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Optimized parallel tempering simulations of proteins SIMON TREBST, Microsoft, Project Q, and Kavli Institute for Theoretical Physics, Santa Barbara, CA 93106, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, CH-8093 Zurich, Switzerland, ULRICH HANSMANN, John-von-Neumann Institute for Computing, Forschungszentrum Julich, D-52425 Julich, Germany — We introduce an adaptive algorithm that systematically improves the efficiency of parallel tempering or replica exchange methods in the numerical simulation of small proteins. Feedback iterations allow us to identify an optimal set of temperatures/replicas which are found to concentrate at the bottlenecks of the simulations. A measure of convergence for the equilibration of the parallel tempering algorithm is discussed. We test our algorithm by simulating the 36-residue villin headpiece sub-domain HP-36 where we find a lowest-energy configuration with a root-mean-square-deviation of less than 4 Å to the experimentally determined structure.

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