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Simulation of diffusion in a crowded environment: The application of the Dynamic Lattice Liquid Model (DLL)

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Extensive and systematic simulation studies of two-dimensional fluid motion in a complex crowded environment were performed. In contrast to other works we focused on cooperative phenomena that occurred where the motion of particles takes place in a dense crowded system. Our main goal was to answer the question how do fluid molecules move in an environment which has a complex structure and taking into consideration the fact that motion of fluid molecules is highly correlated. The Dynamic Lattice Liquid (DLL) model, which can work at the highest fluid density, was employed. It became the basis for a parallel algorithm, which took into account coincidences of attempts of elementary molecular motion resulting in local cooperative structural transformations. Within the frame of the DLL model we considered cooperative motions of fluid particles in an environment that contained static obstacles. We studied the dynamic properties of the system, like the mean square displacement and the relaxation time of the position as a function of the concentration of obstacles. The changes of hydrodynamic interactions were also investigated by studies of the distribution of cooperative loop length. The subdiffusive motion of particles was found in the crowded system. It was also shown that the percolation threshold determined from the dynamic behavior of the mobile particles was considerably lower than that determined from the cluster analysis.

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