Special purpose parallel hypercomputer for modeling of supramolecular systems based on the Dynamic Lattice Liquid

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Computer modeling is nowadays one of the most important sources of information about details concerning behavior of complex molecular and macromolecular systems at the molecular or atomic scale. Main obstacles in exhausting the possibilities in this field concern limitations in computational speed and in limits of spatial resolution of considered models. Possibilities to overcome these problems are both in development of appropriate efficient software, as well as, in development of suitable super fast hardware. Recent modeling techniques allow simulating systems over time intervals not exceeding 7 orders of magnitude and with spatial resolution not exceeding two orders of magnitude in the one-dimensional size scale. In most problems concerning material development as well as in biological systems both molecular or macromolecular dynamics and organization exceed considerably these scales. Recently, very effective methods of atomistic, molecular or macromolecular modelling have been developed (Pakula and co-authors), named the Cooperative Motion Algorithm (CMA) and Dynamic Lattice Liquid (DLL) model [1,2] which allows for dynamic simulations in dense systems of complex molecules or macromolecules by considering natural possibilities of cooperative molecular rearrangements. The main advantages of these methods are: physically reasonable simplifications of the dynamics and structures, applicability to dense systems, flexibility in representation of various molecular topologies and high computational efficiency. Whereas, the CMA method is super efficient on traditional sequentially working hardware (e.g. even single PC or PC clusters), the concepts of the DLL models can directly serve as basis for a parallel special purpose computer system for a super fast molecular modelling and can open new possibilities to improve spatial resolution of models by decoupling it from limitations imposed by computational speed. The main aim of this work is the construction of a dedicated computer (realizing the DLL architecture) with enormous computation power. The success of the discussed simulation methods has been demonstrated in numerous applications in which dense packing, specific interaction, complex molecular structures and complex hierarchical dynamics have important effects on behavior of modelled systems [1,3]. The already tested or potential applications concern all fields of science and technology in which atomistic, molecular, macromolecular and supramolecular structural and dynamic consideration are of importance or of interest.

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