An algorithmic approach to protein folding

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Abstract

In this work we have tested an algorithmic approach to solve the protein folding problem in a cubic lattice. The principle of the approach is to use several simple algorithms to produce more or less random building blocks, which are then joined into a trial conformation. The preliminary tests show that the algorithms producing secondary structure resembling motifs produce more conformations at low energies. The conformation energy optimization is done using a population based method: the most fit conformations of a set of randomly generated trial conformations are re-evaluated by slightly modifying them in a Monte Carlo fashion. The simple building blocks include: an α-helix (both left- and right-handed), β-sheet, and random turns. A local hill climbing scheme was used to aid otherwise random search. It was observed to give about 10^6 times faster search speed when compared to random search. Residue types can be tailored freely by giving pairwise interaction energies. The current test version includes the following residue types: H (Hydrophobic), P (Polar), A (An intermediate type), and I (Inert). Two solvent types: water (polar) and lipid (membrane) are available.

The results presented are mostly preliminary, mainly qualitative, and only lay ground for further studies with the implemented lattice model program Lattice.

Keywords: artificial intelligence, combinatorial and computational geometry, global optimization, lattice model, protein folding.