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Lab experiment optimisation using coupled Finite Element Analysis and Machine Learning

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Abstract

The inside of a fusion energy device is one of the most challenging environments known about, with temperatures exceeding 100,000,000 °C in the centre of the plasma. The Heating by Induction to Verify Extremes (HIVE) testing facility at the UK Atomic Energy Authority (UKAEA) uses high heat flux experiments to research and develop plasma-facing components which experience the most severe thermal loads in such a machine. Induction heating is used to deliver up to 20 MW/m² of surface power to a component while high-pressure coolant passes through it.

Performing these experiments is expensive due to their high-power usage and the setup time required by technicians. It is imperative therefore that each experiment provides as much insight as possible about a component's performance. Experimental parameters, such as induction coil design, frequency or power, are decided based on the memories, experience and gut-feeling of an experienced operator. In the era of High-Performance Computing (HPC), Big Data and Machine Learning (ML) the optimal parameters can be deduced utilising these methods. Moreover, ML algorithms have proved to be excellent at gaining insight from high-dimensional data, which is a common struggle for the human mind.

A fully automated Virtual Twin (VT) of HIVE has been developed using VirtualLab, an open-source package created by the authors used to perform virtual experiments. Simulation results provide data points across the parameter space which VirtualLab's ML routine can use to gain valuable insight, including the optimal experimental parameters. Utilising VirtualLab's multi-node and High Throughput Computing (HTC) capabilities, a large number of simulations are performed for a variety of experimental parameters in a very short space of time, allowing rapid iterations of the engineering design cycle.

This is an example of human-machine collaboration guiding, but not making, decisions which is becoming an increasingly important and useful tool in a wide variety of fields.

Key words: *Machine Learning, Virtual Twin, HPC, Neural Network, Surrogate Model*

1. Introduction

Fusion energy has the potential to supply the ever-growing energy requirements of humanity with a clean, abundant energy source [1]. The fusion of lighter nuclei to form a heavier nucleus releases energy, and it is this process which powers the stars of the solar system. To replicate this behaviour on Earth the hydrogen isotopes deuterium and tritium are combined and heated to over 100,000,000 °C, creating a plasma where their nuclei combine to form a helium nucleus, releasing energy in the process. This process produces no carbon emissions, while there is an abundance of the required fuels, with deuterium extracted from water and tritium produced from lithium inside the power station itself.

While the benefits of fusion energy are clear, there are several challenges to overcome before becoming a widely adopted energy source [2]. One of these is the construction of a commercially viable machine which can routinely withstand the extreme environments fusion requires. The Heating by Induction to Verify Extremes (HIVE) testing facility at the UK Atomic Energy Authority (UKAEA) was established to research and develop the plasma-facing components (PFC) which experience the most severe thermal loads [1]. Induction heating delivers up to 20 MW/m² of surface power to a component to replicate in-service loads, while components are actively cooled using high-pressure coolant.

HIVE's main goal is to develop PFCs with improved component lifespan that diffuse the surface thermal loads through the component, in a way which reduces thermal expansion related stresses particularly in the regions of geometric features or bonding between dissimilar materials.

Performing these experiments is expensive, therefore, to maximise the impact each experiment has it is crucial that the experimental parameters, such as induction coil design, coolant temperature and coil power, are correctly chosen to ensure that the desired behaviour is delivered. Parameters are currently chosen based on the previous experience of a HIVE operator; however, this work shows how Machine Learning (ML) can assist this process by finding the optimal settings in an automated way, reducing the reliance on the memories and gut-feeling of operators.

2. Problem description

Due to the multi-physics nature of HIVE there are several parameters which can be altered for each experiment. Each experimental parameter results in an additional dimension in the parameter space. Given that the human mind struggles to visualise more than three dimensions, it is often the case that the optimal parameter settings would not be identified in scenarios with more dimensions. Over the past two decades ML has shown to perform excellently at gaining insight from high-dimensional data [3]. ML is becoming an increasingly useful tool for engineering applications, often used to create surrogate models to replace time-consuming simulations [4].

While there are a plethora of experimental parameters which can be optimised for, this work focuses on the coil design and configuration which gives the optimal power & uniformity for a component. The design of the induction coil significantly effects the heating profile imposed on the surface of the component [Fig. 1]. Moving the coil closer to the component increases the power delivered to the sample, however it also increases the unevenness of the heating profile. The thermal loads experienced by PFCs in a fusion device during normal operations are locally uniform with variations occurring over a larger length scale. Therefore, it is desirable to achieve as uniform a heat load as possible with HIVE to better replicate these conditions.

The configuration of the component with respect to the coil has 4 degrees of freedom (DoF); displacement in x, y and z and rotation along the y-axis, along which the coolant pipe sits [Fig. 2]. A Multi-Layer Perceptron (MLP), a type of Neural Network (NN), uses simulation data to map these 4 DoFs (the inputs) to values for the power and uniformity (outputs). This NN is then used to find values for the inputs which optimise for power and/or uniformity.

To collect the simulation data a Virtual Twin (VT) of the HIVE experiment has been developed using VirtualLab, an open-source package developed by the authors which enables parameterised and fully automated virtual experiments to take place. It combines the open-source packages SALOME, CodeAster and ERMES to generate CAD geometries and perform FEA analysis [5]. Due to VirtualLab's modular nature, a different FEA package can be included and used to perform analysis.

This simulation data is then analysed using VirtualLab's ML package in an automated and seamless manner. Given that ML requires large quantities of data, VirtualLab has multi-node and High Throughput Computing (HTC) capabilities, meaning that it can be used on High Performance Computing (HPC) clusters to generate the required data in a fraction of the time.

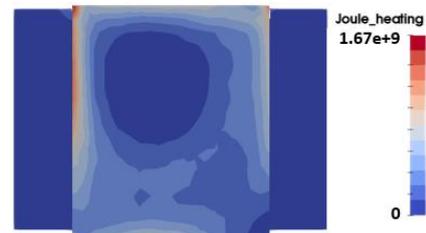


Fig. 1: Non-uniform heating profile generated due to coil design

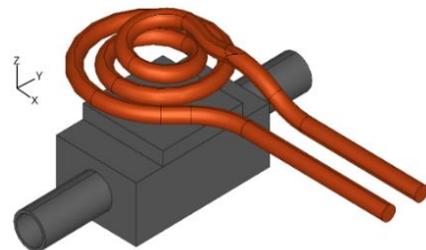


Fig. 2: Sample orientation with respect to coil.

3. Numerical results

Training any ML algorithm requires a substantial amount of data. Since simulation data is used to train the NN an efficient sampling technique is desirable, one where each points in the parameter space provides valuable information. The sampling techniques considered are:

Grid: Sample points are chosen at regular grid intervals across the parameter space [Fig 3a].

Random: Sample points are chosen at random from the parameter space using a uniform distribution [Fig 3b].

Halton: Quasi-random sample points are chosen based on the Halton sequence [6] [Fig 3c].

Adaptive: Each new sample point is decided based on the previously collected sample points [Fig 3d]. In this example there is a peak at the origin, resulting in increased sampling there.

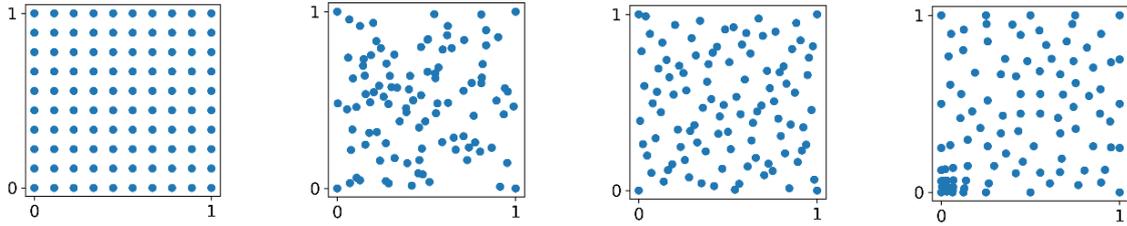


Fig. 3: Sampling techniques in 2D; a) Grid (left), b) Random, c) Halton d) Adaptive

The architecture of the NN used for this work are detailed in Table 1 along with hyperparameters used for training. The accuracy of the NN is measured using the mean squared error (MSE) of the predicted value compared with the actual value on the test dataset [Fig. 4]. Since their accuracy is influenced by their initial weights, 10 identical NNs are trained for each dataset to average out this variability, with the mean MSE highlighted along with the best and worst performing. These results show the grid method to be considerably the worst performing. For fewer data points the adaptive method performs the best, followed by Halton, with all performing similarly as the number of points increase. Unfortunately, the adaptive method is substantially slower than the others due to the need to locate sparsely populated areas in the parameter space to generate each new sampling point.

Table 1: NN architecture & hyperparameters

Number of neurons in input layer	4
Number of neurons in output layer	2
Number of neurons in hidden layers	32-128-16
Activation function	Leaky ReLu
Batch-size	32
Number of epochs	10,000 (max)
Test-split	0.3

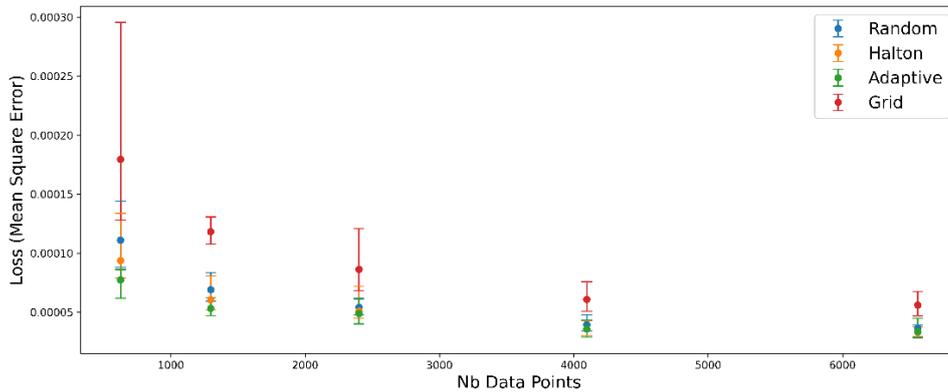


Fig. 4: Best, worst and average MSE value for 10 NNs using different sampling methods. Training dataset sizes are; 625, 1296, 2401, 4096 and 6561 and are chosen for comparability with the grid method.

While MSE infers the accuracy of the NN across the entire parameter space, to ensure the optimal configuration is found it is essential that it is highly accurate at these locations. Fig. 5 shows the power that each NN identified as the optimum, highlighting that no sampling technique is highly accurate in

this regard, although generally a better optimum is identified as the number of data points increase. To overcome this, a coupled Simulation-ML approach is considered, where after running an initial number of simulations, a NN is trained and regions of interest in the parameter space are located and data collected here to improve the NN accuracy in this region. This process continues until a convergence criteria is met.

Initially, 2000 data points are collected using the Halton sampling technique, where an optimal power around 520 W was identified, which is consistent with the findings in Fig. 5. However, as the training data is updated with data points in the region of interest there is a clear improvement in its performance [Fig. 6]. By collecting fewer than 250 additional data points in this region, giving a total of 2250, a configuration resulting in 526 W of power is identified, which is superior to any configuration identified using the original sampling methods alone, even with 6561 data points.

While the coupled Simulation-ML procedure presented here has focused solely on the location where the power attains its maximum value, this can easily be adapted to include additional regions of interest where data points can be densely sampled to ensure a higher accuracy. Doing so may however lead to poor and possibly erratic behaviour in regions further away from these regions of interest and will be investigated in future work.

4. Conclusions

This work has presented how combining simulation data with ML can maximise the effect of experimental facilities. Using NNs trained on simulation data, regions of interest within the parameter space to be identified. While standard sampling techniques were able to identify these regions, their accuracy were often unsatisfactory, however using NNs to advise the regions to densely sample resulted in a substantial improvement in performance.

Acknowledgements

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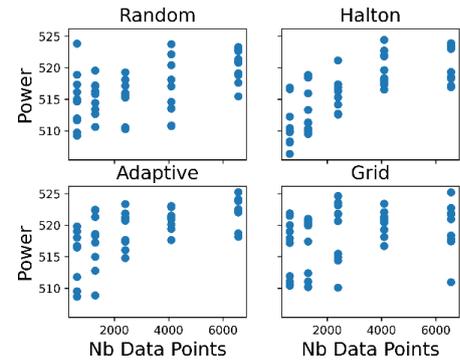


Fig. 5: Max. power discovered by NNs trained with different sampling techniques and dataset sizes.

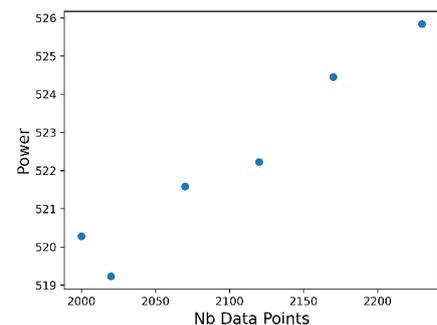


Fig. 6: Maximum power discovered by NN using the coupled Simulation-ML approach