Global optimization of Morse clusters with a heuristic algorithm based on the Strongin method

A N Kovartsev¹, D A Popova-Kovartseva¹

¹Samara National Research University, Moskovskoe Shosse 34, Samara, Russia, 443086

e-mail: kovr_ssau@mail.ru

Abstract. This article presents a new heuristic method for the global optimization of Morse clusters. The algorithm uses multieextremal optimization of a function of one variable, a known method developed by R. G. Strongin. The proposed approach to the parametrization of the problem of structural optimization of Morse clusters makes it possible to significantly reduce the complexity of the original multidimensional problem of global optimization of the Morse cluster and reduce it to the problem of one-parameter optimization. The proposed method is largely based on the ideas of constructing genetic algorithms. First of all, this refers to the proposed method of encoding information as well as to reducing the problem of structural optimization to the task of optimizing a function of one variable. In this case, instead of the usual genetic operations, such as mutation and crossover, we used the R. G. Strongin method for global optimization of a function of one variable. This significantly reduced the algorithmic complexity of the problem being solved.

1. Introduction
Information about the structure of atomic clusters is of major importance in many fields such as metals modeling, protein-folding studies, calculation of electronic and dynamic characteristics of nanomaterials, and development of new light sources [1]. A key problem in this area of research is finding the geometrical structure of an atomic cluster (cluster conformation) that corresponds to the minimum of the interaction energy of the atoms in that cluster.

In simpler cases, the chemical bond between atoms is disregarded. For Morse clusters, only pairwise interactions of atoms are considered. The interactions are described by the potential function

\[ v(r_{ij}) = e^{\rho(t - r_{ij})} - 2, \]

where \( r_{ij} \) is the distance between atoms \( i \) and \( j \); \( \rho \) is the parameter expanding or narrowing the potential well of pairwise interactions in the Morse cluster [2]. As a rule, \( \rho \) falls within the range 3–14.

The interaction energy of all atoms in the cluster can be calculated as the sum of pairwise interactions' energies:
\[ v(X) = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1 \atop i \neq j}^{m} \beta_{ij} r_{ji}^{1/2} \sqrt{r_{ij}^{1/2}}, \]

where \( X = (x_1, \ldots, x_m)' \) and \( x_i \in \mathbb{R}^3 \) are the coordinates of the atoms’ centers.

Figure 1 shows plots of the Morse potential function. As the figure shows, the function depends on the distance between atom pairs and is not convex. As study [2] has illustrated, function (2) obtained by adding together the contributions of pairwise interactions’ energies is a nonconvex multimodal function of spatial coordinates of \( m \) atoms. Thus, the problem of finding atomic clusters’ optimal conformations reduces to the problem of global optimization (GO) of potential function (2).

Unfortunately, direct GO methods yielding accurate solutions to the problem of optimization allow one to find solutions for functions with 20–30 variables [3], while global optimization of atomic clusters involves over 900 optimizable variables.

![Morse potential of pairwise interaction.](image)

This necessitates developing heuristic optimization algorithms that use various additional information about the subject under study [4].

The first methods for optimizing cluster structures were based on the use of geometrical properties of known atomic clusters [2]. For instance, for Morse clusters, atom arrangements in optimal conformations were reported to gravitate toward a symmetrical spherical shape [5]. This led to the development of geometrically sound methods for the GO of Morse clusters. The concept has been repeatedly revisited [6–9]. In [6], for instance, icosahedral, dodecahedral, or face-centered cubic structures were used as cores of initial cluster conformations.

Local stochastic methods based on the basin-hopping technique [2] constitute a larger group of methods for cluster optimization. These methods are premised on the notion that for potential function (2), local extrema accumulate in a limited number of basins. In each of those basins, the funnels of local minima lie so close to one another that a gradual transition from local extrema to a global one is possible through random perturbations of the coordinates of the cluster’s atoms. This concept has been repeatedly elaborated [10–12], and this resulted in finding global heuristics for large-sized clusters [11].

Finally, we should mention population algorithms for GO [13–15]. In some cases, these have significantly increased the efficiency of heuristic algorithms for the GO of Morse clusters.

2. Genetic GO algorithm based on the Strongin method

2.1. Icosahedral nonlattice packing

As the algorithmic complexity of local optimization is of a polynomial nature, almost all known GO methods for atomic clusters use the technique of local optimization of the cluster from the position close to the optimal solution. It is long known [16] that icosahedral or nearly icosahedral structures are
good initial approximations for searching for the global minimum of the cluster’s potential energy through local-optimization methods. Based on this information, study [17] proposes a simple and reliable method to form optimal icosahedral structures for Morse atomic clusters of almost arbitrary size for the magic numbers $m = 55, 147, 309, 561, 817, 923, 1415$, and so on. The record conformations built for the magic numbers provide, in turn, a useful orientation for forming clusters of intermediate size. Such conformations can be built by expanding the preceding full icosahedron or by disassembling the next. This causes atom conformations to deform significantly, which, in turn, requires using other heuristics.

An analysis of cluster structures from the Cambridge Cluster Database [18] and its extension [19] for $6 \geq \rho$ and the number of atoms in the range $12 < m < 240$ showed that at $\rho = 6$, atomic structures with globally optimal energy potential mostly have an icosahedral structure. At $\rho = 14$, however, dodecahedral and icosahedral structures predominate, although face-centered lattices and close-packed configurations occur often as well [18, 19].

An important finding obtained from the analysis of Morse atomic clusters with globally optimal energy potential is that clusters can be expanded along the $z$ axis so that their atoms form an indistinct layered structure. An indistinct layer is understood here to be an arrangement of an atom (circle) group whereby the atom centers lie not on the plane but in a sufficiently “thin” layer—$z_j \pm \Delta z_j$.

Another important finding is that in the plane projection $x0y$ all allocated layers in optimal clusters form an icosahedral nonlattice packing. We will refer to it as an icosahedral grid (see figure 2).

![Figure 2. Plane projection of icosahedral nonlattice circle packing.](image)

### 2.2. Making an icosahedral spatial grid

An icosahedral grid is fairly easy to make.

In the center of the packing, there is a circle with a radius of $r$. Here, $r = 0.5$. The plane is split into five equal parts by beams extending from the coordinate origin. The angle between the beams is $\varphi = 2\pi / 5$. Let us assume that $\alpha = \varphi / 2 = \pi / 5$. Then let us place circle centers on the lines of regular pentagons drawn around the central circle. In the first pentagon each sector contains two circle halves (i.e., one whole circle); in the second, each sector contains four circle halves (two whole circles), and so on. In this case, the coordinates of the circles located on the $0x$ axis ($y = 0$) can be easily calculated for each pentagon from the equation

$$x_k = kr / \sin \alpha = kr / \sin(\pi / 5),$$

where $k$ is the pentagon number.

For the other circles, coordinates can be found geometrically. If, for purposes of this discussion, we assume that the central circle is the zero pentagon and form each layer by merging, using pentagonal configurations with only even or odd numbers, then, placing the layers one over another, we can...
obtain an icosahedral nonlattice circle packing. Note that the even and odd layers penetrate each other almost halfway so that the odd layers are inside the even ones. In [19], the method for making an icosahedral nonlattice circle packing is discussed in detail.

2.3. Genetic GO algorithm

Most atomic-cluster conformations with a size between magic numbers result from deformation of symmetrical figures (regular icosahedrons). But atoms themselves always lie within the points of the icosahedral grid. Therefore, a globally optimal structure can be located with atom locations known in advance.

Let us assume that $X_{set} = \{X_1, X_2, ..., X_M\}$, $X_i = (x_i, y_i, z_i)$ is an icosahedral grid for potential locations of atoms of an optimized conformation with a size of $m < M$ (see figure 2). To encode the locations of the optimized cluster’s atoms, we will introduce a bit vector for the $M$ size: $\vec{b} = (b_1, b_2, ..., b_M)$. It is evident that

$$\sum_{i=1}^{M} b_i = m.$$  \hspace{1cm} (4)

Then a problem of structural geometrical optimization can be posed:

$$\nu(\vec{b}) \rightarrow \min_{\vec{b}} x,$$
$$\sum_{i=1}^{M} b_i = m,$$  \hspace{1cm} (5)

where $\nu(\vec{b})$ is the optimization criterion.

Figure 3. Numbering of atoms of the icosahedral structure $X_{set}$.

The structural-optimization problem (5) can be converted to a problem of parameter optimization with the standard information-encoding technique used for genetic algorithms. For that purpose, we will assume that each $S$ string corresponds to the parameter

$$y = \sum_{i=1}^{M} b_i 2^{(M-i)}.$$  \hspace{1cm} (6)

This gives us the problem of one-dimensional parameter optimization

$$\nu(y) \rightarrow \min_{y} x,$$
$$y \in [a, b],$$
$$\sum_{i=1}^{M} b_i = m.$$  \hspace{1cm} (7)
To solve that problem, we will use R. G. Strongin’s characterization method [20]. Without going into detail on the method (for a thorough description, refer to literature), we will mention its main components. The Strongin method [20] realizes the global optimization of continuous, smooth functions of one variable. The search region \([a, b]\) is iteratively split into half-intervals with dots: 
\[y_0 = a, y_1, y_2, ..., y_L = b\]. For each half-interval \([y_i, y_{i+1})\), the characteristic function \(R(i)\) is calculated. As a result, in every further step, a half-interval is selected that has the maximal value of \(R(i)\). That half-interval is then split further. The method’s unique feature is that the value of the characteristic function for each interval is proportional to the posterior probability that the interval holds the global optimum.

The Strongin method makes it possible to reduce notably the initial multidimensional problem of Morse cluster GO (2) toward the problem of one-parameter optimization (6). In the initial optimization problem, the number of parameters was proportional to \(3m\) at \(m > 20\), while currently research is underway to find optimal conformations for \(m > 300\). Such GO problems are of a significantly large scale.

The method, however, is not that simple. In problem (7), parameter \(x\) is not a continuous variable, and because of the limitation \(\sum b_i = m\) it changes discretely. Further, the objective function \(F(x)\) is not even a continuous function. But experiments have shown that the Strongin method fairly quickly locates prospective regions for search for the global extremum of the function \(F(x)\) and, therefore, locates as well favorable initial conformations of Morse atomic clusters. We will proceed from this observation.

Figure 4 is a schematic of the relationship between the problem of global optimization of a function of one variable and the structural optimization of conformations of Morse atomic clusters.

2.4. Parallel GO algorithm
For problem (7), the Strongin method cannot locate the global extremum because of the nuances outlined above. It is, however, easily parallelizable, and the parallelization serves not so much to improve the algorithm’s efficiency as to improve search efficiency.

The Strongin method quickly locates structural configurations of clusters that appear to achieve global optimality. The reason is that during optimization, the high-order bits (high orders of variable \(y\)) of vector \(\nu(b)\) are registered first. For purposes of obtaining search results, optimization must be performed with very high accuracy. This involves actually adjusting the low-order digits of the
variable under optimization to the result—a very inefficient procedure equivalent to complete enumeration. If an initial section is split into \( L \) parts \([a, b]=\bigcup_{i=1}^{L}\left[c_{i}, c_{i+1}\right]\), a search for the global optimum can be conducted on \( L \) processors in parallel, collecting into a separate group all “champions” from each search section \( X_{l} =\{X_{l1}, X_{l2}, \ldots, X_{lL}\} \) and \( X'_{l} =\{\hat{X}_{l1}, \ldots, \hat{X}_{lL}\} \), where \( \hat{X}_{l} \) denotes quasi-optimal conformations in the first optimization phase on the \( j \) th section \( \hat{X}_{j} =\{c_{j}, c_{j+1}\} \).

Depending on optimization accuracy, in each candidate \( \hat{X}_{jk} \) the first \( m \) unit bits of string \( \hat{b} \) can be registered. Then the zero bits to the left of the \( m \)th bit of the number can be deleted. It is evident that these bits will not be used in the further elaboration of the optimal cluster conformation. Thus, we can reduce the length of the bit string by \( m + n_{0} \) units. Here, \( n_{0} \) is the number of zero bits deleted.

The second stage involves considering similar problems for the truncated bit string \( \tilde{b}_{n} = (b_{1}, b_{2}, \ldots, b_{M-m_{n} - n_{0}}) \) and a smaller representation of the variable under optimization (4).

The process is repeated until complete enumeration of reduced bit vectors becomes possible. As a result, we obtain a multitude of initial approximations for optimal conformations \( X^{*} =\{\hat{X}_{1}, \ldots, \hat{X}_{K}\} \).

At the last stage, parallel local optimization can be organized by using the initial approximations from \( X^{*} \). The best result will determine the optimal cluster of a given size.

### 3. Computational experiments

The practicability of the proposed GO method for the most complicated case, \( \rho =14 \), was first tested on simple sample conformations with the number of atoms equal to \( m = 15, 16, \ldots 20 \). It is interesting to note that besides globally optimal conformations, even these simple cases yielded locally optimal conformations that had not been registered in the known Cambridge database [19] or its extension [18]. The results obtained are presented in table 1. Cells listing newly found Morse cluster conformations are shaded in gray.

#### Table 1. Energy levels of optimal Morse clusters for \( \rho = 14 \).

| \( N \) | Energy   | \( N \) | Energy   |
|-------|----------|-------|----------|
| 15C   | -44,806437 | 17E   | -52,822588 |
| 15-1  | -44,8062  | 17-1  | -52,7959  |
| 15D   | -44,087741| 17F   | -52,100584|
| 15B   | -44,08633 | 17D   | -51,837537|
| 16C   | 48,814517 | 17C   | -51,440588|
| 16-1  | -48,8143  | 17B   | -51,329559|
| 16-2  | -48,7878  |       |          |
| 16D   | -48,094020|       |          |
| 16B   | -47,831957|       |          |

Further, globally optimal conformations have been found that contain more atoms than reported in the database [18]. Table 2 presents the results obtained.

#### Table 2. Energy levels of optimal Morse clusters for \( \rho = 14 \) (\( N > 240 \)).

| \( N \) | Energy   | \( N \) | Energy   |
|-------|----------|-------|----------|
| 241C  | -1155,08651| 247C  | -1186,12051|
| 242C  | -1160,10568| 247D  | -1184,3192|
| 243C  | -1166,118587| 260C  | -1254,29839|
| 243D  | -1162,41193| 318D  | -1560,11539|
| 244C  | -1172,13148| 389D  | -1935,87887|
4. Conclusion
This article presents a new method for optimizing Morse clusters. The method is based on the original reduction of the GO problem for multivariable functions to the multextremal optimization of a function of one variable. The proposed method is largely based on genetic-algorithm concepts. First of all, this includes the encoding method we used as well as the reduction of the structural-optimization problem to one of parameter optimization. But instead of conventional genetic operations such as mutation and crossover, we used R. G. Strongin’s method for the global optimization of a function of one variable. This significantly reduced the algorithmic complexity of the problem.

The method’s efficiency can be greatly increased by including in it the evolution patterns identified from known databases for globally optimal conformations of Morse clusters.

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