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Fast Three-Dimensional Inner Volume Excitations Using Parallel Transmission and Optimized k-Space Trajectories

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Abstract

Purpose—To design short parallel transmission (pTx) pulses for excitation of arbitrary three-dimensional (3D) magnetization patterns.

Methods—We propose a joint optimization of the pTx radiofrequency (RF) and gradient waveforms for excitation of arbitrary 3D magnetization patterns. Our optimization of the gradient waveforms is based on the parameterization of k-space trajectories (3D shells, stack-of-spirals, and cross) using a small number of shape parameters that are well-suited for optimization. The resulting trajectories are smooth and sample k-space efficiently with few turns while using the gradient system at maximum performance. Within each iteration of the k-space trajectory optimization, we solve a small tip angle least-squares RF pulse design problem. Our RF pulse optimization framework was evaluated both in Bloch simulations and experiments on a 7T scanner with eight transmit channels.

Results—Using an optimized 3D cross (shells) trajectory, we were able to excite a cube shape (brain shape) with 3.4% (6.2%) normalized root-mean-square error in less than 5 ms using eight pTx channels and a clinical gradient system ($G_{\max} = 40$ mT/m, $S_{\max} = 150$ T/m/s). This compared with 4.7% (41.2%) error for the unoptimized 3D cross (shells) trajectory. Incorporation of B_0 robustness in the pulse design significantly altered the k-space trajectory solutions.

Conclusion—Our joint gradient and RF optimization approach yields excellent excitation of 3D cube and brain shapes in less than 5 ms, which can be used for reduced field of view imaging and fat suppression in spectroscopy by excitation of the brain only.

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SUPPORTING INFORMATION

Additional Supporting Information may be found in the online version of this article.

Keywords

Parallel transmit; spatially selective excitation; inner volume excitation; B0 robustness; k-space trajectory optimization

INTRODUCTION

In MRI, spin excitation is usually performed using either spatially nonselective or slice- or slab-selective radiofrequency (RF) pulses. Encoding using gradients is then performed in order to disentangle the signal coming from different voxels in the excited volume. In some applications, it may be beneficial, however, to excite more complex three-dimensional (3D) magnetization shapes than slabs or slices. For example, excitation of cubic target regions may be used to reduce the volume that needs to be encoded using gradients in order to form an image. This may result in shorter acquisition times at constant resolution or, equivalently, improved resolution at constant acquisition times, as well as reduction of the echo train length (1,2). Other applications could benefit from exciting volumes of magnetization that are not necessarily cubic. For example, vessel-specific arterial spin labeling could be performed by inversion of the spins flowing in a specific artery [although it is not clear that such a strategy would outperform existing arterial spin labeling territory mapping techniques that phase-encode the perfusion territories of the carotid and vertebral arteries (3)]. Another potential application of noncubic spatially selective excitations is fat suppression in spectroscopic imaging by excitation of the brain only (4).

A simple approach for excitation of a cubic target region in spin echo pulses is to excite the spins (90° pulse) in one slice, followed by refocusing of an orthogonal slice (5). This strategy is limited to rectangular target profiles and spin echo pulses [a significant exception is the STEAM pulse that uses a series of slice-selective excitation pulses in orthogonal directions for 3D rectangular localization of the stimulated echoes (6,7)]. It has long been recognized that 2D and 3D spatial excitations of arbitrary shapes can be achieved by design of the RF and gradient waveforms used for excitation (8–11). However, the potential of these approaches has not yet been realized clinically because of the long duration of the resulting waveforms.

Schneider et al (12) designed fast (3.2 ms) 3D shells and stack-of-spirals trajectories for excitation of small target regions (rat brain and kidneys) using a powerful gradient system for small animal imaging ($G_{\max} = 660$ mT/m, $S_{\max} = 5600$ T/m/s). Malik and Hajnal (13) attempted to extend this approach to a clinical imaging system with lower gradient performance ($S_{\max} = 180$ T/m/s) and used pTx to accelerate the excitation pulse (eight channels). Using unoptimized 3D shell trajectories, they were able to excite cubic regions of reasonable quality in 12 ms. This pulse duration is still relatively long despite the pTx acceleration, which makes the resulting pulse sensitive to off-resonance effects (the authors minimized this problem by using the pulse in a turbo spin echo sequence with non-selective refocusing pulses).

This previous work shows that pTx can help reduce the duration of these complex excitation pulses, but the problem of exciting arbitrary 3D magnetization patterns is extremely

demanding for conventional eight-channel pTx systems, and additional degrees of freedom (DOF) are needed. Increasing the number of transmit channels and using a gradient system with better performance can help, but this is a costly approach. Another source of DOF is the k-space trajectory itself. Chen et al (14) attempted to exploit the excitation DOF in the k-space trajectory by parameterizing 2D k-space trajectories with approximately 150 control points, the positions of which were optimized using a greedy optimization approach. This process resulted in highly convoluted trajectories with many turns that are not efficient from a k-space sampling and gradient performance perspective. Deniz et al (15) and Sun et al (16) extended this approach to 3D selection. As in the 2D work of Chen et al, the highly convoluted nature of the resulting gradient waveforms limited the quality of the excitations (15% normalized root-mean-square-error [NRMSE]) achievable in a short time [3.8 ms]). Additionally, no information about the performance of such pulses in presence of off-resonance effects is given (the measurements reported in these studies were performed in homogeneous spherical or cylindrical phantoms that are easy to shim).

In the present study, we propose a joint optimization of the pTx gradient and RF waveforms that yields fast (less than 5 ms) and smooth 3D k-space trajectories with few turns that, together with the RF waveforms, are tailored to the B_1^+/B_0 maps at hand as well as the 3D target excitation pattern (17,18). In contrast with trajectories computed using greedy approaches (14–16), the gradient trajectories optimized by our algorithm are not highly convoluted and are efficient from a k-space sampling and gradient performance perspective. This is achieved by optimizing a small number of shape parameters that control the overall structure and shape of the trajectory instead of the position of the individual control points.

The specific contributions of this work include:

- An efficient parameterization of three fast 3D k-space trajectories: shells, stack-of-spirals, and cross. Our parameterization of these 3D trajectories greatly reduces the dimensionality of the gradient optimization problem while preserving enough DOF for the optimizer to dramatically improve the excitation quality.
- A stable and locally convergent method for optimization of the k-space trajectories shape parameters. We use a standard optimizer for optimization of the shape parameters along with finite differencing for estimation of the Jacobian of the objective function. Key ingredients of the method are 1) a highly stable gradient waveform design method (given a set of control points) and 2) careful handling of integer parameters that, together, ensure that the objective function is smooth and amenable to gradient-based optimization.
- A study of the influence of the target magnetization profile, type of k-space trajectory, and off-resonance effects (spatio-spectral pulse design) on the optimized excitation pulse using Bloch simulations (based on measured B_1^+ and B_0 field maps) and experiments at 7T.

- The full MATLAB code of our joint design approach is available at <http://martinos.org/~guerin/>.

METHODS

Joint Optimization of Gradient and RF Waveforms

Formally, our joint RF and gradient design approach stated as

$$\min_{\varphi, \mathbf{b}} \left\{ \underbrace{\|A(\varphi)\mathbf{b} - \mathbf{m}^{\text{tar}}\|_2^2 + \alpha \|\mathbf{b}\|_2^2}_{\psi(\varphi, \mathbf{b})} + f_\beta(T(\varphi)) \right\}, \quad [1]$$

where $A(\varphi)$ is the small tip angle encoding matrix relating the RF waveform vector $\mathbf{b}$ (all channels are stacked in a single column vector) to the transverse magnetization. The target magnetization vector is denoted $\mathbf{m}^{\text{tar}}$. The vector φ contains the shape parameters of the k-space trajectory which are optimized along with the RF waveform (the encoding matrix $A(\varphi)$ depends on these parameters). Two regularization terms are added to the least-squares objective for control of the total RF power $\|\mathbf{b}\|_2^2$ (regularization strength controlled by α) and the duration of the RF/gradient pulse $T(\varphi)$ (controlled by a regularization function f_β).

The RF power regularization parameter α was chosen so as to restrict the peak RF power below the maximum amplifier peak power. This parameter was set by computing RF pulses with values of α varying from 10^{-5} to 10^{-2} in a logarithmic manner using the initial guess of the k-space trajectory. In other words, the search for the regularization parameter α was performed only once at the beginning of the optimization and a constant value of α was then used during the optimization of the shape parameters. For regularization of the pulse duration, we use the penalty function:

$$f_\beta(T) = \begin{cases} 0 & \text{for } T < T_{\text{max}} \\ \beta \sqrt{\varepsilon^2 + (T - T_{\text{max}} + \varepsilon)^2} & \text{for } T \geq T_{\text{max}} \end{cases}, \quad [2]$$

where T_{max} denotes the pulse duration limit, β denotes the regularization strength, and ε denotes the transition width between the two phases of the penalty function. For durations $T < T_{\text{max}}$, the function vanishes and the objective function is not penalized. For durations $T \geq T_{\text{max}}$, the function f_β is roughly equal to $\beta(T - T_{\text{max}})$. Therefore, the function f_β is a smoothly varying increasing function for pulse durations greater than T_{max} with a transition width between the constraining and nonconstraining phases controlled by ε . In this study, we found that a value of the parameter ε of 1.5 ms worked well for all pulses. The parameter β , on the other hand, controls the strength of the pulse duration penalty. Empirically, we found that our optimization results did not depend strongly on the specific value of β and that a value of $\beta = 2$ consistently yielded pulses shorter than 5 ms for all trajectory types.

We solve the problem in Equation [1] using a nested optimization approach, ie, we break down the joint optimization in an inner optimization loop (fast) over the RF waveform with a fixed gradient waveform and an outer optimization loop (slow) over the k-space shape parameters

$$\min_{\varphi} \left\{ \underbrace{\min_{\mathbf{b}} \{ \psi(\varphi, \mathbf{b}) \}}_{\text{Inner Loop: RF}} + f_{\beta}(T(\varphi)) \right\}, \quad [3]$$

Outer Loop: Shape Parameters

where $\psi(\varphi, \mathbf{b})$ denotes the regularized flip angle error, as depicted in Equation [1].

In the small flip angle regime, and for a fixed k-space trajectory $\mathbf{k}(t)$, the transverse magnetization is given by (19,20)

$$M_T(\mathbf{r}) = i\gamma M_0 \sum_{c=1}^C s^{(c)}(\mathbf{r}) \int_0^T b^{(c)}(t) e^{i\gamma \Delta B_0(\mathbf{r})} e^{i\langle \mathbf{k}(t) | \mathbf{r} \rangle} dt, \quad [4]$$

where $s^{(c)}(\mathbf{r})$ and $b^{(c)}(t)$ denote the spatial sensitivity and the RF waveform of the c -th transmit channel, respectively, and $B_0(\mathbf{r})$ is the off-resonance map converted in Tesla. Discretization of the continuous integral and concatenation of the spatial locations at which Equation [4] is evaluated yields a well-known system of linear equations between the RF pulse $\mathbf{b}$ and the magnetization $\mathbf{m}$:

$$\mathbf{m} = A(\varphi) \mathbf{b}, \quad [5]$$

where the elements of $A(\varphi)$ are easily deduced from Equation [4]. For a given target magnetization $\mathbf{m}^{\text{tar}}$ and a fixed gradient waveform (φ is constant), the RF design problem, therefore, reads

$$\min_{\mathbf{b}} \left\{ \|A(\varphi) \mathbf{b} - \mathbf{m}^{\text{tar}}\|_2^2 + \alpha \|\mathbf{b}\|_2^2 \right\}. \quad [6]$$

Note that Equation [6] can be reformulated as an unconstrained optimization problem using the normal equations

$$C = A(\varphi)^H A(\varphi) + \alpha^2 I \text{ and } \mathbf{d} = A(\varphi) \mathbf{m}^{\text{tar}} \quad [7]$$

with $(\cdot)^H$ denoting the complex conjugate transpose and I denoting the identity matrix. We solve this problem using the conjugate gradient algorithm as implemented in MATLAB R2014b (Mathworks, Natick, Massachusetts, USA).

To enforce robustness with respect to off-resonance effects in our pulses, we design the gradient and RF waveforms not only at the Larmor frequency but also at two off-resonance frequencies (± 50 Hz), referred to as *spatio-spectral* RF pulse design (21). This is simply implemented by stacking three encoding matrices computed at fixed off-resonance deviations (these are added to the B_0 map), namely

$$A = \begin{bmatrix} A_{-50Hz} \\ A_{0Hz} \\ A_{+50Hz} \end{bmatrix} \text{ and } \mathbf{m} = \begin{bmatrix} \mathbf{m}^{\text{tar}} \\ \mathbf{m}^{\text{tar}} \\ \mathbf{m}^{\text{tar}} \end{bmatrix}. \quad [8]$$

The problem of optimization of the RF waveforms on a fixed k-space trajectory is a linear least-squares problem that can be solved relatively quickly. In contrast, optimization of the gradient shape parameters is nonlinear and, therefore, more difficult and slow. We solve the outer optimization loop (over the k-space trajectory shape parameters) of Equation [3] using a nonlinear constrained sequential quadratic programming algorithm as implemented in MATLAB (using the function “fmincon”). The derivatives of the outer objective function with respect to ϕ are computed via finite differencing with a constant step size ($\epsilon = 0.02$). This minimization is performed subject to constraints on minimum ($\widetilde{\varphi}$) and maximum ($\hat{\varphi}$) values of the shape parameters ϕ :

$$\widetilde{\varphi}_q \leq \varphi_q \leq \hat{\varphi}_q \text{ for } q=1, 2, \dots \quad [9]$$

For positive shape parameters, such as the number of shells or the number of revolutions per shell, an obvious choice for the respective constraint is $\widetilde{\varphi}_q=0$ to impose that the shape parameters are never set to negative values by the optimization process. For other parameters, the tolerated upper and lower bounds were adjusted so as to avoid excessively long pulse durations (eg, longer than 20 ms). In this study, which was focused on brain imaging, we limited the extent of all k-space trajectories to a box in 3D k-space with a maximum k-space extent of 100 m^{-1} in all dimensions (this corresponds to $\hat{\varphi}_{1/2/3}=100 \text{ m}^{-1}$ for all trajectories). On the other hand, lower bound constraints on the k-space extent shape parameters were set to small values to prevent the trajectory from collapsing on itself (we used $\widetilde{\varphi}_{1/2/3}=100 \text{ m}^{-1}$). In practice, the lower and upper bound constraints on k-space extent were never reached (ie, they were nonbinding constraints). More details on the shape parameters definitions and their upper and lower limits can be found in the Supporting Information online.

Parameterization of 3D k-Space Trajectories

Given a set of shape parameters, control points are placed in 3D k-space using simple geometry rules outlined in Figure 1. These control points form the skeleton of the k-space trajectory, but we do not optimize their individual locations. In this study, we analyzed 3D shells, stack-of-spirals, and cross trajectories.

Shells Trajectory

The shells trajectory (Fig. 1, first row) consists of a number of concentric shells (the number of shells is optimized in our approach) that are parameterized using seven shape parameters. The first three shape parameters compress or stretch the entire trajectory in k_x , k_y , and k_z (ϕ_1 , ϕ_2 , ϕ_3). Two shape parameters vary the number of shells (ϕ_4) and the number of revolutions per shell (ϕ_5). The last two parameters control the local sampling density of the k-space trajectory: ϕ_6 controls the number of revolutions of the centermost shells, whereas ϕ_7 controls the relative distance between concentric shells. For example, increasing ϕ_7 causes the rate of variation of the radii of concentric shells (from inner to outer shell) to increase and thus results in a decrease of the sampling density at the periphery of k-space compared with the center (this is similar to the parameterization of variable-density spirals). Note that the parameters ϕ_4 and ϕ_5 are of integer type (we explain how these are handled in the optimization process in the following section).

Stack-of-Spirals Trajectory

We also parameterize stack-of-spirals trajectories (Fig. 1, second row) using seven shape parameters. As with shells trajectories, ϕ_1 , ϕ_2 , and ϕ_3 control the extent of the entire trajectory in k_x , k_y , and k_z . ϕ_4 is the distance of consecutive spirals in k_z which, together with the k_z extent (ϕ_3), controls the number of spirals in the stack. ϕ_5 is the number of revolutions per spiral, which, together with the extent in k_x (ϕ_1) and k_y (ϕ_2), controls the in-plane sampling density. ϕ_6 controls the rate of variation of the distance between spirals in k_z (increasing ϕ_6 increases the distance between consecutive spirals as one moves away from the k-space center, which in turn decreases the sampling density at high k_z compared with $k_z = 0$). ϕ_7 controls the rate of variation of the radial velocity of each spiral and, therefore, affects the sampling density in the periphery of (k_x , k_y) compared with the center (variable density spirals). Because ϕ_3 and ϕ_4 can change the number of spirals in the stack they are considered integer parameters.

Cross Trajectory

The final trajectory that we study is the cross (Fig. 1, third row). This trajectory densely samples k-space along the k_x , k_y , and k_z axes in a way that resembles the Fourier transform of a cube (we, therefore, hypothesize that this trajectory is well suited for cubic target regions). The trajectory consists of three distinct segments covering the k_x , k_y , and k_z axes. The segments themselves consist of concentric 2D elliptic curves that sample a roughly cylindrical region around each k-space axis. Each segment is parameterized by two shape parameters. The first parameter (ϕ_1 for k_x , ϕ_3 for k_y and ϕ_5 for k_z) controls the extent of the trajectory along the axis under consideration while the second (ϕ_2 for k_x , ϕ_4 for k_y and ϕ_6 for k_z) specifies the diameter of the segment in the direction perpendicular to the k-space axis. All six parameters for this cross shape are continuous (ie, there are no integer parameters).

Gradient Trajectory Design

Depending on the anticipated pulse duration and the type of trajectory, up to ≈ 50 control points are then placed in k-space. For the shells and stack-of-spirals trajectory, we use four control points per shell/spiral revolution positioned at 90° from each other. For the cross

trajectory, we place control points at the tips and at the center of each k-space axis segment, also resulting in four control points per revolution along the axis of the segment. We provide the exact one-to-one mapping between the shape parameters and the control point positions of each type of trajectory studied in the Supporting Material available online.

We compute the shortest smooth gradient trajectory $\mathbf{k}(t)$ connecting these control points in the order prescribed in a way that satisfies the gradient amplitude ($\|\dot{\mathbf{k}}(t)\|_{\infty} \leq G_{\max}$) and slew rate limitations ($\|\ddot{\mathbf{k}}(t)\|_{\infty} \leq S_{\max}$) using a novel semianalytical method we published recently (22,23). In short, this approach stitches together piecewise linear gradient segments, which results in piecewise quadratic k-space segments. The duration and slope of the gradient segments are optimized using a minimization algorithm subject to the gradient system performance constraints. Optimization of the individual G_x , G_y , and G_z segments is performed such that the k-space trajectory passes through all control points in the shortest time (the trajectory shape between control points is not predetermined and is optimized by the algorithm). This semianalytical optimization approach is fast (5 s on a single CPU for the design of a 10 ms 3D k-space trajectory) and highly stable. In other words, small perturbations of the control points positions result in small perturbations of the gradient waveforms without oscillations and divergence problems (22,23) which can affect other approaches such as optimal control techniques (24–27). We have found that high numerical stability of the gradient waveform design is crucial in our method. Indeed, instabilities such as oscillations and small violations of the gradient system performance constraints result in discontinuous variations of the objective function in Equation [3] and, therefore, cause premature termination of the optimization process and poor excitation performance of the pulse.

Integer Shape Parameters

As explained in the previous section, some shape parameters are of integer type. Because we use a gradient-based solver for optimization of these variables, which only handles continuous parameters, integer parameters are converted into continuous parameters (for example, a value of the parameter ϕ_4 in a shells trajectory equal to 3.9 means that the trajectory contains three shells). Because these parameters are varied by the optimizer, to avoid discontinuities of the objective function as these parameters are varied by the optimizer, we have found it necessary to use the following strategy. When an integer parameter is increased by the optimizer so that it crosses an integer quantity (eg, ϕ_4 in a shells trajectory increases from 3.9 to 4.1, which signifies that the number of shells increases from three to four), the additional entity created by this increase (eg, the new shell in our previous example) is associated with an infinitely small k-space extent. As a consequence, as this new entity is created, the objective function and pulse duration do not vary in a discontinuous manner. Alternatively, one might decide to remove such integer parameters from the optimization; however, we have found these to be powerful DOF used by the optimizer to fine tune the local sampling density of the trajectory to the magnetization pattern and B_1^+ maps at hand. For the stack-of-spirals trajectory, when changing ϕ_3 and ϕ_4 such that a new spiral needs to be added to the stack, we add two spirals in a symmetric fashion at $\pm k_{\max}$.

Evaluation of the Proposed Method

We evaluated our optimization framework for head imaging at 7T using an eight-channel pTx system (“Step 2” pTx system, Magnetom 7T; Siemens, Erlangen, Germany) loaded with a realistic 3D-printed head phantom with three compartments (bone, brain, and everything else) that we have described elsewhere (28). The B_1^+ and B_0 maps were measured using the product saturated Turbo-FLASH B_1^+ mapping (29) and the gradient echo field mapping sequences, respectively, at a matrix size of $128 \times 128 \times 20$ in a field of view of $20 \times 20 \times 12$ cm³ (Fig. 2). To reduce the computation time in the optimization process, the B_1^+ and B_0 maps were undersampled by a factor of two in the x and y directions (no undersampling in the slice direction), resulting in an effective voxel size of $3.0 \times 3.0 \times 6.0$ mm³. The pulses were evaluated by Bloch simulation using these measured field maps as well as experiments. All pulse optimizations were performed on a 64-bit Windows machine with an Intel Xeon CPU W 3565 processor with eight cores (3.2 GHz) and 16 GB of RAM.

We optimized shells, stack-of-spirals, and cross trajectories for two 10° flip angle excitation targets: excitation of a $4 \times 4 \times 4$ cm³ cube for reduced field of view imaging and excitation of the brain only for fat suppression (Fig. 2, top left). Both targets were blurred with a Gaussian kernel with $\sigma = 3$ mm and $\sigma = 1$ mm for the cube and brain target, respectively. The initial shape parameters of the three k-space trajectories were chosen so as to uniformly sample k-space up to $50\text{--}60$ m⁻¹ in the three directions in less than 5 ms, which corresponds to a sixfold undersampling. This is done in two steps: First, the spacing between sampling points (ie, the sampling density) in 3D k-space is chosen so as to roughly match the ratio of number of channels and the size of the FOX. In other words, we undersample in k-space by a factor equal to the number of transmit channels. Second, keeping this sampling density constant, the extent of the trajectory in k_x , k_y , and k_z is increased in a uniform manner (same extent in all three spatial directions) until the pulse duration constraint is equal to the maximum duration tolerated (5 ms in this study).

Additionally, we designed RF pulses using SPINS trajectories as proposed by Malik et al (30). SPINS are analytical 3D spherical spiral k-space trajectories with parameters controlling the maximum extent, radial velocity, and sampling density of the trajectory at the center and periphery of k-space. These SPINS trajectories as well as shells trajectories optimized by our method were used for flip angle uniformization (whole head) as well as excitation of a cube target magnetization pattern. SPINS pulses were initially proposed only for flip angle uniformization and, in their original implementation by Malik et al, were kept very short (less than 1 ms). For the purpose of spatially selective excitation (eg, excitation of the cube pattern), we increased the length of the SPINS pulse to 5 ms in order to sample the periphery of k-space as well.

All trajectories were designed with $G_{\max} = 40$ MT/m and $S_{\max} = 150$ T/m/s. RF and gradient waveforms were designed with temporal sampling of 10 μ s. The RF power Tikhonov regularization strength (α in Eq. [1]) was adjusted so as to limit the peak voltage to 150 V for all pulses per channel (this results in peak B_1^+ field strengths of 6.2, 6.2, 5.3, 6.6, 6.2, 6.2, 5.8, 6.2 μ T for transmit channels 1 to 8). The pulse duration regularization parameters (Eq. [2]) were adjusted so as to yield pulses with a duration shorter than 5 ms. The performance

of the RF pulses is characterized in terms of NRMSE. Denoting the achieved and the target flip angle distributions as FA_p and FA_p^{tar} (p denotes the pixel index), we compute the RMSE and NRMSE [%] as

$$RMSE = \sqrt{\frac{1}{P} \sum_{p=1}^P (FA_p - FA_p^{\text{tar}})^2}$$

$$NRMSE = 100 \cdot \frac{RMSE}{FA_{\text{max}}^{\text{tar}} - FA_{\text{min}}^{\text{tar}}} \quad [10]$$

RESULTS

Convexity Analysis

Figure 3 shows the results of our analysis of the convexity of the optimization problem in Equation [3] for the shells, stack-of-spirals, and cross trajectories and the two different target magnetizations (cube target in the top row, brain target in the bottom row). For all six pulses, we show the flip angle NRMSE as a colormap and the pulse duration (iso-contour lines of constant pulse duration) as functions of some of the shape parameters being optimized.

These results show that the flip angle error and pulse duration metrics vary continuously as a function of all parameters, even the integer parameters that control the number of shells (ϕ_4) and the number of spirals in the stack-of-spirals trajectories (ϕ_4). The well-conditioned overall topology of the flip angle error objective and pulse duration penalty make them well suited for optimization, which is due to our careful handling of noncontinuous integer shape parameters as well as the numerical stability and robustness of the gradient trajectory design method (22,23). The topology of the objective function (flip angle error plus pulse duration) clearly depends on the target magnetization profile and the type of gradient trajectory. In general, we do not expect it to be a convex function of the shape parameters, which is clearly visible for the cross trajectory/brain target panel (bottom right) of Figure 3. In this case, the objective function seems to show a slight worsening of the non-convexity problem (ie, the number of local minima seems to increase) at long pulse durations.

Figure 4 shows graphs of the pulse duration and flip angle error as a function of integer parameters controlling the number of shells and spirals in the shells and stack-of-spirals trajectories, respectively. The pulse duration and flip angle metrics are plotted as computed with our proposed approach for handling integer-type parameters (see Methods) and a naïve approach that does not handle integer shape parameters in any particular way (in this approach, when a new “entity” is created [eg, a shell or a spiral], it is not associated with zero k-space extent). This figure shows that naïve handling of integer parameters leads to discontinuities in both the pulse duration and flip angle error metrics, a problem that is easily solved by using our proposed approach.

Trajectory Optimization

Figures 5, 6, and 7 show the results of our joint optimization approach applied to shells (Fig. 5), stack-of-spirals (Fig. 6), and cross trajectories (Fig. 7). Each trajectory was optimized for excitation of the cube (left) and brain (right) target patterns. For each type of trajectory and

each target pattern, we show results for the unoptimized trajectory (first column), the trajectory optimized at Larmor frequency (no off-resonance constraints other than the B_0 map, second column), and the optimized trajectory using the spatio-spectral RF pulse design (with off-resonance constraints at ± 50 Hz in addition to the B_0 map, third column). For each of the 18 pulses (3 trajectories $\times$ 2 targets $\times$ 3 optimization strategies), we show the k-space trajectory (top), the achieved flip angle map (center), and the off-resonance performance in terms of flip angle NRMSE as a function of the offset frequency (bottom). Table 1 summarizes these results as well as computation times. In Figure 8, the RF and gradient waveforms of the optimized shells pulse for brain-only excitation are shown.

For both target magnetization patterns and all three types of trajectories, optimization of the k-space trajectory resulted in a significant improvement of the flip angle pattern (the flip angle performance improvement ranged from $\times 1.4$ to $\times 2.3$ for the cube target and $\times 2.4$ to $\times 6.6$ for the brain target when optimizing the gradient waveforms at Larmor frequency [ie, without off-resonance constraints]). For the cube magnetization target (left-hand side of Figures 5, 6, and 7), the overall best performance was achieved by the cross trajectory (NRMSE 3.4%, performance improvement $\times 1.4$), followed by the shells (NRMSE 3.6%, performance improvement $\times 2.3$) and the stack-of-spirals trajectory (NRMSE 3.7%, performance improvement $\times 2.1$). The performance improvement was less pronounced for the cross trajectory ($\times 1.4$) and the cube magnetization target, which is due to the acceptable performance of the unoptimized pulse in this case. Although the three trajectory types generated similar flip angle patterns, they have widely different k-space profiles, which emphasizes the nonconvexity of the gradient optimization problem. For the brain magnetization target (right-hand side of Figures 5, 6, and 7), the best performance after shape optimization at the Larmor frequency was achieved by the shells trajectory, which almost completely suppressed signal outside the brain in these simulations (NRMSE 6.2%, performance improvement $\times 6.6$). This followed by the cross (NRMSE 9.8%, performance improvement $\times 4.6$) and the stack-of-spirals trajectories (NRMSE 10.7%, performance improvement $\times 2.4$).

Enforcing robustness to off-resonance effects during trajectory optimization (spatio-spectral) reduced the accuracy of the achieved flip angle maps at the Larmor frequency but improved the excitation quality over the $[-50$ Hz, $+50$ Hz] frequency range. Compared with optimization at the Larmor frequency, the spatio-spectral design resulted in shorter trajectories with increased sampling density in the center of k-space at the cost of decreased sampling density at higher k-space frequencies, resulting in a slight blurring of the achieved magnetization pattern compared with pulses optimized at the Larmor frequency alone.

In Figure 9, we show a comparison of two SPINS pulses with 1 ms and 5 ms duration with optimized shells trajectories. These three trajectories (1 ms SPINS, 5 ms SPINS, 5 ms shells) were used for two excitation scenarios: Flip angle uniformization in the whole head (**a**) and excitation of a cube target pattern (**b**). The 1-ms SPINS pulse performs well for the flip angle uniformization problem, but is obviously a poor choice for the spatially selective excitation problem. On the other hand, the 5-ms SPINS pulse is able to sample k-space up to 60 m^{-1} and has a surprisingly good performance for excitation of the cube pattern (interestingly, the 5-ms SPINS performs less well than the 1-ms SPINS pulse for flip angle

uniformization due to its lower k-space sampling density at the center of k-space. As a result of this trajectory not spending a lot of time at the center of k-space, the RF power used at these locations is high and, therefore, the pulse is strongly peak power limited, which explains its poor flip angle performance). For the more challenging spatial selection problem (cube target), the use of optimized pulses proved especially beneficial. This is shown by the histogram of flip angle values outside the cube mask (Figure 9, c) showing a much lower signal level with the optimized shells trajectory than with the unoptimized 5-ms SPINS pulse.

Finally, we evaluated our optimized RF pulses on our 7T eight-channel pTx system; Supporting Figure S1 shows two GRE images corresponding to RF pulses based on an unoptimized k-space trajectory (shells trajectory) and a trajectory optimized using our approach. The target excitation pattern is a cube with a flip angle of 10° . We also show the Bloch simulation of the optimized pulse. The trajectory shape optimization significantly reduces residual signals outside of the field of excitation. Deviations between the GRE image and the Bloch simulation for this pulse (center and right) are clearly visible, which are likely due to eddy current effects. As was suggested by the work of several authors (13,31), this is due to the fact that we did not map the actual gradient waveforms played on the system.

All pulses computed in this study were shorter than 5 ms, which shows that accurate excitation of complex 3D magnetization patterns is possible using eight pTx channels and a clinical gradient system using reasonable excitation pulse duration, even when enforcing robustness to off-resonance effects.

Because a number of RF pulses need to be computed at every iteration of the shape parameter optimization loop, our joint RF and gradient optimization was rather time consuming. Computation times ranged from 0.8 to 3.5 h for the shape optimization at Larmor frequency and from 1.3 to 7.7 h for the spatio-spectral design. All computations were performed without acceleration and could be significantly shortened using multithreaded CPU or graphical processing unit (GPU) implementations.

DISCUSSION

In this study, we presented a joint optimization of gradient and pTx RF waveforms for improved excitation of arbitrary 3D excitation patterns. Our gradient trajectories are parameterized using a small number of shape parameters that are optimized numerically using a nested optimization process (the inner optimization loop is the RF design on a constant k-space trajectory, the outer loop is the k-space trajectory optimization). We found that reducing the dimensionality of the gradient optimization problem by optimization of global shape parameters as opposed to the position of individual control points (there are 50 control points in a typical trajectory) was critical to yield smooth trajectories with few sharp turns. This yielded fast trajectories that used the gradient system at maximum performance and, in turn, accurate excitations using pulses shorter than 5 ms using a conventional clinical gradient system ($G_{\max} = 40$ mT/m, $S_{\max} = 150$ T/m/s).

Although our k-space trajectories are parameterized using a small number of shape parameters, the precise contour of these trajectories in 3D k-space is defined using control points (there is a one-to-one mapping between a given set of shape parameters and the position of the individual control points in 3D k-space). Therefore, a key ingredient of our approach is a gradient trajectory design tool that is able to compute trajectories passing through the control points at maximum speed while satisfying the maximum gradient and slew rate constraints of the gradient system. For this, we use a method that we have published recently (22,23) based on a representation of the gradient waveforms using piecewise linear segments (this results in piecewise quadratic k-space segments). A major advantage of this approach is its high numerical stability. In other words, small perturbations of the position of the control points yield only small changes in the optimal gradient waveforms in this method, which in our experience is not always the case with other gradient waveform design strategies such as optimal control methods (24–27). Advantages of our approach include its high numerical stability, the fact that gradient performance limits are exactly satisfied (ie, no $G_{\max}/S_{\max}$ violation) and that the trajectory is guaranteed to exactly traverse all the prescribed control points [For an extensive comparison between this gradient trajectory design approach and optimal control, see Figs. 9 and 10 of Davids et al (23), which show better performance of our semianalytical approach in these three metrics compared with optimal control]. We note that because we use a numerical optimization of the trajectory shape parameters, excellent numerical stability of the gradient waveform design method must be guaranteed for a large class of possible trajectories, including complex nonsmooth trajectories that may not be optimal but still need to be explored by the optimization process to converge to the final solution. In our experience, the presence of small oscillations, numerical instabilities, and small violations of the gradient system constraints in the gradient waveform design step (which are difficult to avoid when using optimal control) prevented convergence of the k-space trajectory optimization process.

We found in this study that optimization of the shape parameters had a profound effect on the k-space trajectories. The optimization process resulted in trajectories that sample 3D k-space in a highly heterogeneous manner in an apparent effort to focus the RF energy in k-space regions that maximally impact the flip angle distribution. For the shells and stack-of-spirals trajectories, the result of the trajectory optimization was a compression of the overall trajectory compared with the unoptimized case. This is likely due to the fact that the coil used in this study has only one row of eight channels and therefore creates only mild variations of B_1^+ in the z-direction, which in turn prevents the algorithm from undersampling k-space in this direction. Under the constraint of limited pulse duration, increasing the sampling density along the z-direction causes $k_{z,\max}$ to decrease for the shells and stack-of-spirals trajectories. This result was also observed when using a cross trajectory to excite the brain (Fig. 7) but not when using the cross to excite a cube of magnetization. This is probably due to the fact that the cross trajectory almost perfectly matches the energy deposition pattern in 3D k-space of a cube, and the algorithm does not change the initial cross trajectory significantly in this case. We also found that when robustness to off-resonance effects is enforced, the shape optimization procedure concentrated the energy of the trajectory at the center of k-space. This reduced the resolution of the achieved excitation profile, but improved the off-resonance performance due to the shorter pulse duration.

The parameterized trajectories analyzed in this study allow the optimizer to adjust the k-space sampling density in a way that is highly nonuniform and tailored to the B_1^+ maps as well as the target magnetization pattern. However, an unwanted property of the optimization problem of Equation [1] is the dependence of the optimized result on the initial value of the trajectory shape parameters. In our experience, properly setting up the initial values of the shape parameters is crucial, which is related to the fact that the optimization problem that we attempt to solve is highly nonconvex. In order to initialize the optimization process, we choose the shape parameters so as to sample the k-space volume defined by the outer portion of the 3D trajectory more or less uniformly. In our experience, a choice of initial shape parameters that should be avoided is one associated with a level of k-space undersampling beyond the acceleration capability of the transmission coil array (eg, for an eight-channel transmit array, the initial level of undersampling must not exceed a value of 8). Another important consideration is to choose an initial trajectory with duration below the maximum tolerated duration. Otherwise early iterations are used to reduce the pulse duration without improvement in the flip angle error, which increases computation time unnecessarily.

We found that implementation details were important to ensure fast convergence of the proposed method. As discussed previously, a robust and numerically highly stable gradient trajectory design algorithm is crucial. Additionally, we found that trajectory shape parameters that were of integer type warranted special treatment in the optimization process. Indeed, these parameters control noncontinuous features of the trajectory such as the number of shells or the number of spirals per stack. As we showed in Figure 4, a naïve implementation of the optimization of these parameters leads to large discontinuities in the optimization metrics (both the flip angle NRMSE and the pulse duration, which we penalize in the objective function), which would cause the algorithm to diverge or stop prematurely. A simple solution to this problem is to vary these integer parameters in such a way that the creation of a new entity, such as a new shell or new spiral, does not cause discontinuities in the objective function. We do this by initializing the newly created entities with infinitely small k-space extent (see Methods).

The topology of the least-squares objective function optimized in this study as a function of the shape parameters depends heavily on the type of gradient trajectory and the target flip angle pattern. It is clear from these investigations that the objective function is continuous but not convex and has several local minima. Therefore, convergence of the proposed approach is limited to local minima (ie, we do not claim to be able to find the best of all possible gradient waveforms satisfying the maximum pulse duration constraint of 5 ms). At any rate, the local pulse solutions found by our algorithm seem to be good enough, because they yield significantly improved flip angle profiles compared with unoptimized gradient waveforms.

A significant limitation of our approach is its rather long computation time: For the shape optimization at the Larmor frequency, computation times ranged from 0.8 to 3.5 h. Enforcing robustness to off-resonance effects further increased runtime (1.3–7.7 h), because of the increased complexity of the RF design problem. In its present form, therefore, the technique is not suitable for patient-specific joint optimization of RF and gradient trajectories. However, computation time could be easily decreased using multithreaded

implementations, especially using GPUs. For example, an acceleration factor of 100, which is common for applications amenable to GPU acceleration, would yield computation times between 0.5 and 2.1 min. We note that matrix operations are highly parallelizable; therefore, optimization of the RF waveform on a constant gradient trajectory, which is the computational bottleneck of our approach, could probably be widely accelerated in this way.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Visual depiction of the effect of shape parameters on the k-space trajectories analyzed in this study (first row, shells; second row, stack-of-spirals; third row, cross trajectories). The effect of each parameter is shown by comparison with an “undeformed” trajectory on the left (the illustrated parameter changes are relatively large in order to facilitate visualization of the effect of each parameter).

FIG. 2.

Target magnetization profiles, B_0 map, and B_1^+ maps used in this work for evaluation of the proposed approach. A different slice is shown for the B_0 map that shows the characteristic B_0 frontal lobe hot spot (this slice is part of the stack being optimized). The cubic target has a dimension of $4 \times 4 \times 4 \text{ cm}^3$. The brain target covers the whole brain and excludes other tissues such as the skull, dura, fat, muscle, and so forth. Both target flip angle distributions are uniform within the excited volumes and equal to 10° .

FIG. 3.

Topology of the objective function in Equation 3 as a function of a subset of the shape parameters for the shells, stack-of-spirals, and cross k-space trajectories. The flip angle (FA) error (colormap) and pulse duration (isocontours) metrics, which are combined to form the total objective function used in our optimization framework, are shown for both the cube and brain target magnetization patterns. Although these optimization metrics are not convex with respect to the shape parameters, they vary continuously with respect to these variables and are, therefore, well suited for optimization.

FIG. 4.

Plot of the pulse duration and flip angle NRMSE metrics as a function of the integer shape parameters for the shells and stack-of-spirals trajectories. These integer shape parameters control noncontinuous features of the trajectories such as the number of shells (ϕ_4) and the number of spirals (ϕ_4) in the shells and stack-of-spirals trajectories, respectively. For each trajectory and optimization metric, we show two ways of computing the metrics. In the first naïve way, the integer parameters are varied in the same way as other continuous parameters. In the second way, which we use in our approach, every time the integer parameter crosses a value that triggers the creation of a new entity (eg, a new shell or a new spiral), the resulting new entity is created with zero k-space extent. This simple strategy removes large discontinuities in the objective function and thus renders it more suitable to optimization.

FIG. 5.

k-space trajectories and flip angle profiles obtained with the shells trajectory for excitation of the cube and brain-only target patterns (10°). For each target, three sets of results are shown corresponding to optimization of the RF waveform alone (left), joint optimization of the RF and gradient waveforms (center), and joint optimization with enforced off-resonance robustness (right). The two white numbers give the flip angle NRMSE in the entire FOX and outside of the cubic/brain-only target region (in parentheses). For each set of results, the off-resonance performance was evaluated in terms of the flip angle NRMSE as a function of the offset frequency (bottom).

FIG. 6.

k-space trajectories and flip angle profiles obtained with the stack-of-spirals trajectory for excitation of the cube and brain-only target patterns (10°). For each target, three sets of results are shown corresponding to optimization of the RF waveform alone (left), joint optimization of the RF and gradient waveforms (center), and joint optimization with enforced off-resonance robustness (right). The two white numbers give the flip angle NRMSE in the entire FOX and outside of the cubic/brain-only target region (in parentheses). For each set of results, the off-resonance performance was evaluated in terms of the flip angle NRMSE as a function of the offset frequency (bottom).

FIG. 7.

k-space trajectories and flip angle profiles obtained with the cross trajectory for excitation of the cube and brain-only target patterns (10°). For each target, three sets of results are shown corresponding to optimization of the RF waveform alone (left), joint optimization of the RF and gradient waveforms (center), and joint optimization with enforced off-resonance robustness (right). The two white numbers give the flip angle NRMSE in the entire FOX and outside of the cubic/brain-only target region (in parentheses). For each set of results, the off-resonance performance was evaluated in terms of the flip angle NRMSE as a function of the offset frequency (bottom).

FIG. 8.

Gradient (top) and RF waveforms (bottom) for an optimized shells trajectory exciting the brain target (this pulse corresponds to the results of Fig. 5). Shown are the concatenated RF magnitude and phase waveforms for the eight-channel transmit coil (ie, the intervals separated by red dashed vertical lines corresponds to a full pulse duration of 4.5 ms). The piecewise linear gradient segments yield piecewise quadratic k-space segments.

Head Magnetization Target **Cube** Magnetization Target

FIG. 9. k-space trajectories and flip angle profiles for the 1-ms SPINS pulse, 5-ms SPINS pulse, and optimized shells trajectories obtained using our approach. Results are shown for both a uniform excitation in the whole head **(a)** and excitation of a cubic pattern **(b)**. All pulses use the gradient system at maximum performance. The two white numbers give the flip angle NRMSE in the entire FOX and outside of the cubic target region (in parentheses; does not apply for the head target). The optimized shells trajectory shows improved performance compared with the SPINS trajectories for the spatial selection problem, which is quantified by the histogram of values outside the target mask **(c)**.

Table 1

Performance of the unoptimized and optimized RF pulses

Target/Trajectory	Unoptimized Trajectory		Trajectory Optimization (at Larmor Frequency)			Trajectory Optimization (Spatio-Spectral Design)		
	NRMSE (Duration, ms)		NRMSE (Duration, ms)	Improvement Factor	Runtime, h	NRMSE (Duration, ms)	Improvement Factor	Runtime, h
Cube								
Shells	8.4% (4.9)		3.6% (5.0)	×2.3	3.5	5.2% (3.2)	×1.6	5.1
Stack-of-Spirals	7.6% (4.9)		3.7% (4.8)	×2.1	2.3	6.5% (2.9)	×1.2	2.5
Cross	4.7% (5.1)		3.4% (5.0)	×1.4	2.7	4.6% (5.0)	×1.0	7.7
Brain								
Shells	41.2% (4.9)		6.2% (4.5)	×6.6	2.5	12.8% (4.4)	×3.2	3.9
Stack-of-Spirals	26.2% (4.9)		10.7% (4.4)	×2.4	0.8	18.8% (3.1)	×1.4	1.3
Cross	45.3% (5.1)		9.8% (4.1)	×4.6	1.1	15.4% (3.1)	×2.9	2.6

Flip angle NRMSE, pulse duration, performance improvement factor, and computation time for the 18 pulses designed in this study. The performance improvement factor is the ratio of the flip angle NRMSE with and without optimization of the gradient trajectory.