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Multi-replica swap optimization of replica exchange method

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The replica exchange Monte Carlo method, or parallel tempering, is a widely used extended ensemble method to overcome the difficulty of sampling from a complex multi-modal target distribution typical in frustrated spin systems and protein folding. Replicas having different model parameters, such as the temperature of a system, are stochastically swapped using the Metropolis algorithm. Enhancing the replica swap probability and the round trip rate is crucial to the success of the replica exchange method. In the meantime, nonreversible Markov chains can generally outperform reversible chains and enhance sampling efficiency. The lifting technique and the probability optimization beyond detailed balance have been applied to various physical and chemical systems. In this work, we propose combining these approaches to enhance the replica swap efficiency and the round trip rate in the replica exchange method. The multi-replica swap probability is maximized beyond the Metropolis algorithm. Our approach can be combined with any local update method for each temperature.

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