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An adaptive immune optimization algorithm for energy minimization problems

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Based on the immune theory of biology, a novel evolutionary algorithm, adaptive immune optimization algorithm (AIOA), is proposed. In AIOA, density regulation and immune selection is adopted to control the individual diversity and the convergence adaptively. By an application of the algorithm to the optimization of test functions, it is shown that the algorithm is a highly efficient optimization method compared with other stochastic optimization methods. The algorithm was also applied to the optimization of Lennard-Jones clusters, and the results show that the method can find the optimal structure of $N \leqslant 80$ with a very high efficiency. The proposed algorithm may be a good tool for fast global optimization in chemical or biological molecular simulations.
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I. INTRODUCTION

Global optimization is one of today's rapidly growing fields of science with many important applications. In general, the global optimization of an arbitrary function requires a search through the whole configurational space. The problem is nondeterministic polynomial-time (NP)-hard due to the fact that the space grows exponentially with the problem size. Determination of global energetic minima of large molecular or atomic clusters is a NP-hard problem. To solve the problem, many optimization methods have been proposed, such as genetic algorithms (GAs),[1–3] simulated annealing (SA),[4–6] basin-hopping method,[7,8] fast annealing evolutionary algorithm (FAEA),[9,10] random tunneling algorithm (RTA),[11] quantum annealing,[12] potential deformation,[13] and hierarchical search,[14] etc.

In recent years, the study on the novel algorithms based on biological immune mechanisms has become an active research field.[15–21] The biological immune system is an efficient natural protection system that can generate multiple antibodies from antibody gene libraries and keep it alive even if the foreign pathogens is unknown. The primary immune theory model is the regulation theory of the biological immune system, which includes immune density regulation mechanism and network regulation mechanism.[22,23] The theory shows that the biological immune system can regulate the generation of antibodies and balance the quantity of the multiple kinds of antibodies. When antigens invade, the antibodies that match these antigens are activated and generate more antibodies to restrain the antigens. Then the immune system reaches a new balanceable state.

In this paper, an adaptive immune optimization algorithm (AIOA) is proposed. Based on the density regulation mechanism and the immune selection mechanism, the algorithm can adaptively balance individual diversity and convergence speed. In order to evaluate the algorithm, a set of standard test functions were used and the results were compared with some other stochastic methods. We also applied the algorithm to the optimization of Lennard-Jones (LJ) clusters.[24–26] It is shown that the algorithm is a good tool for energy minimization problems.

II. METHODS

A. Adaptive immune optimization algorithm (AIOA)

Genetic algorithms (GAs) are known as a new kind of optimization technique for tackling complicated optimization tasks.[27,28] A population of random bit (or digital) strings is used for staring solution trails. Then, a circular process of evaluation, selection, recombination, and mutation is repeated to yield an optimized solution.

AIOA adopts the basic frame of GAs, and regards the evolution individuals as antibodies and the increment of population fitness as the antigen. It controls the recruitment of antibodies according to the immune density regulation mechanism at a genetic operation level and reaches its dynamic balance according to the immune selection mechanism. Therefore, whenever the population fitness changes, the system is dynamic balance between the population convergence and the diversity.

Like GAs, the local search ability of AIOA is not so strong, so a highly efficient local search method, called limited memory quasi-Newton algorithm (L-BFGS),[29] is adopted for local minimizations.

The density regulation is a key essence of designing the proposed algorithm. In the regulation, the density of the antibody can be denoted by the affinity,[15] which can be calculated by information entropy.[15] As shown in Fig. 1, supposing there are N antibodies, the coding length of each antibody is L, the size of symbolic aggregate is S, then the information entropy $H_j(N)$ of the antibody gene located at position j can be defined as

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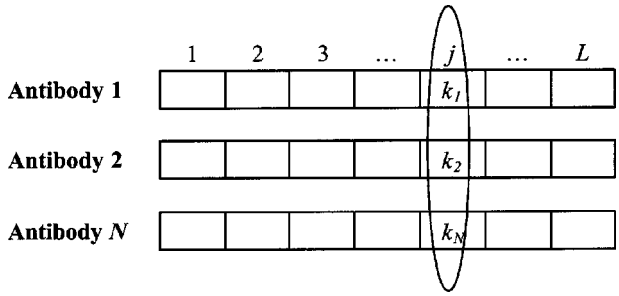

FIG. 1. Concept of information entropy.

$$H_j(N)=\sum_{i=1}^{S} -p_{ij}\log p_{ij}, \tag{1}$$

where p_{ij} is the probability of the ith symbol appearing on the gene location j. Thus the average colony entropy $H(N)$ can be obtained by

$$H(N)=\frac{1}{L}\sum_{j=1}^{L} H_j(N). \tag{2}$$

According to the concept of entropy, the affinity, or similarity, between antibody u and v can be defined as $A_{u,v}$

$$A_{u,v}=\frac{1}{1+H(2)}, \tag{3}$$

where $H(2)$ is the information entropy between two antibodies u and v. In this study, binary coding method is adopted, thus the size of symbolic aggregate is 2, $H_j(2)$ can be summarized as

$$H_j(2)=\begin{cases} 0 & u_j=v_j \\ \log 2 & \text{otherwise}, \end{cases} \tag{4}$$

where u_j and v_j are the value of gene location j of antibody u and v, respectively, which are 0 or 1.

With $A_{u,v}\in(0,1)$, the greater the value of $A_{u,v}$, the greater the affinity and similarity between the antibody u and v. If $A_{u,v}=1$, then the gene codings of u and v are the same. Therefore, the density of the antibody u, C_u, can be defined as

$$C_u=\frac{1}{N}\sum_{v=1}^{N} ac_{uv}, \tag{5}$$

where

$$ac_{uv}=\begin{cases} 1 & A_{u,v}\geqslant Tac \\ 0 & \text{otherwise}, \end{cases}$$

and Tac is a threshold. Therefore, the antibody density, C_u, is the proportion of the similar antibodies in the population.

After calculating the density of each antibody, the regulation of activating and suppressing of antibodies can be achieved by immune selection mechanism. On the base of the traditional selection mechanism of the fitness proportion, by increasing the regulation probability factor based on density, the selection probability of individual v, e_v, is determined by two sections, the fitness and the density,

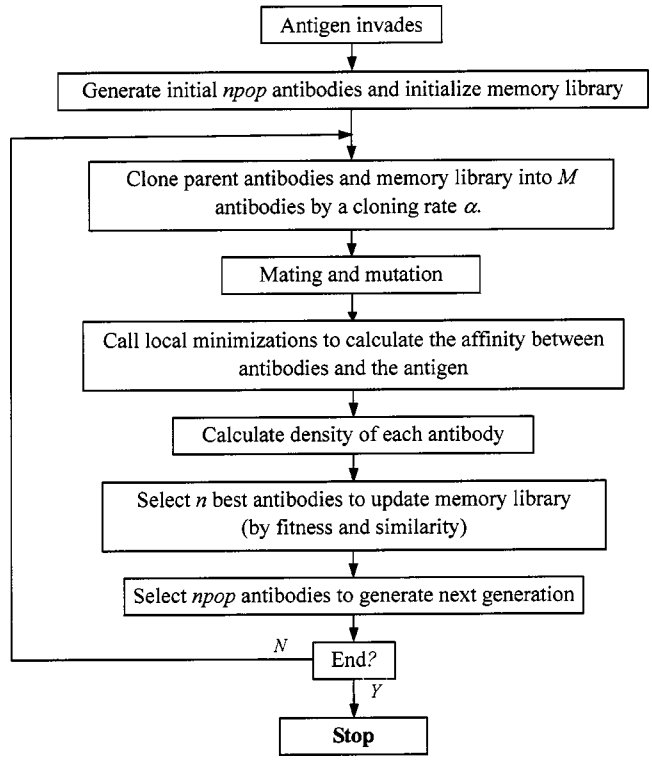

FIG. 2. Flowchart of the adaptive immune optimization algorithm (AIOA).

$$e_v=\frac{\text{fit}(v)}{C_v}. \tag{6}$$

This equation indicates the greater the individual fitness, the higher the selection probability it possesses; the greater the density of an antibody, the lower the selection probability it possesses. Thus AIOA cannot only maintain the individuals of high affinity, but also guarantee the diversity.

B. Flowchart of AIOA

Figure 2 shows the flowchart of the proposed AIOA, which includes the following steps:

(1) Antigen invades, which means a problem to be solved.
(2) Initialize *npop* solutions stochastically to generate initial parent antibodies A_1, where *npop* is population size. And initialize *msize* antibodies stochastically to compose memory library, where *msize* is the size of memory library.
(3) Perform clone operation on the kth *npop* parent antibodies (A_k) and memory library to obtain M antibodies (B_k) simply by a cloning rate α. The size of B_k is $M=a*(npop+msize)$.
(4) Perform mating operation on B_k to obtain C_k by a mating rate $materate\in(0,1)$, then perform mutation operation on C_k to obtain D_k by a mutation rate $mutrate\in(0,1)$.
(5) Evaluate each individual of D_k by the local search procedure L-BFGS and obtain the affinity between each antibody and the antigen, which is defined as the value of the evaluation function. For minimization of functions, the function itself can be directly used as the evaluation

function. For optimization of Lennard-Jones clusters, the evaluation function is LJ potential energy[30] as in Eq. (7),

$$V(r)=4\epsilon\sum_{i=1}^{n}\sum_{j>i}^{n}\left(\left(\frac{\sigma}{r_{ij}}\right)^{12}-\left(\frac{\sigma}{r_{ij}}\right)^{6}\right), \tag{7}$$

where r_{ij} represents the distance between each pair of atom (i,j), which can be determined by the position of each atom, and the values of ϵ and σ used in this study are 1.

(6) Calculate the density C_i of each individual with Eqs. (1)–(5).

(7) Replace the antibodies in the memory library with those in D_k whose fitness is higher than that of the former one, and keep the affinity between individuals in memory library lower than the threshold Tac.

(8) Based on the selection probability (e_v) given by Eq. (6), perform immune selection operation on D_k to obtain *npop* antibodies to compose next parent antibodies A_{k+1}.

(9) If the global minimum is obtained or the iteration reaches the preset number *maxit*, stop the calculation. Otherwise, go to step (3).

III. RESULTS AND DISCUSSION

A. Minimization of test functions

To evaluate the performance of the AIOA, it is applied to the minimization problems of several multidimensional test functions with multiple minima.[31] The test examples used in this study are listed below.

$f1$. Hartman's function:

$$-\sum_{i=1}^{4} c_i \exp\left(-\sum_{j=1}^{n} a_{ij}(x_j-p_{ij})^2\right),\quad 0\leqslant x_j\leqslant 1.$$

It has four local minima, one of which is a global minimum $f_{\min}=-3.8627$ for $n=3$, and global minimum $f_{\min}=-3.3223$ for $n=6$.

$f2$. Rastrigin's function:

$$nA+\sum_{i=1}^{n}[x_i^2-A\cos(2\pi x_i)],\quad A=8,\quad -5.12\leqslant x_i\leqslant 5.12.$$

The test function is highly multimodal. It has more than 50 local minima for $n=2$, one of which is a global minimum at $x_i=0$ with $f_{\min}=0$.

$f3$. Schwefel's function:

$$-\sum_{i=1}^{n} x_i\sin(\sqrt{|x_i|}),\quad -500\leqslant x_i\leqslant 500.$$

It has next best local minima at $x_i=420.9687$, $i=1,...,n$, $i\neq j$, $x_j=-320.5232$, which are from its global minimum at $x_i=420.9687$ with $f_{\min}=-n\times 418.982887$.

$f4$. Griewank's function:

$$\sum_{i=1}^{n} x_i^2/4{,}000-\prod_{i=1}^{n}\cos(x_i/\sqrt{i})+1,\quad -600\leqslant x_i\leqslant 600.$$

It has many widespread local minima, one of which is a global minimum at $x_i=0$ with $f_{\min}=0$.

$f5$. Goldstein–Price's function:

$$(1+(x_1+x_2+1)^2(19-14x_1+3x_1^2-14x_2+6x_1x_2+3x_2^2))$$
$$\times(30+(2x_1+3x_2)^2\times(18-32x_1+12x_1^2+48x_2$$
$$-36x_1x_2+27x_2^2)),\quad -2\leqslant x_i\leqslant 2.$$

It has four local minima, one of which is a global minimum at $x_1=0$, $x_2=-1$ with $f_{\min}=3$.

$f6$. Camelback function:

$$4x_1^2-2.1x_1^4+x_1^6/3+x_1x_2-4x_2^2+4x_2^4,\quad -5\leqslant x_i\leqslant 5.$$

It has six local minima, two of them are global minimum $f_{\min}=-1.0316285$.

$f7$. Function f_{11} in Ref. 32:

$$(\pi/n)\left\{k_1\sin^2(\pi y_1)+\sum_{i=1}^{n-1}(y_1-k_2)^2\right.$$
$$\left.\times[1+k_1\sin^2(\pi y_{i+1})]+(y_n-k_2)^2\right\},$$

where $y_i=1+(x_i+1)/4$, $k_1=10$, $k_2=1$, $-10\leqslant x_i\leqslant 10$.

When $n=3$, it has 5^3 local minima, one of which is a global minimum at $x_i=-1$ with $f_{\min}=0$.

$f8$. Function f_{12} in Ref. 32:

$$k_3\left\{\sin^2(\pi k_4x_1)+\sum_{i=1}^{n-1}(x_i-k_5)^2[1+k_6\sin^2(\pi k_4x_{i+1})]\right.$$
$$\left.+(x_n-k_5)^2[1+k_6\sin^2(\pi k_7x_n)]\right\},$$

where $k_3=0.1$, $k_4=3$, $k_5=k_6=1$, $k_7=2$, $-5\leqslant x_i\leqslant 5$.

When $n=5$, it has 15^5 local minima, one of which is a global minimum at $x_i=1$ with $f_{\min}=0$.

$f9$. Shubert's function:

$$\left\{\sum_{i=1}^{5} i\cos[(i+1)x_1+i]\right\}$$
$$\times\left\{\sum_{i=1}^{5} i\cos[(i+1)x_2+i]\right\},\quad -10\leqslant x_i\leqslant 10.$$

It has 18 global minima with $f_{\min}=-186.7309$.

$f10$. Branin's function:

$$\left(\frac{5x_1}{\pi}-\frac{5.1x_1^2}{4\pi^2}+x_2-6\right)^2+\left(10-\frac{10}{8\pi}\right)\cos x_1+10,$$
$$-5\leqslant x_1\leqslant 10,\quad 0\leqslant x_2\leqslant 15.$$

It has three global minima at $(-\pi,12.275)$, $(\pi,2.275)$, $(3\pi,2.475)$ with $f_{\min}=5/(4\pi)$.

The examples were tested within a tolerance 10^{-6} for the function evaluation. In optimization of $f1-f10$, the following values of the parameters are used: *npop*$=10$, cloning rate $\alpha=2$, *msize*$=4$, *Tac*$=0.90$, *muterate*$=0.01$, *materate*$=0.8$ and *maxit*$=200$. The stop criterion of AIOA for each function is $|f-f_{\min}|<10^{-6}$. The results of AIOA optimization of the test functions listed in Table I are the average outcome of 100 continuous runs, in which the performance

TABLE I. Number of function evaluations in global optimization of ten test functions by AIOA and other stochastic global optimization methods.

Function, dimension	PRS[a]	SA1[b]	SA2[c]	EA[d]	IA[e]	TUN[f]	TS[g]	MAG[h]	FAEA[i]	AIOA[j]
$F1$, $n=3$	5 280	3 416	1459	3416			508		488	68
$F1$, $n=6$	18 090	3 975	4648				2845		2229	156
$F2$, $n=2$	5 964			2408			540		544	1 128
$F2$, $n=5$								9 000	2762	5 506
$F3$, $n=2$								8 787	680	806
$F3$, $n=5$								13 000	3848	4 180
$F4$, $n=2$								29 251	7804	10 616
$F5$, $n=2$	5 125	5 439	563	460			486		490	113
$F6$, $n=2$		10 822			326	1 469			303	150
$F7$, $n=3$								5 509	503	235
$F8$, $n=5$								37 000	1006	6 405
$F9$, $n=2$	6 700	241 215	780		7424	12 160	727	7 200	446	483
$F10$, $n=2$	4 850	2 700	505	430	1354		492		394	30

[a]PRS: Pure random search (Ref. 33). Results are from Ref. 9.
[b]SA1: Simulated annealing based on stochastic differential equations (Ref. 34). Results are from Ref. 9.
[c]SA2: Simulated annealing (Ref. 34). Results are from Ref. 9.
[d]EA: Evolution algorithm (Ref. 35). Results are from Ref. 9.
[e]IA: Interval arithmetic technique (Ref. 36). Results are from Ref. 9.
[f]TUN: Tunneling method (Ref. 37). Results are from Ref. 9.
[g]TS: Taboo search (Ref. 38). Results are from Ref. 9.
[h]MGA: Modified genetic algorithm (Ref. 39). Results are from Ref. 9.
[i]FAEA: Fast annealing evolutionary algorithm (Ref. 9). Results are from Ref. 9.
[j]Results of AIOA are the average results over 100 continuous runs.

of AIOA is compared with other stochastic optimization methods. The number of function evaluations is used in the comparison, however, the number for AIOA is the sum of function evaluations and gradient evaluations. In each run of AIOA, the global minimum was successfully obtained. From Table I, it can be seen that function evaluations number of AIOA is apparently lower than that of other methods, except for $f2$, $f3$, $f4$, and $f8$, in the optimization of which the numbers are higher than that of FAEA. The reason for the results is due to the high local search ability of L-BFGS and not so many local minima for most of these functions. However, the $f2$, $f3$, $f4$, and $f8$ are more complex than the others. The convergence speed is not so high because AIOA emphasizes more of the individual diversity to guarantee the success of the optimizations. This indicates that AIOA should have high performance for complex problems, though it may take longer computation time. For the more complex problems, such as Lennard-Jones problem that will be discussed in the next section, it can be expected to benefit from the individual diversity regulated by the density.

In order to investigate the efficiency of the density regulation, the density trajectories of AIOA with and without density regulation for function $f2$ was compared in Fig. 3. It can be seen that AIOA with density regulation is apparently superior to AIOA with density regulation. At the beginning of the circulation, they both have a low density, but the latter has a higher increasing rate than the former, and reaches a premature state quickly. Therefore, AIOA with density regulation can keep the colony with a lower density, and the colony will has a good individual diversity.

In addition, the comparison of colony information entropy, $H(N)$, of AIOA with and without density regulation for function $f2$ was shown in Fig. 4. According to the concept of information entropy, higher colony information entropy means better information quantity, and better information quantity means higher individual diversity. At the beginning of the circulation, the first generation antibodies are generated stochastically, they have the highest $H(N)$, which is near 1. Then it decreases quickly due to the convergence of the algorithm, but the decreasing speed of the former is lower than that of the later, and $H(N)$ of the former is obviously higher than that of the later when they reach a stable state. Therefore, this indicates that AIOA can adaptively control the individual diversity and the convergence speed, and, as a result, can avoid prematurity successfully.

B. Energy minimization of Lennard-Jones clusters

The LJ cluster is not only interesting as a model for heavy inert gases but also serves as a popular benchmark

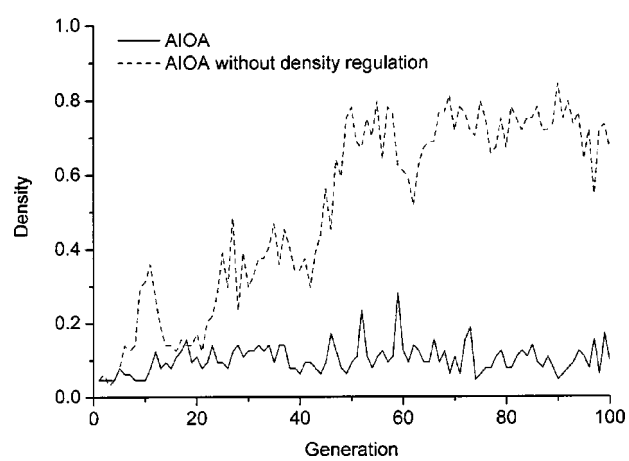

FIG. 3. Comparison of density trajectories for AIOA and AIOA without density regulation for function $f2$, where the dimension space is 5.

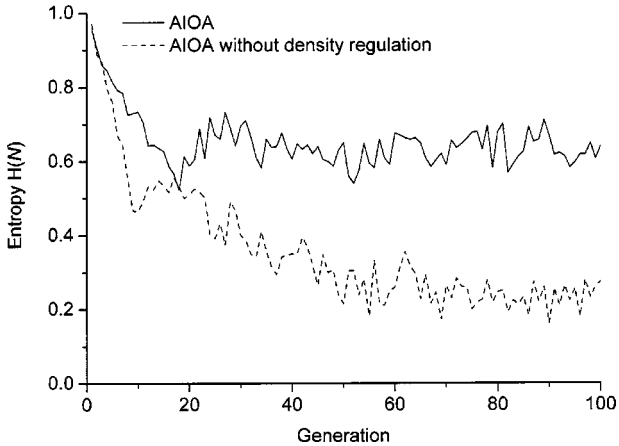

FIG. 4. Comparison of colony information entropy, $H(N)$, for AIOA and AIOA without density regulation for function $f2$, where the dimension space is 5.

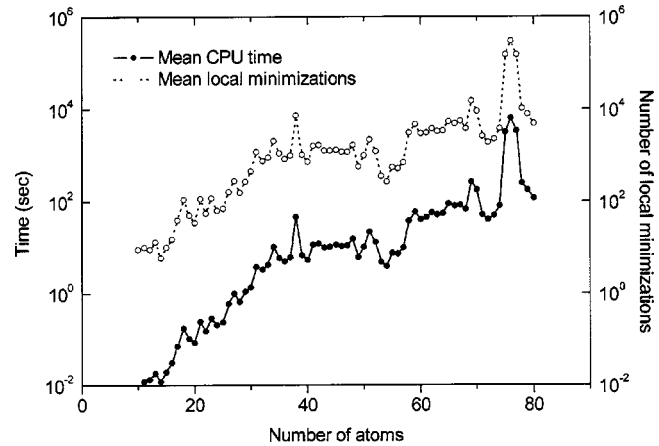

FIG. 5. Average CPU time (s) and average number of local niminization per hit of the global minimum for clusters with $10 \leqslant N \leqslant 80$. The CPU time corresponds to a 1.5 GHz Intel Itanium2 Madsion processor.

system for a putative global optimization algorithm. Most global minima for LJ clusters containing fewer than 80 atoms are based on icosahedral packing.[40] The exceptions, LJ_{38} (truncated octahedron) and LJ_{75-77} (Marks decahedron) serve as particularly interesting test cases. At these magic numbers, the global minimum lies in a very deep funnel on the LJ potential energy surface, while the lowest-energy icosahedral one acts as a trap in a much wider funnel. Therefore, to obtain the global minima of the magic numbers, population diversity is very important for an evolutionary method. In Ref. 2, a GA method is applied to LJ clusters, and the similarity of two local minimum configurations is measured directly by the gap of their potential energy. The global minimum of LJ_{38} is reproduced by this method, but failed in LJ_{75-77}. In Ref. 24, an efficient similarity checking method using the concept of niches is presented to maintain the diversity, and the global minima of LJ_{38} and LJ_{75-77} are successfully located.

To further test the applicability of the proposed method, AIOA was also applied to the global optimization problem of LJ clusters. The potential energy for the N-atom cluster is determined with Eq. (7). The radius of the container that encloses all atoms can be calculated by radius $=(3N/4\pi\sqrt{2})^{1/3}$.[40] The stop criteria for optimizations of LJ clusters are $|V_{\mathrm{cal}}-V_{\mathrm{min}}|<10^{-5}$, where V_{cal} is the calculation result by AIOA, V_{min} is the global minimum in Cambridge Cluster Database (CCD).[40]

All the LJ clusters with atom number $N \leqslant 80$ were investigated by AIOA. It was found that the algorithm successfully located all the known global minima listed in CCD. The AIOA parameters used for optimization are $npop=20-60$, cloning rate $\alpha=1-2$, $msize=10-30$, $Tac=0.90$, $muterate=0.02$, and $materate=0.5$. The hit rate of finding out the known global minima is 10 out 10 runs except for LJ_{75-77}. In the optimization of LJ_{75-77}, the algorithm frequently converges at the icosahedral funnel even using a larger population and larger number of generation (*maxit*). Therefore, for LJ_{75-77}, the efficiency is guaranteed by using a larger number of runs with a smaller *maxit*. The successful rates of hitting the global minimum are 6/100, 3/100, and 6/100, respectively. Figure 5 shows the average number of local minimizations and mean CPU time of hitting the global minimum for $10 \leqslant N \leqslant 80$. For the partly successful cases (LJ_{75-77}), the average includes the part of failure runs. As most of the best cluster optimization algorithms make use of local minimization, the average number of local minimizations can be taken as a criterion to measure a global optimization algorithm. Furthermore, the successful rate is another important criterion to evaluate an evolutionary algorithm. The average number of local minimizations needed by one hit and the successful rate in the optimization of some selected clusters is compared with the monotonic sequence basin-hopping (MSBH) (Ref. 25) and RTA (Ref. 11) in Table II. It can be seen that, average number of local minimizations of AIOA is larger than that of MSBH for most of cases, but for the most difficult case (LJ_{75}) the values are in the same level. It also can be seen that, the successful rate of AIOA is much higher than that of MSBH and RTA. The results indicate that, to guarantee the diversity, the convergence speed of AIOA is not so high as MSBH, which is a kind of greedy method, but as an evolutionary method, AIOA shows its high efficiency in successful rate.

TABLE II. Mean local minimizations per hit of global minima and successful rate for selected clusters of AIOA and some other unbiased global optimization methods.

	MSBH		RTA		AIOA		
N_{atom}[a]	N_{LM}[b]	R_{hit}[c]	N_{pop}[d]	R_{hit}[c]	N_{pop}[d]	N_{LM}[b]	R_{hit}[c]
30	739	0.387	2	4/10	50	451	10/10
38	2 875	0.124	30	9/10	60	7 400	10/10
40	279	0.849	30	10/10	50	743	10/10
50	460	0.868	30	5/10	50	994	10/10
60	388	0.948	30	1/10	60	2 976	10/10
70	1 526	0.630	30	3/10	60	8 905	10/10
75	152 000	0.004	240	1/50	80	149 000	6/100
80	2 009	0.420	30	4/10	60	4 796	10/10

[a] N_{atom}: the atom number of LJ cluster.
[b] N_{LM}: average number of local minimizations per hit of global minimum.
[c] R_{hit}: successful rate of hitting the global minimum.
[d] N_{pop}: the population size used.

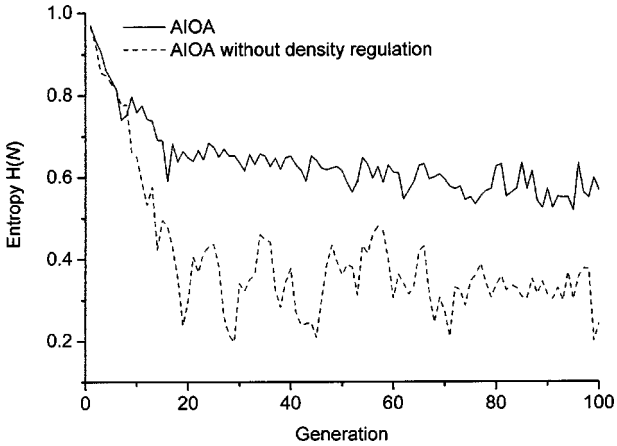

FIG. 6. Comparison of colony information entropy, $H(N)$, for AIOA and AIOA without density regulation for LJ clusters at $N=80$.

AIOA successfully gets over the first two hurdles, LJ_{38} and LJ_{75},[7] of the LJ problem without any specific technique to the system. FAEA can reproduce all the known global minima up to 74 atoms, but failed for LJ_{75} even if some specific techniques, seeding and moving the outside atoms, were used.[10] This indicates AIOA has higher efficiency than FAEA with a much more complex problem.

In order to investigate the performance of the density regulation to the optimization of LJ clusters, the colony information entropy trajectories of AIOA with and without density regulation for optimization of LJ_{80} was also compared in Fig. 6. It can be seen that, for the structural optimization problem, AIOA with density regulation is also apparently superior to AIOA without density regulation as shown in Fig. 4 in the case of function optimization.

IV. CONCLUSION

An adaptive immune optimization algorithm (AIOA) is proposed, in which density regulation and memory library are adopted. By application of the algorithm to optimization of test functions, it is shown that the algorithm has good performance. By comparison of density and colony information entropy trajectories, it is shown that the colony diversity of AIOA with density regulation is much better than AIOA without density regulation. We also applied the algorithm to determine the minimum configurations of LJ clusters. The algorithm successfully got over the two hurdles, LJ_{38} and LJ_{75}, which shows AIOA is a good method for global optimization.

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