Molecular Modeling - A New Approach

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Molecular modeling is indispensable in theoretical research in chemistry, molecular physics, structural biology, new materials development, and other fields. To productively use molecular modeling methods, their theoretical basis must be understood and the appropriate method must be chosen for solving a given problem. Computer simulation methods have been developed primarily in the direction of increasing the simulation lengths and the size of modeled systems, that allows a greater understanding of the relationship between the structure and function in biological macromolecules. The length of simulations has to exceed the nanosecond scale to correspond to the time scale of the chemically and biologically interesting processes, which occur on the microsecond scale.

Among the main theoretical methods of investigation of the dynamic properties of molecular systems are computer simulations and quantum chemical computations. Molecular dynamics is obviously a powerful tool for simulating molecular motion. A complementary computational method to examine molecular behavior is the normal mode analysis that examines motion in the harmonic limit.

In this contribution I will present the survey of our past and current endeavor on molecular modeling algorithm development. In particular, I will describe new symplectic integration algorithms for the numerical solution of molecular dynamics equations and methods for the determination of vibrational frequencies and normal modes of large systems.

We propose an analytical treatment of the internal high-frequency molecular vibrations in the molecular dynamics simulations using a new form of the classical Liouville propagator. The essence of the work lays in the construction of the second-order integrating algorithm that is useful for all-atom molecular dynamics simulations of molecular systems described by flexible models. We apply this algorithm to the molecular dynamics simulations of liquid water providing the evidence about its superior numerical characteristics over the standard approach. The accuracy of the method was confirmed, in particular, by computing the IR spectrum of water in which no blue shifting of the stretching normal mode frequencies is observed as occurs with the standard method.

We have also developed a computer program for molecular dynamics simulation that implements the split integration symplectic method and is designed to run on specialized parallel computers. The molecular dynamics integration is performed by the new integration method, which analytically treats high-frequency vibrational motion and thus enables the use of longer simulation time steps. The low-frequency motion is treated numerically on specially designed parallel computers, which decreases the computational time of each simulation time step. We study the computational performance of simulation on specialized computers and provide a comparison to standard personal computers. The combination of the new integration method with two specialized parallel computers is an effective way to significantly increase the speed of molecular dynamics simulations.