Diffusion and Percolation Transport by Molecular Dynamics Simulations and Random Walks

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Abstract

The continuous and discrete random processes, represent an computationally attractive choice to modelling nonequilibrium complex systems, such as, nucleation, agregation, percolation, growth and diffusion phenomena. In this work, the diffusion and percolation of particles, by molecular dynamics simulation, on a distributed network of colloids with orderly and fractal geometry, is presented. Our intention is that the system can be compared with systems of percolation. Thereby, adjusting the internal parameters of simulation system, we can make a calibration with respect to the values used in the models of percolation. In a second step, the parameters that are difficult to calculate in percolation systems are modeled in our simulation and allow us to calculate the coarse grained dynamic properties of the system. Finally, simulations and numerical results related with Riemann and Weierstrass walks, two discrete random processes for modeling normal and anomalous diffusion dynamics, are included.

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