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An Application of Symplectic Integration on an N-body, with evaluations of Hamiltonian Mechanics interpretations.

Molecular Dynamics (MD) is the numerical simulation of a large system of interacting molecules, and one of the key components of an MD simulation is the numerical estimation of the solutions to a system of nonlinear differential equations. Such systems are very sensitive to discretization and round off error, and correspondingly, standard techniques such as Runge-Kutta methods can lead to poor results. However, MD systems are conservative, which means that we can use Hamiltonian mechanics and symplectic transformations (also known as canonical transformations) in analyzing and approximating solutions. This is standard in MD applications, leading to numerical techniques known as symplectic integrators, and often, these techniques are developed for well-understood Hamiltonian systems such as Hill's lunar equation. In this presentation, we explore how well symplectic techniques developed for well-understood systems (specifically, Hill's Lunar equation) address discretization errors in MD systems which fail for one or more reasons. (Received September 22, 2015)