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Master Thesis: Building a 25 MHz NMR Spectrometer

Maximilian Stabel

September 12, 2023

ETH Zürich

2023-09-12 magnETHical

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"What I cannot create, I do not understand"

—Richard Feynman

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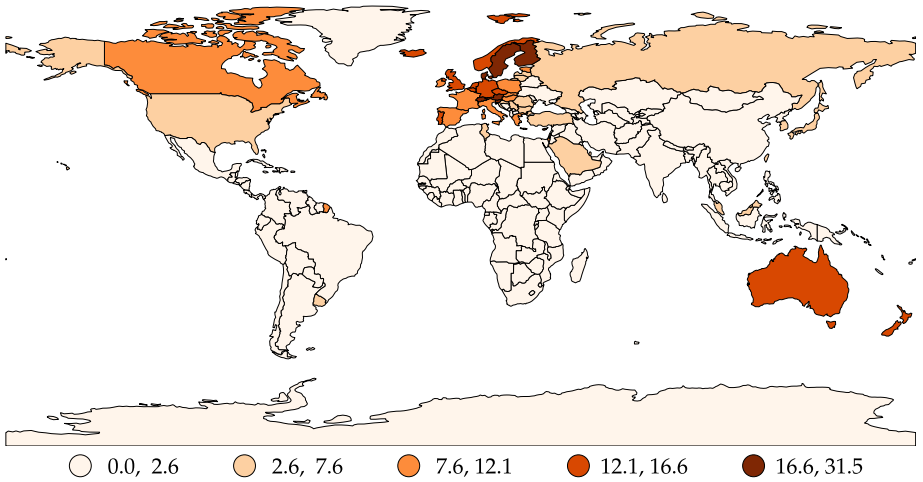
"What I cannot create, I do not understand"

—Richard Feynman

1. In the spirit of Richard Feynman…
2. My master thesis is about building an NMR spectrometer
3. I'm Max and I'll be your host for today
4. Speaking of understanding…

There is not a lot of NMR research in the Global South



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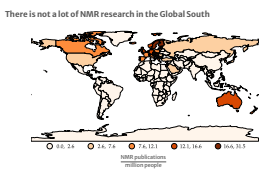

Reminder: What is NMR spectrometer

Nuclear Magnetic Resonance

- Nuclei absorb radio waves at a certain frequency when inside a magnetic field
- The nuclei emit radio waves at that same frequency when excited this way
- $f \sim B_0$ and surroundings

- You: Understanding for own experiments
- The better we know the better we can use
- Push NMR development — better machines
- Transition: if not about you personally — more globally: applications

Nuclear Magnetic Resonance
- Nuclei absorb radio waves at a certain frequency when inside a magnetic field
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NMR is used across various fields

- Research (Structure Analysis, Drug Discovery, ...)
- Medicine (Imaging, Diagnosis, ...)
- Industry (Process Control, Drug screening, ...)
- Education (Quantum Mechanics, Quantum Computing, ...)

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1. Some of you already know, but here are some reasons why NMR is useful

Build an accessible NMR spectrometer

1. **The goal of my thesis was...**

Preview

Preview

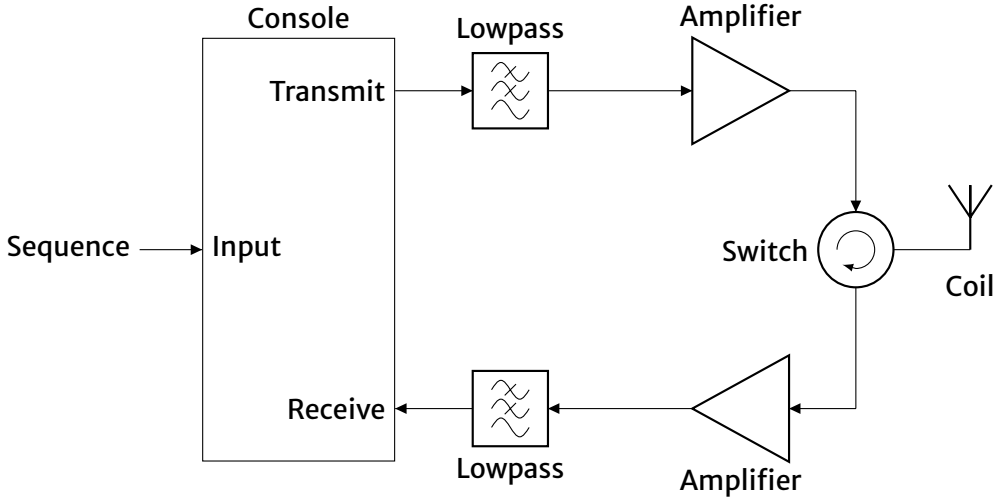
The parts

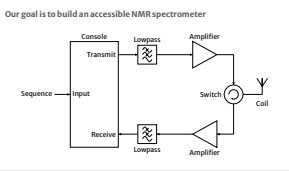
The complete setup

Experimental Results

THE PARTS

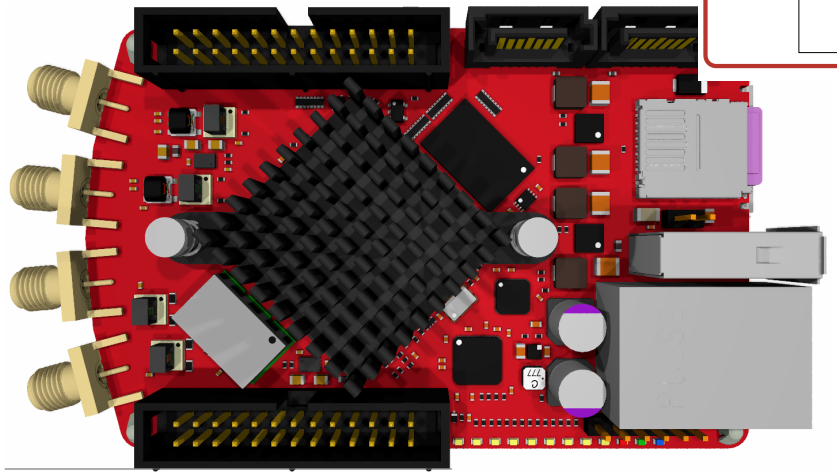
Our goal is to build an accessible NMR spectrometer

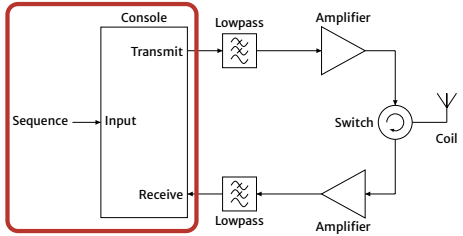




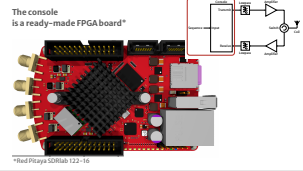
1. Go through the parts left to right
2. Our switch only, others might include more analog processing

The console is a ready-made FPGA board*



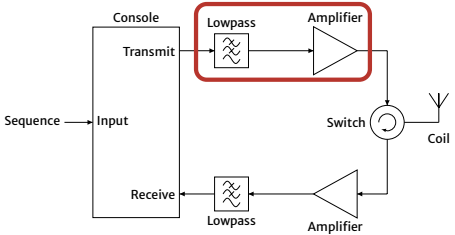


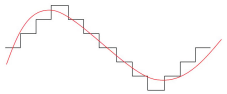
*Red Pitaya SDRlab 122-16

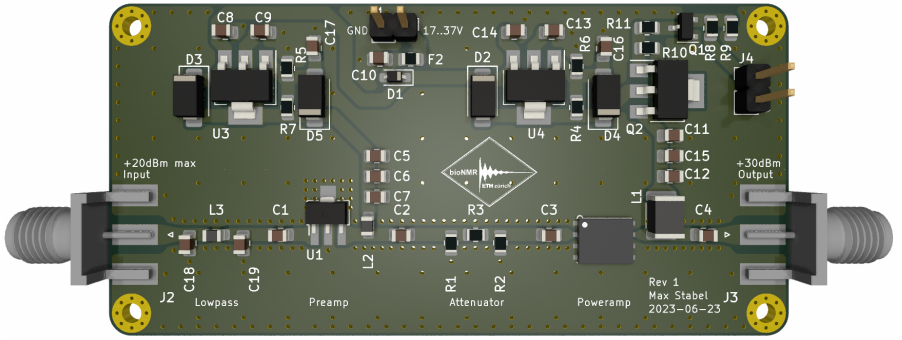


1. FPGA == programmable hardware, very fast
2. oversampling
3. CIC filter (decimation, low pass filter, moving average)
4. The signal needs to be filtered and then amplified: Next Slide

The power amplifier has two stages







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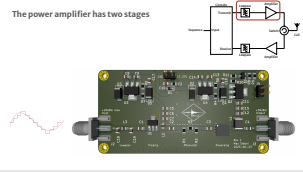
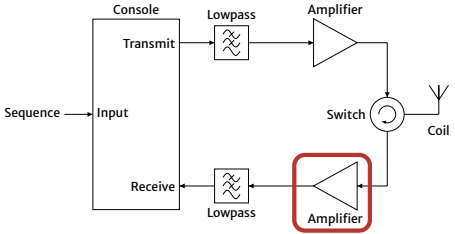
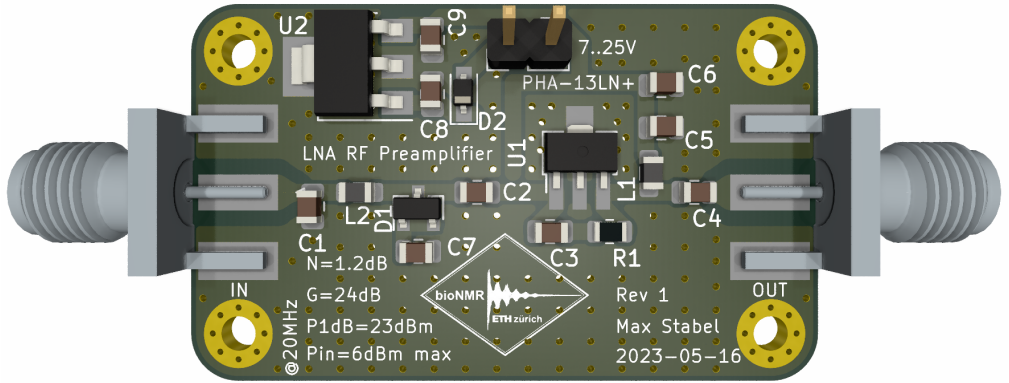
The parts

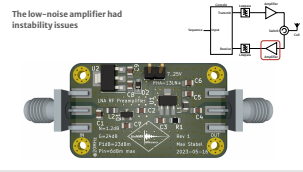


1. We want cheap, so using a simple is the obvious first approach
2. Unfortunately there's a lot to do:
   - Input/Output Impedance Matching
   - Bias Tee
   - DC coupling
   - stability calculations
   - feedback
   - temperature compensation (current feedback)
3. A complete amplifier is quite expensive
4. Solution: Use monolithic (integrated) amplifier
5. Take care of heat dissipation (Class-A)
6. dB is logarithmic unit

The low-noise amplifier had instability issues

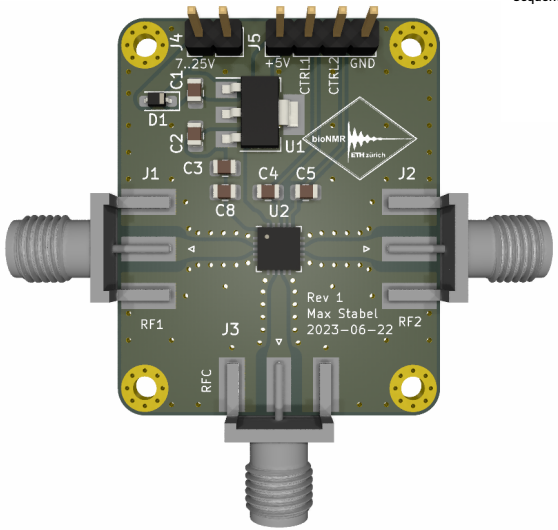


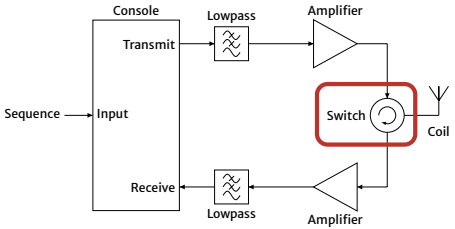


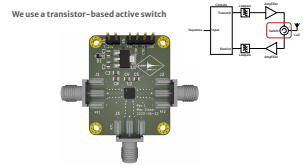


1. Low-noise
2. Feedback loop — stray capacitance
3. Solution: Smaller housing, shorter loop
4. We need 3x for enough gain

We use a transistor-based active switch

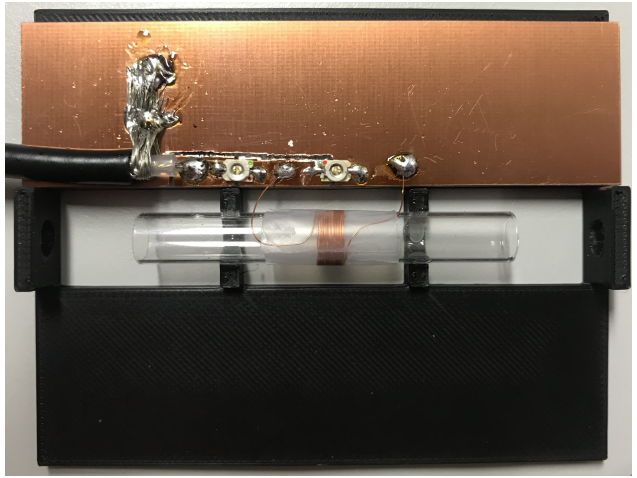


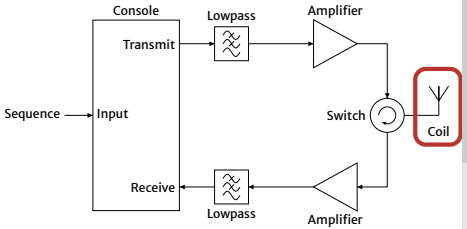


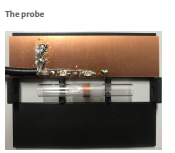


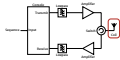
1. Active
2. Isolation: 60 dB
3. Silicon-on-insulator (not pHEMT GaAs) i.e. FET tech, not PIN-Diode
4. PIN-Diode switch also possible, but
   - usually higher leakage
   - slower switching
   - harder to integrate on a chip
   - but higher power capabilities

The probe



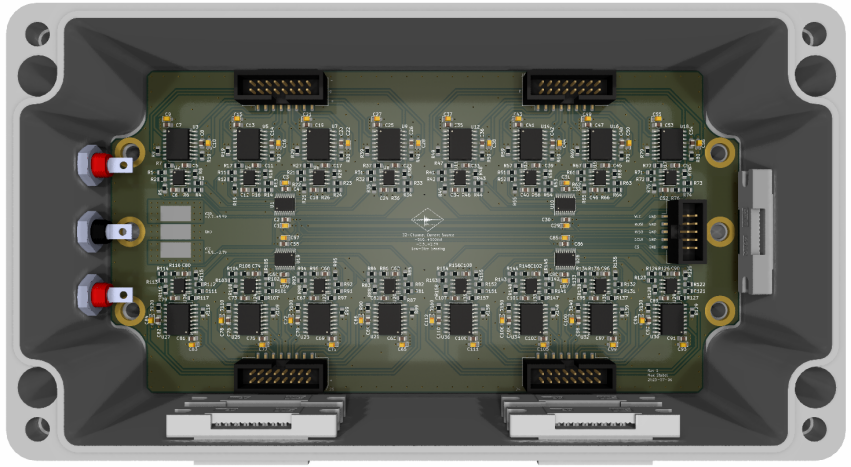






1. Many turns — high inductance — low capacitance — sensitive to stray capacitance

A 32-channel current supply is designed but untested



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The complete setup

Our NMR is affordable ...

	600 MHz‡	mini-circuits	*magnETHical*
Power Amplifier	50 000	323.49	36.01
Switch	-	82.06	20.05
Probe	100 000	-	≈15.00
Low-Noise Amplifier	50 000	409.38	73.11
Shim Driver	-	-	257.08
Console	200 000	-	662.53
Magnet	1 000 000	-	≈9000.00
Sum			**10 142.80**

‡estimated costs
Prices incl. VAT [CHF]

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	Superconducting	Benchtop	*magnETHical*
Price [k CHF]	200–18 000	50–150	≈10
Frequency [MHz]	300–1200	40–125	25
Resolution [Hz]	≈0.2	0.2–1	≈2.5/50[†]
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[†]with/without shims
For 5mm standard NMR tubes

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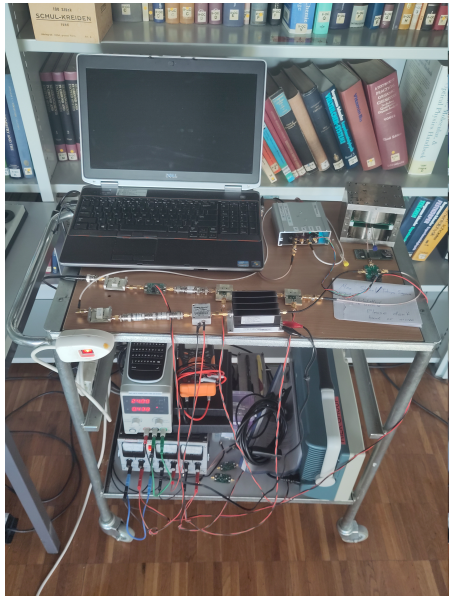
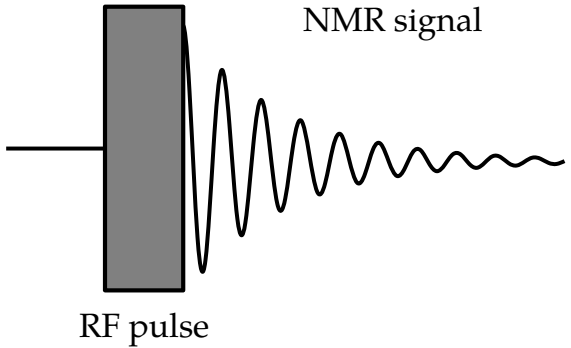


… and portable

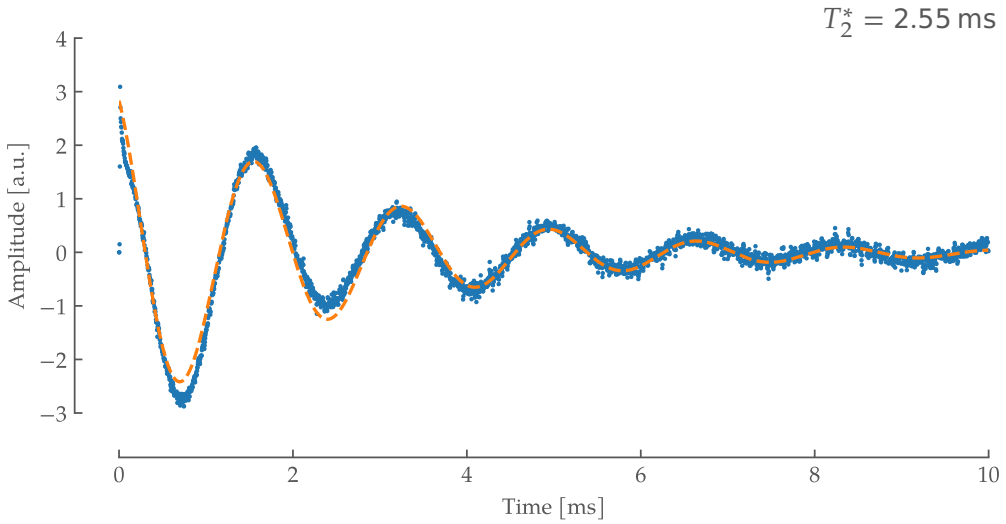
Experimental Results

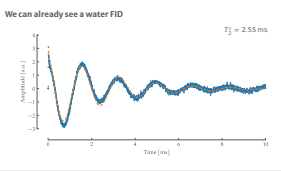
Simple Pulse Sequence



Simple Pulse Sequence
NMR signal
RF pulse

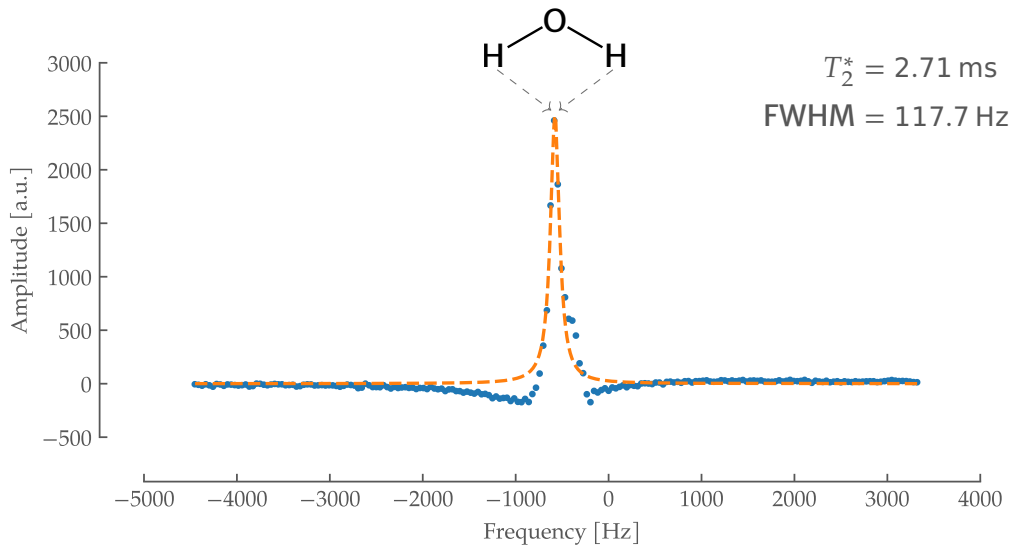
We can already see a water FID

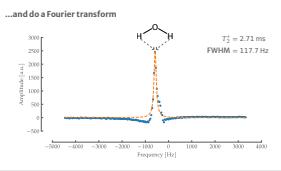




1. Outliers at the beginning are due to CIC filters

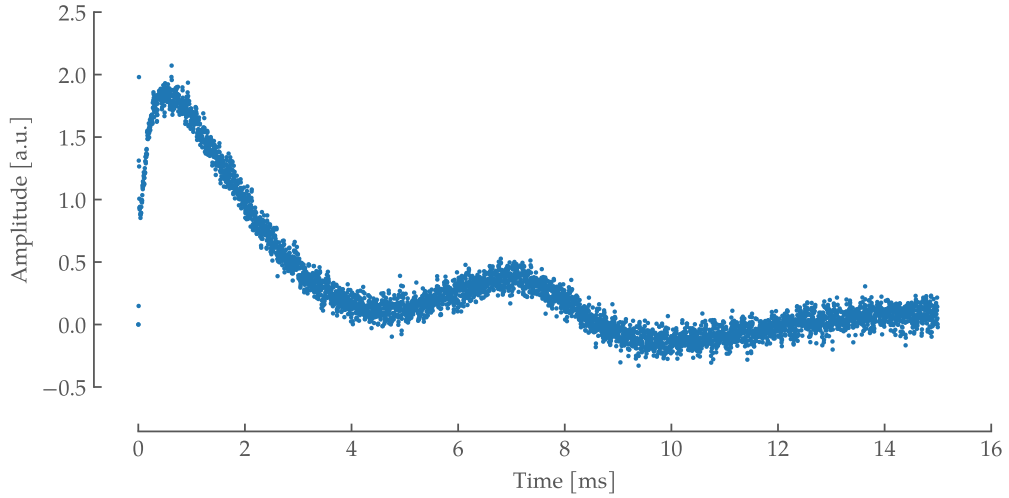
...and do a Fourier transform

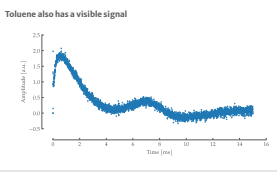




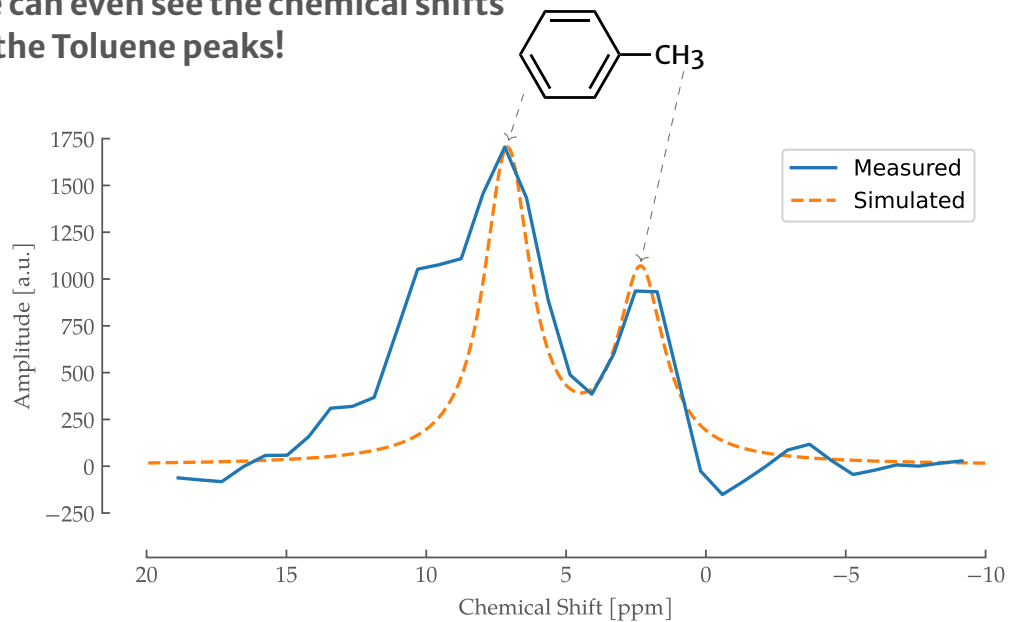
1. Not Lorentz because of missing shimming/inhomogeneities
2. Measured input signal of -92dBm/15.8uV resulted in amplitude of 2200
3. SNR of around 350, With FWHM 2.5Hz/1ppm we estimate snr of 11000

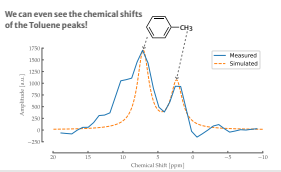
Toluene also has a visible signal





We can even see the chemical shifts of the Toluene peaks!

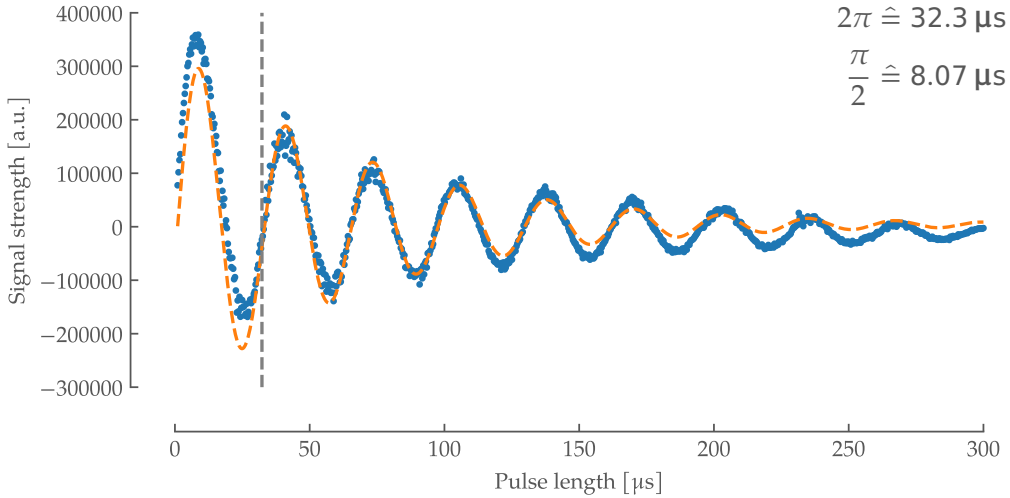


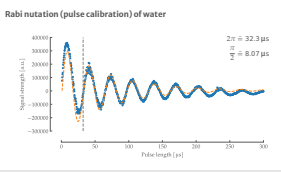


It's a full tube of toluene, not a solution

1. Reasons for sidepeak: no apodization (truncation of FID), no shimming, inhomogeneities/not centred

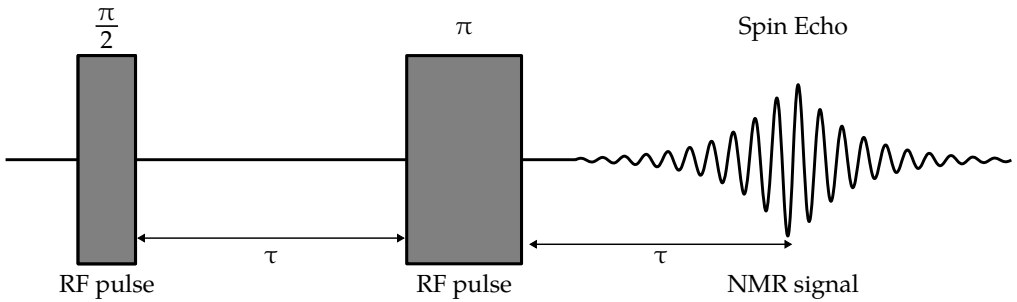
Rabi nutation (pulse calibration) of water

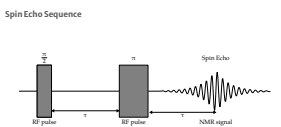




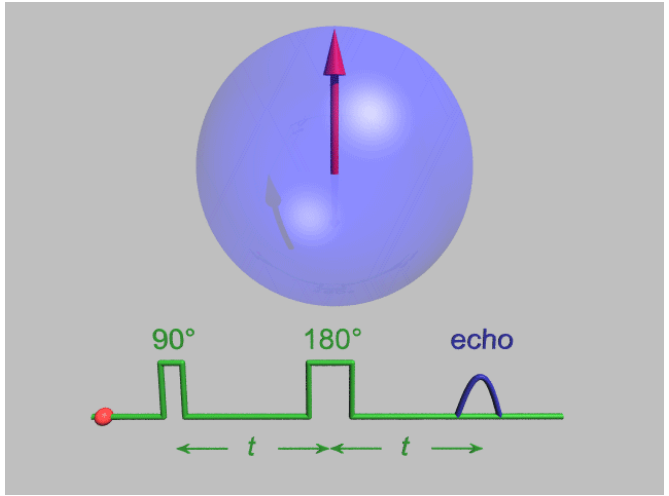
1. $T_{period} = 32\,\mu s$
2. $T_{\frac{\pi}{2}} = 8\,\mu s$

Spin Echo Sequence



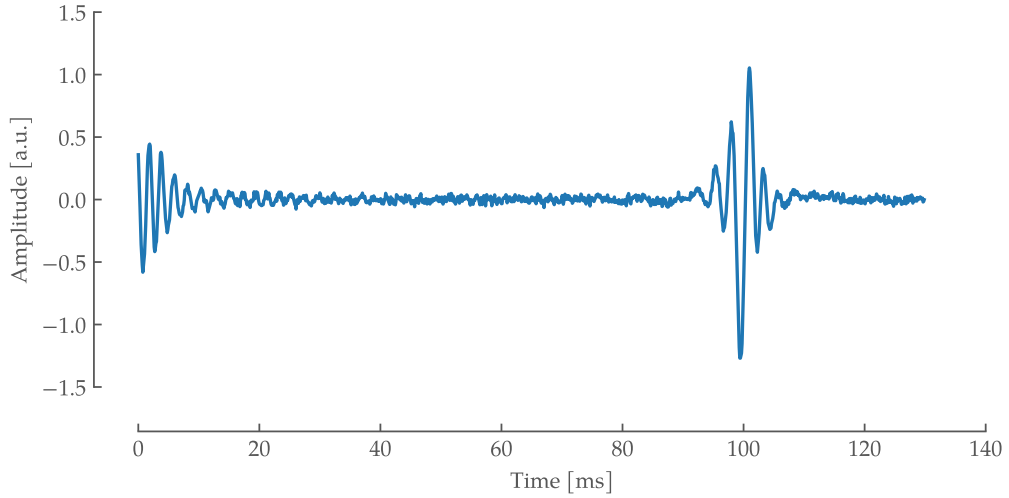


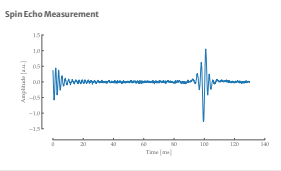
Spin Echo Animation



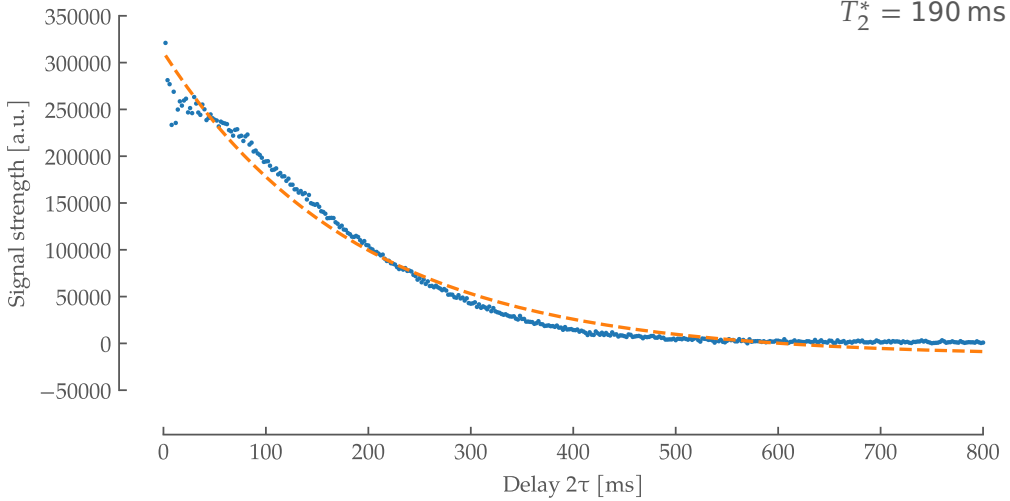
Spin Echo Animation

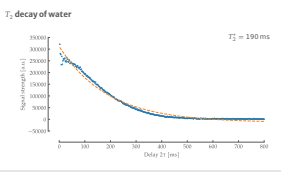
Spin Echo Measurement





T_2 decay of water





1. $T_2 =$

Demo time!

Demo time!

Review

- Why?
- The parts
  - Console
  - Amplifiers
  - Switch
  - Probe
- Capture & Process Software
- Experimental Results
- Demonstration

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Outlook

- Shim Driver
- Shielding
- Improve any part individually
  - Cheaper Magnet
  - Better Probe
  - Software (CIC compensation filter, frequency adjustment during pulse, ...)
- Investigate temperature stability
- Sell it to NexMR (or do Photo-CIDNP ourselves)

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"I have not yet lost that sense of wonder, and of delight, that this delicate motion should reside in all ordinary things around us, revealing itself only to him who looks for it."

"There the snow lay around my doorstep — great heaps of protons quietly precessing in the Earth's magnetic field."

— E.M. Purcell

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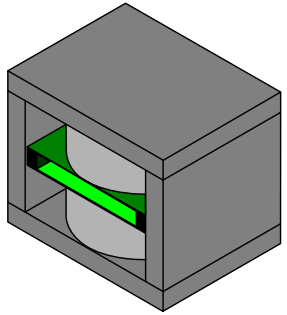
1. Circling back to the beginning, I would like to end with a quote by E.M. Purcell
2. I wouldn't have thought I would get a glimpse of this wonder that Purcell describes when starting my thesis here, but I'm glad I did.
3. And I hope none of you have lost it yet

Thank you!



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Find everything on

https://gitlab.ethz.ch/mstabel/nmr-spectrometer

Thank you!
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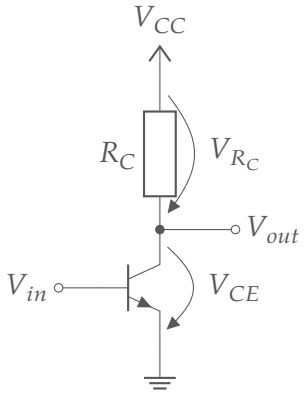
Backup

An amplifier is basically just a transistor

- Transistor:
  voltage-controlled current source
- higher voltage → higher current
  → higher voltage V_{R_C}
  → lower voltage V_{CE}
  → 180° phase shift



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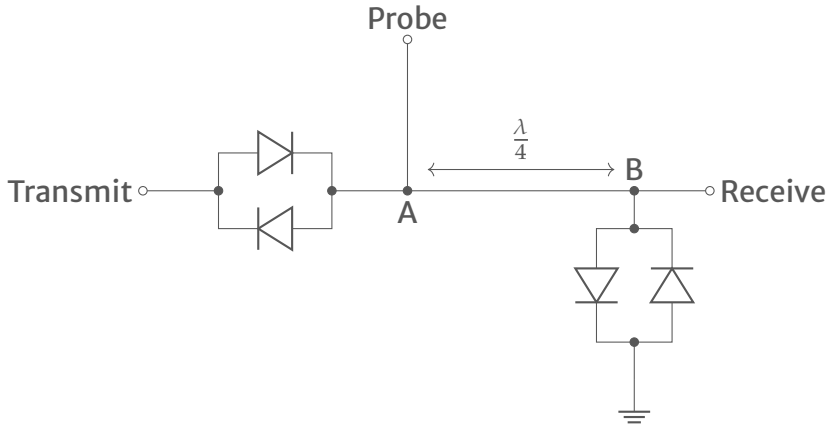
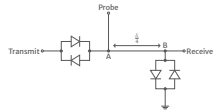
5. Take care of heat dissipation (Class-A)

The passive approach leaked too much power



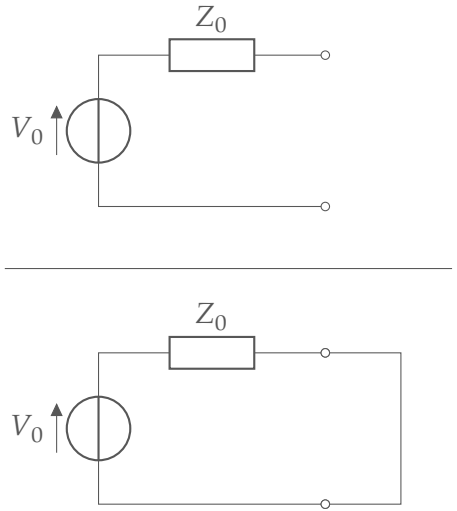
└The passive approach leaked too much power

The passive approach leaked too much power

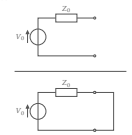


1. So called "video feedthrough"
2. Especially noise during reception phase, leaking through turned off amplifier
3. "Traditional" passive design by Lowe and Tarr
4. Leads to distortion of low-power pulses
5. Same design can be used with PIN-Diodes (effectively current-controlled resistor)
6. But PIN Diodes often need higher frequencies (mid MHz), size of intrinsic semiconductor

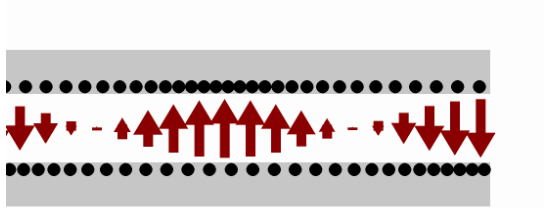
A transmission line transforms impedance

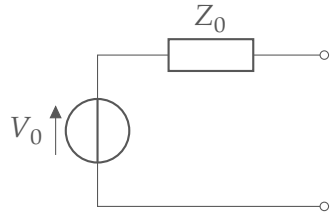


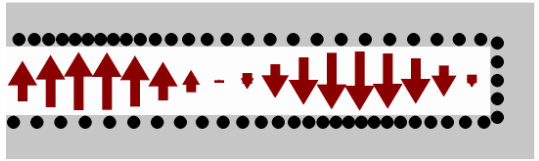
A transmission line transforms impedance

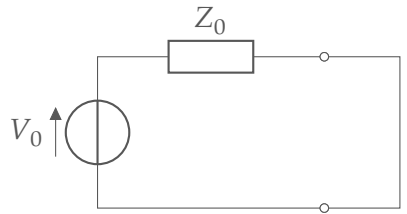


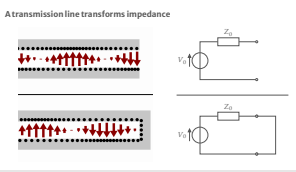
A transmission line transforms impedance



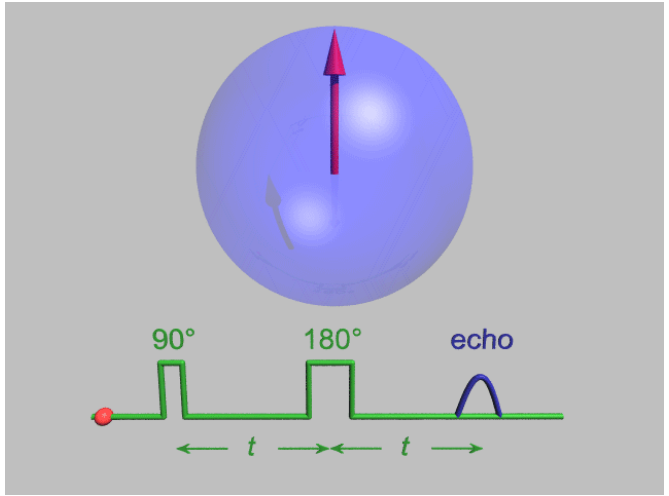






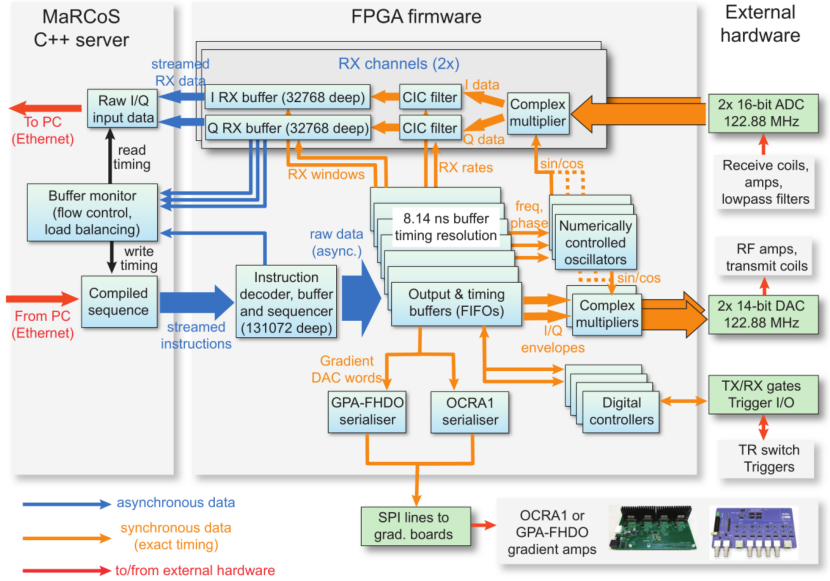


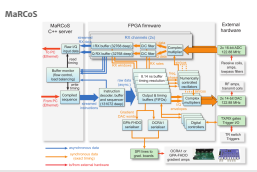
T_2 Decay Animation



T_2 Decay Animation
Gavin Morley — CC BY-SA 3.0

MaRCoS


MaRCoS
C++ server
FPGA firmware
External
hardware
streamed
RX data
RX channels (2x)
I RX buffer (32768 deep)
Q RX buffer (32768 deep)
CIC filter
CIC filter
I data
Q data
Complex
multiplier
2x 16-bit ADC
122.88 MHz
Receive coils,
amps,
lowpass filters
To PC
(Ethernet)
Raw I/Q
input data
read
timing
RX windows
RX rates
sin/cos
Buffer monitor
(flow control,
load balancing)
write
timing
8.14 ns buffer
timing resolution
freq,
phase
Numerically
controlled
oscillators
raw data
(async.)
RF amps,
transmit coils
sin/cos
From PC
(Ethernet)
Compiled
sequence
Instruction
decoder, buffer
and sequencer
(131072 deep)
Output & timing
buffers (FIFOs)
Complex
multipliers
2x 14-bit DAC
122.88 MHz
streamed
instructions
I/Q
envelopes
Gradient
DAC words
GPA-FHDO
serialiser
OCRA1
serialiser
Digital
controllers
TX/RX gates
Trigger I/O
TR switch
Triggers
asynchronous data
synchronous data
(exact timing)
to/from external hardware
SPI lines to
grad. boards
OCRA1 or
GPA-FHDO
gradient amps


MaRCoS