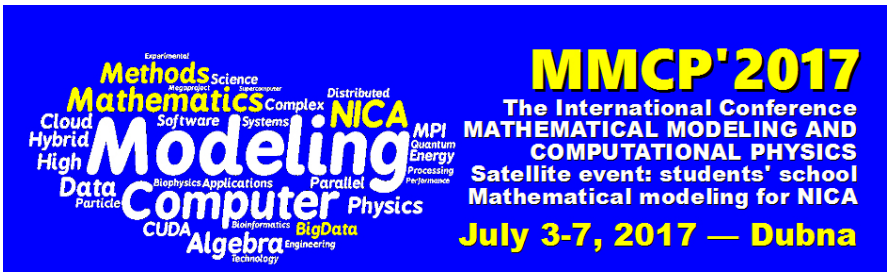

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Development of swarm optimization methods for the structural bioinformatics problems on the basis of the model problem of graph drawing

Monday, 3 July 2017 17:00 (30 minutes)

Our research is related to the problems of predicting the spatial structure of polypeptide molecules and their complexes. Our approach is based on the solution of the corresponding optimization problem, in which the objective function is the potential energy of the corresponding atomic ensemble, and the parameters of optimization are such geometric characteristics as bond lengths, valence and torsion angles. Distinctive features of this kind of optimization tasks are their high dimension and a long calculation time of the objective function, which determines the high requirements to the speed of convergence of the optimization algorithm. Our preliminary studies have shown that the absolute majority of existing optimization algorithms solve this task very badly. The development of new algorithms (or optimization of existing ones) is obstructed by the high computational complexity of the problem itself - typical calculation time is measured in hours and even days. In addition, the calculation of the objective function (energy) requires the installation of very serious software. For these reasons, we proposed to use the simpler related problem of graphs drawing to develop new optimization algorithms. The results of numerical investigation of several classical algorithms of swarm and evolutionary optimization are presented on the solution of such a model problem.

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