Effective diffusion tensor computed by homogenization

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Introduction

Diffusion MRI can give useful information on cellular structure and structural change (for a review see [1]).We show the effective diffusion tensor obtained by mathematical homogenization theory (see e.g. [2,3]) is a good approximation to the long time apparent diffusion tensor under realistic DMR scanning conditions for both isotropic and anisotropic diffusion and general geometries. The homogenized diffusion tensor is obtained by solving three steady-state Laplace equations, which is a more computationally efficient approach than long time simulation in the time domain, either via Monte-Carlo simulation or numerical solution of the time-dependent Bloch-Torrey PDE.

Theory

In the two-compartment model, we consider the two compartments, Ω^i and Ω^e, to be the ensemble of cells and the extra-cellular compartment, respectively. The two compartments have the same intrinsic diffusion coefficient D. The cell membrane is modeled by an infinitely thin permeable interface characterized by permeability κ. Given the diffusion gradient with profile $f(t)$ and gradient strength $\vec{g} := \vec{q}/\gamma$, where γ is the gyro-magnetic ratio, the DMRI signal attenuation is $\Psi(\vec{q},t)$, from which we define the apparent diffusion tensor D^A from the Taylor expansion in $\vec{q}$:

$\log\Psi(\vec{q},t) = -\vec{q}^T D^A \vec{q} \int_0^t du \left(\int_s^u f(s)ds \right)^2 + O\left(\|\vec{q}\|^4 \right)$. The long time limit of D^A can be well approximated by the effective diffusion tensor of homogenization,

$D^{eff} = \begin{pmatrix} D_{11}^{eff} & D_{12}^{eff} & D_{13}^{eff} \\ D_{21}^{eff} & D_{22}^{eff} & D_{23}^{eff} \\ D_{31}^{eff} & D_{32}^{eff} & D_{33}^{eff} \end{pmatrix}$ where $D_{jk}^{eff} = D\int_\Omega \nabla v_j \bullet \vec{e}_k \, d\vec{x}$, $\vec{e}_k$ is the unit vector in the kth coordinate direction and the unknown function v_j can be found by solving the Laplace equation on the right over the box $\Omega = [0,l_1]\times[0,l_2]\times[0,l_3]$ which contains a representation sample of the cellular structure . In an nearly isotropic medium, D^{eff} is nearly diagonal and all the diagonal entries are close to each other. But in the general anisotropic case, the eigenvalues of D^{eff} are not equal to each other.

$$
\begin{aligned}
&\nabla \cdot D\nabla \vec{v}_j^{\,\ell}(x) = 0, \ x \in \Omega^\ell, \ \ell = i,e, \\
&\nabla v_j^i(y) \bullet \vec{n}^i(y) = -\nabla v_j^e(y) \bullet \vec{n}^e(y), \ y \in \Gamma^{ie}, \\
&\nabla v_j^i(y) \bullet \vec{n}^i(y) = \kappa(v_j^e(y) - v_j^i(y)), \ y \in \Gamma^{ie}, \\
&v_j(y + l_j\vec{e}_j) = v_j(y) + l_j, \ \{y, y + l_j\vec{e}_j\} \in \partial\Omega, \\
&v_j(y + l_k\vec{e}_k) = v_k(y), \ \{y, y + l_k\vec{e}_k\} \in \partial\Omega, \ k \neq j
\end{aligned}
$$

Results and discussion

Simulated DMRI signals were obtained for the PGSE sequence with δ=10ms and Δ=10ms, 30ms and 50ms in two gradient directions $\vec{q}/\|\vec{q}\|^2$ =[1,0], and [0,1] (2D case) and δ=10ms and Δ=10ms and 90ms in three gradient directions $\vec{q}/\|\vec{q}\|^2$=[1,0,0], [0,1,0] and [0,0,1] (3D case) by numerically solving the two-compartment Bloch-Torrey partial differential equation on a sample $\Omega = [-40;40]^d$ $(d = 2,3)$ containing numerous convex cells in two dimensions with volume fraction v^i=0,88, average surface to volume ratio S/V=0,51μm^{-1} (Fig 1) and convex-shaped cells in three dimensions (Fig 2) with v^i=0,66, S/V=0,34μm^{-1}. The average radius of cells is 3.9μm for 2D and 8,8μm for 3D. We simulated the DMRI signal for D=2,8.10^{-3} μm^2/μs and κ=10^{-5}μm/μs and κ=10^{-4}μm/μs, giving computed ADCs of between 0,5.10^{-3} and 2,2.10^{-3} μm^2/μs (3D case). In Table 1 and 2 we see the simulated apparent diffusion tensor D^A approaches the steady-state tensor D^{eff} computed by the homogenization method described above. The convergence of D^A to D^{eff} is faster at higher permeability. The calculation of D^{eff} for 3D took between 10 minutes to two hours for spatial discretizations of between 80x80x80 and 160x160x160 on a Dell Latitiude E6410 laptop computer (Intel(R) Core(TM) i7 CPU M640 @ 2,8GHz).

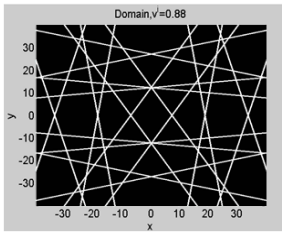

Fig 1. Convex cells with average radius 3.9μm, volume fraction v^i=0,88

	κ=10^{-4} μm/μs				κ=10^{-5} μm/μs			
	$\vec{q}^{\,t} D^A \vec{q}$			$\vec{q}^{\,t} D^{eff} \vec{q}$	$\vec{q}^{\,t} D^A \vec{q}$			$\vec{q}^{\,t} D^{eff} \vec{q}$
$\vec{q}$	δ=10,Δ=10	δ=10,Δ=30	δ=10,Δ=50		δ=10,Δ=10	δ=10,Δ=30	δ=10,Δ=50	
(1,0)	1,1.10^{-3}	9,0.10^{-4}	8,3.10^{-4}	7,1.10^{-4}	8,3.10^{-4}	5,5.10^{-4}	4,5.10^{-4}	2,6.10^{-4}
(0,1)	1,1.10^{-3}	9,4.10^{-4}	8,8.10^{-4}	7,6.10^{-4}	8,9. 10^{-4}	5,9. 10^{-4}	4,8. 10^{-4}	2,7.10^{-4}

Table 1. The simulated apparent diffusion tensor D^A approaches the steady-state tensor D^{eff} computed by homogenization (2D case).

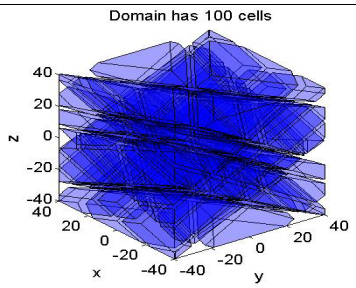

Fig 2. Convex cells with average radius 8,8μm and volume fraction v^i=0,66.

	κ=10^{-4} μm/μs			κ=10^{-5} μm/μs		
	$\vec{q}^{\,t} D^A \vec{q}$		$\vec{q}^{\,t} D^{eff} \vec{q}$	$\vec{q}^{\,t} D^A \vec{q}$		$\vec{q}^{\,t} D^{eff} \vec{q}$
$\vec{q}$	δ=10,Δ=10	δ=10,Δ=90		δ=10,Δ=10	δ=10, Δ=90	
(1,0,0)	1,7.10^{-3}	1,6.10^{-3}	1,5.10^{-3}	1,4.10^{-3}	1,0.10^{-3}	0,8.10^{-3}
(0,1,0)	2,2.10^{-3}	2,1.10^{-3}	2,0.10^{-3}	2,0.10^{-3}	1,5.10^{-3}	1,2.10^{-3}
(0,0,1)	1,2.10^{-3}	1,0.10^{-3}	1,0.10^{-3}	0,84.10^{-4}	0,5.10^{-3}	0,4.10^{-3}

Table 2. The simulated apparent diffusion tensor D^A approaches the steady-state tensor D^{eff} computed by homogenization (3D case).

References

[1] LeBihan (2007) Phys Med Bio 52. [2] Bensoussan et al. (1978) Asymptotic analysis for periodic structures, North-Holland, Amsterdam. [3] Cheng et al (1997) Proc Math Phy Engin Sci 453:145—161.