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# A parametric finite element solution of the generalised Bloch–Torrey equation for arbitrary domains

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ABSTRACT

Nuclear magnetic resonance (NMR) has proven of enormous value in the investigation of porous media. Its use allows to study pore size distributions, tortuosity, and permeability as a function of the relaxation time, diffusivity, and flow. This information plays an important role in plenty of applications, ranging from oil industry to medical diagnosis. A complete NMR analysis involves the solution of the Bloch–Torrey (BT) equation. However, solving this equation analytically becomes intractable for all but the simplest geometries.

We present an efficient numerical framework for solving the complete BT equation in arbitrarily complex domains. In addition to the standard BT equation, the generalised BT formulation takes into account the flow and relaxation terms, allowing a better representation of the phenomena under scope. The presented framework is flexible enough to deal parametrically with any order of convergence in the spatial domain. The major advantage of such approach is to allow both faster computations and sensitivity analyses over realistic geometries. Moreover, we developed a second-order implicit scheme for the temporal discretisation with similar computational demands as the existing explicit methods. This represents a huge step forward for obtaining reliable results with few iterations. Comparisons with analytical solutions and real data show the flexibility and accuracy of the proposed methodology.



## 1. Introduction

Nuclear magnetic resonance (NMR) is a powerful and non-invasive technique that allows to study the translational motion of molecules in solution, either by diffusion or fluid flow, by using magnetic field gradient methods. The study of this motion reflects properties of the media and its surrounding environment, making NMR an extremely valuable methodology for probing the complex microstructure of natural and artificial materials [1]. A complete analysis of this phenomena involves the solution of the generalised Bloch–Torrey (BT) equation [2,3]. This equation describes the evolution of the transverse magnetisation due to diffusion and flow in the media, spin–spin relaxation, and the gradient field encoding scheme. The problem of solving this equation in arbitrary domains is of primary interest when relating variations in the acquired signals to the underlying structures.

There has been many attempts to solve the BT equation, which can be grouped into analytical and numerical approaches. The first group comprises solutions given by mathematical formulae relating the output signal with parameters of interest. These solutions are obtained by proper manipulation of the mathematical expressions describing the physical phenomena. Then, different forms of the solution can be found depending on the mathematical framework used and the approximations made [1,4–7]. These solutions have been shown to be very important to study the physical basis of experimental results (e.g. [5]), as well as to perform other mathematical analysis due to their parametric nature [1]. However, since the difficulty of such manipulation increases with the complexity of the domain, there exist solutions only for simple geometries, as multi-layered slabs (1D), cylinders (2D), and spheres (3D). This limits the application of these solutions to arbitrary domains, restricting their usefulness to idealised models. These disadvantages are addressed by numerical methods. This group is composed by the entire family of approximations of the true signals obtained by the application of a numerical algorithm. Such algorithms have the advantage of being unrestricted to simple geometries. However, they have many disadvantages when

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compared to the analytical solutions, such as their non-parametric nature and the intrinsic approximations and errors associated with them. Although the latter can be reduced in principle, it comes at the expense of computational effort, which can be prohibitive.

There exist many numerical methods that have been used to solve the BT equation explicitly, albeit none of them considers the flow term (see Section 4). This comprises solutions obtained by the finite difference method [8–10], the finite volume method [11], and the finite element (FE) method [12,13]. The latter is generally preferred owing to its flexibility for spatially discretising the domain. However, many proposed solutions based on the FE method rely on strong assumptions (e.g. narrow pulse limit approximation) that limit their general applicability. Recently, a flexible FE formulation of the standard BT equation (i.e. without flow and transverse relaxation terms) has been proposed [14]. There, the authors present a FE approach using first-order basis functions in space and an explicit second-order approximation in time, which does not make such constraining approximations. To the best of our knowledge, this latter paper by Nguyen et al. [14] is the first to do so. Even though their approach allows to consider arbitrary geometries inside the volume of interest, it still has limitations in the way the meshes have to be generated, imposing a hard constraint as the symmetry of the nodal positions on the outermost faces. This adds an extra difficulty for building and testing *ad hoc* models.

In this paper, we present a numerical FE framework for the solution of the complete BT equation in arbitrarily complex domains. We extend the formulation given in [14] by considering the flow and relaxation terms, allowing a better representation of the phenomena under scope. We obtain parametric expressions of the corresponding matrices considering basis functions of arbitrary order. This means that we derive closed-form formulas for all the matrices involved in the numerical algorithm, relating explicitly the output (i.e. the resulting NMR signal) as a function of input parameters defining the particular scenario to be tested (as diffusivities and permeabilities). These expressions are specially useful when performing sensitivity analyses of the acquisitions to a specific parameter, as well as to speed-up the computations [24]. Also, we broaden the formulation to deal with both linear and parabolic spatial profiles of the magnetic field [1]. Finally, we present a second order implicit method for the temporal discretisation. Unlike explicit schemes, implicit methods are unconditionally stable no matter the time-step selected [26]. This is crucial for achieving reliable solutions with a minimum number of iterations. We introduce an implicit scheme to solve the BT equation with similar computational load as the explicit method used in [14], which makes it highly competitive in the field. The presented framework is built on the basis of arbitrary discretisations without imposing special constraints to the geometrical meshes to be used.

The paper is organised as follows. In Section 2 we present the mathematical basis of the problem and the corresponding FE solution. First, we review the differential formulation in Section 2.1. Then, in Section 2.2, we present the variational formulation and the FE spatial discretisation. In Section 2.3 we define the volume and area coordinate systems, which have a key role in the parametric formulation detailed in Section 2.4. The temporal discretisation of the BT equation is described in Section 2.5. In Section 3 we show the capabilities of the numerical framework and compare them with analytical solutions and real data. Finally, in Section 4, we discuss the results, limitations of the approach, and further work.

*Notation:* In the following, we denote vectors with boldface lower case letters and matrices with boldface capital letters. We use $\mathrm{vec}(\cdot)$ to refer to the operator that, given a matrix, returns a vector with the matrix elements stacked columnwise, taking the columns in order from first to last. We express the Kronecker matrix product by $\otimes$, and the $n$th Kronecker product of $\boldsymbol{A}$ with itself by $\boldsymbol{A}^{\otimes n}$. Finally, we denote the $n \times n$ identity matrix as $\boldsymbol{I}_n$, and the $m \times n$ matrix full of ones as $\mathbf{1}_{m,n}$.

## 2. Methods

The generalised BT equation represents the evolution of the magnetisation as a function of the spatial location and time in the absence of the RF field. Basically, it relates the evolution of the complex-valued transverse magnetisation with four mechanisms: diffusive migration of the spin-bearing particles, magnetic field encoding, transverse spin–spin relaxation, and flow [1,2]. The problem statement is completed after selecting the corresponding boundary and initial conditions. These conditions allow to represent arbitrary situations where to study the phenomena. Once the solution is found, it is used to describe the macroscopic signal formed by the spin ensemble.

As mentioned in Section 1, solving the BT equation analytically becomes intractable for all but the simplest geometries. In this section, we describe the numerical framework used to solve the aforementioned equation in arbitrary geometries and conditions. The advantages of the formulation are explained in detail.

### 2.1. Differential formulation

Let $\Omega$ be the domain under analysis, which can be split into $L$ subdomains, such that $\Omega = \bigcup_{l=1}^{L} \Omega_l$. Also, let $\Gamma_l^e$ be the external boundary of $\Omega_l$, and $\Gamma_{ln}$ the boundary between $\Omega_l$ and $\Omega_n$. Then, under generally valid assumptions (such as considering normal or Fickian diffusion, intermediate layers infinitely thin, incompressible flow, and absence of susceptibility effects and hardware imperfections; see [2,6] for a detailed discussion), the evolution of the complex transverse magnetisation $m_l(\boldsymbol{r}, t)$ in the rotating frame is described by [2,15]

$$\begin{aligned}\frac{\partial m_l(\boldsymbol{r},t)}{\partial t} &= \nabla \cdot (\boldsymbol{D}_l(\boldsymbol{r}) \nabla m_l(\boldsymbol{r},t)) - \mathrm{i}\gamma B(\boldsymbol{r},t) m_l(\boldsymbol{r},t) - \frac{1}{T_l} m_l(\boldsymbol{r},t) \\ &\quad - \boldsymbol{v}(\boldsymbol{r},t) \cdot \nabla m_l(\boldsymbol{r},t) \quad (\boldsymbol{r} \in \Omega_l), \end{aligned} \tag{1}$$

subject to the boundary conditions (BCs)

$$\boldsymbol{D}_l(\boldsymbol{r}) \nabla m_l(\boldsymbol{r},t) \cdot \boldsymbol{n}_l(\boldsymbol{r}) = \kappa_{ln}(m_n(\boldsymbol{r},t) - m_l(\boldsymbol{r},t)) \quad (\boldsymbol{r} \in \Gamma_{ln}, \ \forall n), \tag{2a}$$

$$\boldsymbol{D}_l(\boldsymbol{r}) \nabla m_l(\boldsymbol{r},t) \cdot \boldsymbol{n}_l(\boldsymbol{r}) = -\kappa_l^e m_l(\boldsymbol{r},t) \quad (\boldsymbol{r} \in \Gamma_l^e), \tag{2b}$$

and the initial condition (IC)

$$m_l(\boldsymbol{r},0) = \rho_l(\boldsymbol{r}), \quad (\boldsymbol{r} \in \Omega_l), \tag{3}$$

where $t \in [0, T_E]$ with $T_E$ echo time, $\gamma$ is the gyromagnetic ratio of protons ($2.675 \times 10^8$ rad T$^{-1}$ s$^{-1}$ for $^1$H), $\boldsymbol{D}_l(\boldsymbol{r})$ is the diffusion (rank-2) tensor, $T_l$ is the spin–spin relaxation time, $\boldsymbol{v}(\boldsymbol{r},t)$ is the velocity field of the spins due to flow of the medium, $\boldsymbol{n}_l(\boldsymbol{r})$ is the unitary outward pointing normal to $\Omega_l$, $\kappa_{ln}$ ($\kappa_l^e$) is the permeability constant in $\Gamma_{ln}$ ($\Gamma_l^e$), and $B(\boldsymbol{r},t)$ is the effective magnetic field. In the following analysis we considered $T_l$ constant in each subdomain $\Omega_l$ and the same permeability in both directions of the same membrane, i.e. $\kappa_{ln} = \kappa_{nl}$.

Eq. (1) states that the transverse magnetisation evolves due to diffusion (first term), encoded through the applied magnetic field (second term), bulk relaxation (third term), and flow (last term). The BC (2a) accounts for the creation of the diffusive flux by the drop in magnetisation between layers. It can be seen that it also accounts for the conservation of the magnetisation flux between adjacent layers, i.e.

$$\boldsymbol{D}_l(\boldsymbol{r}) \nabla m_l(\boldsymbol{r},t) \cdot \boldsymbol{n}_l(\boldsymbol{r}) = -\boldsymbol{D}_n(\boldsymbol{r}) \nabla m_n(\boldsymbol{r},t) \cdot \boldsymbol{n}_n(\boldsymbol{r}) \quad (\boldsymbol{r} \in \Gamma_{ln}).$$