

**Cluster Optimization Using
Extended Compact Genetic Algorithm**

**Kumara Sastry
Guanghua Xiao**

IlliGAL Report No. 2001016
January, 2001

Illinois Genetic Algorithms Laboratory (IlliGAL)
Department of General Engineering
University of Illinois at Urbana-Champaign
117 Transportation Building
104 S. Mathews Avenue, Urbana, IL 61801

Cluster Optimization Using Extended Compact Genetic Algorithm

Kumara Sastry
Department of General Engineering
ksastry@uiuc.edu

Guanghua Xiao
Department of Material Science & Engineering
gxiao@uiuc.edu

University of Illinois at Urbana-Champaign
Urbana, IL 61801

Abstract

This paper presents an efficient cluster optimization algorithm. The proposed algorithm uses extended compact genetic algorithm (ECGA), one of the competent genetic algorithms (GAs) coupled with Nelder-Mead simplex local search. The lowest energy structures of silicon clusters with 4-11 atoms have been successfully predicted. The minimum population size and total number of function (potential energy of the cluster) evaluations required to converge to the global optimum with a reliability of 96% have been empirically determined and are $\mathcal{O}(n^{4.2})$ and $\mathcal{O}(n^{8.2})$ respectively. The results obtained indicate that the proposed algorithm is highly reliable in predicting globally optimal structures. However, certain efficiency techniques have to be employed for predicting structures of larger clusters to reduce the high computational cost due to function evaluation.

1 Introduction

One of the challenging problems in computational chemistry is the determination of lowest energy structures of atomic and molecular clusters. This can be attributed to the presence of a large number of minima such clusters can possess. A cluster of only 13 atoms has more than 10^3 local minima (Niesse & Mayne, 1996). Some studies (Hoare, 1979; Northby, 1987) estimate that the number of local minima increase as rapidly as $\exp(n^2)$, where n is the number of atoms in a cluster. Wille and Vennik (1985) have proved that the determination of lowest energy cluster, interacting under two-body central force, is an NP-hard problem. Therefore an exhaustive search of all possible structures is not feasible, thus necessitating usage of global optimization techniques.

One of the promising global optimization techniques are Genetic algorithms (GAs) (Goldberg, 1989). GAs are search methods inspired by nature and are based on Darwin's principle of *survival of the fittest*. GAs employ a population of candidate solutions and utilize genetic operators like *reproduction*, *recombination*, and *mutation* to create new candidates with higher fitness. Recently a class of GAs called *competent* GAs have been proposed (Goldberg, 1999) which are far superior to the conventional GAs. *Competent* GAs are defined as GAs that can solve *hard problems* quickly, reliably and accurately. In essence, competent GAs take problems that were intractable with earlier GAs and renders them tractable.

The objective of the current study is to employ extended compact genetic algorithm (ECGA) (Harik, 1999), one of the competent GAs for the task of cluster optimization and to evaluate its effectiveness in predicting globally optimal structures. Silicon clusters are taken as a test case. We have successfully predicted optimal structures for small clusters ($n = 4-11$) and efforts are currently under way to predict structures of bigger clusters. This paper is structured as follows: First we

present a brief literature review followed by a note on the atomic potential used in the present study. Section 4 describes the parameter encoding procedure and a brief description of ECGA is presented in section 5. The cluster optimization algorithms is described in section 6 and the results obtained are discussed in section 7 followed by conclusions.

2 Literature Review

Recently there has been considerable interest in employing GAs for solving cluster optimization problems (Niesse & Mayne, 1996; Gregurick & Alexander, 1996; Zeiri, Fattal, & Kosloff, 1995; Iwamatsu, 2000; Hartke, 1993; Hartke, 1995). Judson (1997) has shown that GAs outperform the traditional Monte Carlo based simulated annealing method. Zeiri (1997) reports that GAs are superior to simulated annealing in predicting the geometry of Ar_nH_2 . GAs were successful in predicting the optimal structure for C_{60} (Deaven & Ho, 1995) atom and simulated annealing failed for the same case. In the above study the authors used a *geometric* crossover to create new individuals. Hartke (1993) used a simple GA to predict the structure of Si_4 and Si_{10} on a semi-empirical potential. Gregurick *et al.* proposed a hybrid GA, in which they combined a binary coded GA and a conjugate gradient local search. They reported significant improvement in the performance when compared a GA without local search method. Niesse and Mayne (1996) modified this hybrid GA by encoding real values instead of binary. Iwamatsu (2000) used a Nelder-Mead simplex (Press, Flannery, Teukolsky, & Vettering, 1989) instead of a conjugate gradient technique to predict the cluster structure of Si_n ($n = 3-15$).

In most of the studies on cluster optimization with GA, researchers have used operators like *proportionate selection*, *single point crossover*, etc. Proportionate selection has various drawbacks, the scaling problem being the foremost. Single point crossover is known to disrupt good building blocks and thereby increase the convergence time as well as population size required. It has been shown in recent works (Goldberg, Thierens, & Deb, 1993; Thierens, 1994; Thierens & Goldberg, 1993) that ensuring effective building block (BB) mixing is an integral part of efficient GA design. These studies also showed that this could be achieved through a tight linkage of the set of alleles belonging to a BB. Based upon this concept many novel *competent* GA designs have been proposed which can be broadly classified into three groups; (1) Perturbation techniques like fast messy GA (FMGA) (Goldberg, Deb, Kargupta, & Harik, 1993), gene expression messy GA (GEMGA) (Kargupta, 1996), Linkage identification by nonlinearity check/Linkage identification by detection GA (LINC/LIMD GA) (Munetomo & Goldberg, 1999), (2) Linkage adaptation techniques like linkage learning GA (LLGA) (Harik & Goldberg, 1997), and (3) Probabilistic model based techniques like extended compact GA (ECGA) (Harik, 1999) and Bayesian optimization algorithm (BOA) (Pelikan, Goldberg, & Cantu-Paz, 2000). Sastry and Goldberg (2000) successfully applied ECGA for optimizing a binary fluid power cycle formulated as a nonlinear constrained problem. They also reported semi-empirical relations for the convergence time and the population size required.

3 Silicon Potential

Many researchers have used either the empirical potential proposed by Stillinger and Weber (1985) (SW) or the Tersoff potential (Tersoff, 1988) for calculating the potential energy of silicon clusters. Tersoff potential is a two body potential where as SW potential is a two and three body potential. However, although these potentials have satisfactorily predicted some bulk phase properties, they are not accurate in predicting the structural properties (Gong, 1993). The three-body term in SW potential becomes zero only for the perfect tetrahedron angle ($\sim 120^\circ$). On the

contrary, *ab initio* molecular dynamics calculations indicate a large peak at 60° and a smaller peak at 100° (Gong, 1993). The Gong potential, based on SW potential, contains a correction in the three-body term to incorporate not only the tetrahedral angle but also the preferred angle. The Gong potential is of the following form

$$U_{\text{tot}} = \sum_{i<j}^n v_2(i, j) + \sum_{i<j<k}^n v_3(i, j, k) \quad (1)$$

$$v_2(i, j) = A \left(B r_{ij}^{-p} - r_{ij}^{-q} \right) \exp \left[(r_{ij} - a)^{-1} \right], \quad |r_{ij}| < a, \quad (2)$$

$$v_3(i, j, k) = h(r_{ji}, r_{ki}) + h(r_{kj}, r_{ij}) + h(r_{ik}, r_{jk}), \quad (3)$$

$$h(r_{ji}, r_{ki}) = \lambda \exp \left[\gamma \left((r_{ij} - a)^{-1} + (r_{ki} - a)^{-1} \right) \right] \left(\cos \theta_{jik} + \frac{1}{3} \right)^2 \left[(\cos \theta_{jik} + c_0)^2 + c_1 \right], \quad |r_{ij}|, |r_{ki}| < a, \quad (4)$$

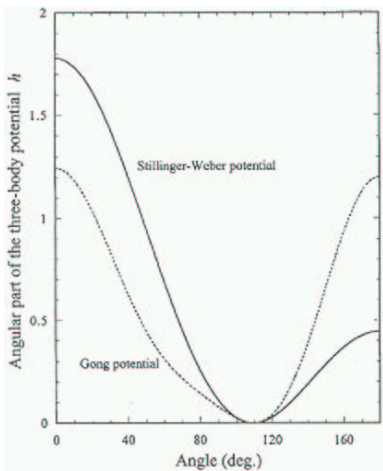


Figure 1: Angular part of the three-body term of SW and Gong potential. Reproduced from Iwamatsu, M. *J. Chem. Phys.* **112** 10976 (2000)

where U_{tot} is the potential energy of the cluster, $v_2(i, j)$ is the two-body term, $v_3(i, j, k)$ is the three-body term, $r_{ij} = |\vec{r}_i - \vec{r}_j|$, and θ_{jik} is the angle subtended by r_{ji} and r_{ki} with the vertex at i . A , B , p , q , a , λ , γ , c_0 , and c_1 are the empirical parameters determined by fitting to the bulk-phase data and *ab initio* calculations. The angular part of the Gong potential is given by the term $\lambda \left[(\cos \theta_{jik} + c_0)^2 + c_1 \right]$ and it incorporates the preferred bond angle. A comparison of the three-body term of SW and Gong potentials for different angles is shown in fig. 1. Gong reported that the structural properties predicted by his proposed potential agreed very closely with those obtained by *ab initio* studies and also was a significant improvement over other potentials. Iwamatsu (2000) has compared the optimal structures predicted by the two-body, two-and-three-body SW potentials and the Gong potentials for Si clusters ($n = 3-15$). In the current study we have used Gong potential with both two-body and three-body terms to calculate the total potential energy of a given cluster.

4 Parameter Encoding

Traditionally GAs encode the variables into binary strings (Goldberg, 1989). However, recently some researchers have employed real values instead of binary encodings for solving cluster optimization problems (Zeiri, Fattal, & Kosloff, 1995; Niesse & Mayne, 1996; Iwamatsu, 2000). They have reported significant improvement over binary coded GAs. However, in this study, we have used binary codings since all the competent GAs proposed so far are for binary coded GAs and linkage learning in real-coded GAs are still in the preliminary stages (Tsutsui, Goldberg, & Sastry, 2000).

The other choice to be made is the representation of the clusters. Earlier studies have employed internal coordinates (inter-atomic distances), where as some of the recent studies have employed space-fixed cartesian coordinates (Niesse & Mayne, 1996; Gregurick & Alexander, 1996; Zeiri, Fattal, & Kosloff, 1995; Iwamatsu, 2000). The space-fixed coordinates require $3n$ variables, whereas the internal-coordinates have $n(n-1)/2$ variables. Therefore, the space-fixed coordinates are more

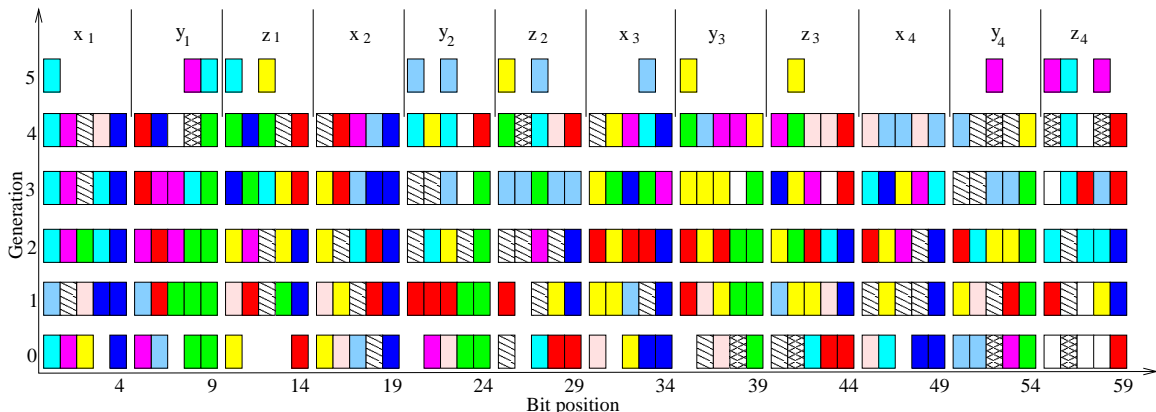


Figure 2: BB identification for the Si_4 case. Same colored box refers to the genes belonging to a BB. Vacant spots indicate that the gene is independent.

compact (require less variables) than the internal-coordinate representation for clusters with more than 6 atoms. Even though there can be infinitely many optimal structures in space-fixed coordinates (due to translation, and rotation), all the studies have shown that space-fixed representation is better than the internal-coordinate representation in terms of the algorithm efficiency. In the present study each atom is represented by cartesian coordinates (x, y, z) . Each coordinate is represented by a 5 bit binary string. For eg., a 4 atom cluster is fully represented by a 60 bit string length.

Niese and Mayne (1996) state that “the representation in space-fixed coordinates is plainly contradictory to the spirit of Goldberg’s “building block(BB) hypothesis”; none of the coordinates stand alone as a meaningful BB.”. This observation is incorrect, a BB need not be meaningful in the physical sense. A particular allele or set of alleles (of lower order) that have significant effect on the fitness of individuals form a BB. It might happen that in a given population some genes are highly correlated and hence form a BB. This claim is illustrated in fig. 2, where the BBs are as identified by ECGA for the case of 4 atom Si cluster. As can be seen in the figure in the initial generation the higher order bits of each coordinate form BBs and in the later generations the lower order bits form BBs. This clearly indicates the domino convergence effect (Thierens, Goldberg, & Pereira, 1998). This also shows that any crossover operator that does not respect the BBs result in poor performance. This is mostly the case with single point crossover.

5 Extended Compact Genetic Algorithm (ECGA)

ECGA, proposed by Harik (1999) is based on a key idea that the choice of a good probability distribution is equivalent to linkage learning. The measure of a good distribution is quantified based on minimum description length(MDL) models. The key concept behind MDL models is that given all things are equal, simpler distributions are better than the complex ones. The MDL restriction penalizes both inaccurate and complex models, thereby leading to an optimal probability distribution. Thus, MDL restriction reformulates the problem of finding a good distribution as an optimization problem that minimizes both the probability model as well as population representation. The probability distribution used in ECGA is a class of probability models known as marginal product models (MPMs). MPMs are formed as a product of marginal distributions on a partition of the genes and are similar to those of CGA (Harik, Lobo, & Goldberg, 1998) and PBIL (Baluja, 1994). Unlike the models used in CGA and PBIL, MPMs can represent probability distributions

for more than one gene at a time. MPMs also facilitate a direct linkage map with each partition separating tightly linked genes. Hence, in the current study each gene partition would refer to a BB.

The MPM concept is illustrated as follows: consider 4 bit problem and chose the following partition [0,2], [1], [3]. This partition implies that 0th and 2nd bit are jointly distributed and the 1st and the 3rd bits are independently distributed. Therefore [0,2] can take the following four values, 00, 01, 10, and 11. The probability distribution for this partition is simply the frequency of individuals with those bit values. Similarly [1] and [3] can take either 0 or 1 and the proportion of individuals have on 1 and 0 in the 1st (and similarly in the 3rd bit) is the probability distribution for that partition.

A flowchart of ECGA procedure is given in fig. 3. Two things need further explanation, one is

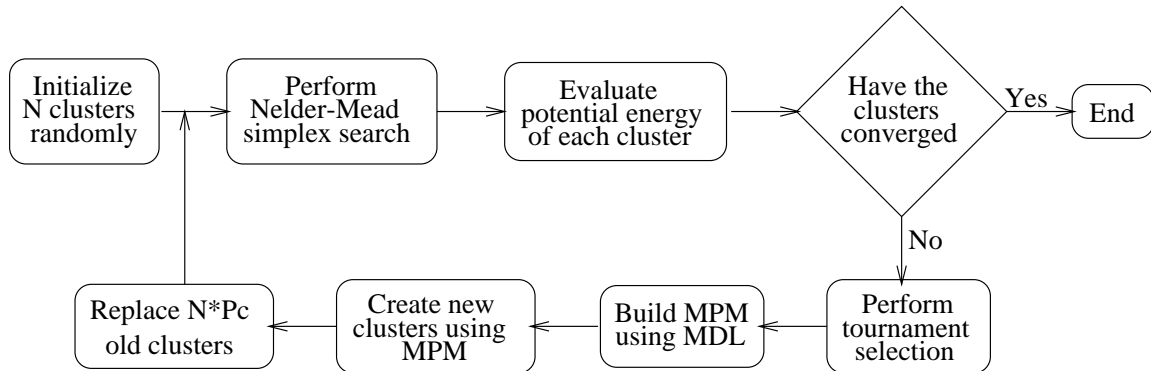


Figure 3: ECGA procedure

the identification of MPM using MDL and the other is the creation of a new population based on MPM. The identification of MPM in every generation is formulated as a constrained optimization problem,

$$\text{Minimize} \quad C_m + C_p, \quad (5)$$

Subject to

$$2^{\ell_{bb,i}} \leq N_p \quad \forall i \in [1, N_{bb}], \quad (6)$$

where C_m is the model complexity which represents the cost of a complex model and is given by

$$C_m = \log_2(N_p + 1) \sum_{i=1}^{N_{bb}} \left(2^{\ell_{bb,i}} - 1 \right), \quad (7)$$

and C_p is the compressed population complexity which represents the cost of using a simple model as against a complex one and is evaluated as

$$C_p = \sum_{i=1}^{N_{bb}} \sum_{j=1}^{2^{\ell_{bb,i}}} N_{ij} \log_2 \left(\frac{N_p}{N_{ij}} \right), \quad (8)$$

N_{bb} in the equations represent the number of BBs, $\ell_{bb,i}$ is the length of BB $i \in [1, N_{bb}]$, N_{ij} is the number of chromosomes in the current population possessing bit-sequence $j \in [1, 2^{\ell_{bb,i}}]$ ¹ for BB i . The constraint (eqn. 6) arises due to finite population size.

¹Note that a BB of length k has 2^k possible sequences where the first sequence denotes be $00 \dots 0$ and the last sequence $11 \dots 1$

A new population is generated based on the optimal MPM as follows, population of size $N_p(1 - P_c)$ where P_c is the crossover probability, is filled by the best individuals in the current population. This differs from the original ECGA procedure (Lobo & Harik, 1999) in which $N_p(1 - P_c)$ individuals were taken to be the last $N_p(1 - P_c)$ individuals of the current generation irrespective of their fitness. The rest $N_p P_c$ individuals are generated by randomly choosing subsets from the current individuals. These subsets are the gene groups identified by the current MPM. This procedure is also different from the original ECGA procedure in which the subsets were chosen by probabilistic polling. The original procedure leads to a stochastic method were as the one used in the current study is a deterministic method in which the frequencies of the bit sequence of a particular subset remains constant. However, it has been observed that the outcome of both the methods are similar and in fact the deterministic method is computationally much faster.

6 Algorithm Description

The objective of the cluster optimization problem is to minimize the total potential energy and thereby determine the lowest energy structure. As stated before we have encoded the positions of the atoms in cartesian coordinates using a 5 bit binary string for each coordinate. The initial population is generated randomly, with each coordinate sampled uniformly between $(0, \sigma \sqrt[3]{6n})$, where $\sigma = 2.0591$. These structures are then relaxed using a local search method, in our case a Nelder-Mead simplex method. Nelder-Mead simplex requires $m + 1$ initial points for an m variable problem. The initial points for every individual in a population is generated by adding a uniform random variabe between $(0, 0.1 * \sigma)$ to one of variables. For eg. if we are solving for a 4 atom cluster, then we have 12 variables. Therefore we need 13 initial clusters for the simplex method. A given individual would account for one initial value, and the rest 12 are generated by adding a uniform random value to one of the 12 variables of the given individual.

Unlike Iwamatsu (2000) who ran the simplex algorithm till a tolerance of 10^{-6} was reached, we just run it till a tolerance of 10^{-3} is reached. There are two ways of incorporating the solution obtained by the local search, one is just to assign the fitness of the local search to individual without changing the structure (Baldwinian approach) and the other is the assign both the fitness as well as the structure to the individual (Lamarckian). A rule of thumb states that Baldwinian approach should be applied for 95% of the time and Lamarckian for the rest 5%. However the present case seems to be an exception, because a preliminary study indicated that a fully Lamarckian approach is superior to the 95% Baldwinian approach. Therefore in the remainder of the study we have used a 100% Lamarckian approach.

These relaxed structures are then subjected to a tournament selection without replacement. i.e., a given number of individuals are selected from the current generation and the individual with minimum potential energy is transferred to a mating-pool. This procedure is repeated till the mating pool has exactly N_p individuals. In the present study we used tournament sizes of 8, 16, and 20. All the results reported in the present study, unless otherwise mentioned, are averages of 25 independent runs. The Nelder-Mead simplex algorithm was adopted from (Press, Flannery, Teukolsky, & Vettering, 1989).

The convergence criteria used were as follows (1) the variance of fitness of the population is less than 0.1, or (2) the variance of bit values of the population is less than 0.1, whichever occurs first. The minimum population size, convergence time and the number of function evaluations were evaluated when the ECGA failed at most once out of 25 runs. Therefore the reliability of the algorithm was set to 96%. These criteria are much more stringent than those existing in literature that just require one out of 10 runs (reliability of 10%) to reach the global minima.

7 Results and Discussion

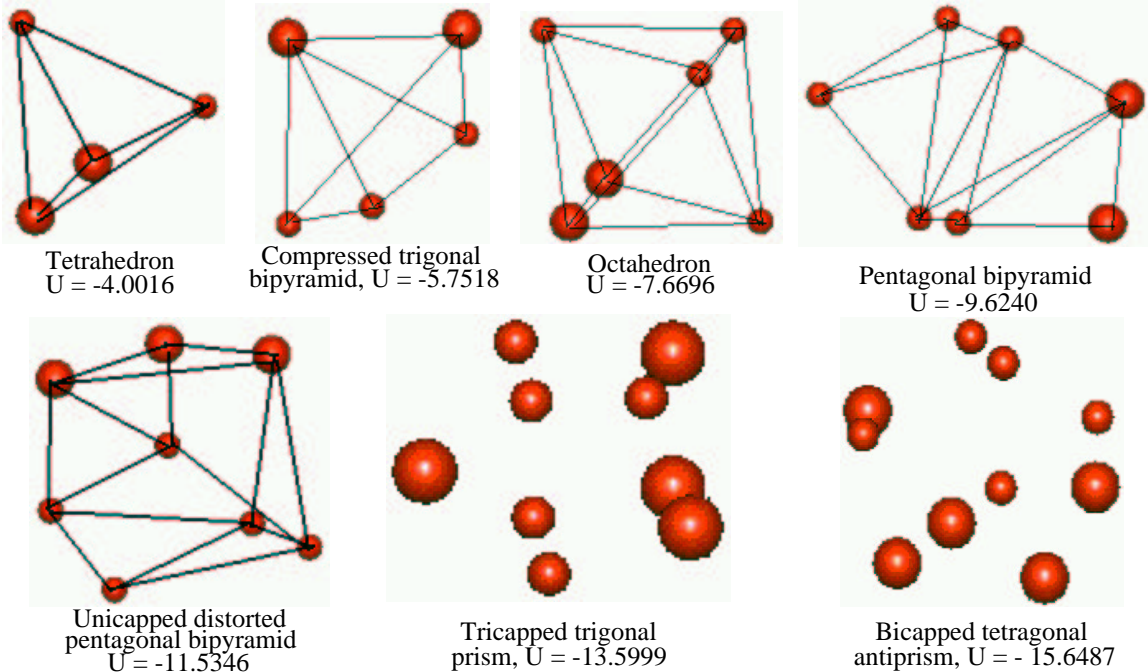


Figure 4: Optimal structures and their total potential energy (in units of $\epsilon = 2.17$ eV) predicted by ECGA for different cluster sizes.

The optimal structures obtained for different cluster sizes along with their potential energy (in units of $\epsilon = 2.17$ eV) are shown in fig. 4. All the structures predicted by ECGA agree with those in literature (Iwamatsu, 2000) indicating that ECGA was successful in reaching global optimum effectively. Illustrations of a single GA run for the case of 6 and 7 atom clusters are given in figs. 5 and 6 respectively. It can be seen in both cases that in the initial generation the structure is very bad, but ECGA quickly converges to a structure close to the optimal structure and then slightly modifies it to reach the global structure. The energy variation is only in the second or third decimal place in those stages.

The minimum population size required for different cluster sizes is shown in fig. 7. The minimum population size scales up with the size of the cluster as $\mathcal{O}(n^{4.2})$. The number of generations taken by ECGA for different cluster sizes is shown in fig. 8. The results show that ECGA converges much faster than those existing in literature, even though the reliability and convergence criteria are much more stringent. This emphasizes the effectiveness of having good operators that preserve good BBs. Finally the number of function evaluations taken by ECGA for different size clusters is shown in fig. 9. The number of function evaluations scales up with the size of the cluster as $\mathcal{O}(n^{8.2})$. It has to be noted that the high reliability constraint is the reason why the algorithm scales so badly. In fact, if the reliability constraint is reduced to 80%, then the minimum population size scales up as $\mathcal{O}(n^{0.86})$ and the number of function evaluations scales up as $\mathcal{O}(n^{2.1})$. As far as we know all the reliability restrictions of all the other existing cluster optimization algorithms are very low (about 10%).

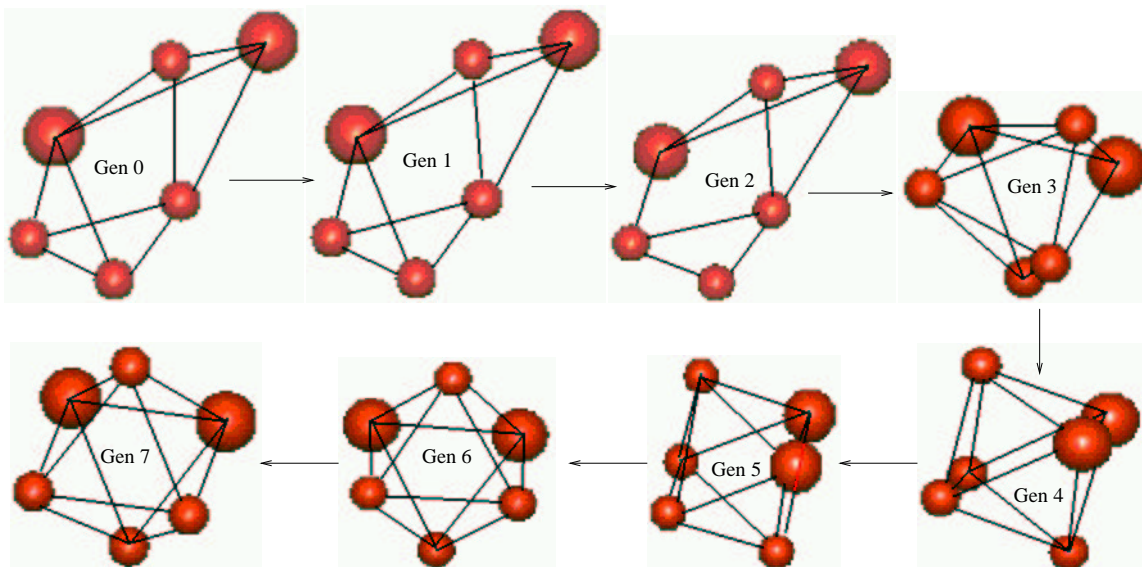


Figure 5: Example of single GA run for 6 atom cluster.

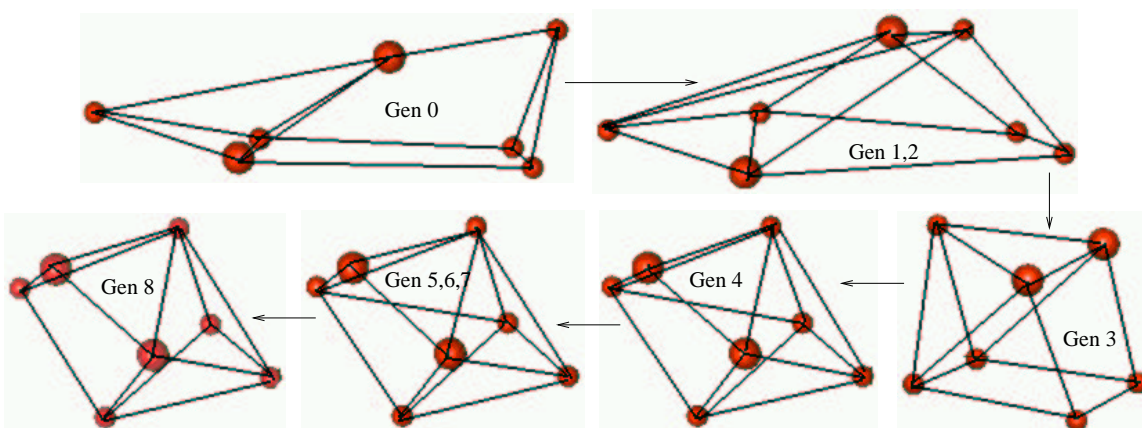


Figure 6: Example of a single GA run for 7 atom cluster.

8 Conclusion

We have developed a hybrid competent genetic algorithm that utilizes Nelder-Mead simplex algorithm for optimizing small silicon clusters. We have successfully predicted optimal structures for clusters of size 4-11. These results agree with those in literature. Furthermore, we have empirical evidence that the number of function evaluations and the population size increase with the number of atoms in a cluster as $\mathcal{O}(n^{4.2})$ and $\mathcal{O}(n^{8.2})$ respectively. The results indicate that more efficient algorithms have to be designed that retain the high reliability of the proposed technique but would have a better scale-up behavior.

Acknowledgments

The first author was sponsored by the Air Force Office of Scientific Research, Air Force Materiel Command, USAF, under grant F49620-00-1-0163. Research funding for this work was also provided

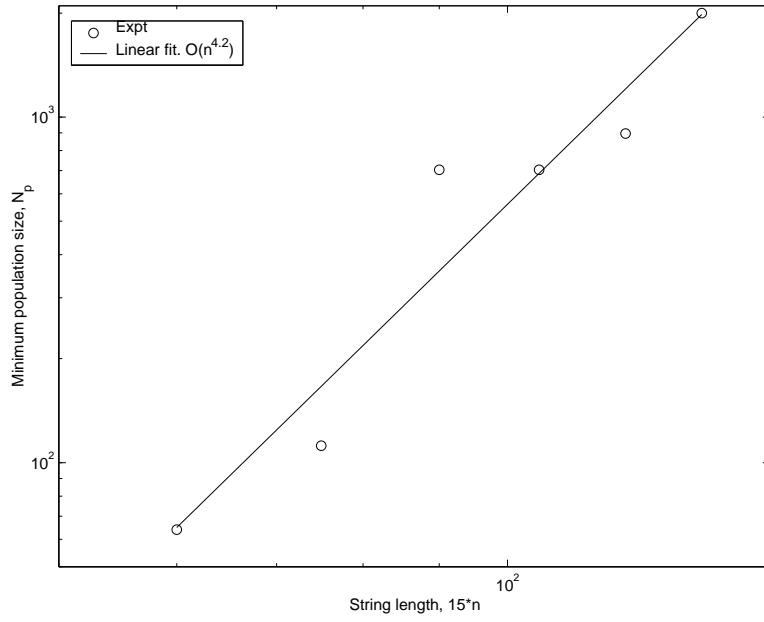


Figure 7: Minimum population size required to reach the global optima for different cluster sizes.

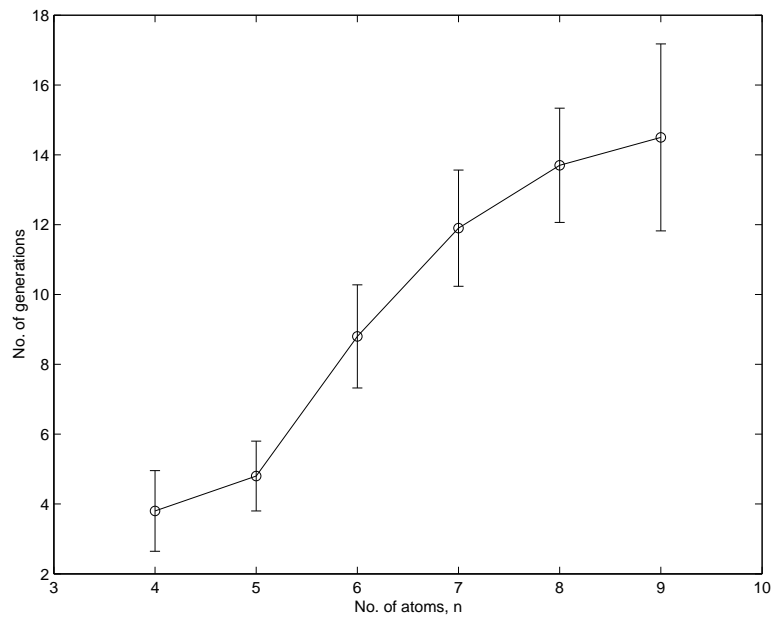


Figure 8: Convergence time to reach the global optima for different cluster sizes.

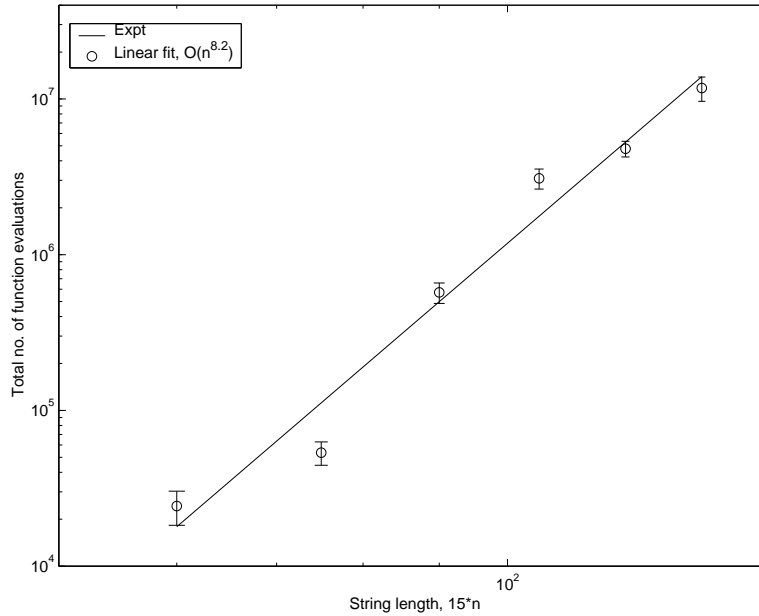


Figure 9: Number of function evaluations required to reach the global optima for different cluster sizes.

by the National Science Foundation under grant DMI-9908252. Support was also provided by a grant from the U. S. Army Research Laboratory under the Federated Laboratory Program, Cooperative Agreement DAAL01-96-2-0003. The U. S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation thereon.

The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research, the National Science Foundation, the U. S. Army, or the U. S. Government.

We thank Prof. Ceperley for his useful suggestions and comments. Thanks are also due to Prof. Goldberg.

References

- Baluja, S. (1994). *Population-Based Incremental Learning: A Method of Integrating Genetic Search Based Function Optimization and Competitive Learning* (Technical Report CMU-CS-94-163). Carnegie Mellon University.
- Deaven, D., & Ho, K. (1995). Molecular Geometry Optimization With A Genetic Algorithm. *Phy. Rev. Let.*, 75, 288–291.
- Goldberg, D. (1989). *Genetic algorithms in search optimization and machine learning*. Reading, MA: Addison-Wesley.
- Goldberg, D., Deb, K., Kargupta, H., & Harik, G. (1993). Rapid, Accurate Optimization of Difficult Problems Using Fast Messy Genetic Algorithms. In *International Conference on Genetic Algorithms* (pp. 56–64). San Mateo, CA: Morgan Kaufmann.
- Goldberg, D., Thierens, D., & Deb, K. (1993). Toward a Better Understanding of Mixing in Genetic Algorithms. *J. Soc. Instrument and Control Engineers*, 32(1), 10–16.

- Goldberg, D. E. (1999). *Evolutionary design by computers* (Chapter 4. The Race, the Hurdle, and the Sweet Spot: Lessons from Genetic Algorithms for the Automation of Design Innovation and Creativity, pp. 105–118). San Mateo, CA: Morgan Kaufmann.
- Gong, X. (1993). Empirical-Potential Studies on the Structural Properties of Small Silicon Clusters. *Phys. Rev. B*, 47(4), 2329–2332.
- Gregurick, S., & Alexander, M. (1996). Global Geometry Optimization of $(\text{Ar})_n$ and $\text{B}(\text{Ar})_n$ Clusters Using A Modified Genetic Algorithm. *J. Chem. Phys.*, 104(7), 2684–2691.
- Harik, G. (1999, January). *Linkage Learning via Probabilistic Modeling in the ECGA* (IlligAL Report No. 99010). Urbana, IL: University of Illinois at Urbana-Champaign.
- Harik, G., & Goldberg, D. E. (1997). Learning Linkage. In Belew, R., & Vose, M. (Eds.), *Foundations of Genetic Algorithms*, Volume 4 (pp. 247–262). San Francisco, CA: Morgan Kaufmann Publishers, Inc.
- Harik, G., Lobo, F., & Goldberg, D. E. (1998). The Compact Genetic Algorithm. In *IEEE Conference on Evolutionary Computation* (pp. 523–528). Piscataway, NJ: IEEE Service Center.
- Hartke, B. (1993). Global Geometry Optimization of Clusters Using Genetic Algorithm. *J. Phys. Chem.*, 97, 9973–9976.
- Hartke, B. (1995). Global Geometry Optimisation of Clusters Using a Growth Strategy Optimized by a Genetic Algorithm. *Chem. Phys. Lett.*, 240, 560–565.
- Hoare, M. (1979). Structure and Dynamics of Simple Microclusters. *Adv. Chem. Phys.*, 40, 49–135.
- Iwamatsu, M. (2000). Global Geometry Optimization of Silicon Clusters Using the Space-Fixed Genetic Algorithm. *J. Chem. Phys.*, 112(24), 10976–10983.
- Judson, R. (1997). Genetic Algorithms and Their Use in Chemistry. *Rev. Comput. Chem*, 10, 1–73.
- Kargupta, H. (1996). The Gene Expression Messy Genetic Algorithm. In *International Conference on Evolutionary Computation* (pp. 814–819). Piscataway, NJ: IEEE Service Center.
- Lobo, F., & Harik, G. (1999, January). *Extended Compact Genetic Algorithm in C++* (IlligAL Report No. 99016). Urbana, IL: University of Illinois at Urbana-Champaign.
- Munetomo, M., & Goldberg, D. (1999). Linkage Identification by Non-Monotonicity Detection for Overlapping Functions. *Evolutionary Computation*, 7(4), 377–398.
- Niese, J., & Mayne, H. (1996). Global Geometry Optimization of Atomic Clusters Using A Modified Genetic Algorithm ins Space-Fixed Coordinates. *J. Chem. Phys.*, 105(11), 4700–4706.
- Northby, J. (1987). Structure and Binding of Lennard-Jones Clusters:13. *J. Chem. Phys.*, 87(10), 6166–6177.
- Pelikan, M., Goldberg, D. E., & Cantu-Paz, E. (2000). *Bayesian Optimization Algorithm, Population Sizing and Time to Convergence* (IlligAL Report No. 2000001). Urbana, IL: University of Illinois at Urbana-Champaign.
- Press, W., Flannery, B., Teukolsky, S., & Vetterling, W. (1989). *Numerical recipes in c*. Cambridge: Cambridge University Press.
- Sastry, K., & Goldberg, D. (2000). *On Extended Compact Genetic Algorithm* (IlligAL Report No. 2000026). Urbana, IL: University of Illinois at Urbana-Champaign.

- Stillinger, F., & Weber, T. (1985). Computer Simulation of Local Order in Condensed Phases of Silicon. *Phys. Rev. B*, *31*(8), 5262–5271.
- Tersoff, J. (1988). New Empirical Approach for the Structure and Energy of Covalent Systems. *Phys. Rev. B*, *37*(12), 6991–7000.
- Thierens, D. (1994). *Analysis and Design of Genetic Algorithms*. Doctoral dissertation, Katholieke Universiteit Leuven, Leuven, Belgium.
- Thierens, D., & Goldberg, D. (1993). Mixing in Genetic Algorithms. In Forrest, S. (Ed.), *International Conference On Genetic Algorithms* (pp. 38–45). San Mateo, CA: Morgan Kaufmann.
- Thierens, D., Goldberg, D. E., & Pereira, A. G. (1998). Domino Convergence, Drift, and the Temporal-Salience Structure of Problems. In *IEEE International Conference on Evolutionary Computation* (pp. 535–540). Piscataway, NJ: IEEE Service Center.
- Tsutsui, S., Goldberg, D., & Sastry, K. (2000). *Progress Toward Linkage-Identification in Real Coded GAs with Simplex Crossover* (IlligAL Report No. 2000033). Urbana, IL: University of Illinois at Urbana-Champaign.
- Wille, L., & Vennik, J. (1985). Computational Complexity of the Ground-State Determination of Atomic Clusters. *J. Phys. A*, *18*(8), L419–L422.
- Zeiri, Y. (1997). Study of the Lowest Energy Structure of Atomic Clusters Using a Genetic Algorithm. *Comput. Phys. Commun.*, *103*(1), 28–42.
- Zeiri, Y., Fattal, E., & Kosloff, R. (1995). Application of Genetic Algorithm to the Calculation of Bound States and Local Density Approximations. *J. Chem. Phys.*, *102*(4), 1859–1862.