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**● Parallel Multiscale Modeling of Biopolymer Dynamics with Hydrodynamic Correlations****Maria Fyta**

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**ABSTRACT**

We employ a multiscale approach to model the translocation of biopolymers through nanometer size pores. Our computational scheme combines microscopic molecular dynamics with a mesoscopic lattice Boltzmann method for the solvent dynamics, explicitly taking into account the interactions of the molecule with the surrounding fluid. We describe an efficient parallel implementation of the method that exhibits excellent scalability on the Blue Gene platform. We investigate both dynamical and statistical aspects of the translocation process by simulating polymers of various initial configurations and lengths. For a representative molecule size, we explore the effects of important parameters that enter in the simulation, paying particular attention to the strength of the molecule-solvent coupling and of the external electric field which drives the translocation process. Finally, we explore the connection between the generic polymers modeled in the simulation and DNA, for which interesting recent experimental results are available.

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