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Multi-scale simulations with a combined Lattice-Boltzmann/Molecular Dynamics approach

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ABSTRACT

We recently proposed a computational method to simulate model nano-sized systems, such as a polymer embedded in a fluctuating hydrodynamic solvent and colloidal systems in non-equilibrium conditions [1]. In these systems non-trivial effects arise from the coupling of the molecular motion to hydrodynamics. In the talk different computational experiments for DNA translocation across nanopores in single file or multiple file conformations will be presented. The achievement of petascale-enabled LBMD simulations on the BlueGene/L parallel computer is described with applications to up to 32,000 processors.

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