Novel Approaches to the Timing of FFC-NMR experiments

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Introduction

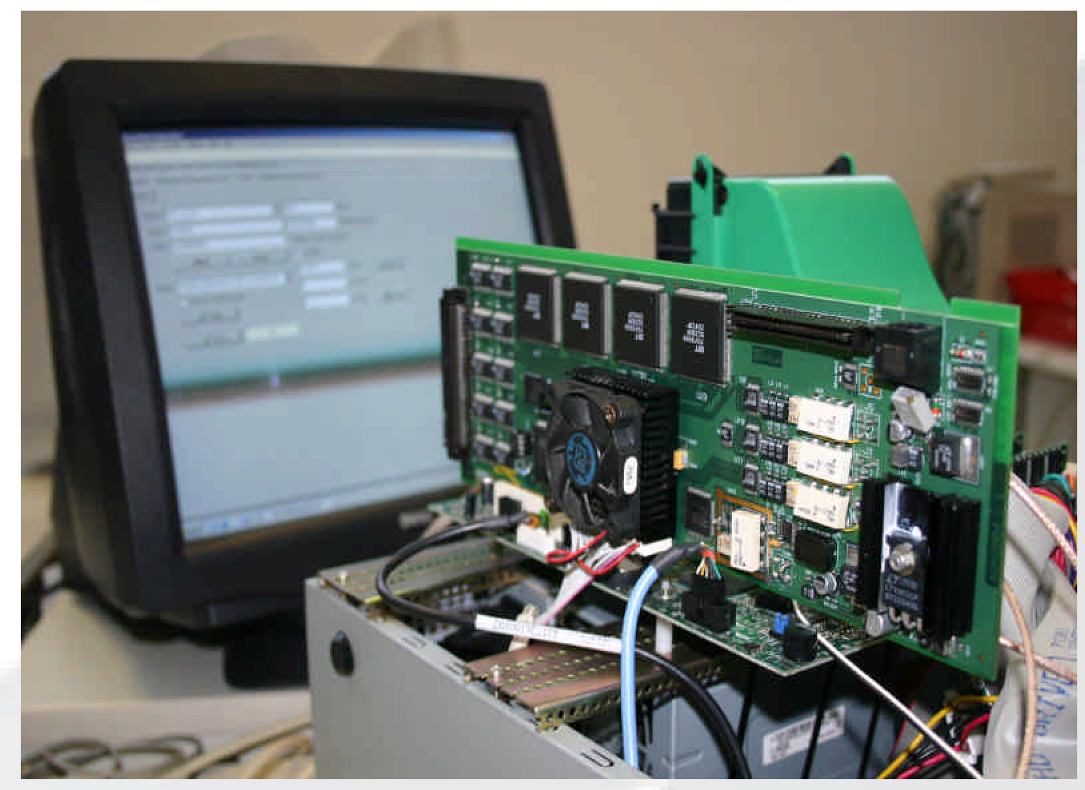
Compared with an HR-NMR spectrometer, a Fast-Field-Cycling NMR Relaxometer imposes a number of extra requirements on the timing of acquisition sequences [1]. With the ongoing development of variable-field relaxometry field-switching cycles become more sophisticated. It is no longer sufficient to use just the classical polarisation, relaxation and acquisition field pulses with constant slew rates during switching intervals. Many experiments would be carried out in a more precise and versatile way if we could use both adiabatic and non adiabatic field switching or be able to profile every magnetic field pulse, giving it the best shape for each chosen experiment. Another peculiarity of FFC-NMR is the growing tendency to investigating all kinds of samples, including liquids, solids and all kinds of heterogeneous and structured materials. This means that we must deal with very different types of FIDs, requiring sampling rates from 1kHz to 10 MHz.

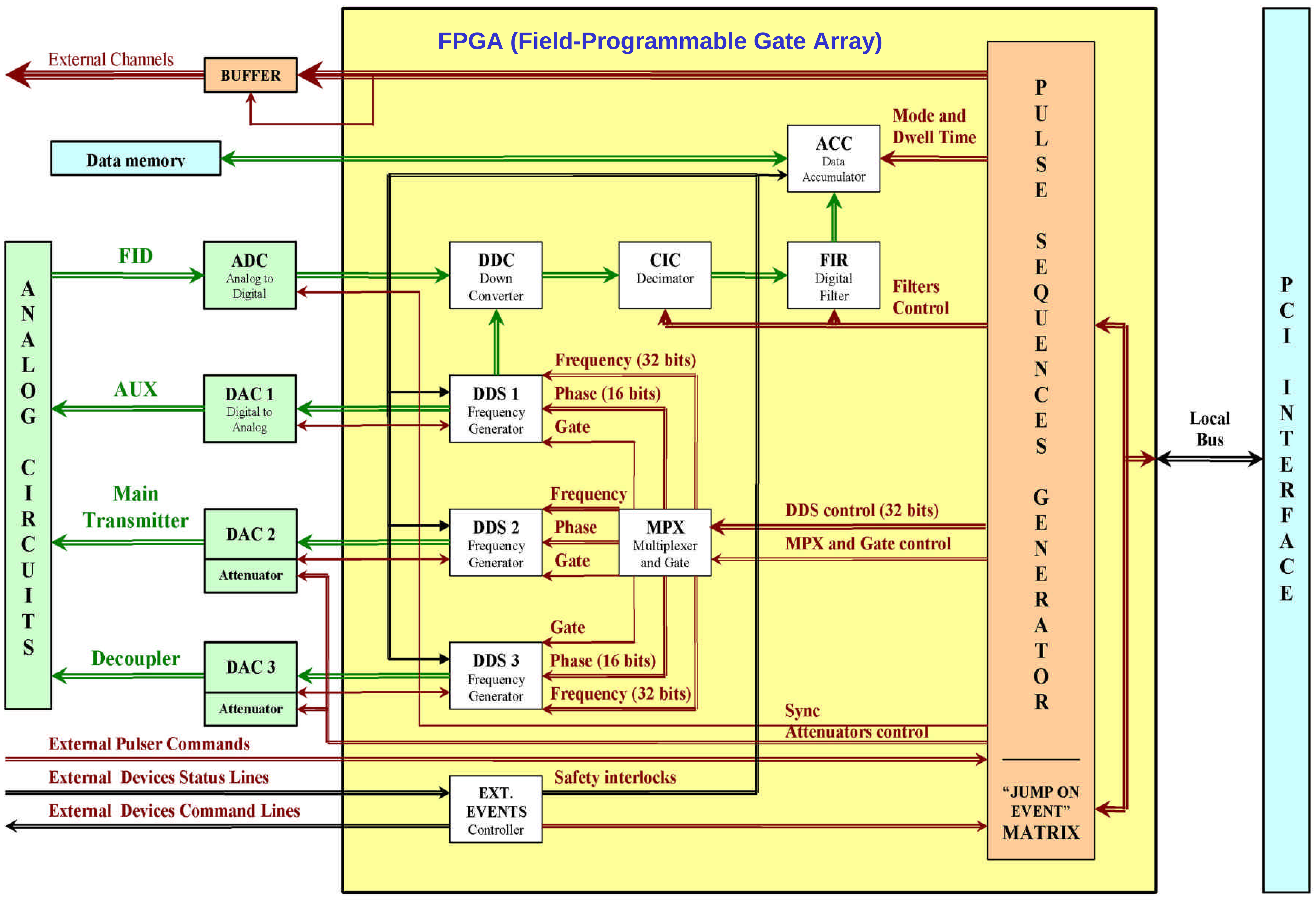
Consider, for example, samples with several phases (e.g., a rigid matrix, a bulk water phase, and an adsorbed water layer). Their signals can be very different in spectral width and in intensity. The solid phase usually needs very short dwell time and very open filters. Applied to the liquid phase the same parameters would lead to an excessive amount of correlated data and possibly exceed the capacity data accumulation buffers. One solution of this dilemma is to optimize the experiment separately for each sample component and perform as many experiments as there are sample components with different types of signals.

Since this is time consuming, we have implemented the possibility to split the multi-segmented FID into two or more temporal windows and apply in each of them quite different signal-acquisition parameters (such as the dwell time and filter width values). In such a way one can, in fact, optimize the final S/N ratio of each sample component [2]. Sometimes it could be convenient to divide a FID in multiple logarithmically spread temporal windows withdrawing the necessity of predicting a priory the sample's phases decay. This approach implies, however, a run-time control of the dwell time, filter settings and other receiver parameters in every window.

Regarding the RF part of FFC relaxometer, we expect that there will soon arise the need for a second and even third RF irradiation channel and that all such channels will need to be synchronized with the rest of the system. We therefore provide dynamically controlled (not just digitally pre-settable) frequency, phase and amplitude of all the channels and thus offer the User additional possibilities such as composite, profiled and chirp pulses.

Stelar Single board NMR console





System implementation

To meet all these requirements, we have adopted a number of innovative engineering solutions, centered around the modern FPGA based **system-on-chip (SOC)** concept. We also placed all the most speed critical discrete electronic devices in proximity on the same board in order to optimize RF and switching parameters.

The heart of the system is the powerful FPGA chip with a clock rate of up to 210 MHz. A **single chip** system provides us with considerable timing advantages such as **direct signal digitization up to 90 MHz** and a **complete control of all relevant acquisition parameters** with **temporal resolution of 20 ns.** Moreover, all hardware devices implemented within the chip **can be easily reprogrammed** and updated in order to meet any future requirements.

The FPGA chip is located on a **PCI board** together with **pulser controlled ADC, DAC's, RF attenuators, RAM** and relative analog and digital circuits.

In order to control slower devices such as magnetic field waveform generators, it was found more expedient to use **dedicated small pulse sequencers** placed on the corresponding remote device board(s) and synchronized by means of the main pulser's external hardware-control channels.

The FPGA chip incorporates:

- **Quadrature Digital Down Converter** (phase detector), followed by **pulser controlled digital CIC and FIR filter blocks**.
- A versatile **pulser controlled data accumulator** with an ample **choice of accumulation modes [2]**.
- Three independent, **pulser-controlled** digital RF-generation channels.
- Safety interlocks and external events controller **interfaced with pulser**.
- Pulse sequences generator, implemented as a **hard-wired sequence-timing sub-processor** with **128 bits wide "words"**, specifically designed to handle all the tasks discussed above as well as many others.

Pulse sequences generator

The pulse generator has **96 output channels** available for hardware control which permit synchronization of all the FPGA chip devices as well as all other boards and external devices.

It supports **unconditional and conditional jumps** to any preprogrammed subroutine and **run-time programming**. It also supports **nested cycles** to a depth of 7 levels, ensuring **very compact and fast loading scripts of sequences**. The **running sequences can be dynamically updated and reprogrammed**. The sequencer **can react in sophisticated ways to run-time internal and external events** such as signal overflows, safety interlocks and timing triggers.

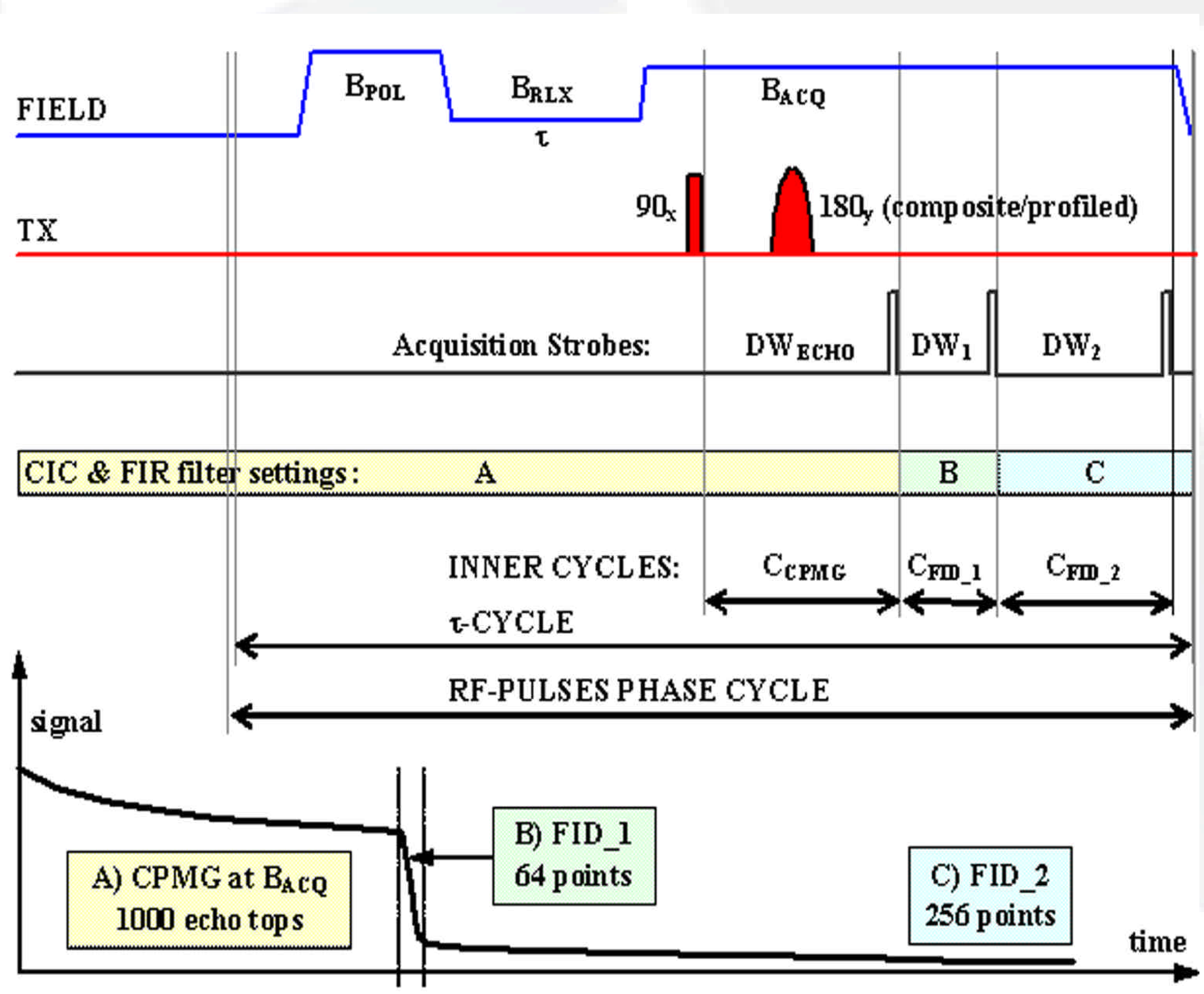
An **elementary pulser interval range is 40 ns to 85.9 s, with a resolution of 20 ns.** If need be, however, the duration of any logical step in a sequence can be extended practically to infinity by means of the cycling feature.

Example of a novel FFC acquisition sequence which can be easily implemented on new Stelar board

Here, the usual pre-polarized FFC cycle is combined with a signal-detection period composed of three sub-intervals. **(A)** A CPMG sequence with short echo spacing (e.g., 50 µs) but a large number of echoes, followed by an FID starting from the top of the last echo. **(B)** Fast acquisition period tailored to catch an FID component with a rapid decay and **(C)** a slow acquisition period (DW2 > DW1) to detect the slow-decaying FID section. The sequence is designed to separate various sample magnetization components according to their T2's at Bacq and T1's at Brlx (it could be also used to monitor magnetization transfer from a liquid phase to a solid matrix).

In the current context, the salient features are: **(a)** limited use of pulser resources, since the code for the three inner cycles takes just a few pulser steps, **(b)** run-time re-programming of filter settings, **(c)** possibility of programming the outer τ-cycle either within the pulser (possibly using a table of pre-defined values), or resorting to run-time re-programming of the single pulser address whose contents vary, **(d)** possibility of having the data read out by the CPU and saved elsewhere even while the acquisition is in progress (the synchronization between the pulser and the CPU is achieved by means of programmable pulser interrupts).

The combination of features (c) and (d) guarantees that there is no hardware limit on the number of data points to be acquired and/or number of τ-blocks and pulse-phase settings even in the improbable case of reaching the top capacity of the pulser or of the acquisition RAM.



1) Ferrante G., Sykora S., *Technical Aspects of Fast Field Cycling*, in Adv.Inorg.Chem., Ed.Rudi van Eldik, Vol.**57**,p.405-470,(2004).
2) D. Canina, A. Galkin, S. Sycora and G.M. Ferrante, *Novel approach to Signal Acquisition and Accumulation in FFC-NMR experiments,* poster at 4th Conf.FC Relaxometry-Torino-2005.