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Evolutionary Strategies for Protein Folding SRINIVASA MURTHY GOPAL, WOLFGANG WENZEL, INT, Forschungszentrum Karlsruhe — The free energy approach for predicting the protein tertiary structure describes the native state of a protein as the global minimum of an appropriate free-energy forcefield. The low-energy region of the free-energy landscape of a protein is extremely rugged. Efficient optimization methods must therefore speed up the search for the global optimum by avoiding high energy transition states, adapt large scale moves or accept unphysical intermediates. Here we investigate an evolutionary strategies(ES) for optimizing a protein conformation in our all-atom free-energy force field([1],[2]). A set of random conformations is evolved using an ES to get a diverse population containing low energy structure. The ES is shown to balance energy improvement and yet maintain diversity in structures. The ES is implemented as a master-client model for distributed computing. Starting from random structures and by using this optimization technique, we were able to fold a 20 amino-acid helical protein and 16 amino-acid beta hairpin[3]. We compare ES to basin hopping method.
[1]T. Herges and W. Wenzel,Biophys.J. **87**,3100(2004)
[2] A. Verma and W. Wenzel *Stabilization and folding of beta-sheet and alpha-helical proteins in an all-atom free energy model*(submitted)(2005)
[3] S. M. Gopal and W. Wenzel *Evolutionary Strategies for Protein Folding* (in preparation)

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