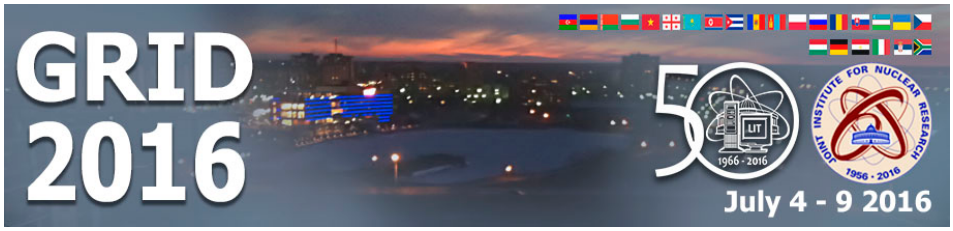

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Distributed evolutionary optimization algorithms for peptide structure prediction

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This work presents an approach to the construction of distributed stochastic evolutionary optimization algorithms for peptide secondary structure prediction. The prediction can be formulated as optimal peptide structure search in continuous space of torsion angles. The optimal peptide structure corresponds to the global minimum of free energy. Two main regular peptide secondary structures are considered: alpha-helix and beta-sheet. The authors proposed a scheme for application of evolutionary algorithms to this problem by changing non-covalent force-field term during optimal structure search. Results of numerical experiments for model and real peptides are presented.

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