Co-Evolutionary Global Optimization Algorithm
Masao Iwamatsu
Department of Information and Computer Engineering
Kisarazu National College of Technology
Kisarazu City, Chiba 292-0041, Japan

Abstract – A hybrid global optimization method, the co-evolutionary global optimization algorithm, is proposed which utilizes the self-organized critical state as the mean of diversification of search and the traditional conjugate gradient local minimization method as the mean of intensification of search. The former has been recently used by Boettcher and Percus (Artificial Intelligence 119 (2000) 275) to solve discrete combinatorial optimization problems. The proposed method has been tested to locate the lowest energy conformation of atomic clusters. It was found that the method was effective not only to locate the lowest energy state but also to enumerate all the low-lying metastable states.

I. INTRODUCTION

Global optimization is the task of finding the lowest minimum point in the rugged landscapes in high dimensions. In order to design an algorithm to solve such a problem, an efficient combination of diversification (exploration) and intensification (exploitation) of search are necessary. Along this principle, many heuristic methods have been designed [1]. Among those, the simulated annealing (SA), tabu search (TS), genetic algorithm (GA), and evolutionary programming (EP) seem most popular and have been applied to many engineering and scientific problems.

They are roughly classified into two categories; one which tries to improve single solutions, and another which uses the metaphor of evolution theory and considers multiple solutions in parallel to try to improve the population of solutions rather than just a single solution.

A common principle of these algorithms, however, is to improve the solution or try to breed the best member in the population. In fact it is well known that the success of the evolutionary algorithms such as GA and EP depends strongly on their strategies that preserves the best member called the elite [2].

Very recently, Boettcher and Percus [3] proposed a new algorithm called “extremal optimization.” (EO). Their algorithm is classified as the first category. However, instead of trying to improve the solution in SA or TS, EO does not try to improve the solution directly. Exploiting the idea of the Bak and Sneppen model [4], which shows self-organized critical phenomena, EO algorithm tries to improve the solution indirectly by replacing the worse element in the system with a randomly created new element. The probability that the \( n \)-th worst element is chosen is \( P(n) \propto n^{-\tau} \), where \( \tau \) is the parameter of the algorithm. Then, the system is allowed to relax towards the optimum state. Replacement of the worse element affects the whole system and may induce the collapse of the system. Thus, this algorithm realizes the self-organized critical state. In contrast to SA where the system moves toward equilibrium, or TS where the system wanders between local minima and saddles, the system never reaches equilibrium in EO and is always in a far-from equilibrium state characterized by a large fluctuation.

Boettcher and Percus used this EO algorithm for typical combinatorial optimization problems, the graph partition problem and traveling salesman problem, and found a fair amount of success.

In this article, we are going to develop the co-evolutionary global optimization algorithm for continuous...
optimization problems by combining the extremal optimization (EO) algorithm with the traditional conjugate gradient local minimization algorithm.

In our co-evolutionary algorithm, the worse element of the system is replaced by a new element, then all the elements of system are allowed to relax toward equilibrium by conjugate gradient method. Thus, all the elements participate in searching and achieve the co-evolutionary optimization.

II. CONFORMATION OPTIMIZATION PROBLEM

The problem we consider in this article is the global optimization of the conformation of atomic clusters [5], for which traditional heuristics such as GA [5,6] or EP [5,7] have been adopted.

The system consists of \( N \) atoms, and the optimum arrangement (conformation) of atoms corresponds to the global minimum of the total potential energy \( U(x) \) of the \( N \)-atom cluster defined by

\[
U(x) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} v(r_{ij})
\]

(1)

where \( v(r_{ij}) \) is the pair potential that represents the inter-atomic interaction between two atoms \( i \) and \( j \) in the cluster. In this work we used the Lennard-Jones potential

\[
v(r_{ij}) = 4\epsilon \left( \frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right)
\]

(2)

where

\[
r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}
\]

(3)

is the distance between two atoms \( i \) at \( (x_i, y_i, z_i) \) and \( j \) at \( (x_j, y_j, z_j) \). \( \epsilon \) is the material parameter and will be fixed to \( \epsilon=1 \) throughout this paper. We choose this Lennard-Jones clusters as the target problem since not only the global optimum structures [8] as well as the low-lying meta-stable structures for small clusters are well documented [9, 11].

In this problem, the element of the system is atoms and we can assign the energy contribution of \( i \)-th atom by

\[
u_i = \sum_{j=1}^{N} v(r_{ij})
\]

(4)

Then the total energy (1) is given by the sum of the contribution \( u_i \) of all atoms:

\[
U(x) = \frac{1}{2} \sum_{i=1}^{N} u_i
\]

(5)

Now, it is possible to rank the atoms according to their energy \( u_i \); the higher their energies the worse they are. The worst atom has the highest energy. The worse atoms naturally locate mostly on the surface of the cluster because they are surrounded and attracted by smaller number of atoms.

III. CO-EVOLUTIONARY ALGORITHM

The co-evolutionary algorithm we propose here for finding the lowest-energy conformation of the cluster that consists of \( N \) atoms is as follows:

1) Prepare the initial \( N \)-atom cluster by placing \( N \) atoms at random position within a given cube (of side length 1). When “seeding” strategy is used, the initial cluster is prepared by attaching one atom to the lowest energy structure of \((N-1)\)-atom cluster obtained from previous run of our co-evolutionary algorithm. In the latter case, the added atom is again place at the random position within the cube. In order to eliminate the translational and rotational degrees of freedom of the cluster, one atom is fixed at the origin, the second on the \( x \)-axis and the third on the \( x-y \) plane [9].

2) The cluster is local minimized using the conjugate gradient method. We use the routine \texttt{fprmn.c} in [10]. Record the total energy as the lowest energy.

3) Evaluate the energy \( u_i \) of each atom from (4) and rank the atoms according to their energies.

4) Choose the \( n \)-th worst atom according to the selection probability \( P(n) \propto n^\tau \) [3]. If \( \tau \) is large (infinite) the worst atom is always chosen.
5) Remove the chosen atom and place one atom anew at random position within the cube using the same procedure as that used to make the initial configuration in 1).

6) The new cluster thus obtained is local minimized [10]. Record the total energy if it is lower than the lowest energy so far.

7) Stop if the halting condition is satisfied, otherwise go to step 3).

At the step 5), the replacement of a single atom having higher energy (worse atom) might cause the relaxation of whole atoms in the cluster. Therefore the small perturbation on the cluster induces the avalanche in the cluster sometimes, and all atoms rearrange co-evolutionary. Using this co-evolutionary algorithm, we will try to determine the lowest-energy structure of Lennard-Jones cluster LJ$_N$ ($N=13-39$), and will compare the results with published results obtained by other methods [8].

IV. RESULT AND DISCUSSION

Fig.1 shows the evolution of the energy of 19-atom LJ$_{19}$ cluster during the search of our co-evolutionary algorithm. The figure shows the highly fluctuating state that is maintained during the search. A newly created cluster by replacing a worse atom might have high energy, but it can have very low energy by the co-evolutionary collapse of relaxation of all atoms in the cluster. This highly fluctuating state makes the exploration of the search space effective.

We should note that this algorithm is not a random search where all the atoms have equal chances to be updated because the worse atoms with higher energies have more chance to be removed. In addition, the local minimization is executed every time in our algorithm.

In order to examine the effect of the exponent $\tau$ of the selection probability on the performance of the algorithm, we compare the lowest energies per atom obtained from 10 independent runs of our co-evolutionary algorithm with $\tau=0$ (random replacement), $\tau=5$, and $\tau=\infty$ (only the worst atom is replaced) compared with the exact results in the literatures [8].

![Fig. 1 The evolution of the energy of LJ$_{19}$ during the search with $\tau=5$. Occasional co-evolutionary avalanches of relaxation produce deep minima. The highly fluctuating state is achieved by our co-evolutionary algorithm.](image)

![Fig. 2 The lowest energies per atom of Lennard-Jones clusters LJ$_N$ plotted as the functions of number of atoms $N$ obtained from our algorithm with $\tau=0$ (random replacement), $\tau=5$, and $\tau=\infty$ (only the worst atom is replaced) compared with the exact results in the literatures [8].](image)
various $\tau$ in Fig. 2. We use the “seeding” strategy in the initialization step 1) and run the algorithm 2000 steps for LJ$_{13}$-LJ$_{19}$, 3000 steps for LJ$_{20}$-LJ$_{29}$, and 5000 steps for LJ$_{30}$-LJ$_{39}$. The best algorithm seems the one with $\tau=5$, though we do not pursue the optimization of $\tau$. The strategy $\tau=\infty$ which replaces only the worst atom is comparable. Naturally, the strategy $\tau=0$ which gives all atoms an equal probability is not effective. In Fig. 2, we also compare our results with exact results [8]. Our co-evolutionary algorithm can find the global minima up to LJ$_{30}$ in spite of the small number of steps (maximum 5000) examined.

Finally, in order to show another potential ability of our co-evolutionary algorithm, we examine the low-lying meta-stable states. Figure 3 shows the evolution of energy during the search for a LJ$_{7}$ cluster, for which all 4 metastable states (isomers) with energies $E=-16.505$, -15.935, -15.593 and -15.533 are well documented [11]. Our co-evolutionary algorithm can clearly identify the 4 isomers. Therefore our co-evolutionary algorithm can be used not only to find out the global minima but also to enumerate all possible low-lying meta-stable states.

V. CONCLUSION

In this paper, we proposed a new global optimization algorithm based on the concept of co-evolution. We applied the algorithm to the conformation optimization of Lennard-Jones clusters and found that the method is effective.

Our algorithm has some similarity to the extension of Monte Carlo method called the Basin-Hopping algorithm [8]. However, Basin-Hopping chooses atoms to be moved at random and also uses usual Metropolis criterion to accept the move. Since our co-evolutionary algorithm chooses mainly those atoms on the surface and accepts any kind of move irrespective of any physical constraint, our algorithm is expected to be more effective than that of the Basin-Hopping [8]. Our algorithm also has some similarity to the symbiotic genetic algorithm proposed by Michaelian [12], though ours is much simpler and easier to apply to many kind of problems.

REFERENCES


* After 1/4/2002: Faculty of Engineering, Musashi Institute of Technology, Setagaya-ku, Tokyo 158-8557, Japan