

Why Does Molecular Dynamics Work?

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Abstract

First, it is acknowledged that a number of scientists do not believe that molecular dynamics does work, including some who accept the validity of molecular mechanics. Second, this presentation does not address the accuracy of classical force fields as an approximation to quantum mechanics, nor is it primarily concerned with defects in the ergodic hypothesis. Rather, the concern is that computed trajectories are overwhelmed by the effect of finite step size (and finite precision) due to the chaotic nature of the Hamiltonian systems and the very long integration times. The best-behaved numerical simulations are generally those that employ symplectic integrators. For these it can be proved that the numerical solution is very nearly the exact solution of a modified Hamiltonian system on a limited time interval. However, from examining the numerical trajectories of one-dimensional systems, it is not apparent that this result extends to very long time intervals. The aim of the presentation is to give a plausible mathematical basis for long time numerical integration using the concept of weak convergence.