STUDIA UNIVERSITATIS BABES-BOLYAI, PHYSICA, L, 4a, 2005

EVOLUTIONARY OPTIMIZATION OF MOLECULAR CLUSTERS

Ioan Zaharie[1], **Daniela Zaharie**[2]

[1]*Physics Department, "Politehnica" University,*
Piata Regina Maria, nr. 1, 300004, Timisoara
izaharie@etv.utt.ro
[2]*Computer Science Department, West University,*
bv. V. Pârvan, nr. 4, 300223, Timisoara
dzaharie@info.uvt.ro

Abstract. The aim of this work is to analyze the ability of a hybrid evolutionary algorithm (obtained by combining a crowding version of differential evolution with a local search procedure) in finding the global minimum of potential energy functions used in modeling atomic and molecular clusters. Results for Lennard-Jones, Morse and Dzugutov potentials are presented.

1. Introduction. Clusters optimization has as aim the identification of stable atomic or molecular structures and is of practical importance in semiconductor industry and in structure-based drug design. Frequently used models of cluster structures are those based on potential energy functions. Different variants of potential functions, modeling structural behavior relevant to rare gases, metals and molecular clusters bound by dispersion forces, have been proposed and used in the past decades. These potential functions generate different cluster models, e.g. Lennard-Jones clusters, Morse clusters, Dzugutov clusters [2]. The problem of identifying the global minimum of the energy function is notoriously difficult, mainly due to the fact that classical optimization methods are easily trapped in local minima which correspond to metastable structures. Different methods for cluster optimization have been proposed lately. Some of them use the idea of finding the global optimum by identifying attraction regions of different optima and refining the approximation by a local search (e.g. basin hopping method [2]). Other methods, e.g. simulated annealing, are based on the idea of escaping from the local optima by accepting structure modifications which, temporarily lead to an increase of the energy. In the last decade another approach, based on evolutionary algorithms, proved to be adequate in identifying optimal structures mainly in the case of large clusters [1,4,5,6,7].

Evolutionary optimization is a paradigm based on the idea of using a population of configurations, each one representing a trial structure, and evolving this population toward better configurations by applying some nature inspired operations: crossover, mutation and selection. Despite the fact that evolutionary algorithms proved to be robust global optimization tools, difficulties (especially related with slow convergence), can arise in applying them for cluster optimization. To eliminate this problem, Deaven and Ho [1] proposed the use of a hybridization

between a genetic algorithm and a local search method. On the other hand, because of the huge number of local minima in the energy landscape in the case of large structures even the evolutionary algorithms have difficulties in identifying the global minimum. In order to reduce the risk of convergence to a local minimum diversity preservation mechanisms should be applied. Their effect is that the population will eventually contain elements grouped in regions of attractions of different optima. Starting a local search from each attraction region increases the chance of identifying the global minimum. This is the underlying idea of the approach presented in this paper. In the next section we shortly review the potential functions used in the numerical experiments while in the other two sections we present the evolutionary approach and some numerical results.

2. Potential functions. The general form of potential energy functions is:

$$f(x_1, x_2, ..., x_n) = \sum_{i<j} V(d(x_i, x_j)) \quad (1)$$

where x_i denotes the spatial position of particle i (a triplet of Cartesian coordinates) and d denotes the Euclidean distance. Different expressions of the potential function, V, lead to different models. Some of the most used potentials are [2]: Lennard-Jones, Morse and Dzugutov. The Lennard-Jones potential, in its scaled version, is:

$$V_{LJ}(r) = \frac{1}{r^{12}} - \frac{1}{r^{6}} \quad (2)$$

It provides a reasonable description of the interatomic interactions of rare gases[2]. The Morse potential can be expressed by [2]:

$$V_M(r) = \exp(\rho(1-r))(\exp(\rho(1-r)) - 2) \quad (3)$$

where $\rho>0$ is a parameter which determines the range of the interparticle forces. When $\rho=6$ the Morse potential is similar to the Lennard Jones potential. Small values of ρ correspond to long range-interactions (as in alkali metals) while large values correspond to short-range interactions (as for C60 molecules which can be modeled by the Morse potential with $\rho=13.62$). The parameter ? influences the difficulty of the optimization task (values for which it is known to be difficult to find the global minimum are $\rho=10$ and $\rho=14$). Another potential for which have been recently obtained results [3] is the Dzugutov potential defined by:

$$V_D(r) = A(r^{-m} - B)\exp\left(\frac{c}{r-a}\right)\theta(a-r) + B\exp\left(\frac{d}{r-b}\right)\theta(b-r) \quad (4)$$

where θ is the Heaviside function ($\theta(x)$ is 1 if $x>0$ and 0 otherwise) and the other parameters are: $A=5.82$, $a=1.87$, $B=1.28$, $b=1.94$, $c=1.10$, $d=0.27$ and $m=16$. Systems interacting according to Dzugutov potential have been found to be good glass-formers.

3. A differential evolution-based approach for cluster optimization. In the last decade a lot of evolutionary algorithms have been applied to the global minimization of energy landscapes, especially to Lennard-Jones clusters and

occasionally to Morse clusters [1,5,6,7]. Most of the evolutionary approaches are based on a hybridization between an evolutionary search process and a local minimization procedure used to refine the results provided by the evolutionary algorithm. One of the main issues in applying evolutionary algorithms to cluster optimization is the computational cost of the process. This could be reduced by using evolutionary algorithms with fast convergence. Differential evolution (DE) [8] is such a simple and fast algorithm. Its basic idea is to generate new trial individuals from the elements of the current population by randomly selecting three so-called parents X_1, X_2 and X_3 and by combining them as follows: $Y=X_1+Fx(X_2-X_3)$. The vector Y is then probabilistically crossed over with an element of a population, X, and the result, Z, is compared with X. If Z is better than X then it will replace X in the population. A first adaptation of this algorithm to cluster optimization problems is presented in [4] (DELP). The particularities of this approach are: (i) at each generation the candidate, Z, is refined by applying a local search procedure; (ii) it is an iterative approach in the sense that the initial population corresponding to n particles is generated from the local minimizers obtained for the case of $n-1$ particles filled in with randomly generated components. The results reported in [4] (Lennard-Jones and Tersoff potentials) suggest that a lot of function evaluations are needed in order to obtain a good approximation of the global optimum. Starting from this remark we tried to modify the approach in [4] such that the computational cost is reduced. The particularities of our approach are: (i) the standard DE algorithm is replaced with a crowding-based DE [9] characterized by a higher exploration power and ability to identify many potential optima; (ii) the local optimization procedure (a simple descent gradient or the Nelder-Mead method) is applied only after the evolution not during the evolution (thus the number of functions evaluations could be reduced); (iii) the population initialization is also different as that in [4]: the initial population corresponding to the case of n particles is generated by randomly perturbing the estimation of the optimum found at the previous stage (for $n-1$ particles).

4. Results and discussion. In this section we present some results obtained for Morse (Table 1) and Dzugutov cluster (Table 2) by using the following control parameters: crossover probability: p=0.1, perturbation factor: F=0.5, population size: m=50, 1000 generations. Because of smaller populations and fewer calls of the local minimization procedure the algorithm which we used lead to fewer function evaluations than DELP [4]: for instance, in the case of Lennard-Jones cluster, for n=10, DELP needs 4653885 function evaluations to find the global optima while our approach used only 121876 functions evaluations to obtain an estimation within 0.0001 precision.

At least for small clusters the proposed approach gives a good estimation of the optimal structure by using fewer function evaluations than in [4]. The variant involving a simple gradient descent method seems to give better results than that based on the Nelder-Mead method. However the variant with Nelder-Mead method can be applied also for non-differentiable potential functions (e.g.

Dzugutov). Results in Table 2 suggest that for small clusters the method which we propose leads to better structures than those reported in [3]. However this is no more true for clusters having more than 8 particles.

Table 1.

Results obtained for the Morse potential (?=10)

n	**Global optimum**			**No. of function evaluations**	
	DE+Gradient descent	**DE+Nelder-Mead**	**Reported in [10]**	**DE+Gradient descent**	**DE+Nelder-Mead**
5	-9.003539	-9.003537	-9.003565	71656	92842
6	-12.009623	-12.009609	-12.094943	96876	117200
7	-15.956481	-15.956282	-15.956512	108800	197493
8	-18.964599	-18.913307	-18.964638	126248	242955
9	-22.850722	-21.876290	-22.850758	136426	409852
10	-25.861408	-26.582537	-26.583857	173340	484672

Table 2.

Results obtained for the Dzugutov potential

n	**5**	**6**	**7**	**8**	**9**	**10**
DE+Nelder-Mead	*-5.2204*	*-6.9472*	*-9.2187*	*-10.9383*	-12.1024	-11.5231
Reported global opt. [3]	-5.1949	-6.8954	-9.1104	-10.8009	*-13.0043*	*-15.1822*

References:

[1] D. M. D e a v e n, K. M. H o, *Molecular Geometry Optimization with a Genetic Algorithm*, Phys Rev Lett 75, 1995, pp 288.

[2] J. K. D o y e, *Physical Perspectives on the Global Optimization of Atomic Clusters*, in Global Optimization-Selected Case Studies, ed. J.D. Pinter, Kluwer, 2005, (online version: http://xxx.lanl.gov/abs/cond-mat/0007338).

[3] J. K. D o y e, D. J. W a l e s, S. I. S i m d y a n k i n, *Global optimization and the energy landscapes of Dzugutov clusters*, Faraday Discuss., 2001, 118, 159-170

[4] N. P. M o l o i, M. M. A l i, *An Iterative Global Optimization Algorithm for Potential Energy Minimization,* Journal of Computational Optimization and Applications, Vol.30, 2005,pp.1-14.

[5] S. D. M u l l e r, N. N. S c h r a u d o l p h, P. K o u m o u t s a k o s, *Evolutionary and Gradient-Based Algorithms for Lennard-Jones Cluster Optimization*, in A. Barry (ed.), Proc. of the Genetic and Evolutionary Computation Conference, 2003.

[6] C. R o b e r t s, R. L. J o h n s t o n, N. T. W i l s o n, *A genetic algorithm for the structural optimization of Morse clusters*, Theor. Chem. Acc (2000) 104: 123-130.

[7] K. S a s t r y, G. X i a o, *Cluster Optimization Using Extended Compact Genetic Algorithm*, IlliGAL Report No. 2001016, 2001.

[8] R. S t o r n, K. P r i c e, *Differential Evolution; A Simple and Efficient Heuristic for Global Optimization over Continuous Spaces*, Technical Report TR-95-012, ICSI, 1995.

[9] R. T h o m s e n, *Multimodal Optimization Using Crowding-Based Differential Evolution*, Proc. of the IEEE Congress on Evolutionary Computation, Portland, June 20-23, 2004.

[10] D. J. W a l e s, J. P. K. D o y e, A. D u l l w e b e r, M. P. H o d g e s, F. Y. N a u m k i n, F. C a l v o, J. H e r n á n d e z-R o j a s, T. F. M i d d l e t o n, *The Cambridge Cluster Database*, URL http://www-wales.ch.cam.ac.uk/CCD.html.