Improved Pulsed RF Signal Generation and Acquisition for NMR Excitation and FID Capture

White Paper

Rev. 1.0

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Document Revision History

Table 1.1 Document Revision History

Revision	Date	Description (Style Table Heading)	Author
1.0	13-Dec-2023	• Original version.	Joan Mercade

Acronyms & Abbreviations

Table 1.2 Acronyms & Abbreviations

Acronym	Description
µs or us	Microseconds
ADC	Analog to Digital Converter
AM	Amplitude Modulation
ASIC	Application-Specific Integrated Circuit
ATE	Automatic Test Equipment
AWG	Arbitrary Waveform Generators
AWT	Arbitrary Waveform Transceiver
BNC	Bayonet Neill–Concelm (coax connector)
BW	Bandwidth
CW	Carrier Wave
DAC	Digital to Analog Converter
dBc	dB/carrier. The power ratio of a signal to a carrier signal, expressed in decibels
dBm	Decibel-Milliwatts. E.g., 0 dBm equals 1.0 mW.
DDC	Digital Down-Converter
DHCP	Dynamic Host Configuration Protocol
DSO	Digital Storage Oscilloscope
DUC	Digital Up-Converter
ENoB	Effective Number of Bits
ESD	Electrostatic Discharge
EVM	Error Vector Magnitude
FPGA	Field-Programmable Gate Arrays
GHz	Gigahertz
GPIB	General Purpose Interface Bus
GS/s	Giga Samples per Second
GUI	Graphical User Interface
HP	Horizontal Pitch (PXIe module horizontal width, 1 HP = 5.08mm)
Hz	Hertz
IF	Intermediate Frequency
I/O	Input / Output
IP	Internet Protocol
IQ	In-phase Quadrature
IVI	Interchangeable Virtual Instrument
JSON	JavaScript Object Notation
kHz	Kilohertz

Acronym	Description
LCD	Liquid Crystal Display
LO	Local Oscillator
MAC	Media Access Control (address)
MDR	Mini D Ribbon (connector)
MHz	Megahertz
MIMO	Multiple-Input Multiple-Output
ms	Milliseconds
NCO	Numerically Controlled Oscillator
NMR	Nuclear Magnetic Resonance
ns	Nanoseconds
PC	Personal Computer
PCAP	Projected Capacitive Touch Panel
PCB	Printed Circuit Board
PCI	Peripheral Component Interconnect
PRBS	Pseudorandom Binary Sequence
PRI	Pulse Repetition Interval
PXI	PCI eXtension for Instrumentation
PXIe	PCI Express eXtension for Instrumentation
QC	Quantum Computing
Qubits	Quantum bits
RADAR	Radio Detection And Ranging
R&D	Research & Development
RF	Radio Frequency
RT-DSO	Real-Time Digital Oscilloscope
s	Seconds
SA	Spectrum Analyzer
SCPI	Standard Commands for Programmable Instruments
SFDR	Spurious Free Dynamic Range
SFP	Software Front Panel
SMA	Subminiature version A connector
SMP	Subminiature Push-on connector
SPI	Serial Peripheral Interface
SRAM	Static Random-Access Memory
TFT	Thin Film Transistor
T&M	Test and Measurement
TPS	Test Program Sets
UART	Universal Asynchronous Receiver-Transmitter
USB	Universal Serial Bus
VCP	Virtual COM Port
Vdc	Volts, Direct Current
V p-p	Volts, Peak-to-Peak
VSA	Vector Signal Analyzer
VSG	Vector Signal Generator
WDS	Wave Design Studio

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1 Abstract

The direct to/from RF multi-channel architecture of the Tabor Electronics Proteus AWT (Arbitrary Waveform Transceiver) results in huge improvements in terms of cost, size, and signal-to-noise ratio in multiple application areas. One of those is NMR (Nuclear Magnetic Resonance). The test architectures used in traditional NMR gear use analog modulators and demodulators combined with external elements such as frequency converters, local oscillators, and mixers. The Proteus AWT can replace all these components by implementing all their functionality digitally and remove all the impairments and noise issues attached to traditional NMR gear. This white paper describes the benefits of using the Proteus AWT for NMR applications.

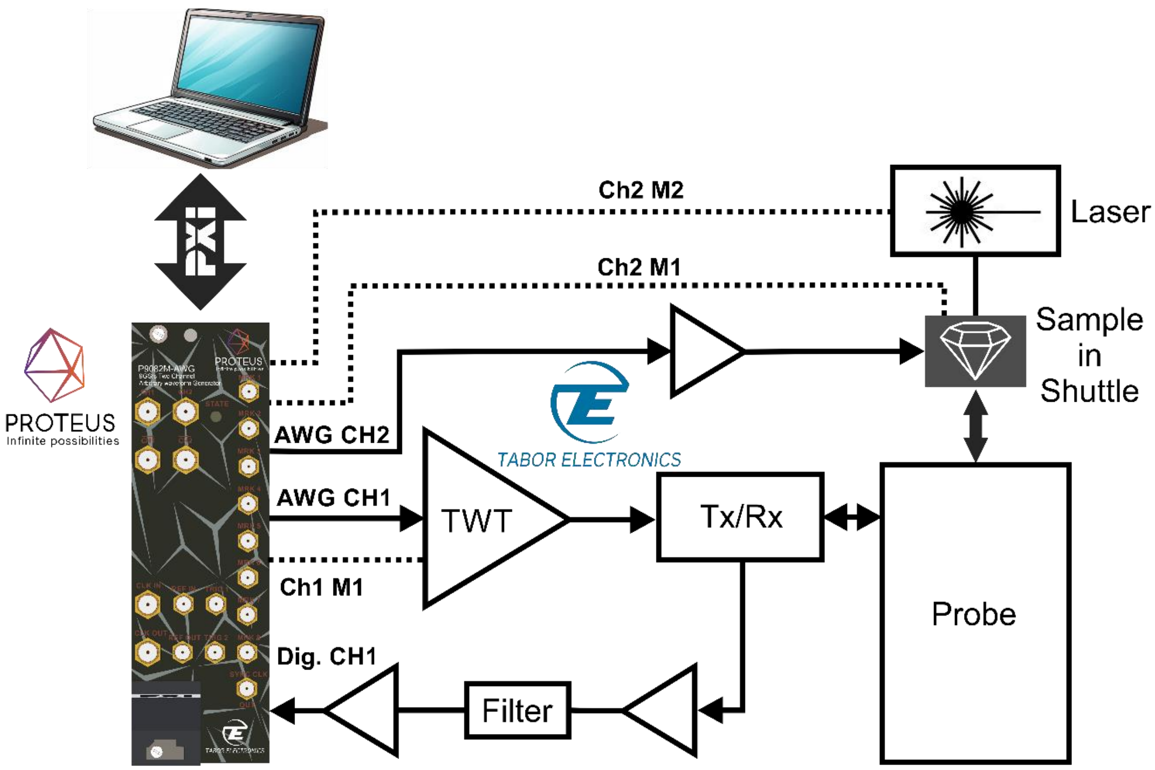

Figure 1.1 Proteus AWT Integrated in an NMR System

The Proteus AWT can be integrated in an NMR system where it can generate the excitation pulses, capture, and process the FID signal coherently with the exciter, and replace the “pulse blaster” controlling the execution of a complete experiment. The improvements achieved in terms of size, speed, signal-to-noise ratio, and cost are significant.

2 Pulsed RF Signal Generation for NMR Excitation

2.1 Introduction

NMR (Nuclear Magnetic Resonance) tests consist in the emission of some RF pulses to some sample while being surrounded by an extremely strong static magnetic field in order to excite transitions between the Zeeman energy levels. The transmitted frequency is that of the resonant frequency associated to the strength of the magnetic field and close to the Larmor frequency. This frequency grows linearly with the intensity of the magnetic field. The response of the sample being analyzed consists in a series of echoes whose amplitude and phase (respect to the transmitted pulse phase) evolves in time in an approximately exponential decay fashion (or FID, Free Induction Decay). The NMR system must read the echoes and estimate the amplitude and sometimes the phase of the echoes.

Excitation of the sample for NMR requires the generation of powerful RF pulses (at frequencies equal to the Larmor frequency) to be transmitted towards the sample. Pulse duration and amplitudes must be calibrated so the right effect on sample polarization is accomplished. Ideally, calibration should find the duration and/or amplitude resulting in 90 degrees shift of the polarization of the sample. Often, calibration consists in finding the amplitudes/durations resulting in a 180- or 360-degrees rotation as zero crossings are easier to detect accurately. The 90 degrees pulse characteristics can be obtained by just dividing the 180 degrees result by two (2) or by four (4) for the 360 degrees results.

Linearity and accuracy of the signal generator is extremely important as any deviation will show up as additional noise in the results. Duration for pulses range typically from a few up to several tens of microseconds while carrier frequency can range from a few tens of MHz up to 1GHz or even more. The traditional approach to the generation of these pulses is combining a CW (Continuous Wave) synthesizer tuned at the target excitation frequency with some modulation hardware, typically a switch or a modulator. This scheme is known as “coherent” as the carrier frequency phase is continuous over time as the synthesizer does not stop operation during the tests. Using an amplitude modulator instead of a switch allows for the control of the duration and amplitude of the excitation RF pulse (and even the shape of the edges) and a much easier calibration of the system. Although analog amplitude modulators can work very well, it may be quite difficult to completely switch off the carrier at the output between active pulses. The residual carrier can inject power into the sample and interfere with the acquisition of the FID signal, adding noise. The ON/OFF ratio can go from 60 to 100dB. Although this number results in the reduction from three to five orders of magnitude, it is important to understand that the excitation pulse may be of hundreds of watts while the FID can be in the microwatt range.

Some NMR systems may require using different excitation channels (1-D, 2-D, 3-D NMR) or different frequencies in each channel (e.g. for proton channel, carbon channel, ion-channel excitation) and or different magnetic field intensity), even during the same experiments. This may be quite challenging for traditional CW Generator/modulator solutions, and typically may require one set of those for each frequency and channel.

2.2 Proteus as the Ultimate Excitation Pulse Generator for NMR Applications

The Tabor Proteus AWT (Arbitrary Waveform Transceiver) family of products are the ideal solution to generate excitation pulses for NMR. It is offered in modular (PXIe) and standalone form factors, and it consists in the combination of a multi-channel RF-Oriented AWG and Digitizer in a single device. The AWG section incorporates up to 4 channels per PXIe Module or up to 12-channels per benchtop or desktop unit. There are models with up to 2.5GS/s or up to 9GS/s and they incorporate two DUC (Digital Up-Converters) per channel. These are some of the specifications and features and how they can improve the usability of this device in the NMR field:

- Continuous frequency range from DC to >9GHz with 30µHz resolution allows for the direct generation of the RF excitation pulses right at the Larmor frequency without the need for any upconverter and local oscillator. Just a power amplifier and some filters may be necessary.
- Multichannel of up to 4 channels per PXIe module allows for the generation of multiple excitation channels simultaneously allowing 1-D, 2-D, and 3-D NMR experiments.
- DUC architecture: Synthesis and modulation of the carrier and the envelopes is performed digitally (Figure 2.1) so accuracy, repeatability, and flexibility are perfect. Both amplitude and phase of the carrier can be controlled with better than 1ns time resolution (111ps after real-time interpolation). ON/OFF ratio is infinite by design as multiplication by the envelope is numerical. Coherence between pulses is preserved as the CW carrier is generated by a free-running NCO that can be set with 30µHz resolution from DC up to 9GHz.
- Two DUCs per channel: This allows for the generation of two sets of excitation pulses at two completely different frequencies through the same channel over the full tuning range while preserving the coherence for both carriers.
- Reduced waveform size for the envelope waveforms as real-time interpolation is applied as part of the numerical up-conversion (Figure 2.2). The 16 GSample memory combined with advanced sequencing capabilities allows for the complete automation of test with durations ranging from a few microseconds to hours or even days.
- Availability of 8 markers (digital outputs) per module (24 per benchtop unit) to control external devices. These outputs are synchronous with the pulse generators and are also controlled by the sequencer. These outputs can be used as a replacement for the “pulse blaster” consoles used in typical NMR systems.

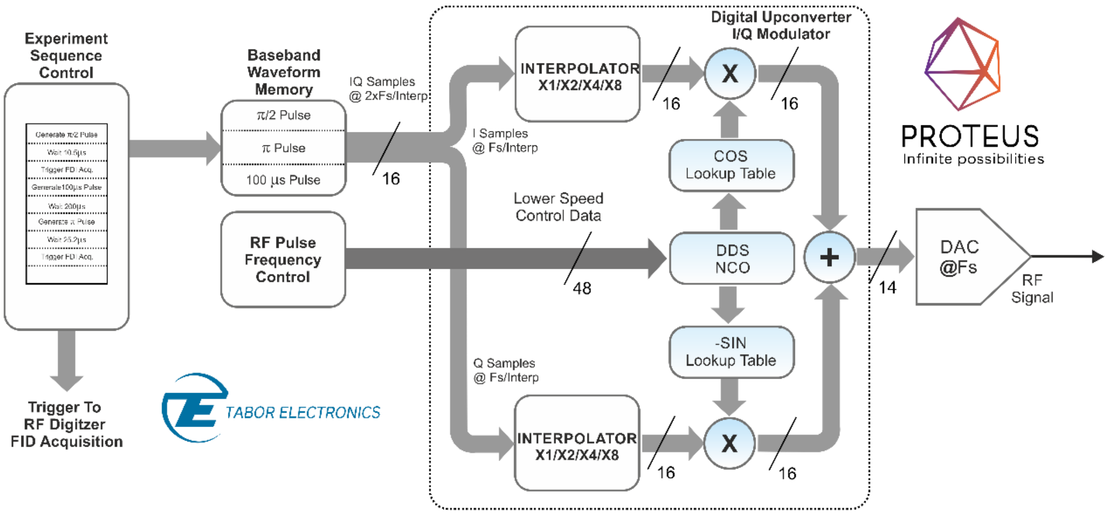

Figure 2.1 Proteus AWG Channels Block Diagram

This is the simplified block diagram of one of the AWG channels in Proteus. Just one of the two DUCs (Digital Up-Converter) is shown for simplicity. The full digital architecture of the DUC results in perfect linearity, high-resolution independent control of pulse characteristics and carrier frequency, coherent operation, ideal ON/OFF ratio, and excellent spectral purity at the output. The embedded real-time sequencer allows for the full automation with sub-microsecond resolution of any experiment involving any number of channels, including the control of mechanical components in the system through the associated digital marker outputs.

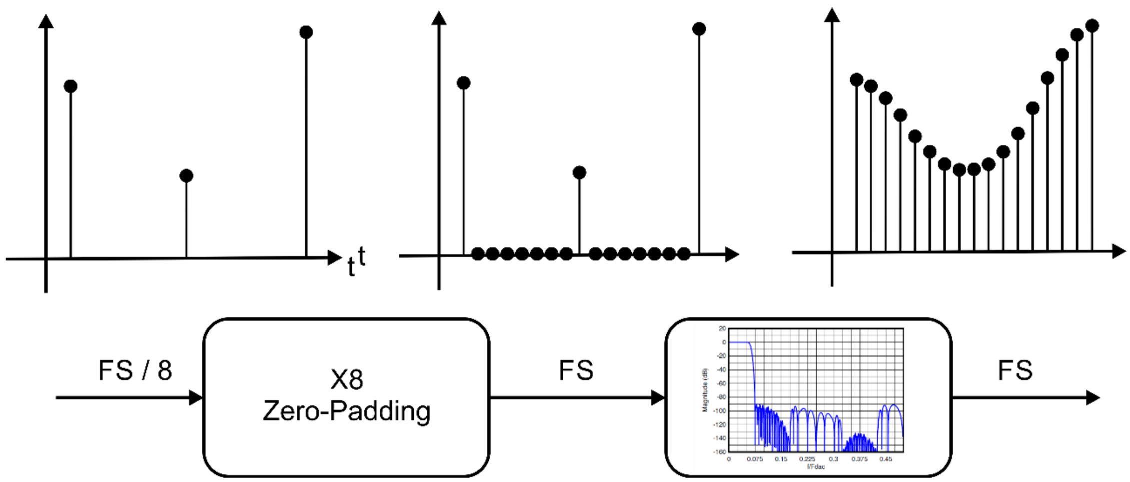

Figure 2.2 Real Time Interpolation of the Pulse Envelope Waveform

Real Time Interpolation of the pulse envelope waveform in Proteus results in simplified, shorter waveforms. The interpolation process allows for the definition of pulses with better than 1ns resolution and controlling the shape of the edges to limit interference and noise. The interpolator increases the timing resolution to 111ps so the DAC can work at the maximum speed so signal quality and image attenuation is optimized.

2.3 Acquisition of FID Signals

The traditional way to capture FID signals is by mixing the response from the sample with two quadrature carriers derived from the same synthesizer used to generate the excitation pulses. These carriers must have a 90 degrees phase difference and they must be applied to phase-sensitive detectors (basically mixers) as shown in Figure 2.3. The output of these two detectors (I, or In-phase, and Q, or Quadrature) can be handled as a complex signal. The instantaneous amplitude will be the module of the complex signal, while the phase can be obtained by calculating the four-quadrant arc-tangent to the IQ signal pair. Generally speaking, the output will consist in an amplitude decaying exponentially in a period up to several seconds long, and a phase-rotation caused by the difference between the actual output frequency of the sample and the carrier frequency being set for the excitation pulses (Figure 2.4). The output of the detectors should be filtered out to remove noise. However, any imbalance of difference between the I and Q signals will show up as noise in the measurement system, reducing accuracy. Linearity of the phase-sensitive detectors is especially important here as AM/AM and AM/PM distortion can also affect the accuracy of the system.

The above scheme may be a very simplified scheme. Actual FID acquisition systems can consist in super-heterodyne receivers where additional mixers and L.O. (Local Oscillator) may add additional non-linearities, impairments, and noise, including phase-noise. Noise figures for active downconverters can be quite high (10 to 25dB) when compared to Low-Noise Amplifiers (LNA). Passive mixers may offer a better noise figure but with a much higher conversion loss. Given the low power of FID signals, noise budget is an important issue.

The availability of high-resolution, high-speed digitizers makes possible the implementation of the FID acquisition system without using the quadrature phase-sensitive detectors described above. Instead, a fast enough ADC can acquire the FID signal directly or at some IF (Intermediate Frequency) after down-conversion (or up-conversion in some cases). If sampled at enough speed, all the information relative to the FID signal can be captured and recovered. Under this scheme, the FID signal is sampled at a high enough sampling rate (e.g. > 2.5 x Larmor Frequency) after applying a good enough antialiasing filter at the input. This filter must be tuned for each sampling rate and sampling rate should be selected according to the target Larmor frequency. This solution seems to be near ideal on paper. However, there are several issues that must be addressed. The first one is the amount of data to be captured for each FDI signal. For a Larmor frequency of 500MHz, and a sample rate of 1.25GS/s, a 10 seconds acquisition will require 12.5GSamples of memory. This information must be stored for further analysis as often processing time will be much larger than the time between two consecutive FID signals. At the end, the acquired samples must be transferred from the digitizer (if enough internal memory is available) to some computer and stored in some hard drive for later processing and analysis. Transferring such a big waveform to an external computer can take a very long time so this will reduce the throughput of the system or the time resolution for the results. The only way to solve this issue is by performing some data reduction in real-time through the usage of proprietary HW implemented in an ASIC or FPGA. The real-time analysis can consist in implementing the phase-sensitive demodulation of the incoming FID signal digitally. The first step of this process consists in mixing the carrier of the FID signal with the carrier of the excitation pulses. However, the only way to get this carrier is by acquiring it through a separate digitizer channel, doubling the memory and throughput limitations of the system. It would be possible to synthesize internally a virtual carrier with a near perfect frequency, but the relative phase information would be lost. Using the FFT as a filter to capture then amplitude and phase (and the delta frequency) of the acquired FID signal is possible although it may be extremely difficult and slow to obtain the required frequency resolution.

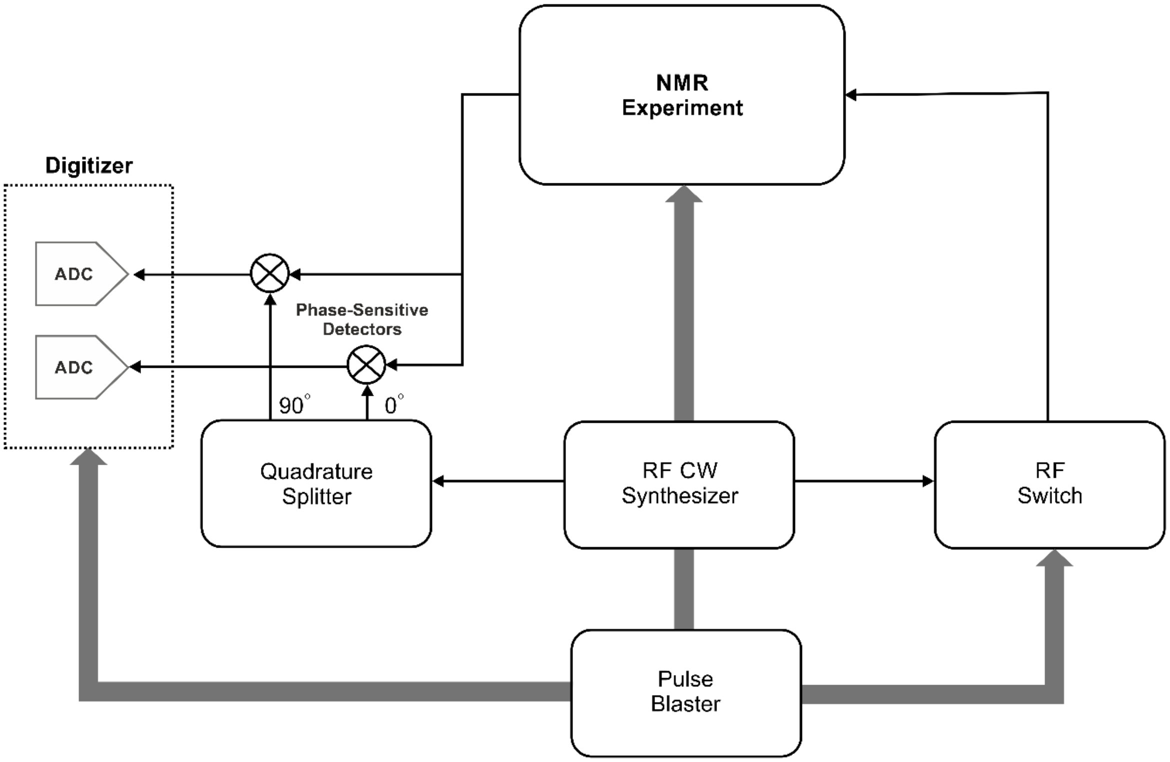

Figure 2.3 Traditional FID Complex Waveform Acquisition

Traditional NMR FID acquisition is made through two phase-sensitive detectors fed the signal coming out from the NMR probe and two quadrature CW signals derived from the same RF synthesizer used for excitation. The output of both detectors (I and Q) is acquired by two ADC and the decay, frequency, and phase characteristics of the output RF signal can be established. Any deviation from ideal alignment for detectors, quadrature of the carriers, skew, and detector linearity will result in errors in the measurements. The Proteus AWT system can implement all the blocks shown fully using digital techniques so component impairments and non-linearities can be removed from the NMR system.

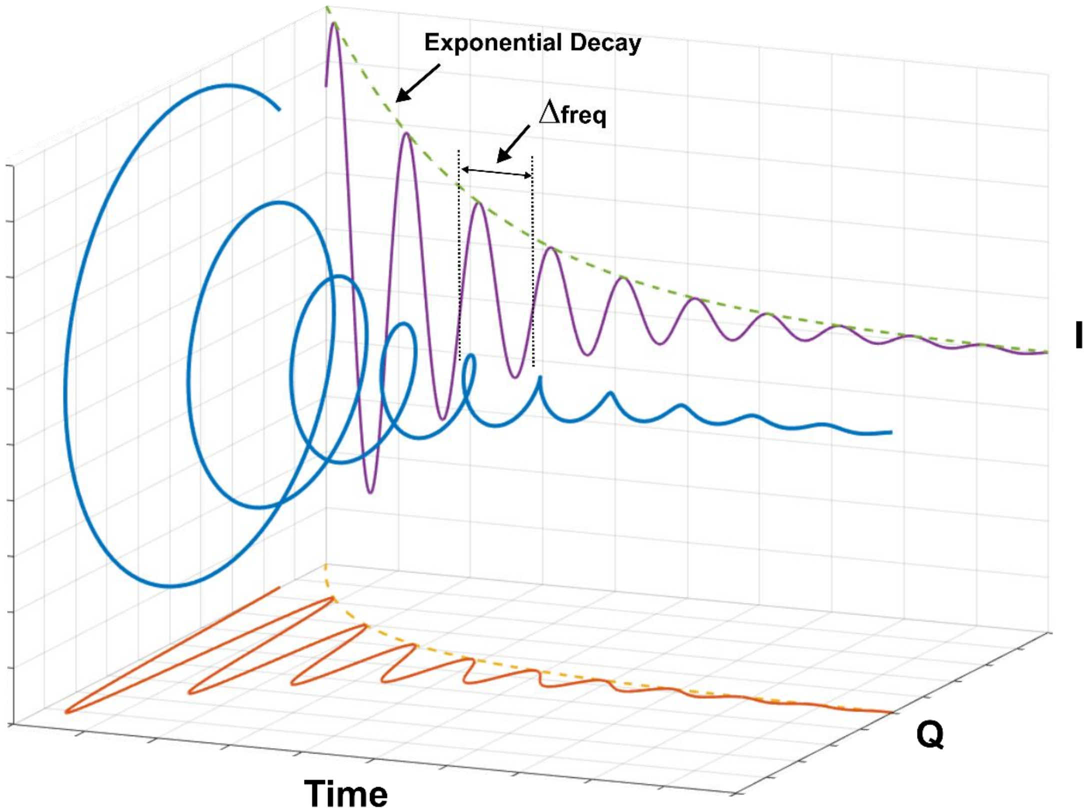

Figure 2.4 FID Raw Signal

The FID raw signal consists of a decaying RF pulse with a frequency close to the one of the excitation RF pulse. The output of the two phase-sensitive detectors carries all the information about the amplitude of the RF signal, the exponential decay it experiences, and the relative phase respect the excitation RF pulse. Noise and impairments in the processing chain will cause errors in the estimation of any of the signal parameters. Here, the I and Q signals are shown individually and as a complex (I+jQ) signal in the time domain.

2.4 Proteus as the Perfect FID Acquisition and Analysis Device for NMR Applications

The digitizer section of the Tabor Proteus AWT family can effectively acquire two RF channels per PXIe module or benchtop unit (Figure 2.5). Frequency range goes from DC up to 8GHz and it can cover from DC up to 1.35GHz in the first NZ as sampling rate is 2.7GS/s. The architecture of the digitizer is designed for RF applications. These are some of the characteristics of the Proteus Digitizer that makes it so successful when applied to NMR applications:

- Frequency range allows for the direct acquisition of the FDI at the Larmor frequency without the need for any frequency converter, local oscillator, and/or mixer.

- DDC (Digital Down-Converter) architecture is implemented for each channel so the complete mixing/detection/filtering/decimation process is made in real-time. Although the signal is sampled up to 2.7GS/s, the complex waveform data is stored at 16x lower sampling rate after applying a near-ideal digital low-pass-filtering/decimation process.
- The NCO (Numerically Controlled Oscillator) attached to the DDC can be coherent with the NCOs in the DUCs of the AWG channels used for the generation of excitation RF pulses, so the complex IQ FID signal is obtained as it would be using ideal quadrature mixers. As all the processing is done numerically, quadrature or non-linear distortions cannot happen.
- Both DDCs can be attached to a single channel so two completely different FID at two different frequencies can be obtained, even simultaneously.
- Triggering for acquisitions can be tightly controlled by the sequencer in the AWG so acquisitions can be done exactly when necessary with ns accuracy. As demodulation is coherent, trigger jitter does not affect the phase information for the acquired FID signal. This strategy can be used for further data reduction as the digitizer section can be set up to take snapshots of the I and Q waveforms at intervals ranging from a few microseconds to several seconds.
- The huge waveform memory in Proteus combined with the real-time data-reduction processing described above results in the capability of the instrument to autonomously handle experiments lasting for seconds, minutes or even hours without any intervention from the control computer.
- The data transfer speed between Proteus and the control computer enables transferring giga samples in a matter of seconds.

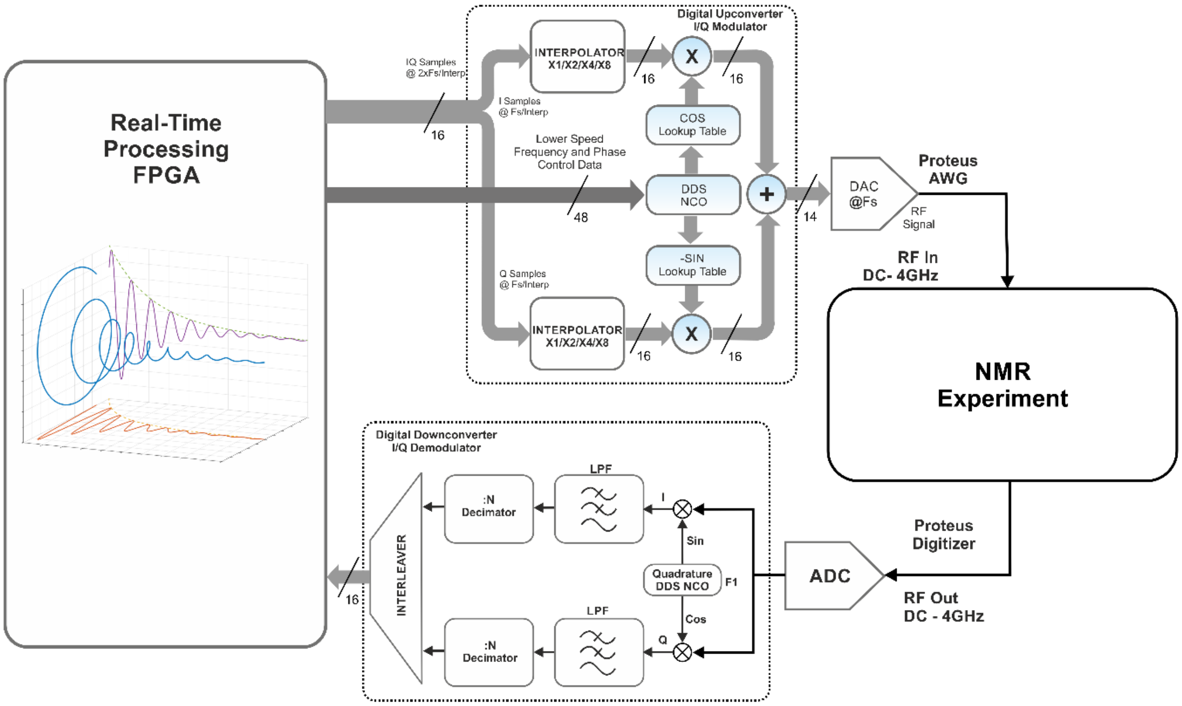

Figure 2.5 FID Raw Signal

The Proteus AWT can implement a complete NMR measurement system including excitation RF pulses, FID acquisition, and even control of all the components in the process (Pulse Blaster functionality). The excitation RF signal generation and the FID acquisition is completely coherent and any of the components is tuned to a single frequency so it can be adapted at the full range of channels and 1-D, 2-D, or 3-D NMR experiments. Real-time processing and data reduction techniques, combined with extremely large generation and acquisition waveform memories, allow for ultra-long fully automated experiments without compromising data integrity.

3 Appendix Proteus SCPI MATLAB Script Example

The MATLAB script listed below will generate the FID complex signal three-dimensional representation as depicted in the figure below.

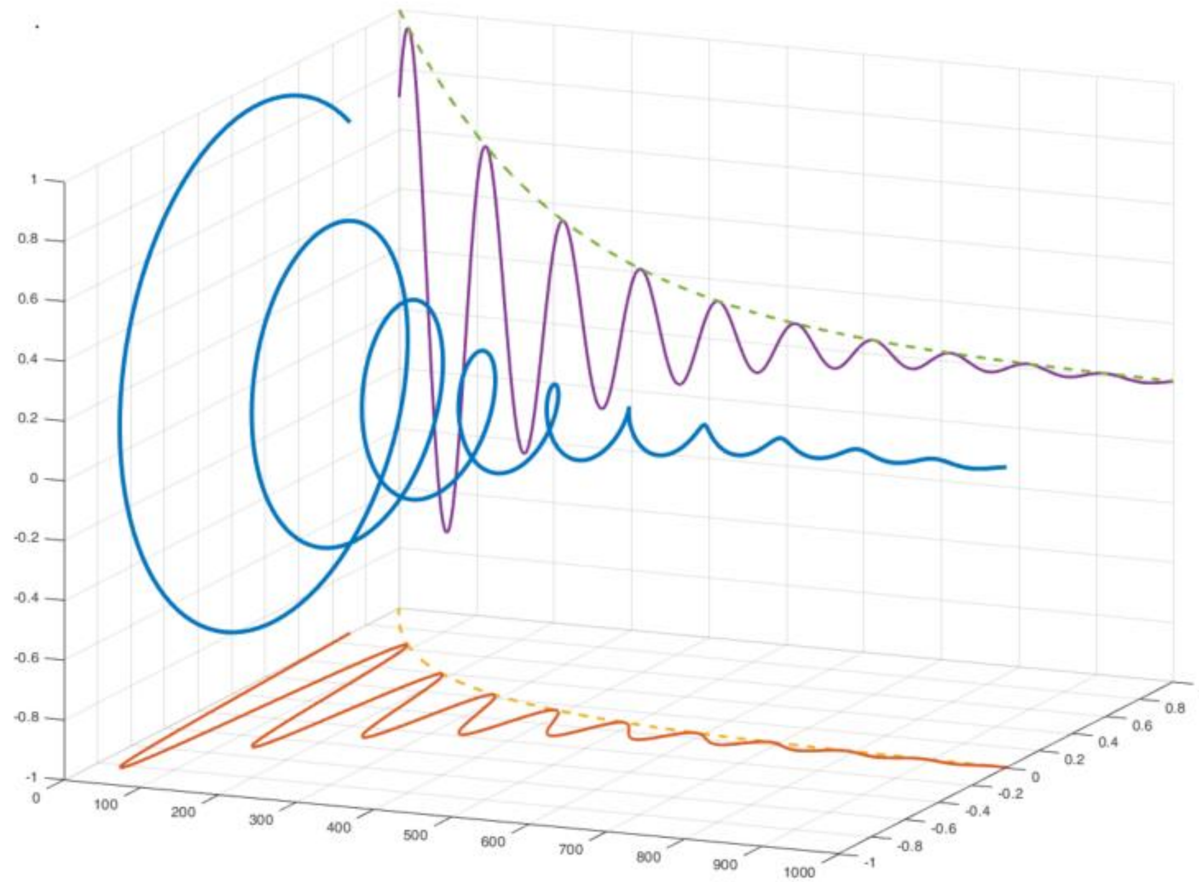

Figure 3.1 FID Complex Signal Three-Dimensional Representation

3.1 NMR_FID_SIMUL.m

```
% NMR Phase Sensitive Detector Output simulation

num_of_samples = 1000;

decay = -0.005;

freq = 0.01;

init_phase = pi / 4;
```

```
x_wfm = 1:num_of_samples;
x_wfm = x_wfm - 1;
zero_wfm = zeros(1, length(x_wfm));

iq_wfm = exp(1i * init_phase + x_wfm * (decay + 1i * (2 * pi *
freq)));

% plot(real(iq_wfm));
% hold;
% plot(imag(iq_wfm));

p = plot3(x_wfm,real(iq_wfm),imag(iq_wfm));

p.LineWidth = 3;

grid on;

hold;

q = plot3(x_wfm,real(iq_wfm),zero_wfm - 1);

q.LineWidth = 2;

q = plot3(x_wfm,abs(iq_wfm),zero_wfm - 1, '--');

q.LineWidth = 2;

r = plot3(x_wfm,zero_wfm + 1,imag(iq_wfm));

r.LineWidth = 2;

r = plot3(x_wfm,zero_wfm + 1,abs(iq_wfm), '--');

r.LineWidth = 2;
```