Semianalytical Integration Method for Macromolecular Simulations

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1 Introduction

Molecular dynamics (MD) simulation, in which the classical equations of motion for all particles of a system are integrated over finite period of time, is one of the theoretical methods to investigate dynamical properties of molecular systems [1]. The problem which arises in performing MD simulations of such systems is that only short simulations can be performed due to the high-frequency motion which requires the use of a small integration steps in MD simulations. The efficiency and thus the scope of MD is increased if methods which permit the MD integration over larger time steps are developed [2, 3, 4, 5].

2 Method and Results

A new semianalytical Split Integration Symplectic Method (SISM) for MD Integration is presented.

The approach in this paper uses the idea of composition methods [6]; it is to split the total Hamiltonian of the system into two pieces, each of which can be solved exactly or more conveniently than by using standard approaches. The individual solutions are then combined in such a way as to approximate the evolution of the original equation for a time step, and to minimize errors.

The SISM for MD simulation of macromolecular system is based on factorization of the Liouville propagator and is quite distinct from other approaches using the fractional-step methods owing to the analytical treatment of high-frequency motions.

The SISM involves splitting of the total Hamiltonian of the system into the harmonic part and the remaining part in such a way that both parts can be efficiently computed. The Hamilton equations of motion are then solved using the second order generalized leapfrog-Verlet (LFV) integration scheme in which the high-frequency motions are treated analytically by the normal mode analysis which is carried out only once, at the beginning of the calculation. SISM requires only one force evaluation per integration step. The computation cost per integration step is approximately the same as that of the standard leapfrog-Verlet method, and it allows an integration time step up to an order of magnitude larger than can be used by other methods of the same order and complexity.

The SISM was applied to the MD of the linear chain molecules of the form H-(-C≡C-)$_2$-H. These molecules were chosen as a bench mark system because the primary restriction on time step usually in macromolecular simulations arises from the presence of strong chemical bonds and angles.

In order to compare the efficienty of the SISM with the standard LFV method, we compared computational performance for the same level of accuracy. Figure 1 displays the error in total energy for test molecules. It shows that SISM is by an order of magnitude faster than standard method.

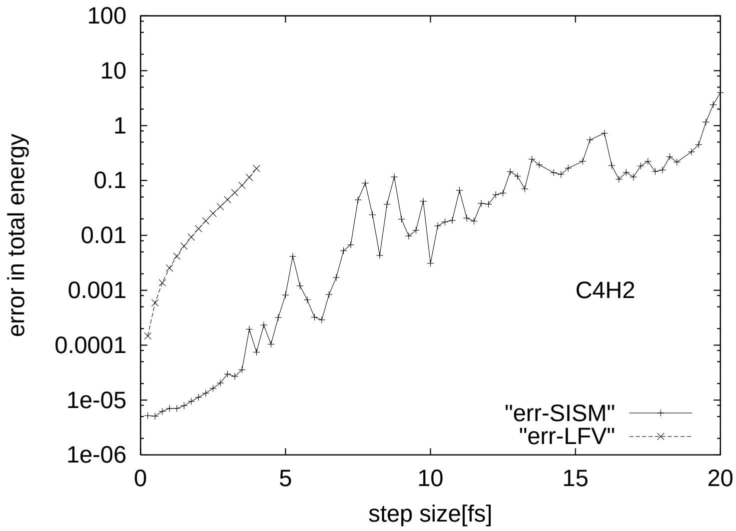

Figure 1: Error in the total energy of the system of 128 molecules of butadiine (H-(-C≡C-)$_2$-H) for SISM and LFV: ρ=0.001g/cm^3, $L = 220$Å.

N	t(SISM)[s]	t(LFV)[s]
10	6.53	6.19
50	155.58	154.21
100	618.65	616.69
128	1012.54	1010.78

Table 1: CPU time [s] for SISM and LFV for 100 MD steps of the system of butadiine molecules for different system sizes N for equal time steps of $1fs$ on the PII/450MHz.

In Table 1 the CPU time required by the two methods (LFV and SISM) for 100 MD steps computed on the PII/450MHz are compared for the same model system. The computational cost per integration step is approximately the same for both methods so that the speed up of the SISM over the LFV algorithm is determined mainly by the difference in step size which is significant.

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