Simulation of spin dynamics: a tool in MRI system development

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Abstract. Magnetic Resonance Imaging (MRI) is a routine diagnostic tool in the clinics and the method of choice in soft-tissue contrast medical imaging. It is an important tool in neuroscience to investigate structure and function of the living brain on a systemic level. The latter is one of the driving forces to further develop MRI technology, as neuroscience especially demands higher spatiotemporal resolution which is to be achieved through increasing the static main magnetic field, $B_0$. Although standard MRI is a mature technology, ultra high field (UHF) systems, at $B_0 \geq 7$ T, offer space for new technical inventions as the physical conditions dramatically change. This work shows that the development strongly benefits from computer simulations of the measurement process on the basis of a semi-classical, nuclear spin-$1/2$ treatment given by the Bloch equations. Possible applications of such simulations are outlined, suggesting new solutions to the UHF-specific inhomogeneity problems of the static main field as well as the high-frequency transmit field.

1. Introduction

In the past five years the number of ultra-high field (UHF) MRI systems (7 T and higher) has grown rapidly. Neuroscientists have particular interest, since UHF is an important tool to investigate structure and function of the living brain with increased spatiotemporal resolution. Additionally, new contrast mechanisms arise at UHF, providing additional structural information not available with conventional MRI at clinical field strength [1]. Especially functional MRI benefits, as not only the BOLD contrast increases, but also new imaging techniques with enhanced spatial specificity of the functional contrast are feasible [2]. One field of research in MRI method development is to avoid susceptibility-induced artefacts in fast imaging acquisitions, since subject-induced distortions of the main field are much more pronounced at UHF. However, most challenging is to master a homogeneous high-frequency excitation across the region of interest: at UHF the RF wavelength gets shorter than the size of the human head, leading to unwanted wave effects in the acquired image [3]. In both situations MRI simulations help to optimise the acquisition process.

Numerical simulation of MRI experiments, based on the Bloch equation, is an essential tool for a variety of different research directions. In the field of pulse sequence optimisation, e.g. for artefact detection and elimination, simulations allow differentiation between effects arising principally from MRI physics and those due to hardware imperfections. If the simulation environment is able to simulate hardware malfunction, then the results may be used for the optimisation of the
Another prominent application is the design of specialised RF pulses which is often based on numerical simulations of the excitation process. In general, the interpretation and validation of experimental results benefits from comparisons to simulated data. Another important application is image generation for the purposes of medical image processing – here, complete control of the properties of the input data allows a tailored design of image processing algorithms. Last but not least, MRI simulations give an extraordinary insight to the complex physics of MR signal generation and the encoding of spatial information with imaging gradients. Especially interesting is the observation of aspects which are hidden in the real experiment – for instance the time evolution of the longitudinal magnetisation. With regard to the latter point, therefore, controlled numerical MRI experiments are also highly valuable for educational purposes.

This work concentrates on new techniques for MR image homogenisation at UHF by means of MRI simulation. The next section gives a brief description of the MRI measurement process from the viewpoint of computer simulation. Afterwards section 3 presents two possible applications of MRI simulations in order to mitigate the above-mentioned inhomogeneities typically occurring at UHF.

2. MRI Simulations

All MRI simulations in this paper are performed with the recently published software package jemris which is freely available under http://www.jemris.org. All details on the numerical implementation of jemris are to be found in [4]. This section describes the most important physical principles as implemented in jemris, reflecting the hardware of a modern MRI scanner, i.e. including the possibility to transmit and receive with multiple channels. Examples of spin dynamics and signal formation are illustrated.

2.1. Spin dynamics

MRI simulations are mostly based on the semi-classical description of nuclear magnetic resonance as described by the Bloch equations [5], providing an exact concept for the description of non-interacting spin isochromats under the influence of an external magnetic field. This driving field decomposes into a strong static component as well as a temporally and spatially varying field along the same direction (the “imaging gradients”) and rapidly varying components in orthogonal directions (the RF field). A mathematical treatment is simplified in the rotating frame of reference, precessing at Larmor frequency, \( \omega_0 = \gamma B_0 \), where \( \gamma \) denotes the gyromagnetic ratio of the nucleus. Here, the effect of the main field, \( B_0 \), can be ignored and the magnetic field at time \( t \) and position \( x \) is given by:

\[
B(x, t) = [G(t) \cdot x + \Delta \omega(x, t)]e_z + \sum_{n=1}^{N} (B_{1x}^n(x, t)e_x + B_{1y}^n(x, t)e_y),
\]

(1)

where \( e_{x,y,z} \) denote unit Cartesian vectors, \( B_{1x,y}^n(x, t) \) are the excitation RF components of the \( n \)-th transmit coil, \( G(t) \cdot x \) is the linear gradient field, and \( \Delta \omega(x, t) \), accounts for various off-resonance effects such as chemical shift of the nucleus, macroscopic field inhomogeneity, and microscopic field fluctuations. The numerical integration of a dynamic system is demanding if the solution changes rapidly as the Cartesian components of the transverse magnetisation. Instead, the Bloch equation in cylindrical coordinates, \( (M_r, \varphi, M_z) \), is very well suited for numerical implementation,

\[
\begin{pmatrix}
M_r \\
\varphi \\
M_z
\end{pmatrix}
= \begin{pmatrix}
\cos \varphi & \sin \varphi & 0 \\
-\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix}
\cdot \begin{pmatrix}
0 \\
0 \\
M_0
\end{pmatrix}
+ \begin{pmatrix}
-\gamma B_x & \gamma B_z & -\gamma B_y \\
\gamma B_z & \gamma B_x & -\gamma B_y \\
-\gamma B_y & \gamma B_y & -\gamma B_y
\end{pmatrix}
\cdot \begin{pmatrix}
M_r \cos \varphi \\
M_r \sin \varphi \\
M_z
\end{pmatrix}
\]

(2)
where the transverse magnitude, $M_r$, is only subject to $T_2$ decay and oscillations are described by smooth phase evolution, $\varphi(t)$. Figure 1 depicts an example of the magnetisation dynamics during so-called adiabatic inversion [6], an important concept for $B_1$-insensitive manipulation of $T_1$ contrast.

\[ S_n(t) = \int x w_n^*(x) M_r(x,t) e^{i\varphi(x,t)} d^3x. \]  

(3)

where $w_n^*(x)$ denotes the spatial sensitivity of the $n$-th receiver coil. Apart from the size of the spin system, other effects need to be considered in order to simulate realistic MR signals. Field inhomogeneities lead to off-resonance: the well-known $T_2^*$ effect is based on the fact that a real sample will always distort the magnetic field on mesoscopic scales of neighbouring isochromats. This effect is realistically simulated by adding small Lorentzian distributed random off-resonance terms to each simulated isochromat, given by the inverse Cauchy-Lorentz cumulative distribution function:

\[ \Delta \omega(x) = R'_2 \tan \left[ \pi \left( X(x) - \frac{1}{2} \right) \right]. \]  

(4)

Here, $X(x)$ denotes a uniformly distributed random variable and $R'_2$ is the reversible component of the total relaxation rate, i.e. $1/T_2^* = 1/T_2 + R'_2$. The corresponding dephasing of isochromats leads to an exponentially reversible signal decay which can be refocused with a spin echo. A common example of MRI echo generation is depicted in figure 2, showing that three excitation pulses yield five MR echoes.
Three RF Pulses: $60^\circ - \tau_1 - 90^\circ - \tau_2 - 90^\circ$

Figure 2. MR signal simulation for a pulse sequence consisting of three RF pulses: $60^\circ - \tau_1 - 90^\circ - \tau_2 - 90^\circ$ with delay times $\tau_1=10\text{ms}$ and $\tau_2=15\text{ms}$. The object parameters were $T_1=T_2=50\text{ms}$ and very short $T_2^*=1\text{ms}$, resulting in the well-known five echo signals: three spin echoes at $2\tau_1$, $\tau_1 + 2\tau_2$, $2(\tau_1 + \tau_2)=20$, 40, 50 ms, one reflected spin echo at $2\tau_2=30\text{ms}$, and the stimulated echo at $2\tau_1 + \tau_2=35\text{ms}$, respectively. RF pulses (dashed lines) rotate the magnetisation around the $x$-axis, resulting in signal on the $y$-axis.

3. Application of MRI simulations in UHF-MRI system development

UHF-MR image quality suffers from patient-induced distortions of the main field as well as short-wavelength of the high frequency excitation field [7]. This chapter illustrates that MRI simulation support the understanding as well as the exact quantification of these effects, directly supporting the technical development to mitigate the according image inhomogeneities. Whereas section 3.1 gives outlook to the performance of not yet available hardware, i.e. the possibility to dynamically pulse higher order correction fields for $B_0$-homogenisation, section 3.2 shows how MRI simulations support RF pulse calculation in case of multichannel RF transmit, which is already available on most recent UHF systems.

3.1. Shimming the main field

Curved spatially-varying magnetic fields have a strong impact on MRI, especially in the context of correcting magnetic field inhomogeneities (shimming) [8]. Conventional methods are well established, but new progress from hardware and sequence development intends to overcome certain limitations, e.g. by the use of higher-order shim coils or the application of spatially-selective dynamic shimming [9]. Beyond field corrections, curved field gradients are currently also under discussion for region-specific zoomed spatial encoding with reduced hardware demand and peripheral nerve stimulations at higher switching rates [10]. However, the gains from such strategies depend on many factors and are hardly predictable without simulations [9, 10].

The simulator jemris was extended by the ability to spatially shape any involved pulsed gradient through a user-defined analytical formula. In this way, the functionality of arbitrary nonlinear gradient shapes directly applies down to each explicit gradient module of the framework. The approach is demonstrated for shimming a human brain phantom with susceptibility-induced field inhomogeneities mimicking 9.4 T. Ultra-fast EPI imaging, which is especially prone to susceptibility-induced artefacts [11], was simulated for the cases of the homogeneous $B_0$ field, the uncorrected inhomogeneous field, and shim-corrected inhomogeneous fields up to $2^{nd}$ and $3^{rd}$ order ellipsoidal harmonics [12], respectively. The correction fields were optimised to dynamically mitigate field inhomogeneities during the pulse sequence, thus, different correction terms were pulsed during frequency and phase encoding, respectively. Figure 3 depicts the simulation results with and without field inhomogeneities and dynamic shim corrections, respectively. The results enable exact prediction of shim performance.
3.2. Multichannel selective excitation pulse computation through time-reversed simulation
Spatial inhomogeneous excitation at high field results from short wave length of the RF transmit field. Compensating the inhomogeneity is possible by means of spatially selective excitation with multiple transmitting RF coils with varying spatial sensitivities [13]. Common formulations to derive the needed RF waveforms require the solution of a huge inverse problem [14]. This section shows that it is also possible to calculate the waveforms through forward integration of the Bloch equation followed by spatial integration of all isochromats.

As introduced by Pauly et al. [15], in selective excitation the magnetisation is investigated under the limits of the small tip-angle approximation (STA), \( \frac{dM_z}{dt} \approx 0 \) and \( M_z \approx M_0 \). Using complex notation \( m = M_x + iM_y \) and \( B_1 = B_x + iB_y \) and the conventional definition of the k-space vector, \( k(t) = \gamma \int_0^t G(\tau) d\tau \) and assuming a self-refocussed k-space trajectory, \( k(T) = 0 \), the STA solution of equation (2) after an RF pulse of duration \( T \) is

\[
m(T) = i\gamma M_0 e^{-T/T_2} e^{-it\Delta \omega} \int_0^T B_1(\tau) e^{\tau / T_2} e^{it\Delta \omega} e^{i k(\tau) \cdot x} d\tau
\]  

for the initial value \( m(0) = 0 \) (equilibrium). Now consider the MR signal following selective excitation

\[
s(t) = \int_{\mathbb{R}^3} e^{-t / T_2} e^{-it\Delta \omega} m(T, x) e^{-ik'(t) \cdot x} d^3 x
\]

where \( k'(t) \) denotes a k-space trajectory during signal acquisition. If now spatially uniform relaxation and off-resonance is assumed, and defining the exponential function \( E(t) = \exp[-t / T_2 - it\Delta \omega] \) to summarise these effects, then the time-reversed simulation of the signal in equation (6) along the excitation process yields the wanted \( B_1 \) in order to spatially excite the target pattern of transverse magnetisation, \( m(T, x) \). Time reversal of the selective excitation encoding, see figure 4, requires one to set \( k'(t) \to k(T - t) \) and \( E(t) \to E(-t) \) in equation (6). Inserting then equation (5) into equation (6) yields

![Figure 3. Top row: EPI simulations without and with 9.4T field inhomogeneities. Bottom row: Additional simulation of dynamic shim-corrections up to 2nd and 3rd order ellipsoidal harmonics, respectively.](image)
\[ s(t) = i\gamma M_0 E(T) E(-t) \int \int B_1(\tau) E(-\tau) e^{i[k(\tau) - k(T-t)] \cdot x} d\tau d^3x \]
\[ = i\gamma M_0 E(T-t) \int B_1(\tau) E(-\tau) \delta[k(\tau) - k(T-t)] d\tau = i\gamma M_0 B_1(T-t) \quad (7) \]

where the integration over the $\delta$-function requires a non-crossing k-space trajectory with unique mapping $t \mapsto k(t)$, ensuring that $k(\tau) = k(t)$ if and only if $t = \tau$.

Denoting the Fourier Transform (FT) operator from image space to k-space as $F[\cdot]$, equations (6) and (7) imply $B_1(k(t)) \propto F[m(T, x)]$, stating the well-known FT relationship between excitation pattern and RF pulse in STA selective excitation. In general, equations (5,6,7) show that the wanted $B_1$ waveform for a given target excitation pattern, $m(x)$, and a given self-refocussed, non-crossing k-space trajectory, $k(t)$, is obtained by the time-reversed solution of the Bloch equation for each isochromat, followed by spatial integration over all isochromats. This dependency is now generalised to the case of multiple transmitters with $N$ perfectly decoupled transmit channels, each with spatial sensitivity weighting, $w_n(x)$, and temporal modulation $b_n(t)$. The total $B_1$ transmit field is then given by

\[ B_1(x,t) = \sum_{n=1}^{N} w_n(x)b_n(t) , \quad (8) \]

where both the sensitivities and the pulseshapes are complex quantities, i.e. $w_n, b_n \in \mathbb{C}$. Now consider the simulation of $N$ time-reversed signals, $s_n(t)$, $n = 1 \ldots N$, stemming from the excitation in equation (5) with time reversal as described above and with complex conjugated receiver sensitivities, $w_n^*$:

\[ s_n(t) = E(-t) \int w_n^*(x) m(x, T) e^{i[k(T-t) \cdot x]} d^3x \quad (9) \]

Inserting equations (8) and (5) into (9) yields

\[ s_n(t) = i\gamma M_0 E(T-t) \sum_{m=1}^{N} \int_0^T E(-\tau) b_m(\tau) \left( \int w_n^*(x) w_m(x) e^{i[k(T-t) - k(\tau)] \cdot x} d^3x \right) d\tau \]
\[ = i\gamma M_0 E(T-t) \sum_{m=1}^{N} \int_0^T E(-\tau) b_m(\tau) \hat{w}_{nm}(k(T-t) - k(\tau)) d\tau \quad (10) \]
with $\hat{w}_{nm}(k)$ denoting the FT of the spatial-sensitivity quadratic form $w_{nm}(x) = w_n^*(x)w_m(x)$. If the transmit coil sensitivities $w_{nm}(x)$ are known from experiments [16], equation (10) can be solved for the wanted $b_n(t)$ waveforms by means of exact multichannel deconvolution techniques. A surprisingly good estimate is already given by

$$s_n(t) \approx i\gamma M_0 b_n(T - t)$$

which follows from equation (10) by assuming spatially disjoint sensitivities, i.e. $|\hat{w}_{nm}(k)| \gg |\hat{w}_{nm}(k)|$ for $n \neq m$, and approximating $\hat{w}_{nm}(k) \approx \delta(k)$. An example of a corresponding 3D selective excitation experiment is depicted in figure 5. Here, an inner volume selective excitation was performed on a 4 T human MR scanner (Bruker MedSpec4T, Bruker BioSpin GmbH, Rheinstetten, Germany). The RF pulse according to the target region (c.f. figure 5(b) top) were obtained through jemris simulation along a 4-fold accelerated 3D spiral trajectory and a duration of 5.12 ms (c.f. figure 5(a)). The according coil sensitivities were acquired with the Actual Flip-angle Imaging method (AFI) [16] and fed as the $w_{nm}(x)$ into the simulation. The simulated receiver channels were then time-reversed and used as the $b_n(t)$ for exciting the target pattern along the same 3D spiral trajectory in a second experiment on the MR scanner. Acquisition was done with standard gradient echo imaging and with pseudo-parallel setup [17], as parallel transmit hardware is not available on this system. The resulting inner volume imaging (c.f. figure 5(b) bottom) shows good suppression of the outer regions.

4. Discussion and Conclusion
This manuscript describes applications of MRI simulations to current problems in ultra-high field MRI. The simulations were performed with the new software environment jemris. After a general introduction to the physical background of MRI simulation, it was shown how MRI system development gains from such simulations.

The simulator jemris can treat multiple off-resonance effects such as the susceptibility-induced
field variations at high magnetic field. Further, pulsed spatially encoding fields – the gradients – may be driven with arbitrary nonlinear field dependence. Together, it is therefore possible to test the performance of higher order pulsed correction fields (shimming), which is not yet available on current MRI systems. In section 3.1 the method was successfully tested for the fast imaging sequence EPI. Generally, new strategies involve new hardware development, which should be subject to preceding extensive simulations in order to maximise application-specific efficiency of the concepts. The presented approach allows such simulations with few limitations on the complexity of the physical processes: it enables simple definition of spatially arbitrarily-shaped, non-linear gradient pulses in combination with the most general numerical Bloch equation simulations. Such an approach may lead to new developments in MRI; that is, simulation-driven development of MRI hardware which then feeds directly into the development of new techniques.

Finally MRI simulations were applied to calculate the waveforms of RF pulses in multichannel selective excitation. Whereas current available approaches to this problem rely on the inversion of a large system matrix [14, 17], it is shown here that the time-reversed MRI signal equation can be formulated to represent the excitation process. In this way the waveforms directly correspond to the simulated signals and, therefore, no matrix inversion is needed. Hence, massive parallelisation of such calculations is possible. This and other possible advantages of the approach will be investigated in the future.

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