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Optimization algorithms of multiparameter reactive force field

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Molecular dynamic methods that use ReaxFF force field allow one to obtain sufficiently good results in simulating large multicomponent chemically reactive systems. Here are represented two algorithms of searching optimal parameters of molecular-dynamic force field ReaxFF and their implementations. These algorithms allow one to search force field parameters for arbitrary types of chemically reactive systems. For the optimization process the program uses data obtained by accurate quantum chemical computations of characteristics (training set) of simple models of chemical compounds. The first algorithm is based on the one-parameter search method. The second one is the multidimensional algorithm of global search. The advantage of the second algorithm is its good scalability useful for running it on distributed parallel computers. Based on the optimized parameters obtained earlier, we compare efficiency of these two methods, namely speed and proximity to the expected result.

Primary authors: Mr SHEFOV, Konstantin (Saint Petersburg State University); Dr STEPANOVA, Margarita (SPbSU)

Presenter: Dr STEPANOVA, Margarita (SPbSU)

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