First exit times for model shapes of porous media

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Diffusive transport in porous media is ubiquitous in biology and material sciences. For instance, the geometrical structure of a cement paste essentially determines the related physico-chemical processes and the consequent hardening and mechanical strength of the material. Given the complexity of these porous materials, the guiding idea is to decompose the whole structure into "elementary" pores, to study restricted diffusion inside and between adjacent pores, and to get a coarser description of the diffusive transport in an effective network of elementary pores.

This internship aims at developing these ideas through numerical simulations in model shapes of elementary pores. An off-lattice Monte Carlo algorithm will be implemented for simulating restricted diffusion in several model shapes: sphere, connected spheres, vycor glass, etc. These simulations will allow one to determine first exit times statistics: how long does it take for a diffusing particle started inside a pore to reach some parts of the pore boundary. This statistics obviously depends on the geometry of the pore. The main question will be: how different shapes of the pore can influence this statistics? For instance, whether the mean exit time is fully determined by the surface-to-volume ratio of the pore, or not? The numerical and theoretical work with model shapes is a necessary step for a better understanding of transport processes in real porous media.