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Angular momentum form of Verlet algorithm for rigid molecules
MIYABI HIYAMA, CREST, Toyota Central R&D Labs., Inc., TOMOYUKI KINJO, SHIAKI HYODO, Toyota Central R&D Labs., Inc. — We seek to make an algorithm based on the Verlet method which could be applied to non-Hamiltonian and explicit time dependent Hamiltonian systems for rigid molecules. For the first step of this aim, we will propose an algorithm based on the Verlet method for rigid molecules and investigate the characteristics of this algorithm for simple system. In our algorithm, the equations of motion for rigid molecules are integrated by Verlet framework in the angular momentum form. This simple algorithm is named 'the angular momentum Verlet algorithm'. We will show the results of MD simulations for 125 carbon tetrachloride molecules using the angular momentum Verlet algorithm. The relative total energy fluctuations are compared with those using the standard leap-frog and the Gear predictor-corrector algorithms. The energy drift using the angular momentum Verlet algorithm is smaller than that using the leap-frog or the Gear predictor-corrector algorithms, especially in the case of MD simulation with the large time interval.

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