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Sandia National Laboratories Early Career University Faculty Mentoring Program in International Safeguards

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ABSTRACT

Recent years have seen a significantly increased focus in the areas of knowledge retention and mentoring of junior staff within the U.S. national laboratory complex. In order to involve the university community in this process, as well, an international safeguards mentoring program was established by Sandia National Laboratories (SNL) for early career university faculty. After a successful experience during 2019, the program continued into 2020 to include two new faculty members who were paired with SNL subject matter experts based on the topic of their individual projects: one to work on advanced laboratory work for physics, technology, and policy of nuclear safeguards and nonproliferation, and the other to look at machine learning applied to international safeguards and nonproliferation.

There is a two-pronged purpose to the program: fostering the development of educational resources available for international safeguards and exploring new research topics stemming from the exchange of mentor and mentee. Further, the program as a whole allows for junior faculty members to establish and expand a relationship network within international safeguards. In addition, programs such as this build stronger connections between the academic and the national laboratory community.

Thanks to the junior faculty members that now have new connections into the laboratory community and potential for collaboration projects with the laboratories in the future, safeguards knowledge can actually increase far beyond just individually engaging students using this new and efficient avenue.

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NOMENCLATURE

Abbreviation	Definition
ASIC	application-specific integrated circuit
ATF	accident tolerant fuel
CT	computed-tomography
DA	destructive analysis
DNN	deep neural networks
DNN R&D	DOE NNSA Defense Nonproliferation Research and Development
DOE	U.S. Department of Energy
DS	Data Science
DT	deiterium-tritium
FBP	filtered back-projection
HPGe	high purity germanium detector
IAEA	International Atomic Energy Agency
ML	Machine Learning
NDA	on-destructive analysis
NEUP	Nuclear Engineering University Program
NNSA	National Nuclear Security Administration
PDS	pulse shape discrimination
PM	process monitoring
SiPM	silicon photomultiplier
SNL	Sandia National Laboratories
SNM	special nuclear materials
UF	University of Florida
UIUC	University of Illinois at Urbana-Champaign

1. INTRODUCTION

In 2019, Sandia National Laboratory has started a mentoring program to connect young faculty with scientists at the Laboratory to help to directly expose early-career faculty to the research performed in the context of nuclear safeguards.

Given the successful experience in 2019 [1], the program continued in 2020, with the involvement of two new faculty members, Angela Di Fulvio, Assistant Professor in the Nuclear, Plasma, and Radiological Engineering Department at the University of Illinois at Urbana-Champaign (UIUC), and Kyle C. Hartig, Assistant Professor of Nuclear Engineering in the Department of Materials Science and Engineering at the University of Florida (UF).

The program had the twofold purpose of fostering the development of educational resources in safeguards-related areas and also exploring research topics of mutual interest of faculty and their mentors. A mentor was assigned to both faculty. Mentors advised the faculty in the course development and held virtual meetings to discuss ongoing research projects and identify potential mutual interests for the development of joined publications or proposals.

2. EDUCATION

The two faculty members focused on different curriculum development tasks: complete course versus flexible course content that could be developed into stand-alone course or integrated into existing coursework. Thus, while there was some overlap in their efforts for this mentoring program, their course material creation was done individually. The material developed by each professor is described separately, below.

2.1. CURRICULUM DEVELOPMENT AT UIUC

A new course was developed at the University of Illinois at Urbana-Champaign, entitled "Advanced Laboratory on Physics, Technology, and Policy of Nuclear Safeguards and Nonproliferation". The course is meant to be an advanced laboratory and will be offered in the Spring 2021 semester, as a graduate elective course. Four students already attended the course as an independent study in the Spring 2020 and Fall 2020 semesters. The laboratory course focuses on the science, technology, and policy associated with nuclear safeguards, security and verification. The course consists of two parts: a lecture component where technical fundamentals and history of nonproliferation are reviewed and discussed, and an immersive lab section. Throughout the semester, the students will design and develop selected experimental systems, among those listed below, which can be used to identify, characterize, image, and quantify special nuclear materials. The lab sessions implement a unique model where students need to fully develop selected experiments, from design to validation and testing. Students will become familiar with experimental techniques employed in contemporary research and industrial laboratories, and learn different software, CAD, and hardware tools, depending on the specific experiment, including programming languages e.g., as C++ and Python, simulation environments, e.g., GEANT4 and MCNP, and engineering CADs, e.g., SolidWorks and Cadence. Each lab will give them the opportunity to learn and become familiar with specific software and hardware tools. The laboratories are:

- Lab #1 Neutron Activation Analysis. This lab concerns the neutron activation analysis using deuterium-tritium fusion neutrons. Students will examine the delayed gamma-ray response of Th-232, U-238, and U-235. High-resolution gamma-ray spectra will be acquired and analyzed to estimate the half-lives and fission yields of detected fission products, such as Se-86, Rb-90, and Cs-144. A pneumatic system will be used to remotely control the irradiated samples and transfer them from the irradiation location to the front face of the HPGe detector.

- Lab #2 Chemistry of liquid organic scintillators. Organic scintillators are suitable for non-proliferation and safeguards applications because they can detect both neutrons and gamma rays and discriminate between them. Additionally, they exhibit a fast response and can be produced in large sizes. In this lab, the students will go through the purification and synthesis stages to produce liquid scintillators, with particular emphasis on pulse shape discrimination capability.

- Lab #3 Stand-off neutron imaging system. Students will operate and analyze data acquired by a stand-off imager capable of imaging neutrons and gamma-rays emitted by radiation sources available in the lab, such as Cs-137 and PuBe. They will learn the application of scattering kinematics to Compton cameras for gamma-ray detection and neutron scatter cameras. Students will quickly become familiar with the operating principles of the system using a virtual reality tool suitably developed to guide them through this laboratory.
- Lab #4 Compact gamma imager based on silicon photomultipliers and CsI(Tl) pixelated detector. Students will operate and analyze data acquired by a compact system capable of imaging gamma-rays emitted by radiation sources available in the lab. They will learn the application of scattering kinematics to Compton cameras for gamma-ray detection. Students will learn gamma-imaging reconstruction methods and will design software and hardware strategies to optimize the system energy and position resolution.
- Lab #5 Multiplicity counting for non-destructive assay of special. nuclear materials based on combined gamma-ray and neutron detection Neutron multiplicity counting is a well-established measurement tool for characterizing and verifying fissile material. In this lab, students will learn how to implement neutron and gamma-ray multiplicity counting to estimate the fissile mass and multiplication of an unknown sample. The counting electronics is based on an open-hardware microcomputer (Red Pitaya). Students will learn to process detectors' signal onboard by programming the open FPGA embedded on the Red Pitaya.
- Lab #6 Muon lifetime and use of muons to detect special nuclear materials. The muon is a heavy, unstable elementary particle similar to the electron, with a lifetime of approximately 2.1 ms. Cosmic rays in the upper atmosphere create a muon flux at sea level of approximately 1 muon/cm^2/minute. In this lab, students will detect cosmic-ray muons using a photomultiplier in a tank of liquid scintillator. They will estimate muon lifetime by measuring the time difference between the first neutron interaction and the appearance of the decay electron. They will also become familiar with the application of muon to nuclear safeguards and nonproliferation by measuring the muon-induced fission neutrons in uranium samples using a separate detector array.
- Lab #7 Raman spectroscopy for nuclear forensics applications. Raman spectroscopy is a very important practical tool for the identification of molecules and minerals. The Raman effect arises when a photon is incident on a molecule and interacts with the electric dipole of the molecule. The resulting shift in photon energy gives information about the vibrational modes in the inspected sample. Students will use a Raman spectrometer to inspect uranium ore samples, of different origin and with a wide range of impurity content. They will be able to analyze the acquired data and identify the compound type, and identify process-related impurities observed in the samples.
- Lab #8 Gamma spectroscopy and deconvolution methods for isotopic identification. Gamma-ray spectroscopy is one of techniques of choice for the identification of unknown radionuclides because each radionuclide exhibits a characteristic gamma-ray spectrum. However, confidently identifying unknown radionuclides is a challenging problem, when assaying real-world samples.

In this lab, the students will use a High-purity Germanium detector to acquire spectra of different nuclides, including uranium bearing samples. The students will then implement new algorithms for unfolding and classification of gamma-ray spectra and, upon availability, compare their performance with available expert systems.

Figures 2-1 and 2-2 show the detector configuration that one student arranged and the reconstructed image of a 30-minute acquisition of a PuBe 1-Ci source. The source was placed approximately 2-m away from the detector panel. These data were acquired while lab access was still possible during the Spring 2020 semester. The development of a relatively complex experiment, encompassing mechanical design, data acquisition, and analysis, is an example of the NPRE advanced laboratory course.

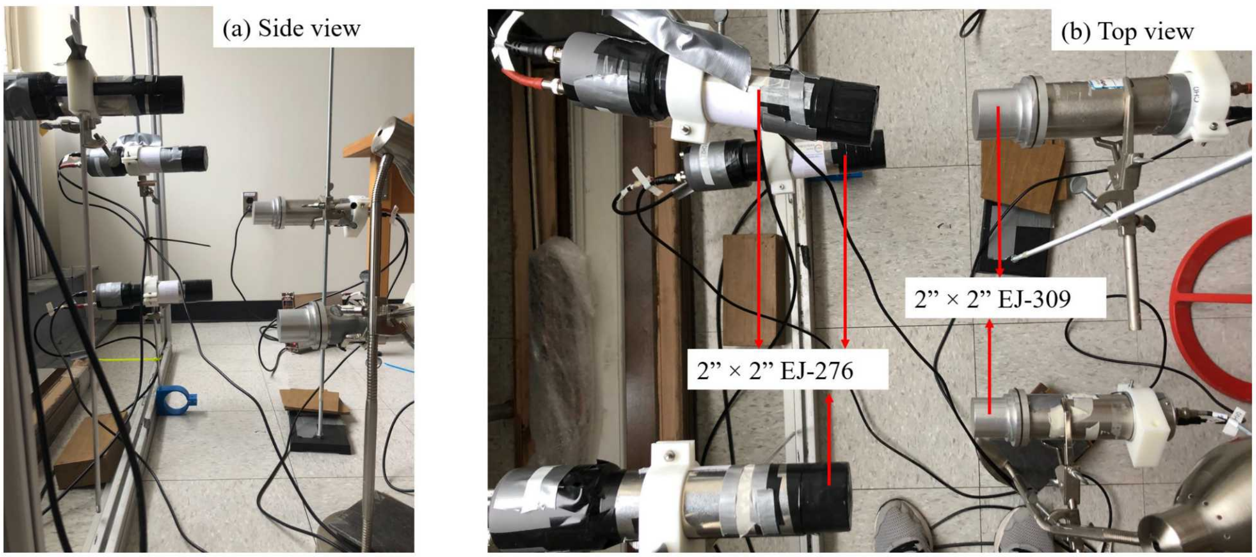

Figure 2-1. Experimental setup of a five-detector neutron scatter camera.

The other three students involved in the independent study developed and demonstrated: a fast-neutron multiplicity counter for active interrogation of depleted uranium; a Raman spectrometry protocol for nuclear forensics; and an internet-of-things based pneumatic system for DT-neutron sample activation.

Recorded lectures will be made available online by the end of the Spring 2021 semester. These will include a review of the history and policy of safeguards and nonproliferation, and several tutorials to introduce the students to the use of the software tools needed to implement the various labs.

2.2. CURRICULUM DEVELOPMENT AT UF

The UF faculty member had prior experience with course development (having previously developed a course in Nuclear Forensics at UF), but creating this course under the guidance of an SNL mentor with expertise in machine learning provided invaluable insight into the essential topics. The mentoring also included input on the best methods of material presentation, contributing to a stronger course. These contributions provided a broader, more comprehensive base for the course. The most important

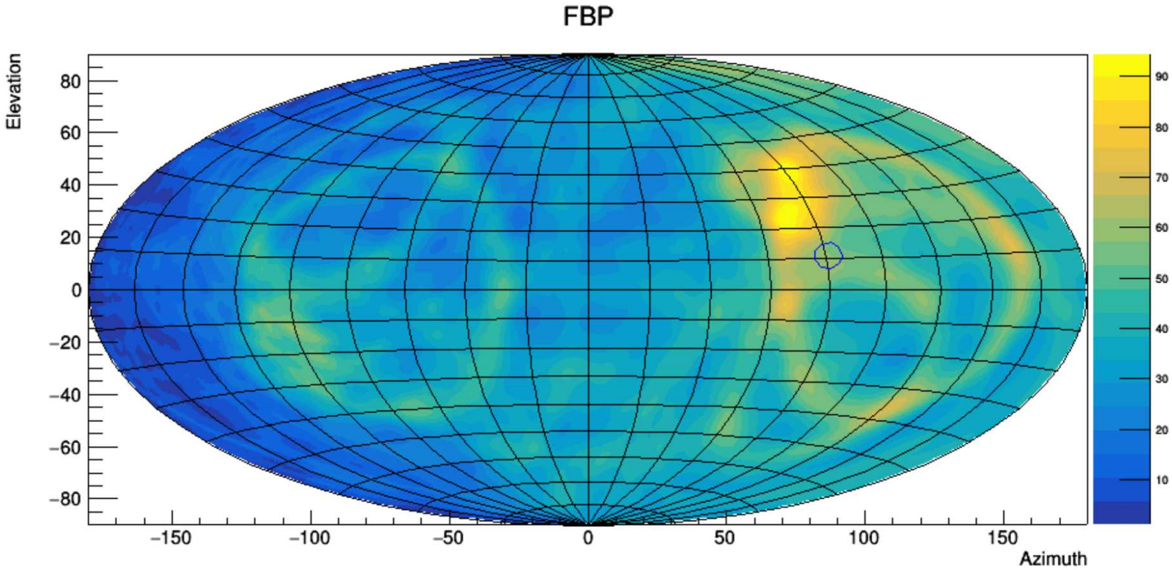

Figure 2-2. Filtered back-projection (FBP) reconstructed image as acquired by the neutron scatter camera. The blue circle indicated the actual source location.

changes to note are the addition of information related to additional datasets that are publicly available and relevant to international safeguards and nonproliferation as well as a focus on the foundations of machine learning and data science. The latter point is extremely important and largely overlooked when developing a new specialized course in a niche subject area.

Flexible course content was and continues to be developed by the UF faculty member that could either be included into existing courses or further developed into a new, specialized course alongside components of existing course material in international safeguards and nonproliferation. From discussions with the SNL mentor, it was determined that mastery of the fundamentals of data science and machine learning is important for the success of any broader application of machine learning to problems of interest (e.g. international safeguards and nonproliferation); therefore, a fundamental list of machine learning and data science topics was developed and is shown in Table 2-1. The UF Faculty member has included a subset of these identified topics as introductory lectures in the Senior Undergraduate Radiation Detection and Instrumentation course he is teaching in Fall 2020, and he plans to develop the full list as a major component of a stand-alone course in "Nuclear nonproliferation, safeguards, and security science" in the spring or fall 2021 semester as a cross-listed graduate and undergraduate level course.

As stated above, the ultimate goal for the flexible course material is development into a stand-alone course. To accomplish this goal, specific datasets will have to be produced, developed, and acquired that are relevant to international safeguards and nonproliferation on which machine learning concepts taught in the course can be practiced and applied. With the help of the SNL mentor, the UF faculty member is in the process of acquiring well-defined datasets that can be developed for use as example datasets for application to international safeguards and nonproliferation. The challenge here is that most of these datasets are not specifically related to nuclear (e.g. credit card fraud datasets); however,

Table 2-1. Machine learning topics to be covered in proposed coursework.

Lecture Topic
Probability, Gaussian Models, Bayesian Statistics
Overview of Supervised Learning
Linear Methods for Regression
Linear Methods for Classification
Model Assessment and Selection
Model Inference and Averaging
Additive Models, Trees, and Related Methods
Deep Learning and Neural Networks
Support Vector Machines
Unsupervised Learning
Random Forests
Ensemble Learning
Graphical Models

concepts of machine learning can be demonstrated quite well with these datasets, and, with some development, similarities of the information to safeguards and nonproliferation information can be made (e.g. shipper and receiver and material control and accountability logs and flow sheets). Additionally, the UF faculty member is working to develop a unique "pattern of life" dataset that would represent real-time radiation field and environmental conditions present in the radiation detection teaching lab during weeks when experiments are taking place as well as off periods, which would produce a unique pattern of life dataset that could be used as a similitude for performing machine learning analysis on the operations of real facilities and processes. Applied projects are a key aspect of the design of the flexible course content, and, ultimately, will form the pillars that are built on the foundation of mastery of the fundamental concepts of machine learning in the stand-alone course. These applied projects are currently being developed; however, several are provided below as examples.

- **Image processing.** Students will utilize existing broad image datasets (e.g. ImageNet) and specialized datasets (e.g. IAEA Tomography Challenge & UF TRISO x-ray images datasets) to develop image classification, change detection, and identification algorithms.
- **Pattern of life.** Students will utilize the already collected pattern of life on the UF radiation detection and instrumentation teaching lab to classify specific activities (e.g. experiment day vs non-experiment day), anomalous activities (e.g. high background, after hours activity, etc.), and nefarious activities (e.g. radiation field present outside experiment periods). Additionally, students will work to develop additional pattern of life datasets through experimental effort and high-fidelity modeling.
- **Data classification.** Utilizing the IAEA database of interdicted nuclear material samples (a heterogeneous and disparate data-set), students will run regression algorithms to classify the samples and discover possible hidden similarities or trends in the characteristics of interdicted materials.

- **Anomalous/nefarious activity detection.** Students will utilize the Credit Card Fraud Detection dataset to apply machine learning concepts for the detection of nefarious activities. The dataset is highly unbalanced, the positive class (frauds) account for 0.172% of all transactions and can be thought of as being analogous to shipper-receiver or material control and accountancy information the IAEA or a domestic regulator may collect..

Recorded lectures will be made available online by the end of the Fall 2021 semester. These will include a review of the history and policy of international safeguards, security, and nonproliferation, an introduction to and basics of data science and machine learning, and several tutorials to introduce the students to the use of software tools and datasets needed to successfully address the various projects.

3. RESEARCH

The communication with SNL mentors helped to develop research topics relevant to international safeguards and nonproliferation that were in line with existing projects and interests of the two faculty. Eduardo Padilla and Nathan Shoman were the SNL mentors of Angela Di Fulvio and Kyle Hartig, respectively.

3.1. COLLABORATION WITH DR. DI FULVIO'S RESEARCH GROUP

The identified topic of interest for Dr. Di Fulvio's collaboration was the light readout emitted by scintillators by silicon photomultipliers (SiPMs). Two students were involved in the project, Satwik Pani, senior undergraduate, and Ming Fang, graduate student. Two main aspects were discussed: (1) the development of a detailed SiPM PSpice model to predict the behavior of a given SiPM for radiation detection from its electrical characteristics and (2) the use of an off-the-shelf application-specific integrated circuit (ASIC) system for the readout of a large-number of SiPM channels. A SiPM is an array of single-photon avalanche detector microcells operated in Geiger mode, which are a promising alternative to traditional photomultiplier tubes in safeguards applications for their smaller form factor, good sensitivity, and low-voltage power supply. Their application to safeguards measurements could enable a number of developments, ranging from compact neutron and gamma-ray imaging systems to unmanned vehicles equipped with compact radiation detectors.

Regarding the former effort, a simulated model of a commercial SiPM was developed in PSpice, which allowed to reproduce electrical pulses in response to an external stimulus, as a function of the number of microcells that were activated inside the SiPM (Figure 3-1). The developed model will be compared to experimental data to validate the used electrical constants in the model. Experimental data will be acquired in response both to a well-characterized light source and radiation-induced light. An experimental setup including a monochromatic laser source, a power meter, and the SiPM in a light-tight environment was developed at UIUC to characterize the SiPM response to single-photon irradiation. A manuscript to be submitted to a peer-reviewed journal is currently being prepared to report the results of this project. In addition to Mr. Padilla, Mr. Maierhafer, expert in electronics for radiation detection, provided subject matter expertise on the topic.

Regarding the second project, the interaction with Mr. Padilla, Dr. Marleau, and Dr. Sweany at Sandia was helpful to identify potential strategies to implement pulse shape discrimination (PDS) to discriminate different types of radiation using ASICs that are not designed to perform this type of analysis. Two custom printed circuit boards encompassing 28 SiPMs each are currently being manufactured, which will be used to detect the light emitted by a CsI(Tl) and stilbene pixelated

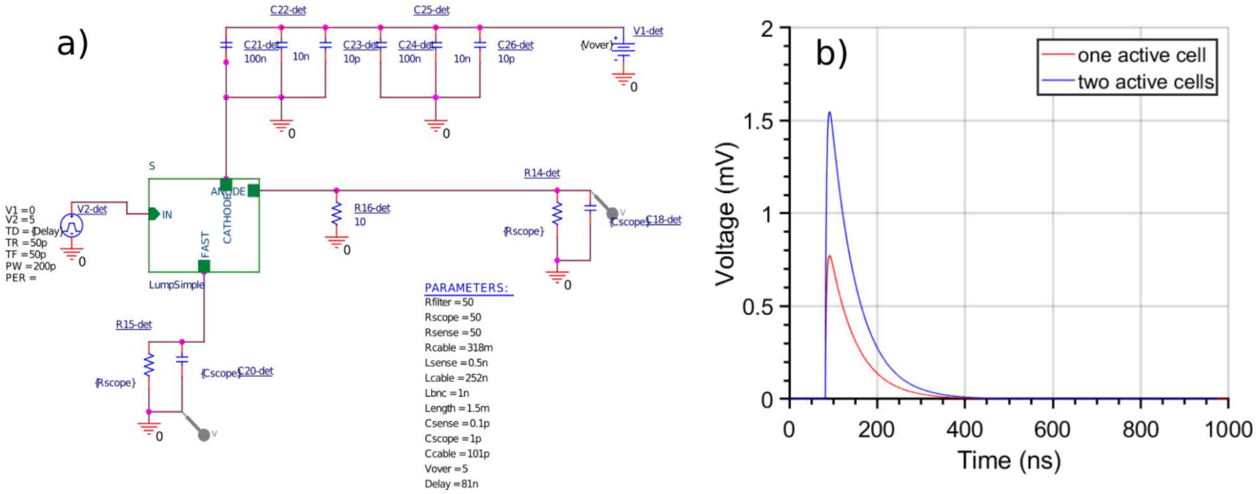

Figure 3-1. (a) Electrical model of the SiPM readout board MicroFC-SMA-60035 by On Semiconductor, the SiPM model is shown by the green-outline square and is simulated simultaneously. (b) Example of simulated output pulses. In the current version of the model, no noise source was included.

detectors. ASICs signal processing will then be performed and imaging and PSD suitability demonstrated for the detection of neutrons and gamma rays in the stilbene case.

3.2. COLLABORATION WITH DR. HARTIG'S RESEARCH GROUP

The identified topic of interest for Dr. Hartig's collaboration was the intersection of data science (DS) and machine learning (ML) with international safeguards and nonproliferation. One graduate student, Emily Kwapis, was involved in this project with Dr. Hartig and SNL laboratory mentor Dr. Shoman.

The collaboration has resulted in the development of a number of research proposals to federal sponsors relevant to international safeguards and nonproliferation, such as DOE NNSA Defense Nonproliferation Research and Development (DNN R&D) and Nuclear Engineering University Program (NEUP) that are outlined below. It is expected that the collaboration will continue and additional proposals, collaborative work, and peer-reviewed articles will be produced either as a continuation of this project or as an extension of it.

Dr. Hartig's group over the past year has initiated several new research efforts related to the application of machine learning to nuclear safeguards and nonproliferation that benefited extensively from the collaboration and advising of the SNL mentor under this program.

One such effort that is focused on application of machine learning to the analysis of 2D and 3D (computed-tomography (CT) images) x-ray images that was under development prior to this collaboration was further developed for material control and accountancy applications at next-generation reactor facilities - specifically to the tagging and tracking of TRISO-fueled pebbles. Currently, TRISO-fueled pebble identities are not tracked because there is no method to identify, or tag, individual pebbles, which poses a problem for application of international safeguards (where verification of individual fuel/SNM items is necessary) at facilities which utilize this attractive accident tolerant fuel (ATF) form. Additionally, maintaining pebble identity offers advantages towards validating computational physics models by measuring pebble transit time as well as determining if any pebbles are retained in the core for unexpectedly long times, which could result in excessive burnup accumulation.

It was identified that during fuel fabrication a unique and arbitrary TRISO-particle distribution pattern (fingerprint) is created when fuel particles are pyrolyzed and compacted into hard graphite spheres. Through X-ray radiography this fingerprint can be imaged. A non-destructive technique using X-ray radiography and automatic image processing for recognition of fuel particles in the fuel-free zone does now exist for safety and quality assurance purposes; 225 to 450 frames are collected for a single fuel pebble within 30 seconds. By optimizing the X-ray tube and detector acquisition settings, image acquisition time can be improved to ≈10 seconds. Combining deep neural networks (DNN) with radiation imaging, these fingerprints can be extracted and compared by targeting the location of the fuel particles. By applying artificial intelligence and exploiting the intrinsic particle fingerprint, our approach is the only approach that leverages the current TRISO-fueled pebble manufacturing process instead of altering it to tag and track these pebbles at facilities for both material control and accountancy as well as international safeguards applications.

Safeguarding and monitoring facilities with high throughput of nuclear material is challenging and often requires many attended measurements. Emerging technologies in the fields of machine learning hold promise in reducing the number of in-person days required to safeguard such facilities, while also enhancing the effectiveness and efficiency of safeguards and verification. Another effort that was explored and developed for submission to NNSA DNN R&D under the university consortia proposal call as part of this faculty development project will investigate the use of data science to improve the efficiency and effectiveness of international safeguards verification and to make robust, scientifically defensible safeguards conclusions. Specifically, we plan to evaluate supervised machine learning methods for automatically integrating cross-domain and disparate data streams representative of existing and possible future sources of IAEA safeguards information for signatures discovery and pattern of life determination. Additionally, this work will evaluate the sensitivity of feature identification to the source and type of data stream included in the analysis to optimize the deployment of resources for collecting facility and process data (i.e. process monitoring (PM) and non-destructive analysis (NDA) vs destructive analysis (DA)). The IAEA has long prioritized the development of safeguards approaches that reduce the need for DA measurements which often require onsite analytical laboratories. The use of PM data combined with NDA and machine learning could reduce the need for burdensome DA measurements by correlating many different PM and NDA measurements.

The primary scientific advancement of this project is the demonstration and maturation of automated data fusion techniques for disparate data streams to answer realistic and safeguards-relevant questions. These data fusion techniques will be developed through a novel combination of cross-domain/disparate synthetic and real data related to a facility's operations and processes. Additionally, this work will produce a tool that could be used to inform the IAEA of the optimum deployment of safeguards resources at a specific facility (i.e. NDA vs DA measurements). The project is highly multidisciplinary, combining expertise in safeguards implementation, facility operations, process modeling and monitoring, radiation detection, wireless sensors, computer science, and statistics, with unique access to a nuclear facility.

The longer-term vision for this work is to provide the IAEA with decision support tools to increase both the productivity of its Operations Divisions and the probability of detecting material diversion or misuse of a safeguarded facility. The aim of our integrated approach is to allow the IAEA to do more with the data they are already collecting and increase confidence in their assessments. While this project has a focus on international safeguards, the science and technology developed in this work can be readily adapted and deployed to support the intelligence and defense missions of NNSA.

Finally, the activities outlined in the above two research examples benefit from the educational component of this project. As an example, the production of a unique data set containing marked-up real-time information on the radiation field and environmental parameters of the teaching lab at the University of Florida, which will be used to provide students a unique opportunity to apply machine learning to identify specific activities/events that occurred in the laboratory and possibly when a non-declared event happened, is invaluable from an international safeguards perspective. This type of data (i.e. pattern of life), even if collected at specific facilities, is rarely shared or available and will augment traditional machine learning data sets available online (e.g. credit card fraud data, image analysis, etc.). Further development of such data sets could be used to develop, demonstrate, and build confidence (from an international safeguards perspective) in this emerging intersection of DS/ML and international safeguards.

4. SUMMARY AND CONCLUSIONS

The second year of the Sandia faculty development program was an extremely beneficial opportunity for faculty with otherwise very limited mentoring in international safeguards. The program supported Drs. Hartig and Di Fulvio in broadening their teaching curricula and developing a network of potential collaborators in the field of international safeguards. The educational material that was created as part of this project is a valuable resource to students who would not otherwise have been exposed to these important topics in nuclear science and engineering. Some of the research projects are also being considered as topics for publications or grant proposals. The two-week visit of the faculty to Sandia National Laboratory, initially planned for July 2020, was canceled because of the travel and operation restrictions due to COVID19. It is the hope of the faculty that the visit will still occur in Fall 2020.

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