# The search for minimum potential energy structures of small atomic clusters. Application of the ant colony algorithm[*]

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The ant colony algorithm has been applied to the problem of finding the minimal potential energy configuration of a small physical system (cluster) of atoms interacting via the Lennard–Jones phenomenological potential. The ants were positively motivated if their activity (displacement of atomic positions) leads to a lower total potential energy of the system. Starting from a random spatial distribution of atoms, during the optimization process, the ants were able to find configurations with energies much lower than the initial ones. The optimized configurations generated by the ant colony algorithm can be used as a good starting point for classical or *ab initio* molecular dynamics (MD) simulations.

Key words: *ant colony algorithm; cluster; potential energy; computer simulations*

## 1. Introduction

The ant colony algorithm has been widely used to solve more and more problems including the famous Travelling Salesman Problem [1, 2], Vehicle Routing Problems [3], etc. The main idea of this algorithm is to duplicate the way the ants search for food and transport it to the ant-hill (using pheromone traces). In other words, it is an adaptation of the natural search behaviour of ants in an ant colony. Usually, at the beginning, the ants use, or try, many random paths. However, after some time – due to mutual exchange of information in the ant society achieved by chemical tracing (pheromone) – a particular path becomes the most preferred, i.e. there is the highest concentration of pheromone on this chosen track. The application of the ant colony algorithm to the important problem of searching for the minimal potential energy configuration of a physical system of interacting atoms is shown.

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## 2. Search procedure

The physical system of interest is a cluster composed of $n$ identical atoms embedded in a cubic box of edge length $a$. To be more specific, let us consider they are argon (Ar) atoms and $n = 7$. The interaction potential $V(r_{ij})$ between a pair of argon atoms is well described by the Lennard–Jones (LJ) equation [4]

$$V(r_{ij}) = 4\varepsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6} \right]$$

where $r_{ij}$ is the distance between an $i$th and $j$th atom. The total potential energy of the system is

$$\varphi = \sum_{i,j=1,j>i}^{n} V(r_{ij})$$

The LJ potential parameters $\varepsilon$ and $\sigma$ for argon are given in Table 1 [5], where $k_B$ is the Boltzmann constant.

Table 1. The Lennard–Jones parameters for argon

| Atoms | $\varepsilon/k_B$ [K] | $\sigma$[Å] | m [$10^{-25}$ kg] |
|-------|-----------------------|-------------|-------------------|
| Ar    | 119.8                 | 3.4         | 0.664             |

The number of ants has been chosen as equal to the number of atoms (interacting sites). The initial position $\mathbf{r}_i = (x_i, y_i, z_i)$ of the $i$th atom has been randomly chosen within the range $[0,a]$ for each component of $\mathbf{r}_i$. In case the positions of neighbouring atoms were too close to each other, the drawing process for these atoms was repeated. This ensures that the system does not explode accidentally. The centre of mass $\mathbf{R}_{CM}$ of the system was calculated. The ants were positively motivated by three factors: pheromone value, drawing the positions of the atoms towards the centre of mass and most importanly, decreasing of the total potential energy. The positions of $n$ atoms can be represented by a graph in three-dimensional space. The vertices of this graph are Ar atoms. Each ant draws one graph's vertex (pick up an atom). Following the ant algorithm procedure [6], the pheromone matrix for this initial configuration must be defined. The pheromone matrix is composed of a pair $(i, j)$ of coefficients characterising the attractiveness of the $(i, j)$ connection (edge) between the $i$th and $j$th vertex of the graph. Since at the begining no ant knows more or less than any other, all coefficients of the pheromone matrix are initialized by the same value $\tau$ between [0,1].

After establishing the initial conditions, the algorithm described starts. This means the first ant randomly moves the position of one of the $n - 1$ atoms (excluding the atom it is associated with) and the Lennard–Jones potential for this perturbed configu-

ration is calculated and memorized. Then the ant puts the just moved atom to its previous position and randomly moves the next one of the $n - 2$ atoms. The LJ potential for this system is again calculated and memorized. The ant applies the same procedure to the remaining $n - 3$ atoms, etc. The described procedure is repeated by all ants.

Now, each ant knows $n - 1$ potential energies (configurations) corresponding to the random displacements of all vertices of the graph (atoms), except the one where the ant actually remains. To consider next move the ant can use one of two possibilities distinguished by a real number $q_0$ ($q_0 \in [0...1]$), which is supplied in the set of the starting parameters (see Table 1). The algorithm randomly draws a number between 0 and 1 and compares it to $q_0$. If this number is smaller than $q_0$, the first possibility is to find a local best minimum [6] defined by the formula:

$$S(i, j) = \arg \max\{[\tau(i, j)][\eta(i, j)]^{\beta}\}$$

where $\tau(i, j)$ is the pheromone coefficient between the $i$th and $j$th vertical (atom), $\eta(i, j) = 1/\varphi$, where $\varphi$ is the total potential energy of the system in which only the position of ($j$th) atom has been changed, $\beta$ is a heuristic parameter which determines the relative importance of the pheromone versus the atomic displacement ($\beta > 0$). The ant will chose the configuration for which the calculated value S($i,j$) is the largest, denoted here by argmax. The other possibility (when the randomly drawn number is larger than $q_0$) is to construct the matrix of probabilities

$$p(i, j) = \frac{[\tau(i, j)][\eta(i, j)]^{\beta}}{\sum [\tau(i, j)][\eta(i, j)]^{\beta}}, \qquad 0 \le p(i, j) \le 1$$

The value of $p(i, j)$ is larger if the LJ potential energy is lower and the pheromone value between the $i$th and $j$th vertex is larger. By definition, the sum over $j$ of $p(i, j)$ must be equal to 1 for any fixed $i$. For fixed $i = i_0$, each $p(i_0, j)$ can be associated with a particular segment from the [0, 1] range. The sum of these segments must be equal to 1 and the whole [0, 1] range is filled. The larger segment of [0, 1] range is associated with the larger $p(i_0, j)$. Then a real number beetwen 0 and 1 is randomly generated, this value falls into one of the segments associated with $p(i_0, j)$, and for that matter with one of the vertices $j$. If the random number indicates the $p(i_0, j')$ segment of [0,1], the vertex to be chosen is $j'$.

Before the algorithm step is completed, the local pheromone update is required, i.e. each ant between $t$, $t + 1$ step, lays a quantity of pheromone on the edge connecting $i$th and $j$th vertices (in our case $i_0$ and $j'$ vertices), following the formula [7]:

$$\Delta\tau_{(i,j)}(t, t+1) = (1 - \rho)\tau_{(i,j)}(t) + \rho k \tau_0 \tag{1}$$

where $k$ is the number of ants that visited the same atom ($i$) and all of them moved another atom ($j$), $\rho$ is a real number between <0,1> which takes care of the intensity of pheromone [7]. The applied ant algorithm parameters are given in Table 2.

Table 2. The applied algorithm parameters

| Parameter symbol | Value |
|:---:|:---:|
| $\beta$ | 5 |
| $q_0$ | 0.65 |
| $\rho$ | 0.23 |
| $\tau_0$ | 1 |

What has been described is one step of the algorithm. The next steps would be essentially similar except that the ant cannot move the vertices already moved in the previous steps. Hence, the total number of steps in the cycle cannot be higher than the number of vertices (atoms) minus one.

At the end of each cycle (composed of maximum $n - 1$ steps), the global pheromone update is performed. This means that the most effective attempt (displacement of atoms) which leads to the lowest LJ potential energy during the cycle, will be marked by an additional amount of pheromone. The formula for global pheromone update is given by [6]:

$$\Delta\tau_{(i,j)}(t, t+z) = (1 - \rho')\tau_{(i,j)}(t) + \rho'\tau_{0(i,j)}(t, t+z)$$

where $\rho'$ has the same meaning as $\rho$ in Eq. (1), $z$ is the sum of steps in a cycle. The most effective try will be used as a starting point for a new cycle.

The number of cycles can be very large, the finite number of cycles is called an experiment. For the interpretation we used the average of many experiments.

# 3. Results

Calculations were performed for a small cluster composed of $n = 7$ argon atoms. Figure 1 shows an example of the initial (randomly chosen) configuration of atoms located in a cubic box (the length of edge $a = 3$ *nm*).
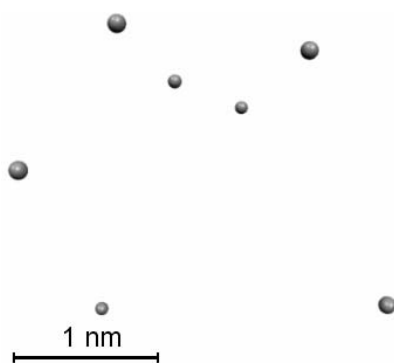


1 nm

Fig. 1. The snapshot of the starting
configuration of $Ar_7$ cluster ($a = 3$ nm)

Several values of *a* have been used for testing the effectiveness of the alghorithm. A natural physical criterion for a stable equilibrium structure is the requirement of minimum potential energy in the system. Guided by this, the ant colony optimalization procedure has been performed. The evolution of potential energy *V* of the $Ar_7$ cluster averaged over $10^3$ experiments as a function of the number of cycles is given in Fig. 2, for several sizes of the cubic box.
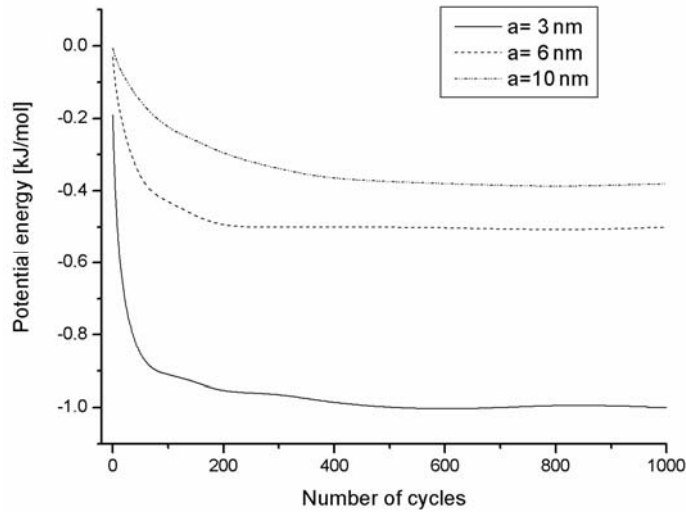
Fig. 2. The average values of the potential energy of $Ar_7$ cluster (*a* = 3, 6, 10 nm)
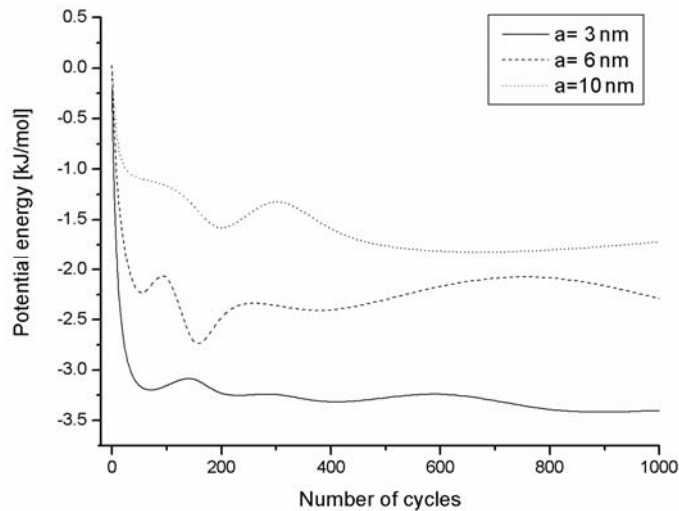
Fig. 3. Examples of potential energy of $Ar_7$ cluster (*a* = 3, 6, 10 nm)

The quick relaxation of *V* towards the required (lower) value can be seen, followed by the saturation. Performing more cycles in the saturation area does not seem

to be effective. The saturated potential energy does depend on the size of the box. The start of optimization procedure in a smaller box leads to a substantially lower energy. Making the box too large generates too many configurations to be checked and the algorithm has the tendency to stop at the local minimum. It is not believed that this type of weakness of the ant algorithm in this context has been reported. Figure 2 shows the average of $10^3$ experiments. Figure 3 presents an example of single optimization (non averaged) which is much better as it shows a lower potential energy than the averaged one. The differences between single optimization could be quite substantial and in Fig. 4 the comparison of two extreme optimizations for $a = 3$ $nm$ is shown.
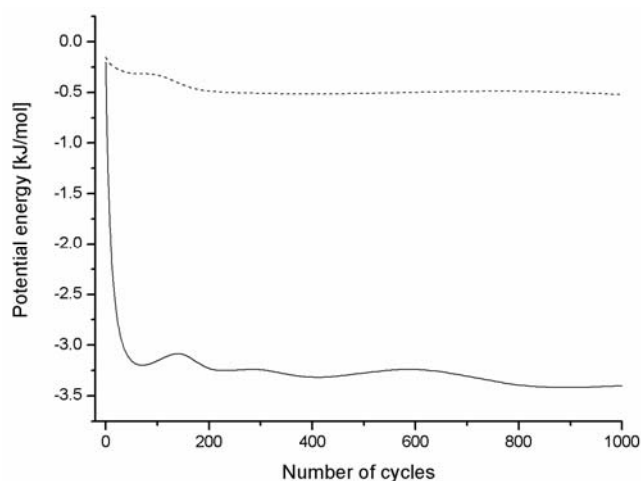


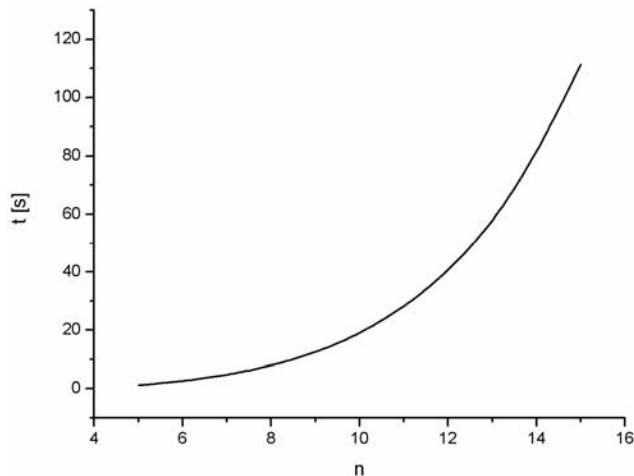Fig. 4. The comparison of two extreme optimalizations of Ar$_7$ ($a = 3$ nm)



Fig. 5. The calculation time of one cycle of optimization for Ar$_n$ clusters
($n = 5, 7, 10, 13, 15$; $a = 3$ nm; CPU AMD Athlon 2GHz)

It was found that the calculation time $t_c$ required for one cycle was dependent on the number $n$ of atoms in the cluster. This is illustrated in Fig. 5, $t_c$ increases rapidly, non-linearly, with the growing number of atoms.
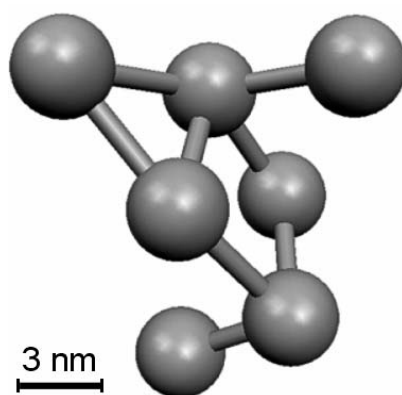


Fig. 6. The snapshot of optimized configuration of $Ar_7$ cluster ($a = 3$ nm)

The final cluster's configuration obtained from the initial positions of argon atoms (shown in Fig. 1) is given in Fig. 6.

# 4. Conclusions

Although the authors cannot guarantee that this is the structure corresponding to the global minimum of potential energy, the increased level of condensation (packing) of the cluster is evident. That was the configuration looked for at the beginning of molecular dynamics or Monte Carlo simulations of the clusters. Starting from this, partially optimized configuration could save computer time for calculations which are solely based on laws of physics (for example molecular dynamics (MD) simulations). This study shows that the ant colony algorithm could be implemented into MD programs as a helpful tool for establishing a reasonable starting configuration. Unfortunately, without additional conditions, one should not expect the ant colony algorithm to guarantee finding the global minimum of potential energy.

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