

NMR-It guide

NMR-It is a user interface for the LabTools NMR system ¹

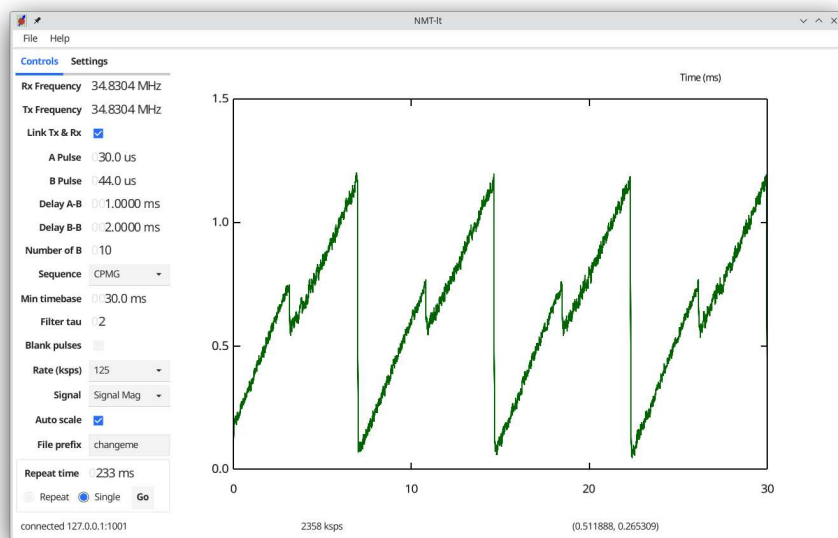


Figure 1: Screenshot of NMR-It

Mouse controls

The numerical controls can be adjusted using the mouse scroll wheel, while pointing at the desired digit, or by selecting the number and using the keyboard arrow keys.

The scroll wheel zooms in to the data plot. Click the middle button to revert to a full view. Click and drag on the plot to get a numerical readout of the coordinates at the bottom of the window.

Controls tab

Tx Frequency This controls the pulses applied to the sample by the transmitter. These should be at the Larmor frequency, $f_L = \frac{\gamma B}{2\pi}$, where B is the field of the permanent magnet, and γ is the gyromagnetic ratio of the proton. Once the Tx frequency is close enough to get a response from the sample, it is easiest to fine tune the receiver before copying its frequency to the transmitter.

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Rx Frequency This controls the centre frequency of the receiver. It should also be set to the Larmor frequency. If it is slightly mis-tuned while looking at an NMR resonance, the signal *magnitude* will be unaltered. However, the phase and quadrature components of the signal will show beats at the difference frequency $f_L - f_{Rx}$. Adjust the Rx frequency until the beat frequency is zero, then copy this value to the transmitter by selecting **Link Tx & Rx**

Link Tx & Rx When selected, this adjusts the transmitter frequency to that of the receiver, and keeps them equal thereafter.

A pulse This determines the duration of the first pulse of a sequence (typically, the $\pi/2$ pulse)

B pulse This determines the duration of all pulses after the first pulse of a sequence (typically, the π pulses)

Delay A-B Time between the A pulse and the first B pulse

Delay B-B Time between successive B pulses, if more than one.

Number of B Determines the number of B pulses. Typically just one to see the Hahn spin echo, or many for a CPMG or more sophisticated sequence.

Sequence This determines the relationship between the phases of the A and B pulses. In the table below, 0, 90, 180 etc. are phases in degrees of the Tx frequency. . . . means repeat from the beginning until all B pulses have finished.

Name	A phase	B phases
CP	0	0, . . .
CPMG	0	90, . . .
x-XY4	0	0, 90, . . .
y-XY4	90	0, 90, . . .
x-XY8	0	0, 90, 0, 90, 90, 0, 90, 0, . . .
y-XY8	90	0, 90, 0, 90, 90, 0, 90, 0, . . .
x-XY16	0	0, 90, 0, 90, 90, 0, 90, 0, 180, 270, 180, 270, 270, 180, 270, 180, . . .
y-XY16	0	0, 90, 0, 90, 90, 0, 90, 0, 180, 270, 180, 270, 270, 180, 270, 180, . . .

CP is from Carr and Purcell², CPMG is from Meiboom and Gill³, and the others are from Gullion et al.⁴ The sequences are intended to preserve the magnetisation of the spins, in the presence of perturbations arising from variation in the field and the precision of the pulses.

²HY Carr and EM Purcell, Phys. Rev. **94** 630 (1954)

³S Meiboom and D Gill, Rev. Sci. Inst. **29** 688 (1958)

⁴T Gullion, DB Baker and MS Conradi, J. Mag. Res. **89** 479 (1990)

Min Timebase In general, the duration of the plotted data is automatically adjusted to accommodate all the B pulses. This control sets a minimum duration that is applied to shorter sequences.

Filter tau The received data are always decimated to no more than 10,000 - 20,000 points, which provides some time averaging at high sample rates. This control provides additional single-pole low pass filtering with a time contrast tau measured in samples. When tau = 0, this filter is inactive.

Blank pulses This setting zeros the data during the pulses, to remove the distracting high spikes caused by breakthrough from transmitter to receiver. To be effective, the pre-blank and post-blank times on the Settings tab need to be adjusted, along with the Trim samples and Fudge timing settings.

Rate (ksps) This sets the receiver sample rate in thousands of samples per second.

Signal This selects which component of the receiver signal is displayed; all components are always acquired, and you can switch between the components after acquisition. The receiver is phase sensitive, so separate in-phase, p and quadrature, q signals are collected, while the magnitude is computed as $\sqrt{p^2 + q^2}$. As well as the signal channel, there is also a pulse receiver, which can be used to verify the transmitter pulses.

Auto scale This switches on and off automatic scaling of the Y axis of the plot. The time axis is autoscaled, as described under Min timebase, above.

File prefix This field sets a prefix for the file names that are proposed by the file saving dialogs.

Repeat time This sets the time between repetitions of the pulse sequence, when Repeat mode is selected.

Repeat/Single/Go In Single mode, one pulse sequence is performed when the Go button is clicked. In Repeat mode, the sequence is repeated after the interval set by repeat time.

Settings tab

Hardware IP This sets the network address of the Spectrometer hardware. If the hardware is not responding, The application attempts to reconnect every two seconds until it succeeds. The connection status is shown at the bottom left of the window.

Trim samples The hardware produces a number of invalid samples at the start of each sequence, while its data processing pipeline initialises. This control removes these samples.

Fudge Rx timing This can help to align the timing of the pulse blanking intervals (see Blank pulses, on the Controls tab) with the position of the

actual pulses. Trim samples and Fudge together offset and stretch the blanking schedule.

Prepulse time This sets an initial delay between the start of data acquisition and the start of the A pulse.

Pre-blank / Post-blank time These extend the duration of the pulse blanking before and after the duration of the pulses. Post-blanking accounts for the recovery time of the receiver after it has been overwhelmed by the transmitted pulse; pre-blanking can help if the Trim and Fudge settings are not quite right.

Menus

The **File** menu allows the saving and loading of all settings, the data currently on the display (as a CSV file), and saving a PDF file containing either one or two copies of the currently displayed data.

The **Help** menu provides information about the version of the application, and a **Crash** function. Guess what that does.

About the system

The digital transmitter and receiver is by Pavel Demin⁵, based on the Red Pitaya FPGA board⁶. The analog hardware is by Lab Tools⁷. The NMR-It application is loosely based on the De Luxe NMR system⁸, itself based on an earlier FPGA design of Pavel's.

⁵https://github.com/pavel-demin/red-pitaya-notes/tree/master/projects/pulsed_nmr

⁶<https://redpitaya.com/>

⁷<http://www.lab-tools.com/lab-tools.html>

⁸MSC