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The parallel replica algorithm: mathematical foundations and recent developments

Abstract:

I will present the parallel replica algorithm, which is an accelerated dynamics method proposed by A.F. Voter in 1998. This technique has been widely used for applications in material sciences. The aim of this algorithm is to efficiently generate trajectories of a metastable stochastic process. Recently, we propose a mathematical framework to understand the efficiency and the error associated with this technique. Generalizations of the original method in order to widen its applicability have been proposed.

References:

- D. Aristoff, T. Lelièvre and G. Simpson, The parallel replica method for simulating long trajectories of Markov chains, *AMRX*, 2, 332-352, (2014)
- A. Binder, T. Lelièvre and G. Simpson, A Generalized Parallel Replica Dynamics, *Journal of Computational Physics*, 284, 595-616, (2015).
- C. Le Bris, T. Lelièvre, M. Luskin and D. Perez, A mathematical formalization of the parallel replica dynamics, *Monte Carlo Methods and Applications*, 18(2), 119-146, (2012).