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Heterogeneous continuous time random walk on graphs

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Solute transport and, particularly, diffusion of particles in porous media is a long standing problem [1]. The general random walks framework has been shown to describe quantitatively the anomalous transport patterns frequently observed in fractured and heterogeneous porous media [2]. One of the major conceptual difficulties consists in a very broad range of time and length scales in the dynamics [3] that prohibits using conventional theoretical approaches or numerical simulation methods.

То

overcome this problem and bridge various scales, we present a new model, Heterogeneous Continuous Time Random Walk model (HCTRW) and suggest to represent a porous medium by an equivalent "porous graph" and then to model the complex dynamics of a particle in the porous medium by a continuous time random walk (CTRW) on that porous graph. The graph

structure accounts for the inter-connectivity of pores, whereas their geometric properties (shapes of pores and of connectivity regions) are, to some extent, captured through the CTRW characteristics, hence connecting the topological and dynamical properties of the system.

In our CTRW approach, the space and time characteristics of individual jumps on a graph are coupled that requires developing new theoretical tools. We present several preliminary results on the long-time asymptotic behavior of a particle on a porous graph. To validate the proposed coarse-graining scheme, we compare the asymptotic behavior of the CTRW on a porous graph with the original continuous dynamics in several models of porous media. In particular, we investigate how topology of a graph (which would correspond to i.e. the interconnectivity of pores) can affect the long-time behavior of HCTRW.

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