TWMS J. App. and Eng. Math. V.11, N.2, 2021, pp. 616-627

A NUMERICAL TREATMENT OF BLOCK NUCLEAR MAGNETIC RESONANCE FLOW EQUATION

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Abstract. The time-dependent Bloch nuclear magnetic resonance flow equation in one dimensional space is investigated numerically. To investigate some physiological and biological properties of living tissues NMR plays pivotal role. In this paper, an applicable approach is used to solve the proposed equation with appropriate initial and boundary conditions. This method is a kind of regularization approaches based on the finite difference and mollification methods. The numerical algorithm is well supported with stability and convergence results and the numerical results for two test problems confirm the ability of the numerical method.

Keywords: NMR, Block Equation, Mollification, Marching Approach.

AMS Subject Classification: 65M06, 65M12, 65M32

1. Introduction

Many industrial and medical processes involve the flow of fluids through porous media. For instance the flow of blood through organ tissues and the transfer of gases to blood within the lung occur through porous materials. Usually the description of media even on a limit basis is not easy. Today it is explored that these flow processes are very important and considerable research activities have been conducted for designing and controlling them [1, 2, 3]. The mathematical simulation plays a pivotal role for making decisions and designing processes with regards to the operation and control of fluids flow through porous environments. Regardless of the applications, many of the issues regarding the mathematical modelling of flow in porous media are similar. In this disciplines, the main challenge is the determination of appropriate properties of these equations in order to predict the process states [2, 3].

Typically the properties of porous media are determined by measuring fluid states outside of the porous media and within porous media [1, 2, 3]. During last decades some methods such as the eradiation, electrical and sonic methods have been used to obtain information regarding fluid states and properties within the media. Although these methods are applicable in many situations but they have significant limitations. Using

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§ Manuscript received: June 25, 2019; accepted: October 31, 2019.
TWMS Journal of Applied and Engineering Mathematics, Vol.11, No.2

nuclear magnetic resonance (NMR) can cover many limitations and determine the states of fluids and porous media properties very well. Due to the abilities of NMR, this method known as a powerful tool to detect and solve various problems in different directions of medicine [2].

For description of the nuclear motion of the substances, Felix Bloch [1] developed a set of coupled differential equations. A modification of Bloch equations has proposed by Torrey [3] to describe the diffusion phenomena observed in all flow systems. Recently it has been explored that determination of diffusion coefficients in the Ficks and Bloch–Torrey equations may gives useful information regards to the structure of the pore. Awojoyogbe et. al. [4, 5, 6, 7, 8, 9, 10] conducted a series of valuable studies on modification and solution of the Bloch NMR flow equations for the analysis of fluid flows through the porous media. The Bloch NMR flow equations, represented as a set of coupled differential equations, model the behavior of the macroscopic magnetization. The effects of the field inhomogeneity, relaxation and precession can be analyzed using these equations. If the magnetization considered as a function of space and time, one may investigate the effects of gradients and diffusion [1, 3, 9].

In this study the coupled Bloch NMR equations proposed by Awojoyogbe is considered in a general form as a parabolic initial-boundary value problem. One may find some theoretical and numerical results regard to these equations in spacial cases in the literature [4, 5, 6, 11, 12]. A numerical approach using marching finite difference and mollification methods will be developed to solve this problem. The mollification method has been used for the stable numerical solution of a wide range of problems in partial differential equations [9, 10, 13, 14, 15, 16, 17, 18]. This paper is organized as follows:

In section 2, the Bloch NMR equation is briefly reviewed. Section 3 contains some results regard to the discrete mollification. In Section 4, a marching mollification approach is established to solve Bloch NMR equation. Section 5 contains some numerical results.

2. Problem description

In this section the mathematical modelling of NMR is briefly reviewed. The objective is to allow us to understand and describe the MR signal and image generation in order to introduce them to processing analysis. One may note that a sample is magnetized when it is placed in a magnetic field. Suppose M_0 denotes the component of magnetization of a sample at equilibrium and $\overrightarrow{M} = (M_x, M_y, M_z)$ be the magnetization vector when it is reached its equilibrium along the field (the $z-$axis). In the presence of the field $\overrightarrow{B_1}$, the magnetization vector $\overrightarrow{M}$ variations can be stated as a system of equations known as Bloch equations as follows [7, 8]

$$\frac{dM_x}{dt} = V(x,t)gradM_x + \frac{\partial M_x}{\partial t} = -\frac{M_x}{T_2}, \quad (1)$$

$$\frac{dM_y}{dt} = V(x,t)gradM_y + \frac{\partial M_y}{\partial t} = \gamma M_z B_1(x,t) - \frac{M_y}{T_2}, \quad (2)$$

$$\frac{dM_z}{dt} = V(x,t)gradM_z + \frac{\partial M_z}{\partial t} = -\gamma M_y B_1(x,t) - \frac{M_0 - M_z}{T_1}. \quad (3)$$

The parameters in these equations defined as

γ: the gyromagnetic ratio of fluid spins,

M_0: the equilibrium magnetization,

T_1: the spin-lattice (longitudinal) relaxation time,

T_2: the spin-spin (transverse) relaxation time,

V: the flow velocity as a result of neuronal activity.

Generally $M_0 \neq M_z$, especially when $B_1(x)$ field is strong. In this situation from equations (2) and (3) one can drive the following equation [7, 8, 9]

$$V^2(x,t)\frac{\partial^2 M_y}{\partial x^2} + 2V(x,t)\frac{\partial^2 M_y}{\partial x \partial t} + \frac{\partial^2 M_y}{\partial t^2} + (\frac{1}{T_1} + \frac{1}{T_2})V(x,t)\frac{\partial M_y}{\partial x}$$
$$+(\frac{1}{T_1} + \frac{1}{T_2})\frac{\partial M_y}{\partial t} + (\gamma^2 B_1^2(x,t) + \frac{1}{T_1 T_2})M_y = \frac{\gamma M_0 B_1(x,t)}{T_1}. \quad (4)$$

Suitable initial and boundary conditions may be available using the real-time experimental arrangements. In this study we consider (4) in one dimensional space. In addition it is supposed that the following initial and boundary conditions are at hand

$$M_y(0,t) = \varphi_1(t),\ t \geq 0, \quad (5)$$
$$\frac{\partial M_y}{\partial x}(0,t) = \varphi_2(t),\ t \geq 0, \quad (6)$$
$$M_y(x,0) = \psi(x),\ x \geq 0, \quad (7)$$

where $\varphi_1(t)$, $\varphi_2(t)$ and $\psi(x)$ are known functions. The main goal of these study is to establish a reliable numerical procedure to solve the foregoing problem. We suppose that the initial and boundary functions are only known approximately as $\psi^\varepsilon(x)$, $\varphi_1^\varepsilon(t)$ and $\varphi_2^\varepsilon(t)$ respectively such that $\|\psi(x) - \psi^\varepsilon(x)\|_\infty \leq \varepsilon$ and $\|\varphi_i(t) - \varphi_i^\varepsilon(t)\|_\infty \leq \varepsilon,\ i = 1,2$. Because of the presence of the noise in the problem's data, implying a regularization process seems to be necessary. Here first we use mollification method to stabilize the problem. To this end let us recall some fundamental results associate with discrete mollification.

3. Method of solution

3.1. **Discrete mollification.** Let $\delta > 0$, $p > 0$, $A_p = (\int_{-p}^{p} e^{-s^2} ds)^{-1}$, $I = [0,1]$ and $I_\delta = [p\delta, 1 - p\delta]$. It is clear that for $p < \frac{1}{2}\delta$, the interval I_δ is nonempty set. Furthermore suppose $K = \{x_j : j \in Z, 1 \leq j \leq M\} \subset I$, satisfying $x_{j+1} - x_j > d > 0, j \in Z$, and $0 \leq x_1 < x_2 < \cdots < x_M \leq 1$, where Z assumed to be the set of integers and d consider as a positive constant. If $G = \{g_j\}_{j\in Z}$ be a discrete function defined on K and $s_j = (1/2)(x_j + x_{j+1}), j \in Z$, Then the discrete $\delta-$mollification of G is defined by [13]

$$J_\delta G(x) = \sum_{j=1}^{M} \left(\int_{s_{j-1}}^{s_j} \rho_\delta(x - s) ds \right) g_j,$$

where

$$\rho_{\delta,p}(x) = \begin{cases} A_p \delta^{-1} \exp\left(-\frac{x^2}{\delta^2}\right), & |x| \leq p\delta, \\ 0, & |x| > p\delta. \end{cases}$$

Notice that $\sum_{j=1}^{M}(\int_{s_{j-1}}^{s_j} \rho_\delta(x-s)ds) = \int_{-p\delta}^{p\delta} \rho_\delta(s)ds = 1$. Let $\Delta x = \sup_{j\in Z}(x_{j+1} - x_j)$, some useful results of the consistency, stability, and convergence of discrete δ-mollification are as follows [13, 14, 15, 16]

Theorem 3.1. (1) *For uniformly Lipschitz function $g(x)$ in I and it's discrete version $G = \{g_j = g(x_j) : j \in Z\}$, there exists a constant C, independent of δ, such that*

$$\| J_\delta G - g \|_{\infty, I_\delta} \leq C(\delta + \Delta x).$$

Moreover, if $g'(x) \in C(I)$ then,

$$\| (J_\delta G)' - g' \|_{\infty, I_\delta} \leq C\left(\delta + \frac{\Delta x}{\delta}\right).$$

(2) *If the discrete functions* $G = \{g_j : j \in Z\}$ *and* $G^\varepsilon = \{g_j^\varepsilon : j \in Z\}$, *which are defined on* K, *satisfy* $\parallel G - G^\varepsilon \parallel_{\infty,K} \leq \varepsilon$, *then we have*

$$\parallel J_\delta G - J_\delta G^\varepsilon \parallel_{\infty,I_\delta} \leq \varepsilon,$$

$$\parallel (J_\delta G)' - (J_\delta G^\varepsilon)' \parallel_{\infty,I_\delta} \leq \frac{C\varepsilon}{\delta}.$$

(3) *For uniformly Lipschitz function* $g(x)$ *in* I *and it's discrete version* $G = \{g_j = g(x_j) : j \in Z\}$, *if* $G^\varepsilon = \{g_j^\varepsilon : j \in Z\}$ *be the perturbed discrete version of* g *satisfying* $\parallel G - G^\varepsilon \parallel_{\infty,K} \leq \varepsilon$, *then*

$$\parallel J_\delta G^\varepsilon - J_\delta g \parallel_{\infty,I_\delta} \leq C(\varepsilon + \Delta x),$$

and

$$\parallel J_\delta G^\varepsilon - g \parallel_{\infty,I_\delta} \leq C(\varepsilon + \delta + \Delta x).$$

Moreover, if $g'(x) \in C(I)$ *then,*

$$\parallel (J_\delta G^\varepsilon)' - (J_\delta g)' \parallel_{\infty,I_\delta} \leq \frac{C}{\delta}(\varepsilon + \Delta x),$$

$$\parallel (J_\delta G^\varepsilon)' - g' \parallel_{\infty,I_\delta} \leq C\left(\delta + \frac{\varepsilon}{\delta} + \frac{\Delta x}{\delta}\right).$$

Denoting the centered difference operator by $\boldsymbol{D}$, *i.e.,* $\boldsymbol{D}f(x) = \frac{f(x+\Delta x)-f(x-\Delta x)}{2\Delta x}$. *Then we have the following results* [13, 15, 16]

Theorem 3.2. (1) *If* $g' \in C^1(R^1)$, *and* $G = \{g_j = g(x_j) : j \in Z\}$ *is the discrete version of* g, *with* G, G^ε *satisfying* $\parallel G - G^\varepsilon \parallel_{\infty,K} \leq \varepsilon$, *then,*

$$\parallel \boldsymbol{D}(J_\delta G^\varepsilon) - (J_\delta g)' \parallel_\infty \leq \frac{C}{\delta}(\varepsilon + \Delta x) + C_\delta(\Delta x)^2,$$

$$\parallel \boldsymbol{D}(J_\delta G^\varepsilon) - g' \parallel_\infty \leq C\left(\delta + \frac{\varepsilon}{\delta} + \frac{\Delta x}{\delta}\right) + C_\delta(\Delta x)^2.$$

(2) *Suppose* $G = \{g_j : j \in Z\}$ *is a discrete function defined on a set* K, *and* $\boldsymbol{D}_0^\delta$ *is a differentiation operator defined by* $\boldsymbol{D}_0^\delta(G) = \boldsymbol{D}(J_\delta G)(x) \mid_K$, *then*

$$\parallel \boldsymbol{D}_0^\delta(G) \parallel_{\infty,K} \leq \frac{C}{\delta} \parallel G \parallel_{\infty,K}.$$

It should be pointed out that concern with the mollification method, one may deal with some limitations. For instance, the implementation of $\delta-$mollification for a noisy function in an interval such as $[0, 1]$ usually requires to extend the values of proposed noisy function to a slightly bigger interval such as $[-p\delta, 1+p\delta]$ or to restrict that function to a subinterval such as $[p\delta, 1 - p\delta]$. Extension to a bigger interval needs an extrapolation technique in conjunction with a minimization processes. On the other hand any limitation on the mail interval may cause one loses some important information of the proposed function. In addition to these limitations, one deals with the challenge of determination of the mollification parameters.

3.2. **Regularized problem and marching scheme.** To establish our interest a numerical procedure, first we consider the regularized form of the problem (4)-(7) as follows

$$V^2(x,t)u_{xx}(x,t) + 2V(x,t)u_{tx}(x,t) + u_{tt}(x,t) + \lambda V(x,t)u_x(x,t) + \lambda u_t(x,t) + (\gamma^2 B_1^2(x,t) + \mu)u(x,t) = \gamma\mu M_0 B_1(x,t),\ x > 0,\ t > 0, \tag{8}$$

$$u(0,t) = J_{\delta_0}(\varphi_1^\varepsilon(t)),\ t \geq 0, \tag{9}$$

$$u_x(0,t) = J_{\delta_0^*}(\varphi_2^\varepsilon(t)),\ t \geq 0. \tag{10}$$

$$u(x,0) = J_{\delta'}(\psi(x)),\ x \geq 0, \tag{11}$$

where $\lambda = \left(\frac{1}{T_1} + \frac{1}{T_2}\right)$ and $\mu = \frac{1}{T_1 T_2}$. Generalized Cross Validation (GCV) method is used to find the radii of mollification such as δ', δ_0 and δ_0^* [13, 14, 17].

In the the problem (8)-(11) it is assumed that $0 \leq x \leq 1$ and $0 \leq t \leq 1$. Suppose M and N are two positive integers and $h = \Delta x = 1/M$ and $k = \Delta t = 1/N$ are the length of mesh sizes of the finite differences discretization of time and space domains ($[0,1]$). Now if one consider the following discrete functions
$U_{i,n}$: the discrete computed approximations of $u(ih, nk)$,
$W_{i,n}$: the discrete computed approximations of $u_t(ih, nk)$,
$Q_{i,n}$: the discrete computed approximations of $u_x(ih, nk)$,
$V_{i,n}$: the discrete computed approximations of $V(ih, nk)$,
$B_{i,n}$: the discrete computed approximations of $B_1(ih, nk)$,
then the algorithm of space marching scheme may be written as follows

(1) Select δ_0,δ_0^*.
(2) Perform mollification of α^ε,β^ε and $f(x)^\varepsilon$ in the interval $[0,1]$

$$U_{0,n} = J_{\delta_0}\varphi_1^\varepsilon(nk),\ Q_{0,n} = J_{\delta_0^*}\varphi_2^\varepsilon(nk), n \neq 0,\ U_{i,0} = J_{\delta'}\psi^\varepsilon(ih),\ i \in \{0,1,\ldots,M\}$$

(3) Perform mollified differentiation in time of $J_{\delta_0}\varphi_1^\varepsilon(nk)$. Set

$$W_{0,n} = \mathbf{D}_t(J_{\delta_0}\varphi_1^\varepsilon(nk))\ (n \neq 0), \quad W_{0,0} = \mathbf{D}_t(J_{\delta'}\psi^\varepsilon(0)).$$

(4) Initialize $i = 0$. Do while $i \leq M - 1$,

$$U_{i+1,n} = U_{i,n} + hQ_{i,n}, \tag{12}$$

$$Q_{i+1,n} = Q_{i,n} + \frac{h}{V_{i,n}^2}[\gamma\mu M_0 B_{i,n} - 2V_{i,n}\mathbf{D}_x(J_{\delta_i}W_{i,n}) - \mathbf{D}_t(J_{\delta_i}W_{i,n}) - \lambda V_{i,n}Q_{i,n} - \lambda W_{i,n} - (\gamma^2 B_{i,n} + \mu)U_{i,n}], \tag{13}$$

$$W_{i+1,n} = W_{i,n} + h\mathbf{D}_t(J_{\delta_i^*}Q_{i,n}). \tag{14}$$

From now on, if $X_{i,n}$ is a discrete function, we denote $|X_i| = \max_n |X_{i,n}|$. We also consider a smoothing assumption $u(x,t) \in C^{2,2}(I \times [0,\infty))$ to discuss the stability and convergence of the scheme.

3.3. **Stability and Convergence Analysis.** In this section, we analyze the stability and convergence of the proposed marching scheme.

Theorem 3.3 (Stability of the Algorithm). *One may find a constant C, such that*

$$\max\{|H_M|, |Q_M|, |W_M|\} \quad \leq \quad C\max\{|U_0|, |Q_0|, |W_0|\}$$

Proof. Let $|\delta|_{-\infty} = \min_i(\delta_i, \delta_i^*)$ and

$$m = \min_{(x,t)\in[0,1]\times[0,1]}\{|V(x,t)|, |B_1(x,t)|\},\ M = \max_{(x,t)\in[0,1]\times[0,1]}\{|V(x,t)|, |B_1(x,t)|\}.$$

Applying Theorem 3.2 yields

$$|\mathbf{D}_t(J_{\delta_i^*}Q_{i,n})| \le \frac{C}{|\delta|_{-\infty}}|Q_{i,n}|,\ |\mathbf{D}_t(J_{\delta_i}W_{i,n})| \le \frac{C}{|\delta|_{-\infty}}|W_{i,n}|,$$
$$|\mathbf{D}_x(J_{\delta_i}W_{i,n})| \le \frac{C}{|\delta|_{-\infty}}|W_{i,n}|. \qquad (15)$$

Now by using (13) and (15) we have

$$\begin{aligned}|Q_{i+1,n}| \le & |Q_{i,n}| + \frac{h}{m^2}[\gamma\mu M_0 M + 2M\frac{C}{|\delta|_{-\infty}}|W_{i,n}| + \frac{C}{|\delta|_{-\infty}}|W_{i,n}| + \lambda M|Q_{i,n}| \\ & + \lambda|W_{i,n}| + (\gamma^2 M + \mu)|U_{i,n}|] \\ \le & \left(1 + h\frac{C_1}{m^2}\right)\max\{C_0, |U_i|, |Q_i|, |W_i|\}, \qquad (16)\end{aligned}$$

where $C_0 = \frac{\gamma M_0 M}{T_1 T_2}$, $C_1 = 1 + (2M+1)\frac{C}{|\delta|_{-\infty}} + \lambda(M+1) + (\gamma^2\mu M + d)$, similarly form (14) and (15) we have

$$|W_{i+1,n}| \le \left(1 + h\frac{C}{|\delta|_{-\infty}}\right)\{|Q_{i,n}|, |W_{i,n}|\},$$

and finally from (12) we have

$$|U_{i+1,n}| \le (1+h)\max\{|U_{i,n}|, |Q_{i,n}|\}, \qquad (17)$$

Letting $C_\delta = \max\left\{1, C_1, \frac{C}{|\delta|_{-\infty}}\right\}$, from (16)-(17) we obtain

$$\max\{C_0, |U_{i+1}|, |Q_{i+1}|, |W_{i+1}|\} \le (1 + hC_\delta)\max\{C_0, |U_i|, |Q_i|, |W_i|\},$$

by iterating this last inequality M times, we have

$$\max\{C_0, |U_M|, |Q_M|, |W_M|\} \le (1 + hC_\delta)^M \max\{C_0, |U_0|, |Q_0|, |W_0|\},$$

which implies

$$\max\{C_0, |U_M|, |Q_M|, |W_M|\} \le (\exp C_\delta)\max\{C_0, |U_0|, |Q_0|, |W_0|\}.$$

This complete the proof of this statement. □

Theorem 3.4 (Formal convergence). *Suppose δ is fixed and h, k and ε tend to zero, then restricted to the grid points, the discrete mollified solution converges to the mollified exact solution.*

Proof. From the definitions of discrete error functions, it follows that

$$\Delta U_{i,n} = U_{i,n} - u(ih, nk),\ \Delta Q_{i,n} = Q_{i,n} - u_x(ih, nk),\ \Delta W_{i,n} = W_{i,n} - u_t(ih, nk).$$

Using Taylor series, we obtain some useful equations satisfied by the mollified solution u, namely,

$$\begin{aligned} u((i+1)h, nk) &= u(ih, nk) + hu_x(ih, nk) + O(h^2), \\ u_x((i+1)h, nk) &= u_x(ih, nk) + \frac{h}{V^2(ih, nk)}[\gamma\mu M_0 B_1(ih, nk) \\ & \quad -2V(ih, nk)\frac{d}{dx}u_t(ih, nk) - \frac{d}{dx}u_t(ih, nk) \\ & \quad -\lambda V(ih, nk)u_x(ih, nk) - \lambda u_t(ih, nk) \\ & \quad -(\gamma^2 B_1(ih, nk) + \mu)u_{i,n}] + O(h^2) \\ u_t((i+1)h, nk) &= u_t(ih, nk) + h\frac{d}{dt}u_x(ih, nk) + O(h^2). \end{aligned}$$

Also,

$$\begin{aligned}\Delta U_{i+1,n} &= \Delta U_{i,n} + (U_{i+1,n} - U_{i,n}) - (u((i+1)h, nk) - u(ih, nk)) \\ &= \Delta U_{i,n} + h(Q_{i,n} - u_x(ih, nk)) + O(h^2) \\ &= \Delta U_{i,n} + h\Delta Q_{i,n} + O(h^2). \qquad (18)\end{aligned}$$

$$\begin{aligned}\Delta Q_{i+1,n} &= \Delta Q_{i,n} + (Q_{i+1,n} - Q_{i,n}) - (u_x((i+1)h, nk) - u_x(ih, nk)) \\ &= \Delta Q_{i,n} + \frac{h}{V_{i,n}^2}[\gamma\mu M_0 B_{i,n} - 2V_{i,n}\mathbf{D}_x(J_{\delta_i} W_{i,n}) \\ &\quad -\mathbf{D}_t(J_{\delta_i} W_{i,n}) - \lambda V_{i,n} Q_{i,n} - \lambda W_{i,n} - (\gamma^2 B_{i,n} + \mu) U_{i,n}] \\ &\quad -\frac{h}{V^2(ih, nk)}[\gamma\mu M_0 B_1(ih, nk) - 2V(ih, nk)\frac{d}{dx}u_t(ih, nk) \\ &\quad -\frac{d}{dx}V_t(ih, nk) - \lambda V(ih, nk)u_x(ih, nk) - \lambda u_t(ih, nk) \\ &\quad -(\gamma^2 B_1(ih, nk) + \mu)u_{i,n}] + O(h^2), \qquad (19)\end{aligned}$$

$$\begin{aligned}\Delta W_{i+1,n} &= \Delta W_{i,n} + (W_{i+1,n} - W_{i,n}) - (u_t((i+1)h, nk) - u_t(ih, nk)) \\ &= \Delta W_{i,n} + \frac{h}{K(ih)}\mathbf{D}_t(J_{\delta_i^*} Q_{i,n}) - hu_t(ih, nk) + O(h^2) \\ &= \Delta W_{i,n} + h(\mathbf{D}_t(J_{\delta_i^*} Q_{i,n}) - u_t(ih, nk)) + O(h^2). \qquad (20)\end{aligned}$$

Now from equalities (17)-(20), using the error estimates of discrete mollification from theorem 3.1

$$\begin{aligned}|U_{i+1,n}| &\leq |\Delta U_{i,n}| + h|\Delta Q_{i,n}| + O(h^2), \\ |\Delta Q_{i+1,n}| &\leq |\Delta Q_{i,n}| + \frac{h}{m^2}\left(2M\left(\frac{C|\Delta W_{i,n}| + h}{|\delta|_{-\infty}} + C_\delta h^2\right)\right. \\ &+ \left(\frac{C|\Delta W_{i,n}| + k}{|\delta|_{-\infty}} + C_\delta k^2\right) + \lambda M|\Delta W_{i,n}| + \lambda|\Delta W_{i,n}| \\ &+ \left.\mu|\Delta U_{i,n}|\right) + O(h^2), \\ |\Delta W_{i+1,n}| &\leq |\Delta W_{i,n}| + h\left(C\frac{|\Delta Q_{i,n}| + k}{|\delta|_{-\infty}} + C_{\delta^*}k^2\right) + O(h^2).\end{aligned}$$

Suppose

$$\begin{aligned}\Delta_i &= \max\{|\Delta U_{i,n}|, |\Delta W_{i,n}|, |\Delta Q_{i,n}|\}, \\ C_0 &= \max\left\{1, \frac{1}{m^2}\left(\frac{(C+1)M}{|\delta|_{-\infty}} + \lambda(M+1) + \mu\right), \frac{C}{|\delta|_{-\infty}}\right\}, \\ C_1 &= \max\left\{\frac{1}{m^2}\left(\frac{h}{|\delta|_{-\infty}} + C_\delta h^2\right) + \left(\frac{k}{|\delta|_{-\infty}} + C_\delta k^2\right), \frac{Ck}{|\delta|_{-\infty}} + C_{\delta^*}k^2\right\}.\end{aligned}$$

Then we obtain

$$\begin{aligned}\Delta_{i+1} &\leq (1 + hC_0)\Delta_i + hC_1 + O(h^2) \\ &\leq (1 + hC_0)(\Delta_i + C_1) + O(h^2), \qquad (21)\end{aligned}$$

Table 1. Relative l_2 error norms for Example 4

M	N	ε	u	u_t	u_x
64	64	0.0001	0.0043119	0.0779168	0.0561945
128	128	0.0001	0.0042946	0.0759839	0.0543272
256	256	0.0001	0.0042752	0.0655975	0.0536547
512	512	0.0001	0.0042553	0.0654142	0.0530131
64	64	0.001	0.0058916	0.0829729	0.0683256
128	128	0.001	0.0058134	0.0861485	0.0661293
256	256	0.001	0.0056368	0.0856221	0.0643106
512	512	0.001	0.0054368	0.0854795	0.0635646
64	64	0.01	0.0075976	0.0977476	0.0762271
128	128	0.01	0.0075222	0.0968234	0.0734151
256	256	0.01	0.0074203	0.0964474	0.0713976
512	512	0.01	0.0063785	0.0962375	0.0699437

and after L iterations

$$\Delta_L \leq \exp(C_0)(\Delta_0 + C_1). \tag{22}$$

Moreover from

$$\begin{aligned}
|\Delta U_{0,n}| &= |U_{0,n} - u(0,nk)| = |J_{\delta_0}\alpha^\varepsilon(nk) - u(0,nk)| \leq C(\varepsilon + k), \\
|\Delta Q_{0,n}| &= |Q_{0,n} - u_x(0,nk)| = |J_{\delta_0^*}\beta^\varepsilon(nk) - u_x(0,nk)| \leq C(\varepsilon + k), \\
|\Delta W_{0,n}| &= |\mathbf{D}_t(J_{\delta_0}\alpha^\varepsilon(nk)) - u_t(0,nk)| \leq \frac{C}{\delta_0}(\varepsilon + k) + C_\delta k^2,
\end{aligned}$$

we see that when ε, h, and k tend to 0, Δ_0 and C_1 tend to 0. Consequently $(\Delta_0 + C_1)$ tends to 0 and so does Δ_L and this complete the proof of this theorem. □

Remark. The numerical algorithm and the stability and convergence results reported in this section can be easily extended for a more general case when in the equation (4), the right hand side contains another source term such as $F(x,t)$.

4. Numerical experiments

The main goal of this section is to investigate the robustness and ability of the proposed mollified marching approach. To this end we examine two standard test problems in general form with a source term function in the right hand side of equation (4). In this problems we consider $p = 3$. Perturbed boundary data are obtained by adding random errors to the exact data functions. For example, for the boundary data function $h(x,t)$, its perturbed version is generated as [13]

$$h^\varepsilon_{j,n} = h(x_j, t_n) + \varepsilon_{j,n}, \qquad j = 0,1,\ldots,N, n = 0,1,\ldots,T, \tag{23}$$

where the $(\varepsilon_{j,n})$'s are Gaussian random variables with variance ε^2.

The relative l_2 error norm defined as follows is used to evaluate the errors between exact and numerical results

$$E = \frac{\left[(1/(M+1)(N+1))\Sigma_{i=0}^M\ \Sigma_{j=0}^N |u(ih,jk) - U_{i,j}|^2\right]^{1/2}}{\left[(1/(M+1)(N+1))\Sigma_{i=0}^M\ \Sigma_{j=0}^N |u(ih,jk)|^2\right]^{1/2}}. \tag{24}$$

Furthermore let R denotes the absolute error norm between the exact and numerical solutions. Using R we approximate the convergence order of numerical results using following formula

$$p \simeq \log_\beta \frac{\|E_h\|}{\|E_{\frac{h}{\beta}}\|}.$$

Example 1. As the first test problem, consider [10]

$$\gamma = 43,\ \mu = 1.5,\ \lambda = 2.5,\ V = 4,\ M_0 = 1.5,\ \omega = 85,$$
$$B_1(x,t) = \cos\omega t,\ \psi(t) = \sin\omega t,\ \phi_i(x) = 0,\ i = 1,2,$$
$$F(x,t) = \cos\omega t(-96.75 + cos\frac{3\pi}{2}x(212.5 + 1849\sin\omega t)$$
$$-3204.42\sin\frac{3\pi}{2}x) + sin\omega t(-7578.81\cos\frac{3\pi}{2}x - 47.1239\sin\frac{3\pi}{2}x).$$

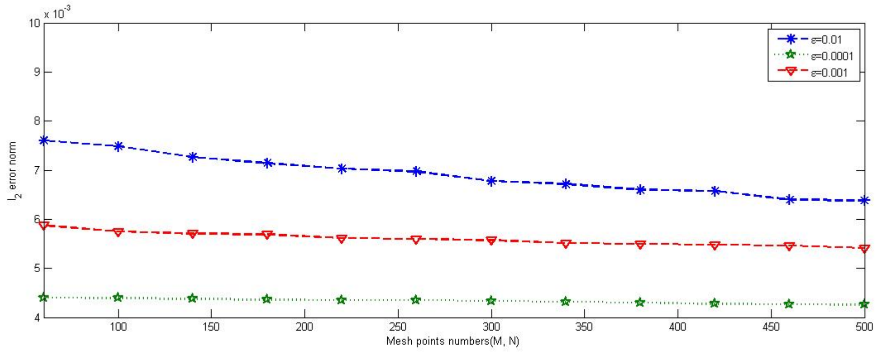

FIGURE 1. The relative l_2 error norm for v for three different noise levels against mesh point numbers in Example 4.

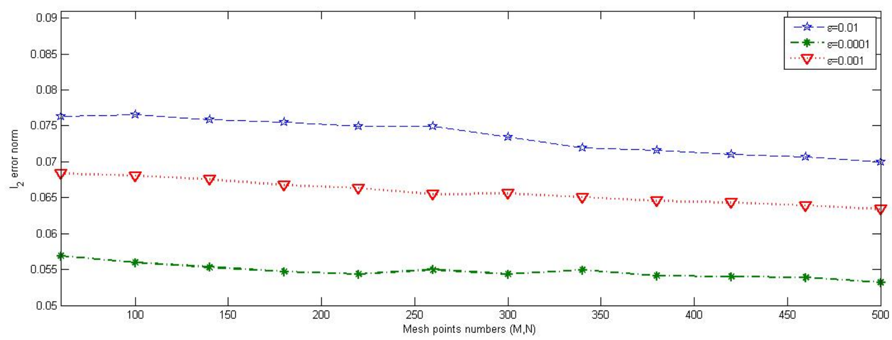

FIGURE 2. The relative l_2 error norm for v_x for three different noise levels against mesh point numbers in Example 4.

The exact solution for this problem may be found as $u(x,t) = \sin\omega t\cos\frac{3\pi}{2}x$. The relative l_2-errors between the numerical and analytical results are shown in Table 1 in three different noise levels for $M,\ N = 64,\ 128,\ 256,\ 512$.

Figures 1, 2 and 3 demonstrate the behavior of l_2 error norm of u, u_x and u_t associate with three different noise levels. It can be observed that decreasing the mash sizes with respect to space and time variables can decrease the l_2 errors.

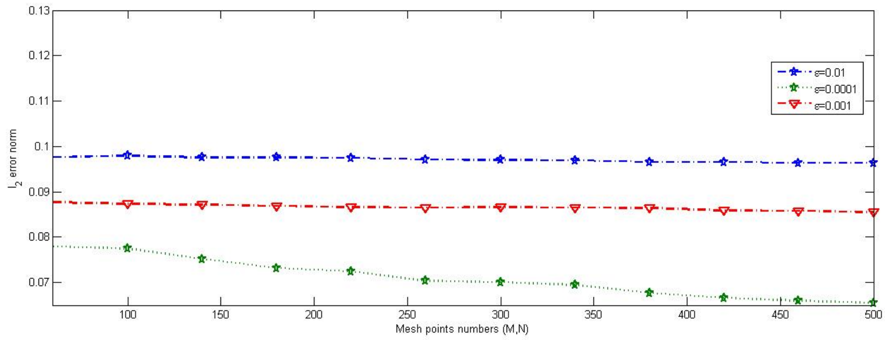

FIGURE 3. The relative l_2 error norm for v_t for three different noise levels against mesh point numbers in Example 4.

TABLE 2. Relative l_2 error norms for Example 4

M	N	ε	u	u_t	u_x
64	64	0.0001	0.0018592	0.0332585	0.0092144
128	128	0.0001	0.0016542	0.0313251	0.0090013
256	256	0.0001	0.0013465	0.0247875	0.0086951
512	512	0.0001	0.0012353	0.0114142	0.0085301
64	64	0.001	0.0039254	0.0522583	0.0099145
128	128	0.001	0.0035345	0.0492568	0.0098985
256	256	0.001	0.0035123	0.0425681	0.0098126
512	512	0.001	0.0033543	0.0358945	0.0097003
64	64	0.01	0.0165914	0.0658947	0.0852459
128	128	0.01	0.0135222	0.0682314	0.0732551
256	256	0.01	0.0098423	0.0548719	0.0689542
512	512	0.01	0.0091375	0.0501252	0.0485962

Example 2. As another test problem we consider the following assumptions [10]

$$\begin{aligned}
&\gamma = 0,\ \mu = 3,\ \lambda = 4.5,\ V = 5,\ M_0 = 2,\ \omega = 8,\\
&B_1(x,t) = e^{-\omega^2 t},\ \psi(t) = \sin \pi x,\ \phi_1(x) = 0,\ \phi_2(x) = \pi e^{-\omega^2 t},\\
&F(x,t) = e^{-2\omega^2 t}(20e^{\omega^2 t} + 1939.93e^{\omega^2 t}) \cos \pi x\\
&-(900 + 3564.26e^{\omega^2 t}) \sin \pi x.
\end{aligned}$$

In this case the exact solution can be derived as $u(x,t) = \sin \pi x e^{-\omega^2 t}$. Table 2 reports the relative l_2-error norms between the numerical and analytical solutions in three different noise levels for $M,\ N = 64,\ 128,\ 256,\ 512$. The behaviors of relative l_2-errors norms of u, u_x and u_t are shown in figures 4, 5 and 6. The numerical results show a good agreement between the exact and numerical solutions.

The numerical results for Examples 1 and 2 explored that for the different values of M and N, when $\varepsilon = 0.01$, the order of convergence of the numerical results (p) varies between 0.35 and 0.75. For $\varepsilon = 0.001$, p varies between 0.55 and 0.95 and for $\varepsilon = 0.0001$, p varies between 0.80 and 1.

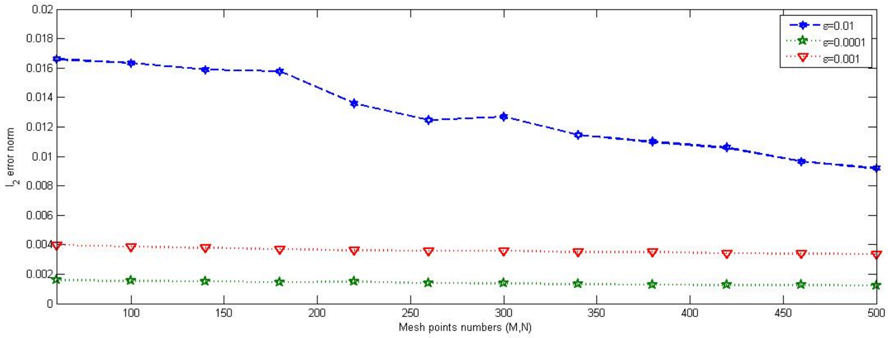

FIGURE 4. The relative l_2 error norm for v for three different noise levels against mesh point numbers in Example 4.

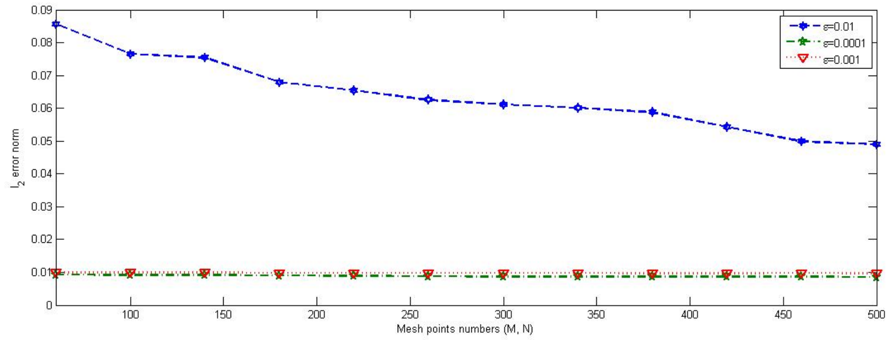

FIGURE 5. The relative l_2 error norm for v_x for three different noise levels against mesh point numbers in Example 4.

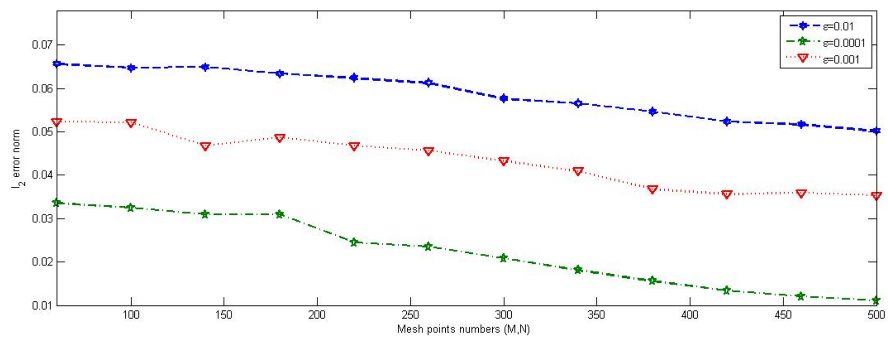

FIGURE 6. The relative l_2 error norm for v_t for three different noise levels against mesh point numbers in Example 4.

5. Conclusion

A stable numerical approach is developed to solve NMR Block Equation in one dimensional case. The numerical approach is based on mollification method as a procedure for filtering the input data noises and space marching method. The convergence and stability results support the applicability of the proposed approach. The numerical results are in good agreement with the analytical solutions for two test cases.

References

[1] Freeze, R.A. and Cherry, J.A., (1979), Groundwater. Prentice-Hall, Englewood Cliffs, NJ.

[2] Ted Watson, A. and Philip Chang, CT., (1997), Characterizing porous media with NMR methods, Prog. Nucl. Mag. Res. Spect. 31, pp. 343–386.

[3] Torrey, HC., (1956), Bloch equations with diffusion terms, Phys. Rev. 104 (3), pp. 563–565.

[4] Awojoyogbe, OB. and Boubarker, K., (2008), A solution to Bloch NMR flow equations for the analysis of hemodynamic functions of blood flow system using m-Boubaker polynomials, Curr. Appl. Phys., Doi:10 1016/j.cap.2008.01.019.

[5] Awojoyogbe, OB., (2007), A quantum mechanical model of the Bloch NMR flow equations for electron dynamics in fluids at the molecular level, Phys. Scr., 75, pp. 788–794.

[6] Awojoyogbe, OB., (2004), Analytical solution of the time dependent Bloch NMR equations: a translational mechanical approach, Physica A., 339, pp. 437–460.

[7] Awojoyogbe, OB., (2002), A mathematical model of Bloch NMR equations for quantitative analysis of blood flow in blood vessels with changing crosssection I, Physica A., 303, pp. 163–175.

[8] Awojoyogbe, OB., (2003), A mathematical model of Bloch NMR equations for quantitative analysis of blood flow in blood vessels with changing crosssection II, Physica A., 323, pp. 534–550.

[9] Awojoyogbe, OB., Faromika, OP., Dada, OM., Boubaker, K. and Fuwape, IA., (2010), Mathematical model of the Bloch NMR flow equations for the analysis of fluid flow in restricted geometries using the Boubaker polynomials expansion scheme, Current. Appl. Phys., 10, pp. 289–293.

[10] Dada, OM., Awojoyogbe, OB. and Ukoha, AC.,(2015), A computational analysis for quantitative evaluation of petrol–physical properties of rock fluids based on Bloch–NMR diffusion model for porous-media, J. Petrol. Sci. Engin., 127, pp. 137–147.

[11] Lin, G. (2018), General pulsed-field gradient signal attenuation expression based on a fractional integral modified-Bloch equation, Commun. Nonlinear. Sci. Numer. Simul., 63, pp. 404 –420.

[12] Liu, F., Feng, L., Anh, V. and Li, J. (2019), Unstructured-mesh Galerkin finite element method for the two dimensional multiterm time-space fractional Bloch-Torrey equations on irregular convex domains, Comput. Math. Appl., 78, pp. 1637 –1650.

[13] Murio, DA. (2002), Mollification and space marching, in: K. Woodbury (Ed.), Inverse Engineering Handbook, CRC Press.

[14] Garshasbi, M., (2019), Determination of unknown functions in a mathematical model of ductal carcinoma in situ, Numer. Meth. Part. Diff. Eq., 35, pp. 2000–2016

[15] Acosta, CD. and Mejia, CE., (2008), Stabilization of explicit methods for convection diffusion equations by discrete mollification, Comput. Math. Appl., 55, pp. 368-380.

[16] Acosta, CD. and Mejia, CE., (2009), Approximate solution of hyperbolic conservation laws by discrete mollification, Appl. Numer. Math., 59, pp. 2256-2265.

[17] Garshasbi, M. and Dastour, H., (2015), Estimation of unknown boundary functions in an inverse heat conduction problem using a mollified marching scheme, Numer. Alg., 68 (4), pp. 769–790.

[18] Garshasbi, M. and Dastour, H., (2016), A mollified marching solution of an inverse ablation-type moving boundary problem, Comp. Appl. Math., 35, pp. 61–73.

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