Part 1

Diffusion in a crowded environment – influence of cooperativity

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We present results of extensive and systematic simulation studies of two-dimensional fluid motion in a complex crowded environment. In contrast to other studies we focused on cooperative phenomena that occurred if the motion of particles takes place in a dense crowded system, which can be considered as a crude model of a cellular membrane. Our main goal was to answer the following question: how do the fluid molecules move in an environment with a complex structure, taking into account the fact that motions of fluid molecules are highly correlated? The dynamic lattice liquid (DLL) model, which can work at the highest fluid density, was employed. Within the frame of the DLL model we considered cooperative motion of fluid particles in an environment that contained static obstacles of various kinds[1,2]. The dynamic properties of the system as a function of the concentration of obstacles were studied. The subdiffusive motion of particles was found in the crowded system. The influence of hydrodynamics on the motion was investigated via analysis of the displacement in closed cooperative loops. The simulation and the analysis emphasize the influence of the movement correlation between moving particles and obstacles.

References

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Part 2

Technology of Real-World Analyzers (TAUR) and its practical application

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As a result of many years of research and testing, at Lodz University of Technology the concept of technology of Real-World Analyzers (in polish: Technologia Analizatorów Układów Rzeczywistych TAUR) was developed [1]. Devices built in this technology can contain up to several hundred million operational cells placed in 3D face centered cubic (fcc) network nodes. These machines are a fully parallel data processing systems equipped with low-latency communication channels, designed for simulations of huge amount of relatively simple elements working in parallel and interacting locally. Devices can support solving problems from various fields of science and technology such as e.g. molecular simulations, artificial intelligence or data encryption.

In frame of TAUR technology the device called Analyzer of Real Complex Systems (in polish: Analizator Rzeczywistych Układów Złożonych - ARUZ) was designed and constructed [2]. This machine is located in Poland in the city of Łódź in BioNanoPark. ARUZ is based on 26 000 reconfigurable FPGA devices (Field Programmable Gate Array) connected in 3D fcc network and working as signal processing units. The DLL algorithm was implemented in ARUZ allowing to study the dynamics of molecular systems on the time scale difficult to access (or unreachable in some cases) for existing computing systems. Currently, ARUZ is intensively used to analyze computationally demanding complex macromolecular systems.

References

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