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Scalability of the Parallel Strongin Algorithm in the Problem of Optimizing a Molecular-Dynamic Force Field

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Strongin's multifactorial global search algorithm (MGSA) allows one to find an absolute minimum of a function of multiple variables on a mesh. In this contribution a parallel program is presented that implements the algorithm above applied to ReaxFF MD force field parameter search.
The MGSA converges the faster, the greater number of mesh points have computed target function value in them. In case of ReaxFF optimization computation time of a target function value significantly exceeds time of data exchange between parallel processes. One is able to speed up computation by obtaining not only one but several function values in various points simultaneously. Our software implements two levels of parallelism. To deal with function of multiple variables, one uses a scan for mapping a multidimensional domain of definition of a function into a one-dimensional segment. To decrease the effect of losing information of multidimensional points proximity, multiple scans are used, the number of which is denoted by N. The algorithm deals with each scan in parallel, computing function value in N different mesh points in a single iteration. This is the first level of parallelism. To define a mesh point of a next iteration, MGSA finds a subinterval with the most probable location of the minimum and computes a target function value in a certain point of this subinterval. If one computes a function value not only in the most probable subinterval but also in (M-1) subintervals with less probability in parallel, one will be able to obtain function values in M different mesh points. This will accelerate the convergence, increasing the amount of data about the target function received every iteration. This is the second level of parallelism. Thus the two levels allow one to compute M * N function values every iteration.
In this contribution we research scalability of our MGSA implementation, namely, the dependence of the number of algorithm iterations it needs to converge on the number of CPU cores used, separately for each level of parallelism.

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