Some New Methods in the Evolutionary Search of Atomic Cluster Shape

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Abstract. The problem of atomic structure optimization related to the minimization of its total energy is a fundamental physical problem as well as hard computational task. For the few last years we have presented some observations concerning the advantages and drawbacks of EA used as a tool to solve such questions. In this paper we would like to present some new approaches devoted to improve the general, not problem oriented part of algorithm. The results obtained for two techniques: population migration and Opposition-Based Learning show that the specific operators, designed for the given problem are still the most important part of algorithm.

1 Introduction

Recently we have presented the results of evolutionary optimization of nanoscopic systems [1-3]. In these works there were studied atomic structures (model and real) which was described by two and three-body potentials. The most important steps during these study can be presented as follows:

- It was created the efficient evolutionary algorithm, performing the optimization of atomic cluster geometry by the minimization of total energy for such systems.
- The implementation of algorithm was tested on the real material samples (monoatomic metallic clusters Au, Ag, Al, C) with three-body interaction.
- The properties of homonuclear argon clusters doped with single potassium ion were studied for cluster sizes up to 60.
- The method of new doped structures searching by means of modification of relative interaction coefficients was proposed.
- There were presented the properties of noble gas clusters doped with two alkali metal ions (up to 36 atoms) described by the total energy model proposed in work.

Atomic clusters are isolated systems of atoms containing from several to even thousands atoms. In the presented papers the size of cluster, understood as a number of atoms was limited to about 60 ($N \leq 60$). For ($N \leq 40$) the single run was sufficient to obtain correct results however the bigger clusters ($40 < N \leq 60$) optimization was repeated few times, because evolutionary process gets stuck in some local optimum. Thus there is the necessity to increase evolutionary algorithm efficiency.

In order to increase the strength our algorithm we tried use two new methods: Migration of populations[4] and different schemes of Opposition-Based Learning [5].

2 Method and tests

From the theoretical point of view geometrical modeling of atomic clusters consists of finding the atoms arrangement with global minimum (GM) of total binding energy which can be found on potential energy surface (PES) , an 3N hypersurface in 3N+1 dimensional space, where N is the number of atoms. The determination of total energy could be realized by *ab initio* molecular theory (like density functional or Hartree-Fock method), molecular dynamics, or analysis of 2 and 3-body potentials describing atomic interactions.

In this paper we show results of evolutionary optimization of 6-atomic clusters described by 2-body Lennard-Jones(L-J) potential. The method of determine the minimum energy is described in detail in our previous papers [1-3].

Because the algorithm is sensitive for the shape of fitness function, its choice is of special importance. In our problem we selected fitness function in exponential form [6]:

$$f(V) = e^{-b\frac{V - V_{\min}}{V_{\max} - V_{\min}}}, \tag{1}$$

where: V - is binding energy of cluster, V_{min} and V_{max} are the lowest and the highest total energy in population, and parameter b - determines the selectivity of the fitness function (b=1 in our work).

In the case of sharp L-J potential the number of candidates for local energy minima on the PES grows exponentially with the number of atoms (according to $exp(0,36N+0,03N^2)$, N is cluster size [7]).

In this work we tested 6-atoms clusters described by L-J potentials, thus we split PES into 4 parts: basin of attractions of global, second and third minima. Optimal energy values from these basins represents structures of atoms which are shown on the Fig. 2. Fourth part of the PES contains all remaining regions corresponding to the systems with low symmetry.

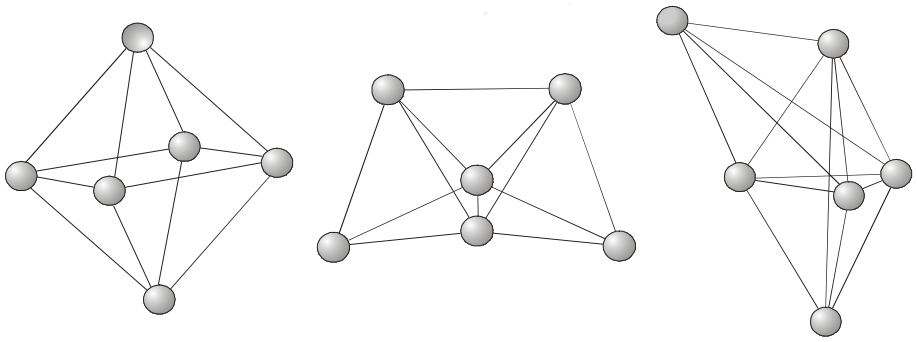

Figure 1. The structures of clusters correspond to global, second and third optimum on the PES.

In order to determine the size of these four regions on the PES we combine method of random search (Monte Carlo) with local optimization (Steepest Descent). The relative percentage of them on the PES shown on the Fig. 3.

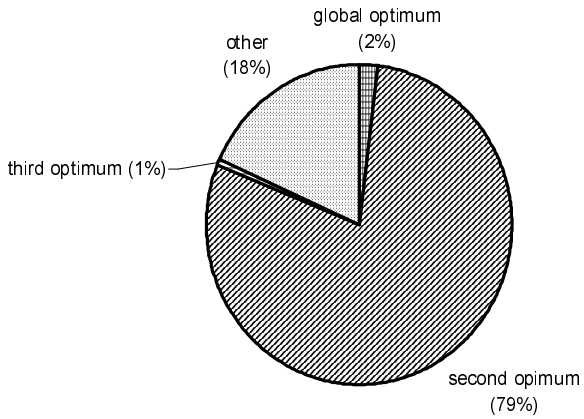

Figure 2. Distribution of global, second, third minimum and others for the PES of 6-atomic clusters.

On the basis of this diagram we can see that the basin of second optimum covers considerable area of PES (it is almost *80%* of whole Potential Energy Surface). The region of global optimum covers only *2%* of PES. This situation leads to premature convergence to local optimum in global optimization problem (that means deceptive problem).

3 Migration of populations method

In this part of work we used algorithm without crossover. Set of task parameters is represented using floating point numbers [8], where each coordinate of the atoms is real number from the range (0,1). For 6-atoms cluster genetic algorithm has to optimize 18-variables function and make evolution process on 20 individuals during 10000 generation.

In our algorithm the reproduction with selection is classical roulette wheel method. The mutation is the uniform mutation with Gauss distribution. We carried out series of 100 independent evolutionary processes for various standard deviations of Gauss function. The situation, when after mutation, the point would be removed from the simulation box was forbidden and the mutation was simply repeated. The averaged quantities of individuals in each optimum basin of attraction during evolutionary process are shown in Fig.3. It means the percentage quantities of individuals in whole population size (*pop_size*) in the function of the age of population drawn in logarithmic scale. This manner makes possible to observe the distributions change in the beginning of evolutionary process.

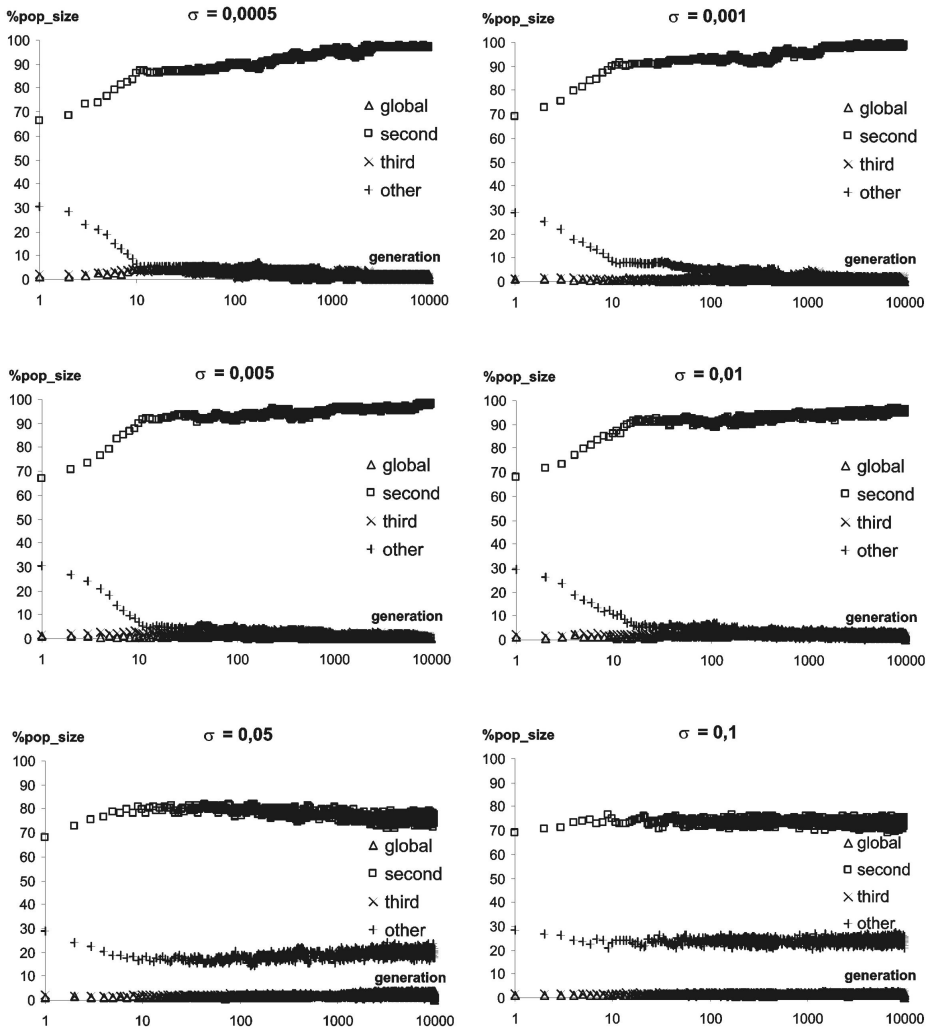

Figure 3. Evolutionary process for various mutation rate.

On the basis of Fig. 3 we can see that, as anticipated, second optimum plays dominant role. The relative number of second optima still grows during the whole evolutionary process. This situation is clearly visible for small range of mutation. For bigger values of deviations distributions are uniform. The decrease of second optimum number is for this case connected with the increase of only one of another groups, this one containing all less important minima (called "other"). Global optimum in the all cases is on the level *1% pop-size*. For all mutation rates the average values of total energy in evolutionary process are shown on the Fig. 4.

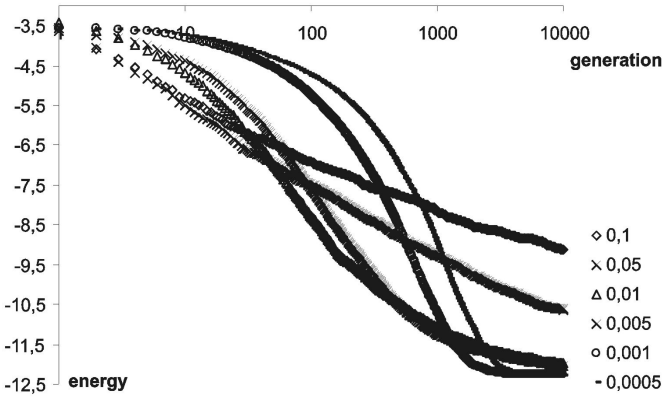

Figure 4. Total energy in evolutionary process for all mutation rates

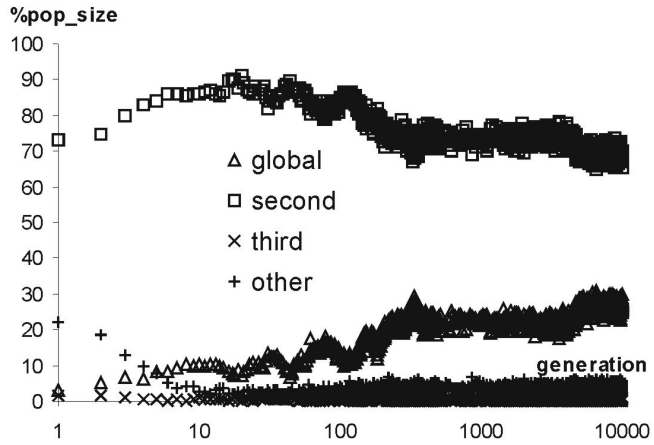

Figure 5. Evolutionary process for the best configuration.

4 Opposition-Based Learning

In order to accelerate the convergence process to global optimum we used new method, called Opposition-Based Learning. This idea was introduced first time as new scheme for machine intelligence[5]. Opposition-Based Learning is based on opposite number definition where: $P(x_1, x_2, ..., x_n)$ is a point in dimensional space ($x_1, x_2, ..., x_n \in R$ and $x_i \in [a_i, b_i]$, $i = 1,2,..., D$). The opposite point of *P* is defined by $\breve{P}(\breve{x}_1, \breve{x}_2, ..., \breve{x}_n)$ where:

$$\breve{x}_i = a_i + b_i - x_i, \tag{2}$$

In our work we used Opposition-Based Learning on two schemes:

– Opposition-Based Population Initialisation, where process of coordinates replacement with opposite points was carried out only for randomly selected individuals in initial

population. Two detailed approaches were used. According to the first one (improving scheme) the replacement was performed only when it led to the better energy. In the second approach (random scheme) energy evaluation wasn't performed and the change was always accepted.

- Opposition-Based Generation Jumping. The EA was modified in such away that during each generation some individuals have the chance to jump to opposite population with probability defined by jumping rate(JR). The replacement occurred also in two manner: in order to improve energy or with random scheme .

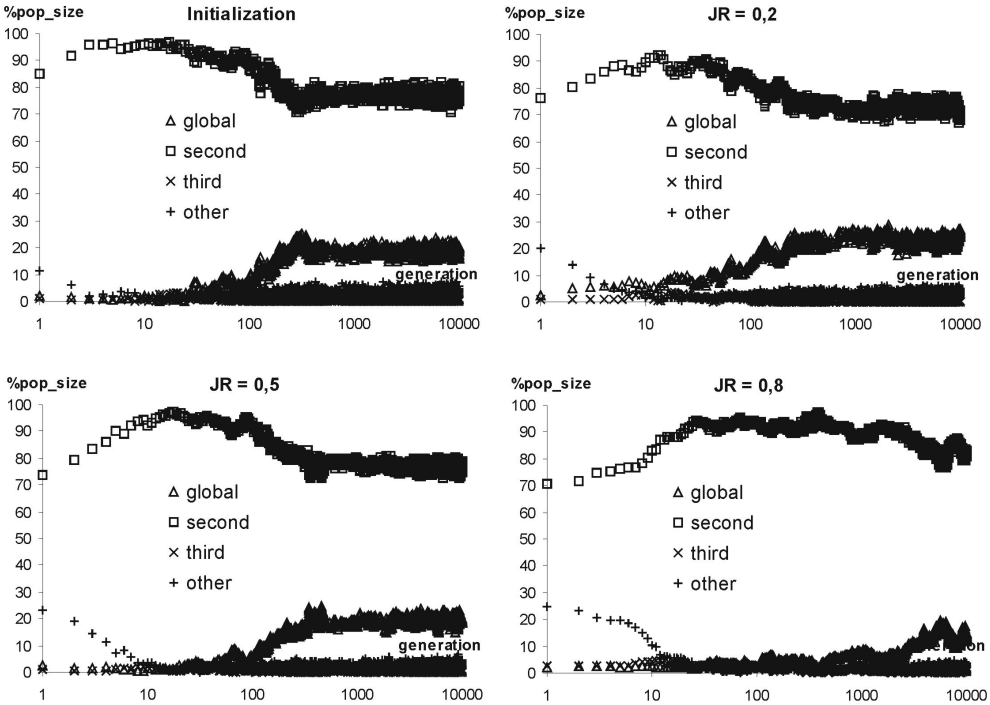

Figure 6. Evolutionary process with various jumping rates and Opposition-Based Population Initialisation.

In this part we carried out series of 100 independent evolutionary processes for various values of jumping rate and for Opposition-Based Population Initialisation. The averaged quantities of individuals in each optimum basin of attraction during evolutionary process are shown in Fig.6.

During the next calculations we tried to determine the percentage factor of reaching the GO in pure evolutionary process and enriched with Opposition-Based Learning in 10000 generations.

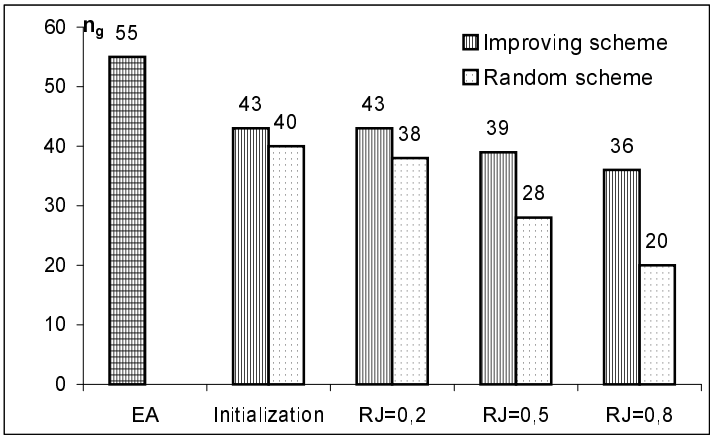

Figure 7. Percentage number of iteration needs to receive the global optimum in evolutionary process and EA with Opposition-Based Learning.

The last section shows how what the Opposition-Based Learning cooperated with evolutionary algorithm with local optimization method (hybrid evolutionary algorithm[1]). Calculations results are presented on figure 8, where is index of population (which can be understood as its age) in which the evolutionary algorithm supported by Steepest Descent[1] local optimization found the global optimum for the first time as t_g.

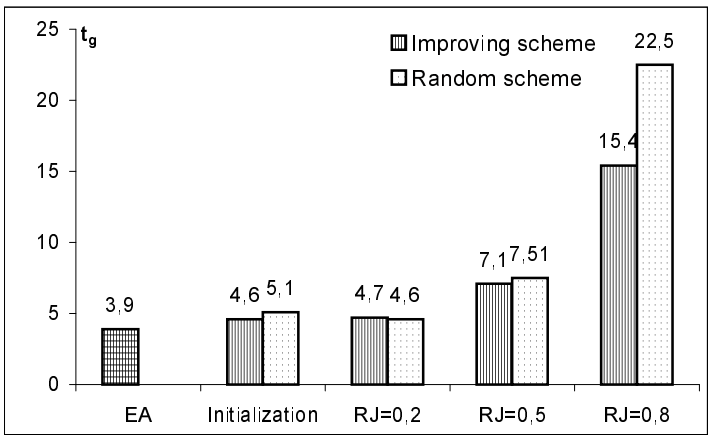

Figure 8. Average values of generation t_g in which the hybrid evolutionary algorithm with Opposition-Based Learning found the global optimum for the first time.

5 Conclusions

In the present paper we showed the effects of newly proposed evolutionary optimization techniques on the computationally hard problem of atomic cluster energy minimization. In our previous papers we pointed out that pure computational attempt isn't efficient tool to solve such a problem. However, with the inclusion of some special operators, like z-sorting,

rotations or mass center shift [1] it used to find very quickly the basin of attraction of global minimum. Unfortunately, with the new operators the general remark about the need to use some special operators should be sustained.

With the population migration algorithm, independently on the mutation range value the algorithm undergoes premature convergence to the local optimum which spreads over large region of PES. For the small mutation ranges the stagnation begins already after about 1000 generations. For the larger ones the population migrates between the basins of attraction of different local minima but the overall influence of this process on the global minimum search is negative. The proof of this is visible in fig.4 where the best obtained energy value averaged over 100 independent runs is presented in the function of generation index. It may be observed that larger mutation range causes the improvement only in the beginning of the diagram and in further part the efficiency significantly decreases.

The similar conclusion should be made when speaking about the Opposition-Based Learning. Indeed we choose this method with the hope that it increases the diversity of population, what is the crucial factor in atomic modeling. The comparison of figures 5 and 6 shows almost ideal compatibility between the shape of curves for the same basin of attraction. Moreover, independently on the shape of these dependencies which describe the general properties of algorithm we can look at the most wanted feature ie. how fast the optimum can be reached. Here, the results are significantly worse especially when the jumping rate increases. This results shows the role of worse adapted individuals in the population. Although it seems that they have very low significance and the probability of their promotion to the next generation is almost negligible, their genetic material is very significant and its worsening causes significant decrease of algorithm efficiency.

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