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The relation between shadowing and weak approximation in molecular dynamics

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Abstract

In computational physics, molecular dynamics refers to the computer simulation of a material at the atomic level. I will consider classical deterministic molecular dynamics in which large Hamiltonian systems of ordinary differential equations are used, though many of the same issues arise with other models. Given its scientific importance there is very little rigorous justification of molecular dynamics. From the viewpoint of numerical analysis it is surprising that it works at all. The problem is that individual trajectories computed by molecular dynamics are accurate for only small time intervals, whereas researchers trust the results over very long time intervals. It has been conjectured that molecular dynamics trajectories are accurate over long time intervals in some weak statistical sense. Another conjecture is that numerical trajectories satisfy the shadowing property: that they are close over long time intervals to exact trajectories with different initial conditions. I will explain how these two views are actually equivalent to each other, after we suitably modify the concept of shadowing.