Statistical analysis of finite-difference scheme errors in molecular dynamics method

Ekaterina Dlinnova, Vladimir Stegailov

HSE

The finite-difference approximation of classical equations of motion introduces errors that accumulate during a molecular dynamics calculation. The proper numerical scheme, however, conserves the average value of the total energy of the system that is why these errors differ significantly from some random noise. The numerical errors lead to the fact that the Newtonian dynamics is conserved in the MD only approximately. The inverse problem consists in finding the equations that satisfy the numerical MD trajectory. We modified the system of Newton's differential equations by adding to the right-hand side additional terms that follow from the finite-difference approximation of the equations of motion and depend on the timestep of the integration. The meaning of these terms is that when they are added, the solutions of the modified equation coincide with the points of the finite-difference numerical solution. In this work we perform the backward error analysis additional terms of the velocities and per-atom forces and show the peculiarities of their statistical distribution.