IMPLEMENTATION OF THE EQUILATERAL TRIANGLE IN THE MULTIPLE CORRELATION FUNCTION APPROACH AS MODEL GEOMETRY FOR RESTRICTED DIFFUSION.

F. B. Laun[1], and B. Stieltjes[2]

[1]Medical Physics in Radiology, German Cancer Research Center, Heidelberg, Baden-Württemberg, Germany, [2]Radiology, German Cancer Research Center, Heidelberg, Baden-Württemberg, Germany

Introduction

Magnetic resonance diffusion weighted imaging finds widespread application, e.g. in medical imaging or porous media research [1] since the measured diffusion is linked to the confining geometry. Although this link is not trivial, efficient techniques like the multiple correlation function (MCF) approach exist [2], that rely on the Laplace eigensystem, and allow for a more efficient computation of diffusion weighted signals than e.g. Monte-Carlo simulations. The main limitation of the MCF approach is the small number of geometries (slab, cylinder, sphere, ring) for which the governing matrices could be computed. The equilateral triangle is one of the few other geometries for which the Laplace eigensystem is known and could thus serve as an interesting model geometry with discrete rotational symmetry. Thus, the aim of this work was to evaluate the equilateral triangle within the MCF approach.

Methods

We follow the notation of [3]. Be λ_{nm} and $u_{nm}(r)$ eigenvalues and eigenfunctions of the Laplace operator satisfying Neumann boundary conditions. $B(r)$ is the magntic field of the diffusion gradients. Here we focus on the geometry describing matrices $B_{n_1m_1,n_2m_2} = \int dr^3 u^*_{n_1m_1}(\vec{r}) u_{n_2m_2}(\vec{r}) B(\vec{r})$. The eigensystem of the equilateral triangle is solved in [4, 5]. For each integer n and $m>n$ an antisymmetric mode $u_{a,nm}(r)$ exists and for each integer n and $m>=n$ a symmetric mode $u_{s,nm}(r)$ is present. Monte-Carlo random walks were performed to validate the results.

$$u_{s,nk}(x,y) = \beta_{nk}\left(\cos[2\pi(-k+n)x/3]\cos\left[2\pi(k+n)y/\sqrt{3}\right] + \cos[2\pi(2k+n)x/3]\cos\left[2\pi ny/\sqrt{3}\right] + \cos[2\pi(k+2n)/3]\cos\left[2\pi ky/\sqrt{3}\right]\right)$$

$$u_{a,nk}(x,y) = \beta_{nk}\left(\sin[2\pi(-k+n)x/3]\cos\left[2\pi(k+n)y/\sqrt{3}\right] + \sin[2\pi(2k+n)x/3]\cos\left[2\pi ny/\sqrt{3}\right] + \sin[2\pi(k+2n)/3]\cos\left[2\pi ky/\sqrt{3}\right]\right)$$

$$\beta_{nk} = \left(2\sqrt{4-2\delta_{nk}}\right) / \left(3^{3/4}\sqrt{(1+\delta_{0n}+\delta_{0k}-2\delta_{0n}\delta_{0k})(1+5\delta_{0n}\delta_{0k})}\right) \qquad \lambda_{nk} = -16\pi^2(n^2+nk+k^2)/9$$

Box 1.: Symmetric and asymmetric Eigenfunctions of the Laplace operator with the equilateral triangle as confining boundary.

Results

While the matrices $B^{x,aa}$, $B^{x,ss}$ and $B^{y,as}$ are zero due to symmetry, the remaining matrices are given by the expressions in box 2 and 3. Note that the indices of a, c and d were omitted for legibility reasons. The expressions for B are well defined, but direct computation yields divergent terms. This may be circumvented by a series expansion around the integer values of n and m. The constants ζ which are important for the second moment (for details see [1]) are presented in Tab. 1. The matrices $B_{00,nk}$ that govern the second moment differ for x- and y-direction. However, their square, namely $B_{00,nk}B_{nk,00}$ is identical. Thus, the second moment, which is closely related to the apparent diffusion coefficient, is independent of the gradient direction. This is also apparent in Fig. 1: For moderate diffusion weightings (b=1000 s/mm²), the ADC is independent of the orientation. For large b-values (b=5000 s/mm²), a clear orientation dependency is observable. Monte-Carlo simulations and the MCF results are in good agreement (Fig. 1).

$$\vec{f}_1(\overline{m},\overline{n}) = \begin{pmatrix}\overline{n}\\ \overline{m}\end{pmatrix}\left(\delta_{|\overline{n}|,2}+\delta_{|\overline{m}|,2}\right) + \begin{pmatrix}1\\1\end{pmatrix}\left(\delta_{\overline{m},1}\delta_{\overline{n},-1}+\delta_{\overline{m},-1}\delta_{\overline{n},1}\right)sign(\overline{n})$$

$$\vec{f}_2(\overline{m},\overline{n}) = \begin{pmatrix}1\\2\end{pmatrix}\left(\delta_{\overline{m},1}\delta_{\overline{n},-1}+\delta_{\overline{m},-1}\delta_{\overline{n},1}\right)sign(\overline{m}) + \begin{pmatrix}1\\-1\end{pmatrix}sign(\overline{m}-\overline{n})$$

$$c = \vec{f}_i(\overline{m}_1,\overline{n}_1)\cdot\begin{pmatrix}m_1\\n_1\end{pmatrix} + \vec{f}_j(\overline{m}_2,\overline{n}_2)\cdot\begin{pmatrix}m_2\\n_2\end{pmatrix}$$

$$\tilde{c} = \begin{cases}1 & \text{if } \vec{f}_i(\overline{m}_1,\overline{n}_1)=0 \,\&\, \vec{f}_j(\overline{m}_1,\overline{n}_1)=0\\ c & \text{otherwise}\end{cases}$$

$$a = \left(\overline{m}_1 m_1 + \overline{n}_1 n_1 + \overline{m}_2 m_2 + \overline{n}_2 n_2\right)$$

$$d = \left(\delta_{\overline{m}_1+\overline{n}_1,3} + \delta_{\overline{m}_1,1}\delta_{\overline{n}_1,-1}\right)\left(\delta_{\overline{m}_2+\overline{n}_2,3} + \delta_{\overline{m}_2+\overline{n}_2,-3} + \delta_{\overline{m}_2,1}\delta_{\overline{n}_2,-1} + \delta_{\overline{m}_2,-1}\delta_{\overline{n}_2,1}\right)$$

Box 2: Auxiliary variables to make the B matrices more readable.

$$B^{y,aa}_{n_1m_1,n_2m_2} = -\frac{81}{128\pi^3}\beta_{n_1m_1}\beta_{n_2m_2}\sum_{\overline{m}_1,\overline{n}_1,\overline{m}_2,\overline{n}_2=-2}^{2}\frac{d}{a}\sum_{i,j=1}^{2}\frac{\sin(2\pi/3\cdot c)}{\tilde{c}^2}(-1)^{2\sin(\pi(\overline{n}_1+\overline{n}_2)/3)/\sqrt{3}}$$

$$B^{y,ss}_{n_1m_1,n_2m_2} = -\frac{81}{128\pi^3}\beta_{n_1m_1}\beta_{n_2m_2}\sum_{\overline{m}_1,\overline{n}_1,\overline{m}_2,\overline{n}_2=-2}^{2}\frac{d}{a}\sum_{i,j=1}^{2}\frac{\sin(2\pi/3\cdot c)}{\tilde{c}^2}$$

$$B^{x,as}_{n_1m_1,n_2m_2} = -\frac{9\sqrt{3}}{128\pi^3}\beta_{n_1m_1}\beta_{n_2m_2}\sum_{\overline{m}_1,\overline{n}_1,\overline{m}_2,\overline{n}_2=-2}^{2}\frac{d}{a^2}\sum_{i,j=1}^{2}\frac{(3a+6c)(1-\cos(2\pi/3\cdot c))-2\pi\cdot ac\sin(2\pi/3\cdot c)}{\tilde{c}^2}(-1)^{\overline{m}_1}$$

$$B^{x,sa}_{00,nk} = \frac{243\sqrt{3}}{16\pi^3}\beta_{00}\beta_{nk}\left(\frac{\sin^2(\pi(k-n)/3)}{(k-n)(2k+n)(k+2n)}\right) \qquad B^{y,ss}_{00,nk} = \frac{729}{32\pi^3}\beta_{00}\beta_{nk}\left(\frac{\sin(2\pi(k-n)/3)}{(k-n)(2k+n)(k+2n)}\right)$$

Box 3: B matrices for the equilateral triangle.

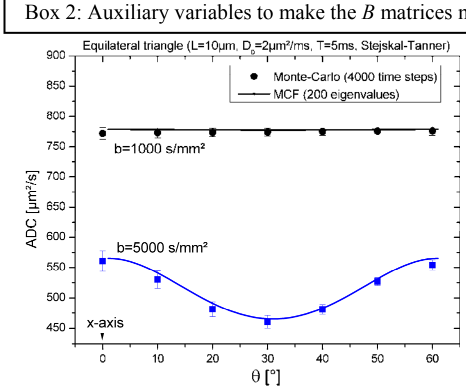

Fig. 1: Apparent diffusion coefficient in dependency of the angle between x-axis and diffusion gradient. The ADC is orientation dependent for large diffusion weightings only.

ζ_2	0
$\zeta_{3/2}$	$4/(3\sqrt{\pi})$
ζ_1	1
ζ_0	1/24
ζ_{-1}	2.29515E−3
ζ_{-2}	−1.3007E−4
ζ_{-3}	7.40495E−6

Tab. 1. ζ constants which are of importance for the second moment. E.g. $\zeta_{3/2}$ is proportional to the surface to volume ratio.

Discussion

Using the expressions of box 3, the B matrices can be computed for arbitrary eigenvalues. This task has to be performed only once. The MCF simulations can then be performed for arbitrary temporal gradient profiles, length scales, diffusion times and free diffusion constants. One interesting finding is that the second moment is orientation independent. This can be explained by the fact that the diffusion tensor of second order has three free parameters in two dimensions and fully describes the orientation dependency of the second moment.

References

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