

# Optimal Pulse Design Of Single Spin Systems (abstract)

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Hard pulses are mostly used in Nuclear Magnetic Resonance (NMR) under the assumption that the rf magnetic field of hard pulses completely dominates all other interactions. However, this is seldom true, particularly with high magnetic fields, strong interactions and delicate cold probes. But 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 [1, 2, 3, 4].

The Bloch equations exactly describe the process of an experiment of single spin systems. By solving Bloch equations and discretizing pulses, optimization models can be constructed for optimal pulse design. Some numerical methods such as simulated annealing and optimal control theory have been applied to solve these problems, but due to the computational cost and the drawbacks of these methods, most of numerical methods only deal with small numbers of variables, or ignore the relaxation terms in the Bloch equations [5, 6, 7, 8, 9]. Optimal control can handle a large number parameters, but it is difficult to design universal optimal refocusing pulses.

We have developed a series of flexible optimization models with exact integration of Bloch equations and exact, efficiently calculated first and second derivatives. Using these models which more fully capture the desirable properties of rf pulses for specific NMR experiments, and the open-source solver IPOPT, we have discovered designs with significantly better performance than existing designs. The following figure shows actual NMR spectra for a rectangular pulse and the estimated results for a comparable optimized pulse.

In this presentation, we will explain the differences between different NMR experiments, and the way that these can be modelled, and present a series of comparisons between the resulting optimized pulses and the best currently available pulses. Since all of the models are highly non-convex, we are not surprised to find many distinct local minima. We will show that using in-depth knowledge of the target experiments leads to models which prefer local minima which are more robust when used in simulations of experiments too long to optimize directly, and in actual experiments themselves. In the future, we will extend these models to multi-spin systems.

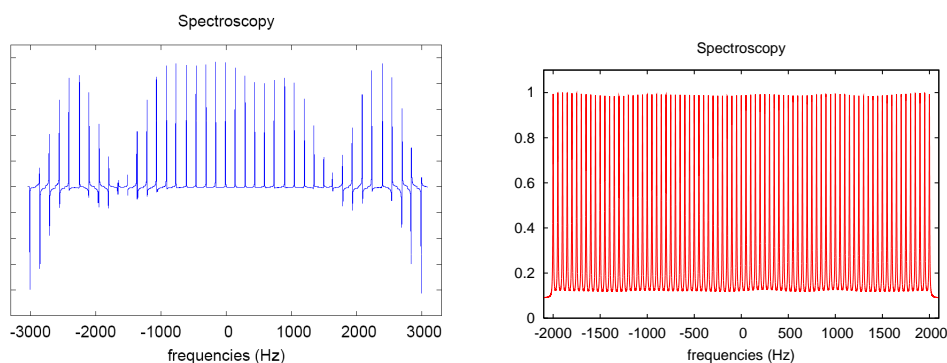


Figure 1: The spectra obtained after a rectangular refocusing ( $\pi$ ) pulse and an optimal pulse which are following a hard  $\frac{\pi}{2}$  pulse.  $\gamma B_1 = 2100\text{Hz}$ ,  $\tau = 250\mu\text{s}$ , the design range of offsets is  $\pm 2000\text{Hz}$ . The goal which we want is to get the uniform spectroscopy without the effect of radio frequency inhomogeneity.

## References

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