Computational statistical physics and hypocoercivity

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I will provide an introduction to molecular dynamics, the computational implementation of the theory of statistical physics. The discussion will be focused on the properties of Langevin dynamics, a degenerate stochastic differential equation, which can be seen as a perturbation of Hamiltonian dynamics. From an analytical point of view, the generator of Langevin dynamics is a degenerate elliptic operator. The evolution of the law of the stochastic process is governed by the Fokker-Planck equation, and its longtime convergence can be obtained via hypocoercive techniques, which I will review. I will also present the implication of these analytical results in terms of error estimates for the computation of average properties of molecular systems by estimating the asymptotic variance of time averages in a central limit theorem..