Population Annealing goes Molecular Dynamics

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We adapt Population Annealing to Molecular Dynamics simulations and show the excellent accelerating performance as well as the massive potential for parallelism. For this we simulate the folding of met-enkephalin, a short peptide commonly used to test the performance of algorithms. A comparison with Parallel Tempering, the *de facto* standard for the simulation of complex systems with a rugged free-energy landscape using Molecular Dynamics, is presented. Further, the impact of choosing the temperatures of the annealing schedule via a constant energy-histogram overlap condition and the influence of the number of update-steps per temperature are checked.