How to measure the relaxation time of an stochastic Markov dynamics in a numerical simulation by using the concept of dynamical temperature

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The computation of relaxation times in generalized stochastic dynamics has shown to be a very elusive aim as it goes beyond any linearized approach or numerical strategy based on some truncation scheme. In Monte Carlo simulations of physical models one normally encodes the stochastic dynamics by using a Markov process, which after to a transient time -called thermalization- drives the system to its equilibrium. In [1] we have found an ensemble-free estimator for the dynamical temperature for spin systems, which allows a direct measure of the thermalization path of the underlying Markov process used in the numerical simulation. It represents a generalization to previous articles on the concept of configurational temperature for spin systems [2], in the sense that it has the useful property to be independent of the ensemble . It further allows to test ergodicity and to measure the absolute errors associated to the statistical fluctuations. Another interesting feature of the present approach is that it gives valuable information about the efficiency of the algorithm and its associated autocorrelation time. In the present article we discuss these ideas by studying the two-dimensional XY-model numerically simulated with a Wolff unicluster algorithm [3].

The main idea is as follows: when performing a Monte Carlo simulation in the canonical ensemble one uses the value of the system temperature or the temperature of the thermal bath -which defines the ensemble- in the weighted Gibbs factor, but on the other side one can directly measure the inverse of the temperature by computing the thermal average of the microscopic estimator found in [1]. This strategy allows us to monitor the thermalization process of the stochastic Markov dynamics, as the measured value for β must coincide with the input β-value used in the Gibbs factor.

This method can be generalized to other ensembles as well as to other spin models, since the microscopic estimator for the inverse of the temperature was proven to be independent of the ensemble.

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