Molecular Dynamics Simulations of Reactive Systems

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Abstract

Classical molecular dynamics has been successfully used to model structural and dynamic properties of complex biological systems. However, these methods cannot simulate chemical reactions, which are essential components of biochemical processes. This is one of the major drawbacks, limiting the scope and application of molecular dynamics techniques. Recently, van Duin et al. have proposed a novel force field, ReaXFF, that aims to mimic chemical reactions using molecular dynamics. This is achieved by establishing relation between bond distance, bond order, and bond energy to accurately model association and dissociation of chemical bonds. Other valence terms in the force field (angle and torsion) are defined in terms of the same bond orders to produce correct behavior with association or dissociation of chemical bonds. ReaXFF also incorporates Coulomb and Morse potentials to describe non–bonded interactions between all atoms. The most compute-intensive part of ReaX-based molecular dynamics is the determination of partial charges on atoms involved in chemical reactions. This in turn requires the solution of a dense linear system of equations. Using our prior work on multipole methods, we develop extremely efficient preconditioned iterative solvers for computing partial charges. Since these solvers are invoked at each time-step, the resulting improvement in complexity and speed are critical to the use of ReaX force fields in real applications. We demonstrate the computational efficiency and modeling accuracy of our methods in the context of real bio-physical systems.

Keywords: reactive force fields, molecular dynamics

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