Numerical Methods in Magnetic Resonance Imaging: The Bloch-Torrey Equation

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In magnetic resonance imaging, insight into different imaging modalities can be gained through the simulation of the magnetic resonance signal measured by the scanner. This signal is modelled as the solution of the parabolic Bloch-Torrey partial differential equation. In this work, I compare various numerical techniques for solving the Bloch-Torrey equation in the presence of highly discontinuous data with the goal of optimising the trade-off between solution accuracy and computation time.

Introduction

In magnetic resonance imaging (MRI), insight into different imaging modalities can be gained through the simulation of the magnetic resonance (MR) signal from first principles. The MR signal which is measured by an MRI scanner within a given region is directly proportional to the magnitude of the net magnetization vector $\mathbf{M}$ within that region. In tissue, $\mathbf{M}$ arises due to the superposition of the magnetic moments of water molecules, also known as *spins* in MRI nomenclature. Ordinarily, $\mathbf{M}$ is zero in tissue as spins are randomly oriented and therefore their vector sum is zero on the average. In MRI, however, there is a large and constant external magnetic field $\mathbf{B_0} = B_0\hat{\mathbf{z}}$ which forces the alignment of the magnetized spins with $\mathbf{B_0}$, taken here to be along the z-direction. This allows for the measurement, and importantly, the manipulation of the otherwise negligible net magnetization $\mathbf{M}$ of the spins.

In one common type of MRI scan, a *gradient echo* scan, $\mathbf{M}$ is initially flipped into the xy-plane through the application of a radio frequency (RF) magnetic pulse. Immediately, $\mathbf{M}$ begins to realign with $\mathbf{B_0}$ exponentially quickly. The rate $R(\mathbf{x})$ at which this realignment occurs, however, depends on local tissue properties. Additionally, there is a characteristic precession of $\mathbf{M}$ about $\mathbf{B_0}$ as it realigns. This precession occurs at a rate $\omega(\mathbf{x})$ which, too, depends on the magnetic properties of the environment. Lastly, spins are free to diffuse within their environment while realigning, which means that they will see varying $R(\mathbf{x})$ and $\omega(\mathbf{x})$ as they move through the tissue.

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The Bloch-Torrey equation

In the continuum limit, the net magnetization $\mathbf{M}$ within a given region is modelled as a continuous vector field, and the complex dynamics which follow the initial RF pulse can be beautifully modelled as solutions to a parabolic partial differential equation (PDE) called the Bloch-Torrey equation [1]:

$$\begin{cases} u_t = D\Delta u - Ru + \omega v \\ v_t = D\Delta v - Rv - \omega u \end{cases} \tag{1}$$

Here, u and v are the x- and y-components of the magnetization $\mathbf{M}$ and D is the diffusion constant. For short simulation times, or *echo times*, T, the z-component of $\mathbf{M}$ does not change appreciably, and we need only consider the transverse magnetization $\mathbf{M}_\perp = (u, v)$.

The transverse Bloch-Torrey equation (1) may be equivalently written as

$$\mathcal{M}_t = D\Delta\mathcal{M} - \Gamma\mathcal{M} \tag{2}$$

where $\mathcal{M} = u+iv$ is the complex magnetization and $\Gamma(\mathbf{x}) = R(\mathbf{x}) + i\omega(\mathbf{x})$ is the complex decay rate. This form is both notationally convenient and conceptually illustrative; now, realignment with $\mathbf{B_0}$ corresponds to the magnitude of the (complex) transverse magnetization $\mathcal{M}$ decaying to zero, and the precession of $\mathbf{M}$ about $\mathbf{B_0}$ corresponds to the rotation of $\mathcal{M}$ about the origin in the complex plane.

Signal simulation

This work will compare three different methods of simulating the signal $S(T)$ measured by an MRI scanner at a time T following an initial RF pulse: finite differences, splitting methods, and finite element methods.

The MR signal $S(T)$ is given by

$$S(T) = \left\| \int_\Omega \mathbf{M}_\perp(T)\,\mathrm{d}x \right\| \tag{3}$$

where $\mathbf{M}_\perp(T)$ is computed by solving (1) or (2). The initial transverse magnetization $\mathbf{M}_\perp(t=0)$ will be taken to be $[0, 1]^T$ without loss of generality.

Geometry

The transverse magnetization $\mathbf{M}_\perp$ will be simulated within a cubic domain Ω of size $3 \times 3 \times 3\,\mathrm{mm}^3$ with a single cylinder of a variable radius a in the centre of the domain, as pictured in Figure 1.

This geometry is chosen for two reasons. First, biologically it represents a single vessel present within a cubic imaging voxel. Second, there exists an exact solution for $\omega(\mathbf{x})$ given the magnetic susceptibility χ of the cylindrical blood vessel. For a cylinder of radius a, we have that

$$\omega(\mathbf{x}) = \begin{cases} \frac{\chi B_0}{2} \sin^2\theta \frac{a^2}{x^2+y^2} \frac{y^2-x^2}{x^2+y^2}, & \text{inside cylinder} \\ \frac{\chi B_0}{6} \left(3\cos^2\theta - 1\right), & \text{outside cylinder} \end{cases} \tag{4}$$

where θ is the angle between the cylinder axis and $\mathbf{B_0}$. An example cross section of $\omega(\mathbf{x})$ can be seen in Figure 1.

Methods

Finite difference methods, splitting methods, and finite element methods will be investigated. First, some basic properties of the Bloch-Torrey equation are described.

Static solution

If $D = 0$, solutions to (2) are simply complex exponentials

$$\mathcal{M}(\mathbf{x}, t) = \mathcal{M}_0 e^{-\Gamma(\mathbf{x})t} = \left(e^{-R(\mathbf{x})t} \left|\mathcal{M}_0\right|\right) e^{i(\phi_0 - \omega(\mathbf{x})t)}, \tag{5}$$

where we have written $\mathcal{M}_0 = |\mathcal{M}_0|\, e^{i\phi_0}$ in polar form. In this form, it is clear to see that the magnitude $|\mathcal{M}| = \|\mathbf{M}_\perp\|$ of the transverse magnetization is exponentially damped at rate $R(\mathbf{x})$ and that the initial phase ϕ_0 changes at the constant rate $\omega(\mathbf{x})$, which can be interpreted as the transverse magnetization rotating about $\mathbf{B_0}$ at a constant angular velocity at each point in space.

Relation to the heat equation

If $\Gamma = 0$, then (1) reduces to two uncoupled heat equations in the transverse magnetization components u and v. This is equivalent to the limit as the magnetic field $B_0 \to 0$, as the magnetic moments of the spins are not forced to realign with an external field and instead are free to diffuse unhindered.

Mathematically, we should expect that solutions to the Bloch-Torrey equation exhibit some of the same properties as solutions of the heat equation, such as exponential suppression of eigenmodes corresponding to large negative eigenvalues.

Positive definiteness

The coupled system of PDEs (1) can be written as

$$\begin{cases} \mathbf{u}_t = -A\mathbf{u} & \text{in } \Omega, \quad t > 0 \\ \mathbf{u}_0 = \mathbf{g} & \text{in } \Omega \end{cases} \tag{6}$$

where $\mathbf{u} = [u, v]^T$, zero Neumann conditions are taken on the boundary $\partial\Omega$, and

$$A = \begin{pmatrix} -D\Delta + R & -\omega \\ \omega & -D\Delta + R \end{pmatrix}. \tag{7}$$

The operator A, although asymmetric, is positive definite as

$$\begin{aligned} \langle \mathbf{u}, A\mathbf{u} \rangle &= \int_\Omega -Du\Delta u + Ru^2 - Dv\Delta v + Rv^2 \,\mathrm{d}x \\ &= \int_\Omega D\left(||\nabla u||^2 + ||\nabla v||^2\right) + R\left(u^2 + v^2\right) \mathrm{d}x \\ &\geq 0 \quad (> 0 \text{ for } \mathbf{u} \not\equiv \mathbf{0}) \end{aligned}$$

where we have used the zero Neumann boundary conditions to drop the boundary terms.

From this, it is then easy to show that the L^2-norm of the solution decreases in time:

$$\begin{aligned} \langle \mathbf{u}, \mathbf{u}_t \rangle &= \int_\Omega u u_t + v v_t \,\mathrm{d}x \\ &= \frac{1}{2} \frac{\partial}{\partial t} \left(\int_\Omega u^2 + v^2 \,\mathrm{d}x \right) \\ &= \frac{1}{2} \frac{\partial}{\partial t} \left\|\mathcal{M}\right\|_{L^2}^2, \end{aligned}$$

and so, for non-zero $\mathbf{u}$ we have that

$$\frac{1}{2} \frac{\partial}{\partial t} \left\|\mathcal{M}(\mathbf{x}, t)\right\|_{L^2} = \langle \mathbf{u}, \mathbf{u}_t \rangle = -\langle \mathbf{u}, A\mathbf{u} \rangle < 0$$

and therefore $\|\mathcal{M}\|_{L^2}^2$ decreases monotonically with time. Note that this does not imply that $S(t)$ decreases monotonically as well, although it does of course go to zero in the limit as $t \to \infty$.

Uniqueness

Suppose for contradiction that $\mathbf{u}_1$ and $\mathbf{u}_2$ are different solutions to (6) zero Neumann boundary conditions on $\partial\Omega$.

Then, let $\mathbf{w} = \mathbf{u}_1 - \mathbf{u}_2$. By linearity, we have $\mathbf{w}$ solves

$$\begin{cases} \mathbf{w}_t = -A\mathbf{w} & \text{in } \Omega, \quad t > 0 \\ \mathbf{w}_0 = \mathbf{0} & \text{in } \Omega. \end{cases}$$

Now, we have that $\|\mathbf{w}\|_{L^2} = 0$, and since we have shown that $\|\mathbf{u}\|_{L^2}$ is non-increasing for all solutions $\mathbf{u}$ to (6), it must be that $\|\mathbf{w}\|_{L^2} \equiv 0$ and therefore $\mathbf{u}_1$ must equal $\mathbf{u}_2$ almost everywhere for all time, a contradiction.

Experimental Procedures

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Results

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Discussion

Solution of the Bloch-Torrey Equation

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Limitations

Limitations

Conclusion

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Acknowledgements

Acknowledgements

References

[1] H. C. Torrey, "Bloch Equations with Diffusion Terms," *Phys. Rev.*, vol. 104, pp. 563–565, Nov. 1956.

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Figures and Tables

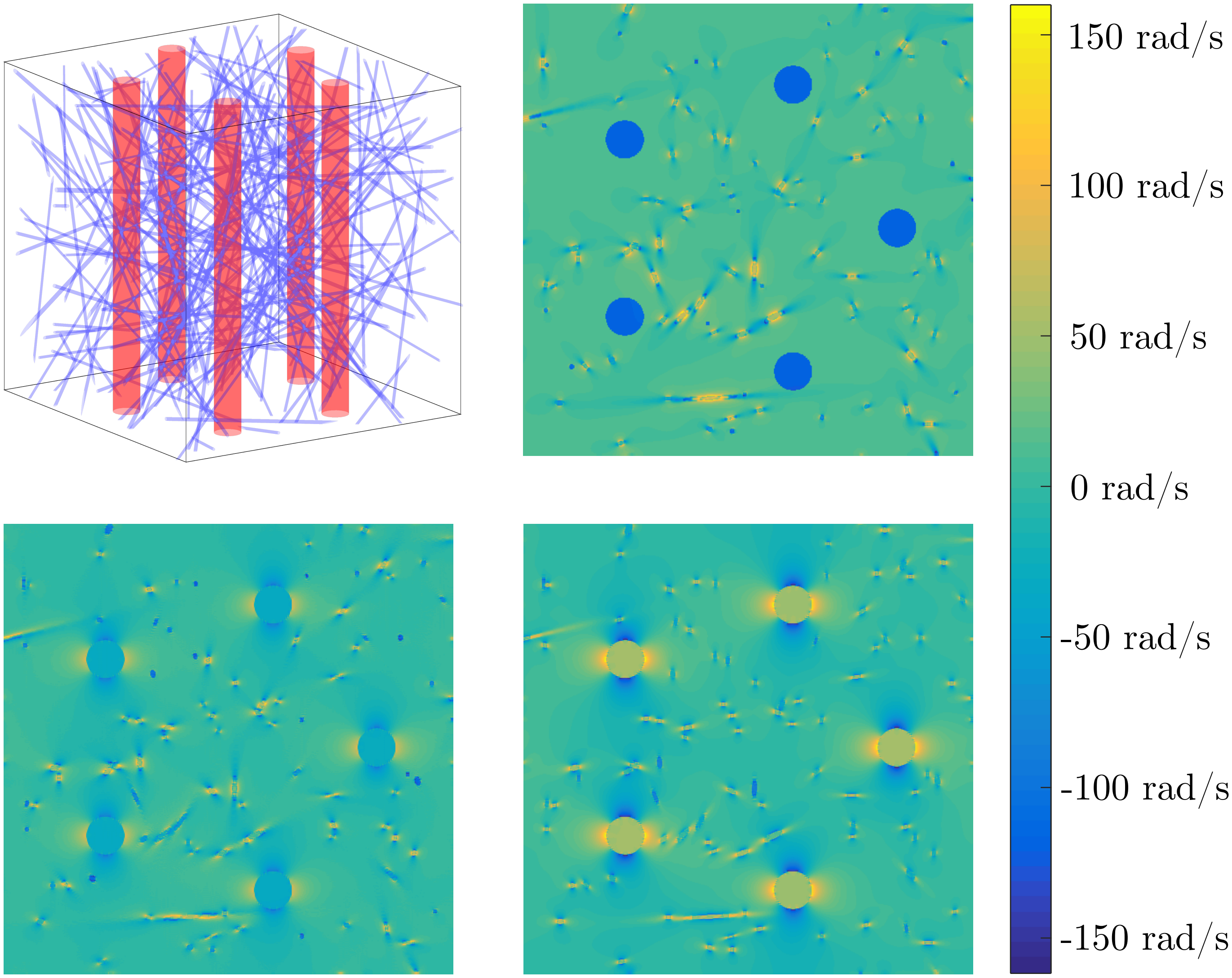

Figure 1: The top-left figure shows an example voxel geometry. The $3 \times 3 \times 3\,\mathrm{mm}^3$ voxel is populated with an isotropic vascular bed and $L = 5$ anisotropic large vessels in the z-direction. The total volume occupied by the blood vessels is determined by the blood volume fraction BVF. The relative fraction of blood contained in the isotropic vascular bed is determined by the isotropic relative blood volume fraction iRBVF, and the amount of blood contained in the anisotropic vessels is then aRBVF $= 1 -$ iRBVF. The magnetic field generated by this configuration is computed by the convolution of the susceptibility map with the unit dipole kernel. Example cross-sections of the frequency shift map $\delta\omega$ are shown for $\alpha = 0^\circ$ (top right), 45° (bottom left), and 90° (bottom right). It can be easily observed that near large vessels, the resonance frequency (i.e. the magnetic field) remains locally relatively constant compared to the resonance frequency near small vessels, which changes rapidly over short distances. Note also the increase in strength and range of inhomogeneities around the large anisotropic vessels as α increases, introducing the dependence on the angle α into the simulations.

Magnetization Propagation Algorithm

1: Initialize: $\mathcal{M}_0 \coloneqq i, \Delta t \coloneqq \mathrm{TE}/30, k \coloneqq 0$

2: **while** $k\Delta t < \mathrm{TE}$ **do**

3: $\quad \mathcal{M}_{k+\frac{1}{2}} \coloneqq e^{-\Gamma(\mathbf{x})\Delta t}\,\mathcal{M}_k$

4: $\quad \mathcal{M}_{k+1} \coloneqq \Phi(\mathbf{x}, \Delta t) * \mathcal{M}_{k+\frac{1}{2}}$

5: $\quad$ **if** $(k+1)\Delta t = \mathrm{TE}/2$ **then**

6: $\quad\quad \mathcal{M}_{k+1} \coloneqq \overline{\mathcal{M}}_{k+1}$

7: $\quad$ **end if**

8: $\quad k \coloneqq k+1$

9: **end while**

10: $S(\mathrm{TE}) \coloneqq \int \mathcal{M}_k \, d^3\mathbf{x}$

Algorithm 1: Magnetization propagation algorithm used to simulate the signal $S(\mathrm{TE})$ for a given set of free parameters $\mathrm{CA}_{\mathrm{PEAK}}$, BVF, iBVF, and L. All four free parameters are encoded solely in the complex decay rate $\Gamma(\mathbf{x})$; the rest of the algorithm does not depend on them. The notation $\mathcal{M}_\nu$ is shorthand for $\mathcal{M}(\mathbf{x}, \nu\Delta t)$ throughout the algorithm. If the $\mathcal{O}(\Delta t^3)$ order evolution equation (**??**) were used instead, line 3 should be modified to decay for only a half time step $\Delta t/2$, line 4 should perform the Gaussian convolution in-place, and an extra line should be added directly following the convolution which decays for another half time step $\Delta t/2$.

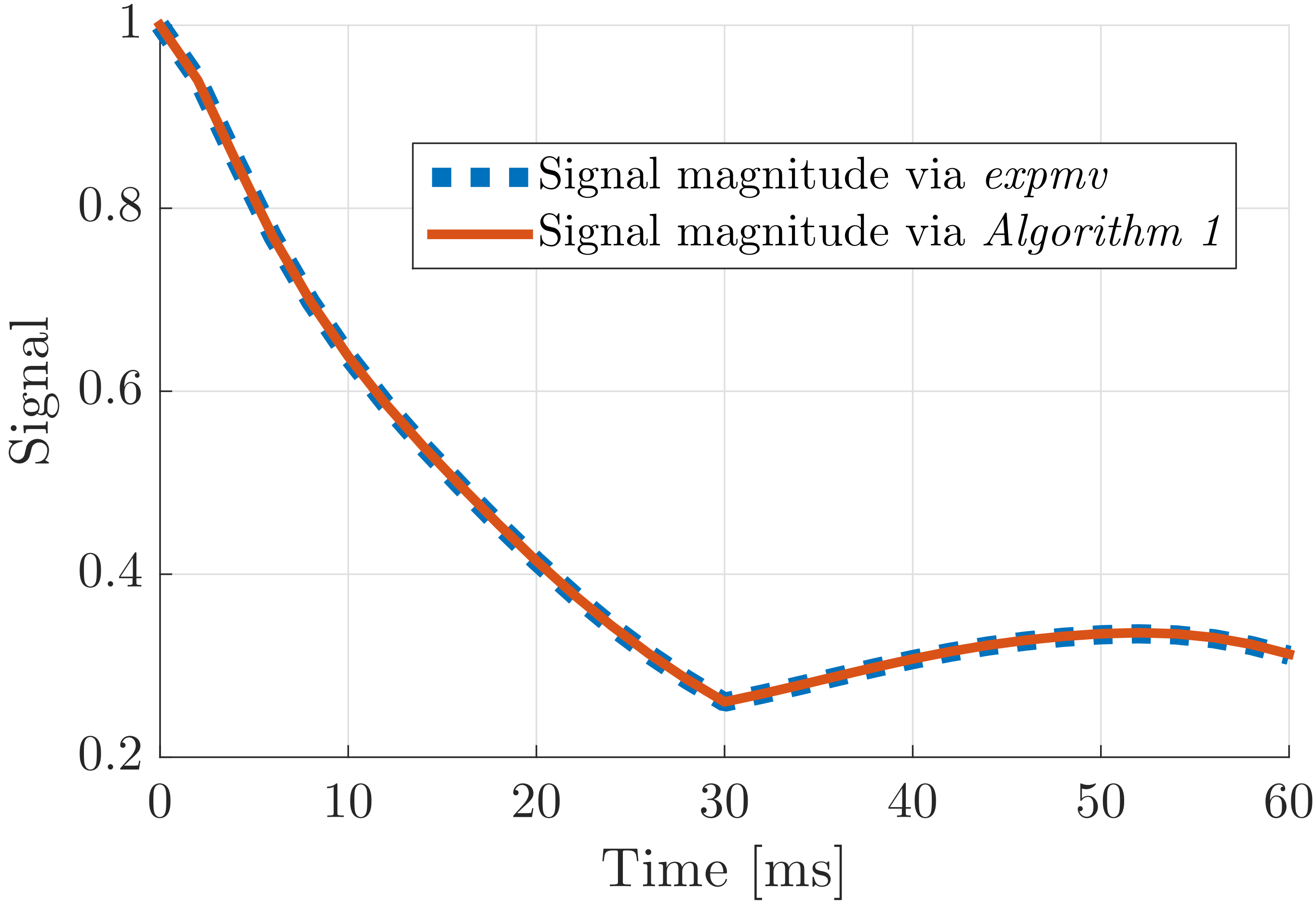

Figure 2: Comparison between solving the Bloch-Torrey equation exactly using the method of lines in conjunction with Higham's *expmv* integrator [2], and solving the Bloch-Torrey equation approximately using the two-step approximate solution as described in Algorithm 1. The signal decay through time calculation shows strong agreement between the two methods, with error values of 0.064% +/- 0.045%; the maximum error value of 0.14% occurs at 60 ms.