

A fast random walk algorithm for computing diffusion-weighted signals in multi-scale porous media

Denis S. Grebenkov¹, Hang Tuan Nguyen² and Jing-Rebecca Li³

¹Laboratoire de Physique de la Matière Condensée, CNRS – Ecole Polytechnique, Palaiseau, France;

²Neurospin, CEA-Saclay, Gif-Sur-Yvette, France; ³Equipe DEFI, INRIA Saclay Palaiseau, France

Introduction: Diffusion-weighted MRI has become an important source of information about the dynamics in and the structure of natural or artificial materials (e.g., rocks, cements, human organs)¹. In spite of intensive research, the relation between the microstructure and the signal formed by diffusing nuclei remains poorly understood, mainly due to lack of efficient algorithms and models for multi-scale porous media². To overcome this limitation, we developed a fast random walk (FRW) algorithm³ with gradient encoding which exploits the multi-scale character of the medium. In this talk, we present an application of this algorithm to a Menger sponge (Fig. 1) which is formed by multiple channels of broadly distributed sizes and often used as a model for soils and materials^{5,6}. Using this model, we investigate the role of multiple scales onto diffusion-weighted signals.

Theory: The basic idea of a FRW algorithm consists in replacing Brownian motion by an equivalent scale-adapted "spherical process" that explores the confining domain as fast as possible⁴. The self-similar structure of a Menger sponge allows one to rapidly compute the jump distances for each move. The algorithm generates successive positions of a diffusing nucleus and its random dephasing φ under the applied magnetic field gradient $\mathbf{B}(\mathbf{r},t)$. The signal is an average over a large number of nuclei: $E = E_0 \mathbb{E}(\exp(i\varphi))$.

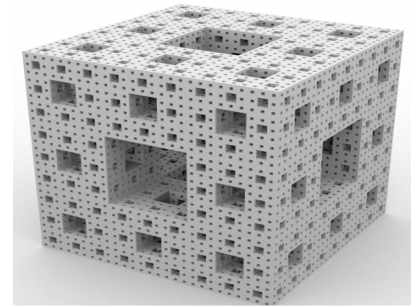


Fig. 1: Level 4 of a Menger sponge: nuclei diffuse in "void" regions and bounce off the "solid" interface

Results and Discussion

The free induction decay (FID) at a constant gradient g is computed for levels 1-4 of a Menger sponge for different times t . Figure 2(left) shows the absolute value of FID for levels 1-4 at a fixed time $t=10$. The presence of multiple channels at length scales from $1/3$ to $(1/3)^4 \approx 0.012$ is reflected in different patterns of these curves. For comparison, the FID from the unit cube is shown by circles, with almost regular diffraction patterns. Figure 2(right) shows the absolute value of FID at times t from 0.1 to 100 for a fixed level 3. At short times ($t=0.01$ and 0.1), the diffusion length $(2Dt)^{1/2}$ is smaller than the width of the smallest channel $(1/3)^3 \approx 0.037$, and the curves are close to each other. In turn, for $t=1$, the diffusion length becomes comparable to 0.037 so that some nuclei start to "feel" the confinement, yielding an increase of the third maximum. At time $t=100$, the diffusion length is comparable to the size of the structure, and the whole pattern is modified. In conclusion, we present an efficient numerical algorithm for simulating diffusion-weighted experiments in three-dimensional porous media, with a broad distribution of length scales. This algorithm allows one to investigate the role of multi-scale character of the medium onto the signal formation.

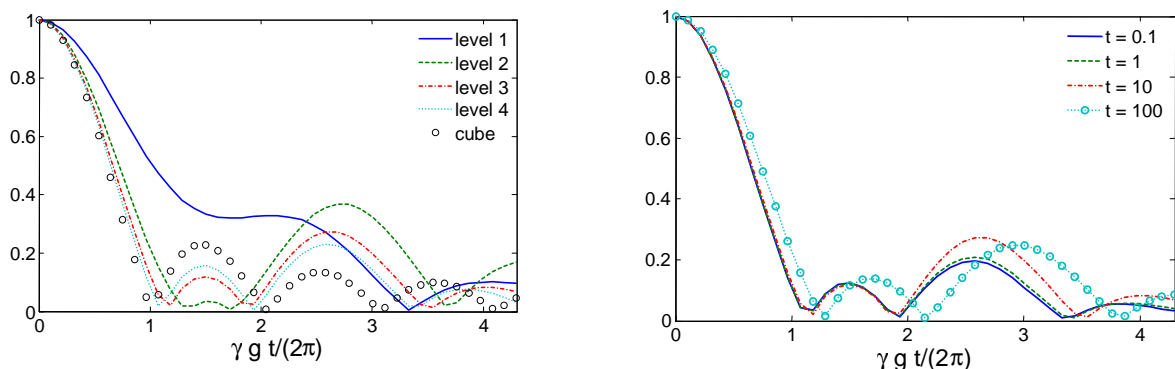


Fig. 2: Absolute value of FID as a function of $q = \gamma gt/(2\pi)$ for levels 1-4 of Menger sponge at time $t=10$ (left), and for level 3 at different times t (right). Units are fixed by setting the size of Menger sponge to 1 and diffusion coefficient D to 0.001.

[1] W. Price, *NMR Studies of Translational Motion*, Cambridge University Press (2009).

[2] D. S. Grebenkov, *Rev. Mod. Phys.* **79** (2007) 1077-1137.

[3] D. S. Grebenkov, *J. Magn. Reson.* **208** (2011) 243-255.

[4] E. Muller, *Ann. Math. Stat.* **27** (1956) 569-589.

[5] E. Perrier, M. Rieu, G. Sposito, G. de Marsily, *Water Resources Res.* **32** (1996) 3025-3032.

[6] C. Atzeni, G. Pia, U. Sanna, N. Spanu, *Construc. Build. Mater.* **22** (2008) 1607-1613.