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# Signal Optimization in Inhomogeneous Fields: Application of Quantum Optimal Control Theory

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## Abstract

We demonstrate that pulses derived using Optimal Control Theory (OCT) techniques can be used to significantly enhance the robustness of the Carr-Purcell-Meiboom-Gill sequence (CPMG) [1,2] to inhomogeneities in the static $B_0$ field. By numerically inverting the Liouville - von Neumann equation, OCT pulses were derived that can be used directly in place of hard pulses in the CPMG sequence to greatly improve the bandwidth of refocusing. To retain the echo stability achieved by the Meiboom-Gill correction to the Carr-Purcell sequence, the refocusing pulses were designed to perform a unitary π-rotation as opposed to just a state inversion transfer. To illustrate this approach we present an example of optimized pulses that show an improved CPMG-like behavior with complete excitation and multiple refocusing over a bandwidth of +/- 2.6 $\gamma B_{1,\mathrm{max}}$ with a pulse duration limited to 10 $t_{180}$.

## Keywords

Inhomogeneous Fields, OCT, NMR, CPMG

## 1. Introduction

The CPMG sequence is widely used in one-sided and stray-field NMR applications to measure transverse relaxation rates. Averaging over the multiple echoes in the sequence improves the signal-to-noise ratio of these measurements. With standard hard pulses, only spins with Larmor frequencies within +/- $\gamma B_1$ of the applied radio frequency are effectively excited, refocused, and detected. We address this limitation by developing novel excitation and refocusing pulses derived from OCT techniques, significantly improving the frequency performance of the Carr-Purcell sequence while retaining the intrinsic stability of the Meiboom-Gill correction.

The idea of using OCT to enhance pulse response has been previously discussed [3], however, the current work focuses on pulse design subject to stringent constraints on pulse duration ($t_p$ < 10 $t_{180}$) and maximum RF amplitude ($\gamma B_{1,\mathrm{max}}$ / 2π < 5 kHz). To ensure the

CPMG echo amplitudes remain asymptotically stable, the refocusing pulses must act as a π-rotation on all spins, regardless of their initial state. This implies a unitary operation is needed.

## 2. Methods

The method used to find optimized pulses was based on the GRadient Ascent Pulse Engineering algorithm (GRAPE) developed by Khaneja [4], which uses gradient ascent techniques to determine locally optimal solutions in a multivariate space subject to a cost functional. To optimize for a desired unitary operation, the Liouville-von Neumann equation, describing the evolution of a density operator, $\rho$, under the action of a time dependent Hamiltonian, Eq. (1), must be inverted.

$$\frac{d\rho}{dt} = -i\left[\rho, H_{tot}(t)\right] \quad (1)$$

The solution to Eq. (1) can be expressed in terms of a unitary propagator, U.

$$\rho(t) = U(t)\rho_0 U^{-1}(t) \quad (2) \qquad\qquad U(t) = e^{-i\int H_{tot}(t)dt} \quad (3)$$

For the current work, we assumed a Hamiltonian consisting of an internal Zeeman interaction and an external RF control field. To simulate an inhomogeneous $B_0$ field, the Zeeman interaction was defined over a distribution function, $P(\omega_0)$, of offset frequencies, $\omega_0$.

$$H_{tot} = \frac{1}{2}\sum_{\omega_0} P(\omega_0)\omega_0\sigma_Z + \frac{1}{2}\omega_1(t)\left[\cos\phi(t)\sigma_X + \sin\phi(t)\sigma_Y\right] \quad (4)$$

Examination of Eq. (2) makes it clear that we can find optimal pulse parameters, $\{\omega_1(t), \phi(t)\}$, by at least two distinct methods. The first approach is to match the simulated density operator to a desired density operator. This was the method used to optimize excitation pulses, with the cost functional defined as the density operator correlation. For the refocusing pulses, the second method, wherein the simulated unitary operator is matched to the desired unitary propagator, was used. In this case, the cost functional was related to the deviation from unit fidelity.

A 1 ms pulse length was used, defined piecewise constant for 10 µs intervals. We chose an initial set of 100 amplitude and phase values then optimized the 200 degrees of freedom in the problem over a uniform distribution function of +/- 13 kHz resonance offset with maximum RF amplitude 5 kHz. Pulse updating at each step in the algorithm was based on derivatives of the appropriate cost functional with respect to the control parameters.

## 3. Results

The amplitude and phase profile for an optimized refocusing pulse is shown in Fig. 1. The complexity of the pulse demonstrates the utility of OCT in pulse design, providing a convenient means to enhance pulse response by optimizing a large number of pulsing degrees of freedom. Such complex solutions are difficult - if not impossible - to find using more conventional methods.

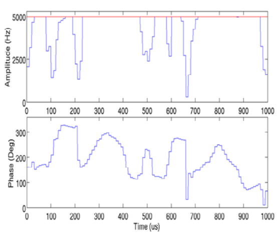


**Fig. 1:** Example pulse profile for an optimized OCT refocusing pulse showing amplitude and phase as a function of time. The noise seen in Fig. 2 is an expected result of the complexity of the pulse and not a simulation artefact.

Simulation results are shown in Fig. 2 for a CPMG-like sequence with 10,000 OCT refocusing pulses, neglecting relaxation effects. The peak echo magnetization shows a flat response over the full range of offset frequencies of interest, +/-2.6 $\gamma B_{1,max}$. This bandwidth greatly exceeds the response obtainable with hard pulses of the same maximum RF amplitude. The additional signal degradation at the time of the 10,000$^{th}$ echo as compared to the 1$^{st}$ echo (not shown here for the sake of space) is negligible. The asymptotic stability of the CPMG sequence using hard pulses is thus maintained, but over a much larger bandwidth.

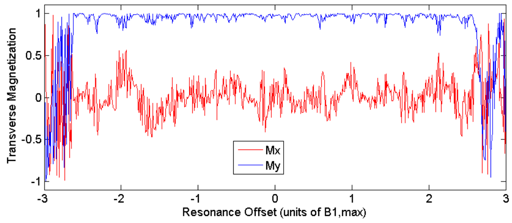


**Fig. 2:** Simulated response of the peak magnetization of the 10,000$^{th}$ echo in a CPMG-like sequence using optimized OCT pulses. The magnetization is almost perfectly aligned along $M_y$ over the range of interest.

As a demonstration of the experimental viability of such complex pulses on real systems we performed preliminary experiments with a spin echo sequence using OCT pulses optimized over a frequency range of +/- 8 kHz and compared the results with standard measurements using hard pulses. In the experiments, the peak echo amplitude was recorded while the transmitter offset frequency was systematically varied in increments of 100 Hz from -10 kHz to +10 kHz. The results shown in Fig. 3 confirm the simulated response.

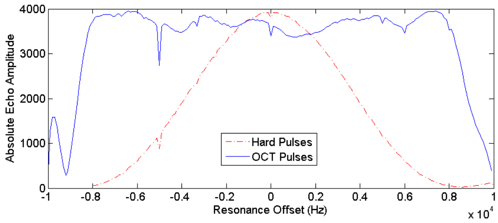


**Fig. 3:** Experimental response of echo amplitude for a spin echo sequence using either hard pulses or OCT pulses. The significant improvement in frequency response of OCT pulses predicted by simulation is clearly confirmed.

## 4. Discussion and Conclusions

We have demonstrated how complex phase and amplitude modulated pulses found through Optimal Control Theory techniques can be directly substituted into the CPMG sequence to significantly enhance robustness to static field inhomogeneities. By demanding a unitary character to the refocusing pulses, the improved sequence remains consistent with the Meiboom-Gill correction to the Carr-Purcell sequence. We have also demonstrated that such modified sequences are experimentally realizable and exhibit the predicted improvement in pulse sequence performance.

While the CPMG sequence was chosen for this demonstration based on its wide applicability and utility in NMR measurements, any sequence, in theory, may be made more robust using the techniques of optimal control to create pulses that generate a desired response.

## References

[1]H. Y. Carr and E. M. Purcell, *Phys. Rev.* **94**, 630 (1954).
[2]S. Meiboom and D. Gill, *Rev. Sci. Instr.* **29**, 688 (1958).
[3]S. Conolly, D. Nishimura, and A. Macovski, *IEEE Trans. Med. Imag., MI*-**5**, 106 (1986).
[4]N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, and S. J. Glaser, *J. Magn. Reson.* **172**, 296 (2005).