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Are numerical trajectories of MD *simulations shadowed by exact solutions?*

Wayne Hayes
School of Information & Computer Sciences
University of California, Irvine
Irvine, CA 92697-3435
USA
[wayne@ics.uci.edu]

Abstract

Numerical trajectories of chaotic systems are suspect because the positive Lyapunov exponent guarantees that numerical errors are exponentially magnified, possibly overwhelming the accuracy of such solutions. Although we like to believe that statistical properties of such solutions are reliable even in the face of exponentially magnified noise, no hard evidence yet exists to support this believe. One avenue that has the potential to partially solve this problem is *shadowing*. A *shadow* trajectory is an exact solution that remains close to a numerical trajectory for a long time. Thus, a numerical trajectory that has a shadow can be viewed as an *experimental observation* of an exact trajectory (namely, the shadow), with the distance between the shadow and the numerical trajectory acting as the "observational error". Although such shadows are not guaranteed to have statistical properties close to those of exact trajectories chosen at random, the existence of a shadow, taken in tandem with the statistical agreement of numerical simulations with experiment, suggests that statistical results of MD simulations with carefully-chosen accuracy parameters may be trustworthy. In this talk, I will review some recent results on shadowing simplified molecular dynamics simulations, including how shadowing times and distances scale with accuracy parameters such as timestep.