



Original contribution

Credit-card sized field and benchtop NMR relaxometers using field programmable gate arrays

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 Low field nmr
 Compact nmr

ABSTRACT

The tools for developing systems for NMR improve each year. Some firmware based designs based on Field Programmable Gate Arrays (FPGAs) have been developed to implement both the core and peripheral apparatus for NMR Relaxometers and NMR Cryoporometers. Hand held in size they are particularly suitable for desktop, mobile and field use.

Software tools now enable the writing of firmware that enable the rapid design of digital and digitised R.F. data and control systems. This firmware can then be loaded into and run on hardware that often is only the size of a credit-card. These devices can include a single-chip Linux computer with an FPGA capable of processing digital RF on the same chip. These can generate RF signals digitally, process RF signals for up- and down-conversion, and can provide an on chip NMR pulse sequencer.

An extremely well tested NMR digital transmitter has been upgraded to use the latest surface-mount Bipolar and Field Effect Transistors. The circuitry is now the size of a book of matches, and interfaces to credit-card sized FPGA modules for RF generation, phase shifting and drive signals. This NMR transmitter design uses digital logic principles rather than conventional tuned R.F. techniques Offering both active-damping and active-quench, a very square R.F. Pulse with fast turn off is achieved, with Mark 1 giving $2.6 \mu\text{s} \pi/2$ and $4.8 \mu\text{s} \pi$ pulses into a 5 mm diameter NMR sample (2.7 mT B_1) at 20 MHz for Protons. $T1\rho$ pulses are stable and consistent.

1. Introduction

1.1. What is an FPGA and why are they useful for instrumentation?

Field Programmable Gate Arrays (FPGAs) are digital logic that contains settable switches to change the connectivity and other properties. Originally often UV erasable, they now mainly employ flash-memory and are electrically programmable and erasable. As well as often having sufficient capacity to have programmed processors, they increasingly contain hard-wired processors, often based on the ARM processor set. A key feature is a basic set of programmable peripherals to interface to the real world.

Increasingly large FPGAs are being produced, with speed, amount of on-chip memory, number of hard-wired multipliers, Giga-Hertz communication channels, etc., continuing to develop. It is therefore important to choose the correct FPGA, or pre-made FPGA module, to implement cost-effective, compact and fast instruments and spectrometers for NMR.

A number of FPGA based NMR components, as well as some completed systems have been described in the literature [1–3]. This paper describes some extremely compact and neat designs of functioning FPGA based NMR relaxometers.

1.2. Choosing a limited set of FPGA modules to work with

1.2.1. Why FPGAs?

Firstly, why use FPGAs to interface to the experiment, rather than microprocessors? The key reasons here are a) that a microprocessor is limited to doing one operation at a time, and has to use interrupts to time-slice between different tasks. Thus while it may be easy to program each task on its own, the grief comes when having to assemble all these parts to all operate harmoniously together. In an FPGA, on the other hand, different areas of the logic circuitry can be carrying out different tasks completely asynchronously with each other, and can be designed separately with no interaction. Further, point b), the different parts of the FPGA circuitry can operate at RF frequencies.

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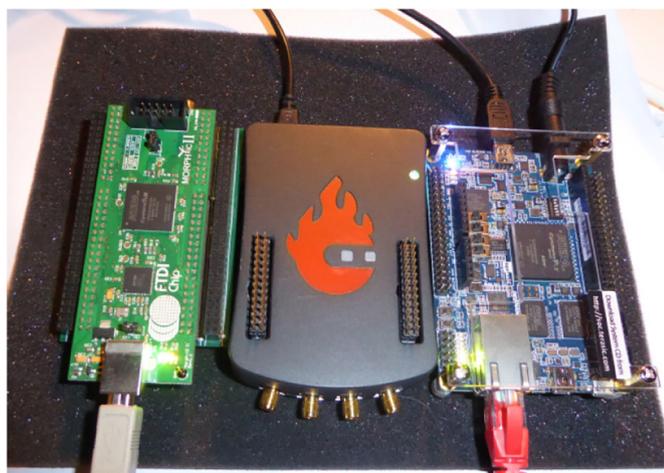


Fig. 1. Three FPGA Modules, A, B, C, as discussed, left to right.

The FPGAs chosen are all very compact “logic engines”, with a minimum in the way of on-board human-interface switches, LEDs etc., but with extensive arrays of connector pins with 0.1” spacing to interface to the apparatus. The assumption being that the human interface is a separate control and data display computer, and that the FPGA is then just a digital interface from that computer, and its programs, to the experiment.

To date Lab-Tools have employed off the shelf FPGA modules, on a convenience, simplicity of design, and cost basis. The three modules used are shown in Fig. 1.

1.2.2. A: morphic II

This is a USB2 interfaced Morph-IC-II module, produced by FTDI [4], with an Altera Cyclone II FPGA chip [5]. This is a compact module, about half a credit-card in size. Its key feature is a single full speed USB2 interface that is used to both upload the pre-compiled binary configuration program, send control information and read data and status information back. This is in contrast to most other similar modules, where a separate USB interface to a specific loader program is needed. In the Lab-Tools modules, the array manipulation program AplX carries out all three operations. The Ancillary NMR Instrumentation discussed in the next section has been implemented using this device. It has also been used to develop the Mark II version of the Digital Transmitter.

1.2.3. B: red pitaya

An Ethernet interfaced FPGA module with on-board RF I/O, the Red Pitaya module [6] has a Xilinx Zynq 7010 Silicon-On-Chip (SOC) FPGA [7], with dual-core ARM Cortex A9 CPU running Linux. Its key feature is research quality (v 125-14) 14bit 125 MHz RF dual D to As and dual A to Ds. A credit-card sized module that is ideal when RF input and output is needed. This module has been used to implement both an NMR Receiver and a Linear NMR Transmitter operating in the 1 to 60 MHz frequency range.

1.2.4. C: DE0-Nano-SoC

An Ethernet interfaced Terasic DE0-Nano-SoC Kit/Atlas-SoC Kit [8] with an Altera Cyclone V FPGA [9] with 800 MHz dual-core ARM Cortex-A9 processor running Linux. Its key features are a much higher performance and larger Cyclone V FPGA than the Cyclone II, Avalon programmable interfaces, has programmable frequency clocks with milli-Hertz precision, and for Lab-Tools, this module can run the same firmware as was implemented in the first FPGA above (Cyclone II), which saves a significant amount of development. It is being used as part of a Digital Transmitter module, operating in the 1 to 30 MHz frequency range.

1.3. How to simplify multi-instrumental designs with an FPGA firmware skeleton

A common requirement of both digital instruments and integrated circuits is the need for a set of registers that are employed to program and define the operation of the instrument/chip, and then to read results back.

A Modular Firmware Skeleton (MFS) design has been created, for the control of multiple instruments in one FPGA, and for the separate access of the results from each instrument. A triple 8-bit bus interface is created between an input/communication module, and as many separate instruments as are needed (each instrument selected by an 8-bit Bank register). Each instrument then has up to 256 8-bit data registers (selected by an 8-bit Address register) – wider registers can easily be accessed using multiple reads or writes, in software.

For the Morph-IC-II with Altera Cyclone II FPGA the MFS registers are accessed from an external computer over the USB bus, either one transfer at a time, or data can also be transferred to and from the instruments in bursts at the maximum transfer rate of a USB2 bus, of 60MByte.s⁻¹. Lab-Tools instrumentation uses the array processing language Apl to both create and control the instrument front-panel Graphical User Interface (GUI) and to communicate via an FTDI DLL

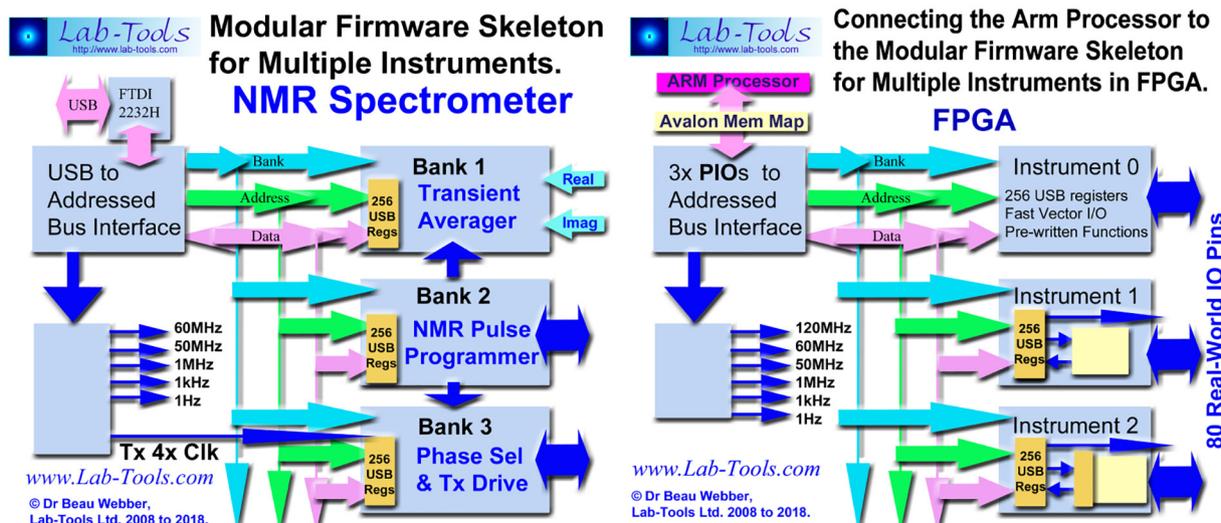


Fig. 2. Modular Firmware Skeletons (MFS): Left: USB interfaced for Morph-IC-II; Right: Connected to ARM processor for DE-Nano-SOC.

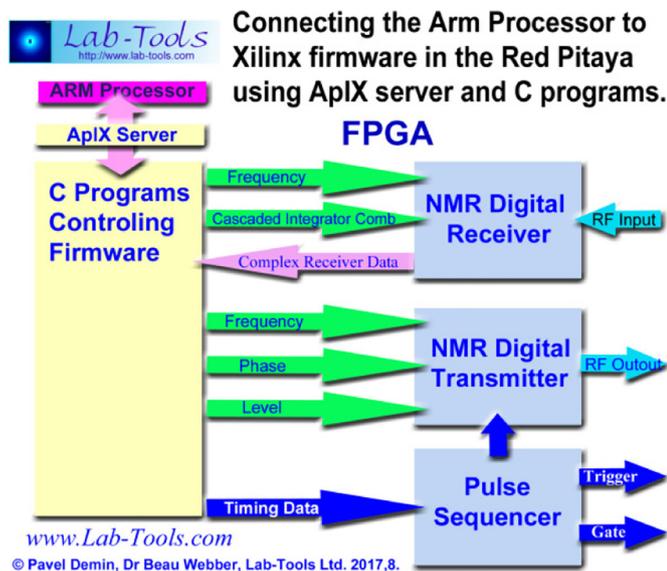


Fig. 3. AplX Server to c programs to firmware interface for Red Petiya.

over the USB interface, as well as analysing and processing the results (Fig. 2).

For the DE0-Nano-SoC with Altera Cyclone V FPGA the MFS registers in the FPGA are accessed from the ARM processor via the Altera Avalon Memory Mapped Interface, via three specially programmed Parallel Input Output (PIO) registers, which then provide the three 8 bit busses and control I/O lines. These may then either be accessed from an

external computer and GUI via data streams over the Ethernet connector, using a language such as Apl, or an AplX Server can be run in the ARM CPU (in Linux) and this can then communicate with the MFS registers in the FPGA using c programs in Linux, under control of an AplX client, and GUI, in the host computer, again over the Ethernet connector.

As yet such a Modular Firmware Skeleton has not yet been created for the Red Pitaya, due to the very different Xilinx firmware.

However, similarly to the DE0-Nano-SoC with Altera Cyclone V FPGA, the firmware in the Xilinx FPGA may be accessed from an AplX server running in the ARM processor via c programs, and this works well, Fig. 3.

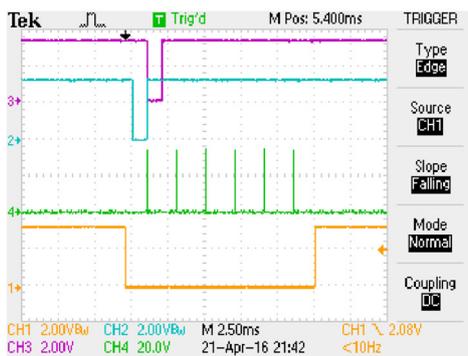
2. Ancillary NMR instrumentation

A range of FPGAs have been employed over a number of years for minor parts in instruments such as Pulsed Field Gradient (PFG) controllers and an Atari to Bruker controller interface. However recently, by employing the Morph-IC-II FPGA a modular range of USB2 interfaced instruments have been implemented, the key ones being as follows:

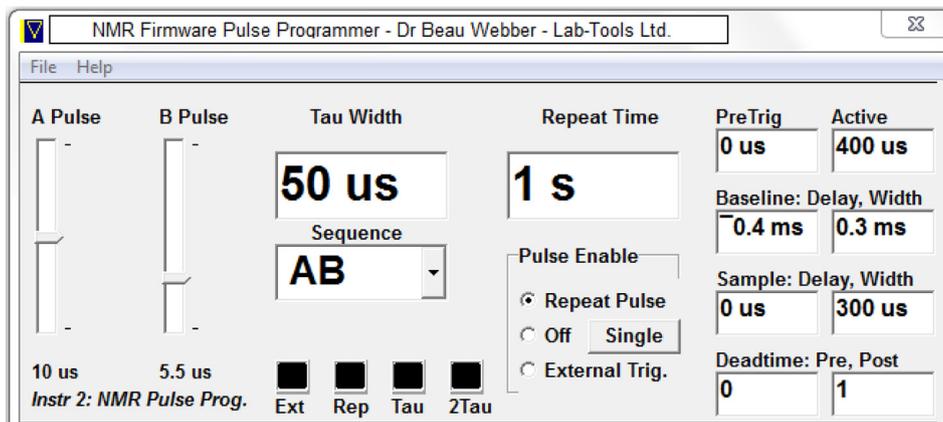
2.1. Precision DVM for NMR cryoporometry

NMR Cryoporometry requires comparative temperature precision of the order of 10 mK or better, and this 5 channel 24 bit digitizing and averaging instrument was created to log the averaged thermocouple EMFs [10].

Used in conjunction with a zero-C reference based on the expansion of a water-ice sample, kept at the bulk melting point of the ice – Omega



a



b

Fig. 4. a: Typical output pulses from NMR Pulse Sequencer. b: GUI Front Panel for NMR firmware Pulse Programmer.

Engineering Ice Point Calibration Reference Chamber Model TRCIIm [11] then highly accurate temperature measurements may be logged with long-term stability.

2.2. Transient signal capture, averaging and processing

This instrument was designed to capture transient real and imaginary base-band signals from an NMR spectrometer, and average and digitally process the signals in firmware, before transferring them to the computer over a USB2 bus [12]. A useful feature is a firmware “magnitude” function, prior to averaging, which enables the averaging of signals that are not phase locked.

2.3. NMR pulse sequence generator

This easy to use pulse programmer [13] implements a basic set of NMR pulse-sequences, as needed for a desk-top relaxation NMR instrument, and generates the 7 sequences: A, B, A- τ -A- τ -Echo, A- τ -B- τ -Echo, B- τ -A- τ -Echo, CP/MG, T1 ρ , Fig. 4b.

As well as the pulses to gate the NMR transmitter, as range of other useful logic pulses are produced as a matter of course, such a Pre-Trig, Active (Ch1, yellow), not τ (Ch2, cyan), not 2 τ (Ch3, magenta), not 2 τ chain (Ch4, green), and a set of signal sampling windows for A and B FIDs, and Echos and Echo chains, in Fig. 4a. This sequencer can be implemented as an “instrument” in an FPGA, alongside one of the other above instruments, without any additional hardware, other than possibly extra output connectors.

3. NMR digital spectrometer

The core components of a Digital NMR Spectrometer (to which the above and other peripheral components may be added) are as follows:

- NMR Receiver
- NMR Pulse Sequencer (discussed earlier)
- NMR Transmitter

For the first NMR system that will be described, the digital components are based on the Red Pitaya FPGA module, described earlier. This is particularly convenient to use because of the on-module RF input and output, directly connected to the FPGA (Fig. 5).

3.1. NMR receiver

3.1.1. NMR digital receiver components

- NMR Low-Noise Linear Receiver
- NMR RF Digitisers (ADC)

- NMR Quadrature RF Oscillator - Direct Digital Synthesiser (DDS)
- NMR Complex Multiplier
- NMR Filters and Decimating Down Convertors – CCIC & FIR

3.2. NMR digital spectrometer to linear amplifier components

- NMR Direct Digital Synthesiser
- NMR Pulse Sequence generator
- NMR Digital to Analogue Converter
- NMR Gated Analogue Linear Amplifier

The NMR Pulse Sequencer GUI Fig. 4. can also be re-used – as part of the AplX Client, which again talks to the AplX Server in the ARM Linux and which via c programs, as shown in Fig. 6 in turn controls the Digital Transmitter Fig. 7. Prior designs have been published, but are more complex and physically larger [14].

3.3. NMR digital spectrometer to digital transmitter components

- NMR Frequency Clock Generator
- NMR Pulse Sequence generator
- NMR Four Phase Gating
- Complementary differential drive for:
- NMR Digital Power Amplifier

4. Current lab-tools spectrometer designs

Lab-Tools have developed two designs of digital NMR spectrometers: a liquids NMR spectrometer, using a linear power amplifier, and also a solids NMR spectrometer, using a digital switching NMR power transmitter (Figs. 8–11).

4.1. Liquids NMR relaxation spectrometer & results

The Lab-Tools liquids digital NMR spectrometer uses the Lab-Tools low-noise amplifier, plugged into a Red Pitaya module, which is running the AplX Server, and Lab-Tools' c programs. The RF from the digital transmitter firmware has to date driven a prototype gated linear power amplifier, to produce the NMR pulses – Fig. 7.

As yet the prototype amplifier does not have a custom metal box, and so is very limited in the power that can be applied, resulting in 800 V Pk-Pk across the probe tuned circuit, giving 15 μ s $\pi/2$ pulses and 30 μ s π pulses into a 5 mm sample tube of water. A suitable box is being 3D printed for the amplifier. Received NMR signals do not seem to be contaminated with noise from the linear power amplifier, the gate signal from the firmware shutting the amplifier down cleanly, Fig. 7.

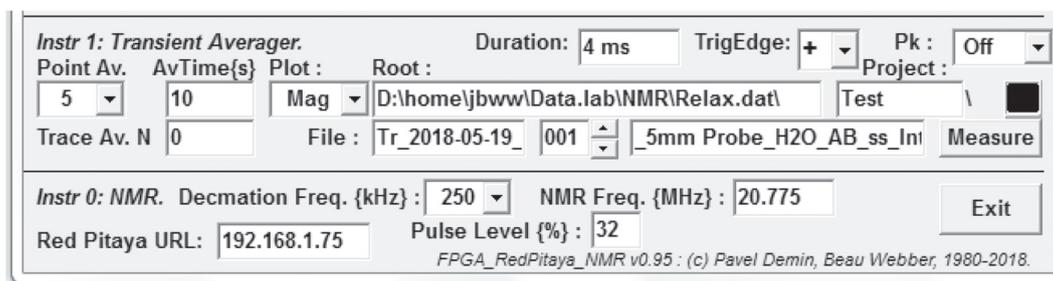


Fig. 5. The Instr 1: section of this receiver GUI is as per the above transient capture – average - process module; the Instr 0: section adds the NMR Frequency control, the filter decimation output rate, and the Ethernet URL.

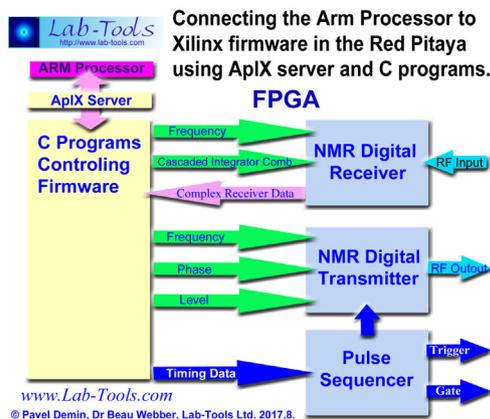
An NMR Low-Noise Amplifier with about 60 dB gain has been developed, and is mounted on a Red Pitaya, using the E1 and E2 connectors. The pre-amp output is then connected to the Red Pitaya RF Input 1.

An AplX Server in the ARM Linux controls the Digital Receiver firmware via c programs.

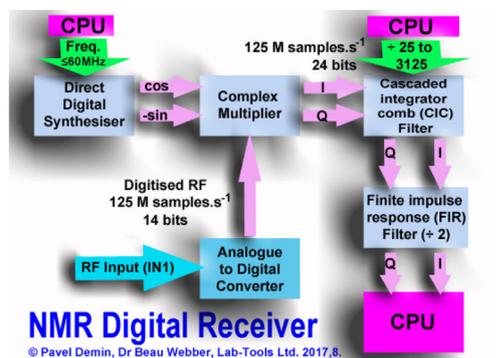
These and the firmware digital section of the receiver in the Red Pitaya FPGA module are shown in Fig. 6.



NMR Low-Noise Amplifier with about 60 dB gain is mounted on a Red Pitaya, using the E1 and E2 connectors. The pre-amp output is then connected to the Red Pitaya RF Input 1.



AplX Server in the ARM Linux, which controls the Digital Receiver firmware via c programs.



The firmware digital section of the receiver in the Red Pitaya FPGA module.

Fig. 6. Component parts of the digital NMR Receiver with low-noise amplifier. The software development was aided by employing the above Transient Capture GUI for the NMR Receiver, as part of the AplX Client, which talks to the AplX Server in the ARM Linux and which in turn controls the Digital Receiver firmware via c programs. For convenience a choice of input impedances are available on both channels: 50 Ω, 9 kΩ, or a high-impedance, high-voltage input capable of being connected directly to the main NMR probe tuning capacitor without needing any matching components. The receiver works well up to 60 MHz.

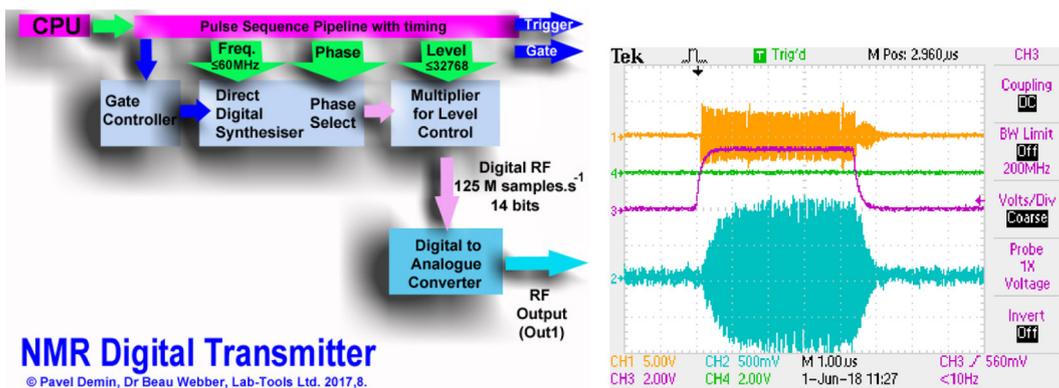


Fig. 7. Left: The firmware digital section of the transmitter, in the Red Pitaya FPGA module. Right: Example RF waveforms with linear transmitter driving into an RF probe and tuning box. Ch2, Purple: Gate signal from firmware; Ch1, Orange: Output of RF Linear Amplifier, note probe ring-down signal after the amplifier is shut down; Ch2, Cyan: RF at 1/100 monitor point across probe tuning capacitor. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
 Note: the ragged amplitudes on the pulse waveforms are both digital aliasing between scope sampling and sampled RF, and also noise due to two successive sets of 1/100 attenuation.

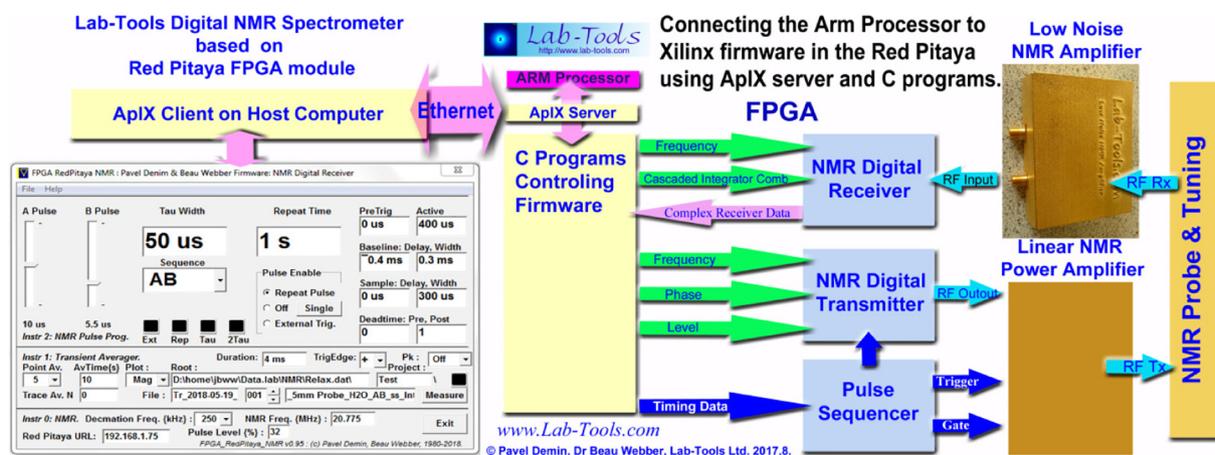


Fig. 8. Overall block diagram of Red Pitaya based Digital liquids NMR Spectrometer.

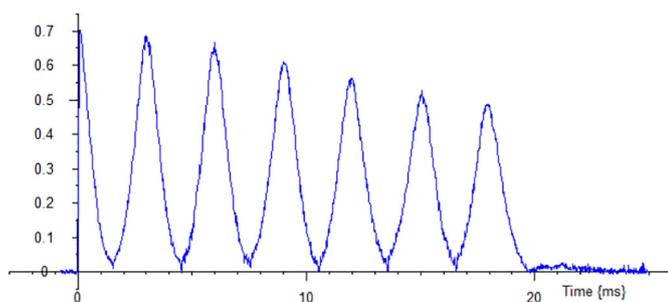


Fig. 9. A single-shot CP/MG echo train for the liquids spectrometer.

4.2. Solids NMR relaxation spectrometer & results

The Lab-Tools solids digital NMR spectrometer also uses the Lab-Tools low-noise amplifier, plugged into a Red Pitaya Xilinx FPGA module, again running the AplX Server, and Lab-Tools' c programs. Currently the Lab-Tools digital switching transmitter module is plugged into an Altera Cyclone II FPGA module, which has a copy of the NMR pulse programmer firmware, receives the trigger pulse from the Red Pitaya and then generates the required NMR pulse waveforms.

This FPGA produces a clock waveform at four times the NMR frequency, and the signals go to phase shifting firmware, gating firmware and firmware that produces the necessary complementary waveform to drive the digital transmitter module. The digital transmitter works well up to at least 30 MHz. For test purposes this transmitter module was plugged into the FPGA module, but this limited the power that could be applied, due to the high circulating RF currents. However NMR signals have been successfully captured with this system. The Digital NMR



Fig. 11. Digital NMR Transmitter under test in 3D printed metal box (1 cm grid).

Transmitter is now being mounted in a very solid 3D printed metal enclosure, and further evaluation will then take place.

5. Conclusion

The key advances being targeted were a significant reduction in size, weight and physical complexity for NMR Receivers and NMR Transmitters, as well as a reduction in cost, so as to allow NMR Relaxation and NMR Cryoporometry to become much more common techniques in commercial laboratories, university laboratories, and even possibly schools. In conclusion, while the final development is still on-going, this original goal of a new highly compact, low-cost and stable NMR relaxation spectrometer design, for desk-top and field use,

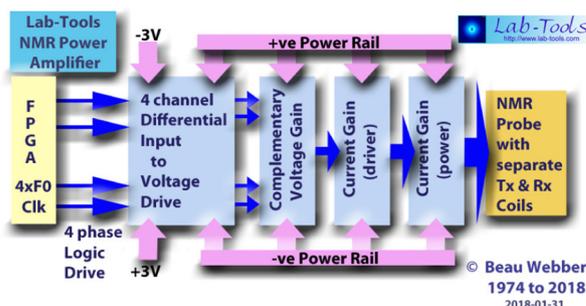
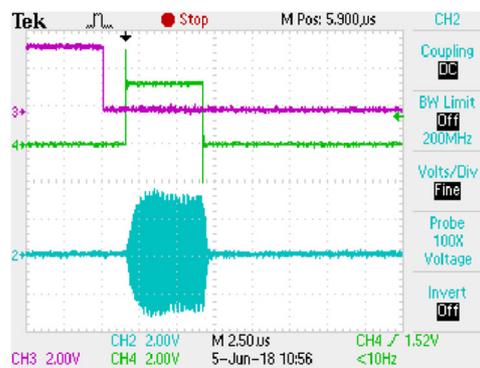


Fig. 10. Left: Digital Power RF Transmitter block diagram. Right: Ch2, Cyan: Preliminary test 20.7 MHz RF pulse into RF probe, at 1/100 monitor across tuning capacitor. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



based on digital firmware in Field Programmable Gate Arrays, has been realised. One of the receivers is in 24/7 use in the Lab-Tools NMR Cryoporometer and is indeed proving to be highly stable. The liquids transmitter module has given good NMR signals, as has the solids transmitter module. Final casing of the transmitter modules is currently underway. Consideration throughout has also been given to their application in a low-cost NMR Cryoporometric instrument for measuring pore-size distributions, which is an on-going part of the final development.

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