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Time-dependent diffusion in one-dimensional disordered media decorated by permeable membranes

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Synopsis

Keywords: Diffusion Modeling, Modelling, disorder, time-dependent diffusion

Motivation: Characterizing water diffusion in its long-time regime is relevant to most medical applications of diffusion MRI. However, this process is challenging to model even for a one-dimensional structure with semipermeable membranes.

Goal(s): Developing methods that predict the asymptotic instantaneous diffusivity from the bulk diffusivity and the membranes' locations and permeabilities.

Approach: We studied the problem theoretically and expressed the instantaneous diffusivity as an infinite sum. An independent numerical scheme is developed. Several types of disorder in the membranes' positions were considered.

Results: Our findings show excellent agreement with simulations. Our methods provide an alternative means for studying time-dependent diffusion.

Impact: This report provides an improved understanding of how tissue organization and disorder may affect water diffusivity, thus making it relevant to diffusion MR studies characterizing tissue microstructure. We also provide methods for readily estimating the instantaneous diffusivity.

Introduction

The water diffusion coefficient is an MR-measurable quantity whose value and time-dependence are influenced by the surrounding medium. Earlier studies in the porous media literature [1,2] have shown that the short-time evolution of the diffusion coefficient is sensitive to the surface-to-volume ratio, while its long-time behavior is determined by the tortuosity and size of the structures. In studies aiming to characterize the microstructure of tissues, the permeability of the membranes is accounted for [3]. Considering the size of the cells, bulk diffusivity of water, and the timescales afforded by conventional MR measurements, the long-time asymptote of the diffusion coefficient as well as how such long-time behavior is approached are critical [1,4]. The latter could indicate the type of disorder present [5].
Here, we visit the simplistic one-dimensional model of permeable membranes with random spacings as illustrated in Figure 1.

Methods

We studied the long-time dynamics of the quantity $\mathrm{u}(\mathrm{x},\mathrm{t})$, which is the probability that a particle initially at the origin traverses to position x over a time interval t (see Figure 2). This quantity is well-represented by a Gaussian at long times [6]. One-half of the time-dependent variance of this Gaussian is denoted by $\tau(\mathrm{t})$, which is determined by requiring that the (time- and position-dependent) slope of the Gaussian is adapted to the time evolution of $\mathrm{u}(\mathrm{x},\mathrm{t})$ by a fitting based on the diffusivity, membrane positions, and the membrane permeabilities. The time derivative of $\tau(\mathrm{t})$ yields the instantaneous diffusivity $\mathrm{D}_{\mathrm{inst}}(\mathrm{t})$.
We also devised an independent numerical simulation framework, which is summarized in Figure 3. The domain is divided into equal-sized bins, and the particle concentration profile, which is initially confined to one such bin, is expressed as a vector. The time evolution for a small time-interval is expressed as a matrix product taking into consideration the possible exchange through the membrane with permeability M. Repeated multiplication by this matrix allows for estimation of the particle distribution at any time.

Results and Discussion

After lengthy derivations, we found that the convergence of the instantaneous diffusivity to its eventual value D_∞ [7] is governed by

$$\frac{\mathrm{D}_{\mathrm{inst}}(\mathrm{t})-\mathrm{D}_\infty}{\mathrm{D}_\infty}=\frac{\mathrm{D}_0}{\mathrm{ML}}\left(1-\sum_{\mathrm{k}}\frac{\mathrm{x}_\mathrm{k}^2\mathrm{L}}{4\sqrt{\pi}\,\tau^{3/2}(\mathrm{t})}\mathrm{e}^{-\frac{\mathrm{x}_\mathrm{k}^2}{4\tau(\mathrm{t})}}\right),$$

where D_0 is the bulk diffusivity and L is the mean separation between adjacent membranes. For disordered media, the positions x_k become stochastic variables.
To assess whether our analytical derivation and computational framework provide consistent results at long diffusion times, we considered realizations of system configurations exhibiting hyperuniform disorder, short-range disorder, and strong disorder [5]. Figure 4 illustrates the result for a particular realization of each of these disorders. As expected, the two methods provide indistinguishable results at long times.
We also considered scenarios involving 200 different membrane realizations for each of the disorder classes. These simulations are compared with the asymptotic formulas derived, and also with our analytical results. We find excellent agreement between our model and our simulations; the latter results are shown in Figure 5. The approach of $\mathrm{D}_{\mathrm{inst}}$ to D_∞ appears to deviate somewhat from the power-law relations in the long-time regime suggested in the recent literature [5], most notably in the case of hyperuniform disorder. We also studied the variance of the quantity $(\mathrm{D}_{\mathrm{inst}}-\mathrm{D}_\infty)/\mathrm{D}_\infty$, which seems to exhibit the same power-law. These findings are obtained by simulations of all disorder classes, and also the numerical evaluation of the sum above for the case of hyperuniform disorder.

Conclusion

With our approach, we present an easy-to-understand model which predicts the asymptotic instantaneous diffusivity for a one-dimensional structure with membranes located according to various statistical models. We expect our methods to facilitate the study of mechanisms that influence the time-dependence of the diffusion process, which ultimately determines the MR signal obtained via different diffusion encoding gradient waveforms.

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Figures

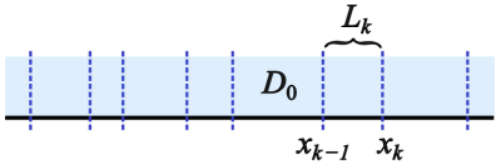

Figure 1: The one-dimensional space is decorated by a sequence of thin membranes with permeability M. The bulk diffusivity of the fluid is D_0. The kth interval, having length L_k, is located between the points $\mathrm{x}_{\mathrm{k}-1}$ and x_k. Following Novikov et al. [5], the positions of the membranes are either regular or they belong to one of the following classes: hyperuniform disorder, short-range disorder, and strong disorder.

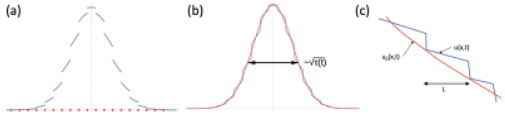

Figure 2: The distribution $\mathrm{u}(\mathrm{x},\mathrm{t})$ of the position of a particle, initially at the origin (a), has an approximately Gaussian distribution $\mathrm{u}_0(\mathrm{x},\mathrm{t})$ at long times (b). The derivative of its halved variance $\tau(\mathrm{t})$ yields the instantaneous diffusivity. We account for the permeability condition at the interfaces by matching the jumps of the piecewise linearized $\mathrm{u}(\mathrm{x},\mathrm{t})$ and its Gaussian approximation $\mathrm{u}_0(\mathrm{x},\mathrm{t})$ when we consider an interval of mean separation L.

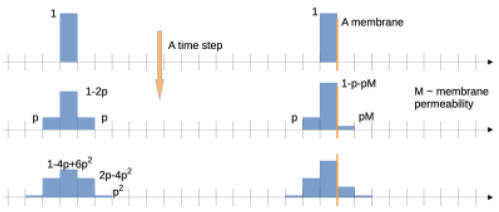

Figure 3: The simulation framework developed to provide an alternative for the estimations of the long-time behavior. At each (small) time step, the probability of the particle leaks to the neighboring bins. If a membrane is to be crossed, this probability is reduced. This evolution can be expressed as a matrix–vector multiplication, with the matrix being tridiagonal. The distribution at any point in time is computed via repeated multiplications.

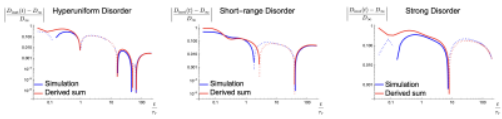

Figure 4: The convergence of the instantaneous diffusivity to its long-time value obtained through two independent methods. The dotted portions of the curves indicate negative values before taking the absolute values. $\tau_\mathrm{r} = \mathrm{L}/2\mathrm{M}$ indicates the residence time. The behavior is dictated by the dimensionless parameter D_0/ML, which we have set to 1.

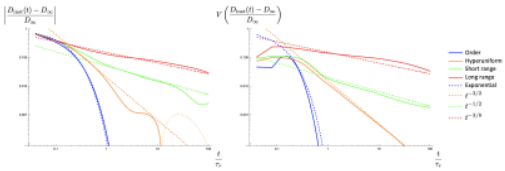

Figure 5: Left: The approach of the instantaneous diffusivity to its long-time value for 200 realizations of each of the disorder classes considered. Also studied is the variance of the deviation of D_{inst} from D_{∞}, which is consistent with power-laws reported in the literature [5].

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