An Improved Imaged-based Finite Difference Method for Studying Water Diffusion in Tissues

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Introduction: The image-based finite difference (FD) method (1) has been proposed for better understanding the factors that affect water diffusion in biological tissues with complex morphologies. However, using conventional boundary conditions for the Bloch-Torrey equation, an edge effect artifact arises with the conventional FD method, which is caused by the introduction of extra artificial boundaries into the computational domain. A hybrid discretization scheme algorithm (HDSA) (2) has been suggested to reduce the edge effect, but this method still induces errors at the boundaries and, moreover, becomes less stable when high *b* values are used. A revised periodic boundary condition (RPBC) method for the Bloch-Torrey equation has been developed in this work to eliminate the edge effect completely for any diffusion-sensitizing gradient waveforms. In addition, a matrix-based FD method that converts the conventional FD approach into a matrix-based algebra is introduced, which not only simplifies the FD formula and increases the computational efficiency, but is also easier to implement using parallel computing (2).

Methods: The conventional FD method assumes impermeable boundaries of the computational domain so that water diffusion is highly restricted by those artificial boundaries. This is called the edge effect and it must either be reduced by additional computation over an extended domain or it becomes a source of significant errors. The HDSA method uses hybrid discretization schemes to reduce the boundary effect but becomes less stable with large *b* values. In contrast, if the structure is assumed to be periodic with the computational domain as the unit cell, a simple relationship between any two corresponding points in different unit cells for any gradient waveforms can be derived as (For simplicity, only 1D formula are shown)

$$m(x,t)=\exp[-\mathrm{i}n\alpha\gamma\int_0^t g(t')dt']\cdot m(x+n\alpha,t), \qquad [1]$$

where *n* is any integer, α is the length of a unit cell. Equation [1], called the revised periodic boundary condition, provides a means to remove the artificial boundaries of the computational domain which can remarkably increase the computing efficiency. For example, to simulate the nerve system model shown in Fig.1, the conventional FD method should simulate the whole image and takes signals from the central barely affected domain for long diffusion times to avoid the edge effect (1); whereas the improved FD method with RPBC only needs to simulate a unit cell (in the black box). For 50ms diffusion time, RPBC method can save 88%(2D) or 96%(3D) computing time compared with the conventional FD method. Note that it is assumed the whole structure to be periodic but the structure inside each unit cell (the computational domain) is usually heterogeneous for biological tissues. To further increase the computing efficiency, the conventional FD method can be converted into a matrix-based method. If grid points are labeled with *1*, *2*, *3*, …, *N* and $\mathbf{M}^n$ denotes a vector containing magnetizations, a matrix-based FD method with explicit scheme (3) can be expressed as $\mathbf{M}^{n+1}=\mathbf{\Phi}^n\otimes(\mathbf{I}+\mathbf{A})\mathbf{M}^n$, where $\mathbf{I}$ is an identity matrix, $\otimes$ denotes the element-by-element vector multiplication, $s_{j\to j-1}$ is the jump probability from point (*j*) to (*j*-1). $\mathbf{\Phi}^n$ is a vector describing the phase accumulation and the transverse relaxation in each time step

$$\mathbf{\Phi}^n=\begin{bmatrix}\exp(-\mathrm{i}\gamma g^n x_1\Delta t-\Delta t/T_{2,1})\\ \exp(-\mathrm{i}\gamma g^n x_2\Delta t-\Delta t/T_{2,2})\\ \exp(-\mathrm{i}\gamma g^n x_3\Delta t-\Delta t/T_{2,3})\\ \cdots \\ \exp(-\mathrm{i}\gamma g^n x_N\Delta t-\Delta t/T_{2,N})\end{bmatrix} \text{ and } \mathbf{A}=\begin{pmatrix} -s_{1\to2}-s_{1\to N} & s_{2\to1} & 0 & \cdots & s_{N\to1}\exp(\mathrm{i}\alpha\gamma\sum_{k=1}^n g^k\Delta t)\\ s_{1\to2} & -s_{2\to1}-s_{2\to3} & s_{3\to2} & \cdots & 0\\ 0 & s_{2\to3} & -s_{3\to2}-s_{3\to4} & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & 0\\ s_{1\to N}\exp(-\mathrm{i}\alpha\gamma\sum_{k=1}^n g^k\Delta t) & 0 & 0 & \cdots & -s_{N\to N-1}-s_{N\to1}\end{pmatrix}. \qquad [2]$$

Results and Discussions: Four types of diffusion-weighted pulse sequences were used to compare the conventional and the improved FD methods: the pulse gradient spin echo (PGSE) with short gradient approximation (PGSE-short), PGSE with finite duration of gradients (PGSE-finite), oscillating gradient spin echo (OGSE) with sine-modulated gradient waveforms (OGSE-sin) and OGSE with cosine-modulated waveforms (OGSE-cos) (4). Fig.2 shows the conventional FD method gives large errors caused by the edge effect and the errors increase when the diffusion time becomes longer which means more and more computational domain are affected by the boundaries. In contrast, all results obtained by the RPBC method have errors smaller than 1% which shows the elimination of the edge effect. In addition, we found that the amplitudes of the applied magnetic gradients affect the results: larger amplitude gradients yield larger errors. A dimensionless factor β is defined as

$$\beta=\max\{\int_0^t g(t')dt'\}\cdot\Delta x/\pi \qquad [3]$$

Fig.3 shows that both the conventional FD and the improved FD method with RPBC have increasing simulation errors with the amplitude of gradient increasing. Furthermore, both FD methods show the same behavior with respect to β (note that results of conventional FD method were only taken from the central region unaffected by the edge effect) which implies this may be an intrinsic property when the FD algorithm is used to solve the Bloch-Torrey equation. In practice, β<0.1 is needed to obtain a simulation error smaller than 1%.

Reference: (1)Hwang, MRM,2003 (2)Xu, ISMRM, 2006 (3)Fletcher C A J, 1988 (4)Parsons, MRM, 2006

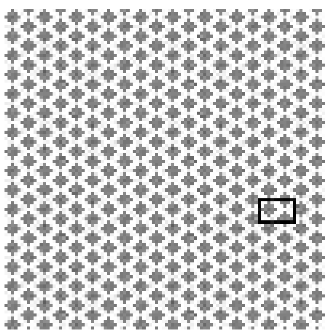

Fig.1 Cross-section of a hexagonal array of cylinders: cylinders (axons) are grey and the surrounding matrix (extracelluar space) is white.

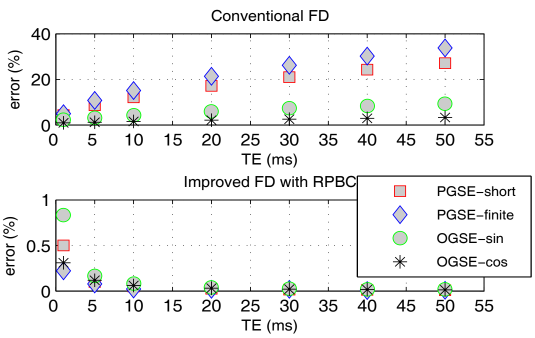

Fig.2 The comparison of the conventional FD and the improved FD with RPBC. Note that the edge effect is completely eliminated by the RPBC method and the small errors were caused by the strong gradients at the short echo times. β<0.1 for all simulations.

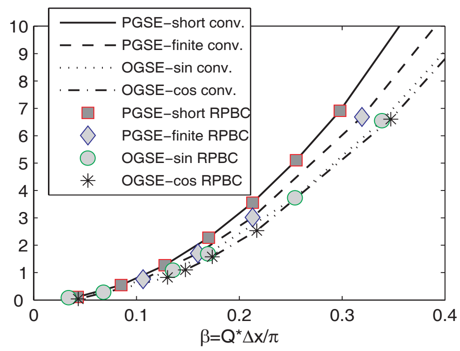

Fig.3 Simulation errors change with respect to a dimensionless factor β. The results of conventional FD method were taken from the central region unaffected by the edge effect.