# Probabilistic AI for Prediction of Material Properties (PROMAP)

University of Strathclyde

Project Duration: 3 months

BEIS ANSIC funding awarded: £25,000

**The PROMAP project performed a review of the use of Artificial Intelligence (AI) within the nuclear industry to understand the opportunities and challenges related to the adoption of this technology. One of the main barriers is the lack of extensive datasets required to train AI models and the poor consideration of the uncertainty.**

**Probabilistic methods have been used to increase the training dataset while retaining the physical dependencies among variables. This has enabled the generation of a large dataset of training data. Then, a set of artificial neural networks have been trained to predict selected properties of material relevant for the nuclear industry, and the results combined using Bayesian statistics. This has increased the accuracy and robustness of the prediction and provided the results with associated confidence. Finally, the approach allows the design of the experimental campaign by defining the input and associated accuracy required to reduce the uncertainty of the output at the desired level.**

**PROMAP has demonstrated the feasibility of integrating probabilistic approaches with AI tools and its applicability for the prediction of material properties relevant to the nuclear industry.**

## Background

Currently, the nuclear sector is falling behind other industries in the implementation of AI technologies. In addition, the nuclear industry faces 2 key challenges: 1) the need to decommission ageing nuclear reactors; and 2) the high costs of building new reactors. This motivates the need for demonstrating the applicability of AI technology in the nuclear sector, and its capability of playing an important part in the designing, construction, operation, and decommissioning of reactors. The role of AI can be divided into 2 aspects: 1) providing technical assistance to humans in solving problems; and 2) introducing autonomised, decentralised decision-making.

This feasibility study focuses on the first aspect of the AI's role, particularly in the context of predicting material properties and behaviour. This is achieved via Artificial Neural Network (ANN) with the eventual aim to help in the development of new materials for future reactor designs (e.g., AMR, Gen IV) while keeping the development cost at a minimum by reducing the necessity for expensive experimental campaigns.

## Project Aims

The aim of this study is to introduce a framework able to combine AI approaches with probabilistic methods. The probabilistic AI approach is expected to:

- improve the robustness by accounting for the unavoidable uncertainty on the training dataset (i.e., experimental data)
- enable ANNs to deal with sparse and noisy data and predict the desired quantity of interest with associated confidence bounds
- allow users to obtain information on the maximum tolerance level on the interval of the input data (i.e., quality and accuracy of the data) given a pre-defined accepted tolerance level of output interval

## Project Steps

The project was carried out in 4 stages:

- Literature review: A literature survey and review have been conducted to study the state of AI and its implementation in the nuclear sector and key challenges faced by the nuclear sector identified
- Data collection and processing: Databases of experimental campaigns performed to characterised material relevant for the nuclear sector have been collected. The data is processed, and a sensitivity analysis is performed to identify key input and output features
- Data enhancement: Synthetic data retaining the original physical relationships have been generated via stochastic approach (using a Gaussian Mixture Model able to capture the variability to the original input data). This has created a huge data set for the training of ANNs
- Merging of AI with uncertainty quantification (UQ) tools: This has been done through the training of a set of Neural Networks and the prediction merged via Bayesian statistics. The approach known as Adaptive Bayesian Model Selection (ABMS[1] has been implemented to determine the ANN model which yields the most reliable predictions with the least uncertainty
- This allows the training of robust AI tools able to predict material properties with the associated level of confidence

## Project Achievements

The main achievements are:

- In-depth review of the current state of AI in the nuclear sector
- Availability of experimental datasets of material relevant to nuclear industry
- Enhancement of the experimental dataset via probabilistic approach able to retain the physical relationship among variables. The enhanced datasets (see Figure 1) increase the number of data points that can be used for training artificial neural networks
- Training a set of ANN using the enhanced dataset for the robust prediction of material properties with associated confidence bounds (see Figure 2). The achieved level of accuracy[2] is between 0.95 and 1.

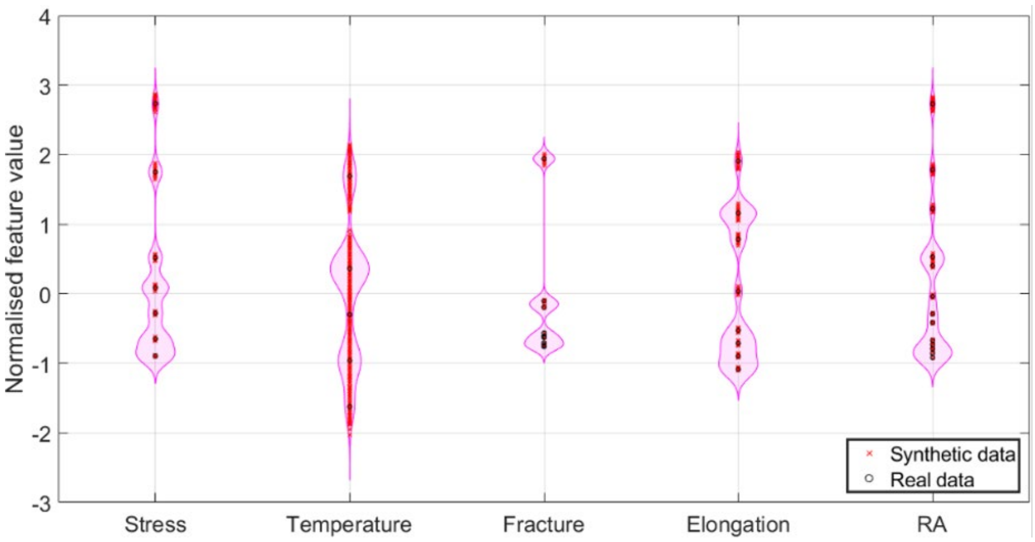


Figure 1: Distribution of selected input parameters (the violin plot) used to generate synthetic data and actual data (blue dots).

[1] S.Tolo, X.Tian, N.Bausch, V.Becerra, T.V.Santhosh, G.Vinod, and E.Patelli (2019). Robust on-line diagnosis tool for the early accident detection in nuclear power plants. Reliability Engineering & System Safety, 186, 110–119. https://doi.org/10.1016/j.ress.2019.02.015

[2] $R^2$ is the most popular performance evaluation measures for regression-based machine learning models. It can be interpreted as share difference between the samples in the dataset and the predictions made by the model.

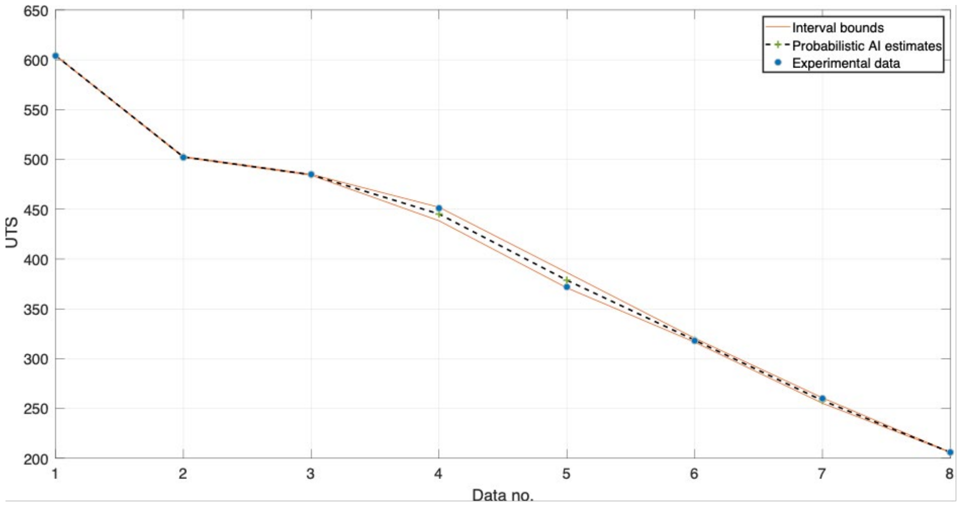


Figure 2: Ultimate tensile strength (UTS) from experimental data and predicted by the probabilistic AI. The red lines show the associated confidence in the prediction.

## Next Steps

The developed tools and algorithm together with the collected dataset will be made available on GitHub as part of the OpenCossan project (https://github.com/cossan-working-group/OpenCossan).

The results of the project will be presented at ESREL2022 (European Safety and Reliability Conference) and a research paper in a peer-reviewed journal will be published.

Further research activities will seek to develop physical-informed probabilistic AI and training Interval Neural Networks able to handle input dataset with data gaps and imprecision modelled as intervals.

## Impact

The main impact of Project PROMAP includes:

1) Availability of a report about the state of the art of AI in the nuclear industry
2) Availability of material database for training and testing AI solutions
3) A robust opensource framework for probabilistic AI for the prediction of material properties as well as quantifying its associated prediction uncertainties
4) A demonstration of the applicability of the approach based on interval predictor models for dealing with the issue of sparse data
5) Publication and presentation of the results at the European Safety and Reliability Conference (ESREL2022) in August 2022.

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