NMR Pulse Design
Using Modern Optimization Methods

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Abstract

Modern NMR consoles give us excellent control over the intensities and phases of RF pulses, This has led to a wide variety of shaped pulses for many purposes. However, perhaps this is an embarrassment of riches. If we have 512 points in a pulse shape, we must optimize over 1000 variables to find the truly "best" pulse. Recently, robust, open-source solvers have become available that can deal with problems of this size. In this poster, we use these methods to design a variety of shaped pulses for a number of applications.

1 Hard Pulses

Hard pulses are the ideal pulses of NMR. They correspond to a rotation, and so are useful for inversion, excitation and refocusing. However, they require infinitely high power, so they are approximated by rectangular pulses with a finite power and magnetic field, γB_1. Because the magnetic field is limited, there are significant off-resonance effects, as in the excitation profile given in Fig. 1. One recent example is the offset dependence of the CPMG T_2 experiment [1]. However, modern consoles give us exquisite control over pulse power and phase, so there have been many designs of composite and shaped pulses to overcome pulse offset effects and other deficiencies. We have applied modern optimization methods to this problem.

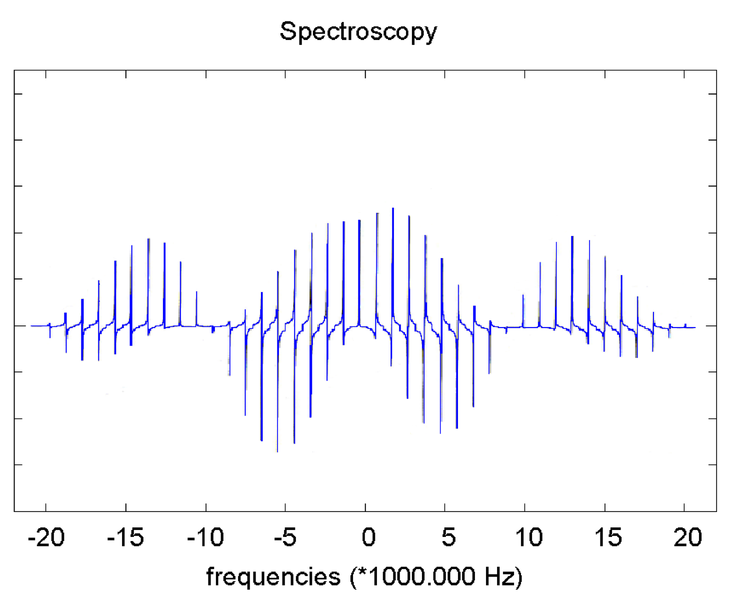

Figure 1: *The spectrum of an excitation ($\frac{\pi}{2}$) experiment using a rectangular pulse. All of the experiments displayed in this poster were done on a Bruker DRX 500 and used one same sample which is dilute $CuSO_4$ in D_2O. $\gamma B_1 = 2100$Hz, $t_p = 100\mu s$, the range of offsets is ± 20kHz, the step size is 1kHz.*

2 Solution

The first step to design an optimal pulse is to break a shaped pulse into steps. Each step has its own phase and intensity, but within each step, the phase and the intensity are constant, so we can deal with each step as a rectangular pulse. Then optimization methods are used to figure out the optimal phase and intensity of every step. Generally, there is lots of scope for variation and lots of variables in the computation, which results in numerical problems.

Anand and Curtis developed a method to efficiently compute the exact integration of Bloch equations and its first-order and second-order derivatives with respect to the RF pulse. The symbolic computation software Maple was used to generate their C code [2]. This calculation did not include relaxation during the pulse, but our present work now incorporates this important feature.

3 Optimization

Since we have a symbolic solution (and its derivatives) to the Bloch equations, we can use this to optimize the steps in the shaped pulse. The main idea is to minimize, for instance, the deviation of the final magnetization obtained from integrating the Bloch equations from the target magnetization. Different formulations of this objective have been developed and profiled. At the same time, all of the models also include the constraints of the total RF energy and the RF amplitude.

The problems we have built are large-scale, non-linear and non-convex. We choose Interior Point OPTimizer (IPOPT) which is an open source solver implementing the interior point method. The interior point method is a proven approach to solving constrained optimization problems. IPOPT can handle very large numbers (thousands) of variables and constraints [3]. In our problems, the cost of function evaluations is far bigger than the cost of the interior point method. For example, on a Power MAC G5 computer (2×2.5GHz, 4G RAM), the pulse in Fig. 4 required 1416.999s for the solver but 42398.557s for function and derivative computation.

4 Results

We will show an optimal refocusing pulse, its simulated spectrum, and experimental spectrum to demonstrate that the effects of resonance offset and rf inhomogeneity are successfully minimized.

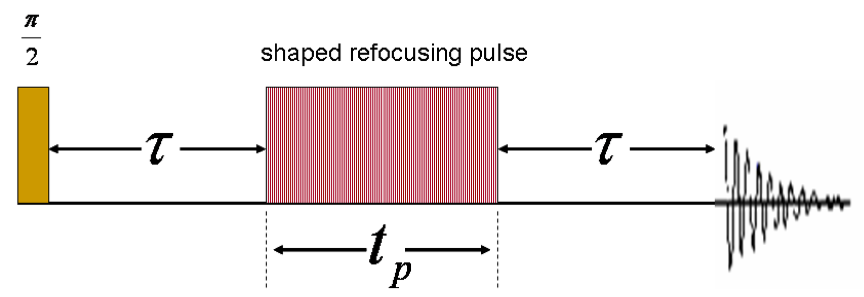

Figure 2: *Refocusing pulse sequence. The first $\frac{\pi}{2}$ pulse is a hard pulse, the second shaped pulse is our optimization target.*

The following experiment which uses the rectangular refocusing π pulse (See Fig. 2) shows the effects of frequency offset on refocusing. The bandwidth here is approximately $\pm 1.5 \times \gamma B_1$.

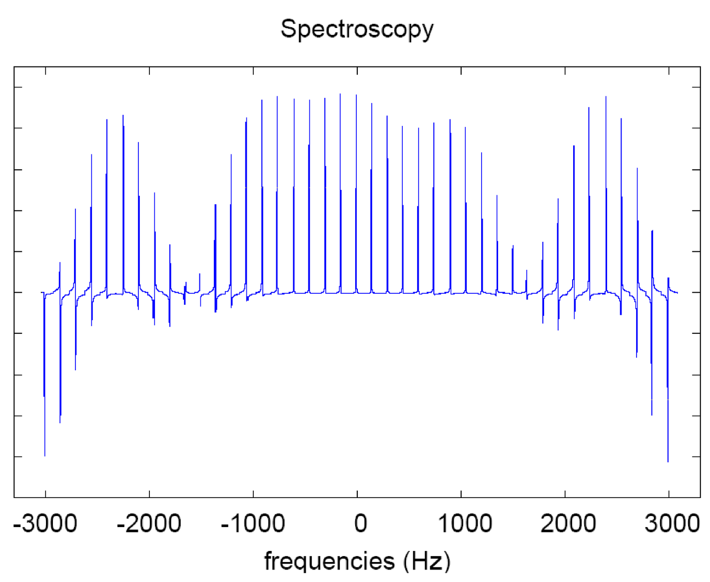

Figure 3: *The spectrum obtained after a rectangular refocusing (π) pulse which is following a hard $\frac{\pi}{2}$ pulse. $\gamma B_1 = 2100$Hz, $t_p = 238\mu s$, the phase of the rectangular pulse is 0, $\tau = 250\mu s$.*

The following optimal refocusing pulse is used to suppress or eliminate the effects of resonance offset and RF inhomogeneity (within some tolerance).

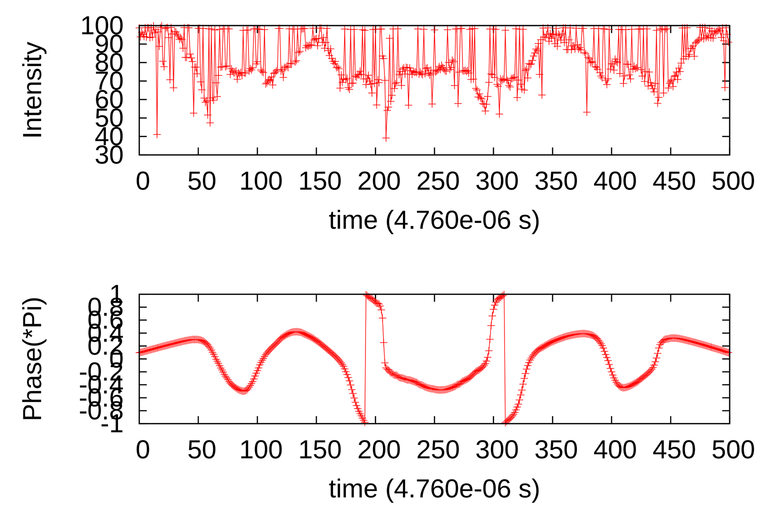

Figure 4: *The optimal refocusing π pulse designed for zero final magnetization phase. The phase of the pulse is almost symmetric with respect to the middle point of the pulse.*

4.1 Details of the Pulse

time steps	500	
t_p	2380	μs
Δt	4.76	μ s
peak RF	2100	Hz
τ	250	μ s
bandwidth	± 2000	Hz
offset resolution	50	Hz
offset steps	81	
T_1	71	ms
T_2	52	ms

The RF scalers α are [0.95,0.975,1.0,1.025,1.05], the weights of RF inhomogeneity are calculated from the Gaussian distribution $exp^{-\frac{(1-\alpha)^2}{2\sigma^2}}$, $\sigma = 0.042$ (the RF scalers and σ are the same as [4]), the initial pulse is a random pulse. The optimal pulse is obtained at the maximum iteration number of the optimization solver which is set to 400. This optimal pulse is also scalable to other RF amplitudes.

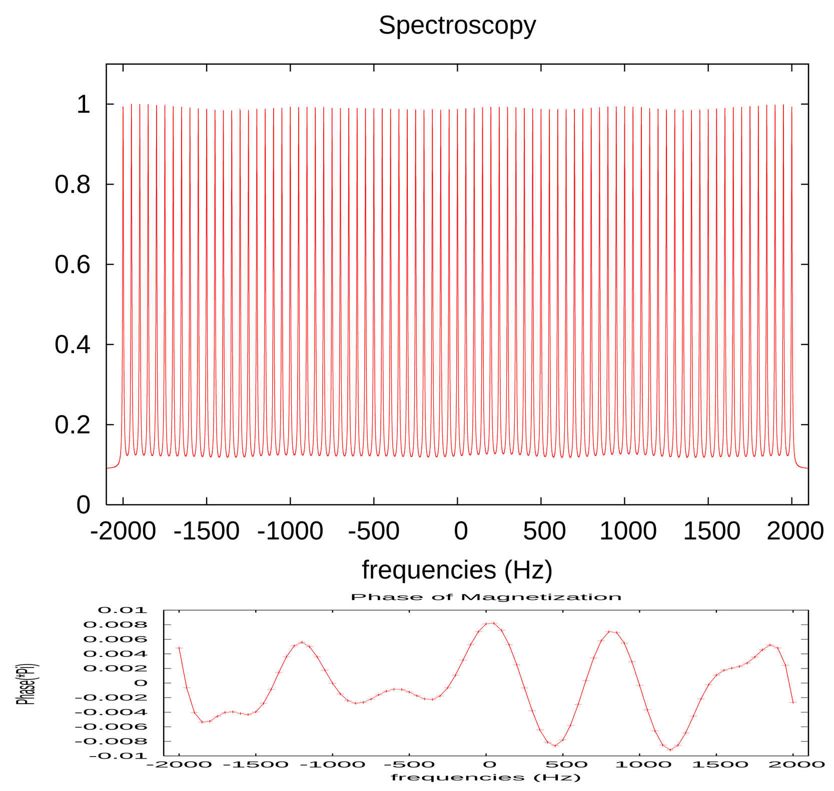

Figure 5: *The simulated spectrum and phase of using the optimal refocusing pulse. The parameters are the same as the design. The maximum phase of the final magnetization in the range of ± 2000Hz is approximate equal to $3.0°$.*

4.2 Comparison

Fig. 6 displays that the optimal refocusing pulse provides considerable improvement comparing with the rectangular π pulse (Fig. 3) in refocusing experiments. These spectra are on the same scale as Fig. 3.

In this poster, we just discuss an optimal refocusing pulse which is solved by minimizing the error of the final magnetization and the target magnetization with the restriction of the RF amplitude, but we can do anything (excitation, inversion, refocusing and pulse sequences) by changing the initial and target magnetization, similar results for excitation pulses are also obtained (not shown).

5 Conclusion

A new approach of different objective functions and constraints to design broadband shaped pulses has been developed. The results of experiments show that the optimal pulses obtained by this new approach can significantly suppress the effect of offsets and the RF inhomogeneity and give the expected spectroscopy. Due to the flexibility of these optimization problems, this approach can be used to design different optimal pulses for different purposes such as phase-modulated, limited total RF energy, specific phase of final magnetization, pulse sequences and so on.

The simulations (not shown) clarify that the optimization solution is better if the designed pulse is longer, the range of offsets is smaller, the RF power is homogeneous, and T_1 and T_2 are bigger. This result matches the result of [5, 6].

In the future, we will compare the performance of this new approach with other methods, explore how to optimize the parameters so as to improve the performance of optimal pulses, investigate the effect of relaxation in the design of optimal pulses, get shorter optimal pulses, apply to more complicated experiments such as reducing the error of the measurements of T_2.

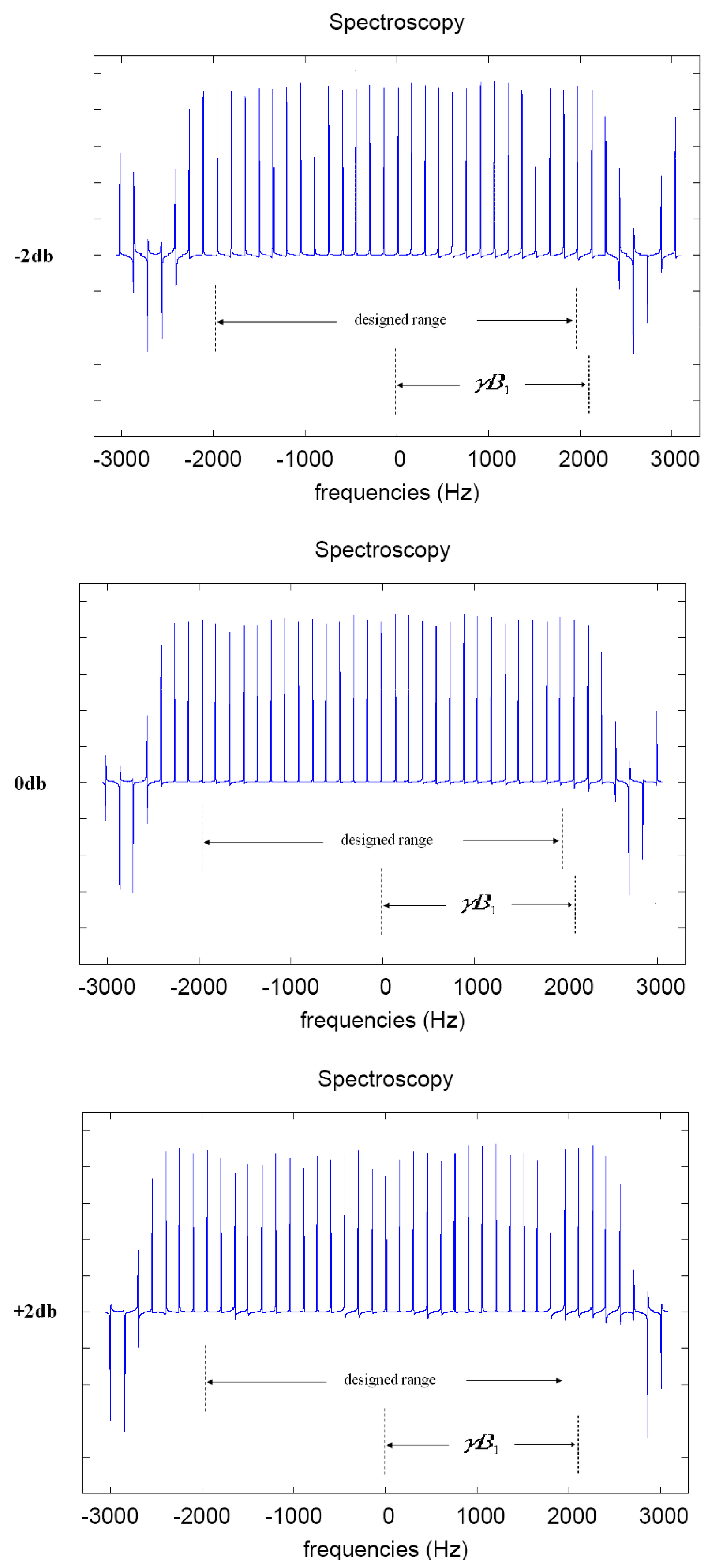

Figure 6: *The spectrum of using the optimal refocusing pulse with respect to the power level (-2db, 0db, 2db). The maximum RF amplitude is calibrated to 2.1kHz (0db) in the experiments. The range of offsets is ± 3kHz which is bigger than the range of the offsets (± 2kHz) designed, the size of the offset step is 150Hz, other parameters are the same as the parameters of the design.*

References

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