Performing massively parallel protein simulations using the SIMONA Monte Carlo framework

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For the theoretical understanding of molecular and nanoscale systems, more and more larger and longer all-atom simulations are needed. Current simulation techniques barely reach the millisecond border, but most interesting processes like protein folding only occur on a millisecond to second timescale. We recently published our new Monte Carlo simulation package SIMONA[1] (SImulation of MOlecular and NAnoscale systems) which is able to fold small proteins to their native state using single threaded MC simulations. For the observation of multiple folding and unfolding events or the folding of bigger proteins, parallel simulation methods are needed.
We successfully applied a GMTM[2] (General Multiple Try Metropolis) method to a proteinous system, where a set of processors simultaneously samples the conformational space of the protein. This leads to much higher acceptance rates and also lower autocorrelation times, in comparison to a conventional Metropolis Monte Carlo simulation.
In addition, we combined this GMTM algorithm with a PT[3] (Parallel Tempering) scheme to sample the systems phase space even more effectively and at different temperatures at once.

[1] Wolf, M. et al. SIMONA: An efficient and versatile framework for stochastic simulations of molecular and nanoscale systems (in revision).
[2] Pandolfi, S., Bartolucci, F. & Friel, N. A generalization of the Multiple-try Metropolis algorithm for Bayesian estimation and model selection. Journal of Machine Learning Research - Proceedings Track 581–588 (2010).
[3] Hansmann, U. H. E. Parallel tempering algorithm for conformational studies of biological molecules. Chemical Physics Letters 281, 140–150 (1997).