Numerical Integration Techniques Based on a Geometric View for Molecular Dynamics Simulations

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To enhance molecular simulation performance, we propose two techniques concerning the integration of ordinary differential equations, including those for the molecular dynamics (MD) simulations. The first one is a method of constituting a phase space time-invariant function. This function is constructed for a suitably defined extended phase space and an extended ODE in which all solutions of the original ODE completely remain. The technique is thus useful in checking the error in the numerical integrating processes used to solve the equation of motion of interest. Aside from this practicality, this idea also provides a conceptual means of uniformly understanding the relation between conserved quantities in many kinds of MD equations. The inspiration for this technique, in fact, has been derived from the special form of the Nose-Hoover MD equation and its related conserved quantity. The second technique is for a numerical integration itself, which is achieved by extending the first technique. Specifically, we have obtained a novel numerical integration technique on a newly defined extended space, and the resulting integrator has the properties of explicit, symmetric, and phase space volume preservation. This method provides a route of easily constructing an efficient integrator for many kinds of ODEs, for example non-Hamiltonian systems, via a new theoretical concept based on a geometric view beyond the symmetric feature. We investigate the theoretical aspects of the texhniques in detail and clarify its efficiency, applicability, differences with respect to other methods, and conditions for validity. We also investigate its efficiencies in numerical simulations of physical systems, including atomic clusters, water molecules, and some complex molecular systems.