Evolutionary Monte Carlo for Protein Folding Simulations

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Abstract

We demonstrate that evolutionary Monte Carlo (EMC) can be applied successfully to simulations of protein folding on simple lattice models, and to finding the native state of a protein. In all cases, EMC is faster than the genetic algorithm and the conventional Metropolis Monte Carlo, and in several cases it finds new lower energy states. We also propose one method for the use of secondary structures in protein folding. The numerical results show that it is drastically superior to other methods in finding the native state of a protein. (This talk is based on a joint work with Wing Hung Wong).