ARTICLE IN PRESS
Computers and Mathematics with Applications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Modelling anomalous diffusion using fractional Bloch–Torrey equations on approximate irregular domains[☆]

Shanlin Qin [a], Fawang Liu [a,*], Ian W. Turner [a,b], Qianqian Yang [a], Qiang Yu [c]

[a] School of Mathematical Sciences, Queensland University of Technology, GPO Box 2434, Brisbane, Qld. 4001, Australia
[b] Australian Research Council Centre of Excellence for Mathematical and Statistical Frontiers (ACEMS), Queensland University of Technology, Brisbane, Australia
[c] Centre for Advanced Imaging, The University of Queensland, St Lucia, Queensland, Australia

ARTICLE INFO

Article history:
Received 20 October 2016
Received in revised form 23 July 2017
Accepted 19 August 2017
Available online xxxx

Keywords:
Irregular domains
Finite difference method
Fractional Bloch–Torrey equations
Stability
Convergence

ABSTRACT

Diffusion-weighted imaging is an *in vivo*, non-invasive medical diagnosis technique that uses the Brownian motion of water molecules to generate contrast in the image and therefore reveals exquisite details about the complex structures and adjunctive information of its surrounding biological environment. Recent work highlights that the diffusion-induced magnetic resonance imaging signal loss deviates from the classic monoexponential decay. To investigate the underlying mechanism of this deviated signal decay, diffusion is re-examined through the Bloch–Torrey equation by using fractional calculus with respect to both time and space. In this study, we explore the influence of the complex geometrical structure on the diffusion process. An effective implicit alternating direction method implemented on approximate irregular domains is proposed to solve the two-dimensional time–space Riesz fractional partial differential equation with Dirichlet boundary conditions. This scheme is proved to be unconditionally stable and convergent. Numerical examples are given to support our analysis. We then applied the proposed numerical scheme with some decoupling techniques to investigate the magnetisation evolution governed by the time–space fractional Bloch–Torrey equations on irregular domains.

1. Introduction

When water molecules interact with obstacles, such as myelin sheath, cell membranes and fibre bundles, they provide significant information about the local physiological and anatomical environment in human brain tissue. Techniques based on magnetic resonance imaging (MRI) provide an ideal platform to non-invasively characterise the diffusion properties of water molecules and reveal important clinical information [1]. The mathematical principle underpinning the origin and properties of the MRI signal is governed by the Bloch equations. The diffusion of water molecules gives rise to an additional MR signal loss. With the consideration of the diffusion process, the basic principle for the dynamics of nuclear magnetisation can be described by the Bloch–Torrey equations, which is defined as follows:

$$\frac{\partial M_{xy}(\mathbf{r},t)}{\partial t} = \lambda M_{xy}(\mathbf{r},t) + D\nabla^2 M_{xy}(\mathbf{r},t), \tag{1}$$

☆ This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

* Corresponding author.
E-mail address: f.liu@qut.edu.au (F. Liu).

http://dx.doi.org/10.1016/j.camwa.2017.08.032
0898-1221/© 2017 Elsevier Ltd. All rights reserved.

where $\lambda = -i\gamma(\mathbf{r} \cdot \mathbf{G})$, γ is the gyromagnetic ratio, $\mathbf{G}$ is the magnetic field gradient, $\mathbf{r}$ is the coordinate; D is the diffusion coefficient; and $M_{xy}(\mathbf{r}, t)$ is the transverse components of the magnetisation $M_{xy}(\mathbf{r}, t) = M_x(\mathbf{r}, t) + iM_y(\mathbf{r}, t)$ with $i = \sqrt{-1}$. Note that the T_1 and T_2 relaxation processes are neglected in Eq. (1) because we focus only on signal intensity changes due to diffusion [2].

A considerable body of work has recently reported that the diffusion-induced MRI signal loss deviates from the monoexponential attenuation derived from the Bloch–Torrey equations [3,4]. In light of obtaining a better description of the diffusion-induced MRI signal, models are modified as biexponential or multi-exponential with distinct relaxation rates by assuming signals can be compartmentalised [5,6]. Although better fitting to the experimental signal loss can be obtained, these models may not provide a concrete and reliable interpretation of the MRI signal given the risk of over-fitting the data and its sensitivity to noise [7]. More importantly, attempts to clarify the biophysical meaning of those models are rare due to the complex and heterogeneous tissue environment [8,9].

As an alternative tool, fractional calculus has had growing success for describing the dynamical processes associated with system memory and heterogeneity due to its endogenous nonlocal property, especially for complex systems [10,11]. Therefore, some recent work has extended the Bloch–Torrey equations to include fractional dynamics through the replacement of the integer derivatives with their fractional counterparts [12–14]. A time–space fractional order generalisation of the Bloch–Torrey equations is given as

$$\sigma^{\alpha-1}\,{}_0^C D_t^{\alpha} M_{xy}(\mathbf{r}, t) = \lambda M_{xy}(\mathbf{r}, t) + D\mu^{\beta-2}\boldsymbol{R}^{\beta} M_{xy}(\mathbf{r}, t), \tag{2}$$

where σ and μ are parameters needed to preserve the units; α and β are the time and space fractional orders with $0 < \alpha < 1$ and $1 < \beta \leq 2$, respectively; and ${}_0^C D_t^{\alpha}$ is the α $(0 < \alpha < 1)$ order Caputo fractional derivative with definition given by [10]

$${}_0^C D_t^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t f'(\tau)(t-\tau)^{-\alpha} d\tau.$$

In Eq. (2), the β-order $(1 < \beta \leq 2)$ two-dimensional Riesz fractional order operator is defined as $\boldsymbol{R}^{\beta} = \frac{\partial^{\beta}}{\partial |x|^{\beta}} + \frac{\partial^{\beta}}{\partial |y|^{\beta}}$ with $\frac{\partial^{\beta}}{\partial |x|^{\beta}}$ (similar for $\frac{\partial^{\beta}}{\partial |y|^{\beta}}$) defined as [15]

$$\frac{\partial^{\beta} u(x, y, t)}{\partial |x|^{\beta}} = -c_{\beta}({}_a D_x^{\beta} + {}_x D_b^{\beta}) u(x, y, t),$$

where $a < x < b$, $c_{\beta} = \frac{1}{2\cos(\pi\beta/2)}$ $(\beta \neq 1)$ and

$$\begin{cases} {}_a D_x^{\beta} u(x, y, t) = \dfrac{1}{\Gamma(n-\beta)} \dfrac{\partial^n}{\partial x^n} \displaystyle\int_a^x \dfrac{u(x, y, t)}{(x-\varepsilon)^{\beta+1-n}} d\varepsilon, \\ {}_x D_b^{\beta} u(x, y, t) = \dfrac{1}{\Gamma(n-\beta)} \dfrac{\partial^n}{\partial x^n} \displaystyle\int_x^b \dfrac{u(x, y, t)}{(\varepsilon-x)^{\beta+1-n}} d\varepsilon. \end{cases}$$

Many numerical methods have been proposed to deal with problems involving fractional order derivatives [16]. For example, first order and second order approximations for the Riesz space fractional derivative can be obtained by using the Grünwald–Letnikov derivative approximation scheme and fractional centred difference method respectively [17,18]. In this work, we generalise these methods for the use on irregular domains. Ervin and Roop presented a theoretical framework for the Galerkin finite element method to the fractional advection dispersion equation [19]. Zeng et al. investigated a spectral method for a two-dimensional fractional nonlinear reaction–diffusion equation [20]. Liu et al. proposed the finite volume method for solving fractional diffusion equations [21–23]. Specific to the time–space fractional Bloch–Torrey equations, Yu et al. proposed several different finite difference methods, including the alternating direction method in high dimensions, and proved its stability and convergence [24–26]. Bu et al. considered the finite difference method in the temporal direction and finite element method in the spatial direction to solve the time–space fractional Bloch–Torrey equations [27].

However, most proposed schemes are only considered in rectangular domains. Arbitrariness and irregularity of the considered domain ubiquitously exist in many real-world problems, such as the human brain. In fact, the effects of simply restricted diffusion have been preliminarily investigated on MR signal formation and lead to a quasi-two-compartment behaviour of the MR signal [28]. Recently, the search for methods that consider the irregularity of the object domain and fractional derivative to capture the spatial heterogeneity and system memory has been addressed [29]. In this work, a finite difference method implemented on approximate irregular domains is proposed to investigate the time–space fractional partial differential equation (PDE) with Dirichlet boundary conditions and then extended to solve the Bloch–Torrey equations.

The Riesz space fractional derivative operator $\frac{\partial^{\beta}}{\partial |x|^{\beta}}$ on an approximate irregular domain is defined as [29]

$$\frac{\partial u^{\beta}(x, y, t)}{\partial |x|^{\beta}} = -c_{\beta}({}_{x_l(j)} D_x^{\beta} + {}_x D_{x_u(j)}^{\beta}) u(x, y, t),$$