Journal of Computational Physics 263 (2014) 283–302

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A finite elements method to solve the Bloch–Torrey equation applied to diffusion magnetic resonance imaging

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A R T I C L E I N F O

Article history:
Received 28 July 2013
Received in revised form 23 December 2013
Accepted 6 January 2014
Available online 21 January 2014

Keywords:
Bloch–Torrey equation
Diffusion magnetic resonance imaging
Finite elements
RKC
Pseudo-periodic
Double-node
Interface problem

A B S T R A C T

The complex transverse water proton magnetization subject to diffusion-encoding magnetic field gradient pulses in a heterogeneous medium can be modeled by the multiple compartment Bloch–Torrey partial differential equation (PDE). In addition, steady-state Laplace PDEs can be formulated to produce the homogenized diffusion tensor that describes the diffusion characteristics of the medium in the long time limit. In spatial domains that model biological tissues at the cellular level, these two types of PDEs have to be completed with permeability conditions on the cellular interfaces. To solve these PDEs, we implemented a finite elements method that allows jumps in the solution at the cell interfaces by using double nodes. Using a transformation of the Bloch–Torrey PDE we reduced oscillations in the searched-for solution and simplified the implementation of the boundary conditions. The spatial discretization was then coupled to the adaptive explicit Runge–Kutta–Chebyshev time-stepping method. Our proposed method is second order accurate in space and second order accurate in time. We implemented this method on the FEniCS C++ platform and show time and spatial convergence results. Finally, this method is applied to study some relevant questions in diffusion MRI.

1. Introduction

Biological tissue is a heterogeneous medium, consisting of cells of various sizes and shapes distributed in the extra-cellular space. The cells are separated from each other and from the extra-cellular space by the cell membranes. Diffusion magnetic resonance imaging (dMRI) is an imaging modality that uses magnetic field gradient pulses in order to access the diffusion characteristics of water molecules over a time period on the order of tens of milliseconds (see a recent review in [1]).

While there have been numerous works on the analysis of the dMRI signal under simplifying assumptions (on the geometry, membrane permeability, pulse sequence), see, e.g., [2–8], in this paper, we focus on a more complete model of the water proton magnetization called the multiple compartment Bloch–Torrey partial differential equation (PDE), that allows the inclusion of general tissue geometries, permeable cell membranes, and arbitrary diffusion-encoding gradient sequences. This numerical model is a generalization of the Bloch–Torrey equation [9] to heterogeneous domains [5,10] and it models the complex transverse water proton magnetization subject to diffusion-encoding magnetic field gradient pulses. The dMRI signal is given as the integral of the magnetization.

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0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2014.01.009

Some previous works that solved the *diffusion equation* to obtain the dMRI signal in the narrow gradient pulse limit (the duration of the pulses is small compared to the measured diffusion time) are [11,12,8], where the spatial discretization is finite elements. To account for the short gradient pulses, the magnetization is pre- and post-multiplied by a spatially-dependent complex factor. The initial condition to the PDE is either the delta function distribution (to obtain the diffusion propagator) or a complex-valued initial distribution describing the magnetization just after the first applied gradient pulse. The PDE solved is the pure diffusion equation (obtained when setting the gradient to zero in the Bloch–Torrey equation), and the simulation starts after the application of the first gradient pulse and ends before the application of the next gradient pulse.

The focus of the work in [11,12,8] is on simulating diffraction patterns of restrictive (or lowly permeable) porous systems, to determine pore size, for example. To produce such diffraction patterns, high gradient amplitudes and long diffusion times (as long as 1 second) are used to probe restrictive geometries. In [8] a second order implicit time-stepping method called the generalized α method [13], which was developed for dissipating high frequencies, was used. Because of the choice of this implicit time-stepping method, the matrix solve at each time step involves the stiffness matrix, whose condition number increases as $O(h^{-2})$, where h is the spatial discretization size. There was also an early work on solving the Bloch–Torrey equation where the pulse duration is not short [14] where the computational domain is one dimensional (restricted diffusion between parallel plates).

The focus of this current paper is not porous systems. Rather, it is biological tissue dMRI, where the diffusion time is much shorter, on the order of tens of milliseconds, and the gradient amplitudes are moderate. Numerical solutions of the multiple compartment Bloch–Torrey PDE for general gradient sequences (no narrow pulse restriction) were reported in [15–18], in which the finite difference method on a Cartesian grid was coupled to the explicit Forward Euler time-stepping method, resulting in first order accuracy in space and time. We found that an *explicit* and *adaptive* second order convergent time-stepping method called the Runge–Kutta–Chebyshev (RKC) method [19] is a much better choice for our application. The RKC method was especially formulated for diffusive PDEs (of which the Bloch–Torrey PDE is an example) to allow for much larger time steps than alternative explicit time-stepping methods such as the Forward Euler method. Explicit stepping methods have an advantage over implicit methods in that the solution of linear systems with the stiffness matrix is not required. Instead, linear systems solutions involve only the mass matrix, whose condition number is $O(1)$, and hence the linear systems are easy to solve. The RKC method is adaptive, in that it allows error control on the ODE solution and adapts the time step size to satisfy the error tolerance during the course of the simulation.

Now we summarize some important requirements of a numerical code for the simulation of biological tissue dMRI:

1. Allows arbitrary diffusion-encoding pulse shapes and sequences, including, for example, pulses that are square (idealized pulsed-gradient spin echo (PGSE) [20]), trapezoid (more realistic PGSE with non-zero rise time), oscillating sine and cosine [21,22], or a yet-determined shape to be optimized [23].
2. Allows generally-shaped cell membranes that are permeable to water passage.
3. Allows the periodic extension of the computational domain so that water can enter and exit the computational domain in a physically reasonable manner, as was done in [16,18].
4. Efficient for large-scale simulations in two and three dimensions.

We tried to satisfy the above requirements by the following choices:

1. The complex-valued Bloch–Torrey PDE (not the diffusion equation) is solved for arbitrary pulse shapes and sequences.
2. Linear finite elements discretization is used to allow generally-shaped compartment interfaces (modeling cell membranes).
3. Additional degrees of freedom are added on the compartment interfaces to allow permeability conditions on generally-shaped interfaces.
4. The periodic extension of the computational domain is an allowed option. To impose this condition the Bloch–Torrey PDE is transformed so that the boundary condition becomes more computationally efficient to implement.
5. The time-stepping method is chosen to be the explicit and adaptive Runge–Kutta–Chebyshev (RKC) method [19].

The combination of linear finite elements and the RKC method makes our approach second order accurate in space and time. For an efficient implementation of finite elements we chose to base our code on the FEniCS Finite Elements platform [24]. The Bloch–Torrey PDE has several unconventional features that cause implementation issues for a standard PDE platform such as FEniCS. We describe these issues and how we resolved them. First, we allowed jumps in the finite elements solution at the compartment interfaces by implementing double-nodes at the interfaces. Second, the pseudo-periodic boundary conditions resulting from the periodic extension of the computational domain are reduced to standard periodic boundary conditions by transforming the Bloch–Torrey PDE, as in [18]. We note, however, that in [18], the discretized PDE using centered finite difference did not take into account first order terms. To obtain second order convergence in space, we had to include all the appropriate first order terms in our discretization. Third, we reformulated the Bloch–Torrey PDE so that the real and imaginary parts of the magnetization are decoupled to allow the solution of two systems of half the number of unknowns compared to a naive implementation. We show accuracy and timing results for our method and use our code to simulate and gain insight into the diffusion characteristics of some complex geometries.