An O(N) Framework for Internal Coordinate Molecular Dynamics Applicable to Molecules with Arbitrary Constraints and Geometries

Molecular Dynamics (MD) is a numerical simulation technique which is used to obtain the time evolution trajectory of a system of interacting particles. Integrating of the equations of motion needs to invert the mass matrix of each molecule. When considering the molecular movements in the space of generalized internal coordinate, the corresponding mass matrix is a dense matrix. Since the direct calculation of mass matrix inversion is cubically scaled with the number of atoms in a molecule, much efficient method is required for macro-molecules simulation.

Fixman's work in 1974 and the follow-up studies have developed a method that can factorize the inverse of mass matrix into an arithmetic combination of three sparse matrices—one of them is positive definite and need to be further factorized by using the Cholesky decomposition or similar methods. When the molecule subjected to study is of serial chain structure, this method can achieve O(n) computational scaling. However, for molecules with long branches, the nonzero structure of this positive definite matrix makes its decomposition in scaling of O(n^3). In this paper we present a new method which can guarantee for no fill-in in doing the Cholesky decomposition, and as a result, the inverting of mass matrix will remain the O(n) scaling, no matter the molecule structure has long branches or not.

Molecular dynamics simulation requires the long time conservation of energy (Hamiltonian). Generally there are two categories of time integrators: non-symplectic integrators, such as Runge-Kutta methods; and symplectic integrators, such as leap-frog and Euler’s symplectic methods. Symplectic integrators preserve the symplectic two-form dp^dq, and thus are better choices for long time simulations of Hamiltonian systems. Symplectic integrators for separable Hamiltonians are already well-developed. However, the internal coordinate molecular dynamics is a nonseparable system, and currently there are no effective time integrator for a large, strongly coupled nonseparable system. We have developed a symplectic time integrator which can be used to integrate a nonseparable Hamiltonian system, and numerical experiments shown that it is at least effective for a system with medium size.

Bio
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