Development of numerical integration scheme and application to molecular dynamics simulations

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We present techniques and the results of molecular dynamics simulations using the recently developed numerical integration scheme for ordinary differential equations (ODEs) [1,2]. These techniques provide an extended ODE possessing a time-invariant function for an ODE that may itself have had no invariant and so enable us to examine the accuracy of the numerical integration. Numerical integrators are developed on the bases of the techniques for divergence-free solvable decomposition of a vector field and symmetric composition of the corresponding maps, so that we have symmetric, explicit, volume-preserving integrators in the extended phase space. Using these techniques, we performed constant temperature molecular dynamics simulations of typical molecular systems, such as vdW particles, water, and protein molecules, with various simulation conditions. By detailed analyses on accuracy, computational cost, sensitivity, and sampling validity, we show the superiority of the current method compared with the conventional methods. Recent developments relevant to these techniques are also provided.

[1] I. Fukuda, H. Nakamura, Phys. Rev. E 2006, 73, 026703. [2] S. Queyroy, H. Nakamura, I. Fukuda, J. Comput. Chem. In press.