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Simulation of DNA Electrophoresis by Coarse-Grained Hybrid Molecular Dynamics Approach[1] RONG WANG, Department of Polymer Science and Engineering, Nanjing University — Simulation of DNA electrophoresis facilitates the design of DNA separation devices. Various methods have been explored for simulating DNA electrophoresis and other processes using implicit and explicit solvent models. Explicit solvent models are highly desired but their applications may be limited by high computing cost in simulating large number of solvent particles. In this work, a coarse-grained hybrid molecular dynamics (CGH-MD) approach was introduced for simulating DNA electrophoresis in explicit solvent of large number of solvent particles. CGH-MD was further applied to the simulation of DNA electrophoresis in polymer solution and in a well-studied nanofluidic device. Simulation results are consistent with observations and reported simulation results, suggesting that CGH-MD is potentially useful for studying electrophoresis of macromolecules and assemblies in nano-fluidic, micro-fluidic, and microstructure array systems that involve extremely large number of solvent particles, non-uniformly distributed electrostatic interactions, bound and sequestered water molecules.

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