Fast Global Optimization of Difficult Lennard-Jones Clusters

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Abstract. The minimization of the potential energy function of Lennard-Jones atomic clusters has attracted much theoretical as well as computational research in recent years. One reason for this is the practical importance of discovering low-energy configurations of clusters of atoms, in view of applications and extensions to molecular conformation research; another reason of the success of Lennard Jones minimization in the global optimization literature is the fact that this is an extremely easy-to-state problem, yet it poses enormous difficulties for any unbiased global optimization algorithm.
In this paper we propose a computational strategy which allowed us to rediscover most putative global optima known in the literature for clusters of up to 80 atoms and for other larger clusters, including the most difficult cluster conformations. The main feature of the proposed approach is the definition of a special purpose local optimization procedure aimed at enlarging the region of attraction of the best atomic configurations. This effect is attained by performing first an optimization of a modified potential function and using the resulting local optimum as a starting point for local optimization of the Lennard Jones potential.
Extensive numerical experimentation is presented and discussed, from which it can be immediately inferred that the approach presented in this paper is extremely efficient when applied to the most challenging cluster conformations. Some attempts have also been carried out on larger clusters, which resulted in the discovery of the difficult optimum for the 102 atom cluster and for the very recently discovered new putative optimum for the 98 atom cluster.

Keywords: Global Optimization, Lennard-Jones clusters, Molecular Conformation

1. Introduction

One of the simplest to describe yet most difficult to solve problems in computational chemistry is the automatic determination of molecular conformation. A molecular conformation problem can be described

as that of finding the global minimum of a suitable potential energy function which depends on relative atom positions. Many models have been proposed in the literature, ranging from very simple to extremely complex, like, e.g., the so-called protein folding problem (Neumaier, 1997). While realistic models of atomic interactions take into account different components of the potential energy function, like pairwise interactions, dihedral angles, torsion, and allow the analysis of composite molecules in which atom of different kinds interact, it is commonly recognized in the chemical literature that a fundamental step towards a better understanding of some molecular conformation problems is the knowledge of the global minimum of the so called Lennard-Jones potential energy model; this model is a sufficiently accurate one for noble gas clusters. Moreover some of the most difficult to find Lennard-Jones structures, exactly those towards which this paper is oriented, were found to represent very closely the structure of nickel and gold clusters (Wales and Scheraga, 1999).

In this model all atoms are considered to be equal and only pairwise interaction is included in the definition of the potential energy. Let $N \geq 2$ be an integer representing the total number of atoms. The Lennard-Jones (in short L-J) pairwise potential energy function is defined as follows: if the distance between the centers of a pair of atoms is r, then their contribution to the total energy is defined to be

$$v(r) = \frac{1}{r^{12}} - \frac{2}{r^6} \tag{1}$$

and the L-J potential energy E of the molecule is defined as

$$E(X) = E(X_1, \ldots, X_N) = \sum_{i<j} v\left(\|X_i - X_j\|\right) \tag{2}$$

where $X_i \in I\!R^3$ represents the coordinates of the center of the i–th atom and the norm used is the usual Euclidean one. An optimum L-J configuration $X^\star = \{X_1^\star, \ldots, X_N^\star\}$ is defined as the solution of the global optimization problem

$$LJ_N = E(X^\star) = \min_{X \in I\!R^{3N}} E(X). \tag{3}$$

Although extremely simplified, this model has attracted research in chemistry and biology, as it can be effectively considered as a reasonably accurate model of some clusters of rare gases and as it represents an important component in most of the potential energy models used for complex molecular conformation problems and protein folding (Neumaier, 1997).

From the point of view of numerical optimization methods, this problem is an excellent test for local and global unconstrained optimization methods; it is one of the simplest models in the literature of test problems (see e.g. Floudas and Pardalos, 1999 pag. 188–193), yet one of the most difficult as it has been conjectured (Hoare, 1979) that the number of local optimum conformations grows at least exponentially with N. Many computational approaches can be found in the literature, ranging from mathematical programming models (Gockenbach et al., 1997), to genetic methods (Deaven et al., 1996), to Montecarlo sampling (Wales and Doye, 1997) and many others. For a recent review of the state of the art in this subject, the reader may consult (Wales and Scheraga, 1999).

Unfortunately very few theoretical results are available which could be used to tune an optimization method for the L-J minimization problem. One notable exception is the result of (Xue, 1997) where it is proven that in any global optimum the pairwise interatomic distance is bounded from below by 0.5: while this result is considered obvious in the chemical literature, only recently it has been proven in a formal way. Very little is a-priori known on the structure of the global optima; even a quite reasonable conjecture stating that the diameter of an optimum N–atoms cluster is $O(N^{1/3})$ is still open. Thus, except for extremely small and easy cases, there are no proofs of global optimality for the putative global optimum configurations known in the literature (see the L-J page on the Cambridge Clusters Database at URL `http://www.brian.ch.cam.ac.uk`). All published results are aimed at confirming, through experimentation, numerical results known in the literature or at improving current estimates of the global optima.

Despite the complexity of the problem, most putative global optima of micro-clusters (with up to 147 atoms) have been discovered by means of a very simple and efficient algorithm first proposed in (Northby, 1987) and further refined in (Xue, 1994), which is based on the idea of starting local optimization from initial configurations built by placing atoms in predefined points in space, according to lattice structures which researchers in chemistry and physics believe are the most common ones found in nature. However quite a few exceptions to regular lattice-based structures do exist; these structures are extremely difficult to discover with general purpose methods. It is to be remarked that new optima are still being discovered, even though at a slower rate than just a few years ago. In August 1999, for example, a new configuration for LJ_{98} was discovered (Leary and Doye, 1999) and possibly other new records will appear even in the range $N \leq 147$ which has been the most thoroughly and extensively studied in the last decade.

In this paper we propose a new methodology aimed at discovering the most difficult structures for Lennard-Jones clusters. Our main aim is not to introduce a general purpose method, but that of defining a new strategy for local searches which can be profitably included in any algorithm which is based on local searches, including the basin-hopping method (Wales and Doye, 1997), the big-bang method (Leary, 1997), Leary's descent method (Leary and Doye, 1999) or genetic algorithms (see (Deaven et al., 1996), (Pullan, 1999)). Our method consists in a modification of the objective function, in the first phase of the descent, which enables a local search algorithm to escape from the enormous number of local optima of the L-J energy landscape; implemented in a straightforward Multistart-like method, our modification improved by at least two order of magnitude the number of local searches required to find the difficult 38 and 75 atom cases and could find the new 98 atom cluster and the difficult 102 case in less than 10 000 local searches. In a series of runs the LJ_{38} optimum was discovered in 56% of the local searches performed, an incredible performance if compared with the best result published so far in which LJ_{38} is found in 0.3% of the attempts (Leary, 1997). In our first attempt to attack the LJ_{98} case, which was discovered only in summer 1999 (Doye et al., 1999a) using "millions of local searches" (Anonymous, 1999), we were able to find the global optimum in less than 10 000 local searches, on average.

2. A new approach to the detection of Lennard-Jones clusters

We consider Multistart-like approaches to the problem of globally minimizing the Lennard-Jones potential function. The pure Multistart method can be described as follows.

Pure Multistart

1. Generate a point $X \in I\!R^{3N}$ from the uniform distribution over a sufficiently large box centered at the origin;
2. perform a local search in $I\!R^{3N}$ using X as a starting point;
3. if a stopping condition is not satisfied, go back to 1, otherwise return the local minimum with the lowest function value.

Of course, we can not expect Pure Multistart to be a feasible method for the solution of the Lennard-Jones problem. Indeed, even though the difficulty of solving a global optimization problem by Multistart is not

actually related to the number of local minima, but to the measure of the basin of attraction of the global minimum, the fact that the number of local minima is exponentially large is a clear indication that Multistart may experience great difficulties in solving this kind of problems. Numerical computations tend to confirm this fact. In Table I we notice that Pure Multistart (PMS) applied to problems with $N \in \{10, \ldots, 30\}$ fails to detect the putative global optimum for $N = 21, 27, 28, 29$ after 1 000 trials and has very low percentage of successes for many other values of N.

Therefore, it seems necessary to modify the basic Multistart scheme in order to be able to solve larger problems. A simple idea is to exploit the special structure of the Lennard-Jones potential function and modify the search mechanism accordingly. Looking at the form of the pairwise interaction function (1) we notice that good solutions should possess some or all of the following characteristics:

- atoms should not be too close each other (also recalling the result in Xue, 1997);
- the distance between many pairs of atoms should be close to 1.0, since at 1.0 the Lennard-Jones pair potential attains its minimum;
- the optimal configuration should be as compact as possible, i.e. the diameter of the cluster should not be too large.

According to these elementary observations, it is possible to substitute the uniform random generation of points (Step 1 in the Pure Multistart method) by a generation mechanism which tends to favor point configuration possessing the above characteristics. As a first attempt in this direction we substituted the uniform random generation procedure with the following:

Point Generation Procedure

1. Start with a single atom placed in the origin, i.e. let $X_1 = 0 \in \mathbb{R}^3$; set $X = \{X_1\}$ and $k = 2$.
2. Generate a random direction $d \in \mathbb{R}^3$ and a point X_k along this direction in such a way that its minimum distance r from every point in X is at least 0.5.
3. If r is greater than a threshold $R > 1$ then X_k is shifted towards the origin along direction d, until its distance from at least one point in X becomes equal to R.

4. Set $X = X \cup \{X_k\}$. If $k = N$, stop; otherwise set $k := k + 1$ and go back to Step 2.

This different point generation procedure slightly improves the performance of Multistart as it can be seen from Table I where the results of Multistart equipped with this generation algorithm are displayed under the heading MMS (Modified Multistart); however even this modified algorithm soon starts failing in detecting the putative global optima of moderately large clusters.

Table I. Number of successes in 1000 random trials by Pure Multistart (PMS) and Modified Multistart (MMS) methods.

N	PMS	MMS	N	PMS	MMS
11	32	36	21	-	-
12	24	53	22	1	3
13	19	32	23	1	5
14	45	91	24	1	5
15	34	73	25	2	3
16	12	34	26	1	-
17	3	9	27	-	1
18	1	1	28	-	-
19	3	6	29	-	-
20	3	7	30	1	-

It might be possible to refine further the Point Generation Procedure in order to produce better starting points, but it is felt that no real breakthrough can be achieved in this direction. It seems more reasonable to attack the problem by changing another component of the Multistart method, i.e. the local search procedure; we are thus led to search for a local optimization method which avoids as much as possible being trapped in stationary points of the Lennard-Jones potential characterized by a high value of the potential energy (2). The idea is that of performing local searches employing a modified objective function which, although related to the Lennard-Jones potential, is in some sense "biased" towards configurations which satisfy the above requirements. The local minimum of this modified potential is then used as a starting point for a local optimization of the Lennard-Jones potential function. This leads to the following version of the Multistart method. Let $ME(X)$ be a suitably defined modified potential function.

Two-Phase Multistart

1. Generate a point $X \in \mathbb{R}^{3N}$ according to the Point Generation Procedure;
2. perform a local minimization of the modified potential function ME in $\mathbb{R}^{3N}$ using X as a starting point; let $\hat{X}$ be the local optimum thus obtained;
3. perform a local optimization of the Lennard-Jones potential (2) starting from $\hat{X}$;
4. if a stopping condition is not satisfied, go back to Step 1; otherwise return the local minimum of E with the lowest function value.

We notice that, in place of the usual local search of the Pure or Modified Multistart method, here we have what we call a *two-phase local search*: first the function ME is optimized, and then the Lennard-Jones potential E. We underline that, even if at each iteration two local searches are started, the computational effort is not doubled: indeed, the local minimum $\hat{X}$ of ME is typically quite close to a local minimum of E, so that the computational effort of the second local search is much lower than that of the first one.

Accordingly we need now to define ME in such a way that the local minima of this function possess the desired characteristics. In what follows two classes of functions, among which ME can be chosen, are introduced. The first class contains functions with the following form

$$\sum_{i<j} g\left(\|X_i - X_j\|\right), \tag{4}$$

where

$$g(r) = \frac{1}{r^{2p}} - \frac{2}{r^p} + \mu r. \tag{5}$$

Here $p > 0$ and $\mu \geq 0$ are real constants; we note that choosing $p = 6$ and $\mu = 0$, g coincides with the Lennard-Jones pair potential (1). In Figure 1 the case $p = 4$ and $\mu = 0.3$ is displayed and compared with the Lennard-Jones pair potential. The parameters p and μ have important effects. By choosing $p < 6$ atoms can be moved more freely; by decreasing p, the effect of the infinite barrier at $r = 0.0$, which prevents atoms from getting too close to each other, is also decreased. The parameter μ has two important effects.

Local effect : it gives stronger penalty to distances between atoms greater than 1.0; actually, it also assigns low penalty for pair distances lower than 1.0, but this is largely overcome by the barrier effect which, as already remarked, prevents atoms from getting too close each other.

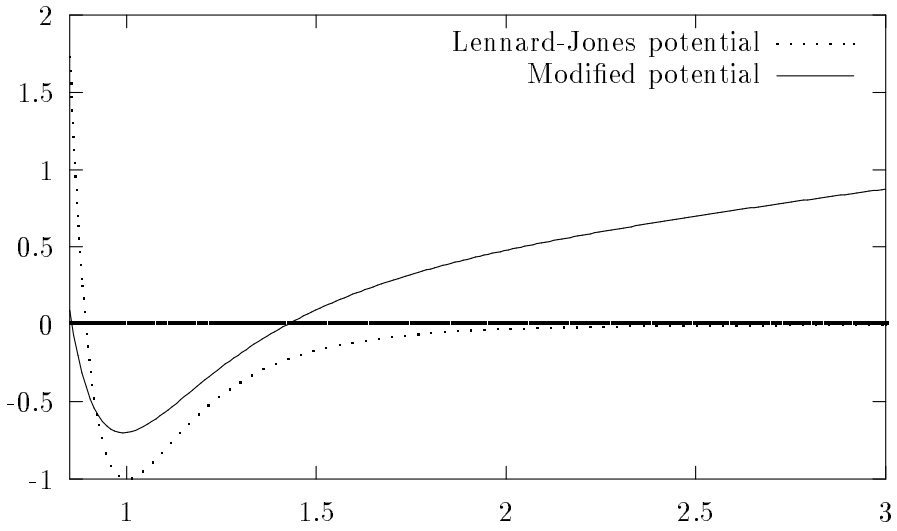

Figure 1. Comparison between Lennard-Jones and Modified potentials.

Global effect : it gives strong penalty to large distances between atoms, e.g. to the diameter of the molecule.

In order to test the feasibility of this approach, a series of numerical experiments have been performed by running 10 000 times the algorithm for $N = 10, ..., 80$. As these experiments were carried out on Pentium II PC's, we did not performed extensive and generalized trials for $N > 80$. In Table II the number of two-phase local searches which led to the putative global optimum are reported. We notice that the percentage of successes is much higher than the one of the Pure or Modified Multistart algorithm. In particular, two important cases are discussed. The first case is $N = 38$, which is considered in the literature a particularly difficult one (Doye et al., 1999a). While most putative global optima in the range $\{10, \ldots, 80\}$ have a so called icosahedral structure, the putative global optimum for $N = 38$ has a FCC (Face Centered Cubic) structure, and many algorithmic approaches, such as the lattice search in (Northby, 1987) and (Xue, 1994), biased towards icosahedral structures, are unable to detect this solution. The new putative global optimum was first observed only recently in (Doye et al., 1995) using a direct approach based on molecular dynamics; more recently, in (Leary, 1997) the putative global optimum was found using the "big bang" global optimization algorithm employing on the average 330 local searches, while for the basin hopping algorithm proposed in

(Wales and Doye, 1997), the expected number of local searches required to first hit this putative global optimum is 2 000. In the new approach, choosing $p = 4$ and $\mu = 0.3$, the expected number of local searches is reduced to 80, but, with the method described later in this paper, we were able to obtain the incredible hitting rate of 1.79 local searches on the average.

As it can be observed from Table II, although quite successful for some configurations, our method fails in several cases; most notably it does not discover, at least in the first 10 000 local searches, the difficult structure of LJ_{75}. This case is the second hard case in the range $\{10, \ldots, 80\}$ and it is much harder than the $N = 38$ case (in order to appreciate the difficulties of both cases see the discussion about multiple funnel landscapes in (Doye et al., 1999b)). As for $N = 38$, the structure of the putative global optimum is non icosahedral (actually the structure is a decahedral one). The putative global optimum has been detected for the first time in (Doye et al., 1995); by employing the Basin Hopping algorithm the reported expected number of local searches to first detect this configuration is over 100 000. Thus our failure in detecting LJ_{75} during the first 10 000 local searches was not a surprise.

However, instead of insisting with an higher number of local searches, a modification of (5) was introduced in order to strengthen the global effect. This lead to the following class of modified functions:

$$\sum_{i<j} h\left(\|X_i - X_j\|\right), \tag{6}$$

where

$$h(r) = \frac{1}{r^{2p}} - \frac{2}{r^p} + \mu r + \beta(\max\{0, r^2 - D^2\})^2, \tag{7}$$

where $p, \mu, \beta, D \geq 0$; D is an underestimate of the diameter of the cluster. In Figure 2 the case $p = 4, \mu = 0.2, \beta = 1, D = 2$ is displayed and compared with the Lennard-Jones pair potential function. We notice that the penalty term $\beta(\max\{0, r^2 - D^2\})^2$ has no influence on pairs of atoms close to each other, but strongly penalizes atoms far away from each other. Thus, the new term does not affect the local properties, but strengthens the global ones. The results for this class of modified functions are reported in Table III. In particular, we note the following results for the two difficult, non icosahedral cases, obtained with suitable choices of the parameters.

- For $N = 38$ the expected number of (two-phase) local searches to first hit the putative global optimum is $\frac{10\,000}{1\,831} = 5.46$, more than 60 times faster, in terms of local searches performed, than Big Bang and 366 faster than Basin Hopping;

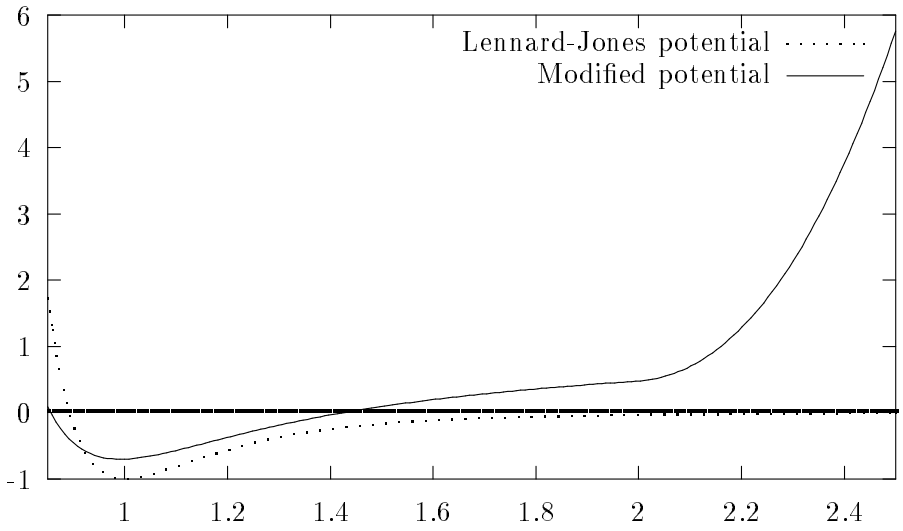

Figure 2. Comparison between Lennard-Jones and modified potentials with diameter penalization.

– for $N = 75$ the expected number of local searches is 3 333, while it was 125 000 for the Basin Hopping algorithm: the improvement factor is thus more than 37.

Given the results of $N = 75$, a better explanation of the failure of our first approach can be given, supported by the observation of the structure of the optimal decahedral structure (see Figure 3) and icosahedral structure (see Figure 4).

In the best icosahedral structure the number of pairs of atoms which are within distance close to 1.0 is 328, higher than what observed in the optimal decahedral structure (319 pairs). In some sense, the icosahedral structure has better local properties than the decahedral one. However, this local disadvantage is compensated by the compactness of the decahedral structure with respect to the icosahedral one: the diameter of the decahedral structure is quite lower than the diameter of the icosahedral one. Moreover, thanks to the compact structure, many pairs of atoms in the decahedral structure have a distance which is equal to the diameter (10 pairs in total, while the icosahedral structure has only 2). In some sense we can say that the decahedral structure has better global properties than the icosahedral one. In view of this comparison, it is now possible to understand the failure for $N = 75$ when (5) is employed. The linear penalty term μr has, as already

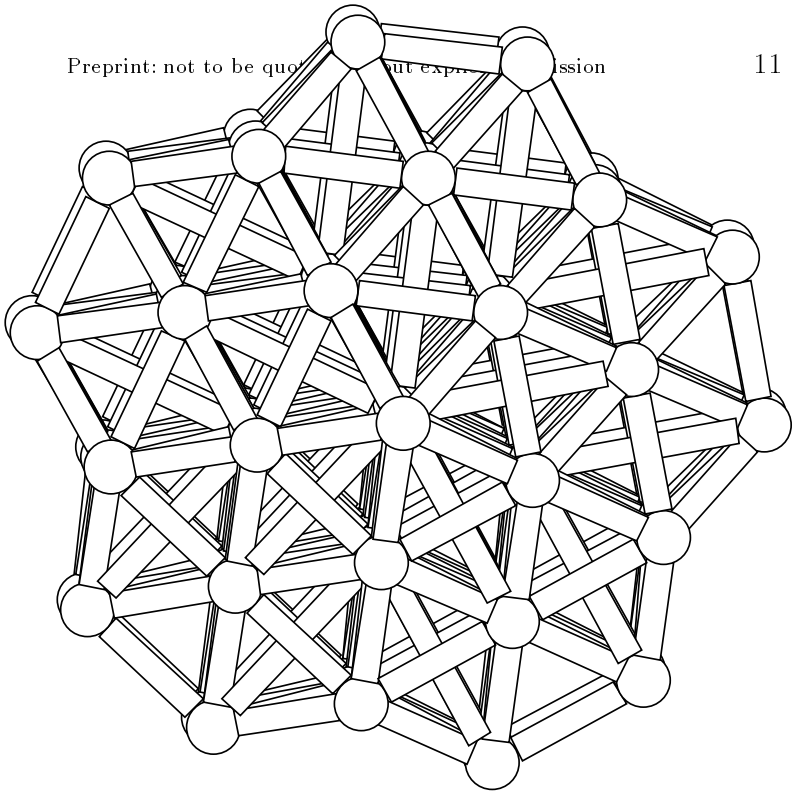

Figure 3. Putative optimum for LJ_{75}

remarked, a double effect: a local effect, rewarding solutions with good local properties (like the icosahedral structure), and a global effect, rewarding solutions with good global properties (like the decahedral structure). What appears to happen for $N = 75$ is that the local effect dominates the global one, thus favoring the icosahedral structure with respect to the decahedral one.

Even though complete computations have been performed only up to $N = 80$, the new approach has been tested for two other difficult cases, for which the putative global optimum is known to be not icosahedral.

- Very recently in (Leary and Doye, 1999) a new, non icosahedral, putative global optimum for $N = 98$ has been detected, displaying a very compact structure; it is reported that this discovery required "millions of local searches" (Anonymous, 1999); our new approach could detect this solution within 10 000 local searches on the average.

- In (Wales and Doye, 1997) a non icosahedral putative global optimum for $N = 102$ has been detected. The new approach was able

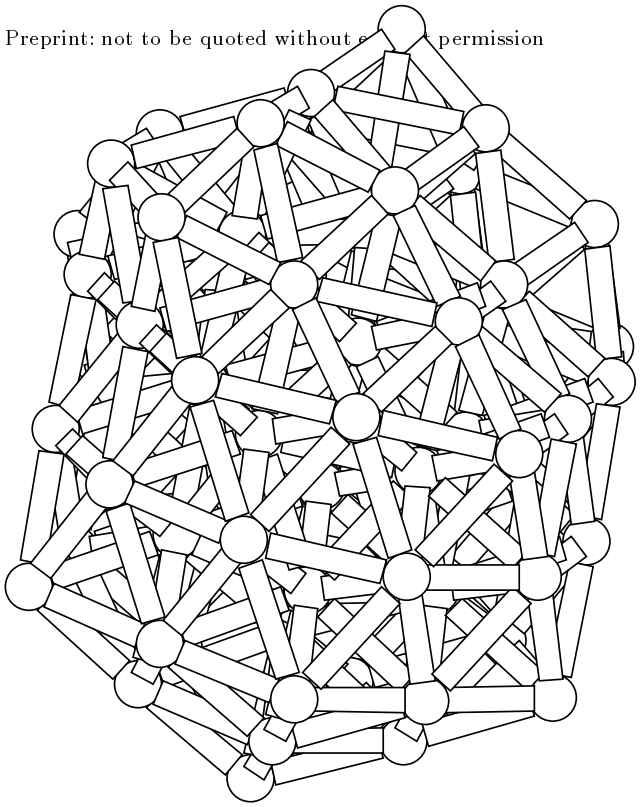

Figure 4. Icosahedral optimum for LJ_{75}

to detect this solution within 10 000 local searches, while the Basin Hopping algorithm could detect the same solution only 3 times out of 500 000 local searches.

In other series of experiments with different parameter settings sometimes better results were found. As a particularly significative instance, for LJ_{38} with parameters $p = 5, \mu = 0., D = 2.25, \beta = 1.$ the incredible result of 56% successes was recorded in 1000 random trials. In practice this means that, with such a parameter setting, the FCC structure of LJ_{38} can be observed after a fraction of a second of CPU time on a normal personal computer.

2.1. Limits of the proposed approach

It is fair to consider the limits of the proposed approach and possible ways to overcome them. The main limits of the approach can be seen from the tables. We notice that for $N > 60$ in many cases the putative global optimum could not be detected. It is not possible to claim that our new approach is a general one to solve problems for *any* value of N.

What can be safely assumed is that it is an extremely successful method in detecting those structures which differ from the icosahedral one; this is particularly important as it is believed that when the number of atoms N is large, compact, non-icosahedral structures prevail. For most tested value of N for which the optimal structure is known to be non icosahedral ($N = 38, 75, 76, 77, 98, 102$) our method is much faster (up to two orders of magnitude) than any other approach found in the literature. It must be again underlined that, in the literature, these cases are considered by far the most difficult ones. However, the approach is not able to detect in an effective way some of the optimal icosahedral structures. In order to detect these optimal structures it is possible to incorporate the two-phase local search on which the new approach is based into some of the approaches proposed in the literature such as the Basin Hopping algorithm: the rationale behind this is that it appears that the use of our modified potential, two-phase local optimization actually enlarges the region of attraction of global optima. In this respect, the choice of imposing a very low penalty on the diameter should be considered safer, as the effect of this penalty is usually so strong that only very compact structures are effectively found (most micro clusters are indeed non compact).

An approach based on a forward procedure followed by a correction procedure, has been tried, which enabled us to detect all the solutions which could not be detected by the previous approach. The forward procedure is already known in the literature and consists of starting the optimization of LJ_N from a good configuration of LJ_{N-1}, adding first a single atom and then optimizing the overall potential; we implemented a variant which incorporates the two-phase local search in place of the regular local optimization. The correction procedure, starting from the best local optimum found, is based upon the displacement of two atoms randomly chosen among those with highest energy contribution into a different position, followed by the usual two-phase optimization. Details on these procedures can be found in (Locatelli and Schoen, 1999), where it is shown that all those configurations which could not be observed through our two-phase Multistart method can be obtained by these more specialized methods.

Another critic to the proposed approach is the difficulty of choosing sensible values for the parameters. Again it has to be remarked that there is no general rule to choose a set of parameters which is sufficiently good for a whole range of clusters. The main reason for this is that, as it has already been remarked, cluster structures vary abruptly around some "magic numbers", like $N = 38, 75, 98, 102$.

In an attempt to find general rules, we performed other experiments, using the following parameters: $p = 5$ (which is an intermediate value

between 4 and 6 used in previous experiments), $\beta = 1$; parameter D, which governs the threshold for diameter penalization, was chosen as a function of N, based upon a regression on the diameters of putative global optima. In particular we choose

$$D = \sqrt[3]{1.3N - 6.5} - 1.1 \tag{8}$$

where the term $\sqrt[3]{1.3N - 6.5}$ comes from a regression analysis of the diameters of putative global optima, while 1.1 is included to force very compact structures during the first phase. Two sets of experiments were carried out choosing respectively $\mu = 0$ and $\mu = 0.1$ in (7). The results of these experiments are not reported here for sake of brevity, but can be obtained through the web page of the second author. Again, with these parameter settings, difficult clusters are found within a number of local searches which is comparable with the results obtained in the other numerical experiments we made; some clusters are found with much greater efficiency using the automatic diameter penalization. For example, clusters with $N = 11, 12, 13, 14$ are generally found in more than 98% of the trials (only LJ_{12} was found in 93% of the trials). LJ_{38} is found (with $\mu = 0.1$) 4 517 times in 10 000 trials, LJ_{51} 1 004 times, LJ_{75} 2 times, and so on; however the automatic diameter choice does not permit to find easy clusters like, e.g., LJ_{15}, which could be found easily without penalty on the diameter; this fact should not be considered a failure of the method: it should be observed that these kind of structures are not particularly spherical, and are thus much more easily detected without imposing any penalty on the diameter. Moreover the regression on diameters we used to set the automatic value was obtained from the diameters of molecules with more than 20 atoms and for low values of N the resulting penalty on the diameter is excessive.

3. Conclusions and further research issues

What we think is the main result presented in this paper is not an original algorithm, although a very efficient method has been analyzed and its performance discussed. The major contribution of this paper is the definition of a new *local* search strategy, composed of two phases, the first of which is built in such a way as to pass over non interesting local minima. Moreover, this local search promises to be very well suited for general approaches for the Lennard-Jones and similar problems in molecular conformation studies; in this paper it was shown how the most difficult configurations for the Lennard-Jones cluster problem can be discovered with much greater efficiency by using a simple

Multistart algorithm in which our two-phase local search is used in place of a standard descent method. Some experiments have already been performed to see if this two-phase local optimization might be useful when substituted in place of a standard local search in a more refined method. Our first results with forward and correct methods are extremely encouraging.

In any case, already from the results presented here it is possible to infer that the penalties and rewards included in the first phase optimization succeed in driving the optimization close to very good, compact clusters, avoiding being trapped in local optima which for a regular local search method display very large regions of attraction. The structures of optimal Lennard-Jones clusters are so radically different in some cases that it seems quite unreasonable to look for general purpose methods capable of discovering all optima in reasonable computer times. Our approach greatly reduces the computational effort required to discover what are commonly accepted as the most difficult configurations. It is hoped that, when applied to larger clusters, this method will succeed in finding better putative global optima. Of course, in case of much larger clusters, the problem arises of efficiently computing the potential as well as the penalized functions and gradients. Using a naive approach, these computations require $O(N^2)$ distances to be evaluated for each iteration during local optimization; for large values of N this cost might be prohibitively large. In order to cope with the curse of dimensionality, it is planned in the next future to explore the possibility of parallelizing energy computations; another possibility, which we did not explore up to now, might be that of using faster approximate potential calculation, based on approaches similar to the one described in (Hingst and Phillips, 1999).

4. Appendix: details on the computational experiments

All of the experiments have been performed either on 266Mhz Pentium II Personal Computers or on a Sun Ultra 5 Workstation. For local optimization a standard conjugate gradient method was employed and, in particular, the implementation described in (Gilbert and Nocedal, 1992) was used with standard parameter settings. For every choice of the parameters, we ran random 10 000 trials. Experiments performed with different parameter settings, like those in tables 1 and 2, were conducted using the same seeds for the random generation mechanism. That is, common random numbers were used for different experiments: this way, in particular for those instances in which finding the global optimum is a rare event, a comparison between

the efficiency of different parameter settings becomes more reliable. The executable code, compiled both for Pentium PC's and for Sun Ultra Sparc Stations, is freely available for research purpose at URL `http://globopt.dsi.unifi.it/users/schoen`.

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Table II. Number of successes in 10 000 trials without diameter penalization

N	$p=4$ $\mu=0.1$	$p=4$ $\mu=0.3$	$p=6$ $\mu=0.3$	N	$p=4$ $\mu=0.1$	$p=4$ $\mu=0.3$	$p=6$ $\mu=0.3$
10	1775	2609	899	46	15	5	2
11	3289	4321	1475	47	28	22	12
12	5855	7513	2436	48	6	6	16
13	6379	8200	2104	49	15	3	5
14	7761	8698	3933	50	1	2	3
15	1866	853	1740	51	100	130	29
16	2381	2201	1050	52	87	133	90
17	585	705	403	53	138	177	208
18	1155	1977	249	54	95	122	192
19	2631	3280	605	55	50	43	59
20	3327	4389	833	56	124	149	141
21	821	1193	309	57	2	2	3
22	2006	2541	644	58	-	-	1
23	1592	2318	336	59	1	-	2
24	1909	2811	530	60	-	-	-
25	2174	3202	827	61	-	-	1
26	942	1938	243	62	-	-	-
27	200	148	45	63	-	1	-
28	417	367	101	64	-	-	-
29	697	1166	105	65	-	-	-
30	66	48	14	66	-	-	-
31	68	53	21	67	-	-	-
32	141	68	44	68	-	-	-
33	104	164	45	69	-	1	-
34	12	5	8	70	-	-	-
35	29	18	20	71	-	-	-
36	24	43	15	72	-	-	-
37	9	8	12	73	-	-	-
38	57	123	24	74	-	-	-
39	32	12	20	75	-	-	-
40	37	19	14	76	-	-	-
41	4	2	8	77	-	-	-
42	4	3	6	78	-	-	-
43	11	6	4	79	-	-	-
44	17	9	16	80	-	-	-
45	16	3	10				

Table III. Number of successes in 10 000 trials with diameter penalization

N	$D=3$ $p=4$ $\mu=0.2$	$D=3$ $p=6$ $\mu=0.2$	$D=2$ $p=4$ $\mu=0.2$	N	$D=3$ $p=4$ $\mu=0.2$	$D=3$ $p=6$ $\mu=0.2$	$D=2$ $p=4$ $\mu=0.2$
10	2686	1223	5172	46	-	-	2
11	4138	1488	6259	47	-	1	4
12	7170	2254	9367	48	63	187	3
13	7858	2185	9931	49	-	-	6
14	8571	3978	9881	50	2	5	6
15	1075	2230	-	51	58	206	97
16	2214	1338	17	52	27	122	23
17	803	540	-	53	13	131	214
18	1851	333	-	54	4	103	26
19	2580	477	19	55	4	40	2
20	3638	804	225	56	1	2	128
21	1302	451	174	57	-	-	4
22	2389	820	4	58	1	15	-
23	2020	428	2854	59	-	-	-
24	2753	968	854	60	-	-	2
25	3459	1597	2191	61	-	4	-
26	2191	564	6840	62	-	-	-
27	52	10	-	63	1	-	-
28	235	58	-	64	-	2	-
29	995	75	5	65	-	-	-
30	42	3	-	66	-	-	-
31	-	13	-	67	-	-	-
32	3	3	-	68	-	-	-
33	10	3	-	69	-	-	-
34	-	-	-	70	-	-	-
35	2	9	-	71	-	-	-
36	6	2	-	72	-	-	-
37	-	-	-	73	-	-	-
38	437	887	1831	74	-	-	-
39	-	-	672	75	-	3	1
40	5	-	9	76	-	4	-
41	-	-	1	77	-	1	-
42	-	-	1	78	-	-	-
43	-	-	1	79	-	2	-
44	-	-	1	80	-	1	-
45	-	1	2				