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Discrete Molecular Dynamics Simulation of Biomolecules

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Discrete molecular dynamics (DMD) simulation of hard spheres was the first implementation of molecular dynamics (MD) in history. DMD simulations are computationally more efficient than continuous MD simulations due to simplified interaction potentials. However, also due to these simplified potentials, DMD has often been associated with coarse-grained modeling, and hence continuous MD has become the dominant approach used to study the internal dynamics of biomolecules. With the recent advances in DMD methodology, including the development of high-resolution models for biomolecules and approaches to increase DMD efficiency, DMD simulations are emerging as an important tool in the field of molecular modeling, including the study of protein folding, protein misfolding and aggregation, and protein engineering. Recently, DMD methodology has been applied to modeling RNA folding and protein-ligand recognition. With these improvements to DMD methodology and the continuous increase in available computational power, we expect a growing role of DMD simulations in our understanding of biology.