Algorithms for global minimum search of atomic–molecular clusters of extremely large dimensions*

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The problem of finding low-potential atomic–molecular clusters is one of the classical problems of computational chemistry. From a mathematical point of view, the problem is reduced to the search for a minimum of potential functions—special models, which have already been created in several hundreds (see, for example, [1]). The main difficulty in this class of problems is their nonconvexity, which is expressed in a huge number of local extrema of potential functions—experts give estimates that, in some cases, prove the exponential growth of the number of local extrema as a function of the number of atoms (optimized variables). The most known and often considered potential functions in the scientific literature are the models of Lennard–Jones, Morse, Keating, Dzugutov, Gupta, and others [2–5]. Since the exact value of the global minimum is unknown in most cases, in the works of this direction the "best of known" principle is used—the presented solution is "probably optimal" (putative) until one of the experts has produced the best solution.

Regular studies of the optimization problems formulated for the potentials of atomic–molecular clusters were initiated in the 1990s by specialists from the United Kingdom and the United States. At this stage, record-breaking indicators of the size of the problems were, for example, for the Morse potential of only 147 atoms (441 variables), but the number of local extrema in record-breaking problems was already estimated to be of the order of 10^{60}.

In recent years, groups of specialists from China and Portugal have joined the correspondence competition to optimize Morse models (see, for example, [6, 7]). Calculations by these groups were performed on powerful supercomputer systems—perhaps the most powerful in their countries. In the publications of the Chinese group, tables of systemic calculation of

*Supported by RFBR, project no. 18-07-00587.

problems for Morse models are presented up to dimensions of 240 atoms (720 variables) inclusive. The Portuguese group, using the original "Big Bang" method, managed to clarify the decisions of the Chinese group for the maximum (in size) Morse cluster of 240 atoms among the presented ones. At the same time, the results obtained by the Portuguese group with careful analysis and visualization are radically different from the record results of the Chinese group both in terms of the physical dimensions of the cluster and in its geometric properties.

The report discusses algorithms and computational schemes that made it possible to replicate the best achievements of the Chinese and Portuguese specialists (240 atoms for the Morse model) and regularly obtain solutions for potential functions of significantly larger dimensions without using parallel computing technologies on a working laptop.

The results of computational experiments for Morse models with dimensions up to 280 atoms (840 variables) are presented.

References

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