Monte Carlo method and the Ising model for magnetized and non-magnetized water as MRI contrast agent

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Abstract: A Monte Carlo algorithm for a two dimensional Ising model is proposed and implemented using Mat lab. It describes a lattice with a discrete number of particles. We study the evolution of the system over time depending on a particular variable called the interaction strength .The results of computer simulations agree with practical experiments showing that there is a change in Energy-Magnetization and strength interaction-Magnetization curves between magnetized water and normal water which means that the magnetized water or Saline changes the properties of the solutions affecting T1 so it can be used as a new contrast agents for MRI.

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- **Introduction**

We can define a Hamiltonian for a system which is dependent on the arrangement of spins on a lattice and from that deduce properties such as Magnetization [1]. Suppose that the Hamiltonian is

$$H = -J \sum_{(ij)} SiSj \; - B \sum_{i} \; Si \qquad (1)$$

Where <ij> means that we sum over the nearest-neighbour pair of spins. This means that the spin at site ij interacts with at i(j ± 1) and (i ± 1)j. The Assuming periodic boundary condition in the model means that every spin will interact with four other spins regardless of their position on the finite lattice. Prefering to figure (1) for better understanding of the proposed system. Here J is the dimensionless interaction strength and B represents the energy involved in the Magnetisation of the lattice and is also dimensionless.

From the Hamiltonian we can calculate the partition function which is

$$Z = \sum_{i} e^{-Hi} \qquad (2)$$

Where we sum over all the particles in the lattice. Then the probability of finding the system in a certain state, denoted S, is

$$P(S) = \frac{e^{-H(S)}}{Z} \qquad (3)$$

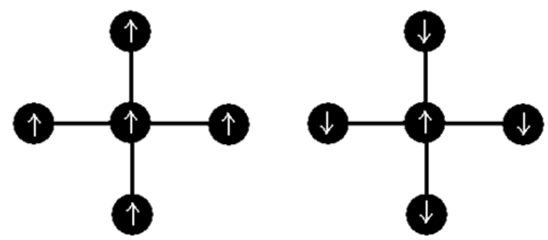

Figure 1. particles on the left all the neighboring particles have the same alignment of spin. and the particle on the right all the neighboring particles have a random spin alignment.

We Quantities such as Magnetization and Energy can be calculated using well known equations from statistical physics. Such as M and E is obtained will give as an estimation of the true value.

$$M = \sum_{S} P(S) \sum_{i} Si \qquad (4)$$

$$E = \sum_{S} P(S) H(S) \qquad (5)$$

It must be pointed out that in the limit of an infinitely large lattice; it is possible to solve the Ising model exactly. If assume that B = 0 the expressions are simplest, it can be seen and we see that the energy and Magnetization are [2,3,4,5].

$$E = -N^2\, J\coth(2J)\left[1 + \frac{2}{\pi}\right]\epsilon K_1\,(k) \qquad (6)$$

$$M = \pm N^2\ \frac{(1+z^2)^{1/4}\,(1-6z^2+z^4)^{1/8}}{(1-z^2)^{1/2}} \qquad (7)$$

$$k = 2\,\frac{\sinh(2J)}{\cosh^2(2J)} \quad \leq 1 \qquad (8)$$

$$\epsilon = 2\tanh^2(2J-1) \qquad (9)$$

$$K_1\,(k) = \int_0^{\pi/2} \frac{d\phi}{(1-k^2\ \sin^2\phi)^{1/2}} \qquad (10)$$

2. Material and Methods

- **Theoretical model**

To understand the model an implementation that declare some physical behavior of hydrogen Atom in magnetized water like magnetization transfer and magnetization curves for diamagnetic material

Magnetization Curves
Any discussion of the magnetic properties of a material is likely to include the type of graph known as a magnetization or B-H curve

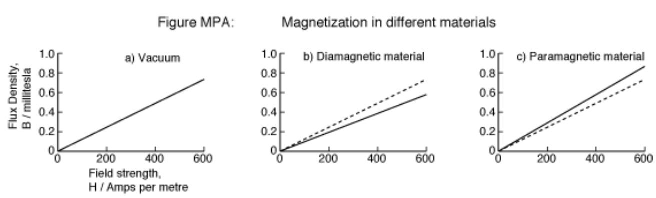

Figure 2. Magnetization Curves

- magnetic field strength as the horizontal axis and the magnetic flux density as the vertical axis.
- Fig. MPA a) is the curve in the absence of any material: a vacuum. The gradient of the curve is 4π.10-7 which corresponds to the fundamental physical constant μ0. b) water as Diamagnetic Material[8]

- **Magnetization Transfer**

Macromolecules have a layer of 'bound' water. Since static or slow changing magnetic fields are dominant in the vicinity of macromolecules, the associated hydrogen pool has a very short T2. The correlated fast de-phasing of the transverse magnetization causes this pool of water to be 'invisible'. However, the magnetization of that 'invisible' water pool is transferred to the visible pool of 'free' water via various mechanisms like chemical exchange or cross-relaxation Fig. (3). The term for these processes is called 'magnetization transfer', MT. Cross-relaxation is a special form of dipole-dipole interaction in which a proton on one molecule transfers its spin orientation to that of another molecule. A short T2 or fast de-phasing is synonymous for a broad range of resonance frequencies, whereas a long T2 is indicative of a narrow range. If there are applicable magnetization transfer mechanisms within the tissue, a saturation of the 'invisible' water pool will affect the 'visible' water pool.[7,9]

The T2 is usually so short that this hydrogen pool is not directly observable, and the signal vanishes faster than the ability to acquire some data. The short T2 corresponds to a significant difference in resonance frequencies causing the rapid de phasing. A significant difference in resonance frequencies is a synonym for a very broad resonance of these unobservable protons. The magnetization of these invisible protons can be transferred to the visible "free" water via a chemical exchange or cross-relaxation, which is a special form of dipole–dipole interaction [10].

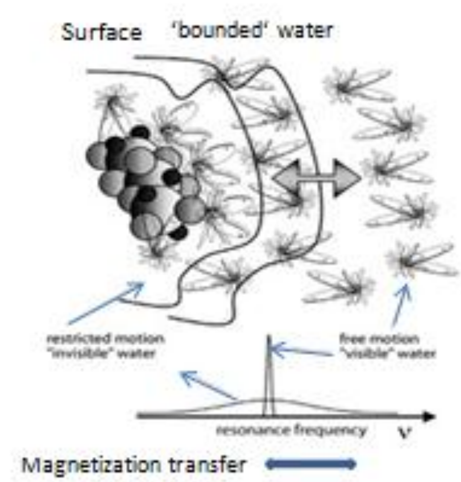

Figure 3. Magnetic Transfer phenomena in Magnetized water

- **The model**

The model is an Ising model in two different cases one with magnetized water(magnetization transfer) , assume the spin is equal 1 or -1,and second case is normal water with random spin, wrote a code in Mat lab that implements the model, a part of the code is borrowed from particularly well written Mat lab code by Tobin Fricke [6].

- **Running the Model**

To begin by creating a square lattice with 128 particles. We also choose a random value between 0 and 1 for the interaction strength and then watch how the system evolves over 1000 steps.. The speed of evolution is controlled by the variable randTol and in this case we decided that randTol= 0.1. A value of 0.1 means that only 10% percent of the originally selected group will have its spin flipped. In essence this parameter tries to mimic the evolution of real systems. Even though a certain particle will have a smaller energy with its spin flipped it doesn't mean that the all the particles in the lattice that follow that criterion will have their spins flipped immediately. We watched the evolution of 1,000 systems and took note of some of the important parameters. We then plot the total energy of the system as a function of interaction, see figure (5).,The computer time needed to finish these computations was approximately 360 seconds in Intel Core 2 Duo CPU 2.67GHZ 4.00GB Ram

- ***practical Method***

Magnetic water phantom Imaging

Two water phantoms used. Each one is constructed of biodegradable latex rubber balloons and filed with 450 ml. one is filled with normal tap water to be used as a reference, where the other is field with magnetic water. Both phantoms are scanned using small body coil of 0.2 Tesla MR (IRIS MATE, Hitachi, Japan). The magnetic water phantom scanned after 4 hours of magnetization figure (4).
The resulted images for both magnetized and non-magnetized water phantoms are quantitatively processed by MATLAP Genetic Algorithms (GAs).
We applied the following signal equation for a repeated spin-echo sequence ,

$$S = k (1 - e^{-TR/T1}) e^{-TE/T2} \quad (11)$$

This equation is only valid when TR >> TE. In our experiment we used TR= 2700, TE=120, and
$k = 8560*10^7$

3. Results

- ***Phantom Imaging analysis***

Quantitative analyses performed using MATLAB Genetic algorithms (GAs) as shown in figure (6) to estimate T1 and T2 for both magnetized and non-magnetized water phantoms based on signal to noise ratio for both images. Table (1) shows imaging parameters in addition to S/N ratio, and results of GAs. We used for both magnetized and non-magnetized images the same calculating parameters as: Function tolerance = 1e-100 ,Generation = 10000 The GAs results shows change in T1, where no changes occurred in T2.

As the positive results obtained from our experiments, the GA in MATLAB show that T1 is Increased to 1.513 s in magnetized phantom instead of 0.672 s in non-magnetized one and T2 did not changed (0.012 s) and S/N increased from 156.3 to 337.5.
The model achieves good confirmation with the expected behavior of magnetization transfer in water although the number of calculated points was not that much. The behavior of the magnetization is plotted in fig.4. The associated energy plot is shown in red.we can note clearly from the model we implement that in non-magnetized water the energy starts from -3 and from magnetized water it starts from -4 indicating changes by 25% also in Magnetized –Energy curves, in magnetic water there is a stable changes in the energy for the system with fixed magnetization ,in no-magnetized water it various so quickly with energy

4. Conclusions

In conclusion, this study clearly indicated a magnetized injection saline and magnetized water as CA enhances MRI. Proved that this technique is a clinically healthy and feasible technique for better diagnosis in MRI Imaging. And we simulate these behavior and results by using Monte Carlo method in Ising model as indicated in many references that Magnetic water is healthy [11-14]

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TABLE 1 WATER PHANTOMS IMAGING PARAMETERS AND RESULTS OF MATLAB GAS

Magnetization	TR	TE	S/N ration	T1	T2
0 Hours	2700	120	**156.3**	672	11
4 Hours	2700	120	**337.5**	1513	12

Non-Magnetized

Figure 4. non-magnetized

4hr Magnetized

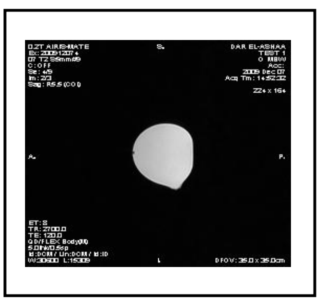

Figure 5. magnetized water

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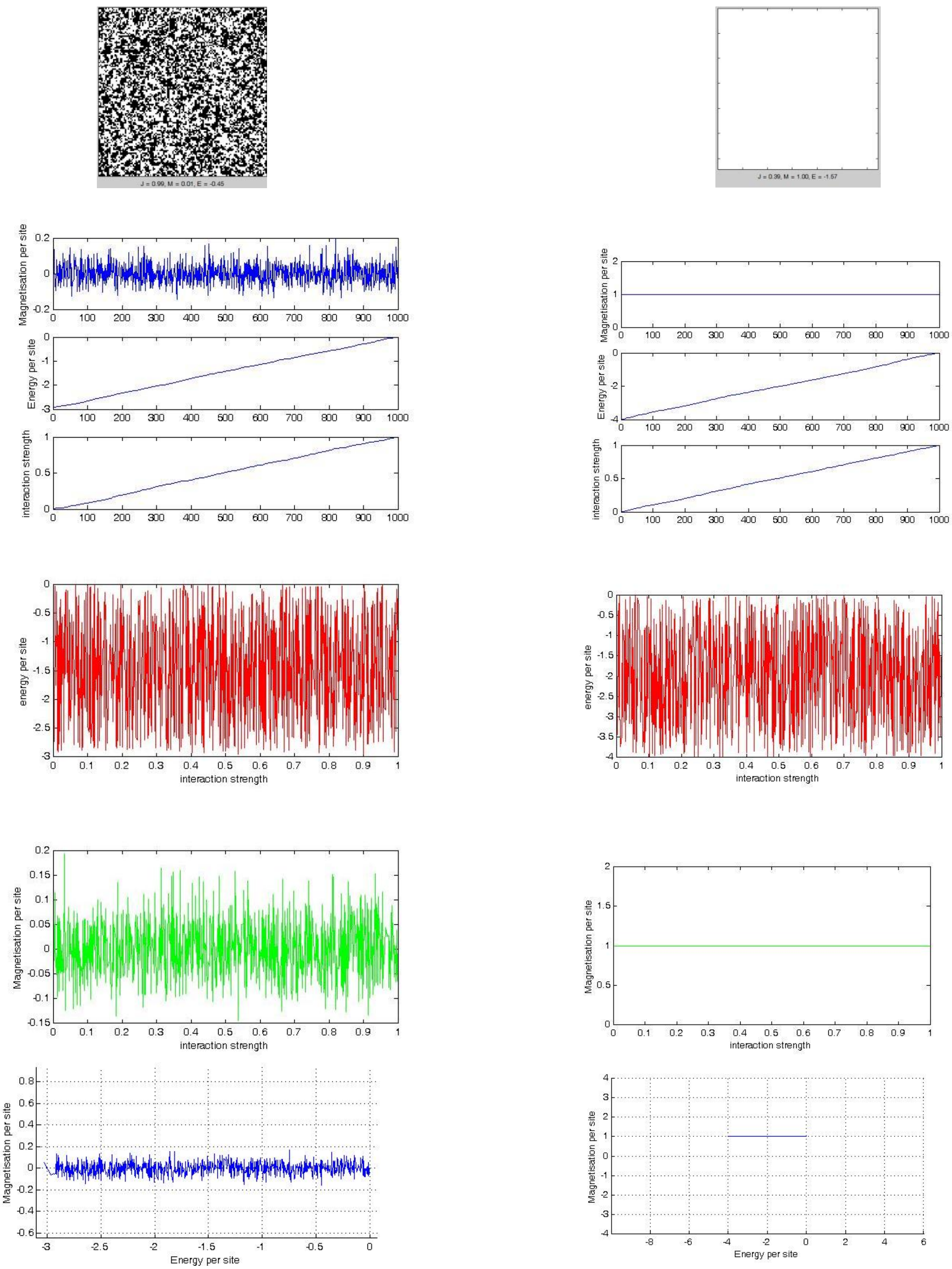

a. Random spin b. spin equal 1

Figure 6. Simulation of the energy behaviour The result fits well with practical expermint

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