BIPM Capacity Building & Knowledge Transfer Programme

2024 BIPM - TÜBİTAK UME Project Placement

REPORT

Project Name	Digital Twin of a Quantum Voltage Standard
Description	The SI volt realization using the Josephson effect requires complex equipment and highly specialized personnel. The development of simulations and real-time control to optimize the system parameters that handle the physics and the measurements is highly desirable. In this context, my PhD thesis entitled "Digital twins applied to quantum metrology" and the EURAMET ViDiT project (having INTI and TÜBİTAK as partners) aims to ensure the reliability of digital twins (DT) in metrology.
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Motivation & Introduction

Implementing a system for realizing the volt using the Josephson effect, as the International System of Units (SI) recommends, requires expensive equipment to obtain and maintain. This implies that any research that may be done on the devices that make this unit through simulation techniques will result in both economic benefits and improvement in understanding the physical and technical processes that occur in these systems. Additionally, optimizing the physical system's configuration parameters will reduce the setup and measurement times and improve the transference of the SI voltage unit to secondary standards. This will also help to comply with the signed CIPM MRA and the CMCs published in the KCBD.

This initiative is supported by Argentina's National Metrology Institute, Instituto Nacional de Tecnología Industrial (INTI), and Universidad Nacional de San Martín (UNSAM), which are collaborating on my PhD thesis titled "Digital Twins Applied to Quantum Metrology." The main objective is to apply digital twin (DT) techniques to the programmable Josephson effect.

With the incorporation of real-time data obtained through instruments and the utilization of Artificial Intelligence (AI) and Machine Learning (ML), a complete representation of that device can be produced, which allows for predicting its behavior, making optimizations without exhaustive measurements, and in some scenarios, anticipating possible failures.

DTs are key technologies that enable the achievement of strategic policies devoted to sustainability and digitalization within the complex framework of Industry 4.0 and the European Green Deal. That is why EURAMET is funding the 22DIT01 ViDiT project [1], to develop methods and tools to ensure DTs' reliability and trustworthiness in metrology. This will enable the traceability of modern measurement systems and boost and strengthen the European lead in this field. To facilitate the uptake of the developed methods, by NMIs/DIs and industrial stakeholders, three good practice guides (GPGs) will be written, and the applicability of the techniques will be demonstrated in twelve case studies covering the industrial metrology applications. INTI and TÜBİTAK UME are partners in this project, and the PhD thesis is one of the case studies.

A DT is a virtual simulation model that accurately replicates a physical system and its characteristics. It includes dynamic updates of the virtual model according to the observed state of its real counterpart. Thus, it consists of two connections: Physical-to-Virtual (P2V) for modeling the system and Virtual-to-Physical (V2P) for implementing control strategies to achieve target accuracy in the physical system. Figure 1 shows a representation of this concept.

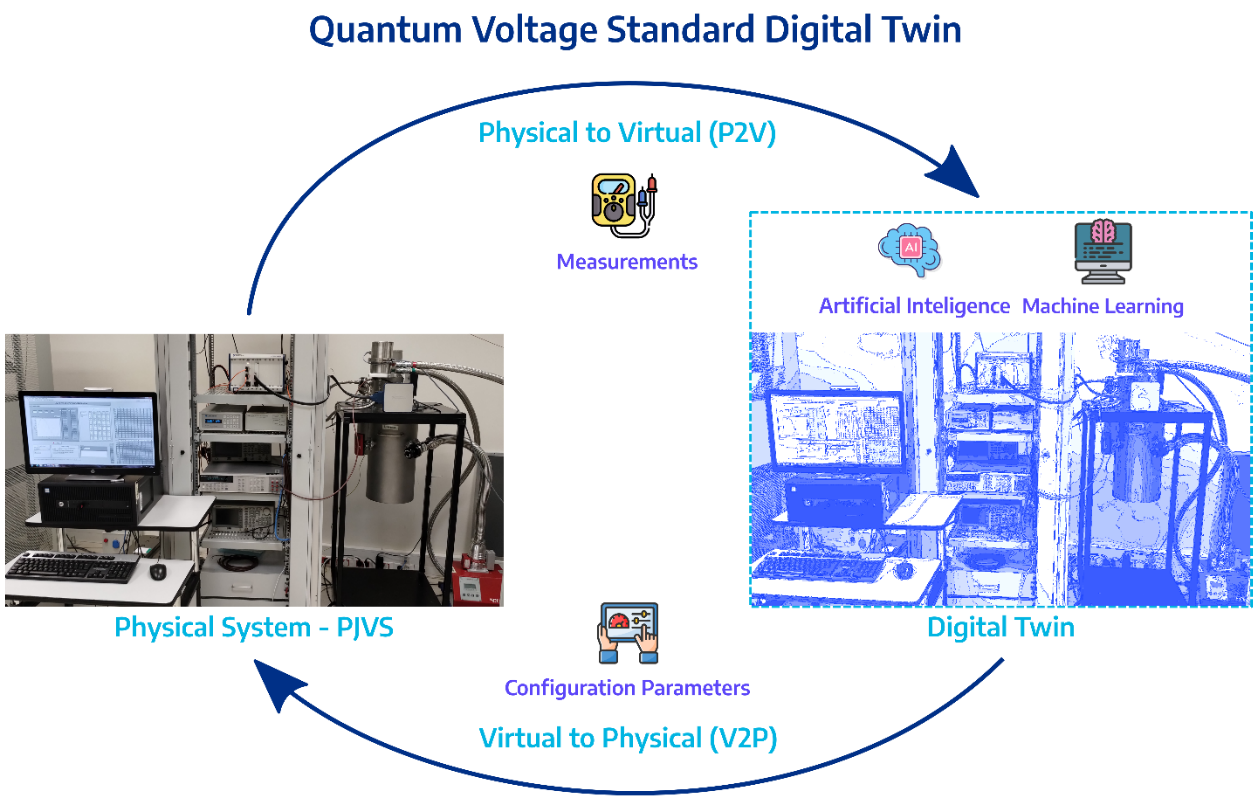

Figure 1. Representation of UME Quantum Voltage Standard Digital Twin.

The P2V connection is determined by measurements on the physical system which feeds the data-driven model. This model predicts the configuration parameters used as control signals in the V2P connection.

Furthermore, time-dependent influences must be considered. Hence, a DT needs to be updated with data from actual measurements collected in real-time, and the evaluation of measurement uncertainty needs to be adapted accordingly to comply with the JCGM:GUM. Otherwise, non-GUM-compliant uncertainty estimation methods should be studied and tested.

A reliable validation procedure needs to be developed to trust the outcomes of a DT. Analyzing and quantifying differences between calibrated standards or data from calibrated instruments and their virtual counterparts is key to making a DT fit for use in metrology, e.g. as substitutes or extensions to certified measurement devices. The model will be updated based on data collected during measurements.

For this work to be carried out, it was necessary to collect a large amount of information on the behavior of the Josephson systems of TÜBİTAK UME. This data was used to predict and model the operation of the device using the previously mentioned techniques.

Developing methods for uncertainty evaluation and validation of a DT are essential for this project and is becoming one of the priorities in the field of metrology, given the current relevance that DTs have acquired.

The proposed objectives of the project are:

- Familiarize with the Josephson systems of TÜBİTAK UME, particularly with the Programmable Josephson Voltage Standard (PJVS), and learn to use a cryocooler.
- Develop a digital twin of a Quantum Voltage Standard to optimize the physical system configuration parameters, reduce the setup and measurement times, and improve the transference of the SI voltage unit, the volt, to secondary standards. The case study will be the generation of quantum DC steps.
- Study of the system's configuration parameters to optimize.
- Study and measure the possible signals to be synthesized by the PJVS.
- Implementation of AI and ML algorithms to train the data-driven model of the DT.
- Develop a method for the validation of the DT, using statistical procedures to assess differences between calibrated standards and the corresponding data from their virtual counterpart.
- Study different approaches for uncertainty quantification for the DT.

Completing these objectives will allow the optimization of the measurements and calibrations at INTI and TÜBİTAK UME, expanding their measurement capabilities. This work will significantly contribute to developing the PhD thesis and the ViDiT project and may lead the way for future collaborations between the laboratories of INTI and UME. It is expected to make joint publications that showcase the results, disseminate the findings of this project, and facilitate the transferability of the developed methods and procedures for uncertainty evaluation and validation in industrial setups. Ensuring direct traceability to the SI DC voltage unit is crucial for the countries involved and the national industry.

Research

The realization of the volt is possible due to the Josephson effect [2], which allows the generation of a voltage that depends only on fundamental constants and a microwave frequency, according to

$$V_J = nf\frac{h}{2e}, \quad (1)$$

where n is a dimensionless quantum number, f is the microwave frequency in Hz, h is the Planck constant in J s, and e is the elementary charge in C. Different types of Josephson systems are in use today, particularly the Programmable Josephson Voltage Standard (PJVS) can be used as a superconducting multi-bit digital to analog converter (DAC), producing time-stepped waveforms whose accuracy is determined by well-defined steps of constant Josephson voltage established by equation 1 [3]. An example is presented in Figure 2.

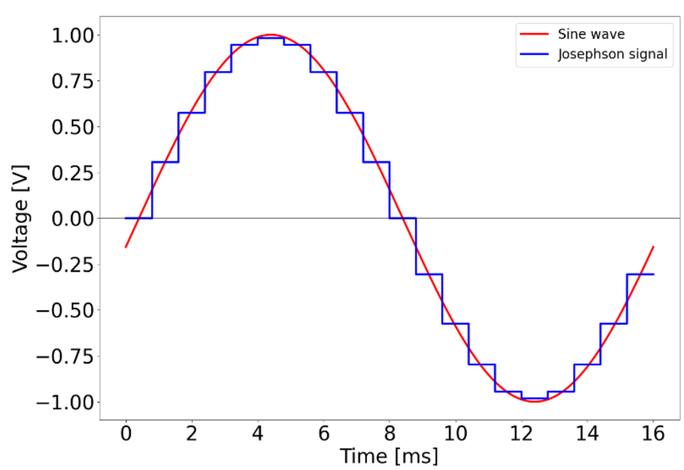

Figure 2. Theoretical Josephson signal. A sine wave with an amplitude of 2 V peak-to-peak and a frequency of 62.5 Hz is shown in red. The theoretical synthesized PJVS counterpart is presented in blue, here 20 steps per period have been used.

UME PJVS System Overview

The work in this project is based on the TÜBİTAK UME PJVS System [4]. The devices that make up the system are presented in Figure 3. Due to the nature of superconductor materials, the PJVS array must be cooled down. To do that, a cryocooler of the brand TransMIT is used, specifically a two-stage 4 K pulse tube cooler PTD-406C (SN 060) with a helium liquefaction unit and chip carrier. This device converts helium from gas to liquid by compressing it. The array is mounted in a special thermal interface, supported on a cold hat. The temperature of the first stage is 40 K, and the second stage drops the temperature to 2 K. As the liquid helium never contacts the array, this is called a dry cooling system. A rotary valve, driven by a frequency converter at 1.2 Hz, compresses the gas automatically. The two cooling stages are built with very thin metallic cylinders to reduce the heat conduction to the coldest zone. Due to this, the operation of the rotary valve produces a mechanical vibration at the frequency of the frequency converter. This translates to a temperature oscillation of ±100 mK in the cold hat. This behavior is intrinsic to system operation and can not be eliminated, but it is reduced by adding a 50 ml reservoir of liquefied helium mounted on the second stage. By this, temperature oscillation is reduced to ±5 mK.

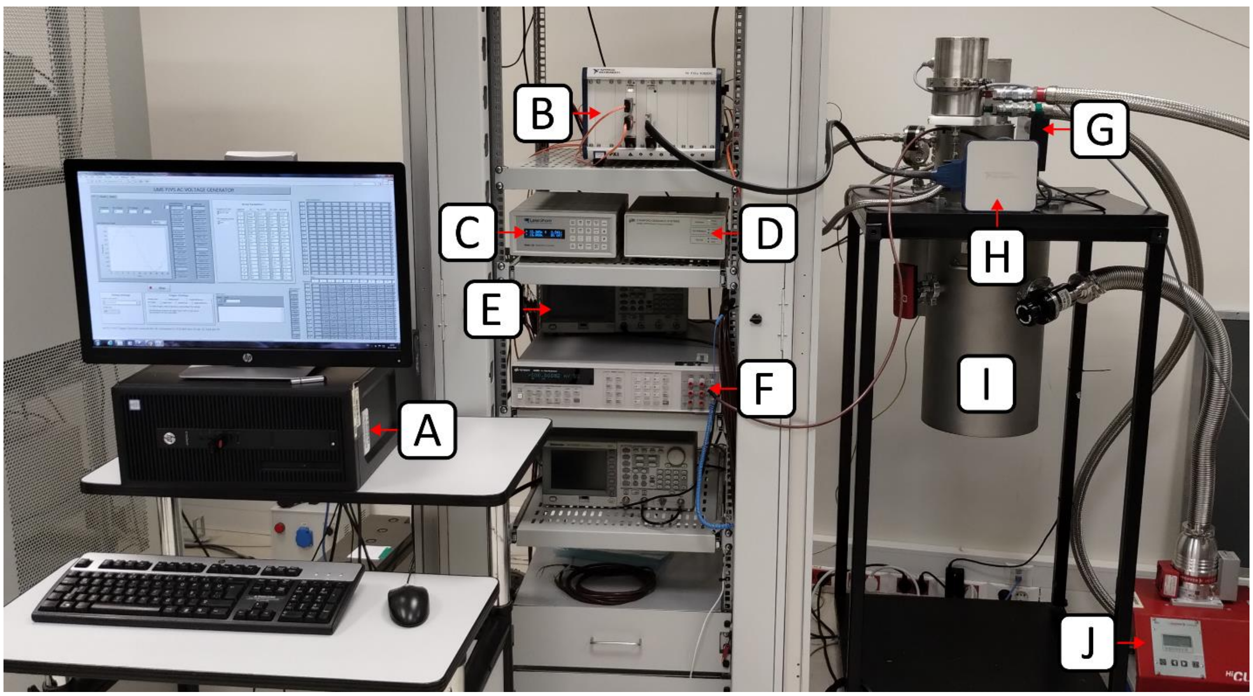

Figure 3. UME's PJVS system. A: PC with PJVS software. B: Bias source. C: Temperature controller. D: Rubidium atomic clock. E: Arbitrary Waveform Generator. F: Digitizer. G: Microwave synthesizer: H: Resistors box. I: Cryocooler when Josephson array is cooled below 4.2 K. J: Turbomolecular pump.

The array used in the PJVS is a 10 V, based on SNS technology, produced by Supracon AG. It contains 69632 Josephson Junctions (JJ) grouped in 18 segments having a nearly binary sequence that can produce a maximum output of ±10.08 V at 70 GHz operating frequency with a resolution of 145 µV. The array is placed in a magnetic shield and mounted on the cryocooler, accommodating all connecting wires and the waveguide. One handy feature of the array package is a small heater installed below the chip which is used to heat the array and remove trapped flux during the system operation. The heater is controlled by a Lakeshore Model 325 temperature controller.

The array is biased with a National Instruments PXIe-6738 32-channel board, mounted in a NI 1082DC PXI chassis. Its main advantage is complete synchronization of all channels on the board. To provide electrical isolation from ground, the bias source is operated by a battery and controlled by a PC via a fiber-optic link. The bias source can produce voltages up to 10.2 V. Because of the low output resistance of the bias source (0.2 Ω), 100 Ω foil resistors with very low inductance are connected in series with each segment and placed inside a special thermal box provided with the bias card. Only for the largest segment 50 Ω is used to reach a total voltage over 10 V.

The total resistance of the bias paths is measured and stored in a file used by the control software. The bias source has a 1 mV resolution, which with the resistance of the bias connections corresponds to the 10 µA (20 µA for the largest segment) current resolution.

Microwave bias is provided by a compact synthesizer produced by TeraHertz Laboratory, a branch of the TÜBİTAK MAM Institute. The synthesizer is directly mounted at the top of the cryoprobe and can produce up to 200 mW of CW power at frequencies between 69 and 71 GHz, with a resolution of 4 kHz. It is locked to a rubidium frequency standard and controlled by the PC via an isolated RS 232 link.

System Setup

Before starting the cooling process, a vacuum must be created in the cryocooler. A two-stage automatic turbomolecular vacuum pump is used. After the vacuum container with the installed cold head has been pumped to a pressure of less than 10^{-3} mbar, the cooler is ready for startup. The frequency converter is turned on to start cooling, and then the compressor is turned on. The system is prepared to operate when the second stage temperature goes below 2.4 K.

The first task is determining the optimum bias currents for all segments of the array and the microwave frequency. Optimum frequency and power are found by sweeping the synthesizer from 69 to 71 GHz, while monitoring the width of the array's 1st and 0th Shapiro steps. V-I characteristics of all segments are measured and centers of the flat voltage regions of the first steps (n = 1) are taken as optimum bias currents. These margins are set in the control software and generally need no change during the system operation; however, bias currents are dithered occasionally to ensure proper quantization. Other data necessary for system software are the number of JJs in each segment and the microwave signal frequency.

The PJVS system can produce stepwise-approximated AC voltages up to a few kilohertz. The frequency of the AC signal and the number of steps per period are controlled by system software. The bias source produces a rise time well below 1 µs on the steps of the stepwise signal, which is enough for sampling-based measurements at frequencies up to 1 kHz. The bias source and its driver offer various synchronization options with the auxiliary instruments. To isolate the bias source, clock & trigger connections are realized through fiber-optic converters.

Troubleshooting

- Cryocooler cleaning

  One of the problems to face at the beginning was that the system was not cooling below 220 K. The compressor and the temperature controller were checked to verify that work properly. The other possible cause is that some impurities were in the helium or clogging the cryocooler’s filter. Cleaning of the helium gas should be performed every 5000 hours of operation. The compressor circulates the gas using the rotary valve across the cryocooler. Then, the gas is expelled and the turbomolecular pump is used to vacuum the chamber. Once a pressure below 10^{-4} mbar is achieved and some time passes, the process is repeated 3 more times. After that, the cryocooler is switched on and the temperature is checked in the second stage. This cleaning solved the cooling issues, and the system was ready to operate.

- Flux trapped in array

  A common issue when working with PJVS systems is the flux trapped in one or more segments. If this occurs, the voltage is not quantized, and the array must be heated to lose its superconducting state. To do that, the bias source and microwave synthesizer should be put on zero, input and output connectors removed, and the temperature controller set to heat up to 12 K for at least ten minutes. Then the heater is switched off and the second stage of the cryocooler should reach a temperature below 2.4 K before connecting and operating the system again.

Measuring system

The experimental measuring setup is shown in Figure 4. The PJVS array is cooled in the cryocooler, and the microwave signal is provided by a microwave synthesizer locked to the frequency of a rubidium clock. The signal travels across a Teflon waveguide which is isolated. The bias source provides the bias currents through the resistors box, the arbitrary waveform generator sends the triggers to the PJVS and the digitizer, and the latter measures the signal. The devices are controlled by a PC and all controlling signals are isolated. Synchronization is possible due to the arbitrary waveform generator AFG3022C, which sends a trigger to generate the PJVS signal and a burst to the digitizer to take measurements in DCV sampling mode.

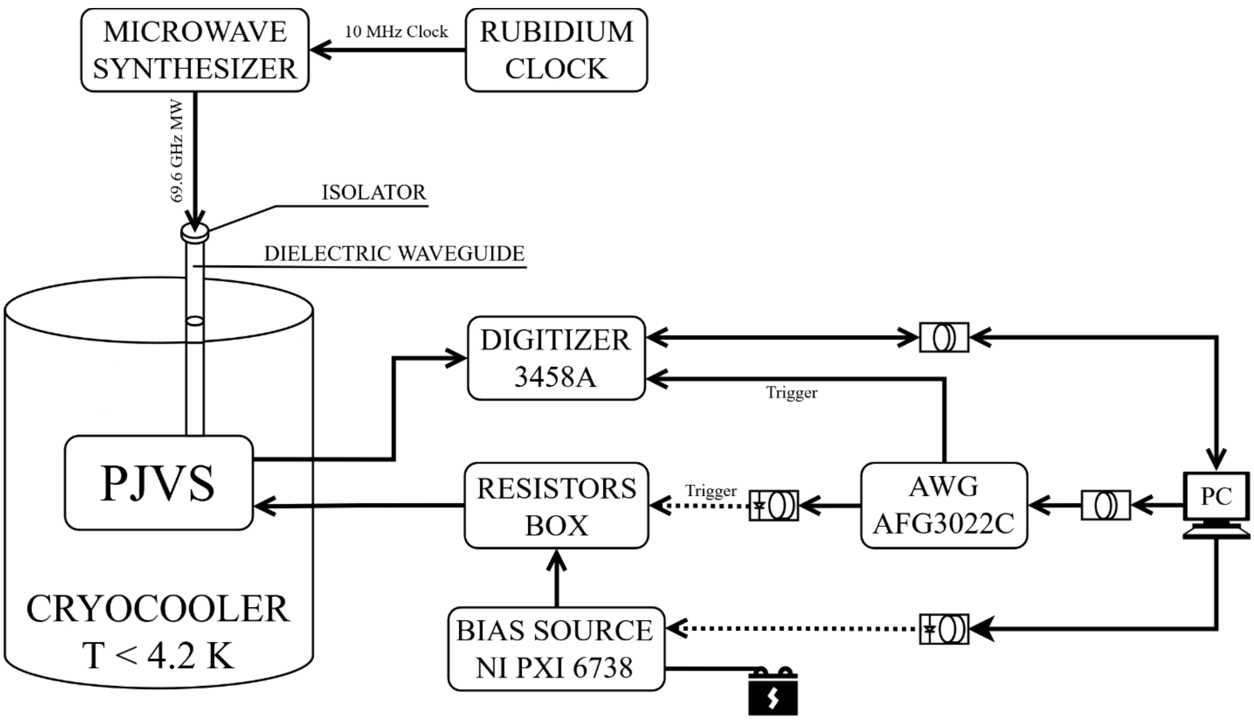

Figure 4. Measuring system. The PC controlling signals, the PJVS trigger, and the microwave signal are isolated to separate the PJVS from the power line ground and perform floating measurements. Dotted lines represent fiber optic cables.

UME's voltage lab has a NI PXI-5922 high-resolution oscilloscope board mounted in a NI 1082DC PXI chassis. This device allows measurements of signals up to 5 V peak amplitude with a sampling rate between 50 kS/s and 15 MS/s. These characteristics make it suitable for differential measurements but for absolute measurements of stepwise approximated signals lacks range and resolution. That is why Agilent 3458 was selected as the primary digitizer to measure the necessary signals to make the data-driven model of the digital twin. The maximum sampling frequency used was 50 kHz and is possible to measure signals of 10 V peak amplitude. The disadvantage is that with a lower sampling rate is difficult to capture the signal transients. Test measurements were performed with both devices, to prove that Agilent 3458 was the best choice for signal digitalization. A comparison of the stability using the overlapping Allan deviation [5] was made by measuring 3000000 points of a 1 V DC value with a 50 kHz sampling frequency, and the Agilent 3458 needs fewer samples to reach an uncertainty of the order of 10^{-6} V, as the Figure 5 shows.

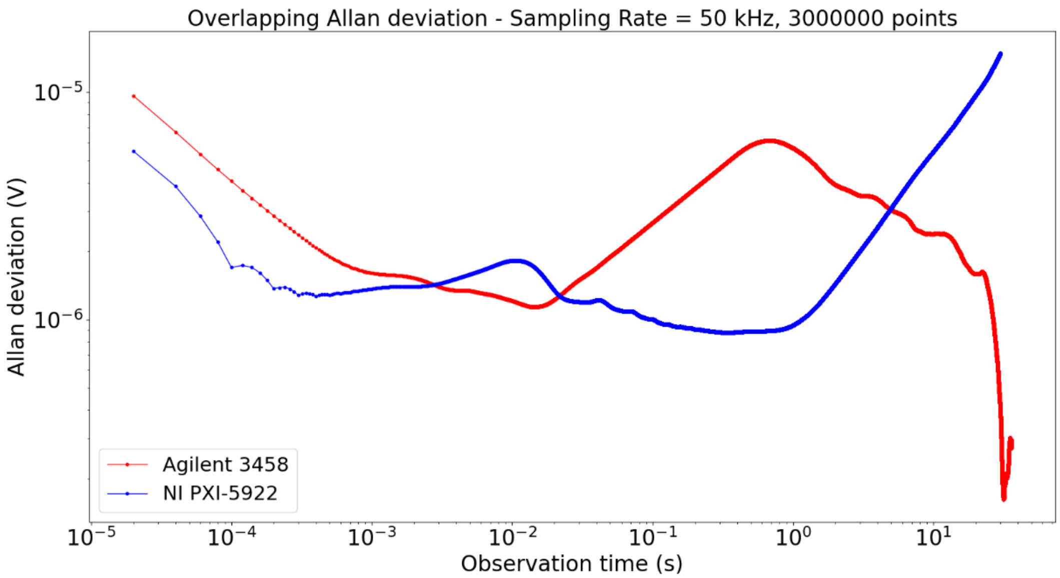

Figure 5. Comparison of the overlapping Allan deviation for a DC voltage of 1 V. Three million points were measured at a sampling frequency of 50 kHz. Agilent 3458 needs fewer samples to reach the minimum uncertainty without low-frequency noise.

Selection of the most relevant features

After getting familiar with the PJVS system and the measurement setup and procedure, the next task was to investigate which system's characteristics impact the stability and accuracy of the signals generated. Based on the knowledge of the system and using the results of measurements of signals with different parameters, the following characteristics were selected as more impactful:

- Output voltage of PJVS
- Critical current of array's segments
- Microwave frequency
- Microwave power
- Number of steps of the signal
- Number of segments of the array
- Amplitude of the signal
- Phase of the signal
- Frequency of the signal
- Sampling frequency

According to the possibilities of the system and considering that the digital twin should take control actions in the Virtual-to-Physical connection to achieve target accuracy in the PJVS output, the parameters selected to be optimized were:

- Output voltage of PJVS
- Critical current of array's segments
- Number of steps of the signal
- Signal frequency of the signal

After creating and validating the model and its predictions, this feature optimization will be performed. The stability of the signal steps and accuracy of the signal RMS value will be used as metrics to evaluate the performance of the model and take control actions that improve system behavior.

Synthetic data generation of PJVS signals

Before start taking measurements, and due to the time consumed for the process of helium cleaning in the cryocooler and some software modifications that had to be made to take the measurements needed, a solution to be able to test different models that allowed making predictions of the system behavior without having the measurements was to generate synthetic PJVS signals to train the neural networks. Python software was programmed to achieve that, Figure 6 presents its block diagram. The variation of the parameters was selected considering the system's characteristics and ensuring that this selection had the most representative variability of the signals, and equation (1) was used to generate the theoretical PJVS stepwise approximated signals. Then, the digitizer effect in the measurement is simulated by multiplying by its gain and adding its offset. Some white noise is added to model the cabling, power line noise, and thermal effects. Finally, a digital FIR filter is convoluted with the resulting signal to add the transients that appear due to the digitizer's output filter response to the transition between adjacent quantum voltage levels of the PJVS.

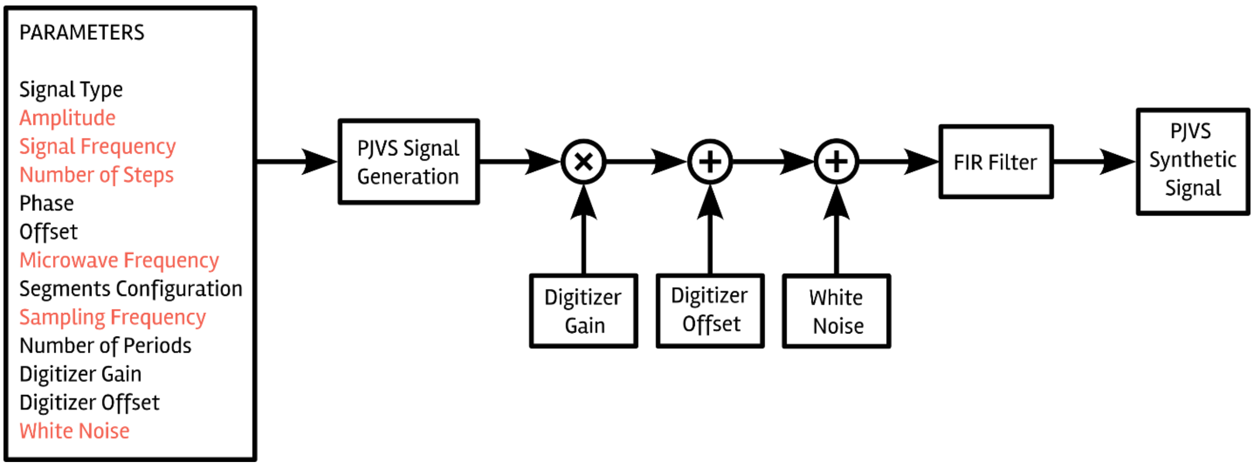

Figure 6. Block diagram of the algorithm to generate synthetic PJVS signals. Marked in red are the parameters modified to add variations and obtain different signals that describe the system behavior.

The variation of the parameters that were used to generate the waveforms was:

- Signal Type: Sine waves
- Amplitude: [1, 5, 10] V
- Signal Frequency: [15.625, 31.25, 62.5] Hz
- Number of Steps: [8, 16, 20]
- Phase: [0] °
- Offset: [0] V
- Microwave Frequency: [69599999998, 69599999999, 69600000000, 69600000001, 69600000002] Hz
- Segments Configuration: [34813, 17406, 8704, 4352, 2176, 1088, 544, 272, 136, 68, 34, 17, 8, 4, 2, 1, 1, 1]
- Sampling Frequency: [10000, 20000, 40000, 50000] Hz
- Number of Periods: [1]
- Digitizer Gain: [1.0]
- Digitizer Offset: [0.000035] V
- White Noise: [2.8e-7, 2.9e-7, 3.0e-7, 3.1e-7] V

The combination of all these features gives a total of 2160 produced signals. Figure 7 depicts an example that compares a test-measured signal with the corresponding synthetic signal generated by the algorithm. The results show that a simple model based on the Josephson equation with the addition of a simulation of the digitizer effect and the noise in the setup, is a faithful representation of the system behavior and could be used to some extent to train the models based on neural networks. The major disadvantage is that not every physical phenomenon that affects the measurements and the system itself is represented in this model. That is why machine learning algorithms were selected to develop the digital twin; because it could be possible to detect patterns not contemplated in this mathematical modeling and describe better the performance of the PJVS.

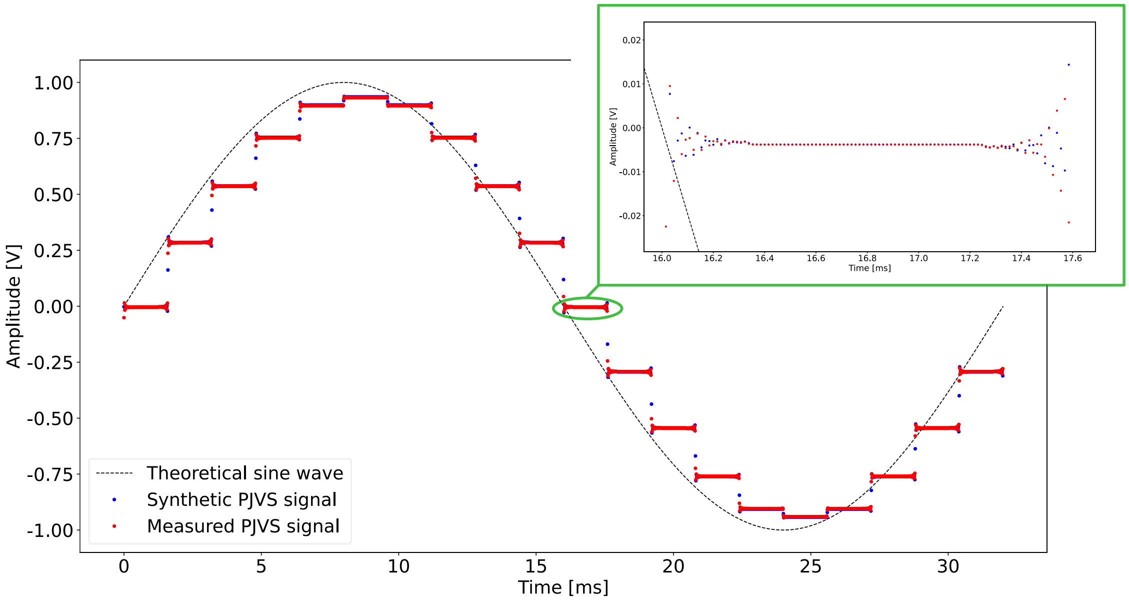

Figure 7. Comparison of a synthetically generated signal with a measured signal. A 1 V peak amplitude, 31.25 Hz test signal (red) sampled at 50 kHz with the corresponding synthetic generated signal by the algorithm (blue) is presented. Here 20 steps per period were used.

Signal measurements with UME PJVS system

Once software modifications and system synchronization were made, sine wave stepwise approximated signals were measured. As stated, Agilent 3458 was used to digitalize the signals generated with the PJVS system. Parameters such as peak-to-peak amplitude, signal frequency, number of steps, sampling frequency, and aperture time were set up manually in the software to take the measurements. The variation of the parameters of the waveforms was:

- Signal Type: Sine waves
- Amplitude peak-to-peak: [1, 1.5, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 19.7] V
- Signal Frequency: [7.8125, 15.625, 31.25, 62.5, 125] Hz
- Number of Steps: [8, 10, 16, 20]
- Phase: [0] °
- Offset: [0] V
- Microwave Frequency: [69600000000] Hz
- Segments Configuration: [34813, 17406, 8704, 4352, 2176, 1088, 544, 272, 136, 68, 34, 17, 8, 4, 2, 1, 1, 1]
- Sampling Frequency: [20000, 40000, 50000] Hz
- Number of Periods: [5]

The combination of all these features gives a total of 1260 measured signals. Figure 8 compares one of the measured signals with its corresponding PJVS theoretical signal. The difference that can be appreciated is that the measured signal has transient points due to the digitizer's output filter response to the transition between adjacent quantum voltage levels of the PJVS, as stated previously.

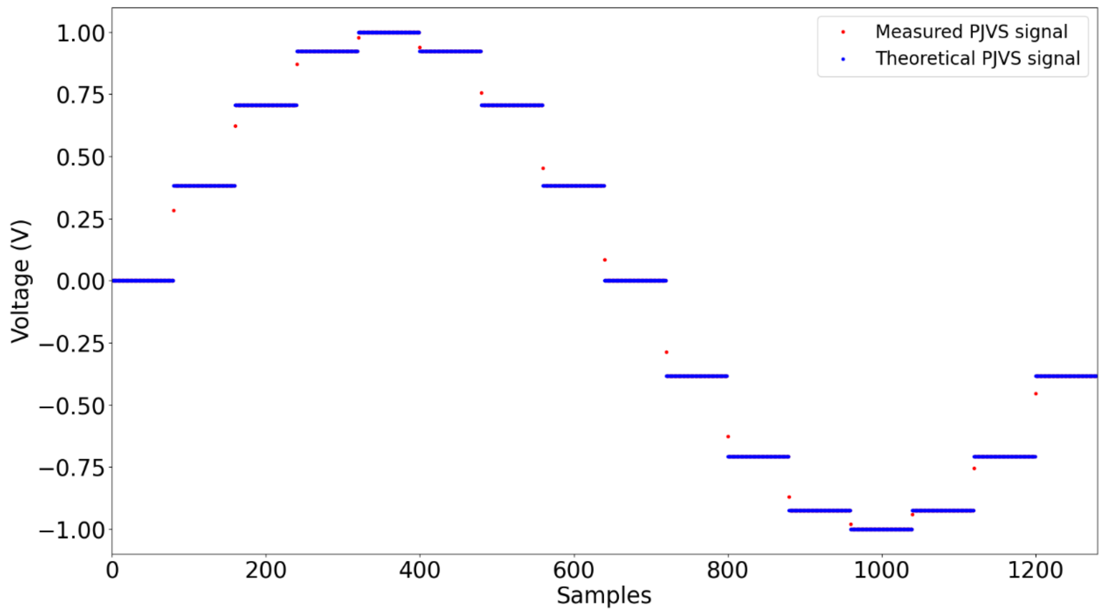

Figure 8. Comparison of a theoretical PJVS signal with a measured signal. A 1 V peak amplitude, 31.25 Hz test signal (red, the steps are at the bottom) sampled at 40 kHz with the corresponding theoretical signal (blue) is presented. Here 16 steps per period were used.

Model architecture and training procedure

To train the model that will make the predictions a dataset was prepared using the most relevant features of the system. These characteristics were selected considering their relevance in system performance, several tests were performed and the results obtained were compared to determine this selection.

Artificial Neural Networks (ANNs) were chosen as the Machine Learning algorithm for the model because of their ability to recognize complex, nonlinear relationships between input and output variables. They are universal function approximators, capable of learning any continuous function given enough data and the right architecture. Unlike traditional physics-based models, which require explicit equations derived from first principles, ANNs are data-driven, making them appropriate for systems with unknown or complex dynamics. Furthermore, they automatically extract features from raw data, reducing the need for manual preprocessing, and they handle noise adequately when trained using techniques such as dropout and regularization. Their scalability allows them to handle high-dimensional datasets like time series or multi-channel measurements, and their versatility makes them excellent for integration into real-time applications [6]. These characteristics make ANNs especially effective for tasks like regression, which need precise predictions of physical quantities such as voltage.

This type of neural network uses supervised learning, so the target (objective of the prediction) must be provided in training. The target selected was the difference between measured and theoretical PJVS voltage, defined as "error" in the dataset.

$$Error_{(measured)} = V_{PJVS\,(measureded)} - V_{PJVS\,(theoric)} \qquad (2)$$

The output of the digital twin becomes the prediction of the error added to the theoretical PJVS voltage, and in that way, PJVS signals can be produced from the prediction of this error.

$$V_{PJVS\,(predicted)} = V_{PJVS\,(theoric)} + Error_{(predicted)} \qquad (3)$$

This gives the future behavior of the PJVS, and this information can be used to optimize the performance of the physical system. Table 1 shows an example of one point of a signal in the dataset. The full dataset consists of 1260 randomly sorted measured sine stepwise approximated signals, using 5 periods for each signal.

Error (V)	V_measured (V)	Amplitude (V)	Signal_freq (Hz)	Steps	MW_freq (GHz)
0.014171063	-0.689885006	1.0	31.25	16	69.6
TARGET	FEATURES				

Table 1. Structure of the dataset used to train the neural networks. Here one point of a signal is represented as an example.

The structure of the dataset is as follows:

- Error: difference between measured and theoretical PJVS voltage, in (V). This is the target of the predictions.
- V_measured: digitizer's measured voltage, in (V).
- Amplitude: programmed signal peak amplitude, in (V).
- Signal_freq: signal frequency, in (Hz).
- Steps: number of steps.
- MW_freq: microwave frequency, in (GHz).

A standard procedure widely used in deep learning was applied for the neural network training [7]. It consists of the following steps:

1. Create a dataset with a representative sample of the signals, randomizing the order. In this case, 1260 signals with 5 periods each were used.
2. Separate target from features.
3. Separate between training (80%) and testing (20%) datasets. Some signals are not used in training so the model can be tested with previously unseen data.
4. Normalize the features using MaxAbsScaler. Normalization prevents overfitting (a situation where the model learns the training data too well and it is not good to generalize the predictions of unseen data). Different scalers were tested, and better performance was reached with MaxAbsScaler, possibly because it considers the effect of negative values:
   - $z = x_i / |x_{max}|$, where x_i = sample i, x_{max} = maximum value. This means that each signal point is divided by the absolute value of the maximum signal value.
5. Create a model of the neural network.
6. Train the model with the train dataset.
7. Evaluate the predictions on the testing datasets and calculate the metrics.

Different models were programmed in Python using TensorFlow [8] and Keras [9] APIs to predict the error of the quantum voltage steps of the signals. A diagram of the structure of the neural network layers is detailed in Figure 9. The input layer has shape = 5 because there are 5 features in the dataset. The number of layers and neurons per layer sets the complexity of the model. Four dense layers with decreasing numbers of neurons are connected, using the Rectified Linear Unit (ReLU) as an activation function. The output layer has 1 neuron and the Linear activation function since the regression target is one value (the error of the measured voltage). Due to this, mean squared error (MSE) is chosen as the loss function and root mean squared error (RMSE) as the metric. After each dense layer, a 20% dropout layer was added to prevent overfitting, and this dropout was used to estimate the uncertainty of the model with the Monte Carlo Dropout method.

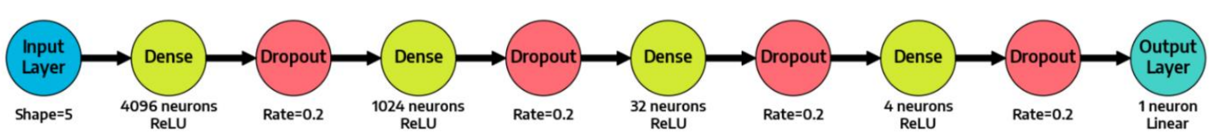

Figure 9. Model architecture of the Artificial Neural Network.

The parameters used in this example are:

- Activation function: Rectified Linear Unit (ReLU).
- Optimizer: Adam, learning rate = 0.0001.
- Loss: mean squared error (MSE).
- Metric: root mean squared error (RMSE).
- Batch Size: 16.
- Epochs: 300.
- Total parameters: 4252841.

An important factor to consider is that these hyperparameters should be optimized to obtain the best results. Updates of the model will include variations to improve the performance.

Results

The test datasets were used to make predictions of signal errors. An example of an 8-step signal is shown in Figure 10. The error predicted depends on the voltage values of the steps, being the higher voltages the ones that differ the most with the measurements.

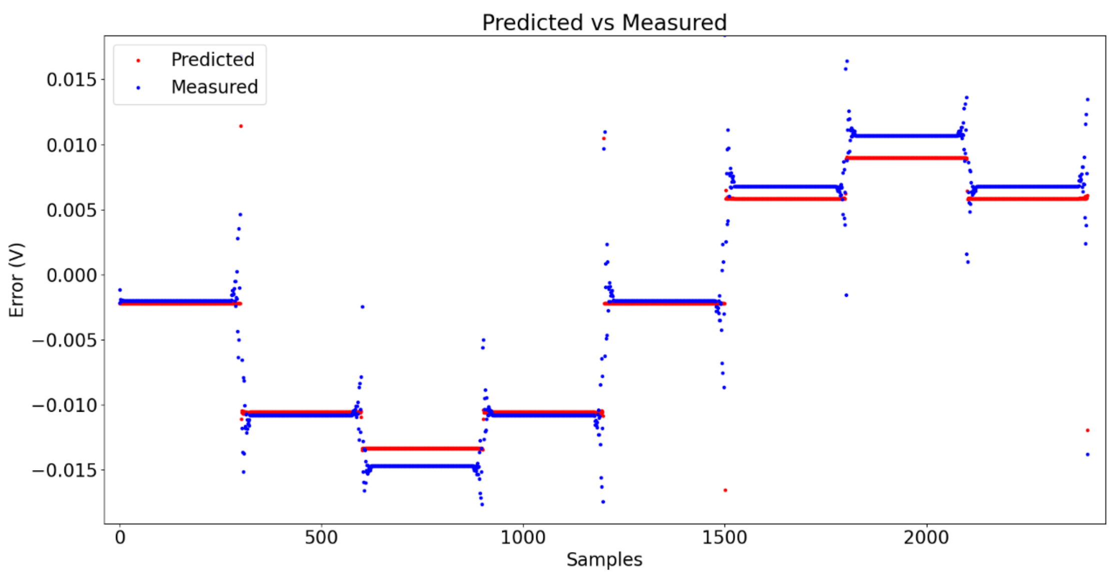

Figure 10. Comparison of the predicted signal error (red) with the measured signal error (blue) of an 8-step signal.

Uncertainty estimation of the model

The uncertainty contribution of the most relevant parameters can be divided into two categories:

1. Errors and uncertainties in the model:

Different sources of errors and uncertainties in neural networks were investigated [10] and identified in these categories:

- Numerical errors result from floating-point round-off errors from different computation orders in the neural network's calculations. This is dependent on the Python libraries used [8, 9].
- Epistemic Uncertainty (Model Uncertainty): This arises from the model's limited knowledge of the data and can be reduced by providing more data.

- Aleatoric Uncertainty (Data Uncertainty): Data bias due to a lack of information and variability in the system parameters. This results from noise inherent in the data and cannot be reduced by adding more data.

2. Errors and uncertainties in the instruments:

In the case of measurement instruments, the sources of error and uncertainty are:

- Digitizer voltage measurements with Agilent 3458A digitizer. The device manual defines the uncertainties and can also be obtained from previous characterizations [11, 12].
- White and power line noise in the system [13].
- Quantization error from Josephson system resolution: ±72.5 μV.
- Microwave frequency measurement. This is related to the stability of the Rubidium clock and can be obtained from a test report of the microwave synthesizer.
- Cryocooler temperature measurements: extracted from calibration certificate, ±4 mK.

The error of the voltage steps will be determined by comparing the predictions of the model with the theoretical voltage of the PJVS signal.

The uncertainty of the neural network will be evaluated using the Monte Carlo Dropout (MC Dropout) method [14].

MC Dropout is a method used to estimate uncertainties in neural network predictions by interpreting dropout, typically used as a regularization technique, as a form of Bayesian approximation. Dropout randomly deactivates neuron connections during training to prevent overfitting. By keeping dropout active during inference and performing multiple forward passes, the predictions become stochastic, effectively sampling from an approximate posterior distribution over the model's parameters.

The procedure to calculate the predictions and its uncertainty is as follows:

1. Keep dropout active during test time (in inference mode).
2. Perform N stochastic forward passes for the same input (typically 100000).
3. Collect the N predictions to compute the mean prediction (average the N outputs to get the final prediction), and the uncertainty (variance or standard deviation of the N predictions).

Figure 11 depicts an example of a 1 V peak-to-peak, 15.625 Hz signal sampled at 40 kHz. The sine wave has 8 steps per period. It can be observed that the uncertainty is higher in the transient points and the higher step voltages, which matches the results of the predictions. The uncertainty can be reduced if the dropout rate is reduced during the model training. Tests with a dropout rate of 15%, 10%, and 5% should be performed to compare the results.

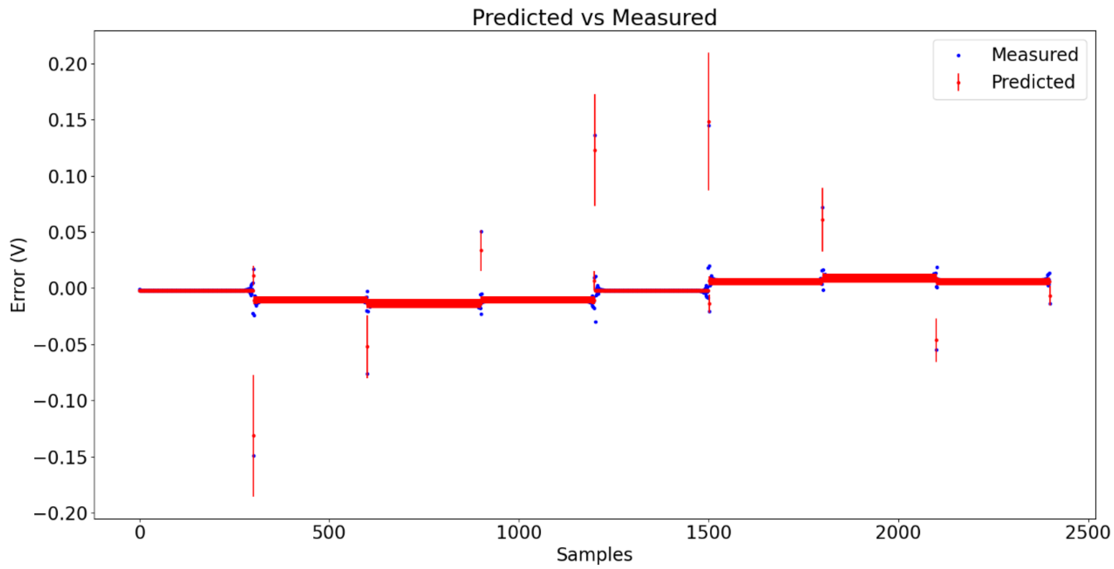

Figure 11. Uncertainty estimation of the model using the Monte Carlo dropout method for an 8-step signal.

Conclusions and Future Work

The possibility of participating in this program represented a significant step toward developing a Digital Twin of the PJVS. Through this work, I gained valuable hands-on experience with the cryocooler and PJVS system operation, optimizing its setup and measurement processes. Critical configuration parameters and signals to be measured were identified, to enable targeted improvements in system behavior. To address limitations at the beginning of the measurement procedure, synthetic signals were generated, which were subsequently used to train various neural network models. These models were tested and evaluated, demonstrating their capacity to predict system deviations.

Measurements of sine stepwise approximated signals were performed to validate the system's operation and enhance the dataset available for training. Methods for validating the DT and quantifying its uncertainty were explored, with Monte Carlo Dropout successfully employed to estimate uncertainty in neural network predictions.

Additionally, participating in the CIPM MRA seminar provided insights into the crucial role of National Metrology Institutes (NMIs) in advancing measurement quality in industries such as health, environment, and science. It also was an excellent chance to engage with colleagues from Bureau International des Poids et Mesures (BIPM) and other NMIs to discuss metrology's challenges and opportunities. This project aligns with the objectives of the CIPM MRA, aiding compliance with its requirements and supporting the expansion of Calibration and Measurement Capabilities (CMCs) in the KCBD. These outcomes are expected to lead the way for declaring additional CMCs, further enhancing metrology's reach and improving traceability to the SI voltage unit.

Moving forward, the next phase of this work will focus on expanding the measurement dataset to train the models more effectively. Testing with different neural network configurations and parameters, including adjustments to the dropout rate (e.g., 15%, 10%, and 5%), will aim to improve the performance and refine uncertainty estimations. The development of the DT will continue with particular emphasis on the Virtual-to-Physical connection, enabling real-time feedback and adaptive control of the PJVS system. Validation of the DT will proceed through comparison with measurements from the physical system, ensuring reliability and robustness in its predictions.

The knowledge gained from this project will be directly applied to advancing the Digital Twin and Artificial Intelligence initiative at INTI, contributing to the progress of my PhD thesis and the 22DIT01 ViDiT EURAMET project. Ongoing collaboration with TÜBİTAK UME's Voltage Laboratory will continue, to publish a paper to disseminate the findings. The methodologies and insights developed here are expected to optimize measurement and calibration processes at INTI and TÜBİTAK UME, expanding their capabilities and promoting innovation in quantum metrology. This work provides a foundation for developing digital twins in electrical metrology, particularly for quantum voltage standards.

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