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Sensitivity Analysis in a problem of ReaxFF molecular-dynamic force field optimization

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In a wide range of modern problems, it is required to estimate an influence of uncertainty of input parameters on uncertainty of an output value of a modeling function. In this contribution, we present algorithms for analyzing the sensitivity of a target function with respect to parameters in the problem of optimization of ReaxFF molecular-dynamic force field. In this particular case it allows one to effectively decrease the number of simultaneously optimized parameters. We compare the Sobol's global sensitivity indexes (SI) approach and the correlation analysis.

Both methods are based on computations of the target function value on the set of pseudo- or quasi-randomly distributed points. The distribution derived is used for further computations of SI using Monte-Carlo technique and correlation coefficients. In the case of optimized ReaxFF force field one may spend up to several seconds to compute a value of the target function in a particular point. That is why it is important to perform calculations in parallel for multiple points. A parallel algorithm has been implemented in C++ using MPI.

We compute Sobol's SI and coefficients of correlation of parameters variation and target function values variation while we optimize the force field for molecules and crystals of zinc hydroxide. We show that using of parameter set sorted by influence allows one to significantly increase convergence speed of the optimization algorithm and even completely exclude those parameters with relatively small influence.

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