Parallelization of the Global Extremum Searching Process

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Abstract—The parallel algorithm for searching the global extremum of the function of several variables is designed. The algorithm is based on the method of nonuniform coverings proposed by Yu.G. Evtushenko for functions that comply with the Lipschitz condition. The algorithm is realized in the language C and message passing interface (MPI) system. To speed up computations, auxiliary procedures for founding the local extremum are used. The operation of the algorithm is illustrated by the example of atomic cluster structure calculations.

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1. INTRODUCTION

In the overwhelming majority of optimization problems, it is required to find the global maximum. However, due to high complexity of these problems, the task is usually limited to finding local solutions. Modern multiprocessor computers considerably broaden possibilities for solving global optimization problems; they also allow using parallel computing algorithms. Transfer of sequential algorithms and design of new parallel computing methods of global optimization have become more urgent. Review of numerous publications on the search for global extremum is given in [1]. Problems of computing parallelization are stated in detail in [2].

In 1971, the method of nonuniform coverings for finding the global extremum of Lipschitz functions was proposed and realized in ALGOL–60. This method was further developed in [4, 5]. In this paper, we consider the parallel variant of the method of nonuniform coverings, give information on its software implementation in C in MPI system. To speed up calculations, auxiliary procedures for finding the local extremum are used. The operation of the algorithm is illustrated by the example of atomic cluster structure calculations. Computing experiments are carried out on systems MVS 6000 and MVS 15 000 [6].

2. FORMULATION OF THE PROBLEM AND THE GENERAL IDEA OF THE METHOD OF COVERINGS

Let us consider the problem of finding the global minimum of the function \( f \) determined and continuous on the compact set \( P \subset \mathbb{R}^n \)

\[
    f_* = \text{glob min}_{x \in P} f(x).
\]
Let $X_*$ is a set of solutions to problem (1); $f_*$ is a minimum value of the objective function $f(x)$. Let us introduce the set of $\varepsilon$-optimal (approximate) solutions to problem (1):

$$X_*^\varepsilon = \{x \in P : f(x) \leq f_* + \varepsilon\}.$$  \hspace{1cm} (2)

Obviously, $X_* \subset X_*^\varepsilon \subset P$. In the most of practical problems, it is sufficient to find at least one point $x_r \in X_*^\varepsilon$ and take the number $f_r = f(x_r)$ as an optimal value of $f_*$. In other words, it is necessary to determine the value of the global minimum of function with the prescribed accuracy $\varepsilon$ and find at least one point $x_r$ where this approximate value is achieved.

Let us introduce a number of sets $B_m = [P_1, P_2, \ldots, P_m]$ from $R^n$ and a set of $n$-dimensional points $N_m = [c_1, c_2, \ldots, c_m]$ such that $c_i \in P_i \subset P$ for all $1 \leq i \leq m$. Let the union $m$ of sets $P_i$ is

$$U_m = \bigcup_{i=1}^{m} P_i.$$  

We say that the union of sets $P_i$ covers the set $P$, if

$$P = U_m.$$  \hspace{1cm} (3)

At each point $c_i$ is computed the value of the function $f$, and by the formula

$$R_m = \min_{1 \leq i \leq m} f(c_i) = f(c_r)$$  \hspace{1cm} (4)

we determine the record point $c_r$ and the record $R_m$.

Assume that the function $f$ and the set $P_i$ are so that for all $x \in P_i$ is met the condition

$$f(x) \geq R_m - \varepsilon.$$  \hspace{1cm} (5)

The basis of the method of nonuniform coverings is the following easy-testable assertion

**Assertion 1.** Let the number of sets $B_m$ and the function $f$ are such that $U_m = P$ and condition (5) is fulfilled for all $1 \leq i \leq m$. Then the record point is $c_r \in X_*^\varepsilon$.

Indeed, if the number of sets $P_i$ completely covers $P$, then each point $x_*$ in $X_*$ will belong at least to one of the sets $P_i$. Let $x_* \in P_s$, $s \leq m$, then taking into consideration (5), we obtain

$$f_* = f(x_*) \geq R_m - \varepsilon = f(c_r) - \varepsilon.$$  

According to (2), the record point $c_r$ belongs to the set of $\varepsilon$-solutions to problem (1).

This assertion expresses the main idea of the method of nonuniform coverings: instead of the global minimum on $P$ are sought global minimums on subsets, whose union coincides with $P$. The sets $P_i$ can be various. For example, on each $P_i$, the function $f$ can meet the Lipschitz condition with its constant $L_i$. The function can be convex or twice differentiable in some domains. It is reasonable to take into accounts all these peculiarities for speeding up computations.

At realizing the method, the sets $B_m$ and $N_m$ are sequentially constructed; after each computation of the value of the function $f$, refinement of the record is conducted. We suppose that the last computation of $f$ was fulfilled at the point $c_m$; the record point was $c_r$; and the record, $R_m$. Determine the following Lebesgue set:

$$L_m = \{x \in P : R_m - \varepsilon \leq f(x)\}. $$ \hspace{1cm} (6)

Let the global minimum on $L_m$ is achieved at the point $x_l$. Then $R_m - f(x_l) = f(c_r) - f(x_l) \leq \varepsilon$ and, hence, as a result of global minimization on $L_m$, the record $R_m$ can be precised no more than $\varepsilon$. Therefore, the set $L_m$ is out of interest and can be excluded from the search domain of $P$.

If the condition $P = U_m$ is not fulfilled after the computations described, then the search for minimum is continued on the set $W_m = P \setminus U_m$. Let $c_{m+1} \in P_{m+1} \subseteq W_m$ are determined, $f(c_{m+1})$