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Research on Genetic Algorithms based on Real Coded and Data Information for Global Optimization

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Abstract

The genetic algorithm is recently developed real number coding used in challenging problems finding the lowest energy structure of the same group of atomic interaction through the wells potential. Find the global optimal this function is difficult, because it has a large number of local extremum, molecular size increase exponentially. The results of the cluster contain 15 atoms, and obtained. The results show the excellent performance of newly developed real number coding genetic algorithm, the earlier published the results.

Keywords: global optimization, real coded , genetic algorithm

1. INTRODUCTION

Find the most stable atom clusters structure is a challenging problem, because it is a highly complex, the complexity increases with the increase of the number of atoms. Usually the maximum energy equivalent to minimum atom clusters stability [1]. This is a challenging global optimization problem is not as the number of the local extremum increase exponentially with the size of the molecular [2]. First, the most efficiency and the most successful method L-J well) introduced the clustering optimization [3] and [4] further refined. This method is based on the idea of local optimization from the initial configuration and began to build the atoms of the random placed in space predefined points, according to the most common lattice structure found in nature.

Also has the hybrid algorithm, combined with monte carlo (MC) or simulated annealing (SA) and genetic algorithm to optimize the model. In different optimization methods are considered, multi-level and terrain single link differential evolution and the genetic algorithm, but it shows that the effective combination of the genetic algorithm, especially local optimization method is rapid, reliable task to find the atoms and molecules structure of the cluster. Technology is developed in recent years to a genetic algorithm hybrid and monte carlo method geometric optimized atom clusters, also is to solve. Rrecently applied parallel particle swarm algorithm is L-J potential problems.

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The research indicates that, in most of the results in [10], and so on. To enrich the function value calculation conditions in [10], use a iterated local search algorithm and based on differential evolution a binary coding genetic algorithm for the L-J potential energy function.

2. PROBLEM DISCUSSION

The problem is that the potential energy L-J atom clusters with two atoms of interaction between the relations of the total, and these interactions are endowed with things L-the size of the J (6-12) strength the potential.

The problem consists of determining the positions $t_1, t_2, \ldots, t_n \in R^3$ of an n atom cluster in such a way that the L-J potential given by

$$V = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(e_{ij}^{-12} - 2e_{ij}^{-6} \right) \tag{1}$$

where e_{ij} is the Euclidean distance between the points t_i and t_j, generated by atomic interactions is minimized. Every atom clusters characteristic is a set of three pieces of real Numbers corresponding to the (x, y, z) position of each atom. The problem is and finds the position of each atom clusters global minimum value corresponding V in (1).

3. REAL CODED GENETIC ALGORITHM

Genetic algorithm is proposed based on heuristic population is used to determine the solving nonlinear optimization problems. Genetic algorithm is a simulation of the main "Darwin's survival of fittest". Use three basic computing algorithm to select, crossover and mutation in moving from one generation to another place. The use of gas real-encoding chromosome called real number coding gas (RCGAs). Four different RCGAs used in this paper, the real number coding operator; Cross (WX wei) and Log-Logistic mutations (LLM) of unpublished "and Laplace cross (LX) given the scheme RCGAs in figure 1.

3.1. Computational Steps

Computational steps of algorithms used are as follows: 1. Generate a suitably large initial set of random points within the domain prescribed only by the bounds on variable i.e. points satisfying $l_i \le x_i \le u_i$.

2. Check the stopping criteria? if satisfied stop; else goto 3.
3. Apply tournament selection procedure on initial (old) population to make mating pool.
4. Apply crossover and mutation to all individuals in mating pool, with probability of crossover p_c and probability of mutation p_m respectively, to make new population.
5. Increase generation ; replace old population by new population ; goto 2.

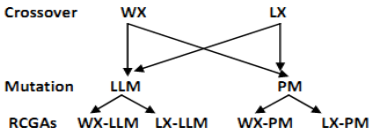

Figure 1. Schematic of all RCGAs used.

3.2. Performance Evaluation Criteria

For evaluating the performance of each method the following are recorded:

1) Average number of function evaluations of successful runs (AFE).

2) Success Rate (SR) = $\frac{Number\ of\ successful\ runs}{Total\ number\ of\ runs} \times 100$

3) Success Performance (SP)= $\frac{(AFE)}{Total\ number\ of\ runs} \times Total\ number\ of\ runs$

4) Average Error (AE) = $\sum_{n} \left(f_{\min} - f_{opt} \right) / n$ where n= total number of runs; f_{min}=best solution obtained by algorithm in a run; f_{opt}=known global minimum of problem.

4. COMPUTATIONAL RESULTS

In this article, we use the numerical results by using RCGAs that all. WX-PM, LX-PM, WX-LLM, LX-the energy function (LLM algorithm in c + + later, and experiments are the different combinations in a core processor in 1.66 MHZ speed and 1 GB WINXP platform exist inside.

For each algorithm are 100 independent operations. Allow the largest number of each generation, it's 5000. For all the algorithm population size five times the number of variables. An operation is considered to be successful if the global minimum known, the differences between made the global minima is strictly is less than 0.01. Global mimina think here, can be found in [21].

The optimal parameter Settings for each RCGA: cross (PC) is the probability of 0.65, 0.7, 0.6 and 0.8; Variation (point) is the probability of 0.06, 0.02, 0.07 and 0.004, the LX-WX-PM, PM WX-LLM and LX-LLM respectively.

From the results of statistical analysis, put forward a table I to IV and figure 2-5, where the best performance RCGA engraved with star. My table shows the average value of the successful operation (AFE). Boxplots function value corresponding to the average of all the gives figure 2 observation RCGAs performance be clear at a glance. Security is proportional to the calculation method of cost. Obviously, LX-LLM perform the most security point of view.

TABLE I. COMPARISON FOR ATOMIC CLUSTER CONTAINING ATOMS FROM 1 TO 10

Number of atoms	GA	WX-PM	LX-PM	WX-LLM	LX-LLM
1	1550	846	386	1020	420
2	3673	1746	1244	1892	1205
3	8032	7437	5929	8431	5158
4	48900	26598	24853	29892	24098
5	121247	38612	32807	39613	31840
6	346397	61807	58498	65448	57731
7	721370	158816	138846	161724	137662
8	-	253963	199814	267389	198436
9	-	302258	280910	326847	271763
10	-	426488	327712	548193	320675

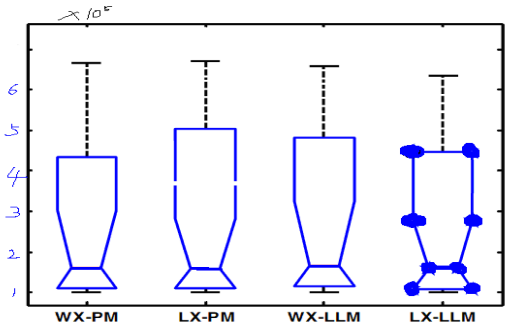

Figure 2. Comparison of Average Function Evaluation.

Table II compares success rate (SR) of all RCGAs considered in this paper for all the cases of the given problem. Success rate is directly proportional to the reliability of the method. The corresponding boxplots are shown in Fig. 3. Again the performance of LX-LLM is best.

TABLE II. COMPARISON OF SUCCESS RATE (SR) FOR ATOMIC CLUSTER CONTAINING ATOMS FROM 1 TO 10

Number of atoms	WX-PM	LX-PM	WX-LLM	LX-LLM
1	100	100	100	100
2	100	100	100	100
3	100	100	100	100
4	100	100	93	100
5	100	98	89	100
6	89	94	78	97
7	93	92	83	96
8	94	91	86	93
9	65	70	62	77
10	81	94	71	86

To observe the consolidated effect on AFE and SR of all the four RCGAs, comparison is done on the basis of success performance (SP). Table III and Fig. 4 present this information.

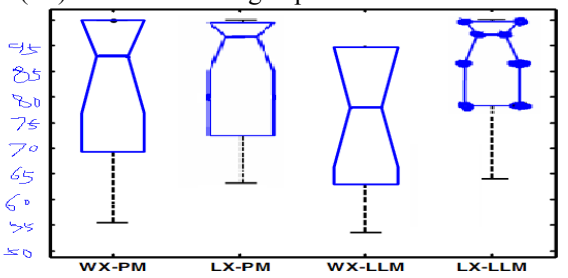

Figure 3. Comparison of Success Rate for all algorithms.

Although LX-one of the best RCGA LLM is observed one important fact is, it is not 100% success, the number of atoms began to increase the success rate (SR) continue to fall.

TABLE III. COMPARISON OF SUCCESS PERFORMANCE (SP) FOR ATOMIC CLUSTER CONTAINING ATOMS FROM 1 TO 10

Number of atoms	WX-PM	LX-PM	WX-LLM	LX-LLM
1	846	386	1020	420
2	1746	1244	1892	1205
3	7437	5929	8431	5158
4	12086	11671	17791	10267
5	26598	25360	33587	24098
6	43384	34901	50786	32825
7	66459	63585	78853	60136
8	168953	152578	188051	148024
9	390712	285449	431273	257709
10	373158	298840	460348	316003

Now the most accurate method is sought. For this purpose the comparison based on average error (AE) of 100 runs is carried out. Table IV shows AE and corresponding boxplots are given in Fig. 5. From Fig. 5 it is clear that on the basis of AE, again LX-LLM performs best.

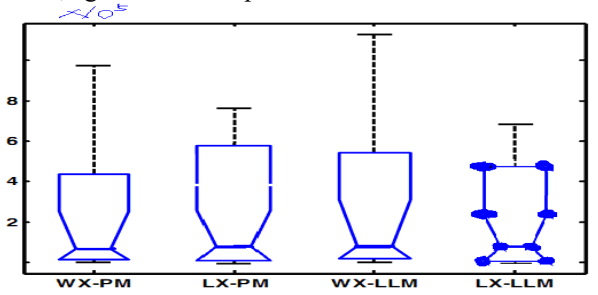

Figure 4. Comparison of Success performance for all algorithms.

TABLE IV. COMPARISON OF AVERAGE ERROR FOR ATOMIC CLUSTER CONTAINING ATOMS FROM 1 TO 10

Number of atoms	WX-PM	LX-PM	WX-LLM	LX-LLM
1	0.00019	0.00016	0.00021	0.00012
2	0.00038	0.00048	0.00039	0.00043
3	0.00071	0.00062	0.00084	0.00057
4	0.00042	0.00031	0.00048	0.00025
5	0.00475	0.00258	0.00661	0.00418
6	0.00517	0.00486	0.00719	0.00393
7	0.00642	0.00513	0.00583	0.00422
8	0.00875	0.00689	0.00976	0.00673
9	0.01613	0.01145	0.01835	0.00919
10	0.01792	0.00933	0.01938	0.00962

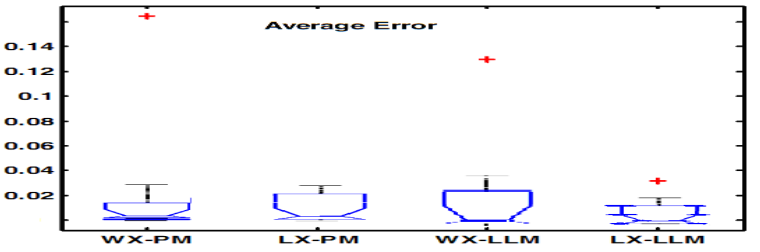

Figure 5.Comparison of Average Error for all algorithms.

5. CONCLUSIONS

A potential atom clusters well 15 atoms very useful minimum molecular structure stability and predict most of its properties. Guide the calculation results; this paper puts forward a new development in the RCGAs namely. WX-PM, LX-PM, WX-LLM and LX-LLM and earlier published results [14] (table 1). Of all the new development of RCGAs LX-LLM is the best performance. It's very important. Note the performance comparison, is based on the function of the values of the operation, the success rate, the number of successful performance and average error, and must realize the global minima and not the whole search method.

This may be because of the fact that L-J problem is highly multimodal transport in nature and without the complexity of the problem with increased number of atoms in the cluster. So these RCGAs hybridization and some local search will certainly help improve their performance.

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