Quantum mechanical simulations in diffusion MRI

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Abstract

Background: Various magnetic resonance imaging simulation packages rely on Bloch equations, Bloch-Torrey equations and the Liouville–von Neumann equation is which a dynamical formulation to simulate a voltage bias across a molecular system and to model a time-dependent current in terms of classical or quantum treatments of magnetic resonance imaging respectively.

Method: The problems in these equations cannot address spin dynamic such as j-coupling and spatial dynamics such as diffusion and flow at the same level. In this study, the Fokker-Planck formalism was used to simulate phantoms that deal with diffusion and flow on the spatial dynamics side and j-coupling in the spin dynamic side using the Spinach simulation package.

Result: The numerical simulation of magnetic resonance imaging has two limits in terms of research. First, a complicated spin system is associated with simple diffusion and flow, such as in spatially encoded NMR experiments. Second, a simple spin system is associated with high dimensional diffusion and flow.

Conclusion: A unique simulation package that deals with the quantum mechanics treatment of spin dynamics and the classical description of diffusion and flow in three dimensions are presented in this work.

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Keywords: *MRI, Diffusion, Quantum mechanical simulation, Fokker-Planck formalism.*

INTRODUCTION

A set of equations describ net magnetization as a time-dependent NMR. These equations are known as Bloch equations or Bloch-Torrey equations, which appear to be the basis of all simulation packages. During the last decay, various magnetic resonance simulation packages have been implemented very well [1]. However, these packages are unable to handle coupled spin systems such as J-coupling. On the nuclear magnetic resonance side, the packages can deal with the coupled spin system but are still insufficient to handle the necessary spatial dynamics such as diffusion and flow. NMR-SCOPE[2] was the first quantum mechanics package to develop a product operator for a coupled spin system. The C++ language then introduces GAMMA [3] for the same purpose. Many packages, such as SIMPSON [4], Bloch-Lib [5], SPINEVOLUTION [6], SIMPLTN [7], NMRSIM [8], Spin-Dynamics [9], and Spinach [10]. In this paper, a unique simulation package that deals with spin dynamics in quantum mechanics vision and the classical description of diffusion and flow was presented.

1. Magnetic resonance imaging

MRI is a noninvasively technique that is generally used for medical purposes. Disorders in muscles and joints, tumors detections, and viewing abnormalities in the brain can be performed very well using MRI. The basic idea of magnetic resonance imaging is the interaction between hydrogen atoms (protons), which are a part of the water molecules. The latter is considered 70% of the entire body. The protons were quantized according to their magnetic moments parallel to the main magnetic field. Subsequently, the radiofrequency pulse was switched on to transfer the magnetization from the transverse plane according to the applied magnetic field. The range of frequencies processed via radiofrequency pulses relies on the power of the magnetic field is strong. Slice can be selected specifically when an additional gradient magnetic field is applied to make the external magnetic field vary from point to point. Each point has will have its own resonant frequency [11].

2. Fokker-Planck equation

Several theoretical approaches describe the magnetic resonance. The selection of a specific approach relies on the application field. The Bloch-Torrey equation [12], can be used for relaxation simulations of an isolated spin 1/2 system. An ensemble spin system simulation experiment can be performed using the Liouville-Von Neumann equation [13]. Most nuclear magnetic resonance theories depend on the Livioulle-von Neumann equation. The latter is based on the density operator formalism, which is described as the dynamics of a quantum system. In general, water molecules with diffusion and flow can be simulated owing to the competition between complicated spatial dynamics and a simple spin system [14]. On the other hand, researchers have good knowledge of the simulation of simple diffusion and flow with a complicated spin system such as spatially encoded NMR experiments. However, the completion of complicated spatial dynamics such as diffusion, flow, and convection in three-dimensional geometry with sophisticated spin systems (J-coupling, cross-correlation, etc.), such as a 3-dimensional phantom combined with typical metabolism, can contain up to seven coupled spin systems.

Methodology

1. Simulation platform

The Fokker-Planck formalism is used to treat an accurate quantum mechanical of spin dynamics such as spin-spin coupling and cross-relaxation coexisting with spatial distribution dynamics such as diffusion, flow, and chemical kinetics [15]. The Liouville-von Neumann equation is the central importance equation that all nuclear magnetic resonance simulation packages rely on in terms of the dynamics of quantum systems description. The Liouville-von Neumann equation can be derived from TDSE:

$$\frac{\partial}{\partial t}\boldsymbol{\rho}(t) = -i\mathbf{H}(t)\boldsymbol{\rho}(t) \quad (1)$$

Where $\boldsymbol{\rho}(t)$ is the density operator and $\mathbf{H}(t)$ is the spin Hamiltonian commutation superoperator [16]. The Hamiltonian can be defined as:

$$\mathbf{H\rho} = [\mathbf{H\rho}] = \mathbf{H\rho} - \mathbf{\rho H} \quad (2)$$

When relaxation and kinetics superoperators present, equation (1) can be updated to:

$$\frac{\partial}{\partial t}\boldsymbol{\rho}(t) = \left[-i\bar{\mathbf{H}}(t) + \mathbf{R} + \mathbf{K}\right]\boldsymbol{\rho}(t) \quad (3)$$

Where $\bar{\mathbf{H}}(t)$ is the Hamiltonian superoperator, $\mathbf{R}$ is the relaxation superoperator [3], which includes the diffusion term, and $\mathbf{K}$ is the kinetics superoperator responsible for the chemical processes in the system. If the thermodynamic equilibrium is non-trivial, the relaxation target must be added:

$$\mathbf{R}\boldsymbol{\rho}(t) \to \mathbf{R}\left\lfloor \boldsymbol{\rho}(t) - \boldsymbol{\rho}_{\mathrm{eq}} \right\rfloor \quad (4)$$

Where $\boldsymbol{\rho}_{\mathrm{eq}}$ is the density matrix in the thermal equilibrium condition.

Indirect representation of the spatial degrees of freedom is the main issue in current magnetic resonance simulation platforms. It is always assumed that spatial dynamics influence the spin Hamiltonian, whereas the latter does not affect the spatial dynamics. Bloch-Torrey equations [17], distributed Bloch equations [18], and k-space Bloch equations [19], etc. are used in current MRI methods. However, these methods are insufficient in terms of J-coupling interactions and some cannot deal with spatial dynamics such as diffusion and flow.

The Fokker-Planck formalism is the only equation that can deal with high spin dynamics including j-coupling interactions and spatial dynamics such as diffusion and flow at the same level. In this communication, we illustrate sufficient Fokker-Plank simulation for some MRI phantoms such as diffusion-weighted images in three dimensions which is required simultaneous treatments of spin dynamics and spatial dynamics at the same level.

2. Diffusion MRI

In the 1-D diffusion formalism for concentration c(x,t), the scalar diffusion coefficient D can rely on the spatial location:

$$\frac{\partial c(x,t)}{\partial t} = \frac{\partial}{\partial x} D(x) \frac{\partial}{\partial x} c(x,t) \quad (5)$$

When we move to the 3-D diffusion equation, all six components have coordinate dependence with a symmetric 3×3 diffusion tensor:

$$q(t) = \int_0^t P(t)\, G(t)\, d \quad (6)$$

Because of high structure structure in biological tissues, even if the diffusion is isotropic, the diffusion coefficient $\mathbf{D}$ will vary from the ideal isotopic diffusion and it will not be the same in all directions.

To understand the formalism of diffusion, we begin with the gradient $s(\varepsilon)$, where $0 \leq \varepsilon \leq 1$. The shape factor σ represent the total effect of the gradient :

$$\sigma = \int_0^1 s(\varepsilon) d\varepsilon \quad (7)$$

Two more type gradient parameters are common:

$$\lambda = \frac{1}{\sigma}\int_0^1 S(\varepsilon) d\varepsilon \qquad \kappa = \frac{1}{\sigma^2}\int_0^1 S^2(\varepsilon) d\varepsilon \quad (8)$$

where $S(\varepsilon)$ is an integral of $s(\varepsilon)$:

$$S(\varepsilon) = \int_0^{\varepsilon} s(\varepsilon) d\varepsilon \quad (9)$$

According to the spin-echo pulse sequence, the coherence can be expressed according to the gradient shape as follows:

$$P(t)G(t)=\begin{cases}\gamma g a(t) & 0\le t\le\delta\\ 0 & \delta\le t\le\Delta\\ -\gamma g a(t-\Delta) & \Delta\le \mathrm{t}\le\Delta+\delta\end{cases}\quad(10)$$

Where $P(t)$ is the coherence in terms of time, $G(t)$ is the gradient variation per unit time, g is the strength of the magnetic field, $a(t)$ is the pulse structure, and δ is the pulse length:

$$a(t)=s\left(\frac{t}{\delta}\right)\quad(11)$$

Substitute equation (12) in equation (11)

$$P(t)G(t)=\begin{cases}\gamma g s\left(\frac{t}{\delta}\right) & 0\le t\le\delta\\ 0 & \delta\le t\le\Delta\\ -\gamma g s\left(\left[\frac{t-\Delta}{\delta}\right]\right) & \Delta\le \mathrm{t}\le\Delta+\delta\end{cases}$$

(12)

Back to the equation(10), we can find:

$$\int_{t_0}^{t} s\left(\frac{[t-t_0]}{\delta}\right)\,dt=\delta\int_0^{s\left(\frac{[t-t_0]}{\delta}\right)} s\left(\frac{[t-t_0]}{\delta}\right)\,d\left(\frac{[t-t_0]}{\delta}\right)=\delta S\left(\frac{[t-t_0]}{\delta}\right)$$

(13)

The amount of dephasing per unit length can be represented as:

$$q(t)=\int_0^{t} P(t)\,G(t)\,dt\quad(14)$$

Put equation (12) in the equation (14):

$$q(t)=\begin{cases}\gamma\delta g S\left(\frac{t}{\delta}\right) & 0\le t\le\delta\\ \gamma\delta g\sigma & \delta\le t\le\Delta\\ -\gamma g\left[\sigma-S\left(\frac{[t-\Delta]}{\delta}\right)\right] & \Delta\le t\le\Delta+\delta\end{cases}$$

(15)

The Einstein diffusion equation contains the square root. Therefore, it is important to introduce the square of Equation (15):

$$q^2(t)=\begin{cases}\gamma^2\delta^2 g^2 S^2\left(\frac{t}{\delta}\right) & 0\le t\le\delta\\ \gamma^2\delta^2 g^2\sigma^2 & \delta\le t\le\Delta\\ \gamma^2 g^2\left[\sigma-S\left(\frac{[t-\Delta]}{\delta}\right)\right]^2 & \Delta\le t\le\Delta+\delta\end{cases}$$

(16)

To integrate Equations (15) and (16) for all pulse sequences, we must define the shape parameters λ and κ

$$\int_{t_0}^{t_0+\delta} S\left(\frac{[t-t_0]}{\delta}\right)\,dt=\delta\int_0^{\delta} S\left(\frac{t}{\delta}\right)\,d\left(\frac{t}{\delta}\right)=\delta\sigma\lambda$$

$$\int_{t_0}^{t_0+\delta} S^2\left(\frac{[t-t_0]}{\delta}\right)\,dt=\delta\int_0^{\delta} S^2\left(\frac{t}{\delta}\right)\,d\left(\frac{t}{\delta}\right)=\delta\sigma^2\lambda$$

(17)

The integral over $q(t)$ is important to show the effects of unidirectional translation E_{transl}

$$\ln(E_{\mathrm{transl}})=\int_0^{\Delta+\delta} q(t)\,dt=\gamma\delta g\left\lfloor\underbrace{\left(\delta\sigma\lambda\right)}_{0\le t\le\delta}+\underbrace{\left(\Delta-\delta\right)}_{\delta\le t\le\Delta}\sigma+(\delta\sigma-\delta\sigma\lambda)\right\rfloor=\gamma\delta\sigma g\Delta\quad(18)$$

where:

$$E_{\mathrm{transl}}=exp\left(iv_z\int_o^{\Delta+\delta} q(t)dt\right)\quad(19)$$

where v_z is the speed of theE_{transl} along the z-axis.

Assessment diffusion effect required integral over $q^2(t)$:

$$ln(E_{\mathrm{diff}})=\int_0^{\Delta+\delta} q^2(t)\,dt$$

$$= \gamma^2 \delta^2 g^2 \times \left[\underbrace{(\delta\sigma^2\kappa)}_{0\le t\le\delta} + \underbrace{(\Delta-\delta)\sigma^2}_{\delta\le t\le\Delta} + \underbrace{(\delta\sigma^2 + \delta\sigma^2\kappa - 2\delta\sigma^2\lambda)}_{\Delta\le t\le\Delta+\delta} \right]$$
$$= \gamma^2\delta^2\sigma^2 g^2 [\Delta + 2(\kappa-\lambda)\delta] \quad (20)$$

where:

$$E_{\text{transl}} = \exp\left(-D\int_0^{\Delta+\delta} q^2(t)\ dt \right) \quad (21)$$

If the gradient has a rectangular shape. The shapes parameters can be written as:

$$\sigma = 1,\ \lambda = \frac{1}{2},\ \kappa = \frac{1}{3} \quad (22)$$

By adding equation (22) to the equation (20), the entire ST equation becomes:

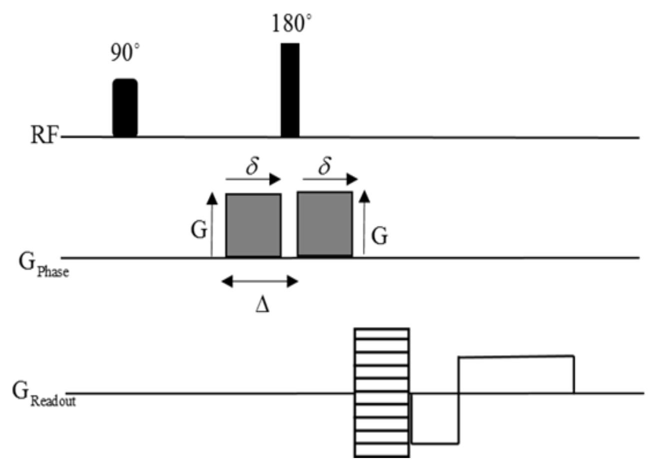
$$E_{\text{diff}} = e^{-D\gamma^2\delta^2 g^2\left(\Delta-\frac{\delta}{3}\right)} \quad (23)$$

In which E_{diff} is the signal intensity. The resulting attenuation is [20]:

$$c = c_0 \exp(-b.D) \qquad b = \gamma^2 G^2 \delta^2 \left(\Delta - \frac{\delta}{3} \right) \quad (24)$$

here c and c_0 are the signal intensities within and without diffusion respectively; D is the coefficient of diffusion; γ is the magnetogyric ratio; G is the strength of the gradient; δ is the duration of the gradient; and Δ is the diffusion timestep. The b factor defines the diffusion sensitivity of the sequence, as shown in Figure 1.

Figure 1: DWI imaging, where G is gradient strength, δ is the gradient duration and Δ is the diffusion interval

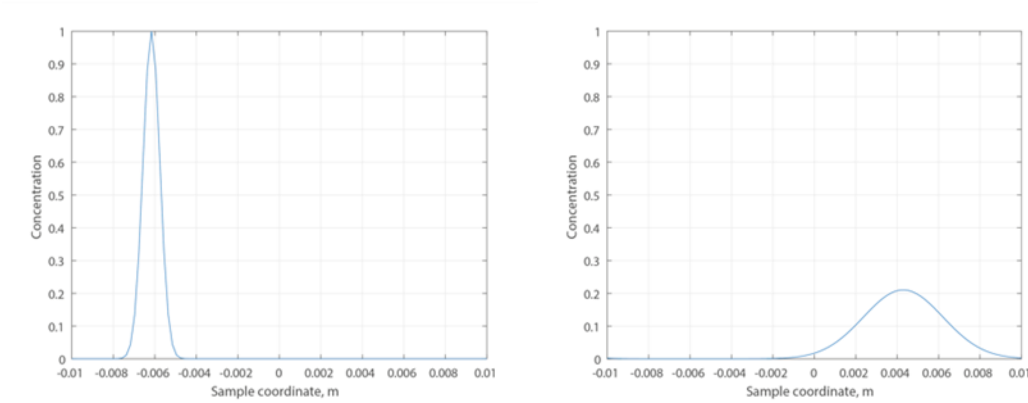


The diffusion-weighted pulse sequence should have two strong gradient fields G separated by time Δ and duration δ. A higher *b* value was obtained when diffusion-sensitive gradients were inserted.

RESULTS

The representations for the numerical solution that includes diffusion and stationary flow simultaneously (Figure 2) are essentially comparable to those applicable for diffusion; the software package is practically identical, and only the velocity distribution data are now given.

Figure 2: A one-dimensional simulation of the interaction of diffusion and flow in Spinach using the Fokker-Planck solver. A symmetrical flow velocity field (0.2 m/s) is utilized, and the diffusion rate is 50 mm2/s



The boundary conditions are a significant issue that must be addressed with flow simulations. The periodic boundary [92] is the only type of border that is not a veritable minefield in terms of the underlying numerical mathematics. At this point in the development, I've decided to merely construct the periodic boundary condition, as shown in Figure 3.

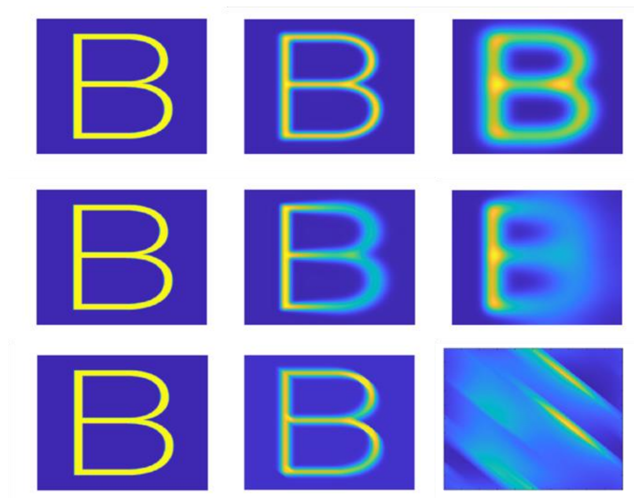
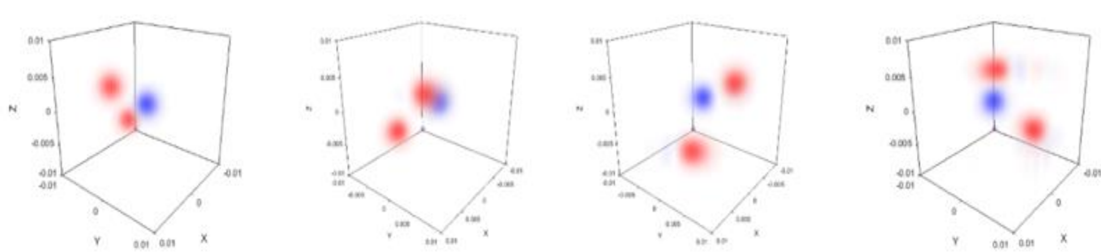


Figure 3: In the case of two-dimensional uniform and isotropic diffusion combined with a linear flow mechanism, the sampling distribution function evolves with increasing diffusion times. D = 5x10-5 m2/s, initial condition displayed in the left panel, periodic boundary values.

Because Spinach claims to be able to mimic three-dimensional MRI procedures in an acceptable amount of time, an instance is necessary (Figure 4).

Figure 4: Images from a three-dimensional diffusion and flow model of three separate elements flowing in a circular flow field. On a modern computer, the simulation takes only a few minutes.



Conclusion

It was impossible to simulate in three dimensional diffusion and flow using numerical simulation. The numerical simulation of magnetic resonance imaging has two limits in terms of research. First, a complicated spin system is associated with simple diffusion and flow, such as in spatially encoded NMR experiments. Second, a simple spin system is associated with high dimensional diffusion and flow. Both cases are well covered by the existing simulation software, and both are well established because the matrix dimension is controllable either directly or by using approximation. In our study using Fokker-Planck formalism with stacking filtering helped us improve the simulation outcomes. Furthermore, the proposed simulation enabled us to obtain a high-dimensional phantom with three-dimensional diffusion and flow [21, 22] to be closer to the real MRI outcomes.

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