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Monte Carlo simulations of (quasi) constrained ensembles

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Resumen

The standard Monte Carlo simulation of systems dysplaing metastability is very inefficient. The standard example is that of first-order phase transitions, but metastibility hampers the simulation of many complex systems (spin glasses, structural glasses, lattice polymers,...). One may use constrained statistical ensembles in order to guide the simulation inside those rare but crucial regions were it does not want to get into. Typical implementations of this idea, such as Multicanonical or Wang-Landau simulations, require the system to perform a one-dimensional in the so-called reaction coordinate space. This random-walk is strongly non-markpovian, and does suffer from exponential critical slowing down. Here we propose a different approache. We combine a generalization of Lustig's microcanonical Monte Carlo, with a fluctuation-dissipation formalism. Thermodynamic integration allows for an accurate reconstruction of the effective potential. Cluster algorithms work fine within this framework. This strategy outperforms random-walks methods in the simulation of disordered systems. The presented work has been (mostly) performed in collaboration [1–5].

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[4] V. Martin-Mayor and D. Yllanes, Phys. Rev. E **80**, 015701(R) (2009).
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