3rd Workshop of Spanish Users on Nuclear Data on "Machine Learning in Nuclear Science and Technology Applications" (video-conference)

May 27, 2021
Universidad Politécnica de Madrid
Instituto de Fusion Nuclear "Guillermo Velarde"
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SUMMARY RECORD

O. Cabellos (UPM/Spain) opened the meeting and welcomed all participants (The Agenda of the Workshop is in Annex 1, and a List of Participants is in Annex 2).

1. Welcome and introduction to the meeting

The chair, **J. Dies** (CSN/Spain) opened the meeting and introduced participants in artificial intelligence (AI) and machine learning (ML) predicting capabilities. These predictive analytical tools may improve reactor safety while offer economic savings. **J. Dies** highlighted the importance of this Workshop to identify and get better understanding of current applications of ML techniques in nuclear science and technology applications.

2. Technical Presentations

- "*ML in radiation metrology: Application of Gamma-ray spectrometry*", T. Kin (Kyushu University, Japan).

  T. Kin presented the current activities on radiation metrology at the Kyushu University. **T. Kin** introduced an example of application for fast gamma-ray spectrometry. This fast technique is useful due to the huge number of samples that must be measured with long measured time required. Examples of activity prediction of 137Cs and 40K were shown using and convolutional neural network to reduce measurement time.

- "Practical cases using Machine Learning applied to education&training, operation and inspection of nuclear power plants", B. Briquez (TECNATOM, Spain)

  B. Briquez gave an overview of the activities in the TECNATOM/DataLab. B. Briquez presented the projects "Baffle Bolts" for nuclear power plan inspections, "Intelligent Optics" for recognition and analysis of colours, shapes and characters to be used in panel identification alarm status and reading indicators. And finally, the "Learning Analytics" with the development of SOUL Analytics used for education and training, and "Virtual Assistants" to provide capabilities of real-time and hand-free analytics using voice recognition.

- "Deep Learning applied to Capture Cross Section Data Analysis", A. Sánchez (CIEMAT, Spain)

  A. Sanchez presented Deep Learning techniques (Neural Network classifier) in the process of capture event discrimination of simulated data for a 197Au sample with Aluminium canning, and a 239Pu sample. This technique gives better results than the traditional method: signal-to-background ratios ~3/5 times larger than traditional cuts, and larger capture efficiencies of ~13/16%, respectively for 197Au and 239Pu samples.

- "Unsupervised learning for nuclear fuel cycle applications", A. Villacorta (CIEMAT, Spain)

  A. Villacorta presented a hierarchical clustering technique to find which selection of technologies provide similar results in nuclear fuel cycle studies, grouping scenarios based on their similarity. **A. Villacorta** used an exercise based on scenario objectives for a nuclear fuel cycle starting with a PWR(UOX) fleet, minimizing and stabilizing the TRU (Pu + MA) inventories. Different configuration of technologies were used (ADS, GFR, SFR, etc…). **A. Villacorta** concluded that hierarchical clustering technique can be used for selecting technologies that are more suitable for given objectives.

- "Machine learning applied to the modelling of nuclear de-excitation cascades", E. Mendoza (CIEMAT, Spain)

  E. Mendoza presented a genetic algorithm to fit the parameters of a model capable of generating neutron capture cascades. The purpose of this work is to calculate the detection efficiency of γ-ray detectors. **E. Mendoza** recognized that there is not straightforward way to generate reliable γ-ray cascades emitted after neutron capture. Then, he proposed to minimize the FoM of N-parameters used in a γ-ray cascade model. He concluded that the genetic algorithm was successful to predict those N-parameters.

- "Surrogate Models for Nuclear Burn-up Calculations and Uncertainty Propagation", Arnau Albà (PSI, Switzerland)

  A. Albà presented a surrogate model which is able to replace depletion calculations of CASMO5 code for fuel assemblies with a specific irradiation history with different nuclear data. This technique is applied for the uncertainty quantification (using stochastic sampling) of burnup calculations which require highly demanding of CPU time. The large number of input variables (nuclear data energy dependent and for different materials/isotopes) might require dimensional reduction techniques, such as PCA or encoder-decoder. Output variables are criticality and isotopic inventory (and related response functions such as decay heat).

- "Predicting the Bias in Calculations of Spent Nuclear Fuel Characteristics", Shama Ahmed (PSI, Switzerland)

  S. Ahmed presented Machine Learning models (neural network, random forest) which are analysed for their predictive performance in spent nuclear fuel calculations, comparing bias model predictions to observed ones. **S. Ahmed** demonstrated that the bias could be predicted from validation data (benchmarks), so this work may support activities such as license applications, and decisions on safety margins.

- "Combining Levenberg–Marquardt and Gaussian Processes for treatment of model defects in nuclear data evaluation", J. Hansson (Uppsala University, Sweden)

  J. Hansson introduced the concept of model defects which adversely may affects nuclear data evaluations. The Gaussian Process (GP) for model defects is presented to model discrepancy functions and to increase model flexibility. **J. Hansson** presented the Maximum a Posteriori Probability (MAP) estimate of linear model with GP discrepancy. He also presented the

Levenberg-Marquardt algorithm (LM) used to improve convergence of this technique. Examples of nuclear data evaluations were shown.

- "Optimisation of used nuclear fuel canister loading using a neural network and genetic algorithm", V. Solans (Uppsala University, Sweden)

  V. Solans presented a study which aims at providing results on the optimization of canister loading using different ML techniques. Firstly, **V. Solans** presented an artificial neural network technique for the prediction of keff values based on SERPENT calculations. Secondly, **V. Solans** presented the optimization algorithm based on genetic algorithm to optimize loading for 212 assemblies into 53 canisters where keff computed values are calculated with the neural network. The goals for this optimization algorithm are the minimizing of keff and decay heat, and with homogeneous distributions both for keff and decay heat.

- "Machine Learning techniques in V&V of Nuclear Data Bases. Examples: EXFOR, JANIS/NEA evaluated data and ICSBEP", G. Clavero, S. Moreno and J. Moreno, INGENIA (UPM, Spain)

  Three different works were presented in this talk. **S. Moreno** presented outlier detection in EXFOR nuclear reactions library using DBSCAN algorithm. The work on nuclear data validation using ML techniques is presented by **J. Moreno** and **G. Clavero**. The NEA databases of JANIS (nuclear data) and ICSBEP (experimental and calculated critical experiments) are used in this exercise. ML techniques such as clustering, modelization (random forest) and selection features are presented. NDaST tool capabilities are also introduced in this work to provide an additional analysis with nuclear data uncertainties. KNIME software is used in this work

- "Machine Learning in Reactor-oriented applications. Examples: optimal design of PWR fuel loading pattern, manoeuvres optimization and modelling and control of xenon oscillations", G. Gabarain, J. A. Monleón and M. Ruiz, INGENIA (UPM, Spain)

  Three different works were presented in this talk. **M. Ruiz** presented an example of fresh fuel reloading optimization for a PWR Westinghouse nuclear plant of 1000 MWe. SEANAP system used for 2D core calculations. Different ML techniques are compared with a brute force calculation: hill-climbing and genetic algorithms showed better results. **J.A. Monleon** presented the work on "optimization of operational manoeuvres in PWRs", the optimization is based of a minimization of levels of boron concentration/dilution in return to power manoeuvres after a few hours of shutdown. Linear regression and random forest techniques are used in this work. **G. Gabarain** presented the work on "Xenon-135 Oscillations' Forecasting in PWR's Operation Manoeuvres" using a genetic algorithm to optimize a sequential neural network that predicts Axial Offsets and cumulative xenon oscillations. The Shimazu's Control Method and Westinghouse Niquist Diagram are tested.

- "Neutron and gamma beam simulation using OpenMC and Python's libraries for Machine Learning", N. Schmidt (CNEA, Argentina)

  N. Schmidt presented a technique to generate more particles in OpenMC code based on multivariate kernel density estimator (KDE) method. A comparison between KDE samples and original tracks shows a good performance of this technique. This work is used for the design of a time-of-flight spectrometry facility in the RA-6 Research Reactor, and the necessity to estimate the neutron current at the exit of the duct.

- "Using Machine Learning Algorithms for Large-scale Nuclear-data Validation", D. Neudecker (LANL, USA)

  D. Neudecker introduced how ML techniques may help to find trends between nuclear-data sensitivities and bias in simulating validation experiments that point towards potential

shortcomings in nuclear data. This can help scientists to resolve issues in nuclear data, or at least suggest future experiments and theory developments to resolve these issues. In this work, random forest model is used to estimate the bias of "C-E" for a suite of 875 criticality experiments and 15 LLNL pulsed sphere neutron-leakage spectra. This bias is model as a function of a large number of features for each experiment: keff-sensitivity coefficients (Δkeff/$\Delta\sigma$) and physical data (geometry, composition, etc…). SHAP index is used for the identification of the most important reaction nuclear data.

- "Announcement: Technical Meeting on Artificial Intelligence for Nuclear Technology and Applications, IAEA virtual-meeting, 25 – 29 October, 2021", G. Schnabel (IAEA/NDS)

  G. Schnabel announced the upcoming meeting on AI/ML organized by IAEA. He invited participants to contribute/participate in the meeting.

O. Cabellos closed the meeting thanking all the speakers and participants, especially for those with different Central European time. He acknowledged the high level of technical presentations providing a good overview of examples of AI/ML techniques in nuclear science and technology applications. Finally, he thanked **INGENIA/UPM students** for the organization of the meeting and their contribution in the technical session.

APPENDIX 1. Agenda

Start - End	*Presenter (Institution)*	*Title*
9:00 – 9:15	*O. Cabellos (UPM)* *J. Dies (CSN)*	*Welcome and Introduction*
9:15 – 9:30	*T. Kin* *(Kyushu University)*	*ML in radiation metrology: Application of Gamma-ray spectrometry*
9:30 – 9:45	*B. Briquez* *(TECNATOM)*	*Practical cases using Machine Learning applied to education&training, operation and inspection of nuclear power plants*
9:45 – 10:00	*A. Sánchez (CIEMAT)*	*Deep Learning applied to Capture Cross Section Data Analysis*
10:00 – 10:15	*A. Villacorta (CIEMAT)*	*Unsupervised learning for nuclear fuel cycle applications*
10:15 – 10:30	*E. Mendoza (CIEMAT)*	*Machine learning applied to the modelling of nuclear de-excitation cascades*
10:30 – 10:45	*Coffee break and photo of participants*	
10:45 – 11:00	*A. Jacas Arnau (PSI)*	*Surrogate Models for Nuclear Burn-up Calculations and Uncertainty Propagation*
11:00 – 11:15	*Shama Ahmed (PSI)*	*Predicting the Bias in Calculations of Spent Nuclear Fuel Characteristics*
11:15 – 11:30	*J. Hansson* *(Uppsala University)*	*Combining Levenberg–Marquardt and Gaussian Processes for treatment of model defects in nuclear data evaluation*
11:30 – 11:45	*V. Solans* *(Uppsala University)*	*Optimisation of used nuclear fuel canister loading using a neural network and genetic algorithm*
11:45 – 12:00	*G. Clavero, S. Moreno and J. Moreno* *INGENIA (UPM)*	*Machine Learning techniques in V&V of Nuclear Data Bases. Examples: EXFOR, JANIS/NEA evaluated data and ICSBEP*
12:00 – 12:15	*G. Gabarain, J. A. Monleón and M. Ruiz* *INGENIA (UPM)*	*Machine Learning in Reactor-oriented applications. Examples: optimal design of PWR fuel loading pattern, manoeuvres optimization and modelling and control of xenon oscillations*
12:15 – 12:30	*N. Schmidt (CNEA)*	*Neutron and gamma beam simulation using OpenMC and Python's libraries for Machine Learning*
12:30 – 12:45	*D. Neudecker (LANL)*	*Using Machine Learning Algorithms for* *Large-scale Nuclear-data Validation*
12:45 – 12:50	*G. Schnabel* *(IAEA/NDS)*	*Announcement: "Technical Meeting on Artificial Intelligence for Nuclear Technology and Applications"* *IAEA virtual-meeting, 25 – 29 October, 2021*
12:50 – 13:00	*Final discussion and closing the meeting*	

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