GEORGE PATRICK, University of Saskatchewan

On converting any one-step method to a variational integrator of the same order

In the formalism of constrained mechanics, such as that which underlies the Shake and Rattle methods of molecular dynamics, we present an algorithm to convert any one-step integration method to a variational integrator of the same order. The one-step method is arbitrary, and the conversion can be automated, resulting in a powerful and flexible approach to the generation of novel variational integrators.