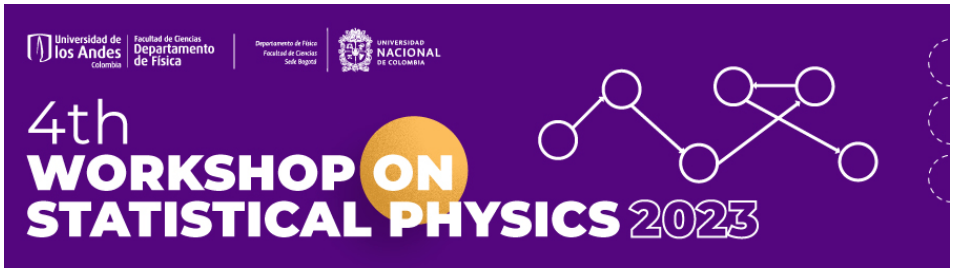

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A review of the stochastic leapfrog thermostat for Langevin dynamics

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In molecular dynamics simulations, thermostats are algorithms known for reproducing the canonical or NVT ensemble on a system of particles, i.e., they reproduce a given temperature in the system. In this work, we review a stochastic thermostat algorithm to reproduce Langevin dynamics according to the equation $\dot{v} = \frac{F}{m} - \gamma v + b\xi$ where F is the total external force, γ is the friction rate, and ξ is a random variable with mean zero and no time correlation.

This algorithm is a modification to the classic leapfrog scheme, it adds the impulsive friction and noise terms $\Delta v = -fv + \sqrt{f(2-f)(k_BT/m)}\xi$ to velocity with $0 \leq f \leq 1$ resulting in the convergence of $\langle v^2 \rangle$ to k_BT/m therefore conserving the temperature. We show that this algorithm not only reproduces the correct average temperature, but it also preserves the canonical distribution of velocity throughout the time integration. Furthermore, we perform simulations to verify these claims by Ornstein-Uhlenbeck processes for different impulsive friction constants f and corroborate its relationship with the friction rate to be $f = 1 - e^{-\gamma \Delta t}$.

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