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Parallel evolutionary optimization algorithms for peptide-protein docking

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In this study we examine the prospect of using evolutionary optimization algorithms in protein-peptide docking. We present the main assumptions that reduce the docking problem to the continuous global optimization problem and provide a way of using evolutionary optimization algorithms. The Rosetta all-atom force field was used for structural representation and energy scoring. We describe the parallelization scheme and MPI/OpenMP realization of the considered algorithms. We demonstrate the efficiency and the performance for some algorithms which were applied to a set of benchmark complexes.

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