Numerical investigation of three types of space and time fractional Bloch-Torrey equations in 2D

Qiang Yu¹, Fawang Liu¹,∗, Ian Turner¹, Kevin Burrage¹,²

1 School of Mathematical Sciences, Queensland University of Technology, GPO Box 2434, Brisbane, Qld. 4001, Australia
2 Department of Computer Science and OCISB, University of Oxford, OXI 3QD, UK

Received 16 January 2013; accepted 27 March 2013

Abstract: Recently, the fractional Bloch-Torrey model has been used to study anomalous diffusion in the human brain. In this paper, we consider three types of space and time fractional Bloch-Torrey equations in two dimensions: Model-1 with the Riesz fractional derivative; Model-2 with the one-dimensional fractional Laplacian operator; and Model-3 with the two-dimensional fractional Laplacian operator. Firstly, we propose a spatially second-order accurate implicit numerical method for Model-1 whereby we discretize the Riesz fractional derivative using a fractional centered difference. We consider a finite domain where the time and space derivatives are replaced by the Caputo and the sequential Riesz fractional derivatives, respectively. Secondly, we utilize the matrix transfer technique for solving Model-2 and Model-3. Finally, some numerical results are given to show the behaviours of these three models especially on varying domain sizes with zero Dirichlet boundary conditions.

PACS (2008): 02.30.Jr, 02.60.Cb, 02.70.Bf

Keywords: fractional Bloch-Torrey equation • fractional centered difference • implicit numerical method • matrix transfer technique • bounded domains

© Versita sp. z o.o.

1. Introduction

The concept of fractional calculus was first proposed by Leibniz in 1695. Since then, many famous mathematicians, such as Euler, Laplace, Fourier, Abel, Liouville, Riemann, Grünwald, Letnikov, Lévy and Riesz, have worked in this field of mathematics and provided important contributions. The main characteristic of fractional order differential equations is that they contain non-integer order derivatives [1, 2]. Fractional models can be used to describe the memory and transmissibility of many kinds of materials, and they play an increasingly important role in science and engineering [3–10]. Metzler and Klafter [4] demonstrated that fractional equations have come of age as a complementary tool in the description of anomalous transport processes. Zaslavsky [5] reviewed a new concept of fractional kinetics for systems with Hamiltonian chaos. New characteristics of the kinetics are extended to fractional kinetics and the most important are anomalous transport, superdiffusion and weak mixing, amongst

∗E-mail: f.liu@qut.edu.au
describe anomalous NMR relaxation phenomena [1] in the context of the classical and fractional order Bloch equations. Making heterogeneous, porous or composite materials [14, 15]. were proposed by Torrey [12] as a generalization of the Bloch-Torrey equations as a function of time [11]. The Bloch-Torrey equations are used for modeling the nuclear magnetization of an appropriate linear system. In time and space are found simultaneously by the solution of an appropriate linear system. In physics and chemistry, specifically in nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI), the Bloch equations represent a set of macroscopic equations that are used for modeling the nuclear magnetization as a function of time [11]. The Bloch–Torrey equations were proposed by Torrey [12] as a generalization of the Bloch equations to describe situations when the diffusion of the spin magnetic moment is not negligible. Bhalekar et al. [13] considered transient chaos in a non-linear version of the Bloch equation that involved a radiation damping model. The fractional Bloch equation provides an opportunity to describe numerous experimental situations including heterogeneous, porous or composite materials [14, 15]. Petrâs [16] proposed numerical and simulation models of the classical and fractional order Bloch equations. Magin et al. [17] considered the fractional Bloch equation to describe anomalous NMR relaxation phenomena ($T_1$ and $T_2$) in Cartilage Matrix Components. Bhalekar et al. [18] considered the fractional Bloch equation with time delays, and analysed different stability behaviors for the $T_1$ and the $T_2$ relaxation processes. Kenkre et al. [19] proposed a simple technique for solving the Bloch–Torrey equations in the NMR study of molecular diffusion under gradient fields. Barzykin [20] derived an exact analytical solution of the Bloch–Torrey equation for restricted diffusion in a steady field gradient and, as a result, for any step-wise pulse sequence. Jochimsen et al. [21] proposed an algorithm for simulating MRI with Bloch–Torrey equations, and showed that the algorithm is efficient and decreases simulation time while retaining accuracy.

Recently, fractional order calculus has been used to examine the connection between fractional order dynamics and diffusion by solving the Bloch-Torrey equation [22–25]. It was pointed out that a fractional diffusion model could be successfully applied to analyzing diffusion images of human brain tissues and provides new insights into further investigations of other tissue structures and the micro-environment. Magin et al. [24] proposed a new diffusion model for solving the Bloch–Torrey equation using fractional order calculi with respect to time and space (ST-FBTE):

$$\tau^{α−1} \frac{∂}{∂ \tau} M_0(r, t) = \lambda M_0(r, t) + \mu G(t)$$ (1)

where $\lambda = -i\gamma(r \cdot G(t))$, $r = (x, y, z)$, $G(t)$ is the magnetic field gradient, $\gamma$ and $D$ are the gyromagnetic ratio and the diffusion coefficient, respectively. $\frac{∂}{∂ \tau}$ is the Caputo time fractional derivative of order $α$ ($0 < α \leq 1$) with respect to $t$, and with the starting point at $t = 0$ is defined as [2]:

$$\frac{∂}{∂ \tau} M(x, y, z, t) = \frac{1}{\Gamma(1 - α)} \int_0^t \frac{M'(x, y, z, τ)}{(t - τ)^α} dτ.$$

$M_0(r, t) = M_n(r, t) + iM_p(r, t)$, where $i = \sqrt{-1}$, comprises the transverse components of the magnetization; and $M_0(t)$ and $M_1(t)$ are the fractional order time and space constants needed to preserve units, ($0 < α \leq 1$, and $1 < β \leq 2$). Magin et al. [24] considered $R^α = (R^α_1 + R^α_2 + R^α_3)$ as a sequential Riesz fractional order operator in space [2], and some authors [26–29] proposed to study the fractional Laplacian operator formulation replacing the Riesz fractional derivative. In this paper, we consider three types of space and time fractional Bloch–Torrey equations in two dimensions (ST-FBTE2D), namely, Model-1: ST-FBTE2D with the Riesz fractional derivative; Model-2: ST-FBTE2D with the one-dimensional fractional Laplacian operator, and Model-3: the space fractional Bloch–Torrey equation with a two-dimensional fractional Laplacian operator. Compared with the considerable work carried out on theoretical analysis, little work has been done on the numerical solution of equation (1). Magin et al. [24] derived analytical solutions with fractional order dynamics in space (i.e., $α = 1$ and $1 < β \leq 2$) and time (i.e., $0 < α < 1$ and $β = 2$). Zhou et al. [31] applied the results from [30] to analyze diffusion images of healthy human brain tissues in vivo successfully at high $b$ values up to 4700 sec/mm$^2$. Yu et al. [23] derived an analytical solution and an effective implicit numerical method for solving equation (1), and also considered the stability and convergence properties of the implicit numerical method. However, due to computational overheads necessary to perform the simulations for ST-FBTE in three dimensions, Yu et al. [23] presented