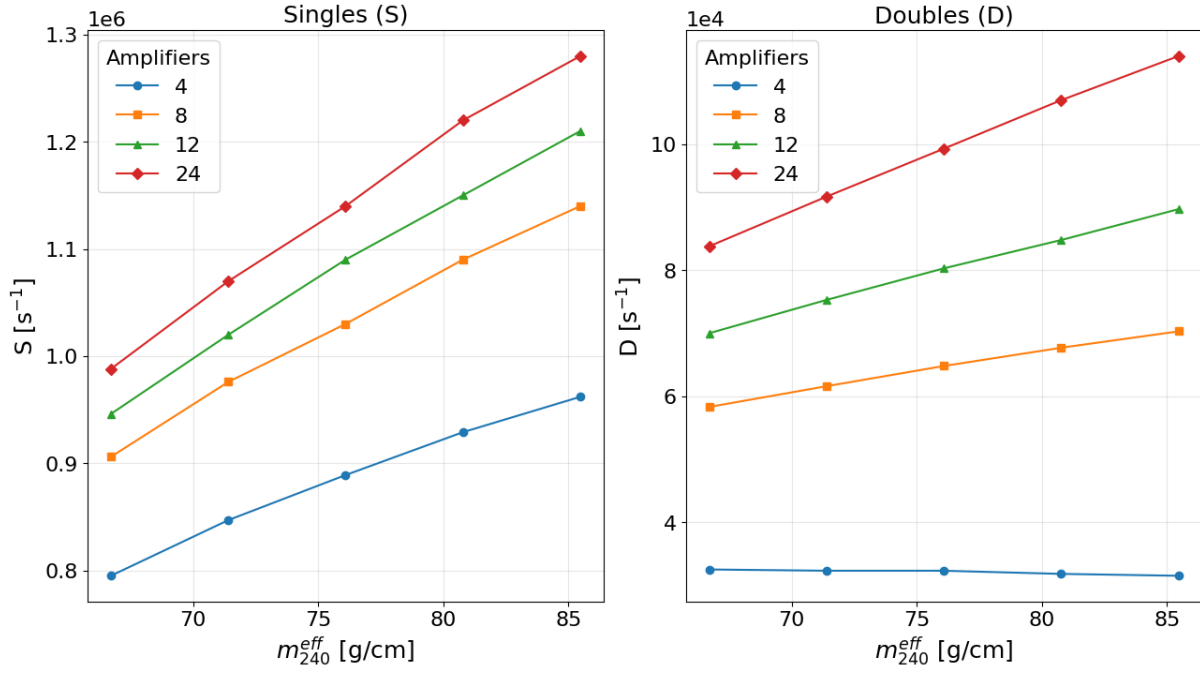


Figure 5.1: Study of the effect of the number of amplifiers on the doubles count rate for the ALFRED fuel assembly varying Pu enrichment. The configuration with a single amplifier for each tube was found to be the most effective in limiting dead-time losses due to signal pileup and OR gate logic.

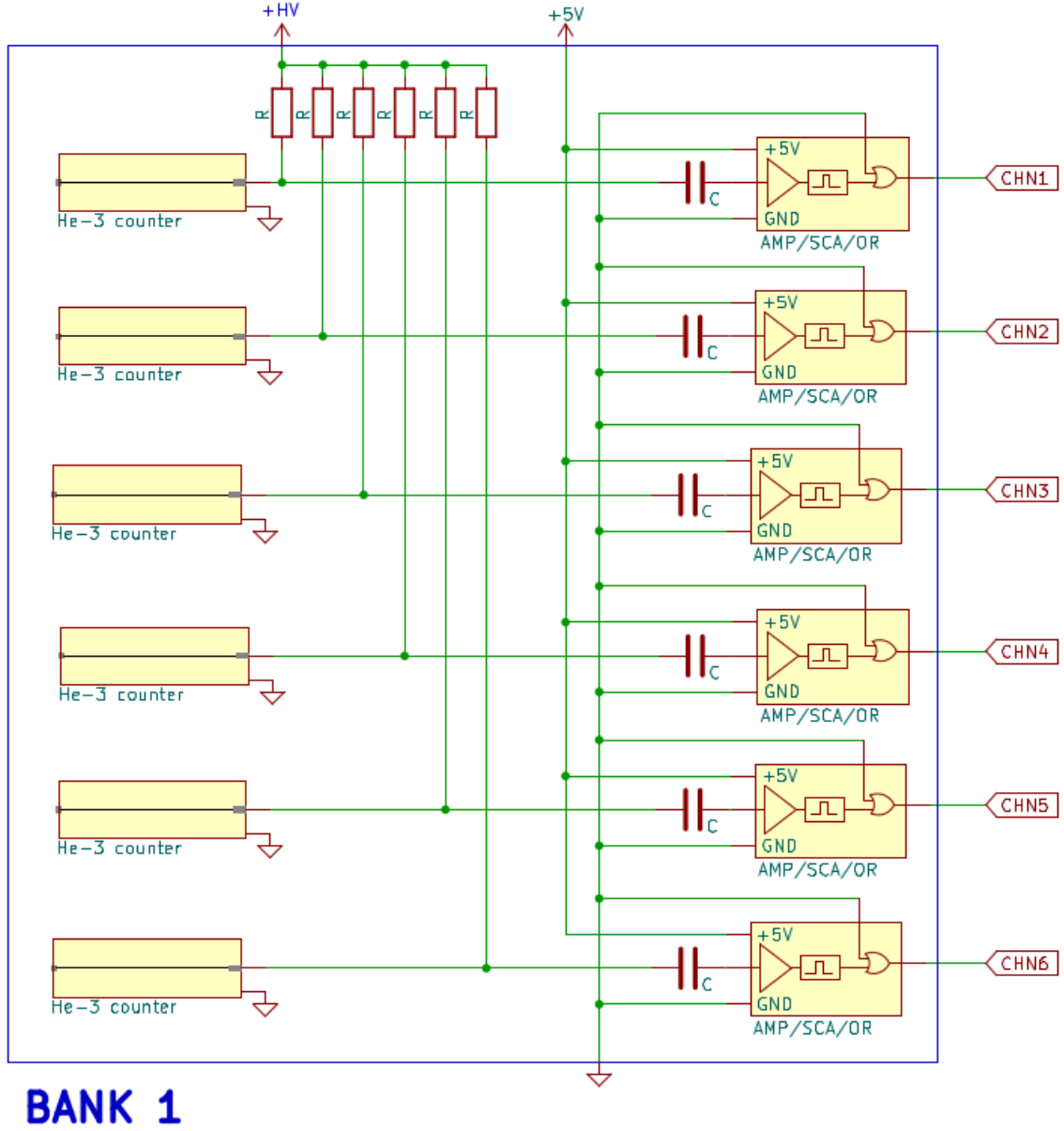


Figure 5.2: Schematic of the electronics acquisition chain for a detector bank in which each tube is connected to a single amplifier, instead of one amplifier for the whole bank. This configuration is used in the simulations of the ALFRED fuel assembly to limit dead-time losses due to signal pileup and OR gate logic. Each output is then connected independently to the shift register module in list mode.

The calibration curve was then computed using one amplifier per tube in fast-mode, by fitting the simulated doubles data with a weighted linear function of the form $D = (a \pm \sigma_a)m_{240}^{eff} + (b \pm \sigma_b)$, where the fit parameters were determined through a weighted least-squares regression using the statistical uncertainties of the simulated doubles rates

summed with the systematic 2%.

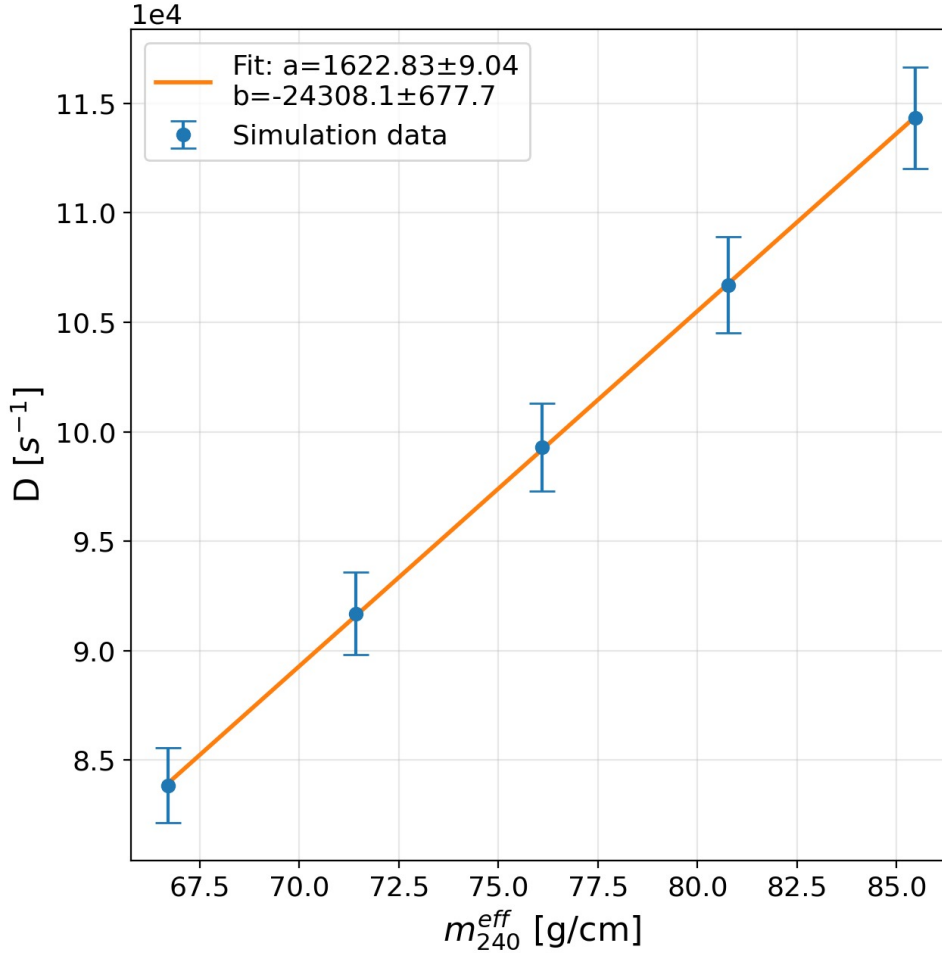


Figure 5.3: Calibration curve for the ALFRED fuel assembly with in fast mode with 24 amplifiers. Linear fit was obtained with weighted least-squares regression using the doubles count rates uncertainties, which were summed with the systematic 2%. NPS 5×10^8 .

5.2. Diversion scenarios: pin removal and replacement

In a IAEA safeguards inspection a defect is defined as a difference between the declared amount of nuclear material and the material actually present (IAEA Glossary, 2001 edition [25]). Three levels of defects are considered

- Gross defect refers to an item or a batch that has been falsified to the maximum extent possible so that all or most of the declared material is missing.

- Partial defect refers to an item or a batch that has been falsified to such an extent that some fraction of the declared amount of material is actually present.
- Bias defect refers to an item or a batch that has been slightly falsified so that only a small fraction of the declared amount of material is missing.

In typical diversion scenarios that involve fresh fuel assemblies defects are created with the removal or replacement of one or more fuel pins. This can lead to nuclear material theft, therefore it is of paramount importance that our detection system is able to verify and quantify all levels of defect, no matter how they are positioned within the fuel assembly.

A reference calculation was performed for the full fuel assembly at 21.7% Pu enrichment, which has a linear ^{240}Pu effective density of 66.19 g/cm and a doubles count rate of 83907 ± 359 (± 1678) counts per second, originating from a total neutron yield (spontaneous fission plus (α, n)) of 7.56×10^6 n/s. All simulations were run with a number of simulated particles (NPS) equal to 5×10^8 . Hence, it would take 66 s for the assembly to emit such number of particles. This is the equivalent physical time represented by the simulation run. To compare the results of the defect scenarios with the reference value, the relative deviation of the doubles count rate was computed as defined in equation 4.1. The uncertainty of the deviation was computed as defined in equation 4.2, which includes both the Monte Carlo statistical uncertainty and the systematic 2% contribution derived from the validation campaign.

For this type of scenarios, a threshold could be defined with a relative deviation compared to the reference value for the full fuel assembly

$$\frac{\text{Dev}(\cdot)}{\sigma_{\text{Dev}}} = 2 - 3 \quad (5.4)$$

in order to have a reliable detection of the defect.

5.2.1. Single pin removal

At first a bias defect scenario was considered, in order to verify the sensitivity to a single pin removed from the fuel assembly. This defect result in a reduction by 0.8% of the total fuel mass. The hexagonal lattice was divided in six rings like shown in figure 5.4. A test with a single missing pin from each ring was conducted.

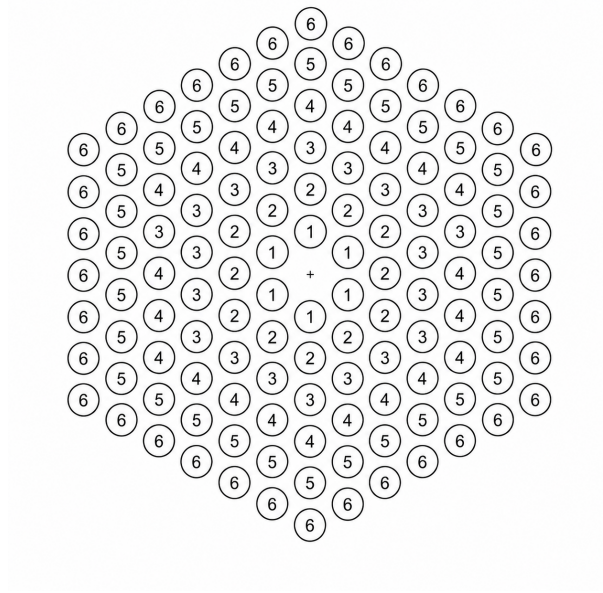


Figure 5.4: Six rings division of the ALFRED fuel assembly. Each pin is identified by its ring index 1 to 6.

In order to limit amplifier losses because of the signal pileup due to the high count rate, a single amplifier was used for each of the 24 ^3He tubes, instead of one amplifier for each bank of 6 tubes.

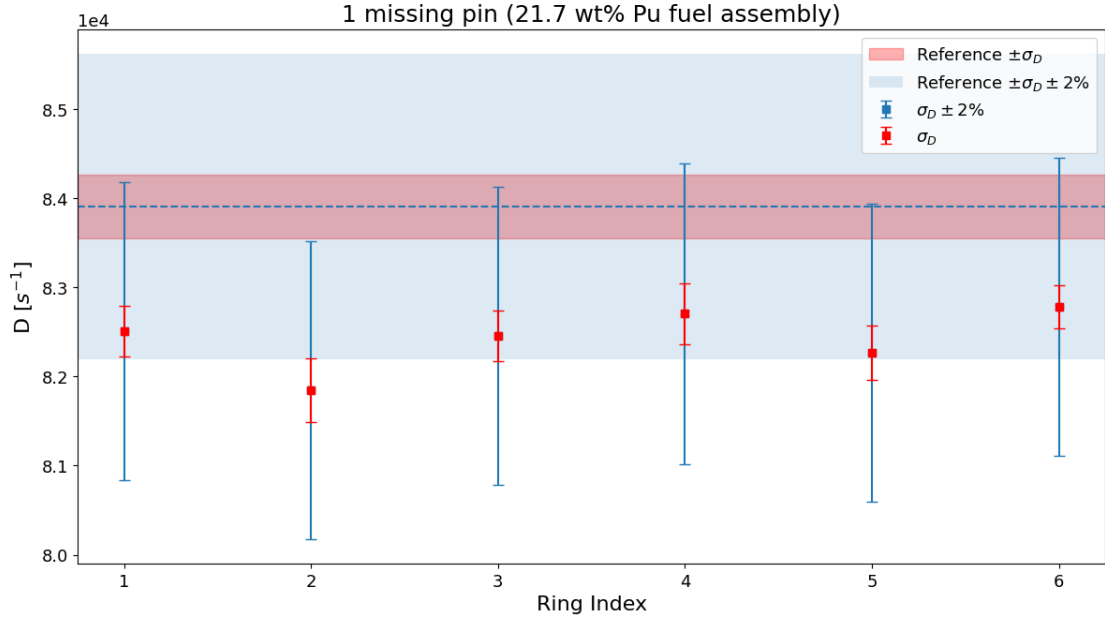


Figure 5.5: Results of the single pin removal test and comparison with the reference value for the full fuel assembly. Both the Monte Carlo statistical uncertainty and the systematic 2% contribution are displayed. NPS 5×10^8 . 24 amplifiers.

Figure 5.5 shows the results of the missing pin test in terms of doubles count rate. The doubles count rate decreases on average of 1.76 ± 0.56 (± 2.83)% for a single pin removed. The average relative deviation is therefore $\text{Dev}(D)/\sigma_{\text{Dev}} = 3.14$ (0.62). Considering the simulations alone, one could think that the system is able to detect a single pin removal from the fuel assembly, since the deviation of the doubles count rate is larger than the statistical uncertainty. However, when considering the additional systematic uncertainty, the deviation becomes not significant, which means that a single pin removal cannot be reliably detected, at least not with such a short measuring time.

5.2.2. Multiple pins replaced with steel

A more complex diversion scenario was simulated here, which involved the replacement of multiple fuel pins with steel pins of the same geometry. The steel used for the simulations was the same as the cladding. In this scenario, a visual inspection cannot detect the diversion, since the replaced pins have the same external geometry as the original fuel pins. However, the neutron emission reduces significantly, which leads to a reduction of the doubles count rate detected by the collar. From the neutronics point of view, steel pins will only have a parasitic scattering and (low) absorption effect. At first 18 replaced

pins were simulated. For this scenario, the expected m_{240}^{eff} is equal to 56.73 g/cm, which corresponds to a reduction of 14.3% compared to the full fuel assembly. The simulations were performed for two cases: in the first one, the replaced pins were located in the inner rings of the fuel assembly, while in the second one they were located in the outermost ring. The results are shown in table 5.1 and figure 5.6.

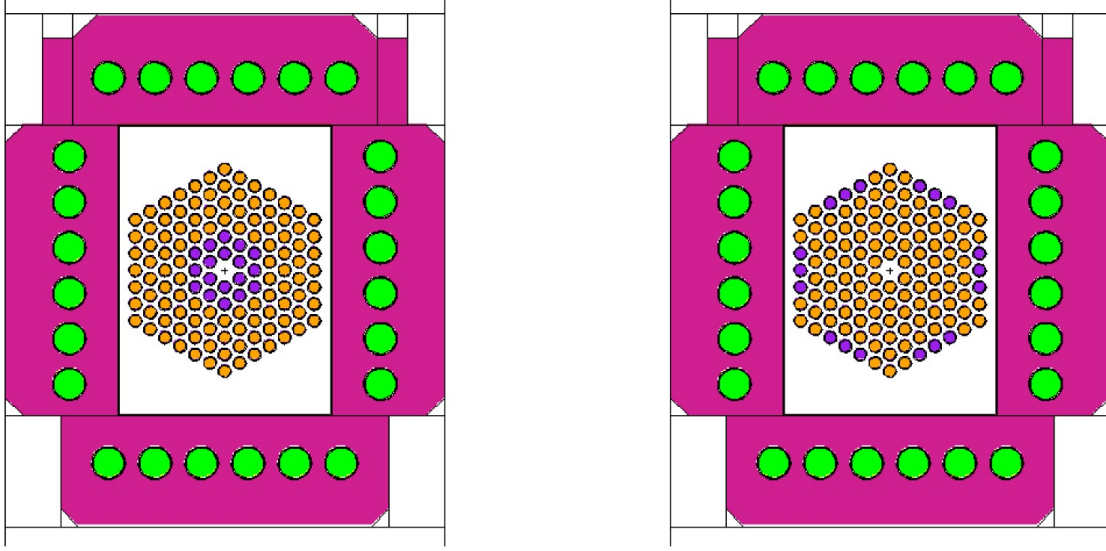


Figure 5.6: Replaced pins (purple) simulations setup. In the first (right) 18 pins in the inner (1,2) are replaced, while in the second (left) 18 pins in the outermost ring (6) are replaced.

Ring	D [cps]	m_{240}^{eff} [g/cm]	Dev(D) [%]	Dev(m_{240}^{eff}) [%]
1,2	66344 ± 237 (± 1348)	55.87 ± 0.54 (± 0.98)	20.93 ± 0.30 (± 1.63)	15.59 ± 0.82 (± 1.48)
6	69274 ± 324 (± 1423)	57.67 ± 0.56 (± 1.02)	17.44 ± 0.40 (± 1.72)	12.86 ± 0.85 (± 1.54)

Table 5.1: Results for the 18 pins scenario. The detected plutonium content was computed with the fast calibration curve and the deviations were calculated with respect to the reference fuel assembly simulation values.

The results show a significant reduction in the doubles count rate, and therefore in the detected m_{240}^{eff} , compared to the reference measurement for both scenarios. The average relative deviation was $\text{Dev}(m_{240}^{eff})/\sigma_{\text{Dev}} = 17.07$ (9.44) which is a clear indication that the system is able to detect this level of defect. The average deviation of the detected m_{240}^{eff} compared to the expected value for 18 replaced pins is 1.59 ± 0.97 (± 1.76).

To stress more the sensitivity of the system, a second simulation was performed with 6 replaced pins instead of 18, which corresponds to a reduction of 4.76% in m_{240}^{eff} (63.04

g/cm). Three simulations were run, with the pins removed at the vertices of ring 1, 3 and 6. The results are shown in table 5.2.

Ring	D [cps]	m_{240}^{eff} [g/cm]	$Dev(D)$ [%]	$Dev(m_{240}^{eff})$ [%]
1	79442 ± 457 (± 1653)	63.94 ± 0.62 (± 1.16)	5.32 ± 0.56 (± 1.90)	3.40 ± 0.93 (± 1.75)
3	78501 ± 377 (± 1615)	63.36 ± 0.59 (± 1.13)	6.44 ± 0.48 (± 1.87)	4.28 ± 0.90 (± 1.71)
6	80025 ± 421 (± 1655)	64.30 ± 0.61 (± 1.16)	4.63 ± 0.52 (± 1.90)	2.86 ± 0.92 (± 1.75)

Table 5.2: Results for the 6 pins scenario. The detected plutonium content was computed with the fast calibration curve and the deviations were calculated with respect to the reference fuel assembly simulation values.

The average relative deviation for this case was $Dev(m_{240}^{eff})/\sigma_{Dev} = 3.84$ (2.02) which indicates that this should be slightly below the limit for a sure detection of such a defect for the given measurement time. The deviation from the expected value of the plutonium content is still relatively small, with an average of 1.31 ± 0.94 (± 1.78).

5.3. Discussion and future developments

The simulated doubles count rates were evaluated using a conservative estimate of the model uncertainty derived from the validation campaign (2%). This uncertainty was combined in quadrature with the Monte Carlo statistical uncertainty to provide a more realistic estimate of the accuracy expected from real measurements.

A 1 mm thick cadmium liner was included in the cavity and a single amplifier was connected to each ^3He tube to mitigate dead-time losses, which otherwise being so significant would have made the measurements useless. The calibration curve obtained for the ALFRED fuel assembly exhibit a linear relationship between the doubles count rate and the effective ^{240}Pu density, which is advantageous for practical implementation and interpretation. Additional simulations or experimental measurements may be required to verify whether this linear behaviour remains valid outside the investigated range of 66.19–85.47 g/cm, corresponding to the minimum and maximum plutonium enrichment considered for the full fuel assembly design.

The sensitivity of the system to diversion scenarios involving fuel pin removal and replacement was assessed through dedicated simulations. The results indicate that a single pin removal (bias defect) cannot be reliably detected under the considered measurement conditions and model uncertainty. In contrast, larger defects, such as the replacement of

18 pins with steel, produced statistically significant deviations in both the doubles count rate and the reconstructed plutonium content relative to the reference fuel assembly and can therefore be detected with good confidence.

The replacement of 6 pins was found to be close to the detection threshold for the selected measurement time. Increasing the measurement duration, or equivalently increasing the number of simulated particles, would reduce the statistical uncertainty of the doubles count rate and improve sensitivity to smaller defects, potentially enabling the detection of scenarios approaching a single-pin diversion.

Further simulations could explore additional diversion scenarios, for example including various asymmetric pin removal patterns, as well as the impact of varying the isotopic composition of the plutonium vector. These studies would provide a more comprehensive understanding of the system's capabilities and limitations in detecting and quantifying nuclear material diversions. A real measurement campaign with a mock-up fuel assembly would be highly beneficial to validate the simulation results and provide additional confidence in the proposed methodology.

The ALFRED fuel assembly was selected as the case study for this work because of its relevance within the European context and the availability of detailed design information. However, once further refined and validated, the proposed methodology could be extended to other Lead-Cooled Fast Reactor (LFR) fuel assemblies employing similar highly enriched plutonium MOX fuels.

During this work, an initiative was proposed to modernize the PTA codebase, which had already been partially updated with new nuclear data, by integrating it into the OpenMC ecosystem [50] as a Python-based framework and extending its capabilities toward multi-core execution.

6 | Developments on deterministic particle transport methods for NDA

Throughout this work, neutron transport simulations have been performed using Monte Carlo methods. For complex three-dimensional systems, Monte Carlo remains the reference approach due to its flexibility in treating arbitrary geometries, material compositions, and interaction physics. However, achieving high statistical accuracy may require substantial computational effort (when a high NPS is needed), motivating the investigation of alternative solution strategies. This is particularly relevant for time-dependent transport problems, where solving transient phenomena can lead to prohibitively long simulation times. In Monte Carlo transport, time is not typically treated as a primary solution variable; instead, temporal behaviour is reconstructed through time-dependent tallies, which can significantly increase statistical requirements and computational cost.

In recent years, deterministic approaches to particle transport have gained renewed interest. Advances in numerical algorithms and high-performance computing have enabled the direct solution of the transport equation in problems that were previously considered computationally intractable. In particular, low-rank tensor methods such as the Tensor Train (TT) decomposition exploit the inherent structure of high-dimensional transport operators and solutions, representing them in a compressed format that can dramatically reduce memory requirements and computational effort.

Motivated by these developments, the NDA team at JRC Ispra has embarked on a research into deterministic particle transport methods, with the goal of developing simulation tools capable of providing accurate results at a fraction of the computational cost of conventional Monte Carlo calculations. Such methods could eventually enable faster analyses, support real-time decision making, and facilitate large-scale parametric studies relevant to safeguards and non-destructive assay applications.

This chapter provides a brief overview of traditional deterministic transport methods

before introducing the Tensor Train approach and its application to high-dimensional transport problems. A representative application case is then presented, followed by a discussion of future developments and potential NDA applications of these techniques.

6.1. Traditional deterministic neutral particle transport methods

The motion of neutral particles which do not interact with one another is described by the linear Boltzmann transport equation, which in its full form is a linear integral-differential equation in a seven-dimensional phase space (three spatial dimensions, two angular dimensions, one energy dimension and time). The primary unknown in the Boltzmann equation is the particle distribution function, which describes the density of particles in phase space at any given time. In practice, it is more common to work with the angular flux, which is related to the distribution function by a factor of the particle velocity.

$$\psi(\mathbf{r}, E, \hat{\Omega}, t) \quad [\text{particles}/(\text{cm}^2 \cdot \text{s} \cdot \text{MeV} \cdot \text{sr})] \quad (6.1)$$

The transport equation for the angular flux is given by [9]

$$\begin{aligned} \frac{1}{v} \partial_t \psi + \hat{\Omega} \cdot \nabla \psi + \Sigma_t(\mathbf{r}, E) \psi = \\ \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\mathbf{r}, E', \hat{\Omega}', t) + S(\mathbf{r}, E, \hat{\Omega}, t) \end{aligned} \quad (6.2)$$

where v is the particle velocity, Σ_t is the total macroscopic cross section, Σ_s is the double-differential scattering macroscopic cross section and S is a source term. Despite the daunting appearance of this equation, it has the straightforward physical meaning of a balance relation for particles across the whole phase space. The first two terms of the left hand side, the time partial derivative and the streaming term $\hat{\Omega} \cdot \nabla \psi$ imply local conservation in an infinitesimal volume around $\mathbf{r}$ along flight direction Ω and energy E . The removal term $\Sigma_t \psi$ is the rate at which particles of energy E are removed by any reaction around the same position. The scattering term in the right hand side is responsible for particle redistribution along the angle and energy variables, via a convolution with the integral kernel $\Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})$. In the case of neutrons in multiplying media, the source includes a fission term, [51] which adds another coupling in the energy variable

$$S(\mathbf{r}, E, \hat{\Omega}, t) = Q(\mathbf{r}, E, \hat{\Omega}, t) + \frac{\chi_p(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \bar{\nu}(E') \Sigma_f(\mathbf{r}, E') \psi(\mathbf{r}, E', \hat{\Omega}', t) \quad (6.3)$$

where Q is an external source, $\bar{\nu}$ is the average number of neutrons produced per fission, Σ_f is the fission macroscopic cross section and χ_p is the prompt fission neutron spectrum. It should be noted that the equation is linear, which greatly facilitates both analytical study and numerical evaluations. Contributions from delayed neutrons can be included by adding additional terms to the source.

The Boltzmann transport equation is notoriously difficult to solve analytically, and many physically justified approximations have been developed to make it more tractable, the most common of which is diffusion theory. Solving the neutron transport equation by applying numerical techniques to the full PDE has also always been a challenging task, especially for realistic three-dimensional problems with complex geometries and detailed energy dependence. The high dimensionality of the phase space, leads to a large number of degrees of freedom when discretized, resulting in significant computational and memory demands. The main numerical techniques for deterministic neutron transport have traditionally combined spatial discretizations — including finite difference, finite volume, and continuous finite element methods — with multi-group approximations in energy and angular discretizations based on discrete ordinates (S_N) or spherical harmonics (P_N) expansions [52, 53]. In these approaches, the phase space is approximated by a tensor-product discretization in space, angle, and energy, leading to a coupled system of algebraic equations whose size scales multiplicatively with the resolution in each variable. In realistic three-dimensional multi-group S_N calculations, this results in extremely large linear systems. This is the so called "curse of dimensionality" which is a fundamental challenge in deterministic transport methods, as the computational cost and memory requirements grow exponentially with the number of dimensions in the phase space [54, 55].

Despite this apparent complexity, modern transport solvers do not assemble the global system matrix explicitly but they instead exploit the structure of the transport operator. By treating scattering and fission contributions as fixed sources, the streaming–collision operator can be inverted direction-by-direction through a process known as a transport sweep [52], in which unknowns are updated sequentially by marching through the spatial grid along the direction of flight. This procedure provides an efficient, matrix-free application of the transport operator and forms the computational backbone of large-scale S_N solvers. For time dependent problems, this is combined with Euler or higher-order time integration scheme.

The classical iterative scheme built on this structure is source iteration, in which scattering and fission sources are evaluated from the current angular flux estimate and a transport sweep is performed to update the solution. While conceptually simple, source iteration converges slowly in optically thick or highly scattering media due to the spectral

properties of the scattering operator [52]. Consequently, substantial research has focused on acceleration techniques. Among the most widely adopted are Diffusion Synthetic Acceleration (DSA), Transport Synthetic Acceleration (TSA) and Coarse Mesh Finite Differences (CMFD). In addition, Krylov subspace methods such as GMRES are increasingly employed, often in conjunction with the fore mentioned acceleration techniques which can serve as a preconditioner for better convergence. [56]

In parallel with advances in iterative solvers, higher-order spatial discretizations have gained increasing attention. In particular, discontinuous Galerkin (DG) formulations provide locally conservative, high-order accurate schemes that naturally incorporate upwind numerical fluxes and remain compatible with sweep-based solution procedures. Such methods are especially attractive for unstructured meshes and complex geometries, and have been incorporated into several modern transport codes.[57, 58]

Beyond standalone deterministic solvers, transport methods are also often embedded within hybrid frameworks. Deterministic solutions of the forward or adjoint transport equation are routinely used to construct importance functions and weight windows for variance reduction in Monte Carlo simulations, thereby combining global phase-space resolution with stochastic refinement in regions of interest. These hybrid deterministic-stochastic approaches play an important role in shielding analysis and reactor applications. [53]

Several approaches have been proposed to improve the computational efficiency of deterministic neutron transport solvers, ranging from hardware-oriented strategies such as parallelization and GPU acceleration, to more recent machine learning-based methods aimed at accelerating solution convergence, surrogate modeling, or reduced-order approximations.[56]

6.2. The Tensor Train approach for high-dimensional transport problems

A promising strategy to address high-dimensional PDEs is to seek low-rank approximations [59], where both the solution and the discrete operators are represented in compressed low-rank formats. In this framework, functions and operators are expressed through combinations of lower-dimensional objects, drastically reducing storage requirements and computational complexity. When PDE operators can be expressed in tensor product format, i.e. when basis functions and the grid can be expressed in tensor product, separable representations and tensor decompositions can be efficiently exploited.

Among the available low-rank formats, the Tensor Train (TT) decomposition [60, 61] has emerged as one of the most successful approaches for high-dimensional scientific computing. TT represents multidimensional tensors as a sequence of low-dimensional core tensors, resulting in memory requirements that scale linearly with the number of dimensions rather than exponentially. This property makes TT especially attractive to overcome the curse of dimensionality in transport simulations. A brief introduction to Tensor Train decomposition is reported in Appendix B. Throughout the *compression ratio* denotes the ratio between the number of elements stored in the TT representation and those required by the corresponding full tensor, providing a direct measure of memory reduction.

The practical success of TT methods for PDEs is also due to the availability of efficient numerical algorithms operating directly in compressed form. Fundamental linear algebra operations—including addition, multiplication, and matrix inversion—can be performed without reconstructing full tensors. In particular, the Alternating Minimal Energy (AMEn) algorithm [62] currently represents one of the most advanced solvers in the TT framework. By combining alternating local optimization with adaptive basis enrichment, AMEn controls tensor ranks dynamically while minimizing the residual at each iteration, leading to robust convergence in high-dimensional settings.

In recent years, considerable effort has been devoted to extending TT methods to transport PDEs. Initial developments demonstrated the feasibility of solving radiative transport problems entirely in compressed format. Gorodetsky et al. [63] developed an SN, first-order explicit finite-volume solver for the grey thermal transport equation in TT format. Although numerical experiments were restricted to stationary problems in two spatial dimensions, the study established the capability of TT methods to handle transport operators while achieving substantial reductions in computational and memory costs.

More directly relevant to the nuclear field, researchers at Los Alamos National Laboratory (LANL) developed a TT-based fixed-point iterative scheme for the k-eigenvalue problem [64]. Their formulation incorporated SN angular discretization and multigroup energy treatment and was validated on one- and three-dimensional benchmark problems using finite-difference spatial discretization on Cartesian grids. The computed solutions agreed with the LANL PARTISN code up to an accuracy of 10^{-5} while delivering significant memory compression.

Subsequent work extended the framework to include spatially varying cross sections [65], addressing one of the main obstacles to applying tensor methods to realistic reactor configurations. While spatial heterogeneities increased tensor ranks and computational effort, substantial compression was still retained, demonstrating the robustness of the approach

under more demanding physical conditions.

A major step forward was recently achieved at JRC Ispra, in collaboration with LANL, through the development of the T²S² (Tensor Train Spectral Superconsistent) solver [66]. This method combined spectral collocation for accuracy, superconsistent grid point placement for stabilization of convection-dominated regimes, and Tensor Train compression for efficient high-dimensional representation. Numerical experiments reported errors as low as $\mathcal{O}(10^{-11})$ while maintaining compression ratios of $\mathcal{O}(10^{-10})$. The superconsistent grid placement was particularly effective in mitigating the Gibbs phenomenon, which can arise in spectral methods when approximating discontinuous solutions, and was for the first time extended to multi-dimensional grid. Furthermore, this work demonstrated that time can be incorporated directly as an additional TT dimension, opening the possibility of avoiding traditional time-marching schemes and solving the entire space-angle-energy-time problem simultaneously in compressed form.

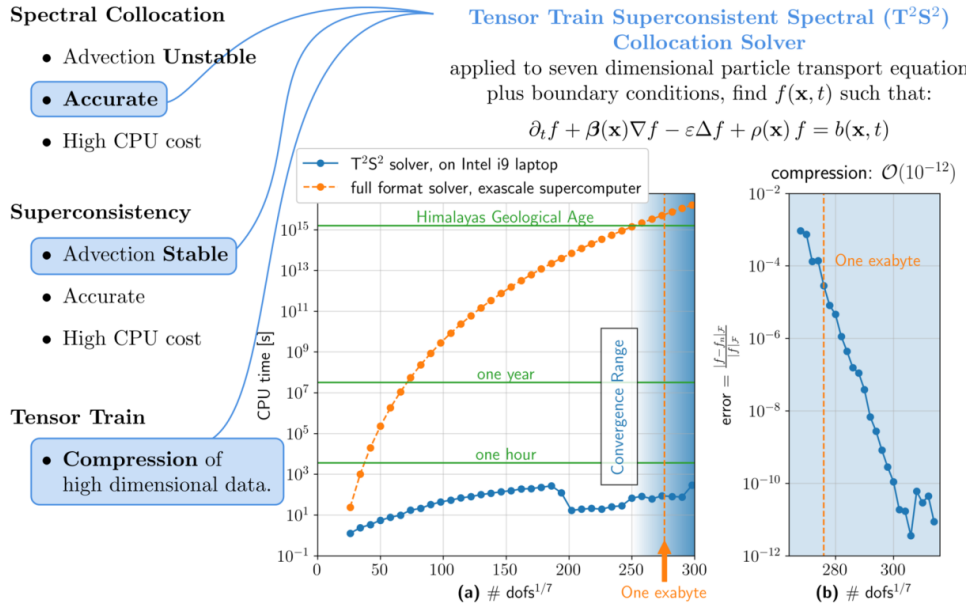


Figure 6.1: Key components of the T²S² solver. (a) Illustrates the compression capabilities, which enables real time solution of a seven-dimensional problem. The same problem with a number of degrees of freedoms (dofs) per dimension resulting in one exabyte of memory required to store the full solution tensor runs in less than 1 hour on a Intel i9 laptop, compared to millions of years on a exascale supercomputer (supposed to run at 2.7 exaFLOPS). (b) Shows the convergence behaviour in which the error decreases exponentially to $\mathcal{O}(10^{-11})$. [66]

Building on these advances, the ongoing research at JRC aims to develop a finite-element Tensor Train solver for time-dependent radiative transfer and neutron transport equa-

tions. The objective is to move beyond idealized benchmark settings and extend low-rank methodologies toward physically realistic transport models.

The preliminary results presented in the next section already provide evidence of the potential of this approach, showing that substantial memory and computational savings can be achieved while preserving the flexibility and accuracy of traditional transport discretization techniques. These findings suggest that Tensor Train methods may represent a viable pathway toward the efficient simulation of previously intractable high-dimensional transport problems.

6.3. Preliminary results for a neutron transport model

To demonstrate the potential of this novel numerical approach for NDA applications, a finite element, Tensor Train based solver was developed for the time dependent, neutron transport equation in a slab of homogeneous, non-multiplying medium. This numerical experiment was implemented in Python using the TorchTT Tensor Train library. [67]

Employing the multi-group approximation in energy the equation can be written as

$$\left(\frac{1}{v_g} \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial x} + \Sigma_{tg} \right) \psi_g(x, \mu, t) = \sum_{g'=1}^G \int_{-1}^1 d\mu' \Sigma_{s,g' \rightarrow g}(\mu', \mu) \psi_{g'}(x, \mu', t) + f_g(x, \mu, t) \quad (6.4)$$

where Σ_{tg} is the total cross section for group g , $\Sigma_{s,g' \rightarrow g}(\mu', \mu)$ is the multi-group scattering differential cross section, v_g is the neutron group velocity and f_g is an external source term. Groups are ordered following decreasing energy, so that $g = 1$ corresponds to the highest energy group and $g = G$ to the lowest energy group. The spatial domain is the slab of length L , while $\mu \in [-1, 1]$ is the direction cosine with respect to the x-axis.

Introducing the transport operator

$$\mathcal{L} = \frac{1}{v_g} \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial x} + \Sigma_{t,g}, \quad (6.5)$$

and the scattering operator

$$(\mathcal{K}\psi)_g = \sum_{g'=1}^G \int_{-1}^1 d\mu' \Sigma_{s,g' \rightarrow g}(\mu', \mu) \psi_{g'}(x, \mu', t), \quad (6.6)$$

the system can be written compactly as

$$(\mathcal{L} - \mathcal{K})\psi_g = f_g. \quad (6.7)$$

The independent variables in this equation are $x \in [0, L]$ for space, $\mu \in [-1, 1]$ which is the direction cosine, $t \in [0, T]$ for time and the energy groups $g = 1 \dots G$. The problem is therefore four-dimensional; even a modest discretization of the phase space would immediately lead to prohibitive computational and memory costs. For example, let's consider the discretization used for the numerical experiments reported in this work, which consists of 1000 spatial degrees of freedom, 100 angular directions, 10 energy groups and 1000 temporal points. This results in a total of 10^{10} degrees of freedom, which would require approximately 80 GB of memory to store the solution tensor in double precision, and around 64 GB for the discrete operator.

Instead by exploiting the natural tensor product structure the discrete operator L and K can be expressed as a sum of a set of 4-dimensional, rank-1 Tensor Train Operators, which are a tensor product of one dimensional operators (matrices) in each dimension.

The discrete operators were constructed by combining a modal Discontinuous Galerkin finite-element discretization in space with upwind numerical fluxes, a discrete ordinates (S_N) angular discretization, the multigroup energy approximation and a backward Euler discretization in time. Unlike conventional time-marching schemes, the temporal dimension is treated as an additional tensor dimension. The resulting linear system is therefore solved simultaneously over the entire space-angle-energy-time domain, allowing the TT representation to exploit correlations not only in phase space but also along the temporal coordinate.

The multi-group differential cross section in angle can be decomposed in a sum of rank-1 terms via Legendre polynomial expansion in the angular variable. This is advantageous because nuclear data libraries often report this type of cross section as continuous energy Legendre coefficients. It is interesting to notice that this treatment of the scattering integral kernel is directly extendible to three dimensional transport, where via the addition theorem for spherical harmonics [9] one can obtain a perfectly rank-1 separable matrix structure in both the polar and azimuthal angles.

A more thorough description of the numerical scheme and the construction of the discrete operators for the following described model can be found in Appendix C.

In order to have a first test of the method, a simplified moderator model was used. The total cross section was set to unity for each energy group, which were spaced logarithmi-

cally in energy, i.e. $\Sigma_{t,g} = 1 \forall g$, so that the double-differential scattering cross section simply represents the probability distribution function per collision. The latter is modeled as being directly separable in energy groups and angle

$$\Sigma_{g' \rightarrow g}(\mu', \mu) = c_{gg'} K_s(\mu', \mu) \quad (6.8)$$

where $c_{gg'}$ is a matrix of scattering coefficients in energy. This was chosen to have the bidiagonal form

$$c_{gg'} = \begin{cases} 0.75 \cdot (1 - c_{a,g'}) & \text{if } g' = g \\ 0.25 \cdot (1 - c_{a,g'}) & \text{if } g' = g - 1 \\ 0 & \text{otherwise} \end{cases} \quad (6.9)$$

where $c_{a,g'}$ is the absorption fraction for group g' which is set to resemble a $1/v$ type absorber, hence it increases with decreasing energy. Group velocities are set to be proportional to the square root of the group midpoint energy, which is consistent with the neutron energy-velocity relation. With this choice of scattering kernel, neutrons can only scatter down in energy, which is a common approximation for moderators and thermal systems.

The angular part was chosen to be the Henyey-Greenstein phase function, [68]

$$K_s(\hat{\Omega}', \hat{\Omega}) = \frac{1 - \gamma^2}{4\pi(1 + \gamma^2 - 2\gamma\hat{\Omega}' \cdot \hat{\Omega})^{3/2}} \quad (6.10)$$

which has anisotropy directly controlled by a single parameter $\gamma \in [0, 1]$. This phase function presents an analytical Legendre expansion in $\hat{\Omega}' \cdot \hat{\Omega}$ and in order to adapt it to a one-dimensional slab geometry, the azimuthal angular dependence can be integrated out, yielding a Legendre series in the direction cosine μ [69]

$$K_s(\mu', \mu) = \sum_{l=0}^{\infty} \frac{2l+1}{2} \gamma^l P_l(\mu') P_l(\mu). \quad (6.11)$$

The following manufactured solution, rank-1 separable in all variables, was proposed

$$\psi_g(x, \mu, t) = E_g \sin(x\pi/L) (a_0 P_0(\mu) + a_1 P_1(\mu) + a_2 P_2(\mu)) (1 - e^{-\alpha t}) \quad (6.12)$$

which is convenient since it is null at $t = 0$ and at the domain boundaries for all angles, hence it allows to test solely the discrete operator without worrying about initial and boundary conditions. These are being currently tested in other experiments (not reported

in this work) and seem to behave correctly. The angular part as a linear combination of Legendre polynomials allows to both test and exploit their orthogonality property.

Applying the operators to this solution we find the source term to use for the numerical test:

$$\begin{aligned}
f &= (\mathcal{L} - \mathcal{K})\psi = \\
&= \frac{E_g}{v_g} \sin(x\pi/L)(a_0 P_0(\mu) + a_1 P_1(\mu) + a_2 P_2(\mu))\alpha e^{-\alpha t} + \\
&+ E_g \frac{\pi}{L} \cos(x\pi/L)\mu(a_0 P_0(\mu) + a_1 P_1(\mu) + a_2 P_2(\mu))(1 - e^{-\alpha t}) + \\
&+ E_g \sin(x\pi/L)(a_0 P_0(\mu) + a_1 P_1(\mu) + a_2 P_2(\mu))(1 - e^{-\alpha t}) \\
&- c_{gg'} E_{g'} \sin(x\pi/L)(a_0 P_0(\mu) + a_1 \gamma P_1(\mu) + a_2 \gamma^2 P_2(\mu))(1 - e^{-\alpha t})
\end{aligned}$$

This is source term, conveniently already in Tensor Train structure, will be the right hand side of the linear system solved by AMEn.

$$A\Psi = F \tag{6.13}$$

where $A = L - K$ is the full discrete operator in TT format.

The grid used for the test case is composed of $N_s = 500$ spatial cells with polynomial order $p = 1$ for the finite element discretization, $N_a = 100$ angular directions, $G = 10$ energy groups and $N_t = 1000$ time points. With such grid the discrete operator in TT format occupied only 40 MB of memory, resulting in a compression ratio of $\mathcal{O}(10^{-12})$ with respect to the full tensor representation.

The parameters used for the test case were $\gamma = 0.5$ for the Henyey-Greenstein kernel, $\alpha = 1$ for the time dependence and $E_g = 1/(g+1)$ for the energy-group dependence. The Legendre coefficients were set to $a_0 = 0.2$, $a_1 = 0.3$ and $a_2 = 0.2$.

Given the low-rank structure and smoothness of the solution, the AMEn solver was able to achieve a residual $\text{res} = \|A\Psi - F\|/\|F\|$ in the order of 10^{-5} in just 3 solver iterations (sweeps). The solution tensor in TT format occupied a mere 155 kB of memory with TT ranks $r = 7$, resulting in a compression ratio of $\mathcal{O}(10^{-5})$

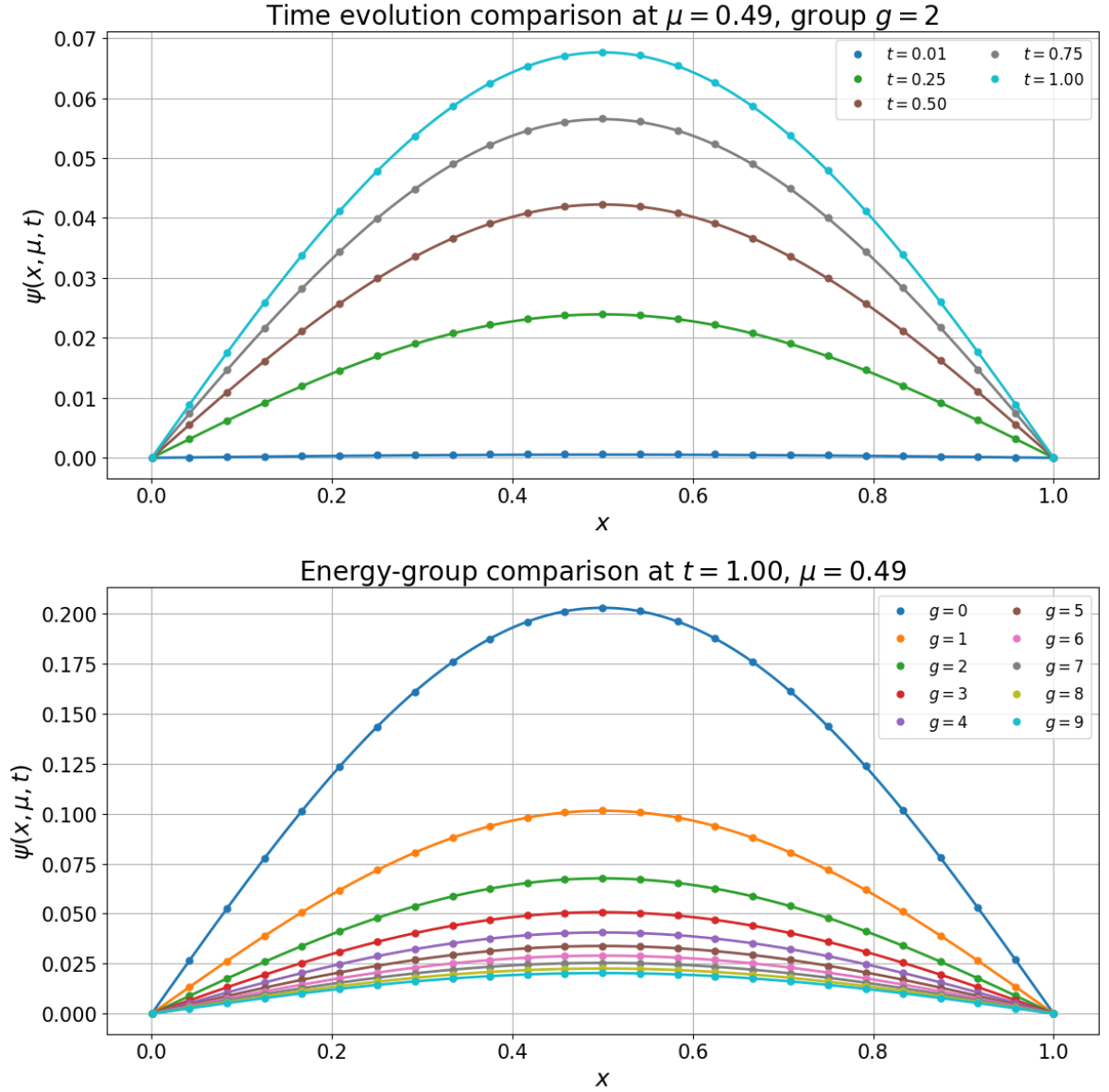


Figure 6.2: TT and manufactured solution comparison at different time points (top) and energy groups (bottom). For these simulations number of spatial elements was $N_s = 500$ with polynomial order $p = 1$, angular directions $N_a = 100$, $\gamma = 0.5$ with Legendre truncation $l_{max} = 10$, $G = 10$ and time points $N_t = 1000$. With such grid the compression ratio of the discrete operator and solution was $\mathcal{O}(10^{-12})$ and the solver achieved a residual of 10^{-5} in just 3 iterations.

For all simulated time points, energy groups and angles on this numerical experiment, the TT solution was found to be in good agreement with the manufactured solution, yielding a L^2 error norm in the order of $10^{-4} - 10^{-6}$.

These preliminary results indicate that the proposed approach behaves consistently for

this simplified benchmark and provide an initial demonstration of the feasibility of solving the time-dependent neutron transport equation using a Tensor Train representation. However, a more comprehensive convergence and performance analysis is required to fully assess the accuracy and computational efficiency of the method. Future work should investigate the effects of spatial and angular discretization, polynomial order, and TT rank truncation on both solution accuracy and compression performance, using multiple error metrics.

6.4. Future work and NDA applications

The Tensor Train (TT) approach has shown promising results in the first set of simulations performed during this work. At the time of writing, additional studies are underway to investigate the influence of boundary conditions and solution discontinuities on rank growth and compression efficiency. Preliminary efforts are also being devoted to extending the methodology to three-dimensional problems on structured spatial meshes, preserving the tensor-product structure required by the TT representation.

Another imminent step forward would be the incorporation of realistic multigroup cross-section data, enabling a more thorough assessment of the method's robustness and performance in practical transport calculations.

Another important research direction is the integration of Tensor Train techniques into existing deterministic transport solvers, such as OpenSN [58], which could sensibly reduce memory and computational costs.

Regarding Non-Destructive Analysis, an interesting application could be found in Multi-Probe Imaging and Signature (MPIS) [70], where multiple particle types (neutrons, photons, ions, muons...) at various energies are used simultaneously to probe a system, to study its composition, physical properties and structural distribution. Simulating this type of experiments would require solving coupled transport equations for each particle type, which could be efficiently handled within the TT framework.

Furthermore, efficient deterministic solutions of the adjoint transport equation could be exploited to quickly generate importance maps for Monte Carlo simulations, providing powerful variance-reduction capabilities and potentially reducing computational costs by orders of magnitude. This may be one of the most plausible applications of these techniques in the near term, even in complex three-dimensional geometries such as a neutron coincidence collar.

Casting our sight beyond NDA applications, the potential impact of this numerical tech-

nique extends to a wide range of physical problems. Many governing equations in physics share common mathematical structures, particularly conservation laws and transport phenomena, making them natural candidates for low-rank tensor methods.

Particle transport, as treated in this work, can find direct applications in fields such as astrophysics and high-energy physics. Within nuclear engineering, these techniques could be employed to reduce the computational cost of thermo-fluid dynamics and coupled neutronics calculations, potentially enabling high-fidelity multi-physics reactor simulations that are currently beyond practical computational limits.

Another promising field is plasma physics. The evolution of charged particles in electromagnetic fields is governed by the Vlasov equations, a high-dimensional equation closely related to the Boltzmann transport equation. As such, it represents a natural application for low-rank tensor methods, with potential impacts on nuclear fusion research. [71].

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A | Appendix A: Extended abstract accepted to the 2026 INMM Annual Meeting (August 2026)

Extended Abstract – INMM 2026

Passive Neutron Coincidence Collar for Non-Destructive Assay of ALFRED Lead-Cooled Fast Reactor Fuel Assemblies

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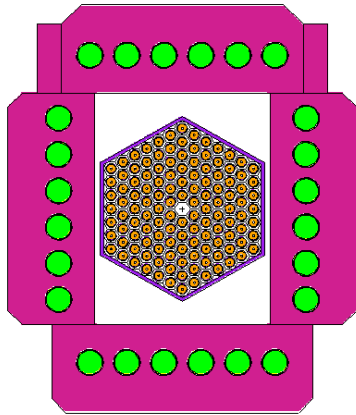
Abstract

The development of Small Modular Reactors (SMRs) and Advanced Modular Reactors (AMRs) has attracted strong interest, potentially contributing to the decarbonisation of hard to decarbonise sectors such as transport, chemical and steel industry, and district heating. In this context, the European Industrial Alliance on SMR aims to accelerate the development, the demonstration and the deployment the first European SMRs by the early 2030s. A candidate is ALFRED, a 300 MWth pool-type lead-cooled fast reactor that will serve as a demonstrator of this technology. Because the lead fast spectrum enables a closed fuel cycle, ALFRED can significantly reduce uranium consumption and transuranic waste. The reactor will use high-Pu-enriched mixed oxide (MOX) fuel (>20 wt% Pu) blended with depleted uranium, creating a substantial spontaneous fission neutron source. To safeguard this fuel cycle, we propose a passive neutron coincidence collar as a non-destructive assay (NDA) tool. The collar relies on the intense spontaneous fission

neutrons from the MOX fuel, eliminating the need for an external interrogating source, as used in traditional neutron coincidence collars. A high-fidelity MCNP-PTA model of the passive neutron coincidence collar, in thermal mode, and a full-scale ALFRED fresh fuel assembly was developed. The results of the collar model simulations were validated against measurements using certified ^{252}Cf and a set of Pu oxide reference materials. The validated model enabled us to predict with confidence the reliable performance of the full assembly, demonstrating that a passive neutron coincidence collar is a viable, cost-effective safeguards instrument for verifying ALFRED nuclear fuel.

Introduction. The development of fast lead-cooled reactors in Europe has gained significant momentum through new strategic alliances. ALFRED (Advanced Lead Fast Reactor European Demonstrator) is an example of a Lead-cooled Fast Reactor (LFR), one of the six reactor technologies identified by the Generation IV International Forum (GIF) for the next generation of nuclear energy systems. In February 2026, the EAGLES Consortium (Ansaldo Nucleare, ENEA, RATEN, and SCK CEN) signed a collaboration agreement with NewCleo to advance the LEANDREA reactor prototype. This prototype, to be built at SCK CEN in Belgium by 2034, serves as a technological precursor to the ALFRED performance demonstrator in Romania. The ALFRED project is central to the roadmap for commercializing the EAGLES-300 reactor by 2039. ALFRED's lead-cooled fast-spectrum and closed fuel-cycle capability promise substantial reductions in uranium consumption and trans-uranic waste [1,2]. To support these advancements and the related nuclear safeguards needs, the development of NDA techniques is essential. ALFRED's fuel is Mixed Oxide (MOX) composition with Pu fractions of 20–30 wt% (up to ~ 13 kg of reactor-grade Pu per fuel assembly) and a high spontaneous-fission rate, particularly from even Pu isotopes. The goal of this study is to develop an NDA system for safeguards verification of the ALFRED fresh fuel, as part of the "NDA 2.0" framework for advanced and small modular reactors.

Methodology. The study utilized the MCNP-PTA (Pulse Train Analysis) code, a JRC-Ispra extension of MCNP4C2 developed for the design of neutron coincidence and multiplicity counting systems. MCNP-PTA implements shift-register logic, allowing the direct modeling of dead time for each component of the electronic chain (including amplifiers, OR chains, or mixers). This capability ensures that simulation results can be compared directly with experimental data [3].



The modeled passive neutron coincidence collar (PNCC) replicates a JCC-71 type collar typically used in BWR mode. To adapt it for the ALFRED fuel cycle, the traditional door, which houses an AmLi neutron source for active interrogation, was replaced with a dedicated front bank of detectors to enable fully passive operation. The system consists of 24 ^3He proportional counters (pressurized to 4 atm) embedded in a polyethylene moderator. The detector geometry follows a 4-bank configuration with an internal cavity measuring 17×23.5 cm and a polyethylene height of 40 cm. These dimensions were specifically optimized to accommodate the hexagonal ALFRED fuel assembly (Fig.1).

Results. The experimental validation demonstrated high accuracy for the simulation framework:

- **^{252}Cf Scans:** Measurements were performed in a low-background neutron scattering laboratory at JRC-Ispira. Total count rates for source positions across the horizontal axis matched simulations with an uncertainty of less than 1%.
- **Plutonium Oxide Validation:** Using certified reference materials spanning a wide range of ^{240}Pu content, the simulations indicated a deviation of less than 1% for Singles and less than 2% for Doubles compared with the actual measurements.
- **Calibration & Diversion:** The validated model is used to generate a reference curve mapping rates to linear plutonium density (g/cm) for the full-scale ALFRED assembly. Furthermore, the model quantified diversion scenarios.

This work is ongoing, and the full set of results regarding diversion sensitivity will be presented at the INMM conference.

Conclusion. The passive neutron coincidence collar fulfills key safeguards requirements for the ALFRED reactor by providing verification of the Pu content and the detection of diversion at the fuel assembly level without an external neutron source. This work supports the development of the "NDA 2.0" needs for the next generation of Advanced

and Small Modular Reactors.

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B | Appendix B: Tensor Train decomposition

This appendix provides a brief introduction to the Tensor Train (TT) decomposition, with emphasis on its application to high-dimensional PDEs. For a more comprehensive treatment of the mathematical theory and algorithms, we refer the reader to the original work of Oseledets [60] and the PhD thesis of Gelß [61].

Consider a function of d variables

$$\psi(y_1, \dots, y_d)$$

discretized on the tensor-product grid

$$\{y_{\nu_i}\}_{\nu_i=1}^{m_i} \quad i = 1, \dots, d$$

The discrete function can be represented as a tensor of order d

$$\Psi \in \mathbb{R}^{m_1 \times \dots \times m_d} \quad (\text{B.1})$$

whose entries are defined through

$$\Psi_{\nu_1, \dots, \nu_d} = \psi(y_{\nu_1}, \dots, y_{\nu_d}) \quad (\text{B.2})$$

Similarly, a discrete linear operator mapping functions defined on $\{y_{\nu_i}\}_{\nu_i=1}^{m_i}$ to functions defined on $\{x_{\mu_i}\}_{\mu_i=1}^{n_i}$ can be represented by a tensor operator of order $2d$

$$\mathcal{L} \in \mathbb{R}^{(n_1 \times \dots \times n_d) \times (m_1 \times \dots \times m_d)} \quad (\text{B.3})$$

with entries

$$\mathcal{L}_{\mu_1, \dots, \mu_d, \nu_1, \dots, \nu_d} = \mathcal{L}(x_{\mu_1}, \dots, x_{\mu_d}; y_{\nu_1}, \dots, y_{\nu_d}) \quad (\text{B.4})$$

Applying the operator to the function equals doing a tensor contraction,

$$\Phi_{\mu_1, \dots, \mu_d} = \sum_{\nu_1=1}^{m_1} \cdots \sum_{\nu_d=1}^{m_d} \mathcal{L}_{\mu_1, \dots, \mu_d, \nu_1, \dots, \nu_d} \Psi_{\nu_1, \dots, \nu_d} \quad (\text{B.5})$$

which is the high-dimensional analogue of a matrix–vector product.

The number of entries in the full tensor representation scales as

$$\mathcal{O}(m^d)$$

for functions and

$$\mathcal{O}(n^d m^d)$$

for operators, assuming $m = \max_i \{m_i\}$ and $n = \max_i \{n_i\}$. This exponential growth is the manifestation of the curse of dimensionality.

Many functions and operators arising in physical applications, however, exhibit low-rank structure and can be approximated efficiently using tensor decompositions.

For a tensor Ψ , the Tensor Train decomposition writes

$$\Psi_{\nu_1, \dots, \nu_d} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} G_{\nu_1, \alpha_1}^{(1)} G_{\alpha_1, \nu_2, \alpha_2}^{(2)} \cdots G_{\alpha_{d-1}, \nu_d}^{(d)} \quad (\text{B.6})$$

where

$$G^{(i)} \in \mathbb{R}^{r_{i-1} \times m_i \times r_i} \quad r_0 = r_d = 1$$

are called TT cores and r_i are the TT ranks.

The storage cost becomes

$$\mathcal{O}(dmr^2)$$

where $r = \max_i r_i$.

Operators can be represented analogously in TT format:

$$\mathcal{L}_{\mu_1, \dots, \mu_d, \nu_1, \dots, \nu_d} = \sum_{\beta_1=1}^{s_1} \cdots \sum_{\beta_{d-1}=1}^{s_{d-1}} A_{\mu_1, \nu_1, \beta_1}^{(1)} A_{\beta_1, \mu_2, \nu_2, \beta_2}^{(2)} \cdots A_{\beta_{d-1}, \mu_d, \nu_d}^{(d)} \quad (\text{B.7})$$

with TT operator cores

$$A^{(i)} \in \mathbb{R}^{s_{i-1} \times n_i \times m_i \times s_i} \quad s_0 = s_d = 1.$$

The corresponding storage requirement is

$$\mathcal{O}(dnmr^2)$$

assuming bounded operator ranks.

The contraction of a TT operator with a TT tensor can also be performed directly in compressed form. The resulting TT tensor $\Phi = \mathcal{L}\Psi$ has cores

$$D_{\gamma_{i-1}, \mu_i, \gamma_i}^{(i)} = \sum_{\nu_i} A_{\beta_{i-1}, \mu_i, \nu_i, \beta_i}^{(i)} G_{\alpha_{i-1}, \nu_i, \alpha_i}^{(i)}, \quad (\text{B.8})$$

where

$$\gamma_i = (\alpha_i, \beta_i)$$

The resulting TT ranks grow multiplicatively as

$$r_{\Phi, i} = r_{\Psi, i}, r_{\mathcal{L}, i}$$

The computational complexity of the operator–tensor product scales as

$$\mathcal{O}(dnmr_{\mathcal{L}}^2 r_{\Psi}^2)$$

which grows linearly with dimension.

Another common operation in which the ranks grow is the addition of two TT tensors. The resulting TT ranks grow additively.

Several algorithms exist to compute TT decompositions. TT-SVD constructs the decomposition through successive singular value decompositions of matricized tensors [61]. Its truncation error is bounded by the root-sum-square of the discarded singular values at each unfolding.

When the full tensor cannot be assembled explicitly, TT-Cross provides an alternative approach by constructing the decomposition from sampled tensor entries only [72].

As shown in this work and in literature, many differential operators admit separable low-rank representations. In such cases, TT operators can often be constructed directly from one-dimensional components without assembling the full multidimensional tensor.

C | Appendix C: Numerical scheme for the neutron transport model

C.0.1. Phase space discretization

The angular variable is discretized using the discrete ordinates (S_N) method. The angular integrals are approximated by Gauss–Legendre quadrature using N_a discrete directions and weights,

$$\{\mu_n\}_{n=1}^{N_a} \quad \{w_n\}_{n=1}^{N_a}$$

The spatial domain is partitioned into N_s finite elements,

$$K_i = \left[x_i - \frac{h_i}{2}, x_i + \frac{h_i}{2} \right]$$

where x_i denotes the cell center and h_i the cell width. Within each element, a local coordinate $\xi \in [-1, 1]$ is introduced through the affine mapping

$$x = x_i + \xi \frac{h_i}{2}, \quad dx = \frac{h_i}{2} d\xi.$$

A modal Discontinuous Galerkin finite-element discretization is employed. The angular flux is expanded locally in a Legendre polynomial basis of order p ,

$$\psi(\xi) = \sum_{a=0}^p \psi_a P_a(\xi).$$

The weak form is obtained by multiplying the transport equation by a test function $P_a(\xi)$ and integrating over each element,

$$\int_{-1}^1 P_a(\xi)(\mathcal{L} - \mathcal{K})\psi_g(\xi)d\xi = \int_{-1}^1 P_a(\xi)f_g\left(x_i + \xi\frac{h_i}{2}\right)d\xi.$$

This procedure yields the elemental mass matrix

$$M_{ab} = \frac{h_i}{2} \int_{-1}^1 P_a(\xi)P_b(\xi)d\xi = \frac{h_i}{2a+1}\delta_{ab}$$

where the orthogonality of the Legendre basis has been exploited.

The streaming term is treated by integration by parts,

$$\int_{-1}^1 P_a(\xi)\frac{\partial\psi_g}{\partial\xi}d\xi = [P_a(\xi)\psi_g^*]_{-1}^1 - \int_{-1}^1 \psi_g\frac{\partial P_a}{\partial\xi}d\xi$$

leading to the elemental streaming matrix

$$S_{ab} = \int_{-1}^1 P_b(\xi)\frac{\partial P_a}{\partial\xi}d\xi = \begin{cases} 2, & a > b, \ a + b \text{ odd}, \\ 0, & \text{otherwise.} \end{cases}$$

Where recurrence relations of Legendre polynomials were exploited. After assembly, the spatial discretization results in a block-structured operator with

$$\text{dof}_s = N_s(p+1)$$

degrees of freedom.

Since the DG approximation is discontinuous across element interfaces, information must be exchanged between neighboring cells through numerical fluxes ψ^* . An upwind flux is employed, ensuring that particle information propagates only from the upstream side of an interface.

For positive angular directions ($\mu_n > 0$), particles travel from left to right and the interface matrices are

$$B_R^+ = P_a(1)P_b(1), \quad B_L^+ = P_a(-1)P_b(1).$$

Using the endpoint properties of Legendre polynomials,

$$P_a(1) = 1, \quad P_a(-1) = (-1)^a,$$

these become

$$B_R^+ = 1, \quad B_L^+ = (-1)^a.$$

Similarly, for negative angular directions ($\mu_n < 0$), particles travel from right to left, yielding

$$B_R^- = P_a(1)P_b(-1) = (-1)^b,$$

and

$$B_L^- = P_a(-1)P_b(-1) = (-1)^{a+b}.$$

These matrices introduce the coupling between neighboring elements required to correctly represent particle transport. Boundary conditions enter naturally through the inflow faces, namely the left boundary for $\mu_n > 0$ and the right boundary for $\mu_n < 0$. The cell boundary vectors which will be used for the implementation of boundary conditions are defined as

$$\mathbf{b}_R = P_a(1) = 1$$

$$\mathbf{b}_L = P_a(-1) = (-1)^a$$

The temporal dimension is discretized using a first-order implicit Euler scheme. Let

$$\{t_k\}_{k=1}^{N_t}$$

be the discrete time points, with

$$\Delta t_k = t_k - t_{k-1}.$$

The time derivative is approximated as

$$\frac{\partial \psi}{\partial t} \approx \frac{\psi_k - \psi_{k-1}}{\Delta t_k},$$

while all remaining terms are evaluated at the new time level t_k .

Rather than performing a conventional time-marching procedure, the entire temporal dimension is retained within the Tensor Train representation. Time is therefore treated as an additional tensor dimension alongside space, angle and energy. The resulting linear system couples all time levels simultaneously, allowing AMEn to exploit low-rank structure not only in phase space but also along the temporal coordinate. The known initial condition appears as a contribution to the right-hand side at the first time level.

For what regards inflow boundary conditions, they are defined for the discrete direction μ_n and time step t_k as

$$\begin{aligned}\psi_g(x=0, \mu_n, t_k) &= \psi_{0,g}(\mu_n, t_k) \quad \mu_n > 0 \\ \psi_g(x=L, \mu_n, t_k) &= \psi_{L,g}(\mu_n, t_k) \quad \mu_n < 0\end{aligned}$$

by integrating by parts the streaming term, the contribution of the boundary conditions is naturally included in the right hand side of the equation for the first and last spatial cells, and only for the inflowing angular directions.

$$\begin{aligned}&+ \mathbf{b}_L \mu_n \psi_{0,g}(\mu_n, t_k) \quad i=1, \mu_n > 0 \\ &- \mathbf{b}_R \mu_n \psi_{L,g}(\mu_n, t_k) \quad i=N_s, \mu_n < 0\end{aligned}$$

The initial condition is defined for the discrete spatial points x_i and angular directions μ_n as

$$\psi_g(x_i, \mu_n, t=0) = \psi_{in,g}(x_i, \mu_n) \quad (\text{C.1})$$

The right hand side of the equation for the first time level will then have a contribution from the initial condition of the form

$$+ \frac{h_i}{2\Delta t_1} \int_{-1}^1 P_a(\xi) \psi_{in,g} \left(x_i + \xi \frac{h_i}{2}, \mu_n \right) d\xi \quad (\text{C.2})$$

C.0.2. Tensor Train representation

To visually highlight the separation of the TT cores the tensor product symbol $\otimes$ will be used. Hence, the solution and source term decomposition can be expressed as

$$\begin{aligned}\psi_g(x_i, \mu_n, t_k) &= \psi^{(1)}(x_i) \otimes \psi^{(2)}(\mu_n) \otimes \psi^{(3)}(g) \otimes \psi^{(4)}(t_k) \\ f_g(x_i, \mu_n, t_k) &= f^{(1)}(x_i) \otimes f^{(2)}(\mu_n) \otimes f^{(3)}(g) \otimes f^{(4)}(t_k)\end{aligned}$$

Where the spatial index $i = 1 \dots N_s$ indicates the finite element cells, and the spatial cores will have block structure in the Legendre modes.

The operator for the whole phase space naturally presents a tensor product structure allowing to decouple operators for each variable in the phase space. L and K will be a sum of rank-1 Tensor Train matrices (TTM) for each term of the equation. The transport operator L will be the sum of the streaming, collision and time derivative operators, and it will result to be fully diagonal in energy group and angle, while bi-diagonal in time and space.

The time derivative term is

$$M\delta_{ii'} \otimes \delta_{nn'} \otimes \frac{1}{v_g}\delta_{gg'} \otimes \frac{1}{\Delta t_k}(\delta_{kk'} - \delta_{k,k'+1})$$

Where M is the mass matrix and δ is the Kronecker delta. For the streaming term let us define

$$\delta_{nn'}^+ = \begin{cases} 1 & n = n' \text{ and } \mu_n > 0 \\ 0 & \text{else} \end{cases}$$

$$\delta_{nn'}^- = \begin{cases} 1 & n = n' \text{ and } \mu_n < 0 \\ 0 & \text{else} \end{cases}$$

to denote the positive and negative angular directions, respectively. The streaming term can then be written as

$$\begin{aligned} & [(B_R^+\delta_{ii'} - B_L^+\delta_{i,i'+1}) \otimes \mu_n\delta_{nn'}^+ + \\ & (B_R^-\delta_{i,i'-1} - B_L^-\delta_{ii'}) \otimes \mu_n\delta_{nn'}^- + \\ & -S\delta_{ii'} \otimes \mu_n\delta_{nn'}] \otimes \delta_{gg'} \otimes \delta_{kk'} \end{aligned}$$

where S is the streaming matrix. The collision term is simply

$$M\delta_{ii'} \otimes \delta_{nn'} \otimes \Sigma_{t,g}\delta_{gg'} \otimes \delta_{kk'}$$

The scattering operator K will be a sum of rank-1 TTM for each term in the Legendre expansion of the scattering kernel. It will be diagonal in space and time, but dense in angle and energy. For the l -th term of the Legendre expansion it will be, reducing the integral to a sum with the angular quadrature weights w_n ,

$$M\delta_{ii'} \otimes \frac{2l+1}{2}\gamma^l P_l(\mu_n)P_l(\mu_{n'})w_{n'} \otimes c_{gg'} \otimes \delta_{kk'}$$

Choosing Gauss-Legendre quadrature for the angular discretization is particularly advantageous since it is exact for polynomials of order up to $2N_a - 1$, which means that the only approximation error in the scattering operator comes from the truncation of the Legendre expansion.

Finally the boundary conditions contribute to the right hand side of the equation for the first and last spatial cells, and only for the inflowing angular directions. From the previous treatment, we can directly express the contributions in TT format by decomposing the 3 dimensional angular, energy group and time dependence in a 3-dimensional TT.

$$\begin{aligned} & + \mathbf{b}_L \delta_{i1} \otimes \delta_{nn'}^+ \mu_{n'} \psi_0(\mu_{n'}) \otimes \psi_0(g) \otimes \psi_0(t_k) \\ & - \mathbf{b}_R \delta_{i1} \otimes \delta_{nn'}^- \mu_{n'} \psi_L(\mu_{n'}) \otimes \psi_L(g) \otimes \psi_L(t_k) \end{aligned}$$

where $\psi_0(\mu_n)$, $\psi_0(g)$, $\psi_0(t_k)$ and $\psi_L(\mu_n)$, $\psi_L(g)$, $\psi_L(t_k)$ are the TT cores for the left and right boundary conditions, respectively.

Similar treatment can be done for the initial condition, which will contribute to the right hand side of the equation for the first time level with a term of the form

$$\frac{h_i}{2} \int_{-1}^1 P_a(\xi) \psi_{in} \left(x_i + \xi \frac{h_i}{2} \right) d\xi \otimes \psi_{in}(\mu_n) \otimes \psi_{in}(g) \otimes \frac{1}{\Delta t_k} \delta_{k1}$$

where $\psi_{in}(x_i)$, $\psi_{in}(\mu_n)$ and $\psi_{in}(g)$ are again the TT cores for the initial condition in space, angle and energy, respectively.

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