Simple integrators for Langevin dynamics

Robert D Skeel
skeel@cs.uiuc.edu
University of Illinois, USA

The best simple method for Newtonian molecular dynamics is indisputably the leapfrog method. The appropriate generalization to simple Langevin dynamics is unclear. We present analytical evidence suggesting that the "impulse method" (half a kick, fluctuate, half a kick) is the best basic method for simple Langevin dynamics. We show how this method and the 1982 method of van Gunsteren and Berendsen can be implemented as efficiently as the BBK method.