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**A Fast Multipole Method and a Metropolis Method for Coarse-grained Brownian Dynamics Simulations of a DNA with Hydrodynamic Interactions**[1] SZU-PEI FU, YUAN-NAN YOUNG, SHIDONG JIANG, New Jersey Inst of Tech — The coarse-grained molecular dynamics (MD) or Brownian dynamics (BD) simulation is a particle-based approach that has been applied to a wide range of biological problems that involve interaction with water molecules. The simulations are often numerically expensive for exploring long-time dynamics over meso-scales due to the amount of water molecules needed for capturing the non-local hydrodynamic interactions (HIs). In this paper a fast multipole method for computing the HIs and a metropolis method for molecular dynamics are validated by comparing against both experiments and simulations of a single DNA molecule in linear flow. In addition, it is shown that the Metropolis integration scheme for self–adjoint diffusions can be used to expedite the time it takes to prepare the initial configuration of the macromolecule for the BD simulations. Further numerical tests show that the fast multipole method scales linearly to the total number $N$ of beads for the long-chain molecule when $N \gtrsim O(10^3)$ while other numerical algorithms scale to $O(N^2)$ (at least).

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