Quantum Sensing

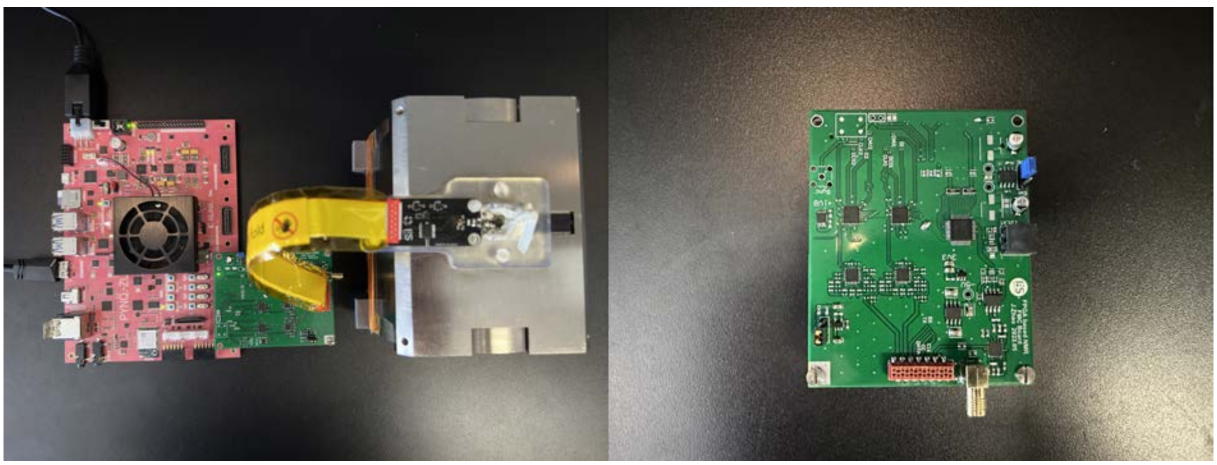
PYNQ based Portable Nuclear Magnetic Resonance Spectrometer Powered by Deep Learning

AMD Xilinx Open Hardware

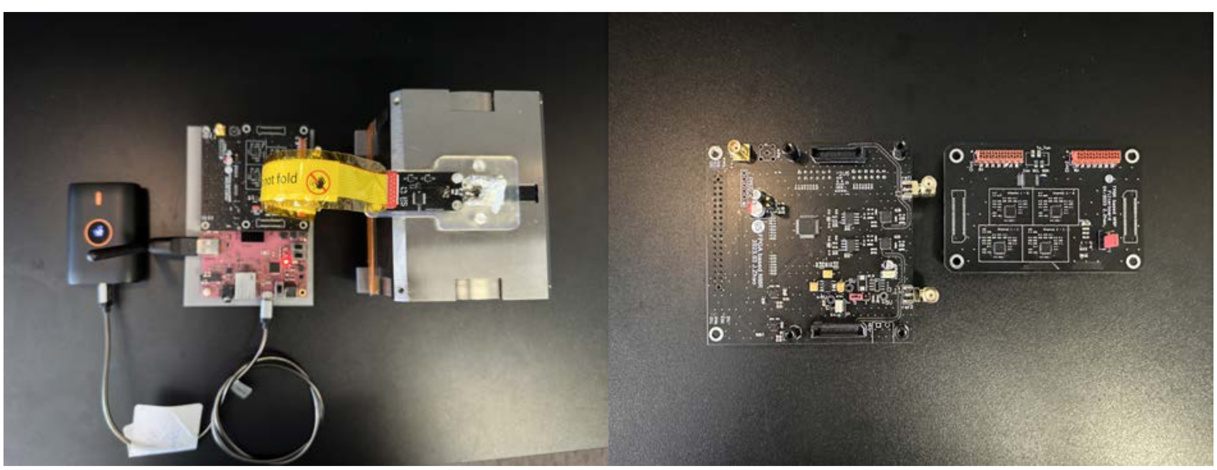
Competition 2023

HARDWARE

The experiment is divided into two parts, both using the hardware and software systems designed for this competition. We designed and tested two hardware systems: PYNQ ZU and our high-performance NMR board based on the FMC interface. Meanwhile, we also designed and tested the peripheral circuits for the PYNQ-Z2 low power, wireless system powered by a power bank.

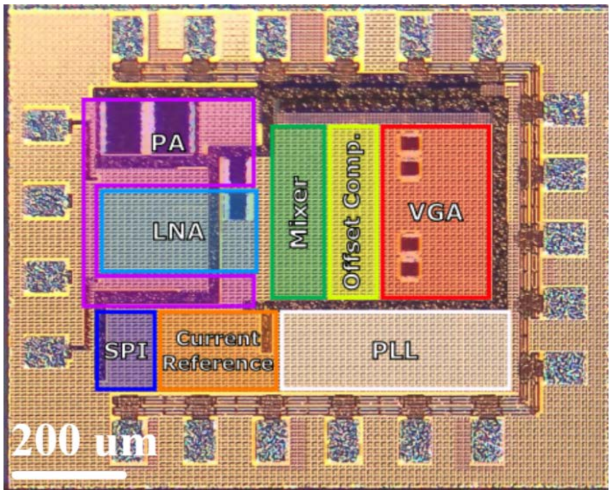


PYNQ ZU and NMR-FMC Board



PYNQ Z2 and NMR Daughterboard

The both daughterboard uses a 125 MSps 14 bits DAC AD9767 to generate spin excitation pulse sequences. After being sent to the ASIC circuit through a low-pass filter, the FPGA implements the switching of the TX and RX control signal for the ASIC chip via the FMC interface, as well as the control of PLL, reference current, and amplification factor, in order to accurately capture information from hydrogen atoms in the sample. The information from hydrogen atoms, after being amplified by the in-chip LNA, is sent to a 4th-order analog Bessel filter circuit and sampled by the ADC chip.



NMR on Chip AISC Chip [1]

The main difference between the PYNQ ZU and Z2 daughterboards lies in the design of the ADC. The ZU daughterboard, based on the ZYNQ UltraScale' s excellent computational performance, I/O, and high-performance FMC interface, uses two 5MSPS 18-bit resolution SAR ADCs AD7960 for the I&Q Channels. The signal and clock use the LVDS interface for transmission. It can better capture weak quantum signals with higher resolution.

The PYNQ Z2 system uses a 2MSPS 16-bit resolution ADC MAX11198. Its purpose was to verify feasibility at the beginning of the competition. However, we did not abandon the development of PYNQ Z2 in the later stage. This is due to the low cost and low power consumption advantages of PYNQ Z2. The cost of the PYNQ Z2 system is around 220 euros, and it can operate outdoors for an extended period. NMR Spectrometers are generally considered expensive laboratory equipment. As medical equipment, their costs, which often reach tens of thousands of euros or more, greatly limit their use in some underdeveloped areas. We are trying to minimize system costs as much as possible by using AMD XILINX's deep learning IP along with superior hardware and signal processing algorithms. We hope to contribute to the popularization of quantum sensing and medical diagnosis in these areas through the platform of this open-source competition.

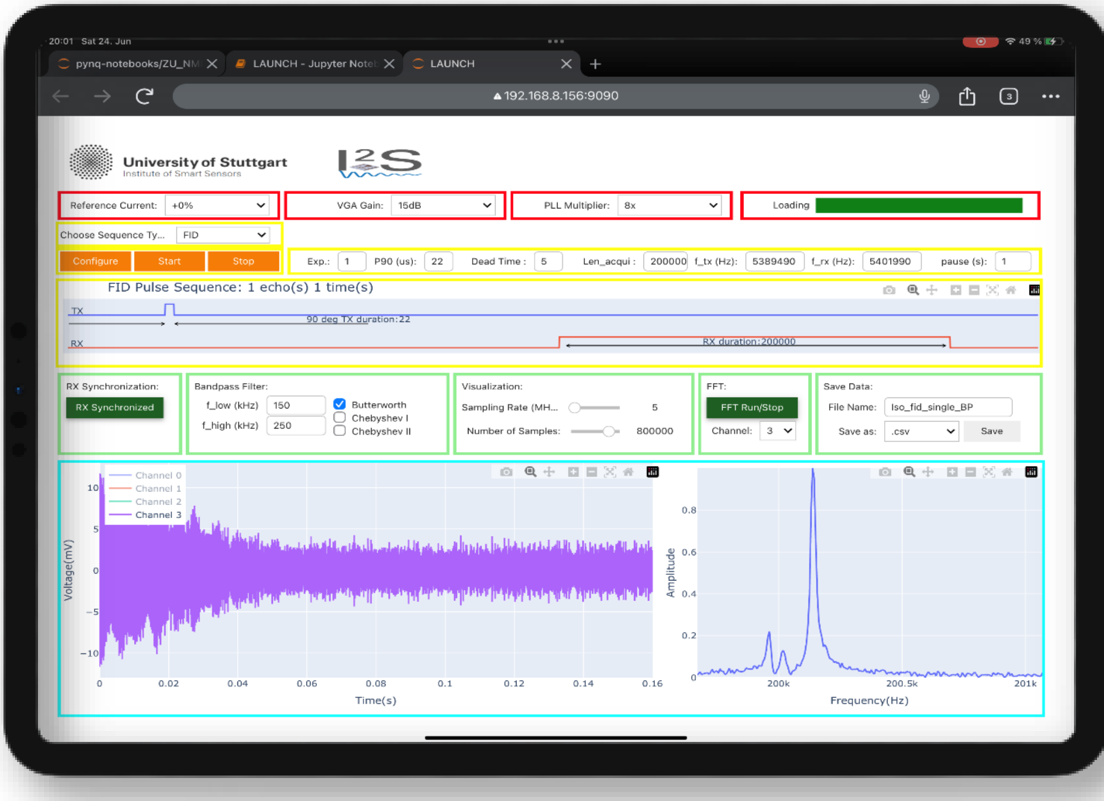
EXPERIMENT

The experiment is divided into two parts. The first part involves FID (Free Induction Decay) measurement. Through this part of the measurement, the hydrogen atom FID signals can qualitatively and quantitatively reflect the composition of the sample. In the two different hardware systems mentioned above, we tested different samples (Ethanol, Isopropyl alcohol, Toluene). During the testing process, the liquid samples were placed in test tubes with a diameter of 0.8mm.

Ethanol NMR FID signal in Time and Frequency Domain

the results for Ethanol (CH3-CH2-OH) displayed on the iPad. We can see the peaks produced by the signals from three different hydrogen atoms in Ethanol. Their proportions are 3:2:1. The lower left image shows the time-domain spin signal.

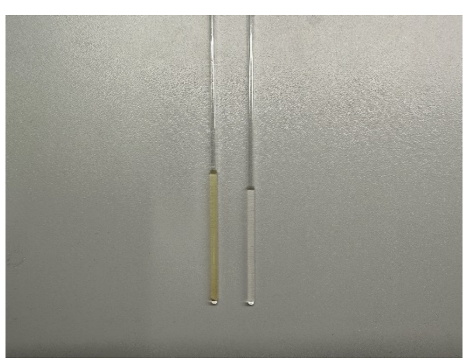
Below is the results for Isopropyl alcohol (CH3)2-CH-COH. We can see a clear difference from Ethanol in the time-domain diagram at the bottom left. If you enlarge the image, you can see two small peaks with almost equal amplitudes on the left side of a main peak. This image perfectly reveals the molecular structure of Isopropyl alcohol from a macro perspective.



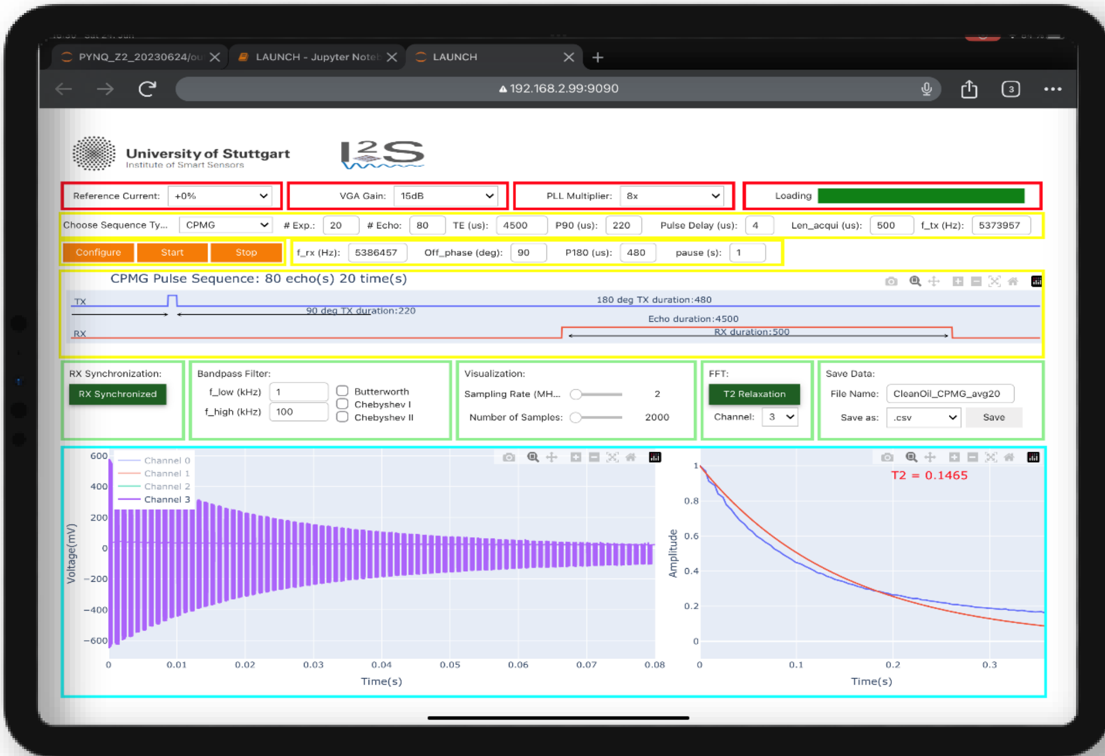
Isopropyl alcohol NMR FID signal in Time and Frequency Domain

Thanks to the excellent compatibility of the web GUI based on Jupyter notebook, this NMR spectrometer can be controlled by almost all laptops, PCs, and tablet. Users don't need to download or install any complex operating software. They can modify the parameters in the open source code according to their own needs. Based on the high-performance computing platform, both the computation and control systems are integrated into the FPGA. The Python code adjusts the system by modifying the parameters in the register interface of the IP core via the AXI bus.

In the second experiment, we demonstrated the application of the CPMG sequence on our designed system. We measured the T2 of cooking oil, which typically reflects the quality of the oil. The results show the unused cooking oil and the cooking oil used for cooking food. It's worth noting that the cooking oil tested here after cooking contains a small amount of water and seasoning.

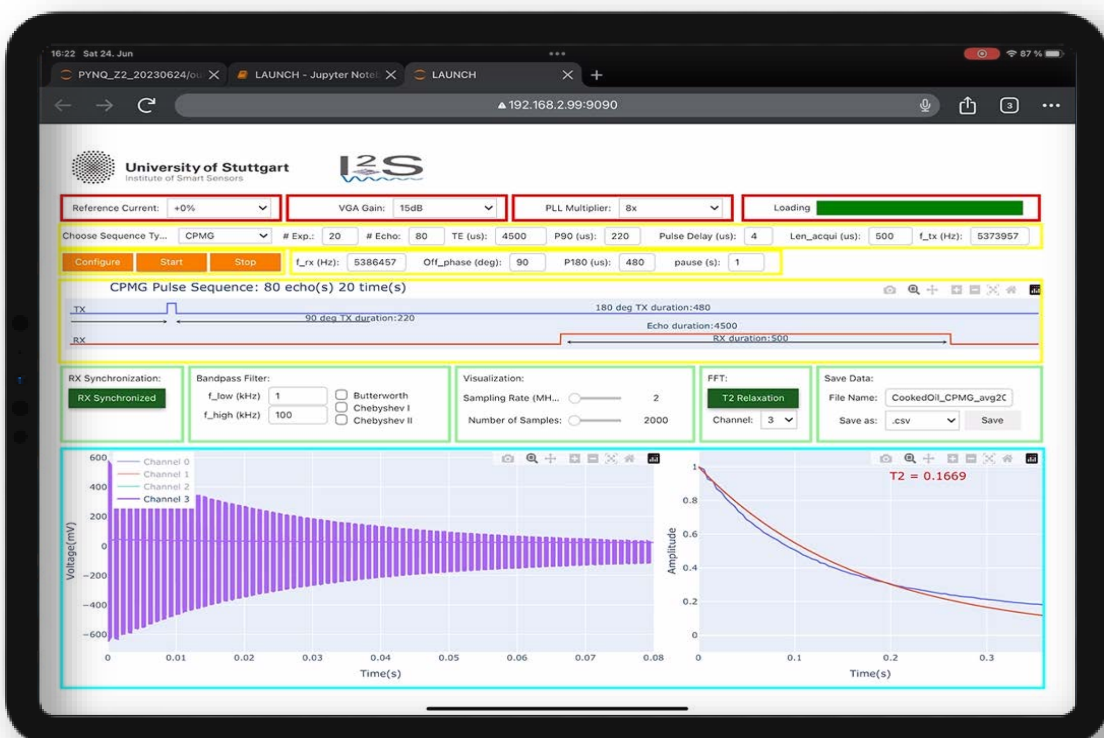


Oil after cooking and cleaning



T2 measurement for clean oil

On the left is the time-domain spin signal of the complex sequence, and on its right is the relaxation curve after calculation and fitting. What we need to note here is that the T2 time length of the clean oil is approximately 146.5 ms.



T2 measurement for the oil after cooking

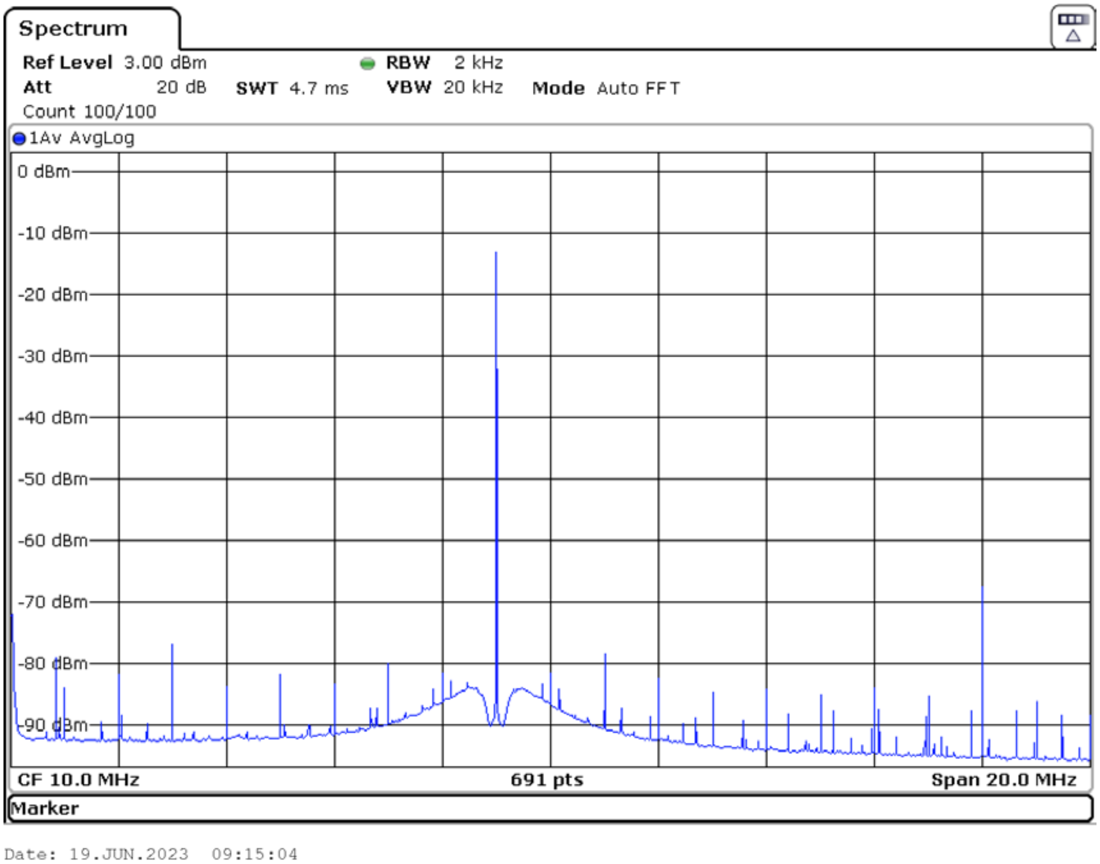
After testing the clean oil, we also measured the oil after cooking. As can be seen, there is almost no difference in the time-domain of the spin signal. However, after the calculation and fitting of T2, it's noteworthy that the time of T2 has increased to 0.1669. This is due to the diffusion of water from the vegetables into the cooking oil during the cooking process.

We also measured solid samples like tires. The degree of wear on tires can also be distinguished by T2. We very much wanted to do some medical-related experiments, such as blood sugar tests. However, due to the fact that our supervisor (me) faint at the sight of blood, we had to abandon this experiment. But we firmly believe that T2 will certainly yield significantly different results. 

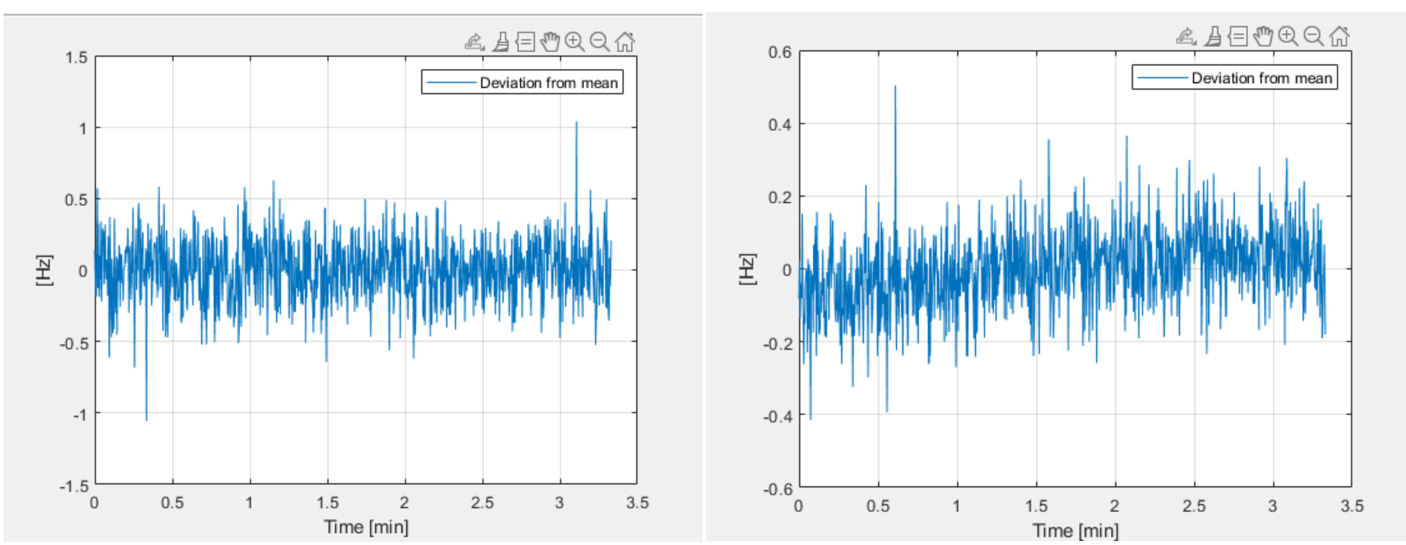
Deep Learning Application:

The chemical shift in NMR spectrometry is extremely sensitive to temperature changes. The influence of temperature can cause the magnet to change its original magnetic field B0, which directly affects the Larmor frequency of the sample. On the spectrum, you will observe some offsets on the original basis. Under normal circumstances, a temperature control box is used to ensure temperature stability, which often makes the equipment heavier. At the same time, a lot of energy needs to be converted into thermal energy. Artificial intelligence has greatly improved this. We first performed spectral recognition, marking the chemical characteristics of substances. Then we calculated the deviation between the theoretical and actual Larmor frequencies, adjusted the TX transmission frequency to ensure that the sample is excited. Then the signal is stacked and averaged again to reduce the system's white noise. Of course, the functionality of deep learning is not limited to this. We hope that our initial exploration and the experience of hardware platform selection will bring you more good ideas.

HARDWARE TEST

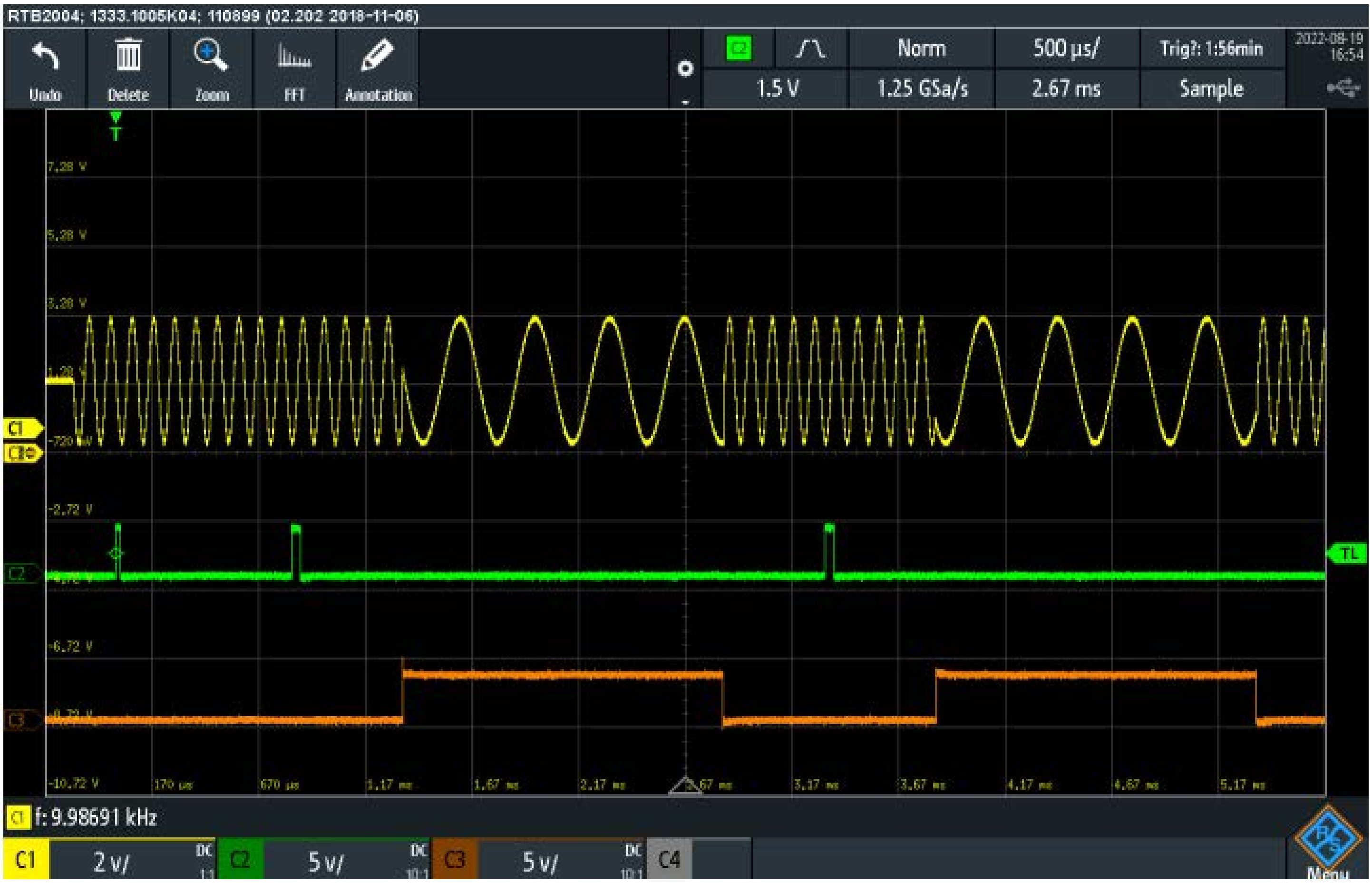


PYNQ Z2 daughterboard Tx pulse generator output testing, read out from signal analyzer Rohde & Schwarz 4 GHz



standard deviation for a single tone, frequency stability analysis

left: PYNQ based Interface, right: Keysight 33500B



Example for using Jupyter Notebook (python 3.0) to control FPGA IP Core and generate real wave from 2 channel DACs (Series AD9767)